Supplementary Information

**Comparison of the reactivity and structures for the neutral and cationic bis(imino)pyridyl iron and cobalt species by DFT calculations**

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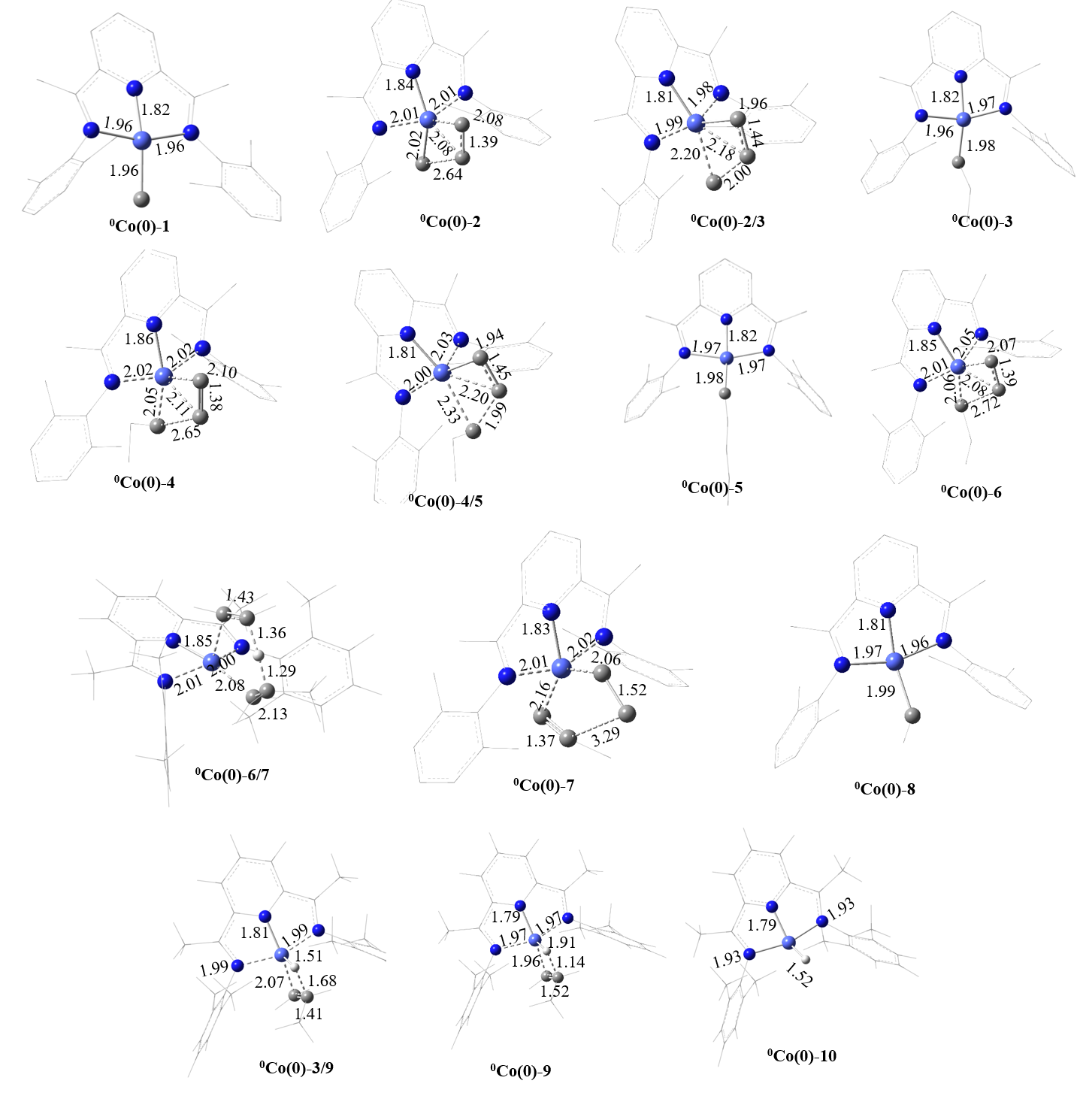
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Tel.: +86-10-6255-7955 (Y.M. & W.-H.S.)

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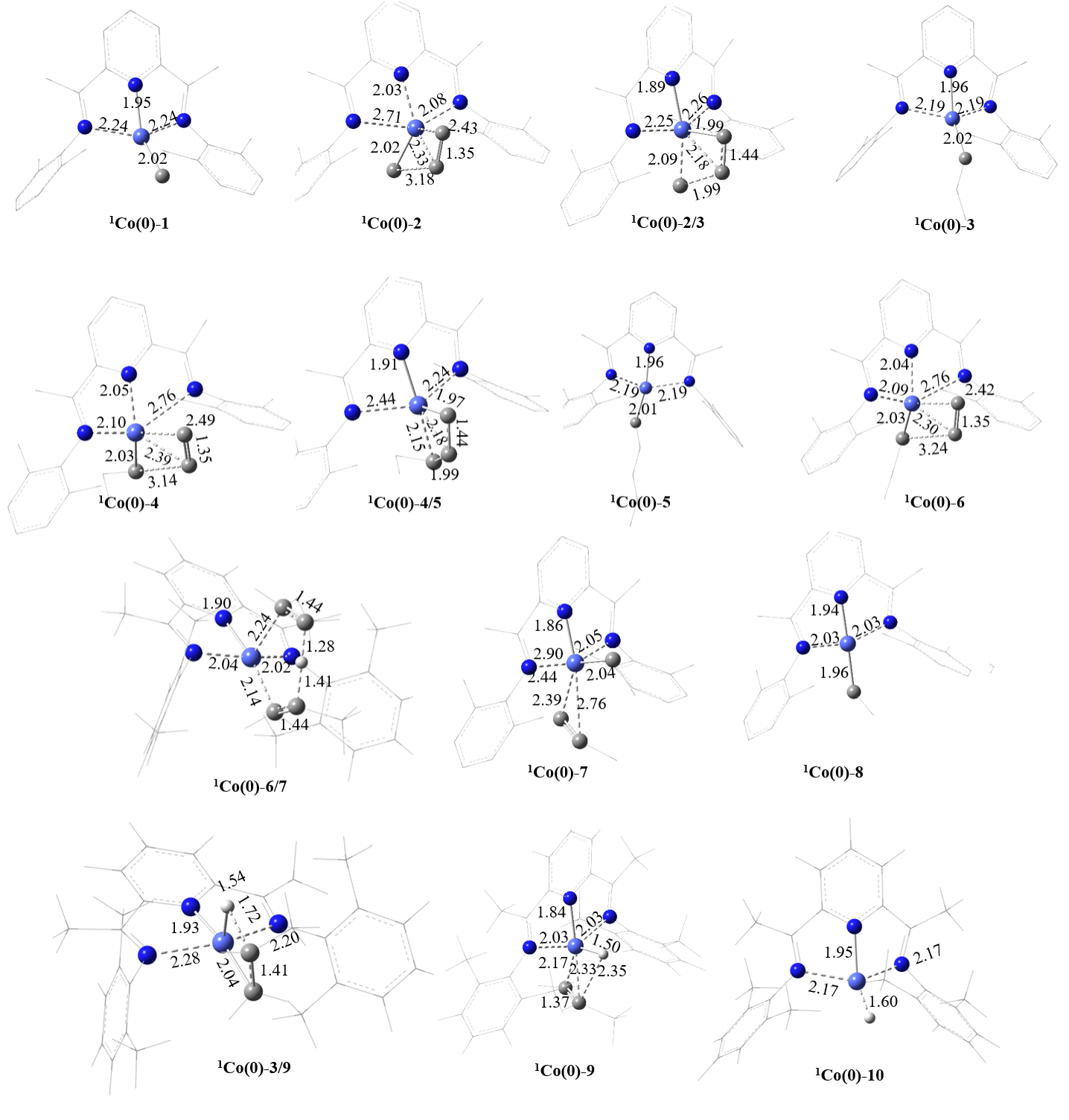
* 1. **Figure S1** The DFT optimized structures of the neutral cobalt system **0Co(0)** in Figure 1. The bond distance is listed for the active center in Å.
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**22.** Coordinates of all optimized structures:

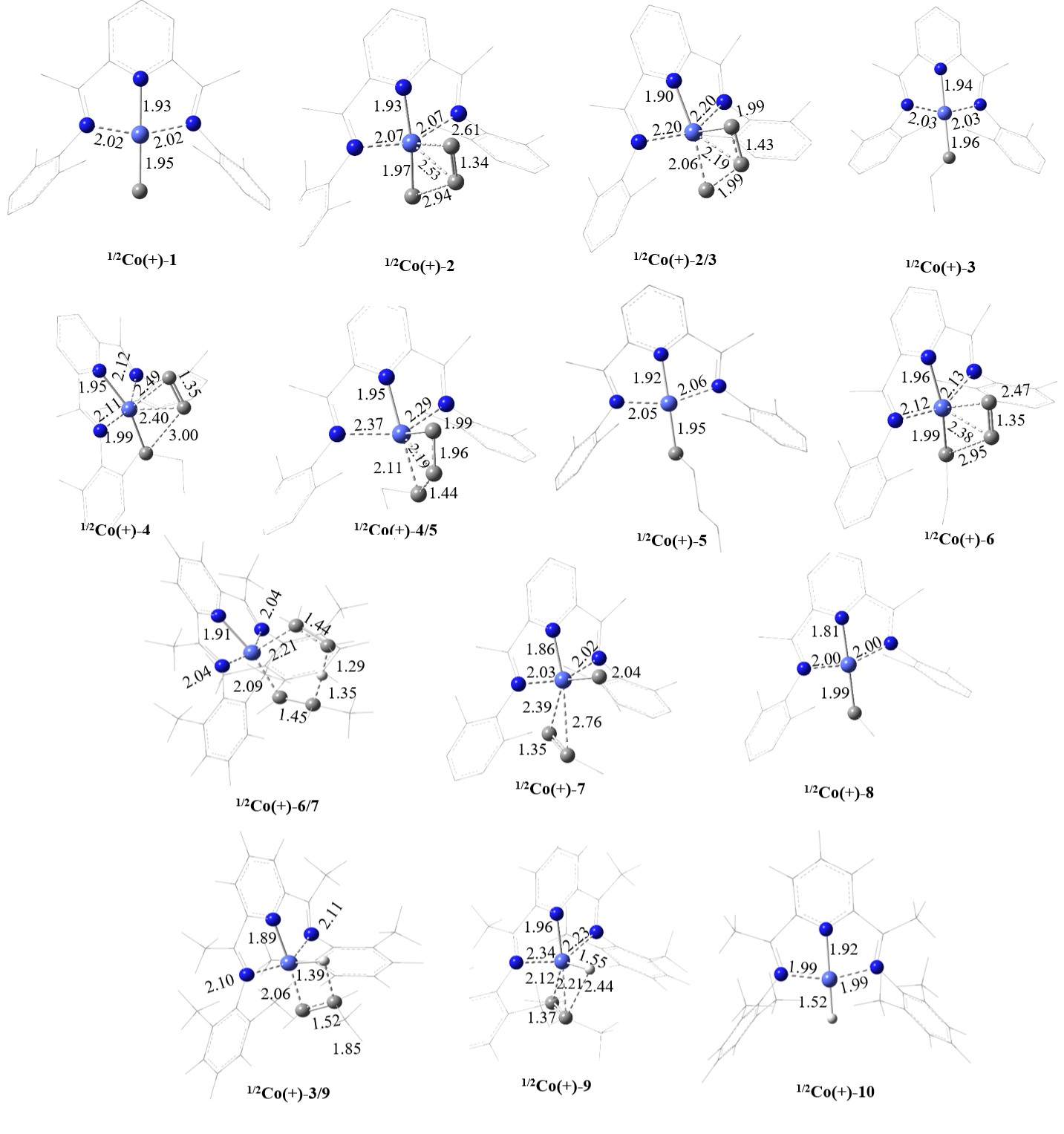
Optimized Structures:



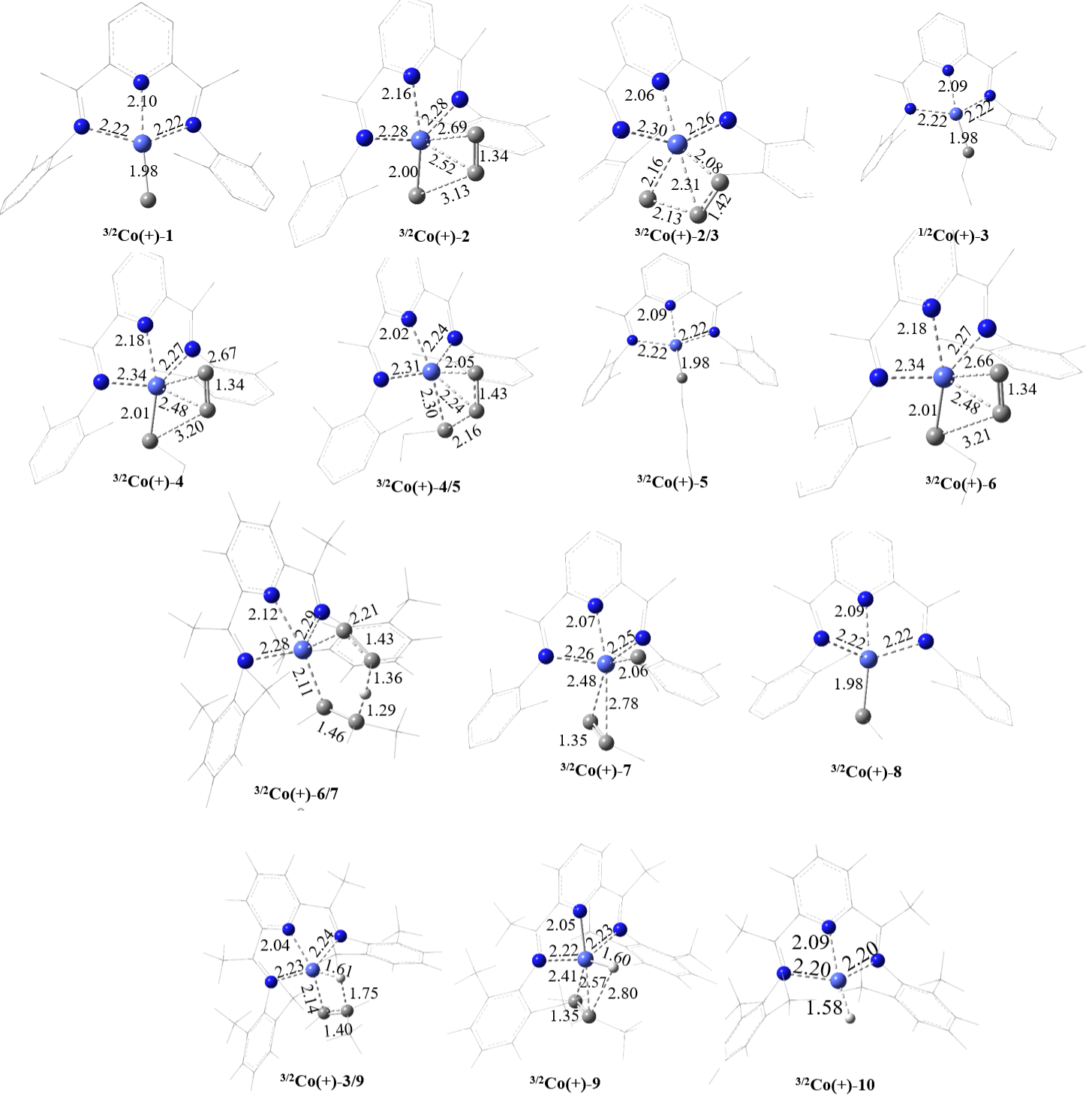
**Figure S1** The DFT optimized structures of the neutral cobalt system **0Co(0)** in Figure 1. The bond distance is listed for the active center in Å.



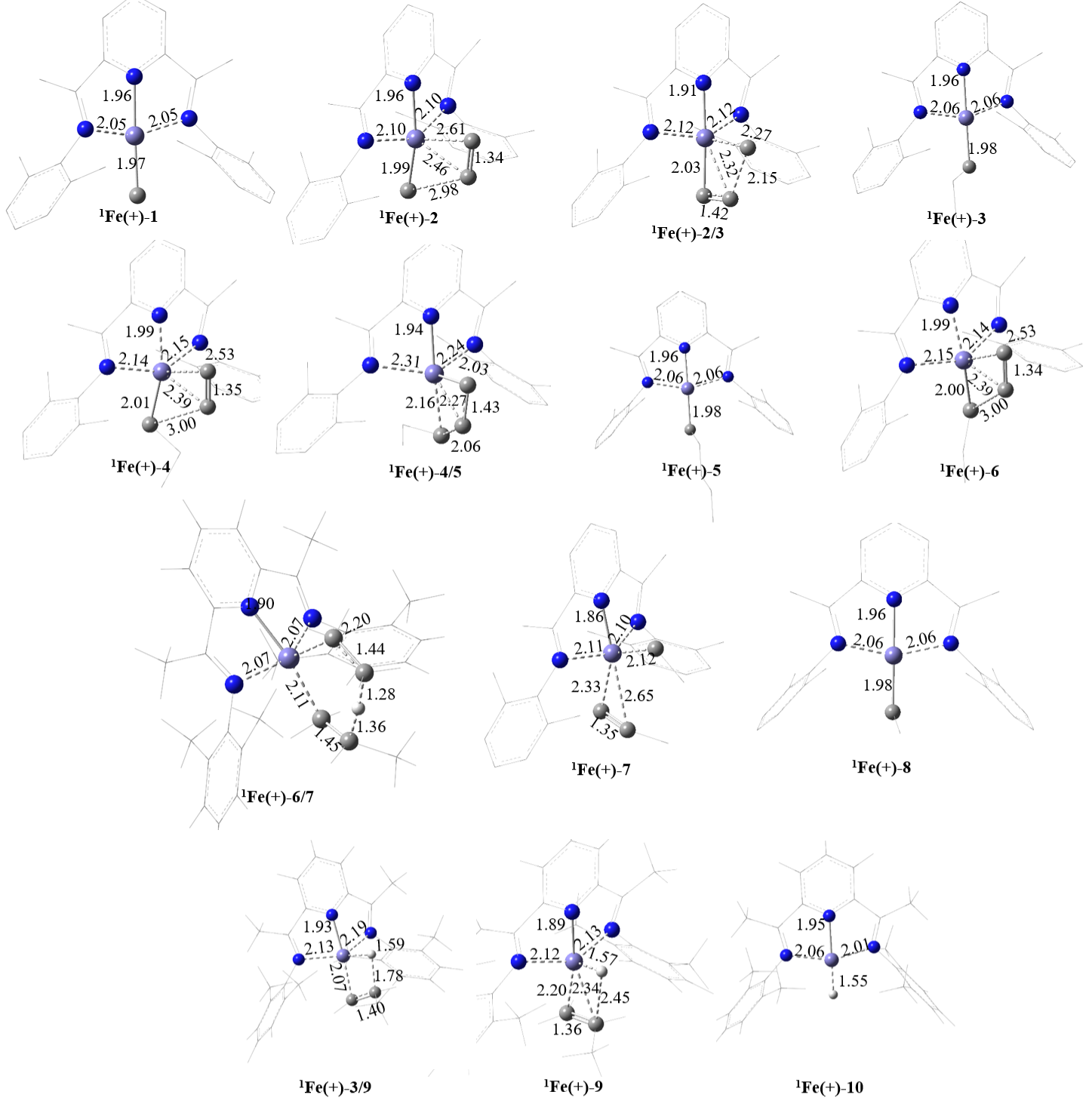
**Figure S2** The DFT optimized structures of the neutral cobalt system **1Co(0)** in Figure 1. The bond distance is listed for the active center in Å.



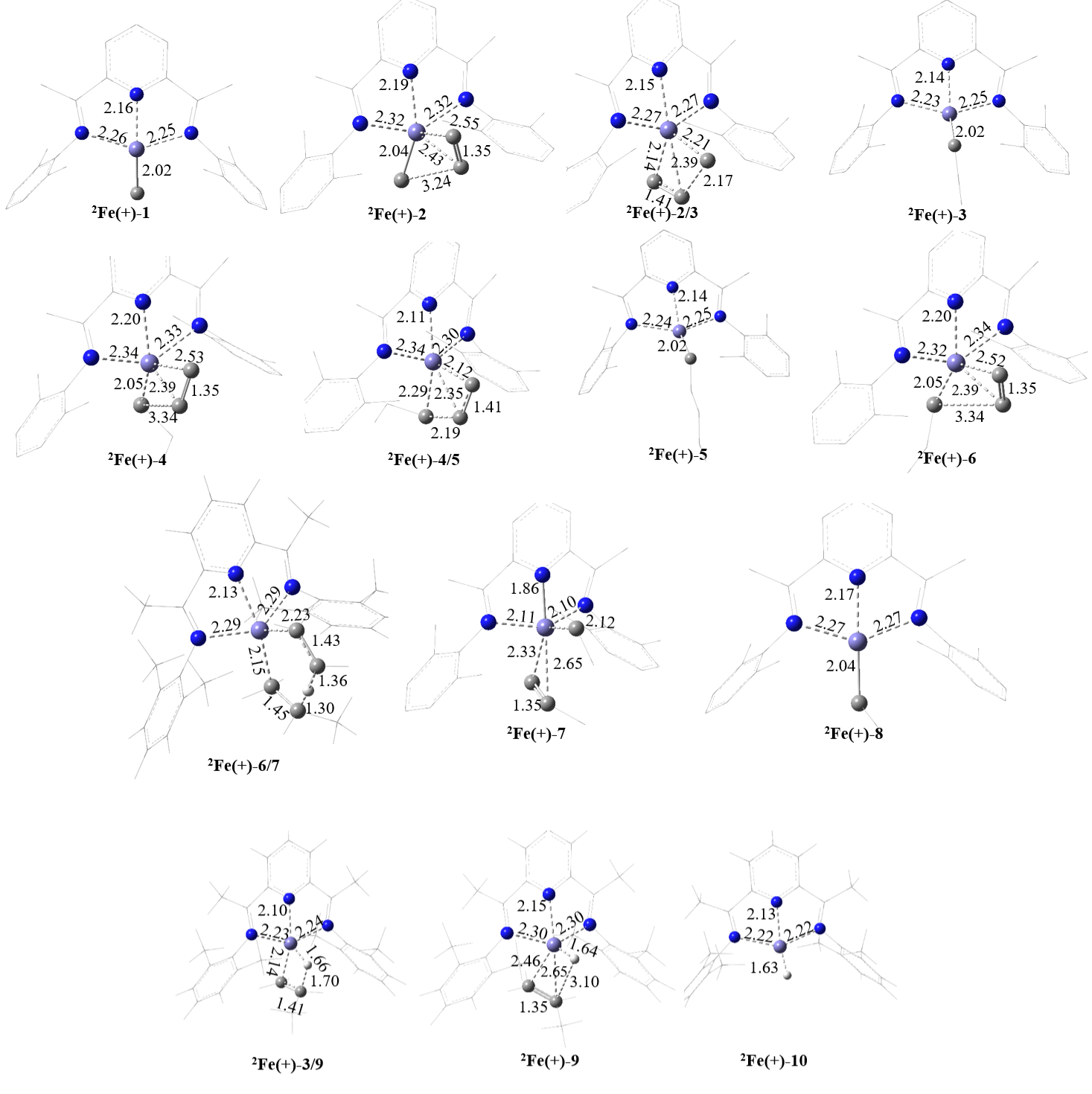
**Figure S3** The DFT optimized structures of the cation cobalt system **1/2Co(+)** in Figure 3. The bond distance is listed for the active center in Å.



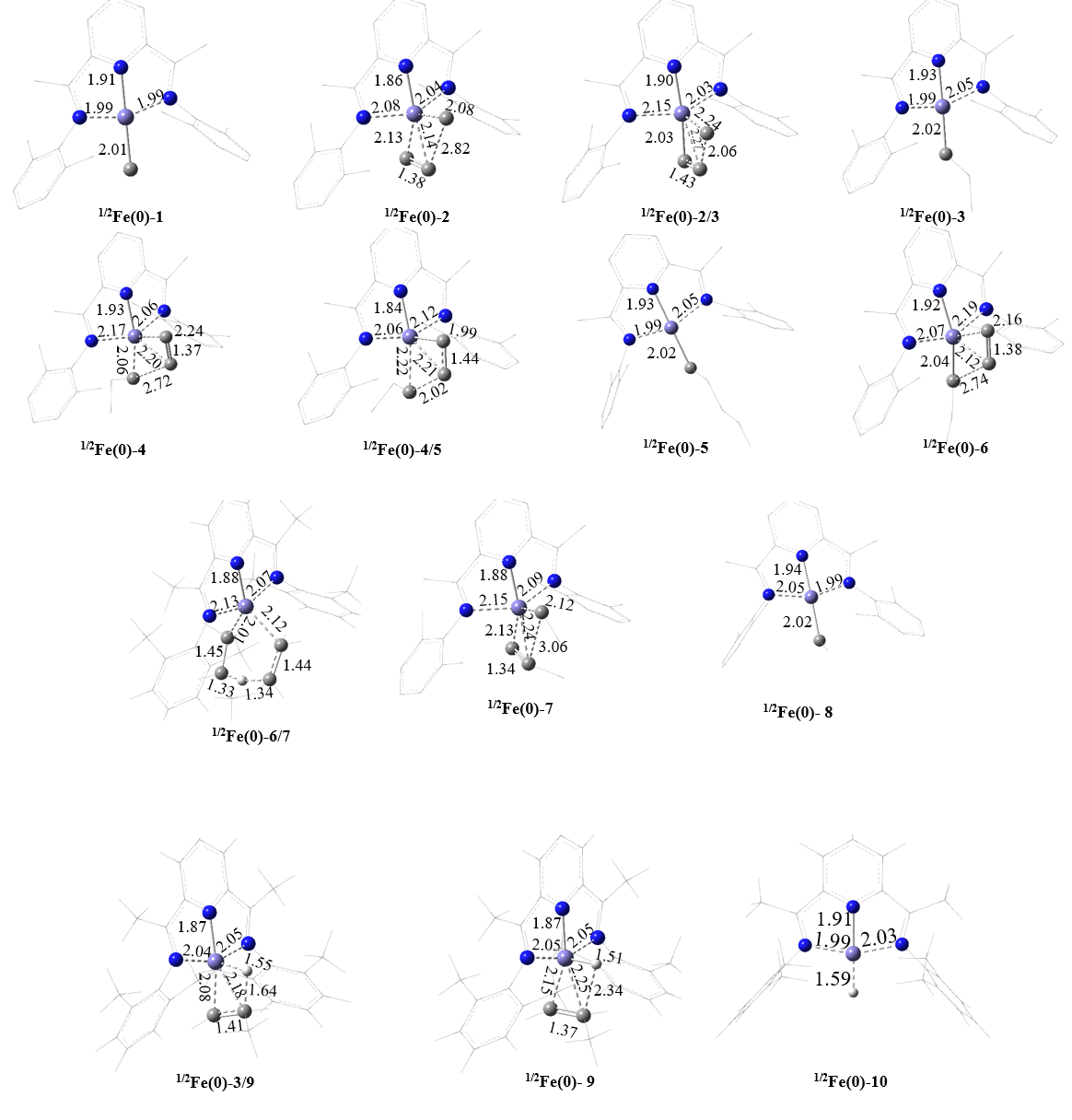
**Figure S4** The DFT optimized structures of the cation cobalt system **3/2Co(+)** in Figure 3. The bond distance is listed for the active center in Å.



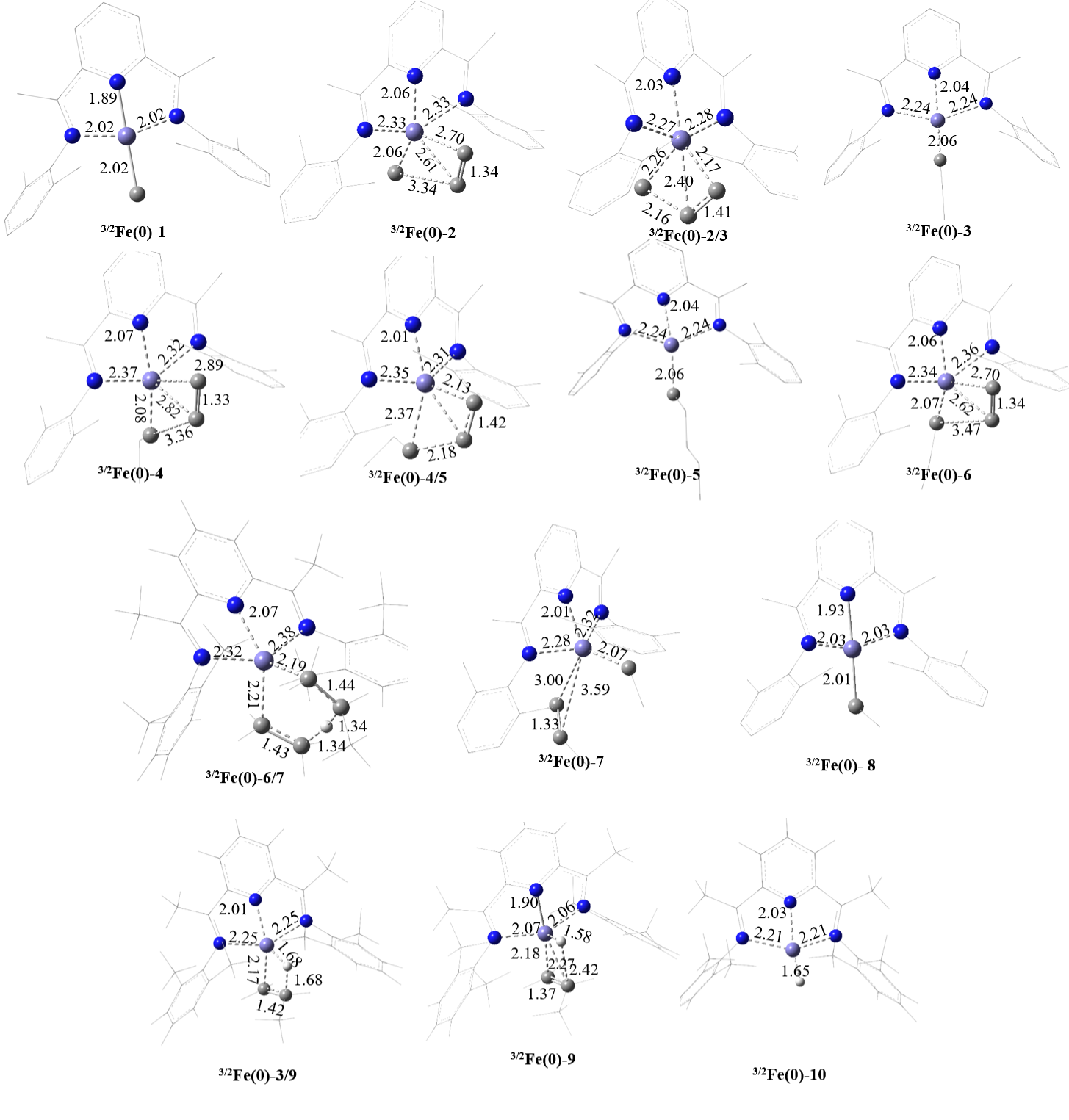
**Figure S5** The DFT optimized structures of the cation iron system **1Fe(+)** in Figure 5. The bond distance is listed for the active center in Å.



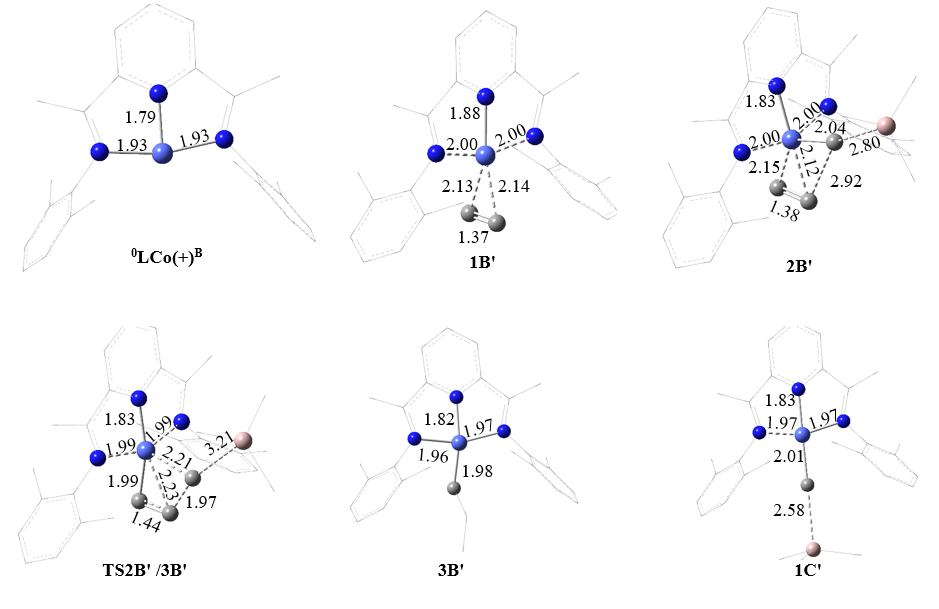
**Figure S6** The DFT optimized structures of the cation iron system **2Fe(+)** in Figure 5. The bond distance is listed for the active center in Å.



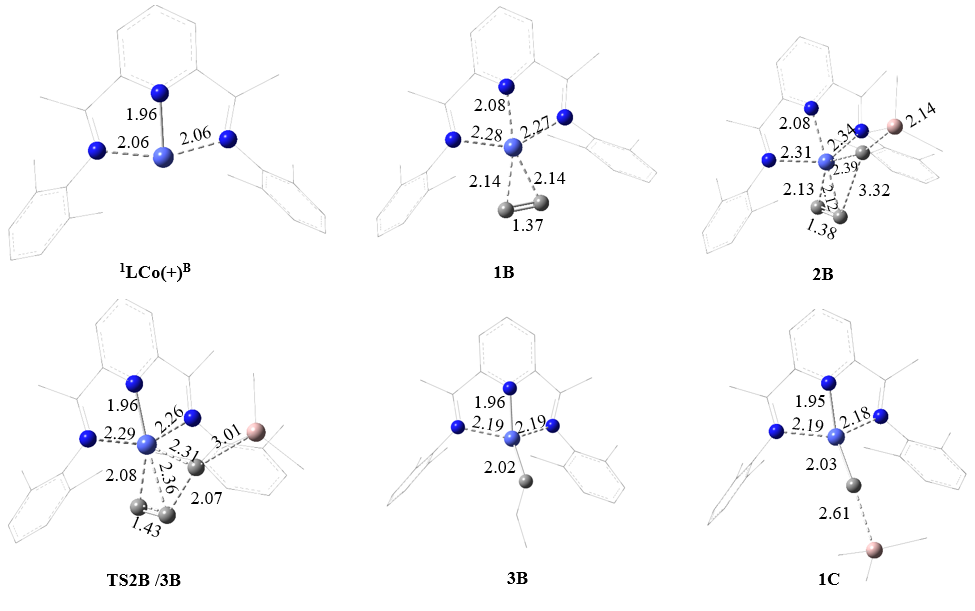
**Figure S7** The DFT optimized structures of the neutral iron system **1/2Fe(0)** in Figure 6. The bond distance is listed for the active center in Å.



**Figure S8** The DFT optimized structures of the neutral cobalt system **3/2Fe(0)** in Figure 6. The bond distance is listed for the active center in Å.



**Figure S9** The DFT optimized structures of the cobalt system **0LCo(+)B** in Figure 9. The bond distance is listed for the active center in Å.



**Figure S10** The DFT optimized structures of the cobalt system **1LCo(+)B** in Figure 9. The bond distance is listed for the active center in Å.

**Table S1** The factors for calculating the structure parameter Δ in **0Co(0)**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **0Co(0)** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| 1 | 1.372 | 1.372 | 1.445 | 1.445 | 1.318 | 1.318 | 0.100 |
| 2 | 1.376 | 1.376 | 1.436 | 1.436 | 1.325 | 1.325 | 0.085 |
| TS-2/3 | 1.384 | 1.385 | 1.424 | 1.423 | 1.340 | 1.341 | 0.061 |
| 3 | 1.374 | 1.374 | 1.442 | 1.442 | 1.320 | 1.320 | 0.096 |
| 4 | 1.373 | 1.373 | 1.436 | 1.436 | 1.328 | 1.328 | 0.086 |
| TS-4/5 | 1.385 | 1.384 | 1.420 | 1.422 | 1.342 | 1.341 | 0.058 |
| 5 | 1.375 | 1.375 | 1.442 | 1.442 | 1.320 | 1.320 | 0.095 |

**Table S2** The factors for calculating the structure parameter Δ in **1Co(0)**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **1Co(0)** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| 1 | 1.372 | 1.372 | 1.461 | 1.461 | 1.304 | 1.304 | 0.123 |
| 2 | 1.368 | 1.383 | 1.484 | 1.441 | 1.285 | 1.323 | 0.123 |
| TS-2/3 | 1.377 | 1.377 | 1.454 | 1.455 | 1.308 | 1.307 | 0.112 |
| 3 | 1.369 | 1.370 | 1.455 | 1.455 | 1.313 | 1.313 | 0.114 |
| 4 | 1.386 | 1.369 | 1.438 | 1.485 | 1.325 | 1.284 | 0.120 |
| TS-4/5 | 1.376 | 1.385 | 1.463 | 1.443 | 1.299 | 1.315 | 0.109 |
| 5 | 1.370 | 1.370 | 1.455 | 1.455 | 1.312 | 1.312 | 0.114 |

**Table S3** The factors for calculating the structure parameter Δ in **1/2Co(+)**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **1/2Co(+)** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| 1 | 1.337 | 1.337 | 1.491 | 1.491 | 1.297 | 1.297 | 0.174 |
| 2 | 1.341 | 1.341 | 1.486 | 1.486 | 1.296 | 1.296 | 0.167 |
| TS-2/3 | 1.349 | 1.350 | 1.485 | 1.486 | 1.290 | 1.290 | 0.166 |
| 3 | 1.337 | 1.337 | 1.490 | 1.490 | 1.297 | 1.297 | 0.173 |
| 4 | 1.343 | 1.342 | 1.484 | 1.483 | 1.295 | 1.296 | 0.165 |
| TS-4/5 | 1.350 | 1.350 | 1.492 | 1.489 | 1.283 | 1.285 | 0.174 |
| 5 | 1.340 | 1.340 | 1.485 | 1.485 | 1.297 | 1.297 | 0.167 |

**Table S4** The factors for calculating the structure parameter Δ in **3/2Co(+)**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **3/2Co(+)** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| 1 | 1.338 | 1.338 | 1.497 | 1.497 | 1.286 | 1.286 | 0.185 |
| 2 | 1.338 | 1.338 | 1.496 | 1.496 | 1.283 | 1.283 | 0.185 |
| TS-2/3 | 1.345 | 1.344 | 1.494 | 1.494 | 1.285 | 1.284 | 0.180 |
| 3 | 1.338 | 1.338 | 1.496 | 1.496 | 1.288 | 1.288 | 0.183 |
| 4 | 1.339 | 1.339 | 1.496 | 1.495 | 1.282 | 1.284 | 0.185 |
| TS-4/5 | 1.345 | 1.345 | 1.487 | 1.485 | 1.290 | 1.292 | 0.168 |
| 5 | 1.338 | 1.338 | 1.495 | 1.495 | 1.288 | 1.288 | 0.183 |

**Table S5** The factors for calculating the structure parameter Δ in **1Fe(+)**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 1**Fe(+)** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| 1 | 1.344 | 1.344 | 1.481 | 1.481 | 1.300 | 1.300 | 0.159 |
| 2 | 1.352 | 1.352 | 1.473 | 1.473 | 1.302 | 1.302 | 0.146 |
| TS-2/3 | 1.357 | 1.357 | 1.467 | 1.467 | 1.305 | 1.305 | 0.136 |
| 3 | 1.347 | 1.347 | 1.476 | 1.476 | 1.302 | 1.302 | 0.150 |
| 4 | 1.352 | 1.352 | 1.471 | 1.472 | 1.300 | 1.301 | 0.145 |
| TS-4/5 | 1.360 | 1.360 | 1.474 | 1.470 | 1.294 | 1.298 | 0.144 |
| 5 | 1.348 | 1.348 | 1.475 | 1.474 | 1.303 | 1.303 | 0.149 |

**Table S6** The factors for calculating the structure parameter Δ in **2Fe(+)**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 2**Fe(+)** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| 1 | 1.337 | 1.337 | 1.498 | 1.498 | 1.285 | 1.285 | 0.187 |
| 2 | 1.342 | 1.342 | 1.492 | 1.497 | 1.284 | 1.283 | 0.182 |
| TS-2/3 | 1.343 | 1.344 | 1.491 | 1.491 | 1.285 | 1.285 | 0.177 |
| 3 | 1.339 | 1.339 | 1.495 | 1.496 | 1.289 | 1.288 | 0.182 |
| 4 | 1.343 | 1.342 | 1.496 | 1.491 | 1.283 | 1.286 | 0.180 |
| TS-4/5 | 1.347 | 1.347 | 1.488 | 1.487 | 1.288 | 1.289 | 0.170 |
| 5 | 1.339 | 1.339 | 1.496 | 1.495 | 1.288 | 1.288 | 0.182 |

**Table S7** The factors for calculating the structure parameter Δ in **1/2Fe(0)**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 1/2**Fe(0)** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| 1 | 1.369 | 1.369 | 1.447 | 1.447 | 1.332 | 1.332 | 0.097 |
| 2 | 1.371 | 1.375 | 1.441 | 1.432 | 1.323 | 1.334 | 0.086 |
| TS-2/3 | 1.365 | 1.381 | 1.458 | 1.431 | 1.31 | 1.341 | 0.095 |
| 3 | 1.375 | 1.356 | 1.432 | 1.461 | 1.346 | 1.313 | 0.099 |
| 4 | 1.362 | 1.376 | 1.462 | 1.431 | 1.306 | 1.337 | 0.101 |
| TS-4/5 | 1.388 | 1.381 | 1.425 | 1.435 | 1.336 | 1.324 | 0.073 |
| 5 | 1.373 | 1.355 | 1.43 | 1.461 | 1.346 | 1.314 | 0.098 |

**Table S8** The factors for calculating the structure parameter Δ in **3/2Fe(0)**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 3/2**Fe(0)** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| 1 | 1.371 | 1.365 | 1.448 | 1.443 | 1.332 | 1.331 | 0.095 |
| 2 | 1.379 | 1.379 | 1.457 | 1.456 | 1.305 | 1.305 | 0.115 |
| TS-2/3 | 1.377 | 1.378 | 1.452 | 1.451 | 1.308 | 1.309 | 0.109 |
| 3 | 1.373 | 1.373 | 1.454 | 1.454 | 1.311 | 1.311 | 0.112 |
| 4 | 1.378 | 1.380 | 1.459 | 1.453 | 1.302 | 1.307 | 0.114 |
| TS-4/5 | 1.375 | 1.379 | 1.456 | 1.447 | 1.306 | 1.315 | 0.107 |
| 5 | 1.371 | 1.371 | 1.454 | 1.454 | 1.311 | 1.311 | 0.112 |

**Table S9** The NBO charge distribution for sM(q)-1 and sM(q)-2, M includes iron and cobalt, s means the spin states and the q refers to the charge number.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **sM(*q*)-1** | **1/2Co(+)** | **3/2Co(+)** | **1Fe(+)** | **2Fe(+)** | **0Co(0)** | **1Co(0)** | 1/2Fe(0) | **3/2Fe(0)** |
| PBI | 0.060 | -0.089 | -0.030 | -0.095 | -0.449 | -0.705 | -0.540 | -0.760 |
| M | 0.746 | 1.060 | 0.837 | 1.090 | 0.428 | 0.911 | 0.617 | 0.818 |
| CH3 | -0.321 | -0.466 | -0.320 | -0.484 | -0.365 | -0.529 | -0.451 | -0.426 |
| 2Ar | 0.515 | 0.496 | 0.514 | 0.492 | 0.385 | 0.327 | 0.374 | 0.369 |
| **sM(*q*)-2** | **1/2Co(+)** | **3/2Co(+)** | **1Fe(+)** | **2Fe(+)** | **0Co(0)** | **1Co(0)** | 1/2Fe(0) | **3/2Fe(0)** |
| PBI | 0.049 | -0.073 | -0.065 | -0.072 | -0.402 | -0.677 | -0.393 | -0.774 |
| M | 0.648 | 1.010 | 0.968 | 1.020 | 0.192 | 0.831 | 0.283 | 0.968 |
| CH3 | -0.294 | -0.488 | -0.272 | -0.469 | -0.201 | -0.485 | -0.248 | -0.549 |
| C2H4 | 0.098 | 0.078 | 0.103 | 0.072 | 0.038 | 0.036 | 0.010 | 0.054 |
| 2Ar | 0.498 | 0.472 | 0.490 | 0.449 | 0.373 | 0.295 | 0.347 | 0.301 |

**Table S10** The factors for calculating the structure parameter Δ in **0Co(+)B**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **0Co(+)B** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| LCo(+)B | 1.350 | 1.350 | 1.477 | 1.477 | 1.302 | 1.302 | 0.150 |
| 1B | 1.343 | 1.343 | 1.479 | 1.479 | 1.299 | 1.299 | 0.158 |
| 2B | 1.375 | 1.375 | 1.435 | 1.435 | 1.327 | 1.327 | 0.084 |
| TS2B/3B | 1.381 | 1.381 | 1.433 | 1.433 | 1.330 | 1.330 | 0.077 |
| 3B | 1.374 | 1.374 | 1.442 | 1.442 | 1.320 | 1.320 | 0.095 |
| 1C | 1.364 | 1.364 | 1.452 | 1.452 | 1.312 | 1.312 | 0.114 |

**Table S11** The factors for calculating the structure parameter Δ in **1Co(+)B**.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **1Co(+)B** | d1 | d1' | d2 | d2' | d3 | d3' | Δ |
| LCo(+)B | 1.334 | 1.334 | 1.497 | 1.497 | 1.298 | 1.298 | 0.181 |
| 1B | 1.342 | 1.342 | 1.492 | 1.492 | 1.283 | 1.283 | 0.180 |
| 2B | 1.346 | 1.345 | 1.484 | 1.485 | 1.288 | 1.288 | 0.168 |
| TS2B/3B | 1.376 | 1.375 | 1.457 | 1.456 | 1.306 | 1.306 | 0.116 |
| 3B | 1.369 | 1.370 | 1.455 | 1.455 | 1.313 | 1.313 | 0.114 |
| 1C | 1.368 | 1.368 | 1.458 | 1.458 | 1.310 | 1.310 | 0.119 |

Coordinate of all optimized structures:

B3LYP/6-311G\*[SDD]

**0Co(0)**

**0Co(0)-1**

Atom x y z

C -1.18944000 2.46497300 0.13456600

C -1.20792100 3.85634600 0.11032400

C 0.00003800 4.55956200 0.10668100

C 1.20798300 3.85632100 0.11037800

C 1.18947800 2.46494900 0.13462600

N 0.00000900 1.78253800 0.17006300

H 0.00004900 5.64323200 0.08689200

H -2.15189700 4.38958900 0.08895000

H 2.15197100 4.38954600 0.08902600

C -2.30239900 1.54378200 0.10287700

C 2.30242100 1.54375000 0.10289100

N 1.93606400 0.27914700 0.03822500

N -1.93607200 0.27917200 0.03815400

C 3.72112400 2.03708100 0.14205400

H 3.95869500 2.61631600 -0.75651500

H 3.87604200 2.69942900 0.99884700

H 4.43216300 1.21623500 0.21152000

C -3.72109400 2.03713400 0.14209300

H -3.87599600 2.69938000 0.99897000

H -3.95865800 2.61648500 -0.75640000

H -4.43214700 1.21629100 0.21146500

C 2.92510800 -0.75630600 0.00804500

C 3.24299700 -1.42675600 1.20172600

C 3.51234400 -1.12009400 -1.21626400

C 4.18181300 -2.45947500 1.15213300

C 4.44457000 -2.16065300 -1.21968600

C 4.78300300 -2.82629600 -0.04703600

H 4.43771500 -2.98377200 2.06829400

H 4.90220800 -2.45448100 -2.15985100

H 5.50647400 -3.63509200 -0.06884200

C -2.92513100 -0.75626500 0.00792900

C -3.51213500 -1.12021500 -1.21644100

C -3.24324900 -1.42656100 1.20164000

C -4.44435400 -2.16078400 -1.21990400

C -4.18204600 -2.45929400 1.15200300

C -4.78300400 -2.82627800 -0.04723400

H -4.90181100 -2.45473700 -2.16011800

H -4.43811500 -2.98347300 2.06818400

H -5.50645800 -3.63508800 -0.06907500

C -3.13696600 -0.41694300 -2.49668000

H -3.52347300 0.60740700 -2.53207600

H -2.05168000 -0.35234100 -2.60547700

H -3.53908600 -0.94664800 -3.36246700

C -2.58813800 -1.04118300 2.50418000

H -1.49840300 -1.10532000 2.43424500

H -2.82083400 -0.01106200 2.79215700

H -2.91690000 -1.69537000 3.31403000

C 3.13739800 -0.41665600 -2.49647600

H 2.05212700 -0.35210400 -2.60547600

H 3.52384200 0.60772400 -2.53164100

H 3.53972500 -0.94620800 -3.36226000

C 2.58763000 -1.04156200 2.50419100

H 2.82022000 -0.01146500 2.79233800

H 1.49791200 -1.10574700 2.43404100

H 2.91627000 -1.69583400 3.31402200

Co -0.00004800 -0.02519700 -0.02513500

C 0.00012500 -1.83613300 -0.76790400

H 0.00001300 -2.45919200 0.14722100

H -0.88856200 -2.12704100 -1.33545600

H 0.88895400 -2.12699900 -1.33524900

**0Co(0)-2**

Atom x y z

C 1.19341500 2.46349400 -0.09732300

C 1.20648500 3.84999700 -0.21801300

C -0.00022100 4.55164400 -0.27494800

C -1.20687000 3.84982400 -0.21779800

C -1.19343800 2.46340300 -0.09711400

N -0.00000300 1.78225400 -0.02749900

H -0.00027600 5.63105800 -0.37311700

H 2.14836600 4.38343600 -0.27895300

H -2.14895100 4.38297400 -0.27850800

C 2.31277500 1.56474300 -0.07977700

C -2.31290100 1.56474000 -0.07950000

N -1.97207500 0.28847000 0.02848200

N 1.97176300 0.28846100 0.02837100

C -3.72397000 2.06280400 -0.24501800

H -3.88447100 2.98391600 0.31941100

H -3.94204600 2.28479000 -1.29563700

H -4.45396000 1.32808900 0.09008100

C 3.72406300 2.06180100 -0.24618100

H 3.94616900 2.27044400 -1.29871700

H 3.88194800 2.98996800 0.30713900

H 4.45336100 1.33183100 0.10075300

C -2.99663400 -0.71140800 -0.09203100

C -3.30103900 -1.20160800 -1.37852700

C -3.68110100 -1.19361400 1.04067000

C -4.23940200 -2.22803400 -1.50082400

C -4.61787500 -2.21793000 0.86835100

C -4.88747300 -2.74758900 -0.38674800

H -4.46363600 -2.62001300 -2.48872700

H -5.14768900 -2.59501400 1.73849700

H -5.61112200 -3.54883500 -0.49820300

C 2.99654800 -0.71121200 -0.09200100

C 3.68117700 -1.19294900 1.04083600

C 3.30109400 -1.20170600 -1.37835100

C 4.61842200 -2.21686300 0.86877200

C 4.23993100 -2.22774500 -1.50037600

C 4.88830100 -2.74668200 -0.38620200

H 5.14835700 -2.59353400 1.73902400

H 4.46425800 -2.61994100 -2.48817600

H 5.61232500 -3.54761500 -0.49746200

C 3.47689400 -0.61546700 2.42238900

H 3.29398900 0.46018700 2.39749600

H 2.63061600 -1.07173900 2.94202200

H 4.36234900 -0.78697600 3.03844000

C 2.67318100 -0.61090200 -2.61669800

H 1.64291800 -0.30582900 -2.44332900

H 3.22408700 0.27665700 -2.95014000

H 2.68841300 -1.32733500 -3.44060600

C -3.47717900 -0.61616200 2.42227800

H -2.63030500 -1.07159500 2.94167000

H -3.29545100 0.45970100 2.39748500

H -4.36233300 -0.78870100 3.03847000

C -2.67357800 -0.60977500 -2.61659800

H -3.22375600 0.27892300 -2.94823100

H -1.64282800 -0.30605200 -2.44366100

H -2.69035600 -1.32500300 -3.44151700

C -0.00005200 -1.81277400 -0.69901300

H -0.00005300 -1.60239200 -1.77373400

H 0.88416400 -2.41303800 -0.47665400

H -0.88430900 -2.41298500 -0.47667200

C 0.00002700 -1.33712400 1.89877000

H 0.91011300 -1.92250600 1.87697000

H -0.90993100 -1.92270400 1.87685200

C -0.00014300 -0.02482800 2.34924900

H -0.91220500 0.46531900 2.66500400

H 0.91178200 0.46553700 2.66506000

Co 0.00000200 -0.03606600 0.27046500

**0Co(0)-2/3**

Atom x y z

C 1.20267100 2.51469200 -0.11794800

C 1.19911600 3.90078100 -0.24317400

C -0.01311700 4.59487600 -0.28465900

C -1.22027700 3.89262000 -0.21275600

C -1.21133800 2.50702200 -0.08870000

N -0.00203400 1.83709900 -0.02247200

H -0.01800500 5.67388500 -0.38872600

H 2.13387100 4.44438400 -0.31717200

H -2.15950900 4.43086400 -0.26442200

C 2.30882400 1.62009000 -0.11194000

C -2.31224700 1.60430100 -0.06306800

N -1.94002400 0.32040400 0.03261500

N 1.94116800 0.33534800 -0.00238500

C -3.74643300 2.03976700 -0.17693800

H -4.33349300 1.73932800 0.69631900

H -3.82792200 3.12194100 -0.27349100

H -4.23558300 1.59138800 -1.04721100

C 3.73954800 2.05891200 -0.24793100

H 3.81197400 3.13163000 -0.42525500

H 4.32390400 1.83202600 0.64973200

H 4.23774400 1.55120900 -1.07900600

C -2.94785500 -0.68832700 -0.10795000

C -3.19626500 -1.19004800 -1.40541900

C -3.66611000 -1.18370400 0.99661100

C -4.13289900 -2.21130500 -1.56773500

C -4.59686800 -2.20794700 0.78696900

C -4.82675400 -2.72887500 -0.47874500

H -4.32041200 -2.60254200 -2.56351700

H -5.15440300 -2.59125900 1.63715600

H -5.55130400 -3.52469200 -0.61967600

C 2.93663300 -0.68542500 -0.13031400

C 3.67150400 -1.14874900 0.97823400

C 3.15539200 -1.23734300 -1.41294700

C 4.57167600 -2.20442400 0.79319400

C 4.06023700 -2.29055000 -1.55002500

C 4.75863900 -2.78522400 -0.45337600

H 5.13921100 -2.56496100 1.64694400

H 4.22164700 -2.72332500 -2.53322200

H 5.45680800 -3.60741200 -0.57491000

C 3.55389900 -0.53222900 2.35370800

H 4.53779400 -0.46844600 2.82601000

H 3.13002500 0.47027500 2.32536300

H 2.92227000 -1.13023800 3.01781200

C 2.46848300 -0.67373300 -2.63292700

H 1.41999600 -0.43814100 -2.44563300

H 2.93788600 0.26345100 -2.95311400

H 2.52680300 -1.37049800 -3.47162100

C -3.48703200 -0.64074900 2.39516100

H -2.74129100 -1.20909400 2.95898800

H -3.16438000 0.40009900 2.39860800

H -4.42503600 -0.70540700 2.95202900

C -2.47613600 -0.62643700 -2.60519300

H -2.73563100 0.42281400 -2.77900100

H -1.39230100 -0.65376200 -2.47662700

H -2.73043200 -1.18481800 -3.50829600

C -0.01984700 -2.09202300 -0.11817500

H 0.24016700 -1.66638400 -1.08894900

H 0.68717500 -2.89640300 0.06172700

H -1.03004100 -2.48515800 -0.16483000

C 0.11415100 -1.53704200 1.79362100

H 1.07016000 -2.02291400 1.94453000

H -0.71645000 -2.19561100 2.02684000

C 0.02451900 -0.17463500 2.25275100

H -0.90279400 0.17516900 2.68837900

H 0.91037500 0.28805700 2.67067200

Co 0.00980500 0.06255000 0.31027000

**0Co(0)-3**

Atom x y z

C -1.19022100 2.69903200 0.09065500

C -1.20735300 4.08769000 0.00535300

C 0.00000000 4.79119800 -0.02662900

C 1.20735400 4.08769000 0.00535100

C 1.19022200 2.69903200 0.09065400

N 0.00000000 2.01600700 0.16461300

H 0.00000000 5.87291900 -0.09399800

H -2.15153800 4.61892900 -0.04276000

H 2.15153900 4.61892800 -0.04276300

C -2.30446000 1.78299600 0.08871100

C 2.30446000 1.78299600 0.08871000

N 1.94226600 0.51438700 0.05862700

N -1.94226700 0.51438800 0.05862800

C 3.72183800 2.28156300 0.12352900

H 3.96964000 2.82413600 -0.79484800

H 3.86562700 2.97785800 0.95474200

H 4.43392700 1.46611300 0.23464300

C -3.72183800 2.28156400 0.12353100

H -3.86562600 2.97785800 0.95474500

H -3.96963900 2.82413900 -0.79484500

H -4.43392700 1.46611500 0.23464300

C 2.93470200 -0.51700000 0.06980300

C 3.20928900 -1.17556200 1.28220100

C 3.57632800 -0.88764200 -1.12540900

C 4.14833000 -2.20879500 1.27967500

C 4.50493000 -1.93131000 -1.08214900

C 4.79362400 -2.58913000 0.10766500

H 4.36988500 -2.72251000 2.21060900

H 5.00217300 -2.23128900 -2.00003600

H 5.51507200 -3.39987800 0.12111200

C -2.93470300 -0.51699900 0.06980300

C -3.57632800 -0.88764100 -1.12540900

C -3.20928900 -1.17556300 1.28220100

C -4.50492900 -1.93131000 -1.08215000

C -4.14833000 -2.20879700 1.27967400

C -4.79362300 -2.58913100 0.10766300

H -5.00217200 -2.23128800 -2.00003700

H -4.36988400 -2.72251200 2.21060800

H -5.51507100 -3.39987900 0.12111000

C -3.28783500 -0.17559600 -2.42416800

H -3.78451900 0.80004800 -2.47138300

H -2.21902700 0.00185900 -2.55616400

H -3.64496800 -0.76086800 -3.27382200

C -2.51468600 -0.76865000 2.55763000

H -1.42689000 -0.81983900 2.45470800

H -2.75036600 0.26212600 2.84046600

H -2.80881900 -1.41710400 3.38517900

C 3.28783400 -0.17559800 -2.42416800

H 2.21902600 0.00185800 -2.55616400

H 3.78451900 0.80004600 -2.47138500

H 3.64496600 -0.76087100 -3.27382300

C 2.51468600 -0.76864800 2.55763000

H 2.75036500 0.26212800 2.84046400

H 1.42689000 -0.81983800 2.45470800

H 2.80882000 -1.41710100 3.38518000

C -0.00000100 -1.52365300 -0.97712000

H -0.87897400 -1.60105400 -1.62855400

H 0.87897200 -1.60105400 -1.62855500

C 0.00000000 -2.72839400 -0.01594600

H -0.87712800 -2.69397500 0.64142400

H 0.87712800 -2.69397500 0.64142400

C 0.00000000 -4.08374500 -0.74323900

H -0.88312800 -4.18430000 -1.38210000

H 0.88312900 -4.18429900 -1.38210000

H 0.00000100 -4.92387500 -0.03852200

Co 0.00000000 0.20716300 -0.01227000

**0Co(0)-4**

Atom x y z

C 1.19275100 2.61014300 -0.33263400

C 1.20730800 3.96768400 -0.64207700

C -0.00007800 4.65222500 -0.80238800

C -1.20744000 3.96764600 -0.64211300

C -1.19283400 2.61010800 -0.33265900

N -0.00003400 1.94587300 -0.18603900

H -0.00009000 5.70686900 -1.05273300

H 2.14941800 4.48881100 -0.76902000

H -2.14957700 4.48872400 -0.76908100

C 2.31243600 1.72431600 -0.17844500

C -2.31249200 1.72429200 -0.17840000

N -1.97159000 0.47042400 0.09400400

N 1.97157000 0.47044400 0.09393000

C -3.72523100 2.20455800 -0.37895600

H -3.87081700 3.18817300 0.07327800

H -3.96906800 2.29982500 -1.44267900

H -4.44804300 1.51985600 0.06160000

C 3.72517800 2.20450600 -0.37914100

H 3.96947100 2.29813700 -1.44290500

H 3.87043300 3.18883000 0.07162900

H 4.44791500 1.52058200 0.06276300

C -2.99409200 -0.53673100 0.02925500

C -3.32213400 -1.06059400 -1.24174900

C -3.65831100 -0.99536000 1.18095300

C -4.24858200 -2.10052500 -1.32086400

C -4.58263100 -2.03806800 1.05282800

C -4.86738200 -2.60359500 -0.18137800

H -4.48799500 -2.51787800 -2.29471700

H -5.09137000 -2.39827500 1.94312200

H -5.57944500 -3.41898900 -0.25965100

C 2.99410300 -0.53667500 0.02904300

C 3.65871900 -0.99501400 1.18064100

C 3.32172800 -1.06085400 -1.24193200

C 4.58301700 -2.03773000 1.05248300

C 4.24816000 -2.10080000 -1.32107600

C 4.86735300 -2.60356900 -0.18167400

H 5.09204900 -2.39771100 1.94270200

H 4.48725500 -2.51840600 -2.29490000

H 5.57939800 -3.41897600 -0.25998800

C 3.48162500 -0.35886300 2.53985600

H 4.44112600 0.01779600 2.90899300

H 2.78743200 0.47737200 2.52126500

H 3.12264600 -1.07932100 3.28044700

C 2.73941800 -0.48801100 -2.51275900

H 1.72090500 -0.12736600 -2.37455800

H 3.33826200 0.35756500 -2.87106700

H 2.73501400 -1.23457600 -3.30960900

C -3.48080400 -0.35954100 2.54026200

H -2.78689400 0.47693200 2.52157600

H -4.44025700 0.01670100 2.90993800

H -3.12123900 -1.08008500 3.28048400

C -2.74014700 -0.48742000 -2.51257500

H -3.33847600 0.35888600 -2.87000400

H -1.72124700 -0.12770700 -2.37474100

H -2.73683000 -1.23350600 -3.30987900

C 0.00008800 -1.83897800 0.26567200

H 0.87775900 -2.23092700 0.79361700

H -0.87649700 -2.23164800 0.79489000

C -0.00071000 -2.42723000 -1.14796100

H 0.87219300 -2.08721400 -1.70964100

H -0.87520000 -2.08858500 -1.70798300

C 0.00045300 -3.96580600 -1.14534300

H 0.88399000 -4.35765600 -0.63106300

H -0.88156400 -4.35896900 -0.62945200

H -0.00018500 -4.37424300 -2.16312700

Co -0.00008600 0.20227700 0.46109500

C 0.00044700 -0.39268200 2.48610800

H 0.91095600 -0.94173900 2.67441100

H -0.90972500 -0.94202200 2.67521600

C 0.00020600 0.98432100 2.40666100

H -0.91235900 1.56059600 2.51044600

H 0.91261800 1.56095000 2.50977300

**0Co(0)-4/5**

Atom x y z

C 1.22933400 2.61767600 -0.26830000

C 1.25028100 3.98570500 -0.52148400

C 0.05165800 4.69127000 -0.65674600

C -1.16445300 4.01638800 -0.52959700

C -1.17942600 2.64810800 -0.27525200

N 0.01674300 1.96083100 -0.14904000

H 0.06590600 5.75507800 -0.86436400

H 2.19488800 4.50686900 -0.62086600

H -2.09557200 4.56035300 -0.63515900

C 2.33234600 1.72976800 -0.14138300

C -2.30157000 1.78617900 -0.15321400

N -1.96636800 0.50619400 0.06923800

N 1.97313500 0.45417500 0.06147000

C -3.72356300 2.25078200 -0.30188400

H -3.78156800 3.33433800 -0.39889400

H -4.20438500 1.81429900 -1.18306700

H -4.33415200 1.96164200 0.55838200

C 3.76545000 2.17466900 -0.24027400

H 4.29570800 1.67053000 -1.05346300

H 3.84101500 3.24760600 -0.41217100

H 4.31747500 1.94753100 0.67709500

C -3.01717700 -0.46665600 0.00311500

C -3.34439800 -1.01208300 -1.25818300

C -3.71243500 -0.88160200 1.15747900

C -4.31785300 -2.01172200 -1.33022900

C -4.68576100 -1.87757100 1.03655200

C -4.98190600 -2.45359800 -0.19253100

H -4.56004800 -2.44103500 -2.29843300

H -5.22255200 -2.19767600 1.92524400

H -5.73560800 -3.23128500 -0.26513000

C 3.01350200 -0.53221000 -0.01317100

C 3.71905900 -0.97606600 1.12130500

C 3.33718500 -1.04602100 -1.29300500

C 4.66630400 -1.99672800 0.97115600

C 4.29420900 -2.05509200 -1.39668900

C 4.94606300 -2.54764200 -0.27003800

H 5.20207700 -2.34585600 1.85011300

H 4.53003000 -2.45915000 -2.37705900

H 5.68067900 -3.34105300 -0.36520200

C 3.56969600 -0.34045100 2.48423900

H 4.52380300 0.09128700 2.80433700

H 2.82996000 0.45503600 2.49211500

H 3.28691700 -1.07123800 3.24766300

C 2.69474100 -0.49382200 -2.54270200

H 1.63204900 -0.29658200 -2.40355000

H 3.15216300 0.45769900 -2.83633200

H 2.81645200 -1.18346500 -3.38066700

C -3.45703200 -0.27035500 2.51435000

H -2.64374100 -0.77466600 3.04377400

H -3.18656600 0.78376300 2.44732200

H -4.34685200 -0.35173400 3.14289900

C -2.70759200 -0.50850200 -2.53176000

H -3.29359500 0.31051000 -2.96538700

H -1.70294400 -0.12230700 -2.36545300

H -2.65899100 -1.29867800 -3.28455200

C -0.26394400 -2.08033900 0.56326300

H 0.15476000 -2.90690900 1.13782600

H -1.34505000 -2.14813200 0.65722900

C 0.15486500 -2.33636800 -0.89142100

H 1.23801200 -2.28354900 -0.98806100

H -0.26457800 -1.58970200 -1.56665300

C -0.31267400 -3.73218900 -1.34051300

H 0.12817800 -4.51804700 -0.71880900

H -1.40027700 -3.82877000 -1.27780000

H -0.01802000 -3.92725000 -2.37695000

Co -0.01036400 0.23501600 0.40592800

C 0.17555700 -1.03086500 2.20052200

H 1.16910800 -1.43156900 2.35658400

H -0.58191400 -1.63404700 2.69114000

C 0.03897300 0.40172600 2.33356100

H -0.89140400 0.79509600 2.72711100

H 0.90725100 0.98290500 2.62445400

**0Co(0)-5**

Atom x y z

C 1.19080900 -3.06892500 0.04151500

C 1.20743800 -4.45501400 -0.07766500

C 0.00000500 -5.15755700 -0.12643500

C -1.20742900 -4.45501700 -0.07766200

C -1.19080300 -3.06892700 0.04151700

N 0.00000300 -2.38788700 0.13356400

H 0.00000600 -6.23729200 -0.22034200

H 2.15155800 -4.98499400 -0.13936100

H -2.15154800 -4.98499900 -0.13935600

C 2.30475700 -2.15342900 0.06080000

C -2.30475300 -2.15343400 0.06080100

N -1.94201300 -0.88422900 0.05837800

N 1.94201500 -0.88422500 0.05837800

C -3.72241100 -2.65181300 0.08702100

H -3.97238900 -3.17361100 -0.84270800

H -3.86542400 -3.36612900 0.90291600

H -4.43371500 -1.83848700 0.21742400

C 3.72241600 -2.65180500 0.08701700

H 3.86542700 -3.36613500 0.90290100

H 3.97239900 -3.17358800 -0.84272000

H 4.43371800 -1.83848100 0.21743600

C -2.93201500 0.14850800 0.09642900

C -3.19294400 0.78662600 1.32294600

C -3.58378700 0.54278900 -1.08575300

C -4.12780400 1.82329600 1.34770000

C -4.50777800 1.58919900 -1.01513000

C -4.78246200 2.22710400 0.18867800

H -4.33902100 2.32078200 2.28977700

H -5.01263300 1.90717700 -1.92275600

H -5.50082600 3.03996500 0.22341400

C 2.93201500 0.14851300 0.09643000

C 3.58378900 0.54279500 -1.08575000

C 3.19293900 0.78663300 1.32294800

C 4.50777800 1.58920700 -1.01512400

C 4.12779700 1.82330500 1.34770400

C 4.78245800 2.22711400 0.18868300

H 5.01263500 1.90718600 -1.92274900

H 4.33900900 2.32079300 2.28978200

H 5.50082000 3.03997600 0.22342100

C 3.31267500 -0.14731900 -2.40009000

H 3.83003300 -1.11109200 -2.46629400

H 2.24829200 -0.34397900 -2.53926300

H 3.65987200 0.46303300 -3.23611700

C 2.48785100 0.35521800 2.58449400

H 1.40091600 0.41025500 2.47423400

H 2.71954900 -0.68144800 2.84816300

H 2.77635900 0.98649700 3.42716700

C -3.31266600 -0.14732500 -2.40009200

H -2.24828000 -0.34396400 -2.53927100

H -3.83000400 -1.11110800 -2.46629000

H -3.65988100 0.46301700 -3.23612000

C -2.48785800 0.35521100 2.58449400

H -2.71955700 -0.68145500 2.84816200

H -1.40092300 0.41024800 2.47423700

H -2.77636900 0.98649000 3.42716600

C 0.00000100 1.15303200 -0.97333600

H 0.87909900 1.23026900 -1.62398300

H -0.87909700 1.23026900 -1.62398200

C -0.00000100 2.35299600 -0.00662200

H 0.87769100 2.31591900 0.65116800

H -0.87769300 2.31591400 0.65116800

C -0.00000400 3.71685900 -0.72255600

H 0.87690100 3.77327500 -1.38069100

H -0.87690900 3.77327100 -1.38069100

Co 0.00000000 -0.57766200 -0.01012800

C -0.00000700 4.91800300 0.22953300

H -0.87599200 4.85769300 0.88791400

H 0.87597800 4.85769600 0.88791500

C -0.00000900 6.26771400 -0.49338600

H -0.00001400 7.10515100 0.21132900

H 0.88187700 6.37591500 -1.13320300

H -0.88189200 6.37590800 -1.13320900

**0Co(0)-6**

Atom x y z

C 1.05483200 2.70133200 0.24281300

C 1.01042000 4.07671600 0.46290800

C -0.22051900 4.72060100 0.58758400

C -1.39729700 3.97294300 0.48938000

C -1.32673800 2.60202600 0.26746900

N -0.11004200 1.97282600 0.14337600

H -0.26392400 5.78886400 0.76548700

H 1.92897800 4.64539000 0.54787600

H -2.36025400 4.45909100 0.59590600

C 2.20854600 1.85958900 0.13999200

C -2.41907600 1.67394000 0.18450100

N -2.04715000 0.42015200 -0.01899100

N 1.92057800 0.57745500 -0.05500800

C -3.84224100 2.12619000 0.38486800

H -4.05834800 2.28355200 1.44729800

H -4.02955200 3.07343200 -0.12532200

H -4.55642800 1.39411000 0.01295500

C 3.60596600 2.38976000 0.31959100

H 3.66189300 3.45078200 0.07465700

H 3.94437000 2.27436100 1.35501300

H 4.32293000 1.86072600 -0.30829100

C -3.05736300 -0.59969900 0.03143300

C -3.75682700 -0.99748800 -1.12441500

C -3.33597400 -1.19156000 1.28102400

C -4.68679800 -2.03679200 -1.01568300

C -4.26925300 -2.22836600 1.33988500

C -4.93443900 -2.66227200 0.19943500

H -5.22981800 -2.34881700 -1.90320000

H -4.47488600 -2.69723900 2.29773100

H -5.65407800 -3.47247400 0.26023300

C 3.00612900 -0.36061000 -0.00114500

C 3.36887400 -0.89253800 1.25296200

C 3.70297400 -0.73363700 -1.16800600

C 4.37542200 -1.85984300 1.30511300

C 4.70941500 -1.69799800 -1.06527500

C 5.03593800 -2.27480100 0.15590400

H 4.64379200 -2.28716800 2.26712200

H 5.24774700 -1.99216000 -1.96177800

H 5.81309900 -3.03025100 0.21323900

C 2.73900600 -0.41158800 2.53873700

H 3.32770400 0.40130800 2.98061500

H 1.72927700 -0.03506200 2.38739100

H 2.69997700 -1.21418800 3.27855000

C 3.43260100 -0.09685600 -2.51127100

H 2.58816100 -0.55783100 -3.02907900

H 3.20873300 0.96803400 -2.42549300

H 4.30371200 -0.20135400 -3.16170200

C -2.67272100 -0.70022200 2.54437100

H -1.61272800 -0.49787300 2.39293400

H -3.13080700 0.23123900 2.89675500

H -2.77375800 -1.43417100 3.34630300

C -3.58091100 -0.30832900 -2.45757200

H -3.48643000 0.77444800 -2.35167000

H -2.69350700 -0.65381500 -2.99259600

H -4.44151700 -0.50334000 -3.10086000

C 0.01746400 -1.71164600 0.49164300

H 0.40739700 -1.49383700 1.49370900

H -1.03356900 -1.97860800 0.61541800

C 0.74302300 -2.93908500 -0.06125600

H 1.78000800 -2.70767800 -0.32366600

H 0.26362800 -3.27558600 -0.98798000

C 0.74424600 -4.11921000 0.92360400

H 1.26110400 -3.85902200 1.85314600

H -0.27631100 -4.41472000 1.18880600

H 1.24632400 -4.99723100 0.50141600

Co -0.03243600 0.17985100 -0.31992400

C -0.05366100 -0.88622000 -2.10189800

H 0.87072400 -1.43654700 -2.20468700

H -0.94423300 -1.50124200 -2.12861900

C -0.10707000 0.47465800 -2.36747400

H -1.04282300 0.97496300 -2.58278200

H 0.78168400 1.02693600 -2.64788700

**0Co(0)-TS6/7**

Atom x y z

C 1.16009900 2.70705900 -0.02135400

C 1.17633700 4.09369400 -0.13443700

C -0.03424900 4.78585000 -0.24347500

C -1.24041400 4.08222200 -0.23516900

C -1.22621100 2.69330200 -0.11457400

N -0.03045100 2.02822100 -0.00488300

H -0.03664100 5.86617600 -0.33371600

H 2.11583300 4.63464300 -0.14098600

H -2.17776300 4.61927300 -0.32078100

C 2.27978500 1.81099300 0.12766500

C -2.33525600 1.77930900 -0.03776400

N -1.97031900 0.50380700 0.03178100

N 1.93803300 0.53172700 0.15815100

C -3.76377800 2.24264500 0.04784500

H -4.18458000 2.04453000 1.03916900

H -3.84983100 3.31264100 -0.13887800

H -4.40323800 1.72258900 -0.66921000

C 3.68578500 2.32809400 0.26748200

H 4.33325000 1.59863700 0.75287900

H 4.12565700 2.55587600 -0.71012500

H 3.70972000 3.24791400 0.85539400

C -2.98869000 -0.46717100 0.31238600

C -3.69885000 -1.10099600 -0.72318200

C -3.24425600 -0.78547200 1.66142800

C -4.66682600 -2.05163500 -0.38536700

C -4.21761800 -1.74347000 1.95294200

C -4.92875000 -2.37611200 0.94000600

H -5.22157100 -2.54174600 -1.18041100

H -4.41514500 -1.99508900 2.99095000

H -5.68231000 -3.11880000 1.18225800

C 2.93906400 -0.45852100 0.42816000

C 3.03455200 -0.96084900 1.74436500

C 3.79111600 -0.93593800 -0.58428000

C 3.95584900 -1.97439600 2.01061000

C 4.69721100 -1.95553700 -0.27219000

C 4.77786400 -2.48197900 1.00938200

H 4.02827700 -2.36801500 3.02026200

H 5.35008300 -2.33332200 -1.05436800

H 5.48242200 -3.27725100 1.23127300

C 2.20061700 -0.38466000 2.86192600

H 2.53251900 0.62575800 3.12543300

H 1.14901400 -0.30197600 2.58353400

H 2.27567300 -1.00031700 3.76046300

C 3.80250900 -0.35172700 -1.97638600

H 2.88555700 0.18345700 -2.20984400

H 4.63338700 0.35363500 -2.09373300

H 3.94315900 -1.13261300 -2.72795700

C -2.47762400 -0.11879900 2.77614800

H -1.40078200 -0.25466200 2.65015200

H -2.65023900 0.96153500 2.80867700

H -2.76599400 -0.53015600 3.74552600

C -3.42869500 -0.79482800 -2.17463700

H -3.38000200 0.27808700 -2.37478900

H -2.47216100 -1.21612900 -2.49168000

H -4.20790100 -1.21911000 -2.81119300

C -0.03972900 -1.88105500 0.07737800

H 0.57088100 -1.85845200 0.98559000

H -1.07303100 -2.13026500 0.32506000

C 0.51798400 -2.79546900 -0.90852200

H 1.59244800 -2.97361900 -0.81725800

H 0.53763100 -2.10700400 -1.99947300

C -0.25163000 -4.03927400 -1.31821100

H -0.23153700 -4.78174100 -0.51217700

H -1.30283800 -3.80697600 -1.51350000

H 0.16851300 -4.51277700 -2.21196100

Co -0.01213900 0.18622700 -0.18740400

C 0.40216800 -1.16340600 -2.96598400

H 1.37940200 -1.28651500 -3.42935700

H -0.38543900 -1.67345300 -3.52117200

C 0.09479300 0.07112300 -2.30857600

H -0.90108400 0.46046900 -2.50161900

H 0.85662100 0.84235400 -2.40955600

**0Co(0)-7**

Atom x y z

C -1.26036600 2.52471000 -0.11679000

C -1.28219500 3.91904200 -0.10824300

C -0.08748600 4.63612900 -0.15715300

C 1.12707300 3.94420800 -0.17991600

C 1.12715400 2.55454000 -0.18288600

N -0.05733700 1.85238900 -0.20222500

H -0.10032100 5.71994900 -0.15566900

H -2.22616100 4.44894000 -0.06050300

H 2.06562500 4.48701600 -0.18976300

C -2.36243400 1.61848000 -0.07755400

C 2.26147900 1.68360100 -0.20050800

N 1.94864800 0.39538400 -0.11022400

N -1.99663300 0.33769900 -0.03108500

C 3.65736700 2.22914400 -0.35632200

H 3.72228300 2.90544200 -1.21314300

H 3.95564700 2.80126900 0.52840200

H 4.38919600 1.43695600 -0.49935800

C -3.79735800 2.06699500 -0.13231200

H -3.88012400 3.15074800 -0.05969600

H -4.28104200 1.76090400 -1.06480400

H -4.38282200 1.63120900 0.68117400

C 2.99931900 -0.56225200 -0.31067200

C 3.78613800 -1.00522400 0.76816000

C 3.23989200 -1.03171100 -1.61859500

C 4.77084600 -1.96782400 0.52933700

C 4.23017500 -1.99883700 -1.81090100

C 4.98687000 -2.47525000 -0.74639200

H 5.37406100 -2.32046900 1.36107300

H 4.41198800 -2.37395700 -2.81397200

H 5.74865800 -3.23038700 -0.91253700

C -3.02274900 -0.64358100 -0.24419400

C -3.33762600 -0.99089100 -1.57932700

C -3.70153900 -1.24953800 0.82801400

C -4.29504900 -1.97935500 -1.80930400

C -4.65605800 -2.23438000 0.54946300

C -4.94842900 -2.60810100 -0.75410300

H -4.53164000 -2.25595400 -2.83279700

H -5.17931900 -2.70464700 1.37772900

H -5.68753600 -3.37840800 -0.95039100

C -2.68978100 -0.29036900 -2.75052500

H -3.18149500 0.66557300 -2.96477900

H -1.63930500 -0.06312500 -2.56485300

H -2.76242800 -0.89830500 -3.65484700

C -3.47593900 -0.84032700 2.26340500

H -2.71882100 -0.06672800 2.35636800

H -4.40398200 -0.46180100 2.70484700

H -3.16244300 -1.69133300 2.87516400

C 2.50193700 -0.46337200 -2.80670700

H 1.45008900 -0.27846800 -2.58739600

H 2.93297200 0.49784400 -3.10974600

H 2.56954800 -1.13375600 -3.66624700

C 3.61769400 -0.42525800 2.14861700

H 4.15946100 0.52295600 2.24470100

H 2.57441200 -0.21840500 2.37433700

H 4.01282000 -1.10127200 2.90993100

C -0.07133800 -1.87968000 -0.72554700

H -0.95626700 -1.80247200 -1.33963200

H 0.85342000 -2.08615100 -1.25163600

C -0.15212600 -2.13042700 0.62345200

H -1.13745500 -2.16512400 1.07688800

H -0.80541400 -1.12418900 3.30255200

C 0.92163500 -2.87741800 1.37130800

H 0.62643400 -3.93274600 1.44233400

H 1.87881700 -2.84697100 0.85227800

H 1.06818800 -2.52468700 2.39085200

Co -0.02051000 0.06810100 0.20532500

C -0.05220000 -0.33722900 3.38427000

H -0.27363800 0.21362300 4.31043900

H 0.90848400 -0.82990100 3.54846200

C -0.03593600 0.61041700 2.18957900

H 0.82793400 1.28041800 2.26541500

H -0.92263700 1.25193000 2.22388300

**0Co(0)-8**

Atom x y z

C 1.19171000 2.55097400 -0.18993400

C 1.20737200 3.94145400 -0.15270900

C -0.00000800 4.64595300 -0.14650800

C -1.20738400 3.94144800 -0.15270600

C -1.19171300 2.55096800 -0.18993200

N 0.00000000 1.86462500 -0.24592500

H -0.00001000 5.72931100 -0.11561100

H 2.15141400 4.47424600 -0.11999300

H -2.15142800 4.47423400 -0.11998500

C 2.30473100 1.63764900 -0.14610000

C -2.30473300 1.63763700 -0.14609900

N -1.94131000 0.37034000 -0.06187900

N 1.94131000 0.37035000 -0.06186600

C -3.72280400 2.13312900 -0.20101700

H -3.97752100 2.69855300 0.70164300

H -3.86328100 2.80715500 -1.05074200

H -4.43332400 1.31401200 -0.29467100

C 3.72280000 2.13314500 -0.20103800

H 3.86328000 2.80711400 -1.05080800

H 3.97750600 2.69863200 0.70158500

H 4.43332500 1.31402600 -0.29463100

C -2.92978900 -0.66328800 -0.02294900

C -3.18077200 -1.39988800 -1.19559800

C -3.59150600 -0.96131200 1.18188900

C -4.11539100 -2.43552500 -1.14378600

C -4.51334400 -2.01195000 1.18932700

C -4.77867800 -2.74514800 0.03910100

H -4.31933000 -3.00762400 -2.04421900

H -5.02432900 -2.25663400 2.11608900

H -5.49591200 -3.55935700 0.06476400

C 2.92979100 -0.66327500 -0.02293000

C 3.59146800 -0.96133000 1.18192400

C 3.18081000 -1.39985100 -1.19558700

C 4.51331300 -2.01196100 1.18936300

C 4.11543300 -2.43548400 -1.14377100

C 4.77868900 -2.74512900 0.03912800

H 5.02427000 -2.25666600 2.11613500

H 4.31939900 -3.00756300 -2.04421100

H 5.49592800 -3.55933300 0.06479300

C 3.33425200 -0.16570700 2.43818500

H 3.88915200 0.77929700 2.43853500

H 2.27759800 0.08204200 2.54934900

H 3.64958600 -0.72434800 3.32171900

C 2.46575000 -1.07246100 -2.48257400

H 1.38005300 -1.14119200 -2.36653200

H 2.67602500 -0.05276700 -2.81923700

H 2.76522500 -1.75651000 -3.27897700

C -3.33434700 -0.16563900 2.43813000

H -2.27770800 0.08216900 2.54930400

H -3.88929600 0.77933700 2.43844000

H -3.64966600 -0.72426700 3.32167700

C -2.46568700 -1.07251100 -2.48257500

H -2.67594400 -0.05281500 -2.81924200

H -1.37999200 -1.14125400 -2.36651400

H -2.76515600 -1.75655800 -3.27898100

C 0.00001900 -1.54644500 1.16670300

H 0.87925800 -1.56732200 1.81910000

H -0.87920400 -1.56729800 1.81912300

C -0.00000800 -2.81636700 0.29254900

H 0.88365600 -2.88065000 -0.35026600

H -0.88369500 -2.88063500 -0.35023600

Co 0.00001100 0.07221600 0.02890300

H -0.00000600 -3.72888000 0.90699500

**0Co(0)-TS3/9**

Atom x y z

C -1.14806300 2.57073500 0.06427900

C -1.14032900 3.96128900 0.08726200

C 0.07196200 4.65397900 0.11689200

C 1.27039900 3.93797000 0.11188700

C 1.25180400 2.54726100 0.08769200

N 0.04433400 1.86685500 0.07855600

H 0.08235000 5.73763100 0.13278400

H -2.07386100 4.51137300 0.07970500

H 2.21474700 4.46934500 0.12332500

C -2.26512300 1.69098400 0.00045500

C 2.35319800 1.64732700 0.04739600

N 1.98553300 0.36714900 -0.00668200

N -1.92422100 0.40209300 -0.03366300

C 3.78859600 2.09511900 0.05452100

H 3.86810800 3.17976800 -0.00569900

H 4.30660800 1.77542700 0.96392900

H 4.34557400 1.67308800 -0.78598100

C -3.68903300 2.17273900 -0.04944900

H -3.73892300 3.25843000 -0.12061300

H -4.22222500 1.75821800 -0.90900900

H -4.25151400 1.87314400 0.83977100

C 3.02062900 -0.61907000 -0.08229800

C 3.57686700 -1.15311600 1.09778300

C 3.45938900 -1.05245000 -1.34957600

C 4.55614000 -2.14379600 0.98481900

C 4.44117100 -2.04487400 -1.41406200

C 4.98508500 -2.59359800 -0.25872400

H 4.98604100 -2.56503300 1.88913300

H 4.78084600 -2.38816200 -2.38709500

H 5.74215800 -3.36847100 -0.32683200

C -2.99182000 -0.54820700 -0.12362000

C -3.39586500 -1.00582200 -1.39366900

C -3.62951300 -1.00338200 1.04675600

C -4.42409700 -1.94932900 -1.46786900

C -4.65691500 -1.94309300 0.92471800

C -5.05112000 -2.42055400 -0.31999300

H -4.73666800 -2.31305200 -2.44253400

H -5.14886300 -2.30558000 1.82288800

H -5.84608500 -3.15581200 -0.39538000

C -2.77507800 -0.45709100 -2.65519100

H -3.17025700 0.53763900 -2.89114500

H -1.69402600 -0.34744200 -2.56104800

H -2.99068700 -1.10262900 -3.50930600

C -3.23322500 -0.48811700 2.40908000

H -2.15574000 -0.33980500 2.48717300

H -3.70253900 0.47828700 2.62544100

H -3.54743000 -1.18064300 3.19290900

C 2.92564700 -0.43124400 -2.61794000

H 1.85745000 -0.22142500 -2.55199400

H 3.41889900 0.52437600 -2.83017700

H 3.10268400 -1.08313900 -3.47608000

C 3.15939800 -0.65712300 2.46154000

H 3.65481400 0.28786200 2.71162300

H 2.08626200 -0.47073600 2.51852900

H 3.43065500 -1.37720100 3.23657700

C 0.02836100 -1.82000300 -0.76003300

H -0.92793900 -2.07047200 -1.20474400

H 0.87958500 -1.87960700 -1.42565500

C 0.21107100 -2.04196100 0.61985800

H 0.04393000 -0.60839900 1.47163700

H 1.23968800 -2.16565200 0.94058000

C -0.75456300 -2.86417400 1.44709100

H -1.78889900 -2.73050700 1.13700900

H -0.50618500 -3.92301200 1.30829100

H -0.67999600 -2.64559600 2.51541100

Co 0.02711400 0.05491400 0.11635000

**0Co(0)-9**

Atom x y z

C 1.28344900 2.58177800 -0.13753300

C 1.31540900 3.97098300 -0.10553800

C 0.12310600 4.70061200 -0.09213800

C -1.09905100 4.02253000 -0.09741600

C -1.12615300 2.63306600 -0.13000300

N 0.06376800 1.91609400 -0.17903200

H 0.14632200 5.78377800 -0.06448000

H 2.26671100 4.49037300 -0.08140600

H -2.02731500 4.58172400 -0.06695200

C 2.36910700 1.66289900 -0.12378000

C -2.24870500 1.76025500 -0.11296600

N -1.90968700 0.46996100 -0.06041800

N 1.97749000 0.38795400 -0.06917300

C -3.66998900 2.24728200 -0.16057600

H -4.14493600 2.22039600 0.82578600

H -3.72202600 3.27382100 -0.52342500

H -4.27925200 1.62713800 -0.82164400

C 3.80903400 2.09157200 -0.17273300

H 3.90449600 3.10599500 -0.56041300

H 4.27557000 2.07110700 0.81792000

H 4.39707300 1.43110000 -0.81320200

C -2.94733500 -0.51420400 -0.06975500

C -3.25063700 -1.16312000 -1.28632400

C -3.63739600 -0.84170600 1.11282300

C -4.23313900 -2.15346300 -1.29140500

C -4.61000000 -1.84675800 1.06160500

C -4.90756400 -2.50273300 -0.12482700

H -4.47205900 -2.65607600 -2.22411800

H -5.13867300 -2.11221900 1.97306100

H -5.66366500 -3.28125400 -0.14405100

C 2.97265500 -0.64007100 -0.06671800

C 3.64331100 -0.98840200 1.12070900

C 3.24612100 -1.31723800 -1.27525000

C 4.56387900 -2.04217800 1.08322300

C 4.17823500 -2.35490700 -1.26723200

C 4.83092000 -2.72548300 -0.09464200

H 5.07718100 -2.32302800 1.99891200

H 4.39474700 -2.87792600 -2.19421800

H 5.54725100 -3.54095700 -0.10320400

C 3.42762500 -0.25039300 2.42163800

H 4.27092200 0.41568100 2.63681300

H 2.52301000 0.35437100 2.40895000

H 3.35713000 -0.94944500 3.25915200

C 2.56464300 -0.91824700 -2.56111300

H 1.47947900 -1.02965600 -2.49735700

H 2.74869100 0.13099200 -2.80962400

H 2.92060600 -1.52831400 -3.39376600

C -3.38389100 -0.13122900 2.42207100

H -2.43765500 0.40668300 2.42334800

H -4.17877100 0.59274200 2.63459400

H -3.37315600 -0.84045700 3.25383500

C -2.55434900 -0.77725800 -2.56850700

H -2.74017100 0.26894300 -2.83009300

H -1.46964500 -0.88205500 -2.49202400

H -2.89985400 -1.39629900 -3.39889500

C 0.00965700 -1.16240500 1.50226800

H 0.85515800 -1.15260600 2.18431100

H -0.92836900 -1.22734700 2.04881500

C 0.12742900 -2.16236300 0.36964400

H 1.15585500 -2.50941800 0.26768300

H -0.05828000 -1.64703800 -0.63312900

C -0.83054600 -3.35927900 0.40728400

H -0.60504100 -3.97591400 1.28233600

H -1.87213700 -3.04680000 0.47964100

H -0.72594200 -3.98744300 -0.48304000

Co 0.02595600 0.14348600 0.04531000

**0Co(0)-10**

Atom x y z

C -1.19939700 2.42431300 -0.16148500

C -1.21006000 3.81360500 -0.11279200

C 0.00001200 4.51591100 -0.11293600

C 1.21007800 3.81360100 -0.11281700

C 1.19940900 2.42430700 -0.16151400

N 0.00000100 1.74620600 -0.25784600

H 0.00001400 5.59905000 -0.07555800

H -2.15211100 4.34862700 -0.05928600

H 2.15213500 4.34861500 -0.05933000

C -2.29981400 1.50062500 -0.08341000

C 2.29981700 1.50061400 -0.08347300

N 1.91054200 0.23798200 -0.00214700

N -1.91055900 0.23799200 -0.00208400

C 3.72988600 1.96109800 -0.09089700

H 3.92303800 2.62320700 -0.93968100

H 3.96572200 2.52578700 0.81748900

H 4.42018700 1.12108000 -0.15040700

C -3.72988100 1.96112300 -0.09081700

H -3.92303200 2.62328000 -0.93956100

H -4.42018300 1.12111300 -0.15039100

H -3.96573100 2.52574600 0.81760500

C 2.85088200 -0.84014600 0.02356100

C 3.39828200 -1.26706200 1.24735000

C 3.15889300 -1.49321800 -1.18418100

C 4.27065900 -2.35815300 1.23593500

C 4.03549900 -2.57987100 -1.14747400

C 4.59021300 -3.01300700 0.05174800

H 4.69839800 -2.69924700 2.17420600

H 4.28087100 -3.09179200 -2.07346900

H 5.26674000 -3.86173500 0.06398700

C -2.85090400 -0.84013200 0.02361100

C -3.15896800 -1.49312200 -1.18416100

C -3.39823100 -1.26713700 1.24739900

C -4.03555100 -2.57979200 -1.14748700

C -4.27059700 -2.35823900 1.23595000

C -4.59020000 -3.01301700 0.05173600

H -4.28095800 -3.09165800 -2.07350300

H -4.69828300 -2.69940400 2.17421900

H -5.26670900 -3.86175900 0.06395200

C -2.56192400 -1.03190400 -2.49127000

H -2.87857500 -0.01652700 -2.74943400

H -1.46930400 -1.01294300 -2.45091700

H -2.86048200 -1.69094800 -3.30877300

C -3.04763000 -0.57425900 2.53865900

H -1.96375800 -0.50380600 2.65748600

H -3.44042900 0.44752000 2.57475800

H -3.45923900 -1.11426600 3.39365100

C 2.56175200 -1.03214800 -2.49129900

H 1.46912800 -1.01338700 -2.45091200

H 2.87823300 -0.01673700 -2.74951800

H 2.86038600 -1.69119000 -3.30877900

C 3.04775400 -0.57409300 2.53858200

H 3.44063900 0.44765600 2.57461400

H 1.96389100 -0.50354900 2.65742800

H 3.45933800 -1.11408400 3.39359600

H 0.00002300 -0.81000700 1.41817600

Co 0.00001100 -0.00345500 0.12451000

**1Co(0)**

**1Co(0)-1**

Atom x y z

C -1.18657500 2.36864300 0.13461400

C -1.20456800 3.75292600 0.26948600

C -0.00000200 4.45991500 0.31884900

C 1.20456400 3.75293600 0.26952200

C 1.18658900 2.36864600 0.13467500

N 0.00001100 1.69254600 0.00696200

H -0.00000500 5.53855500 0.42484800

H -2.14655400 4.28252800 0.34971400

H 2.14654500 4.28254800 0.34975200

C -2.37122400 1.51410400 0.14346700

C 2.37123000 1.51410500 0.14356500

N 2.14346100 0.23042300 0.10936100

N -2.14345300 0.23042500 0.10938700

C 3.74332700 2.13870400 0.21001200

H 3.93258100 2.77734400 -0.65798700

H 3.84243800 2.76721100 1.09970000

H 4.52062200 1.37791900 0.24896800

C -3.74332000 2.13871800 0.20981000

H -3.84256800 2.76695000 1.09968600

H -3.93239400 2.77762800 -0.65801900

H -4.52064200 1.37794500 0.24842000

C 3.19230300 -0.72851100 0.10985800

C 3.44905000 -1.43118500 1.30341300

C 3.88644400 -1.03636900 -1.07669600

C 4.43018000 -2.42370900 1.29881900

C 4.85512500 -2.04256700 -1.03607300

C 5.13370900 -2.73119000 0.13906500

H 4.63806700 -2.96460900 2.21762900

H 5.39253700 -2.29039400 -1.94690700

H 5.88876100 -3.51071100 0.14889900

C -3.19230400 -0.72850200 0.10985700

C -3.88636800 -1.03641300 -1.07674200

C -3.44916000 -1.43108500 1.30342900

C -4.85508200 -2.04257200 -1.03612200

C -4.43033000 -2.42358000 1.29882700

C -5.13377700 -2.73111200 0.13904600

H -5.39243600 -2.29044800 -1.94697600

H -4.63830600 -2.96439900 2.21766400

H -5.88885500 -3.51060800 0.14886500

C -3.58450600 -0.31638600 -2.36738900

H -3.91186600 0.72855700 -2.34366500

H -2.51293100 -0.31399100 -2.57807900

H -4.09354700 -0.79639300 -3.20538200

C -2.67702900 -1.11539400 2.56000500

H -1.59998000 -1.24426300 2.41086600

H -2.82246500 -0.08066300 2.88517200

H -2.98158000 -1.76837800 3.38023600

C 3.58473200 -0.31622100 -2.36731300

H 2.51316800 -0.31367300 -2.57805100

H 3.91221900 0.72867900 -2.34350600

H 4.09375300 -0.79623100 -3.20531700

C 2.67685000 -1.11552400 2.55995400

H 2.82255700 -0.08089200 2.88533400

H 1.59978200 -1.24403400 2.41066800

H 2.98112300 -1.76874300 3.38010000

Co 0.00003600 -0.21477200 -0.38311300

C -0.00002800 -1.56696000 -1.87893800

H -0.88485700 -2.21467400 -1.86271000

H -0.00006900 -1.06149800 -2.85511600

H 0.88479300 -2.21468400 -1.86275000

**1Co(0)-2**

Atom x y z

C 1.18519200 2.34289400 -0.03836600

C 1.18085300 3.74798300 -0.05708000

C -0.01153500 4.43916900 -0.00396200

C -1.20983200 3.70667900 0.03881000

C -1.17695800 2.32051400 0.04131600

N 0.00211200 1.62806800 0.01913200

H -0.02782100 5.52318000 -0.00562800

H 2.11918500 4.28662200 -0.10789100

H -2.15558800 4.23123800 0.05832100

C 2.40087600 1.57077500 -0.07369000

C -2.43444700 1.53366700 0.00388200

N -2.34735800 0.25638900 0.10906200

N 2.26518700 0.25969100 0.03914600

C -3.73988700 2.27828400 -0.19136100

H -3.92730100 2.96493400 0.63911400

H -3.72582000 2.87439500 -1.10728300

H -4.57586900 1.58395400 -0.24591000

C 3.73424800 2.26193800 -0.23323500

H 3.77077100 2.86500200 -1.14557200

H 3.93905400 2.93482700 0.60575500

H 4.54669900 1.53908100 -0.27825900

C -3.47761100 -0.58949500 -0.04457100

C -3.85762100 -0.99673900 -1.34179400

C -4.16005200 -1.07550400 1.08915600

C -4.89769000 -1.91853300 -1.47539900

C -5.20166900 -1.98814400 0.90395400

C -5.56736100 -2.42011600 -0.36519700

H -5.18597600 -2.24144400 -2.47165900

H -5.73320400 -2.36058900 1.77516600

H -6.37330700 -3.13632100 -0.48868600

C 3.39712100 -0.60849400 -0.04512600

C 4.03709800 -1.06052500 1.12495300

C 3.83267600 -1.04884900 -1.31432100

C 5.08816200 -1.97552200 1.00724100

C 4.88071900 -1.96793200 -1.38358400

C 5.50549100 -2.43831900 -0.23346200

H 5.58560700 -2.32286000 1.90870500

H 5.21143200 -2.31508700 -2.35821700

H 6.31929700 -3.15284700 -0.30578500

C 3.62751500 -0.58418600 2.49826100

H 3.22618600 0.42978000 2.48261300

H 2.86099800 -1.23270800 2.93557400

H 4.48036100 -0.59765400 3.18097500

C 3.20161800 -0.52215400 -2.57841400

H 2.11384300 -0.58145900 -2.53736700

H 3.45993400 0.52898500 -2.74943100

H 3.54391600 -1.08728000 -3.44756700

C -3.80189700 -0.62240300 2.48411900

H -2.88326400 -1.09505800 2.84328600

H -3.64867400 0.45819000 2.54315200

H -4.59516700 -0.88245900 3.18799100

C -3.18009900 -0.43113800 -2.56512500

H -3.48994100 0.60350400 -2.75402100

H -2.09514100 -0.42942300 -2.46048400

H -3.43668000 -1.01189400 -3.45329400

C -0.04179500 -1.80753100 -1.42003000

H 0.02316000 -1.44048900 -2.45158200

H 0.72702700 -2.58608800 -1.31686100

H -1.01515900 -2.29774800 -1.30966000

C -0.17780600 -1.81453700 1.75996800

H 0.67235500 -2.48415600 1.67597200

H -1.13014500 -2.20826400 1.42602000

C -0.07501200 -0.61863500 2.37665400

H -0.93602800 0.01740400 2.52963900

H 0.86299900 -0.26723100 2.78561200

Co 0.28410700 -0.38511000 -0.01984000

**1Co(0)-TS-2/3**

Atom x y z

C 1.18988900 2.39933000 -0.20220800

C 1.20525700 3.78742900 -0.29688400

C 0.00455000 4.50068000 -0.31720100

C -1.19848600 3.79228700 -0.28042800

C -1.18694000 2.40410000 -0.18659300

N 0.00061400 1.71178000 -0.11169800

H 0.00632000 5.58268600 -0.38035300

H 2.14893300 4.31627800 -0.36491300

H -2.14105900 4.32468200 -0.33504100

C 2.37695700 1.55927300 -0.24442500

C -2.37585000 1.56749200 -0.21282800

N -2.18139000 0.28740800 -0.02897600

N 2.18284100 0.28035400 -0.05638400

C -3.72539600 2.19178800 -0.48030800

H -3.98741500 2.91382300 0.29936000

H -3.73407600 2.73089500 -1.43200300

H -4.50903900 1.43669100 -0.51300600

C 3.72307200 2.17998200 -0.53670400

H 3.71483000 2.71879100 -1.48853200

H 4.00220100 2.90137000 0.23756500

H 4.50354400 1.42230200 -0.58460100

C -3.23820500 -0.65304400 -0.15271400

C -3.43632000 -1.29074900 -1.39556100

C -4.01945100 -1.00782100 0.96603700

C -4.41238500 -2.28428600 -1.49532200

C -4.98748200 -2.00454400 0.81938300

C -5.18604700 -2.64609900 -0.39808500

H -4.56651600 -2.77694200 -2.45124900

H -5.59362400 -2.27836600 1.67839900

H -5.93984500 -3.42133500 -0.49131900

C 3.23418600 -0.66588400 -0.17527900

C 4.04703500 -0.97999800 0.93359800

C 3.39718400 -1.34931600 -1.39892200

C 5.00166200 -1.99145400 0.80051100

C 4.36392900 -2.35289300 -1.48637300

C 5.16172100 -2.68150200 -0.39584200

H 5.62932900 -2.23675300 1.65267300

H 4.49148300 -2.88053500 -2.42744700

H 5.90576000 -3.46725800 -0.47883900

C 3.91211800 -0.23089100 2.23636100

H 4.16043900 0.82969300 2.12587200

H 2.89388300 -0.27137800 2.62806700

H 4.58077800 -0.64564700 2.99337700

C 2.56442800 -0.98414800 -2.60295800

H 1.49434300 -1.00663400 -2.38159200

H 2.78287700 0.02949600 -2.95509100

H 2.75440700 -1.66941900 -3.43148400

C -3.82530200 -0.33004400 2.29977700

H -2.83537200 -0.53369100 2.71510300

H -3.91414700 0.75765400 2.22731500

H -4.56761300 -0.67578200 3.02204200

C -2.62180500 -0.89490500 -2.60208700

H -2.83837200 0.13014500 -2.92076100

H -1.54904800 -0.93230400 -2.39621200

H -2.83014500 -1.55399500 -3.44727800

C -0.11927300 -2.19313400 0.40293000

H 0.15327700 -1.91482900 -0.63371800

H 0.54687500 -3.01357100 0.66037100

H -1.15096700 -2.53843500 0.41173800

C 0.13138600 -1.34796300 2.18412400

H 1.10411500 -1.78714700 2.37938400

H -0.67338800 -1.96842800 2.56978900

C 0.02236400 0.07527200 2.37336800

H -0.90815700 0.48457700 2.75424400

H 0.90411400 0.62489700 2.68898600

Co -0.00259100 -0.11118800 0.38949500

**1Co(0)-3**

Atom x y z

C 1.18583200 2.67571500 0.10616600

C 1.20677500 4.06507000 0.03196000

C 0.00009800 4.77249000 0.03276400

C -1.20661600 4.06512200 0.03195700

C -1.18572700 2.67577300 0.10617000

N 0.00002700 2.00769300 0.25831300

H 0.00011800 5.85468700 -0.02788900

H 2.14657300 4.59810200 -0.05356500

H -2.14638800 4.59819900 -0.05356500

C 2.33869100 1.79857900 -0.03424000

C -2.33863600 1.79868500 -0.03424700

N -2.05967300 0.52199100 -0.15754700

N 2.05967500 0.52188100 -0.15758000

C -3.73055200 2.37676500 -0.05949200

H -3.99218600 2.82686700 0.90323900

H -3.80972000 3.16383000 -0.81412600

H -4.47265300 1.61497600 -0.29141600

C 3.73064800 2.37654900 -0.05941500

H 3.80990700 3.16361100 -0.81404500

H 3.99229200 2.82661600 0.90332500

H 4.47268900 1.61470000 -0.29133600

C -3.07620400 -0.46536400 -0.29120600

C -3.21970600 -1.09301600 -1.54538200

C -3.84885400 -0.87263800 0.81430800

C -4.16372200 -2.11081300 -1.68210500

C -4.77505500 -1.90403300 0.63291200

C -4.94028100 -2.51858300 -0.60207400

H -4.28437700 -2.59294100 -2.64792300

H -5.36918100 -2.23072500 1.48160900

H -5.66318700 -3.31932700 -0.72086900

C 3.07621000 -0.46549600 -0.29117000

C 3.84876300 -0.87277300 0.81441300

C 3.21984800 -1.09310100 -1.54534300

C 4.77497400 -1.90417000 0.63309100

C 4.16387300 -2.11091000 -1.68199300

C 4.94030600 -2.51871300 -0.60188900

H 5.36900600 -2.23089500 1.48184100

H 4.28462400 -2.59301500 -2.64781000

H 5.66321100 -3.31946800 -0.72062100

C 3.69351600 -0.23103100 2.17159700

H 4.24269300 0.71447700 2.24066500

H 2.64878200 -0.01641300 2.40142300

H 4.08234800 -0.88584500 2.95384600

C 2.37357200 -0.66452000 -2.71722000

H 1.30655000 -0.74220500 -2.48831900

H 2.55477500 0.37878400 -2.99361100

H 2.57777100 -1.28294500 -3.59348300

C -3.69364100 -0.23092400 2.17150900

H -2.64886800 -0.01661600 2.40146900

H -4.24253300 0.71474800 2.24053400

H -4.08276300 -0.88562700 2.95370300

C -2.37327200 -0.66448400 -2.71716200

H -2.55424100 0.37887400 -2.99347000

H -1.30628000 -0.74241400 -2.48817900

H -2.57751000 -1.28280800 -3.59348800

C -0.00008100 -1.59217100 1.58988000

H 0.87493800 -1.59032100 2.25564500

H -0.87489800 -1.59010100 2.25590000

C -0.00039300 -2.89071600 0.76399600

H 0.87524500 -2.91651000 0.10201300

H -0.87623800 -2.91625300 0.10227700

C -0.00041100 -4.17018800 1.61519300

H 0.88218500 -4.20890700 2.26221300

H -0.88284900 -4.20870900 2.26244000

H -0.00058800 -5.07527900 0.99641500

Co 0.00003100 0.05375100 0.42648100

**1Co(0)-4**

Atom x y z

C 1.19426900 2.41273000 -0.52134700

C 1.23531200 3.75138500 -0.87879700

C 0.04223800 4.48102800 -1.02022600

C -1.15321900 3.82786500 -0.81350700

C -1.16682200 2.46960300 -0.44873700

N 0.01292100 1.75989400 -0.29237700

H 0.06543400 5.52973300 -1.29405800

H 2.18346200 4.24027700 -1.05604100

H -2.08907500 4.36016000 -0.92905900

C 2.45206900 1.63141600 -0.41403200

C -2.39011400 1.74659400 -0.22958500

N -2.27302100 0.49429100 0.18827200

N 2.38795000 0.44965500 0.08328900

C -3.71871300 2.42783400 -0.46047300

H -3.83353100 3.29534300 0.19728000

H -3.82297400 2.78836600 -1.48821800

H -4.54753400 1.75270300 -0.25739800

C 3.73298400 2.26450100 -0.92101900

H 3.63519200 2.58095400 -1.96235200

H 3.99276200 3.15152900 -0.33606100

H 4.56365800 1.56531400 -0.85032000

C -3.41593400 -0.35722100 0.26777500

C -3.97169000 -0.89119200 -0.91591900

C -3.95069700 -0.70520000 1.52436500

C -5.02851400 -1.79893000 -0.81229900

C -5.01509600 -1.60794100 1.57946800

C -5.54850800 -2.16457800 0.42326900

H -5.44803500 -2.22173600 -1.72081500

H -5.43121700 -1.87229800 2.54758300

H -6.36956000 -2.87175000 0.48434000

C 3.52141700 -0.40294700 0.14633700

C 4.28479000 -0.47526400 1.32981500

C 3.82570200 -1.22692000 -0.95741200

C 5.32523000 -1.40463900 1.39914000

C 4.87069800 -2.14555100 -0.83836100

C 5.61568600 -2.24536500 0.33088800

H 5.91712500 -1.46256300 2.30820400

H 5.10155300 -2.78849400 -1.68288100

H 6.42211900 -2.96760000 0.40659200

C 4.01556300 0.44418700 2.49623000

H 4.00002000 1.49600900 2.19540900

H 3.05328900 0.23702600 2.97104100

H 4.78715500 0.33305400 3.26059700

C 3.06552900 -1.09845800 -2.25329700

H 1.98972400 -1.04333200 -2.08651500

H 3.35287300 -0.19168500 -2.79870600

H 3.26752700 -1.94735700 -2.90920700

C -3.41354600 -0.10912100 2.80205100

H -2.48163500 -0.59034400 3.11244400

H -3.20634400 0.95826300 2.69972100

H -4.12806700 -0.23628500 3.61809600

C -3.47263200 -0.48209000 -2.28052900

H -3.92647900 0.46132000 -2.60462800

H -2.39174300 -0.34321100 -2.29893000

H -3.72977900 -1.23482200 -3.02843600

C 0.00299600 -2.07678200 -0.38498500

H 1.07227600 -2.30430500 -0.27322900

H -0.50076900 -2.69393600 0.37879600

C -0.48201700 -2.54668200 -1.76119600

H -0.09558900 -1.89322300 -2.55531100

H -1.57205400 -2.45923200 -1.81497200

C -0.09571300 -3.99612500 -2.09515800

H 0.99178900 -4.12527400 -2.08998300

H -0.50733700 -4.69056700 -1.35513900

H -0.46334100 -4.30408900 -3.08133200

Co -0.29214800 -0.18158000 0.28542300

C 0.39315400 -0.84084600 2.47383700

H 1.34917700 -1.27050900 2.20080900

H -0.39487500 -1.54798500 2.70983800

C 0.22405100 0.48493300 2.63177700

H -0.71467300 0.90468000 2.97158000

H 1.03169900 1.18430200 2.46212200

**1Co(0)-TS-4/5**

Atom x y z

C 1.14936700 2.52116500 -0.30167000

C 1.13233900 3.90704500 -0.47066900

C -0.07430100 4.59199400 -0.54061500

C -1.26417500 3.85598600 -0.46315100

C -1.22501400 2.47898100 -0.29224900

N -0.02985200 1.80414400 -0.18907600

H -0.09658100 5.66852700 -0.66414900

H 2.06692100 4.45002800 -0.54911600

H -2.21602000 4.36576500 -0.54633200

C 2.36047800 1.73722100 -0.25466600

C -2.43445000 1.65648900 -0.26051600

N -2.28529200 0.38833100 -0.02043500

N 2.21996700 0.45855500 0.02014700

C -3.77339100 2.30833900 -0.53301300

H -4.00123800 3.06900300 0.21939100

H -3.78446800 2.80556200 -1.50658400

H -4.57637300 1.57358000 -0.51914300

C 3.69356400 2.39822600 -0.52416400

H 3.71384800 2.88319400 -1.50448400

H 3.90881800 3.17137800 0.22020200

H 4.50586700 1.67422300 -0.49076500

C -3.38002000 -0.51344600 -0.08631300

C -3.66862200 -1.14880500 -1.31367800

C -4.12291700 -0.82799100 1.07098700

C -4.66459600 -2.12740800 -1.34894500

C -5.11248000 -1.81054100 0.98778100

C -5.38004900 -2.46923800 -0.20713700

H -4.88246400 -2.62197400 -2.29146700

H -5.68428600 -2.05580700 1.87838300

H -6.14763900 -3.23524300 -0.25013900

C 3.32681900 -0.42878300 -0.04737100

C 4.02785700 -0.77931200 1.12517100

C 3.67197700 -1.01420900 -1.28481900

C 5.04700000 -1.73127100 1.04304400

C 4.69386600 -1.96617900 -1.32023900

C 5.37838000 -2.33166900 -0.16652200

H 5.58914000 -2.00038400 1.94527500

H 4.95684200 -2.42105300 -2.27125600

H 6.16899500 -3.07390800 -0.21081900

C 3.70584500 -0.12265500 2.44414500

H 3.78420300 0.96692100 2.38533900

H 2.68639900 -0.34127500 2.76886300

H 4.38791700 -0.46436200 3.22545400

C 2.97323200 -0.60432500 -2.55811100

H 1.88699600 -0.60602700 -2.44789000

H 3.25077200 0.41055700 -2.86258100

H 3.23517900 -1.27392300 -3.37989500

C -3.89555300 -0.09233900 2.36821800

H -2.86437200 -0.17204400 2.71509900

H -4.10695300 0.97740300 2.26890500

H -4.54538300 -0.48240000 3.15420000

C -2.94793800 -0.75293500 -2.57920900

H -3.28262400 0.22570800 -2.94151300

H -1.86990200 -0.67518100 -2.43055000

H -3.13451600 -1.47486100 -3.37702700

C 0.36928000 -2.08607200 0.81737400

H 1.45796300 -2.13762000 0.85705200

H -0.01825100 -2.93160800 1.38452100

C -0.14898300 -2.23352400 -0.62015500

H 0.06256400 -1.34151100 -1.23677400

H -1.23473700 -2.34487100 -0.61154000

C 0.48907000 -3.44059900 -1.32817900

H 1.57556100 -3.34023400 -1.38509400

H 0.26744000 -4.36667700 -0.78936500

H 0.10365400 -3.54833400 -2.34682700

Co 0.07692600 0.02024500 0.48393800

C -0.14341700 -0.99243600 2.40412300

H 0.63603400 -1.51248200 2.95545500

H -1.11511600 -1.44801700 2.56923600

C -0.09510400 0.44923200 2.39939400

H -1.01411900 0.99931300 2.57782700

H 0.79078600 0.93913400 2.79427400

**1Co(0)-5**

Atom x y z

C 1.18576600 -3.04409300 -0.25373900

C 1.20659900 -4.43518600 -0.27448500

C 0.00006400 -5.14119000 -0.32194000

C -1.20648900 -4.43521400 -0.27446000

C -1.18568800 -3.04412300 -0.25371800

N 0.00002900 -2.36618900 -0.35668800

H 0.00007700 -6.22499900 -0.33442200

H 2.14664500 -4.97261800 -0.22694400

H -2.14652100 -4.97267000 -0.22690000

C 2.34070900 -2.18024000 -0.05985600

C -2.34065100 -2.18029600 -0.05982600

N -2.06526200 -0.91458100 0.15079300

N 2.06529100 -0.91453100 0.15077000

C -3.73098000 -2.76261200 -0.07746200

H -3.97986200 -3.17059100 -1.06190000

H -3.81561300 -3.58297000 0.64048700

H -4.47832600 -2.01457800 0.18054100

C 3.73105200 -2.76252300 -0.07749900

H 3.81571200 -3.58287200 0.64045800

H 3.97993500 -3.17050700 -1.06193500

H 4.47838200 -2.01446900 0.18049000

C -3.08477000 0.06058100 0.34028700

C -3.24115500 0.60395400 1.63129800

C -3.84669700 0.53957800 -0.74407900

C -4.18825500 1.60958200 1.82561200

C -4.77694600 1.55501800 -0.50405900

C -4.95531000 2.08641800 0.76737600

H -4.31873900 2.02719400 2.81978400

H -5.36344500 1.93635800 -1.33503800

H -5.68140200 2.87612300 0.93184500

C 3.08477600 0.06065400 0.34027600

C 3.84668000 0.53969300 -0.74408700

C 3.24116000 0.60400300 1.63129700

C 4.77690200 1.55515500 -0.50405600

C 4.18823400 1.60965300 1.82562300

C 4.95526400 2.08653300 0.76738900

H 5.36338200 1.93652900 -1.33503200

H 4.31871700 2.02724700 2.81980200

H 5.68133500 2.87625500 0.93186700

C 3.67100800 -0.00831100 -2.13926800

H 4.17847300 -0.97049500 -2.26854300

H 2.61849800 -0.16279500 -2.38335800

H 4.09020000 0.67758300 -2.87792800

C 2.40183400 0.10238400 2.77887300

H 1.33371600 0.21645900 2.57019400

H 2.56684500 -0.96180000 2.97312100

H 2.62738200 0.64941700 3.69637900

C -3.67102100 -0.00844500 -2.13925200

H -2.61851000 -0.16293000 -2.38333900

H -4.17848400 -0.97063200 -2.26851700

H -4.09021300 0.67743700 -2.87792300

C -2.40180700 0.10237900 2.77887600

H -2.56682200 -0.96179700 2.97317200

H -1.33369300 0.21643500 2.57016700

H -2.62733000 0.64945000 3.69636400

C -0.00003800 1.34364800 -1.38580000

H 0.87525100 1.40674200 -2.04771000

H -0.87538100 1.40670400 -2.04764400

C -0.00003100 2.55119400 -0.43171300

H 0.87634900 2.50939100 0.23001400

H -0.87636900 2.50935600 0.23006700

C -0.00007800 3.91734600 -1.13962200

H 0.87640800 3.97667500 -1.79884100

H -0.87661100 3.97664600 -1.79878300

Co 0.00001500 -0.40405100 -0.38344600

C -0.00006700 5.11529800 -0.18366100

H -0.87572900 5.05212700 0.47494000

H 0.87564400 5.05215800 0.47487700

C -0.00011800 6.46832100 -0.90011700

H -0.00010800 7.30227600 -0.19134200

H 0.88173800 6.57986000 -1.53944400

H -0.88202400 6.57982700 -1.53938000

**1Co(0)-6**

Atom x y z

C 1.09882700 2.53896500 0.38145700

C 1.06808700 3.91790900 0.65294000

C -0.13615300 4.58482400 0.72464000

C -1.31915000 3.84744100 0.55289300

C -1.26162400 2.48447700 0.30306600

N -0.06939500 1.81996700 0.19685300

H -0.17341400 5.65062900 0.91956800

H 1.99642200 4.45619200 0.79787500

H -2.27427800 4.34873800 0.62898100

C 2.33334700 1.80555600 0.27202000

C -2.51158000 1.68919400 0.20850300

N -2.41814700 0.45314300 -0.12618400

N 2.23574100 0.53615300 -0.08957600

C -3.82198400 2.37373800 0.54470200

H -3.80889600 2.79146300 1.55450100

H -4.02107000 3.19905700 -0.14477900

H -4.65112000 1.67277300 0.47431900

C 3.64788500 2.49454500 0.55451400

H 3.82172900 3.32001700 -0.14327500

H 3.67796000 2.91563400 1.56401400

H 4.48227000 1.80307900 0.45639000

C -3.53770800 -0.41910300 -0.10582000

C -4.21867500 -0.72534700 -1.30198200

C -3.90568700 -1.03732900 1.10883500

C -5.24326600 -1.67391800 -1.26600100

C -4.92840500 -1.98816100 1.09216000

C -5.59422100 -2.31453200 -0.08336600

H -5.77308900 -1.90860200 -2.18491600

H -5.20592200 -2.47446800 2.02300100

H -6.38579000 -3.05686400 -0.07680500

C 3.39740800 -0.29414600 -0.14628500

C 3.87430400 -0.89444500 1.03921100

C 4.02966100 -0.54723000 -1.37871600

C 4.96549600 -1.76182500 0.96175700

C 5.12284100 -1.41818800 -1.40828500

C 5.58844200 -2.03058600 -0.25197300

H 5.32915600 -2.23158000 1.87109400

H 5.61519000 -1.61121000 -2.35735100

H 6.43554900 -2.70776600 -0.29423900

C 3.23320000 -0.60146000 2.37268500

H 3.46294800 0.41250500 2.71863700

H 2.14630800 -0.68139900 2.32165800

H 3.59294800 -1.29423000 3.13589900

C 3.56650000 0.10178000 -2.66076000

H 2.74068100 -0.45322400 -3.11751000

H 3.22117600 1.12520100 -2.50501700

H 4.37598300 0.12775900 -3.39364900

C -3.23735400 -0.66565700 2.40958200

H -2.15522100 -0.58957300 2.30414000

H -3.59596800 0.30070300 2.78356200

H -3.45133700 -1.40866500 3.18029400

C -3.87880900 -0.03481500 -2.60042600

H -3.83228100 1.05234700 -2.49007000

H -2.91106500 -0.35550700 -2.99505600

H -4.62931200 -0.25629600 -3.36183600

C -0.08535800 -1.81799100 0.95029100

H 0.05168200 -1.55439100 2.01106800

H -1.14834900 -2.06972300 0.84178100

C 0.75143700 -3.06681900 0.63596300

H 1.82240500 -2.84103900 0.69768900

H 0.57995700 -3.38163600 -0.40229500

C 0.45050000 -4.26310400 1.55289500

H 0.65216000 -4.01490100 2.60044200

H -0.60270300 -4.55505600 1.48540900

H 1.05742700 -5.13949900 1.29639300

Co 0.27022500 -0.16027600 -0.17141000

C -0.19550400 -1.12908100 -2.20979700

H 0.67145000 -1.77599400 -2.30028700

H -1.13319800 -1.61799700 -1.97401900

C -0.13376500 0.18082200 -2.53400500

H -1.01423300 0.80854400 -2.52954500

H 0.78820800 0.64449500 -2.85982900

**1Co(0)-TS-6/7**

Atom x y z

C 1.26571800 2.67836600 -0.10140100

C 1.32593600 4.06618500 -0.12518800

C 0.12770200 4.79658000 -0.14517800

C -1.09691000 4.12963800 -0.12191200

C -1.12092000 2.73244100 -0.10020500

N 0.06156600 2.04306900 -0.12106600

H 0.15390400 5.88025700 -0.16075800

H 2.27901600 4.58226000 -0.12731600

H -2.01802800 4.70036900 -0.11571700

C 2.37198300 1.74624500 0.00680500

C -2.25406600 1.85112400 -0.00338600

N -1.94922700 0.55429500 0.05192500

N 2.02019900 0.47494800 0.07019000

C -3.66473900 2.36369500 0.10343800

H -3.70846700 3.44817000 0.01237900

H -4.30816300 1.93721800 -0.67038100

H -4.11386800 2.08943300 1.06314000

C 3.79078200 2.24366100 0.07911200

H 3.87364400 3.09881400 0.75372700

H 4.47123100 1.46885100 0.42790700

H 4.13829600 2.57479400 -0.90556800

C -3.00335800 -0.37763100 0.31835400

C -3.76894500 -0.93746000 -0.72144400

C -3.24198900 -0.73863000 1.66057100

C -4.76744500 -1.86029300 -0.39373600

C -4.24697200 -1.66615000 1.94217900

C -5.00851200 -2.22831700 0.92419300

H -5.36423100 -2.29292600 -1.19171400

H -4.43092000 -1.94858400 2.97477000

H -5.78688000 -2.94808400 1.15691600

C 3.01033000 -0.52413800 0.34888300

C 3.15950700 -0.94359900 1.68777500

C 3.79091100 -1.09146000 -0.67396200

C 4.07050100 -1.96112400 1.97478900

C 4.68706400 -2.11262700 -0.34108800

C 4.82564500 -2.55375100 0.96822500

H 4.18559800 -2.29125200 3.00302400

H 5.28597100 -2.56136800 -1.12859000

H 5.52231100 -3.35141400 1.20560300

C 2.37967500 -0.28625700 2.79946600

H 2.65234600 0.76763900 2.91681500

H 1.30363800 -0.30900800 2.61101600

H 2.56694000 -0.78452000 3.75252100

C 3.72714900 -0.59195900 -2.09566000

H 2.73376800 -0.24000200 -2.36194800

H 4.42100600 0.24291400 -2.25046900

H 4.01251800 -1.37733300 -2.79893200

C -2.42835900 -0.13639000 2.77899000

H -1.35954900 -0.31875900 2.63742300

H -2.55232100 0.94927100 2.84112100

H -2.71886600 -0.55971300 3.74251500

C -3.53096700 -0.58339700 -2.16808900

H -4.37497500 -0.89711000 -2.78604800

H -3.38320800 0.48750300 -2.32052600

H -2.63672700 -1.07889600 -2.55222700

C -0.03197300 -1.94664200 0.31692900

H 0.76234800 -1.94112600 1.06470000

H -1.01336100 -2.05740400 0.78023700

C 0.20304400 -2.89796900 -0.73983700

H 1.22407800 -3.27512600 -0.82428600

H 0.24225700 -2.14685100 -1.93223600

C -0.86028800 -3.90959000 -1.11198200

H -0.90651700 -4.71468700 -0.36790700

H -1.85097300 -3.44690900 -1.14208400

H -0.66971800 -4.37451200 -2.08502100

Co 0.01551000 0.14016000 -0.14588600

C 0.18560200 -1.33023300 -2.91202400

H 1.12363000 -1.57306200 -3.41399900

H -0.66535200 -1.75587500 -3.44859500

C 0.03831800 -0.00312000 -2.38092400

H -0.91683000 0.48596600 -2.54200500

H 0.87337800 0.67738600 -2.52807100

**1Co(0)-7**

Atom x y z

C -1.24402500 2.43073400 0.19166000

C -1.30840800 3.81227100 0.28834400

C -0.12544800 4.57373400 0.28732700

C 1.08043600 3.92091900 0.16802400

C 1.11553700 2.51586800 0.07056400

N -0.05070600 1.77256200 0.11108200

H -0.16797000 5.65422600 0.36772400

H -2.26391500 4.31469500 0.35075600

H 2.00597900 4.48349700 0.15248900

C -2.49233500 1.62654400 0.09415600

C 2.33922200 1.77761300 -0.07593600

N 2.23532600 0.45303600 -0.03265100

N -2.38568500 0.36159500 -0.08753100

C 3.65138000 2.50306200 -0.25246600

H 3.63273700 3.17911500 -1.11274800

H 3.89235900 3.10949700 0.62738400

H 4.47062500 1.80072700 -0.39807100

C -3.82046800 2.35322200 0.17526400

H -3.90864600 2.90518200 1.11461800

H -3.93148100 3.07603800 -0.63753900

H -4.64785300 1.64868900 0.11546900

C 3.33546100 -0.38401300 -0.37351500

C 4.06066500 -1.04540800 0.63893200

C 3.64627000 -0.59800500 -1.73384900

C 5.06499100 -1.94257000 0.26893000

C 4.65624200 -1.50832600 -2.05798800

C 5.35988000 -2.18491800 -1.06877600

H 5.62539400 -2.45424400 1.04621000

H 4.89050000 -1.68438000 -3.10424100

H 6.13847100 -2.89170700 -1.33770600

C -3.50398000 -0.46725600 -0.35150000

C -3.94206700 -0.61139200 -1.68567800

C -4.09883900 -1.21712500 0.68376000

C -4.96440900 -1.52138400 -1.96165700

C -5.12170400 -2.11122200 0.36012000

C -5.55445300 -2.27233400 -0.95144700

H -5.30013700 -1.63834900 -2.98825800

H -5.58365100 -2.68846900 1.15606300

H -6.34526900 -2.97803500 -1.18438400

C -3.33830500 0.21306400 -2.79670800

H -3.68143800 1.25333800 -2.76346300

H -2.24802300 0.24612300 -2.73919300

H -3.61569500 -0.18749500 -3.77373100

C -3.65595800 -1.04346600 2.11362700

H -2.57868500 -1.17651900 2.22188200

H -3.88156300 -0.03998100 2.49044500

H -4.15734200 -1.75960300 2.76764200

C 2.93358000 0.15680200 -2.83042700

H 1.87414900 0.29688900 -2.61122200

H 3.35951700 1.15718400 -2.96709900

H 3.02474900 -0.36429200 -3.78606900

C 3.79189800 -0.75907000 2.09450300

H 4.03576900 0.27816400 2.34766500

H 2.74118300 -0.89758800 2.35111400

H 4.39258900 -1.40622800 2.73696100

C 0.04871000 -1.66013500 -1.28047700

H -0.70795800 -1.04767300 -1.75184500

H 1.00985700 -1.73818300 -1.77623800

C -0.22560000 -2.39190100 -0.18121600

H -1.23288200 -2.36265700 0.22588300

H -0.62613100 -2.27421300 3.13893300

C 0.70968900 -3.41287600 0.40432000

H 0.34404500 -4.41933900 0.16755600

H 1.71919700 -3.31939600 -0.00104800

H 0.76246800 -3.34581800 1.49174700

Co 0.37956400 -0.15028800 0.61144000

C 0.10968300 -1.52753700 3.45939100

H -0.08215800 -1.34459300 4.52661400

H 1.09063300 -2.01302700 3.40504000

C 0.04094700 -0.24677600 2.62023100

H 0.76010800 0.48428700 3.02079500

H -0.94184100 0.22283300 2.75959600

**1Co(0)-8**

Atom x y z

C 1.19666600 2.55800900 -0.01270700

C 1.21441600 3.95017900 -0.04884700

C -0.00001300 4.64639800 -0.07164100

C -1.21445400 3.95015800 -0.04874000

C -1.19664100 2.55801100 -0.01261300

N 0.00000300 1.90104300 -0.00563000

H -0.00001700 5.73007400 -0.10243800

H 2.15000100 4.49667900 -0.06349400

H -2.15006500 4.49661800 -0.06331500

C 2.31049300 1.63571000 0.02025400

C -2.31050500 1.63571700 0.02040600

N -1.96662900 0.35255400 0.04697400

N 1.96658600 0.35252500 0.04685200

C -3.73781400 2.10825100 0.01167600

H -3.81391800 3.15510000 0.30514100

H -4.18580700 2.01065300 -0.98316000

H -4.35504000 1.51893500 0.69205400

C 3.73785800 2.10806700 0.01161900

H 4.18676600 2.00794500 -0.98253600

H 3.81388900 3.15559200 0.30265000

H 4.35441000 1.52030000 0.69398200

C -2.99364000 -0.64262600 0.05295700

C -3.52081500 -1.10415600 -1.16623000

C -3.42529200 -1.17496100 1.28178300

C -4.49853700 -2.10182400 -1.13269000

C -4.40838500 -2.16663000 1.26936700

C -4.94546900 -2.62967200 0.07298900

H -4.90820000 -2.47039400 -2.06878500

H -4.74906000 -2.58413800 2.21244300

H -5.70366700 -3.40628100 0.08034600

C 2.99364500 -0.64260200 0.05289400

C 3.42537700 -1.17480200 1.28175400

C 3.52078700 -1.10424500 -1.16626800

C 4.40853500 -2.16640800 1.26939600

C 4.49858400 -2.10184000 -1.13266900

C 4.94560900 -2.62952800 0.07304500

H 4.74926200 -2.58381400 2.21249900

H 4.90822100 -2.47048800 -2.06874400

H 5.70386100 -3.40608400 0.08045000

C 2.83836900 -0.68716900 2.58229500

H 3.02546400 0.37892100 2.74627300

H 1.75306200 -0.82098100 2.59934700

H 3.26016900 -1.23216200 3.42901200

C 3.04668600 -0.54400700 -2.48508600

H 1.95795900 -0.46526600 -2.52056700

H 3.44231100 0.46030900 -2.67230500

H 3.36803700 -1.17792500 -3.31382000

C -2.83833200 -0.68733200 2.58234600

H -1.75299000 -0.82086000 2.59932400

H -3.02570500 0.37869400 2.74643900

H -3.25994900 -1.23252200 3.42902500

C -3.04684300 -0.54371400 -2.48500700

H -3.44255700 0.46059900 -2.67205600

H -1.95812300 -0.46490200 -2.52056400

H -3.36821200 -1.17754200 -3.31380200

C 0.00000500 -1.98624900 0.21918700

H 0.87775700 -2.30340500 0.79866500

H -0.87760200 -2.30339000 0.79889500

C -0.00017700 -2.74940300 -1.11396600

H 0.88207500 -2.51833800 -1.72085600

H -0.88257100 -2.51830600 -1.72063600

Co 0.00000000 -0.00357600 0.06901600

H -0.00017900 -3.83989400 -0.97331200

**1Co(0)-TS-3/9**

Atom x y z

C -1.22413900 2.49189100 -0.01006300

C -1.25398500 3.88030200 0.02525200

C -0.05406900 4.60104100 0.03968200

C 1.14928300 3.90283100 -0.02514200

C 1.14298400 2.50890900 -0.06057100

N -0.03712000 1.80909800 -0.01241100

H -0.06259900 5.68422900 0.07930400

H -2.20114600 4.40640600 0.02904300

H 2.08865300 4.44268700 -0.05312600

C -2.41785000 1.64952000 -0.09422900

C 2.33077100 1.68239700 -0.18402900

N 2.13357600 0.38984600 -0.11559300

N -2.20833900 0.36783700 -0.09204300

C 3.67465400 2.33121900 -0.41082400

H 3.65154700 2.99521500 -1.27965200

H 3.97227800 2.93892600 0.44971400

H 4.44994400 1.58509000 -0.57584500

C -3.77868600 2.29440800 -0.20496100

H -4.00171200 2.89922700 0.67919100

H -3.82928200 2.96048300 -1.07095300

H -4.56169700 1.54516500 -0.30775900

C 3.21041900 -0.52878500 -0.21121700

C 4.01103200 -0.79537100 0.91889500

C 3.41344000 -1.22738000 -1.41930500

C 5.00553400 -1.77161300 0.81848200

C 4.42223100 -2.19098600 -1.47476200

C 5.21505400 -2.46902800 -0.36592800

H 5.62146800 -1.98573100 1.68751900

H 4.58517200 -2.72979400 -2.40391400

H 5.99060400 -3.22600900 -0.42456900

C -3.26499900 -0.57377700 -0.15712800

C -3.53682700 -1.21176300 -1.38498000

C -3.96062600 -0.93529200 1.01489400

C -4.51380600 -2.20812100 -1.41953000

C -4.92692300 -1.94107600 0.93295900

C -5.20665500 -2.57749900 -0.27109900

H -4.73034500 -2.70077400 -2.36320200

H -5.46386500 -2.22812700 1.83276900

H -5.95772100 -3.35973300 -0.31388900

C -2.80253200 -0.80639800 -2.63850600

H -3.04399400 0.21931300 -2.93696100

H -1.71880800 -0.84076000 -2.49839100

H -3.06069000 -1.46224800 -3.47240300

C -3.68082100 -0.24908600 2.33017800

H -2.61131100 -0.09743600 2.48894400

H -4.15026900 0.74009300 2.37915900

H -4.07436000 -0.83304000 3.16483400

C 2.57143400 -0.92413600 -2.63302000

H 1.50618800 -1.05357600 -2.42238900

H 2.69889400 0.11017400 -2.96828100

H 2.83651000 -1.57865200 -3.46588900

C 3.80799900 -0.04213700 2.21096200

H 4.25380200 0.95819100 2.17111100

H 2.74853400 0.09208100 2.43726200

H 4.27472400 -0.56905600 3.04590700

C -0.01102700 -2.13157100 -0.07492800

H -0.86063000 -2.38228900 -0.70456700

H 0.95023700 -2.51151500 -0.41196000

C -0.21684800 -1.93147500 1.30284500

H -1.24506600 -1.98301200 1.65047600

H -0.13741500 -0.25416500 1.68754300

C 0.79978700 -2.37776700 2.33098200

H 0.65497100 -3.44474900 2.53841500

H 1.82009200 -2.25089400 1.96703300

H 0.70029300 -1.83750500 3.27561400

Co 0.00967500 -0.10782300 0.16077000

**1Co(0)-9**

Atom x y z

C 1.20182400 2.48713400 -0.05973400

C 1.23280800 3.87416600 -0.17084900

C 0.03857700 4.59514300 -0.20394600

C -1.16248800 3.89874800 -0.11215200

C -1.15146700 2.50833100 -0.00520400

N 0.02040600 1.80394700 0.00456000

H 0.04726600 5.67546800 -0.29283900

H 2.18039100 4.39570100 -0.22520600

H -2.10341100 4.43536400 -0.12425100

C 2.41671300 1.66239700 0.00342100

C -2.36389100 1.69694900 0.08287800

N -2.18118500 0.41149600 0.09252400

N 2.23792200 0.38460400 0.07720600

C -3.71214600 2.37424200 0.13689800

H -3.76671800 3.08276200 0.96839500

H -3.90757300 2.93863200 -0.78047200

H -4.51245000 1.64650700 0.25833500

C 3.76819400 2.33711700 -0.02676200

H 3.91135200 2.88930300 -0.96057200

H 3.87027200 3.05551800 0.79156900

H 4.57129900 1.60747200 0.05980700

C -3.27511800 -0.49272700 0.14811700

C -3.87536300 -0.93489700 -1.04770500

C -3.68440600 -1.00066000 1.39702500

C -4.88497500 -1.89712500 -0.96739300

C -4.69894900 -1.96015900 1.42833500

C -5.29763800 -2.41182500 0.25718400

H -5.35098100 -2.24659400 -1.88440000

H -5.01911900 -2.35714400 2.38755800

H -6.08018100 -3.16274900 0.29818800

C 3.32202200 -0.52732900 0.13639900

C 3.75030700 -1.00321100 1.39171100

C 3.88170200 -1.02417000 -1.05813100

C 4.74881400 -1.97817000 1.43116900

C 4.87679300 -2.00073500 -0.96920300

C 5.31160500 -2.47933300 0.26201800

H 5.08493800 -2.34920400 2.39530100

H 5.31203100 -2.39136900 -1.88471400

H 6.08178000 -3.24245800 0.31019900

C 3.15669800 -0.45394300 2.66542600

H 3.46330100 0.58300600 2.84234200

H 2.06421600 -0.45161400 2.63415100

H 3.47360500 -1.04074100 3.52989800

C 3.42145600 -0.50970000 -2.39973700

H 2.33226100 -0.44262200 -2.45071400

H 3.80969000 0.49558300 -2.60118900

H 3.77039500 -1.15848500 -3.20585300

C -3.05264700 -0.50348800 2.67337100

H -1.96150700 -0.53473800 2.61940500

H -3.32426100 0.53721900 2.88195700

H -3.37245400 -1.10322300 3.52790900

C -3.44596500 -0.37706400 -2.38196600

H -3.81416900 0.64504700 -2.52849000

H -2.35796800 -0.33603500 -2.46681000

H -3.83859200 -0.98277800 -3.20143700

C -0.19822500 -2.10255400 0.67390300

H 0.45997600 -2.01511200 1.53537600

H -1.23604200 -2.34024600 0.88583500

C 0.32168000 -2.28262100 -0.58541500

H 1.40177500 -2.28848800 -0.70019300

H -0.01761300 -0.13388300 -1.69058800

C -0.45254200 -2.88905500 -1.72546200

H -0.25970900 -3.96945300 -1.76940500

H -1.52826400 -2.75081800 -1.60245400

H -0.16046600 -2.46355700 -2.68714500

Co -0.03419700 -0.15034700 -0.14573100

**1Co(0)-10**

Atom x y z

C 1.18677900 2.37112400 0.07071000

C 1.20880300 3.73077700 0.36482600

C 0.00000000 4.42652800 0.48011500

C -1.20880300 3.73077600 0.36482900

C -1.18677900 2.37112300 0.07071200

N 0.00000000 1.74031800 -0.17481500

H 0.00000000 5.48488500 0.71402900

H 2.14867600 4.24457700 0.53113100

H -2.14867600 4.24457600 0.53113700

C 2.33188700 1.46921600 0.06896900

C -2.33188700 1.46921500 0.06897100

N -2.03739000 0.19220200 0.00715900

N 2.03739000 0.19220200 0.00715600

C -3.73175400 2.02061100 0.15180000

H -4.47074100 1.22271400 0.19424700

H -3.85518900 2.64177000 1.04357700

H -3.95761500 2.65176900 -0.71322900

C 3.73175400 2.02061300 0.15179600

H 3.85519100 2.64176700 1.04357600

H 4.47074200 1.22271600 0.19423900

H 3.95761400 2.65177400 -0.71323000

C -3.04823500 -0.81404000 0.03358500

C -3.70490000 -1.19936400 -1.15054300

C -3.30618600 -1.46373400 1.25528900

C -4.63874200 -2.23622900 -1.08056700

C -4.24971500 -2.49254900 1.27822500

C -4.91601800 -2.87931200 0.12064400

H -5.14929600 -2.54481600 -1.98817400

H -4.45736000 -2.99767300 2.21718700

H -5.64273000 -3.68482800 0.15270700

C 3.04823500 -0.81403900 0.03358500

C 3.30618600 -1.46373100 1.25528900

C 3.70489800 -1.19936800 -1.15054400

C 4.24971400 -2.49254800 1.27822700

C 4.63873800 -2.23623400 -1.08056600

C 4.91601400 -2.87931500 0.12064600

H 4.45735900 -2.99767000 2.21719000

H 5.14929000 -2.54482400 -1.98817300

H 5.64272500 -3.68483200 0.15271100

C 2.57759300 -1.05651800 2.51177200

H 2.81441900 -0.03004600 2.81009900

H 1.49282300 -1.09665500 2.37566000

H 2.83965100 -1.71198300 3.34457400

C 3.39695900 -0.53010000 -2.46620200

H 2.32685100 -0.57345900 -2.68528700

H 3.68523800 0.52654200 -2.46985400

H 3.93298500 -1.01759200 -3.28281900

C -2.57759100 -1.05652500 2.51177100

H -1.49282100 -1.09666200 2.37565700

H -2.81441500 -0.03005300 2.81010100

H -2.83964700 -1.71199100 3.34457300

C -3.39696100 -0.53009300 -2.46620000

H -3.68524000 0.52654900 -2.46985100

H -2.32685300 -0.57345300 -2.68528500

H -3.93298700 -1.01758400 -3.28281900

H 0.00000300 -1.17469800 -1.87940400

Co 0.00000200 -0.14968800 -0.65013400

**1/2Co(+)**

**1/2Co(+)-1**

Atom x y z

C 1.17635900 2.47981300 0.00491500

C 1.21366000 3.87448200 0.00737000

C 0.00066100 4.56623300 0.00829200

C -1.21245800 3.87470400 0.00627200

C -1.17550400 2.47996400 0.00386600

N 0.00040500 1.84466000 0.00340600

H 0.00076700 5.65005400 0.01031400

H 2.15325200 4.41271800 0.00833700

H -2.15190800 4.41312300 0.00641300

C 2.32105000 1.52458800 0.00089400

C -2.32053800 1.52488300 -0.00128700

N -1.98553000 0.27198100 0.00770700

N 1.98546900 0.27201900 0.00989200

C -3.71797400 2.05996600 -0.01711600

H -3.89007600 2.69797200 0.85541500

H -3.87662700 2.68254300 -0.90328000

H -4.45735400 1.26337200 -0.01579400

C 3.71882200 2.05887200 -0.01347400

H 3.87931100 2.68024900 -0.90015100

H 3.88986600 2.69787300 0.85856900

H 4.45774900 1.26187300 -0.00998100

C -3.00054600 -0.75404100 -0.00306800

C -3.44185600 -1.25060000 -1.23891900

C -3.46289000 -1.25932700 1.22185100

C -4.39747400 -2.26905200 -1.22434300

C -4.41863000 -2.27729300 1.18382500

C -4.88646200 -2.77743500 -0.02624000

H -4.75541300 -2.66924200 -2.16739600

H -4.79303000 -2.68372400 2.11772300

H -5.62636900 -3.57016800 -0.03548100

C 3.00020700 -0.75439100 -0.00086900

C 3.45607000 -1.26383600 1.22465300

C 3.44776300 -1.24693800 -1.23621000

C 4.41164800 -2.28198600 1.18833300

C 4.40282900 -2.26596100 -1.21992200

C 4.88540000 -2.77845900 -0.02097100

H 4.78122600 -2.69144500 2.12286000

H 4.76544400 -2.66331100 -2.16241900

H 5.62501300 -3.57146800 -0.02902800

C 2.92663100 -0.74386800 2.53772200

H 3.16090500 0.31443300 2.69342400

H 1.83788300 -0.84541400 2.59810500

H 3.35481200 -1.29569700 3.37487300

C 2.91464500 -0.70737300 -2.54032100

H 1.82343200 -0.77875900 -2.58910100

H 3.17622100 0.34480100 -2.69502500

H 3.31822700 -1.26642900 -3.38486600

C -2.94053200 -0.73578900 2.53634700

H -1.85162200 -0.83198100 2.60108800

H -3.18064500 0.32142800 2.69044300

H -3.36921400 -1.28906400 3.37228900

C -2.90143400 -0.71515400 -2.54167100

H -3.16102800 0.33686800 -2.70056000

H -1.81004000 -0.78775800 -2.58434400

H -3.30096800 -1.27607000 -3.38689400

Co 0.00018300 -0.08428900 0.02603200

C -0.00003600 -2.03166400 0.04887500

H -0.01450600 -2.39141400 -0.99070500

H 0.89528500 -2.44766700 0.51966300

H -0.88441900 -2.44455200 0.54277900

**1/2Co(+)-2**

Atom x y z

C 1.17038600 2.43915600 -0.33753900

C 1.20319800 3.81132600 -0.59074400

C -0.00598300 4.50047300 -0.68225600

C -1.21431300 3.81485400 -0.55842100

C -1.17841900 2.44284800 -0.30562300

N -0.00284600 1.81330600 -0.16275000

H -0.00696600 5.56726400 -0.87320200

H 2.14282600 4.33300900 -0.72116900

H -2.15570700 4.33889300 -0.66464000

C 2.32526800 1.50528700 -0.29840100

C -2.33359500 1.51090400 -0.24435800

N -2.02548200 0.26669100 -0.05037300

N 2.01785200 0.26087600 -0.10564500

C -3.71443500 2.04868100 -0.47152300

H -3.97262600 2.78063600 0.30003100

H -3.76855700 2.56668500 -1.43374800

H -4.46219000 1.25980700 -0.46399800

C 3.70494300 2.04260400 -0.53253600

H 3.74054600 2.61211000 -1.46567500

H 3.99102300 2.72730700 0.27221600

H 4.44414400 1.24746300 -0.58610600

C -3.04939900 -0.75111900 -0.08873000

C -3.21737100 -1.46063000 -1.29108600

C -3.81587300 -1.03376600 1.05474500

C -4.15860200 -2.49144700 -1.31822900

C -4.74122000 -2.07849700 0.97756400

C -4.91010200 -2.80785600 -0.19292000

H -4.30023400 -3.05039300 -2.23754400

H -5.33818000 -2.31664500 1.85198700

H -5.63033700 -3.61772200 -0.22945500

C 3.03925300 -0.75814300 -0.12757400

C 3.84638500 -0.99228000 0.99803400

C 3.15858100 -1.52954800 -1.30025500

C 4.75453900 -2.05557800 0.94075900

C 4.08882800 -2.56798600 -1.31140000

C 4.87460800 -2.84156400 -0.19624600

H 5.37830800 -2.25855600 1.80574000

H 4.19546900 -3.16980500 -2.20801900

H 5.58344600 -3.66196800 -0.21819700

C 3.81708200 -0.12367700 2.23364000

H 4.61458300 0.62706300 2.20319700

H 2.87704700 0.41091800 2.35998500

H 3.98354100 -0.71922800 3.13327300

C 2.34983200 -1.21675600 -2.53418100

H 1.27953200 -1.16887500 -2.32160800

H 2.63456900 -0.25354700 -2.97151900

H 2.50216100 -1.97730900 -3.30059400

C -3.69718600 -0.23003600 2.32685100

H -2.66549600 -0.13356300 2.66660100

H -4.09296200 0.78457300 2.20832100

H -4.26398100 -0.69835900 3.13200500

C -2.44949300 -1.09768600 -2.53778700

H -2.78393500 -0.14122800 -2.95497800

H -1.37714900 -1.00759900 -2.35009400

H -2.58869400 -1.85226700 -3.31261900

C -0.02769200 -2.05367400 0.14838300

H -0.11498100 -2.36554700 -0.90028700

H 0.88908300 -2.49584300 0.54607200

H -0.88530100 -2.47567600 0.67875800

C 0.13449900 -0.54722300 2.66847300

H 1.08896300 -1.05764600 2.68946300

H -0.73675800 -1.18057300 2.77365900

C 0.04289200 0.78977100 2.64220000

H -0.90992200 1.30136400 2.71879000

H 0.92189900 1.42437900 2.63585100

Co -0.00442600 -0.08799400 0.18680800

**1/2Co(+)-TS-2/3**

Atom x y z

C 1.17516800 2.43931000 -0.24115900

C 1.20121900 3.81606100 -0.46642000

C -0.00202400 4.51097700 -0.55049600

C -1.20353900 3.81551900 -0.44810700

C -1.17312800 2.43908100 -0.22160200

N 0.00193800 1.79416100 -0.07368200

H -0.00354100 5.58122000 -0.72052200

H 2.14252800 4.33746900 -0.58210100

H -2.14674500 4.33634700 -0.55009400

C 2.36857100 1.55408300 -0.23914300

C -2.36567700 1.55375100 -0.19830600

N -2.11132500 0.29377000 -0.08753400

N 2.11187300 0.29416500 -0.13602500

C -3.72772900 2.16350700 -0.37228500

H -3.94357600 2.87427500 0.43084500

H -3.78425500 2.71687100 -1.31434500

H -4.50574500 1.40384600 -0.37889900

C 3.73033000 2.16039800 -0.42302200

H 3.76250700 2.76941100 -1.33079300

H 3.98206600 2.81730900 0.41507100

H 4.49754600 1.39365600 -0.50235500

C -3.15131700 -0.69275800 -0.15270000

C -3.30654200 -1.38652700 -1.36805600

C -3.92925900 -1.00276600 0.97871900

C -4.26388800 -2.40077500 -1.43297300

C -4.87103100 -2.02926700 0.86354700

C -5.04065900 -2.72577900 -0.32716400

H -4.39967700 -2.93828800 -2.36599100

H -5.48051600 -2.28081600 1.72558200

H -5.77772600 -3.51847800 -0.39303600

C 3.13559700 -0.70672200 -0.19507600

C 3.95832800 -0.97665300 0.91461300

C 3.22452900 -1.46465600 -1.38078300

C 4.85938600 -2.04224400 0.81808700

C 4.14864300 -2.50827400 -1.43098100

C 4.95653100 -2.80499000 -0.33821700

H 5.49573900 -2.26900700 1.66780200

H 4.23425600 -3.09367900 -2.34085000

H 5.66229100 -3.62672400 -0.39019600

C 3.92740200 -0.14510600 2.17512000

H 4.58873000 0.72484100 2.09635200

H 2.93190900 0.23049000 2.41181600

H 4.27538000 -0.72587500 3.03079200

C 2.39216800 -1.12367000 -2.59232900

H 1.33189000 -1.00487400 -2.35160100

H 2.71342700 -0.18158100 -3.04935500

H 2.47617400 -1.89944100 -3.35424000

C -3.77003800 -0.27443500 2.29153800

H -2.79205800 -0.45695300 2.74427700

H -3.87628900 0.80896000 2.18824700

H -4.52397900 -0.60455100 3.00679900

C -2.49093100 -1.02508100 -2.58480900

H -2.75615100 -0.03677600 -2.97495400

H -1.41887400 -0.99892100 -2.36835600

H -2.65102600 -1.74446200 -3.38863500

C -0.08586400 -2.10384000 0.53782200

H 0.20695600 -1.91082500 -0.51173400

H 0.57009600 -2.90260700 0.87113300

H -1.12109100 -2.43304800 0.57012700

C 0.18817400 -1.14433800 2.26011100

H 1.17847300 -1.53639800 2.45952700

H -0.59554900 -1.76098500 2.68790800

C 0.03344600 0.27734200 2.33542300

H -0.90823600 0.68594400 2.68840100

H 0.89553100 0.87682100 2.61203700

Co 0.00796100 -0.04965700 0.37310800

**1/2Co(+)-3**

Atom x y z

C 1.17470800 2.69827300 -0.08589800

C 1.21225500 4.09101800 -0.16459400

C 0.00017100 4.78233000 -0.20567600

C -1.21196800 4.09110100 -0.16462600

C -1.17451500 2.69836000 -0.08593200

N 0.00007400 2.06124200 -0.05462000

H 0.00020500 5.86439500 -0.26767600

H 2.15199000 4.62815500 -0.19336300

H -2.15166200 4.62830900 -0.19341300

C 2.32346600 1.75177800 -0.02165100

C -2.32330500 1.75191900 -0.02173500

N -1.99775000 0.49924800 0.06103600

N 1.99785900 0.49910800 0.06097800

C -3.71737800 2.29689500 -0.04765500

H -3.86216700 3.00650400 0.77273000

H -3.89534600 2.84493500 -0.97824300

H -4.46234900 1.51033900 0.03885900

C 3.71755600 2.29671000 -0.04742800

H 3.89560100 2.84479100 -0.97797800

H 3.86231300 3.00627500 0.77300000

H 4.46249400 1.51012600 0.03908700

C -3.02372100 -0.51346300 0.11431200

C -3.56707200 -0.99711600 -1.08654100

C -3.40441800 -1.01570700 1.36931300

C -4.52298900 -2.01278900 -1.00314400

C -4.36848400 -2.02546700 1.39986900

C -4.92385300 -2.52313900 0.22612600

H -4.95417400 -2.40629900 -1.91800300

H -4.68089400 -2.42692400 2.35840800

H -5.66645000 -3.31224600 0.26951200

C 3.02377700 -0.51368400 0.11427900

C 3.40440900 -1.01599200 1.36927400

C 3.56714700 -0.99729300 -1.08657400

C 4.36841600 -2.02580500 1.39980500

C 4.52302500 -2.01301000 -1.00320300

C 4.92380200 -2.52344800 0.22605400

H 4.68076400 -2.42735400 2.35832600

H 4.95422000 -2.40648900 -1.91806900

H 5.66635500 -3.31259700 0.26944600

C 2.80555200 -0.47858600 2.64479900

H 3.05847800 0.57417300 2.80922900

H 1.71321700 -0.54987900 2.63903700

H 3.16699500 -1.03663600 3.50892200

C 3.15619700 -0.43968900 -2.42792600

H 2.07191500 -0.33243400 -2.51645900

H 3.59491500 0.54715000 -2.61336900

H 3.48926700 -1.09208000 -3.23569000

C -2.80558600 -0.47825600 2.64483200

H -1.71326500 -0.54978000 2.63918700

H -3.05829900 0.57457800 2.80909400

H -3.16722700 -1.03612300 3.50899000

C -3.15602500 -0.43966200 -2.42792500

H -3.59480200 0.54711200 -2.61356400

H -2.07174400 -0.33232800 -2.51637100

H -3.48895600 -1.09219700 -3.23563000

C -0.00014300 -1.82476600 0.27520700

H 0.88300200 -2.12098300 0.85503300

H -0.88371300 -2.12041900 0.85468900

C -0.00015000 -2.57186300 -1.06433800

H 0.87760900 -2.28894300 -1.65822400

H -0.87728900 -2.28810900 -1.65874800

C -0.00085800 -4.09984400 -0.90012400

H 0.88156300 -4.43565000 -0.34804500

H -0.88388400 -4.43494500 -0.34859300

H -0.00075000 -4.60673400 -1.86995900

Co 0.00002600 0.12638100 0.09084100

**1/2Co(+)-4**

Atom x y z

N -0.12730100 2.01706300 -0.08560000

C -1.32453400 2.60543900 -0.23882700

C -2.45225400 1.64121200 -0.23377500

N -2.11654500 0.39819800 -0.09654700

C -3.12321100 -0.63223400 -0.16987300

C -3.25937300 -1.31581600 -1.39536200

C -2.47422800 -0.90447100 -2.61574900

H -2.62515500 -1.61354200 -3.43031600

C -4.17693600 -2.36312500 -1.46640500

C -4.93580800 -2.73008300 -0.35915600

C -4.79956500 -2.03095800 0.83118900

C -3.90233700 -0.96311900 0.95060300

C -3.85900800 -0.19407400 2.25038800

H -2.97749900 0.43678200 2.34712600

H -5.40322400 -2.30595700 1.69083800

H -4.29509000 -2.89710000 -2.40360500

C -3.84722100 2.15637500 -0.43473100

H -4.14092500 2.80190800 0.39900800

H -3.90644900 2.76036400 -1.34448700

H -4.56889200 1.34746800 -0.51263700

C -1.41541500 3.98313800 -0.44440900

C -0.23950500 4.72794100 -0.51570700

C 0.99430900 4.08716200 -0.42099300

C 1.01699800 2.70691000 -0.21493100

C 2.22068900 1.84046200 -0.19486000

N 1.99175100 0.57403600 -0.04529900

C 3.08738200 -0.36112200 -0.13844700

C 3.33384800 -0.96174600 -1.38561700

C 4.34596700 -1.92166200 -1.46232600

C 5.09855500 -2.26364200 -0.34568700

C 4.85907800 -1.63095000 0.86851500

C 3.85544200 -0.66777300 0.99867600

H 5.45945700 -1.88455500 1.73619700

H 4.54653300 -2.39908900 -2.41608500

C 3.56634500 2.46906000 -0.40945700

H 3.77913800 3.19815600 0.37826500

H 4.36232500 1.72920600 -0.41903000

H 3.58808800 3.01042500 -1.35990000

H 1.91377700 4.65170800 -0.51344700

H -0.28444600 5.79975900 -0.66892500

H -2.37729300 4.46713600 -0.55410500

H 5.87738300 -3.01394600 -0.42321000

C 3.64496500 0.02586000 2.32229500

H 3.84084000 1.10159200 2.25988700

H -5.63615300 -3.55515200 -0.42895800

C 2.58631500 -0.54882200 -2.63033100

H 2.73222100 -1.27595300 -3.43003500

C -0.00111000 -1.87416500 -0.10055400

H -1.04850500 -2.18872100 -0.14103300

H 0.36857700 -1.85821300 -1.13947700

H -1.40189800 -0.85212600 -2.41448000

H -2.78163100 0.08107000 -2.98247700

H -3.87898500 -0.87098700 3.10731200

H -4.73484600 0.45665300 2.34515800

H 4.31875700 -0.37735900 3.07891500

H 2.62637800 -0.09318100 2.69641000

H 2.94105500 0.41736900 -3.00707400

H 1.51235600 -0.44976400 -2.46209900

C 0.86639200 -4.26796900 -0.00107000

C 0.80350500 -2.89926800 0.69551000

H 1.41885900 -4.99424000 0.60239000

H 1.36560700 -4.19666000 -0.97178000

H -0.13536900 -4.67277800 -0.17312800

H 1.82652000 -2.55074700 0.87101900

H 0.35082700 -3.04126600 1.68323900

C -0.18300300 -0.46838600 2.54580700

C -0.13620900 0.87569200 2.57537300

H -1.11991500 -1.01126000 2.55256000

H 0.70831700 -1.06888200 2.66191200

H -1.03462500 1.48132200 2.59450200

H 0.79876700 1.41033900 2.69741400

Co -0.04150600 0.08799900 0.21947100

**1/2Co(+)-TS-4/5**

Atom x y z

C 1.12289400 2.51015400 -0.22669300

C 1.13500100 3.89238700 -0.42432800

C -0.06981000 4.57544600 -0.53037800

C -1.25766800 3.85803100 -0.46228100

C -1.21483300 2.47641700 -0.26367500

N -0.03838200 1.82819000 -0.12668000

H -0.08298400 5.64914800 -0.67678500

H 2.07193800 4.42794700 -0.49640300

H -2.20594600 4.36812900 -0.56417900

C 2.36793100 1.69493400 -0.16588100

C -2.44400700 1.63110600 -0.23937800

N -2.27275100 0.37857100 -0.02258500

N 2.21532900 0.43421000 0.03021900

C -3.77002500 2.29327500 -0.50633300

H -3.98687800 3.04961200 0.25364000

H -3.76954600 2.80000100 -1.47536100

H -4.57870800 1.56616000 -0.50196200

C 3.68760500 2.38966200 -0.37210100

H 3.72312700 2.88889000 -1.34450500

H 3.84286400 3.15836300 0.39056200

H 4.51564700 1.68694200 -0.31901800

C -3.37018800 -0.54344800 -0.09368500

C -3.64958200 -1.15253200 -1.33389500

C -4.09809800 -0.87355500 1.06429300

C -4.63967900 -2.13676900 -1.37935100

C -5.07923900 -1.86437600 0.96660600

C -5.34465300 -2.50251500 -0.23860600

H -4.86189100 -2.61536000 -2.32797200

H -5.64640000 -2.12944800 1.85341500

H -6.10608500 -3.27284400 -0.29160100

C 3.33825400 -0.45773300 -0.03737100

C 4.00093000 -0.85143000 1.13943800

C 3.71316100 -0.96493400 -1.29688800

C 5.03213500 -1.78866200 1.03296400

C 4.74675100 -1.90350700 -1.35026000

C 5.40068500 -2.32060900 -0.19694400

H 5.55562600 -2.09716900 1.93228800

H 5.04383500 -2.30416500 -2.31434100

H 6.20124000 -3.04958500 -0.25743200

C 3.65059700 -0.26219900 2.48355100

H 3.71163500 0.83026300 2.48278000

H 2.63673900 -0.52244600 2.79593400

H 4.33246000 -0.62484100 3.25343900

C 3.05226900 -0.49271500 -2.56990600

H 1.96239600 -0.48019700 -2.49477900

H 3.36293500 0.52389900 -2.83441300

H 3.32206500 -1.13580300 -3.40843200

C -3.90239700 -0.14035700 2.36915700

H -4.31724100 -0.70956500 3.20234900

H -2.85449200 0.06035200 2.58963300

H -4.41476900 0.82845900 2.36028900

C -2.95078700 -0.72524400 -2.60279700

H -3.33626000 0.23337400 -2.96798400

H -1.87445200 -0.60041400 -2.46964500

H -3.10929200 -1.45465000 -3.39831400

C 0.26822300 -2.09504200 0.83350300

H 1.34164000 -2.23512200 0.95144600

H -0.25077500 -2.90629700 1.33580400

C -0.14642700 -2.08426700 -0.63612300

H 0.04498600 -1.09893800 -1.14749000

H -1.21861800 -2.25633200 -0.72459800

C 0.62659300 -3.12988600 -1.45786000

H 1.70429800 -2.96955400 -1.40380200

H 0.41690000 -4.13304500 -1.07965000

H 0.32523300 -3.10062700 -2.50778900

Co 0.00841600 -0.03679400 0.44712800

C -0.19328200 -0.97698200 2.40995600

H 0.56814300 -1.51863200 2.96184100

H -1.18541100 -1.37207200 2.59656000

C -0.06908000 0.45471400 2.34574900

H -0.95161600 1.05599200 2.54443700

H 0.85141100 0.91002700 2.70001300

**1/2Co(+)-5**

Atom x y z

C 1.31877400 -2.97021300 0.34469500

C 1.41400700 -4.33911400 0.59394100

C 0.23494500 -5.07633200 0.71525500

C -1.00354500 -4.44597100 0.58587700

C -1.02745400 -3.07369000 0.33681500

N 0.11798800 -2.38655200 0.22697100

H 0.28138400 -6.14124400 0.91011800

H 2.37637600 -4.82546000 0.69355800

H -1.92021900 -5.01478300 0.67921900

C 2.43148200 -2.00002300 0.17972400

C -2.22028800 -2.20542200 0.16475100

N -1.96569000 -0.95390400 -0.06294500

N 2.06870000 -0.77546800 -0.04816400

C -3.58659500 -2.81063000 0.26084200

H -3.69178100 -3.62580100 -0.46121300

H -3.74273700 -3.24200400 1.25443200

H -4.36792800 -2.07825300 0.07515500

C 3.84533500 -2.48281200 0.28063400

H 4.03508400 -2.90030100 1.27429900

H 4.02491800 -3.28443800 -0.44188800

H 4.55951700 -1.68399100 0.09871200

C -3.03774600 -0.00296200 -0.21947200

C -3.56974100 0.61258500 0.92534600

C -3.47299800 0.31445300 -1.51668900

C -4.56900300 1.57133900 0.74102000

C -4.47593900 1.27762600 -1.64740800

C -5.02010700 1.90356300 -0.53140100

H -4.99385200 2.06276300 1.61032900

H -4.83004100 1.53807400 -2.63955600

H -5.79509800 2.65225000 -0.65365000

C 3.05336100 0.26574200 -0.20540700

C 3.46600300 0.61122100 -1.50288600

C 3.51963000 0.93602900 0.93700900

C 4.37968700 1.65906100 -1.63619900

C 4.42961600 1.97942600 0.75016100

C 4.85764400 2.34049600 -0.52235100

H 4.71489100 1.94272200 -2.62853300

H 4.80267500 2.51431900 1.61758100

H 5.56239300 3.15535800 -0.64639000

C 2.95488800 -0.12915400 -2.71332000

H 3.27325900 -1.17702400 -2.71984400

H 1.86133900 -0.12720900 -2.75889400

H 3.32494200 0.32673100 -3.63200600

C 3.07334700 0.54362800 2.32435500

H 1.98780300 0.43272100 2.39183300

H 3.51420500 -0.40747300 2.64307600

H 3.37550700 1.29487000 3.05464200

C -2.89711300 -0.37218900 -2.72982500

H -1.80669100 -0.28794100 -2.76687600

H -3.13605500 -1.44088300 -2.74886100

H -3.29381100 0.06375700 -3.64709800

C -3.09819800 0.25071500 2.31269600

H -3.45637800 -0.73713400 2.62330600

H -2.00742700 0.23456800 2.38576500

H -3.46810500 0.96811900 3.04581800

C -0.04350600 1.37658900 -0.68072000

H 0.85345500 1.60165500 -1.27059700

H -0.91359100 1.50101700 -1.33749400

C -0.14479400 2.34284700 0.50236200

H 0.71817700 2.22318400 1.16946500

H -1.03310100 2.11562200 1.10429000

C -0.22017700 3.81891400 0.06881200

H 0.67005000 4.06365000 -0.52386100

H -1.07729000 3.94968200 -0.60357400

Co 0.03743900 -0.50842600 -0.17500500

C -0.33855600 4.79795700 1.24203400

H 0.51648700 4.66287000 1.91642500

H -1.22968100 4.55013000 1.83242900

C -0.41187700 6.26135400 0.79995600

H -1.27577400 6.43931500 0.15217600

H -0.49940100 6.93463100 1.65680600

H 0.48219100 6.55473200 0.24135300

**1/2Co(+)-6**

Atom x y z

C 1.02223300 2.70052400 0.23778600

C 1.00001500 4.08038300 0.44714900

C -0.23329700 4.72425000 0.52565700

C -1.40927100 3.98225900 0.43437000

C -1.31861100 2.60531800 0.22382900

N -0.12132000 2.01338700 0.08724800

H -0.27783600 5.79569400 0.68207000

H 1.91922800 4.64187800 0.55444900

H -2.37164700 4.46796600 0.53296700

C 2.22584600 1.83357900 0.23197200

C -2.45024300 1.64598000 0.20439500

N -2.12244500 0.40304400 0.05018300

N 1.99696800 0.56768200 0.08354600

C -3.84056200 2.16767400 0.42371000

H -3.90238500 2.70183300 1.37656900

H -4.11134200 2.88133700 -0.36034000

H -4.57638300 1.36797700 0.43225400

C 3.57084700 2.46126600 0.45218200

H 3.81029300 3.14924400 -0.36472400

H 3.57449100 3.04690800 1.37592200

H 4.35905200 1.71578100 0.51563900

C -3.13879300 -0.61785900 0.13710800

C -3.89024700 -0.97344900 -0.99641400

C -3.32017300 -1.25507200 1.37792800

C -4.81469800 -2.01364700 -0.86707500

C -4.25871600 -2.28615500 1.45598400

C -4.99619100 -2.67191200 0.34325600

H -5.40228100 -2.30422100 -1.73192800

H -4.41004400 -2.78889100 2.40570900

H -5.71632600 -3.47902900 0.42037700

C 3.08949400 -0.37002900 0.17277300

C 3.28412700 -1.02391400 1.40525200

C 3.89573600 -0.64182500 -0.94460500

C 4.28377900 -1.99340400 1.48361600

C 4.88072400 -1.62717400 -0.81606300

C 5.07127800 -2.30514000 0.37979600

H 4.44628000 -2.50744700 2.42544800

H 5.50599600 -1.85802500 -1.67295900

H 5.83708400 -3.06916100 0.45619500

C 2.48550000 -0.65475000 2.63135600

H 2.79006100 0.31970800 3.02979500

H 1.41443200 -0.59457800 2.42851300

H 2.63360700 -1.38674700 3.42603800

C 3.77770400 0.11127900 -2.24856500

H 2.80103700 0.57169200 -2.38960400

H 4.52348300 0.91183300 -2.30696600

H 3.96038800 -0.54857100 -3.09894900

C -2.56128100 -0.82060800 2.60727700

H -1.48356200 -0.78205300 2.43320100

H -2.86831200 0.17598900 2.94336400

H -2.73903800 -1.50784800 3.43500900

C -3.75134400 -0.25252500 -2.31524000

H -4.01852000 0.80642700 -2.23760900

H -2.73490900 -0.29848200 -2.70980500

H -4.41005100 -0.69246000 -3.06443500

C -0.06442800 -1.88239800 0.02462800

H 0.12598200 -1.89048700 1.11178100

H -1.11038200 -2.17509900 -0.11192300

C 0.84282800 -2.90969200 -0.64757500

H 1.88874700 -2.59192300 -0.62336100

H 0.57649900 -3.00939200 -1.70586800

C 0.73767300 -4.29831700 0.00384400

H 1.05266600 -4.27010100 1.05124200

H -0.28979500 -4.67325100 -0.02136400

H 1.37022800 -5.02651800 -0.51223600

Co -0.03826900 0.08540400 -0.24097600

C 0.07458500 -0.45407500 -2.55791900

H 1.05618700 -0.90571800 -2.60796200

H -0.76019700 -1.13738000 -2.64621600

C -0.09168300 0.88149500 -2.57914700

H -1.07127000 1.33640900 -2.66724100

H 0.75240500 1.55963600 -2.63113200

**1/2Co(+)-TS-6/7**

Atom x y z

C 1.20486300 2.68357000 0.02198200

C 1.25277100 4.07272400 -0.09680200

C 0.05092400 4.77803100 -0.16611100

C -1.16624100 4.09762300 -0.11290200

C -1.14869900 2.70791300 0.00606800

N 0.02083500 2.04973100 0.06774500

H 0.06267700 5.85752000 -0.26013900

H 2.19961800 4.59700800 -0.13552100

H -2.10139600 4.64141100 -0.16327500

C 2.33776300 1.74310900 0.13482300

C -2.30261600 1.79088900 0.10459600

N -1.99352100 0.52718800 0.10768500

N 2.00128200 0.48633100 0.13375000

C -3.68419200 2.35980300 0.22924500

H -3.73943400 3.04404000 1.08100100

H -3.94086200 2.94002600 -0.66273800

H -4.43418900 1.58415200 0.36000900

C 3.73129400 2.27818100 0.27095000

H 4.03690700 2.78378100 -0.65082900

H 3.78124400 3.01851700 1.07402600

H 4.44993200 1.48966600 0.48023800

C -3.02423700 -0.46035200 0.33009600

C -3.80028700 -0.94315300 -0.73732300

C -3.19438300 -0.93342900 1.64428100

C -4.75167800 -1.92930100 -0.45872800

C -4.15752500 -1.91892900 1.87066000

C -4.92981100 -2.41936000 0.82931400

H -5.36316200 -2.31177400 -1.26962200

H -4.30169800 -2.29290600 2.87913700

H -5.67319200 -3.18511700 1.02193700

C 3.00338600 -0.53015900 0.35396900

C 3.12833500 -1.04666700 1.65947400

C 3.79967900 -0.99822600 -0.70413100

C 4.04459700 -2.07663300 1.87506600

C 4.69940500 -2.03631100 -0.43750100

C 4.81886800 -2.57939100 0.83438100

H 4.15293700 -2.48467900 2.87476900

H 5.31796400 -2.41348900 -1.24595000

H 5.52056900 -3.38546000 1.01875700

C 2.34239900 -0.47542400 2.81428800

H 2.65252400 0.54890400 3.04661500

H 1.26881300 -0.44102600 2.61138100

H 2.49069000 -1.07072100 3.71578800

C 3.76511300 -0.38870200 -2.08462000

H 2.80457100 0.06371300 -2.32162900

H 4.52799300 0.39134000 -2.18677600

H 3.98284500 -1.13889400 -2.84722500

C -2.38007500 -0.38650800 2.79031800

H -1.30556600 -0.47488300 2.60494600

H -2.58561900 0.67341000 2.97199100

H -2.60176500 -0.92267500 3.71355100

C -3.64232900 -0.43272200 -2.14838900

H -3.72292100 0.65600800 -2.21310700

H -2.67382900 -0.70712500 -2.57099700

H -4.41322200 -0.85151700 -2.79598800

C -0.02744000 -1.92058400 0.16935100

H 0.70941300 -1.98693300 0.97290000

H -1.03009000 -2.14377900 0.53405800

C 0.34620500 -2.74170300 -0.96521800

H 1.40709700 -2.98758100 -1.03681700

H 0.33233100 -1.90969100 -2.02761200

C -0.57339200 -3.83764400 -1.45574300

H -0.53483100 -4.68359600 -0.76034800

H -1.61248400 -3.50087200 -1.49533300

H -0.28605500 -4.21236700 -2.44153300

Co 0.00330000 0.14877100 -0.08520300

C 0.21501600 -1.00623300 -2.93755700

H 1.15246900 -1.18444400 -3.46281900

H -0.63292300 -1.44096000 -3.46767400

C 0.02800200 0.26328300 -2.29230700

H -0.94344000 0.72589500 -2.44020900

H 0.84254600 0.97337100 -2.41790400

**1/2Co(+)-7**

Atom x y z

C 1.25675700 2.61087800 0.09216200

C 1.30335100 4.00122100 0.02239600

C 0.10857700 4.72290900 0.02568300

C -1.11107400 4.04561200 0.07668600

C -1.11203800 2.65460200 0.14430500

N 0.06142400 1.97234400 0.18636900

H 0.12731600 5.80466200 -0.02774500

H 2.25410900 4.51677600 -0.03740400

H -2.04423500 4.59533700 0.05855900

C 2.37363000 1.67538700 0.08852100

C -2.26175900 1.76021200 0.17803800

N -1.95961000 0.48844500 0.07553700

N 2.02171800 0.41430600 0.01386500

C -3.64706300 2.31478400 0.33374200

H -3.70587300 2.97633100 1.20198200

H -3.91823800 2.91049800 -0.54375200

H -4.38935800 1.52887000 0.44781500

C 3.78302200 2.17913600 0.18887000

H 4.01164700 2.83506200 -0.65664300

H 3.92131400 2.76945600 1.09913500

H 4.50626400 1.36753800 0.19208800

C -2.99532500 -0.50191200 0.26189700

C -3.73654600 -0.98937900 -0.82643400

C -3.23028300 -0.96134400 1.57643700

C -4.67044200 -2.00481300 -0.58505500

C -4.17102400 -1.97415200 1.76522600

C -4.87885700 -2.50656600 0.69144500

H -5.24748800 -2.39305000 -1.41884200

H -4.35706900 -2.34121000 2.76950300

H -5.60372300 -3.29641300 0.85563800

C 3.02204200 -0.61187000 0.20396900

C 3.31337500 -1.00792600 1.52746900

C 3.66830900 -1.20415100 -0.89505800

C 4.21224900 -2.05830400 1.72088900

C 4.56290900 -2.25153600 -0.64815300

C 4.82533900 -2.68782500 0.64306300

H 4.43796400 -2.37915300 2.73285200

H 5.06657600 -2.71844200 -1.48900400

H 5.51726800 -3.50562500 0.81226200

C 2.73655000 -0.29363500 2.72851600

H 3.31110300 0.60976500 2.96166700

H 1.70164300 0.02368700 2.58626200

H 2.77532700 -0.93001400 3.61379300

C 3.50625700 -0.70026900 -2.30857000

H 2.62017700 -0.08568900 -2.43931700

H 4.37117000 -0.09221100 -2.59542900

H 3.45581100 -1.52681000 -3.02084300

C -2.54279900 -0.34306100 2.77122000

H -1.47632400 -0.17425100 2.60869800

H -2.97996100 0.63049100 3.01872400

H -2.65344600 -0.97552700 3.65303900

C -3.63278500 -0.41561800 -2.21878700

H -4.53078500 0.16467700 -2.45550000

H -2.77630900 0.24131900 -2.34447800

H -3.56595200 -1.20635500 -2.96964900

C -0.00394500 -2.02400900 0.84550300

H 0.82394600 -1.67945500 1.45213300

H -0.96943800 -2.11742800 1.32715100

C 0.21814000 -2.60362100 -0.35107500

H 1.22881100 -2.58713300 -0.75244100

H 0.73842600 -1.30465700 -3.00175900

C -0.78891500 -3.41560200 -1.10042800

H -0.55183400 -4.47616800 -0.95019200

H -1.80622200 -3.24866400 -0.74486100

H -0.74765500 -3.24277100 -2.17612200

Co 0.01978500 0.14505600 -0.15219600

C -0.08896200 -0.60043700 -3.11206000

H -0.05618000 -0.24171900 -4.15041400

H -1.01848700 -1.15968200 -3.00476400

C -0.00470300 0.56872900 -2.14787400

H -0.85463200 1.24408300 -2.27583900

H 0.90149900 1.15706600 -2.31266400

**1/2Co(+)-8**

Atom x y z

C 1.17463100 2.55914400 0.00898100

C 1.21214300 3.95406400 -0.00041500

C -0.00000400 4.64649200 -0.00732300

C -1.21215100 3.95406300 -0.00041100

C -1.17463800 2.55914300 0.00898400

N -0.00000300 1.92143100 0.00831800

H -0.00000400 5.73029100 -0.01550700

H 2.15183800 4.49203600 -0.00196600

H -2.15184600 4.49203500 -0.00196000

C 2.32348200 1.61060100 0.02786800

C -2.32348800 1.61059900 0.02787200

N -1.99788400 0.35537500 0.04955600

N 1.99787900 0.35537700 0.04953800

C -3.71749700 2.15628600 0.03154900

H -3.86055000 2.82337900 0.88721500

H -3.89694900 2.75107000 -0.86958300

H -4.46263500 1.36653000 0.07949200

C 3.71749100 2.15629000 0.03156400

H 3.89695300 2.75107500 -0.86956400

H 3.86053300 2.82338100 0.88723400

H 4.46262900 1.36653400 0.07951500

C -3.02311900 -0.65927600 0.05427400

C -3.57136400 -1.08145800 -1.16738400

C -3.39696200 -1.22650300 1.28340000

C -4.52492700 -2.10210300 -1.13184000

C -4.35900600 -2.23838700 1.26645200

C -4.91887700 -2.67615900 0.07119000

H -4.95961400 -2.44893700 -2.06376000

H -4.66604300 -2.68943200 2.20443700

H -5.65938400 -3.46836300 0.07715500

C 3.02311700 -0.65927400 0.05427100

C 3.39694100 -1.22649600 1.28340500

C 3.57138200 -1.08145500 -1.16737700

C 4.35898700 -2.23837900 1.26647400

C 4.52494800 -2.10209800 -1.13181500

C 4.91887800 -2.67615200 0.07122200

H 4.66601100 -2.68942200 2.20446500

H 4.95965100 -2.44893200 -2.06372700

H 5.65938700 -3.46835500 0.07720100

C 2.79332100 -0.75355700 2.58199900

H 3.05222600 0.28724700 2.80329200

H 1.70055600 -0.81634800 2.56568200

H 3.14535300 -1.35908300 3.41757800

C 3.16792300 -0.45567000 -2.48069300

H 2.08438900 -0.34185400 -2.56975600

H 3.60878600 0.53859900 -2.61411300

H 3.50426100 -1.06678300 -3.31883200

C -2.79335900 -0.75356700 2.58200400

H -1.70059500 -0.81636700 2.56570300

H -3.05225900 0.28723900 2.80329200

H -3.14541100 -1.35908900 3.41757700

C -3.16788200 -0.45567200 -2.48069400

H -3.60873700 0.53860000 -2.61411800

H -2.08434600 -0.34186400 -2.56974200

H -3.50421200 -1.06678100 -3.31883900

C -0.00000200 -1.97595500 0.14097800

H 0.88313600 -2.30470100 0.70050300

H -0.88316600 -2.30470600 0.70046000

C 0.00003400 -2.63083000 -1.24470300

H 0.88428000 -2.36505000 -1.83235200

H -0.88418400 -2.36505700 -1.83239700

Co -0.00000200 -0.01885300 0.06009900

H 0.00003600 -3.72529100 -1.16814500

**1/2Co(+)-TS-3/9**

Atom x y z

C -1.13248200 2.56200100 -0.08462200

C -1.15020700 3.95339300 -0.17765000

C 0.05892100 4.64495000 -0.17813000

C 1.25769200 3.93728100 -0.12887200

C 1.21823000 2.54623500 -0.03860100

N 0.03612700 1.90012200 0.04024100

H 0.06746900 5.72645700 -0.24496900

H -2.08744400 4.48906800 -0.25608400

H 2.20447000 4.46035600 -0.16940700

C -2.30389900 1.66883100 -0.16481500

C 2.38024900 1.63769800 -0.07646200

N 2.07402900 0.37916800 -0.13944400

N -2.01868800 0.40246500 -0.17945700

C 3.76762500 2.20821200 -0.09046300

H 3.87149000 2.94053600 -0.89596600

H 3.98500200 2.72820900 0.84749800

H 4.51738700 1.43436000 -0.23685400

C -3.67586900 2.26418600 -0.28229800

H -3.94714900 2.80565500 0.62892700

H -3.70748900 2.98378000 -1.10512400

H -4.42972600 1.50293500 -0.46728500

C 3.09078200 -0.63031300 -0.17856800

C 3.81140800 -0.96950400 0.98215100

C 3.28540600 -1.30950700 -1.39839100

C 4.73467100 -2.01670300 0.89340700

C 4.22795900 -2.33700300 -1.43714400

C 4.94606600 -2.69443900 -0.30014700

H 5.29475400 -2.29867100 1.77949700

H 4.39871400 -2.86203800 -2.37142100

H 5.66852100 -3.50196100 -0.34551400

C -3.05624400 -0.58485200 -0.24453800

C -3.17431500 -1.32625600 -1.43752500

C -3.87859400 -0.83841800 0.86988500

C -4.13973500 -2.33117400 -1.49627000

C -4.82066400 -1.86726100 0.76464200

C -4.95515700 -2.60716300 -0.40285500

H -4.25148900 -2.90322700 -2.41163900

H -5.45726100 -2.08455600 1.61660700

H -5.69428100 -3.39854500 -0.46230800

C -2.31213300 -1.01756400 -2.63534700

H -2.51026000 -0.01709200 -3.03270300

H -1.24603800 -1.05355700 -2.38951800

H -2.49272800 -1.73125900 -3.43988000

C -3.78705900 -0.04379600 2.15166000

H -2.78252200 0.33651400 2.34165900

H -4.46701300 0.81482800 2.13778300

H -4.07740100 -0.65709200 3.00628700

C 2.53310200 -0.90923400 -2.64305200

H 1.45312900 -0.86223100 -2.47326600

H 2.83700500 0.07997200 -3.00073900

H 2.71405400 -1.61765700 -3.45219000

C 3.63673900 -0.24189700 2.29516400

H 4.34355100 0.59005900 2.38714300

H 2.63387900 0.16851000 2.42299800

H 3.83357500 -0.91081400 3.13486900

C 0.02870000 -2.03638600 0.13522600

H -0.93318800 -2.41073500 -0.20168900

H 0.88431600 -2.28718100 -0.48348100

C 0.21873900 -1.77822300 1.48949000

H 0.08540800 0.05767800 1.69604000

H 1.24299900 -1.73291400 1.84448000

C -0.79780900 -2.11501900 2.54786500

H -1.81665100 -2.07761000 2.16430000

H -0.61024700 -3.14352900 2.87764700

H -0.72092900 -1.47081200 3.42483300

Co 0.01789200 0.01932700 0.17324600

**1/2Co(+)-9**

Atom x y z

C 1.13729400 2.58467300 0.01901900

C 1.14811400 3.97732000 0.01433400

C -0.06424900 4.66610900 -0.01998400

C -1.26447600 3.95558000 -0.02928200

C -1.22869100 2.56354700 -0.02267200

N -0.03886700 1.91278500 -0.02884400

H -0.07391100 5.74938800 -0.02456100

H 2.08552400 4.51854700 0.04166400

H -2.21205800 4.47962800 -0.03575900

C 2.28313500 1.68586200 0.08853800

C -2.36014900 1.64484700 0.01175400

N -2.01697200 0.38395900 0.06995400

N 1.96410400 0.41680800 0.11505100

C -3.76500400 2.16860200 -0.00850000

H -3.91292100 2.90392100 0.78708000

H -3.97484100 2.67363500 -0.95659000

H -4.49475700 1.37338700 0.12227500

C 3.67544900 2.24050300 0.14184300

H 3.75716200 2.99235900 0.93123700

H 4.41374000 1.46519300 0.33093900

H 3.93248400 2.73434000 -0.80056500

C -3.03592900 -0.63145300 0.12085800

C -3.64299100 -1.07811500 -1.06791100

C -3.37508000 -1.16952900 1.37699000

C -4.58362300 -2.10822800 -0.97349600

C -4.32479900 -2.19269500 1.41800500

C -4.92033000 -2.66610000 0.25395600

H -5.05860300 -2.47113800 -1.87942900

H -4.60106200 -2.61806700 2.37741700

H -5.65112300 -3.46580700 0.30461000

C 3.00842400 -0.57138800 0.17635200

C 3.28800700 -1.16445700 1.42265100

C 3.70782800 -0.92863300 -0.99029800

C 4.27239000 -2.15344500 1.47339000

C 4.68211000 -1.92670800 -0.88758900

C 4.96102700 -2.53935800 0.32797800

H 4.50385700 -2.61967700 2.42560700

H 5.22823100 -2.22153600 -1.77808700

H 5.71949600 -3.31244200 0.38508800

C 2.59249300 -0.71254200 2.68338500

H 2.89980800 0.29845100 2.97084700

H 1.50493000 -0.68861800 2.57383900

H 2.83131800 -1.37302400 3.51771200

C 3.45692200 -0.25501200 -2.31824500

H 2.41053100 0.02095400 -2.45510600

H 4.05206600 0.65947800 -2.41749700

H 3.74567000 -0.90781700 -3.14345000

C -2.78907400 -0.62241800 2.65643400

H -1.70717100 -0.47881900 2.59761600

H -3.21960800 0.35328500 2.90637800

H -2.99476700 -1.28893100 3.49484600

C -3.33526600 -0.45783200 -2.41040300

H -3.93649100 0.44291900 -2.57743600

H -2.28810200 -0.16674500 -2.50887500

H -3.57386900 -1.14928400 -3.22002300

C -0.00104300 -2.03866500 0.40455000

H 0.97707900 -2.29219100 0.79726100

H -0.82703900 -2.04421700 1.10628700

C -0.24125500 -2.09522900 -0.93826200

H -0.01399600 0.14495100 -1.61173300

H -1.27169300 -2.02695800 -1.26846100

C 0.72828100 -2.57349500 -1.97457500

H 1.75795000 -2.57453600 -1.62087300

H 0.46326000 -3.60838700 -2.22391200

H 0.66189800 -1.99839600 -2.89912400

Co -0.02029400 0.07003100 -0.11241800

**1/2Co(+)-10**

Atom x y z

C -1.12754200 2.71011000 0.09644000

C -1.14602300 4.10175800 0.19352300

C 0.07822700 4.77169200 0.26099400

C 1.28392500 4.06642600 0.23234100

C 1.22848400 2.67565400 0.13475800

N 0.04207100 2.06627700 0.07207100

H 0.09278100 5.85283500 0.33670000

H -2.07718300 4.65398600 0.21654800

H 2.22931400 4.59173900 0.28558800

C -2.27815200 1.76043100 0.01002500

C 2.35333200 1.69310000 0.08639800

N 1.98501000 0.45247300 -0.00322700

N -1.94273100 0.51027800 -0.07343600

C 3.76316400 2.18946200 0.13431900

H 3.94299400 2.89708400 -0.68104700

H 3.94700200 2.72754200 1.06969700

H 4.48092400 1.37699700 0.05446100

C -3.67476800 2.29457000 0.02478500

H -3.82495300 2.98958800 -0.80737000

H -4.41186300 1.49906400 -0.04935600

H -3.85743400 2.85624200 0.94638900

C 2.95910300 -0.61205900 -0.04652400

C 3.47376400 -1.11444500 1.15839600

C 3.30317600 -1.14799500 -1.29676200

C 4.38615200 -2.16927600 1.08172700

C 4.22419900 -2.19688300 -1.32092200

C 4.76566900 -2.70316700 -0.14451300

H 4.79646300 -2.57829000 1.99930900

H 4.51083800 -2.62446600 -2.27617900

H 5.47564200 -3.52197500 -0.18270800

C -2.94677800 -0.52425400 -0.16082900

C -3.34942700 -0.96302300 -1.43085600

C -3.43194100 -1.09482100 1.02532600

C -4.29567500 -1.98825300 -1.49148600

C -4.37570200 -2.11798700 0.91204600

C -4.80957900 -2.55974500 -0.33284300

H -4.62523100 -2.34427900 -2.46215900

H -4.76706400 -2.57589600 1.81465500

H -5.54164700 -3.35693400 -0.40015900

C -2.76757700 -0.36866600 -2.68866500

H -2.98577100 0.69968600 -2.78875800

H -1.67815400 -0.48055700 -2.71272800

H -3.16755000 -0.86426500 -3.57356100

C -2.93642200 -0.64403400 2.37664900

H -1.85138400 -0.76597100 2.46328400

H -3.16137600 0.40853200 2.57759800

H -3.39597700 -1.22952000 3.17328100

C 2.68637900 -0.62626700 -2.56931400

H 1.59646100 -0.73873400 -2.55145400

H 2.90124800 0.43406100 -2.73695100

H 3.05855500 -1.17389300 -3.43552100

C 3.04393900 -0.56241400 2.49531200

H 3.38994400 0.46411100 2.65710900

H 1.95416200 -0.55737800 2.59718100

H 3.44593300 -1.16619000 3.30922600

H -0.00505100 -1.35241800 -0.17743100

Co 0.01580500 0.15182700 -0.06767300

**3/2Co(+)**

**3/2Co(+)-1**

Atom x y z

C 1.16931800 2.44969700 -0.11223100

C 1.20663400 3.83274800 -0.29869000

C 0.00000100 4.52487500 -0.37661800

C -1.20663300 3.83274800 -0.29868700

C -1.16931600 2.44969700 -0.11222900

N 0.00000100 1.81281500 0.01430300

H 0.00000100 5.59953900 -0.51870300

H 2.14723800 4.36012300 -0.38996600

H -2.14723700 4.36012300 -0.38996100

C 2.36487900 1.54917100 -0.09690600

C -2.36487800 1.54917200 -0.09689900

N -2.09945600 0.29100800 -0.07713700

N 2.09945600 0.29100800 -0.07713500

C -3.73296600 2.16030800 -0.16208100

H -3.90817100 2.81747300 0.69487000

H -3.83301100 2.77336400 -1.06290500

H -4.50808300 1.39810800 -0.18108300

C 3.73296700 2.16030600 -0.16210500

H 3.83300100 2.77336000 -1.06293200

H 3.90818300 2.81747200 0.69484200

H 4.50808300 1.39810500 -0.18111600

C -3.12725000 -0.71108000 -0.07047700

C -3.33903800 -1.43423700 -1.25702900

C -3.81734300 -1.00460500 1.11886500

C -4.29924600 -2.44669900 -1.24293300

C -4.75977400 -2.03545100 1.08399000

C -5.00680100 -2.74712100 -0.08412600

H -4.48660000 -3.00889800 -2.15201900

H -5.30040000 -2.28420800 1.99143100

H -5.74321300 -3.54311500 -0.08864000

C 3.12724800 -0.71108200 -0.07048100

C 3.81736000 -1.00459700 1.11885300

C 3.33901400 -1.43425200 -1.25702900

C 4.75978800 -2.03544500 1.08397300

C 4.29922000 -2.44671600 -1.24293800

C 5.00679400 -2.74712800 -0.08414000

H 5.30042800 -2.28419500 1.99140700

H 4.48655800 -3.00892500 -2.15202200

H 5.74320400 -3.54312400 -0.08865800

C 3.54635600 -0.26268600 2.40545600

H 3.92451100 0.76485700 2.38400700

H 2.47701300 -0.21159100 2.63006900

H 4.03148500 -0.76100600 3.24512200

C 2.56456700 -1.11868400 -2.51202900

H 1.48362900 -1.17414400 -2.34438600

H 2.77665000 -0.11245800 -2.88767000

H 2.81007200 -1.82217800 -3.30806500

C -3.54631600 -0.26270700 2.40547000

H -2.47697000 -0.21162500 2.63007200

H -3.92446100 0.76484000 2.38403300

H -4.03144100 -0.76102800 3.24513900

C -2.56461100 -1.11865700 -2.51203900

H -2.77670300 -0.11242900 -2.88766900

H -1.48367000 -1.17411400 -2.34441300

H -2.81012600 -1.82214600 -3.30807600

Co 0.00000300 -0.25067100 0.40159600

C 0.00000900 -2.08618400 1.13530400

H 0.00005400 -2.79489200 0.29672400

H 0.88532400 -2.30064800 1.74192900

H -0.88534000 -2.30068200 1.74186600

**3/2Co(+)-2**

Atom x y z

C 1.16488100 2.40490200 -0.36195900

C 1.20222900 3.78313200 -0.58877000

C 0.00003100 4.47749000 -0.68197000

C -1.20218800 3.78324600 -0.58822600

C -1.16488100 2.40499800 -0.36149100

N -0.00000800 1.76260000 -0.21369100

H 0.00004700 5.54838000 -0.84988100

H 2.14403000 4.30463000 -0.69763200

H -2.14399200 4.30483300 -0.69662500

C 2.37747400 1.52898500 -0.33132300

C -2.37754200 1.52914700 -0.33057200

N -2.15543000 0.28104100 -0.13306400

N 2.15538700 0.28093000 -0.13329000

C -3.71978300 2.15126800 -0.59110300

H -3.96493500 2.88774600 0.18008000

H -3.72000800 2.67755400 -1.54996500

H -4.50658700 1.40111300 -0.61284600

C 3.71965000 2.15089500 -0.59263500

H 3.71939000 2.67718100 -1.55149200

H 3.96536100 2.88734600 0.17839900

H 4.50634300 1.40063500 -0.61481200

C -3.21620300 -0.68848900 -0.13952600

C -3.36466900 -1.48536100 -1.28941900

C -4.02453200 -0.86752100 0.99718400

C -4.34927000 -2.47418300 -1.27991200

C -4.98822600 -1.87923700 0.96081700

C -5.15293100 -2.67799700 -0.16386800

H -4.48117000 -3.09368200 -2.16104500

H -5.61730400 -2.03670100 1.83103900

H -5.90605900 -3.45817200 -0.17075900

C 3.21610600 -0.68870600 -0.13969300

C 4.02484400 -0.86719700 0.99681600

C 3.36407300 -1.48618100 -1.28922900

C 4.98839400 -1.87905900 0.96063900

C 4.34855600 -2.47512400 -1.27954100

C 5.15257400 -2.67845500 -0.16367100

H 5.61779400 -2.03611800 1.83070100

H 4.48008500 -3.09508700 -2.16040100

H 5.90559300 -3.45873600 -0.17041300

C 3.89240300 -0.00024100 2.22584200

H 4.28141600 1.01043200 2.06159300

H 2.85572700 0.10455200 2.55181700

H 4.45532400 -0.42361800 3.05823100

C 2.50928400 -1.26508000 -2.51157300

H 1.44392400 -1.33160100 -2.27494300

H 2.68000900 -0.28048900 -2.95967900

H 2.72553500 -2.01158500 -3.27641800

C -3.89144900 -0.00126800 2.22663500

H -2.85461300 0.10315000 2.55222600

H -4.28033900 1.00957200 2.06309600

H -4.45410700 -0.42499700 3.05902300

C -2.51024800 -1.26372500 -2.51191900

H -2.68164200 -0.27921300 -2.95995900

H -1.44480800 -1.32958700 -2.27547600

H -2.72620100 -2.01032600 -3.27675600

C -0.00154800 -2.34604100 0.18630500

H -0.00226200 -2.70930300 -0.84781500

H 0.88217000 -2.77367700 0.67210100

H -0.88604000 -2.77161600 0.67251300

C 0.00080900 -0.59834100 2.77985500

H 0.91782600 -1.17242400 2.84633200

H -0.91603000 -1.17259100 2.84716100

C 0.00067000 0.74106700 2.73549300

H -0.91961500 1.31439800 2.75165000

H 0.92087800 1.31455000 2.75067100

Co 0.00050200 -0.34615200 0.27116600

**3/2Co(+)-TS-2/3**

Atom x y z

C 1.16915700 2.47857100 0.00930000

C 1.19915300 3.87447100 0.02595800

C -0.00297100 4.57353700 0.06166900

C -1.20409300 3.87101300 0.09295900

C -1.16972100 2.47631800 0.07222200

N 0.00014600 1.81483800 0.02306800

H -0.00420000 5.65739700 0.07137000

H 2.13980900 4.40886600 0.01209300

H -2.14557800 4.40264900 0.13293300

C 2.39497300 1.62508000 0.01008900

C -2.39189800 1.61806900 0.12305500

N -2.19499100 0.35165100 0.03533500

N 2.19878300 0.35807000 -0.06117400

C -3.72976800 2.28186800 0.28824000

H -3.74116500 2.91862500 1.17716400

H -3.95362900 2.92166900 -0.57081200

H -4.52557700 1.54661900 0.38098300

C 3.73573100 2.29742600 0.11474600

H 3.89599300 2.97354700 -0.73031700

H 3.80307300 2.89820700 1.02625200

H 4.54229000 1.56807900 0.12380800

C -3.28299100 -0.58577900 0.09357400

C -3.98105700 -0.91890400 -1.08162000

C -3.57570500 -1.19827800 1.32767800

C -4.94529000 -1.92861100 -1.00621600

C -4.55021100 -2.19800600 1.34965400

C -5.22280000 -2.57367000 0.19220800

H -5.48787300 -2.20350500 -1.90542400

H -4.78599300 -2.68163300 2.29236700

H -5.96999000 -3.35884700 0.22739800

C 3.29153200 -0.56991600 0.01629000

C 3.71991000 -1.00800300 1.28344700

C 3.86075900 -1.06539100 -1.17065100

C 4.71275700 -1.99019700 1.33615700

C 4.85338200 -2.04240500 -1.06392700

C 5.27221300 -2.51171200 0.17599100

H 5.05056500 -2.34429100 2.30497200

H 5.30491100 -2.43405200 -1.96991900

H 6.03896200 -3.27612900 0.23759900

C 3.17172800 -0.41304300 2.55877700

H 3.61715200 0.56640500 2.76690300

H 2.08953000 -0.27113800 2.52306800

H 3.39819400 -1.05184600 3.41346800

C 3.46622500 -0.52431200 -2.52304600

H 2.38435200 -0.48830600 -2.65845800

H 3.84032600 0.49461800 -2.67307400

H 3.88222000 -1.13761600 -3.32334000

C -2.93168300 -0.74482200 2.61660100

H -1.88688100 -0.45748900 2.49148900

H -3.45386500 0.12561700 3.03016200

H -2.97637200 -1.52970700 3.37329200

C -3.77675800 -0.18351200 -2.38604400

H -4.48556700 0.64709700 -2.47950800

H -2.77607500 0.23546000 -2.49050600

H -3.95269000 -0.84239100 -3.23832100

C -0.21978200 -1.24780900 -2.04986000

H 0.09839400 -0.21798100 -2.30047100

H 0.39748100 -1.91438400 -2.64348600

H -1.26717800 -1.37405100 -2.30311000

C 0.07624500 -2.53039600 -0.37830000

H 0.96828400 -2.94049400 -0.83320800

H -0.84128600 -3.02837000 -0.66713600

C 0.19553500 -2.00954600 0.93391000

H -0.66257900 -2.09167300 1.59267800

H 1.16635300 -2.05535900 1.41111900

Co -0.01986700 -0.23888000 -0.14517800

**3/2Co(+)-3**

Atom x y z

C -1.17002500 2.70667100 0.00355600

C -1.20720600 4.09756100 0.11815200

C 0.00000000 4.79248000 0.15885100

C 1.20720600 4.09756100 0.11815200

C 1.17002500 2.70667100 0.00355600

N 0.00000000 2.06587300 -0.09461600

H 0.00000000 5.87303100 0.24535200

H -2.14732600 4.62964700 0.18384600

H 2.14732500 4.62964700 0.18384600

C -2.36165000 1.80377800 0.04307000

C 2.36165000 1.80377800 0.04307000

N 2.09363800 0.54582400 0.10675600

N -2.09363800 0.54582400 0.10675600

C 3.73143100 2.41477800 0.06624300

H 3.91005300 3.00741800 -0.83588000

H 3.83097900 3.09162800 0.92013900

H 4.50534300 1.65504900 0.14302000

C -3.73143100 2.41477800 0.06624300

H -3.83097900 3.09162800 0.92013900

H -3.91005400 3.00741800 -0.83588000

H -4.50534300 1.65504900 0.14302000

C 3.12279100 -0.45302200 0.16286400

C 3.32276900 -1.10926400 1.39064500

C 3.82965500 -0.80982500 -0.99948900

C 4.28307500 -2.12021300 1.44399100

C 4.77045800 -1.83809500 -0.89648100

C 5.00307700 -2.48493800 0.31136500

H 4.46142300 -2.62957900 2.38545400

H 5.32282100 -2.13516200 -1.78210900

H 5.73904300 -3.27934600 0.36827300

C -3.12279100 -0.45302200 0.16286400

C -3.82965500 -0.80982500 -0.99948900

C -3.32276900 -1.10926400 1.39064500

C -4.77045800 -1.83809500 -0.89648100

C -4.28307500 -2.12021300 1.44399100

C -5.00307700 -2.48493800 0.31136500

H -5.32282100 -2.13516200 -1.78210900

H -4.46142300 -2.62958000 2.38545400

H -5.73904300 -3.27934600 0.36827300

C -3.58883400 -0.13207100 -2.32703300

H -4.03308900 0.86816700 -2.36905700

H -2.52363600 -0.02490100 -2.54799300

H -4.03345800 -0.70925600 -3.13827100

C -2.53971000 -0.72048600 2.61960900

H -1.45975500 -0.77901300 2.44773700

H -2.75463000 0.30434200 2.93893100

H -2.77587800 -1.37913200 3.45586100

C 3.58883300 -0.13207100 -2.32703300

H 2.52363600 -0.02490100 -2.54799300

H 4.03308800 0.86816700 -2.36905700

H 4.03345700 -0.70925500 -3.13827100

C 2.53971000 -0.72048500 2.61960900

H 2.75463000 0.30434200 2.93893000

H 1.45975600 -0.77901300 2.44773700

H 2.77587800 -1.37913200 3.45586100

C 0.00000000 -1.80170000 -1.22287900

H -0.87813900 -1.88695700 -1.87727500

H 0.87813900 -1.88695700 -1.87727500

C 0.00000000 -2.94115100 -0.19226000

H -0.87760400 -2.85873300 0.46134000

H 0.87760400 -2.85873300 0.46134000

C 0.00000000 -4.33782200 -0.83227000

H -0.88273800 -4.48103600 -1.46225800

H 0.88273800 -4.48103600 -1.46225800

H 0.00000000 -5.12637900 -0.07359800

Co 0.00000000 -0.00610700 -0.38126400

**3/2Co(+)-4**

Atom x y z

N -0.11856100 2.00248500 -0.13863500

C -1.30709700 2.60968200 -0.24096300

C -2.49053300 1.69407600 -0.25435100

N -2.23092700 0.44539900 -0.12506700

C -3.26497400 -0.54817200 -0.20239100

C -3.40516300 -1.25135000 -1.41269400

C -2.57592000 -0.90039100 -2.62244700

H -2.72882000 -1.62573600 -3.42223300

C -4.36038600 -2.26685200 -1.47534100

C -5.14539200 -2.58431300 -0.37270800

C -4.99181500 -1.87425200 0.81171500

C -4.05654300 -0.84154700 0.92202700

C -3.93758000 -0.06801300 2.21303900

H -2.90187600 0.03506900 2.54297000

H -5.60775500 -2.11932300 1.67107100

H -4.48429200 -2.81610100 -2.40308300

C -3.85242100 2.28871200 -0.48057900

H -4.11375500 2.98203300 0.32452600

H -3.87513800 2.85725500 -1.41474300

H -4.61681300 1.51719500 -0.53167800

C -1.39650100 3.99612500 -0.39175100

C -0.22248400 4.73951500 -0.45929400

C 1.00459900 4.08560900 -0.41790400

C 1.01910200 2.69670100 -0.26454000

C 2.26427100 1.86988100 -0.29797900

N 2.10233800 0.60642200 -0.13809300

C 3.21023900 -0.30662200 -0.22602100

C 3.37593400 -1.02015300 -1.42691600

C 4.40689900 -1.95850900 -1.49455200

C 5.24063100 -2.19022000 -0.40618300

C 5.05994900 -1.47053200 0.76848700

C 4.04834400 -0.51312800 0.88344100

H 5.71320900 -1.64924900 1.61647100

H 4.55202200 -2.51542700 -2.41454600

C 3.57208100 2.55533600 -0.57520700

H 3.81395200 3.26721000 0.21983000

H 4.38605200 1.83895200 -0.65378700

H 3.51971600 3.12227900 -1.50896700

H 1.92575600 4.64576500 -0.50950000

H -0.26393100 5.81726000 -0.56767100

H -2.35784900 4.48760300 -0.46278300

H 6.03070500 -2.92988600 -0.47405600

C 3.89668900 0.27417900 2.16254900

H 4.23679000 1.30943100 2.05012200

H -5.87567500 -3.38342700 -0.43652000

C 2.48855600 -0.76617900 -2.61976500

H 2.71916900 -1.45936000 -3.42927800

C -0.10936300 -2.12568300 0.04030600

H -1.13151800 -2.41415000 0.32199600

H -0.06287200 -2.26958100 -1.05141600

H -1.50803300 -0.88023700 -2.39040200

H -2.83620900 0.08525300 -3.02355300

H -4.48771800 -0.56510900 3.01262200

H -4.34857600 0.94377700 2.12612800

H 4.49150200 -0.16911500 2.96170700

H 2.86138100 0.31371500 2.50740200

H 2.61235500 0.24782700 -3.01460000

H 1.43084600 -0.88735300 -2.37069700

C 0.71784200 -4.54127700 0.27947700

C 0.89248100 -3.07720600 0.70739800

H 1.43469400 -5.19646300 0.78412600

H 0.86525100 -4.65754300 -0.79870500

H -0.28752800 -4.90457300 0.51326400

H 1.92037500 -2.76788700 0.48895800

H 0.79034000 -3.02580800 1.79853200

C -0.00090800 -0.42298600 2.75124700

C -0.06594600 0.91639000 2.74223100

H -0.88753300 -1.04372100 2.81091800

H 0.94434200 -0.95021700 2.81225500

H -1.01289000 1.44385300 2.77146800

H 0.82675100 1.53125800 2.77196800

Co -0.00162600 -0.13290900 0.28675800

**3/2Co(+)-TS-4/5**

Atom x y z

C 1.14469600 2.59804800 -0.32304700

C 1.16230400 3.98254400 -0.50016500

C -0.04728700 4.66795900 -0.56539800

C -1.24175600 3.95709900 -0.47841500

C -1.19445000 2.57335300 -0.30332600

N -0.01747200 1.93008600 -0.20882100

H -0.05990800 5.74373500 -0.69525200

H 2.09805700 4.51895300 -0.58896300

H -2.18887700 4.47546800 -0.55134400

C 2.35824900 1.74394500 -0.27662100

C -2.39389400 1.69650000 -0.24491500

N -2.18305600 0.44799700 0.00394400

N 2.16730200 0.49661500 -0.00087300

C -3.74097700 2.31619800 -0.49563700

H -3.95898100 3.07686900 0.26020400

H -3.76679800 2.81443200 -1.46862400

H -4.53467600 1.57404000 -0.46727500

C 3.69227400 2.37420400 -0.56304800

H 3.69191300 2.86345900 -1.54090400

H 3.91893500 3.14424600 0.18078000

H 4.49375200 1.64003600 -0.54417800

C -3.27772600 -0.48853400 -0.03853100

C -3.60221500 -1.07446000 -1.27807600

C -3.97508500 -0.82216000 1.13657300

C -4.60019500 -2.05128800 -1.30607000

C -4.97068300 -1.80027700 1.05387200

C -5.27439800 -2.42407200 -0.14957700

H -4.85478500 -2.51570300 -2.25345600

H -5.52006400 -2.06553200 1.95156900

H -6.04677700 -3.18421900 -0.18952200

C 3.26736700 -0.43297900 -0.03938800

C 3.97270600 -0.74078000 1.13761100

C 3.57460100 -1.05125700 -1.26678600

C 4.97733800 -1.71027500 1.06625000

C 4.58159100 -2.01907800 -1.28371900

C 5.27561400 -2.35527000 -0.12743700

H 5.53452400 -1.95517000 1.96488400

H 4.82728000 -2.50611900 -2.22200000

H 6.05534400 -3.10824400 -0.15942900

C 3.69007200 -0.05294000 2.45126700

H 3.56258300 1.02671900 2.34092400

H 2.78325000 -0.43717000 2.92618300

H 4.51014200 -0.21438600 3.15191100

C 2.87632200 -0.66557500 -2.54861600

H 1.78978200 -0.63949800 -2.44219300

H 3.18512400 0.32643900 -2.89614000

H 3.11491100 -1.37020200 -3.34596100

C -3.71616400 -0.13590600 2.45645900

H -2.81146400 -0.50384500 2.94620200

H -3.60648800 0.94620100 2.34961200

H -4.54367400 -0.31116400 3.14499200

C -2.94016900 -0.63775000 -2.56299200

H -3.32617100 0.32940800 -2.90434600

H -1.85871900 -0.53119700 -2.46360100

H -3.13358300 -1.35526400 -3.36141400

C 0.34093000 -2.23301500 0.59368800

H 1.43084900 -2.25301200 0.59530900

H -0.01487600 -3.06054800 1.20320200

C -0.24163100 -2.37456500 -0.81280200

H 0.02682300 -1.52838700 -1.46189100

H -1.33182400 -2.39540200 -0.76493700

C 0.25985700 -3.66284800 -1.49349500

H 1.34846500 -3.66586500 -1.58797500

H -0.02754900 -4.54411300 -0.91435200

H -0.16819300 -3.76639500 -2.49482200

Co 0.03097300 0.04125700 0.50541800

C -0.06243200 -1.13734200 2.41002500

H 0.79056600 -1.69353300 2.78053200

H -1.00205100 -1.65125400 2.57097700

C -0.04494500 0.28544400 2.53545800

H -0.96562300 0.81099000 2.76261700

H 0.85561300 0.77886800 2.88377300

**3/2Co(+)-5**

Atom x y z

C 1.17023100 -3.08644800 -0.02332000

C 1.20733500 -4.47837500 0.07772300

C -0.00000200 -5.17357400 0.11139900

C -1.20733900 -4.47837400 0.07772300

C -1.17023400 -3.08644700 -0.02332000

N -0.00000100 -2.44510600 -0.11613500

H -0.00000300 -6.25491400 0.18740600

H 2.14736300 -5.01121000 0.13859400

H -2.14736800 -5.01120800 0.13859400

C 2.36122400 -2.18342300 0.02644800

C -2.36122600 -2.18342100 0.02644800

N -2.09257400 -0.92622700 0.10586400

N 2.09257300 -0.92622900 0.10586400

C -3.73138300 -2.79390400 0.04153500

H -3.91045500 -3.37438100 -0.86837600

H -3.83125300 -3.48199800 0.88634700

H -4.50490600 -2.03488100 0.12858100

C 3.73138100 -2.79390700 0.04153600

H 3.83125000 -3.48200100 0.88634700

H 3.91045200 -3.37438400 -0.86837600

H 4.50490400 -2.03488500 0.12858100

C -3.12109900 0.07242200 0.17314300

C -3.31834400 0.71690400 1.40766800

C -3.82993900 0.44122900 -0.98432700

C -4.27770700 1.72802600 1.47275800

C -4.76956500 1.46936500 -0.86948300

C -4.99945900 2.10451000 0.34504800

H -4.45412300 2.22797300 2.41962500

H -5.32333900 1.77550300 -1.75114200

H -5.73485500 2.89875500 0.41114300

C 3.12109900 0.07242000 0.17314300

C 3.82993900 0.44122600 -0.98432700

C 3.31834400 0.71690100 1.40766800

C 4.76956600 1.46936100 -0.86948300

C 4.27770800 1.72802200 1.47275800

C 4.99946000 2.10450600 0.34504800

H 5.32334000 1.77549900 -1.75114200

H 4.45412500 2.22797000 2.41962500

H 5.73485800 2.89875000 0.41114300

C 3.59293900 -0.22370300 -2.31904100

H 4.04477500 -1.22001800 -2.37216800

H 2.52850200 -0.33647500 -2.54048300

H 4.03274800 0.36558300 -3.12420300

C 2.53335900 0.31551800 2.63130700

H 1.45373000 0.37637000 2.45837900

H 2.74736900 -0.71274100 2.93997900

H 2.76857000 0.96521200 3.47480400

C -3.59293900 -0.22370000 -2.31904100

H -2.52850200 -0.33647400 -2.54048300

H -4.04477700 -1.22001500 -2.37216800

H -4.03274700 0.36558700 -3.12420300

C -2.53335900 0.31552100 2.63130700

H -2.74737000 -0.71273800 2.93997900

H -1.45373000 0.37637100 2.45837900

H -2.76856900 0.96521400 3.47480400

C 0.00000000 1.42257900 -1.21893200

H 0.87859800 1.51112400 -1.87174500

H -0.87859800 1.51112500 -1.87174400

C 0.00000200 2.54964100 -0.17556800

H 0.87824000 2.46088200 0.47775100

H -0.87823600 2.46088300 0.47775200

C 0.00000200 3.95972200 -0.79328000

H 0.87638400 4.06306100 -1.44562700

H -0.87638000 4.06306200 -1.44562700

Co 0.00000000 -0.37255100 -0.37935100

C 0.00000300 5.08613800 0.24577600

H 0.87600400 4.97786900 0.89766900

H -0.87599700 4.97787000 0.89766900

C 0.00000400 6.48338400 -0.37887000

H -0.88199800 6.63925900 -1.00763400

H 0.00000400 7.26424000 0.38628400

H 0.88200500 6.63925800 -1.00763500

**3/2Co(+)-6**

Atom x y z

C 1.30679500 2.60941600 0.23650000

C 1.39691600 3.99601500 0.38610200

C 0.22315700 4.73970000 0.45383300

C -1.00415500 4.08611500 0.41223800

C -1.01933500 2.69718200 0.26027500

N 0.11821200 2.00235400 0.13568200

H 0.26479500 5.81745500 0.56195800

H 2.35861200 4.48686300 0.45614800

H -1.92502800 4.64689200 0.50315400

C 2.49031300 1.69390200 0.24864000

C -2.26498400 1.87109600 0.29326600

N -2.10274000 0.60711500 0.13870300

N 2.23169800 0.44512000 0.11734000

C -3.57348000 2.55839600 0.56263000

H -3.52562600 3.12624600 1.49609500

H -3.80955500 3.26965700 -0.23464200

H -4.38906900 1.84341500 0.63755000

C 3.85187600 2.28974300 0.47360800

H 4.11183800 2.98215900 -0.33275800

H 3.87436400 2.85998000 1.40670100

H 4.61720400 1.51926900 0.52514300

C -3.21024100 -0.30622000 0.22730000

C -4.04696200 -0.51656400 -0.88226000

C -3.37713200 -1.01662400 1.43021100

C -5.05612600 -1.47678900 -0.76680600

C -4.40601200 -1.95698400 1.49857000

C -5.23677700 -2.19428300 0.40898500

H -5.70738600 -1.65921300 -1.61559600

H -4.55224700 -2.51105900 2.42010600

H -6.02426000 -2.93667400 0.47704200

C 3.26848500 -0.54631200 0.19673000

C 3.42110200 -1.23677800 1.41280700

C 4.05087300 -0.84910800 -0.93125500

C 4.37953100 -2.24930300 1.47709300

C 4.99087300 -1.87720600 -0.81862700

C 5.15652900 -2.57518600 0.37131300

H 4.51253700 -2.78932300 2.40897200

H 5.60044200 -2.12851500 -1.68069400

H 5.89007300 -3.37112900 0.43706600

C 2.59884500 -0.87952100 2.62550400

H 2.83691400 0.12157400 3.00103700

H 1.52769400 -0.89443200 2.40797100

H 2.78178200 -1.58213800 3.43910600

C 3.91545900 -0.09033800 -2.22917600

H 2.87756200 -0.01673400 -2.56024300

H 4.30086000 0.93211900 -2.15131800

H 4.47813600 -0.58124800 -3.02378900

C -2.49673400 -0.75318400 2.62619700

H -1.43625600 -0.85185300 2.37987700

H -2.64152500 0.25616800 3.02608300

H -2.71616600 -1.45488900 3.43147700

C -3.90159500 0.27155000 -2.16161800

H -4.30609900 1.28520500 -2.06473500

H -2.86084000 0.37145100 -2.47503800

H -4.44543300 -0.20897500 -2.97559000

C 0.10154000 -2.12652900 -0.02099300

H 1.12942500 -2.41806300 -0.27723200

H 0.02943800 -2.26132200 1.07048600

C -0.88555100 -3.08231400 -0.70399200

H -0.75878400 -3.03813200 -1.79294600

H -1.91833600 -2.77224900 -0.51073300

C -0.72100400 -4.54351900 -0.26232500

H 0.28893200 -4.90906600 -0.47167500

H -0.89196600 -4.65219000 0.81316300

H -1.42716600 -5.20184100 -0.77788400

Co 0.00190600 -0.13505200 -0.28345300

C -0.02277600 -0.43318600 -2.74231300

H 0.85088300 -1.07122900 -2.80972500

H -0.97860900 -0.94165700 -2.79499100

C 0.06856200 0.90472600 -2.73409300

H -0.81201700 1.53702600 -2.75690700

H 1.02527900 1.41336600 -2.77154800

**3/2Co(+)-TS-6/7**

Atom x y z

C 1.27119600 2.64747100 -0.03841100

C 1.34898800 4.04069500 -0.11154400

C 0.16542100 4.77210400 -0.16179500

C -1.05783600 4.11058500 -0.09691300

C -1.05978800 2.71512300 -0.02457200

N 0.08656100 2.02711500 -0.04498400

H 0.19646600 5.85374100 -0.22583600

H 2.30510100 4.54783400 -0.12161700

H -1.98324000 4.67184600 -0.09517000

C 2.44605400 1.73801400 0.12666200

C -2.28376200 1.87596500 0.15547600

N -2.07517400 0.61241900 0.26208700

N 2.16361800 0.48930300 0.24016400

C -3.61466800 2.56245200 0.27180100

H -3.59163000 3.30665100 1.07303200

H -3.86243000 3.09339600 -0.65225200

H -4.41094500 1.85396800 0.48715200

C 3.81723600 2.34320300 0.21951800

H 4.08725200 2.84283600 -0.71578200

H 3.84871700 3.09983600 1.00856300

H 4.57034600 1.58993400 0.43815100

C -3.13627500 -0.31966500 0.50937900

C -4.01227900 -0.71346200 -0.51875900

C -3.20757000 -0.88211300 1.79817300

C -4.97572500 -1.68199400 -0.22065100

C -4.19388900 -1.83690300 2.04841200

C -5.07288200 -2.23881800 1.04865400

H -5.65839600 -2.00019200 -1.00210200

H -4.26863800 -2.27035800 3.04055300

H -5.82917700 -2.98745300 1.25752200

C 3.16909500 -0.50636500 0.47059500

C 3.22164000 -1.07803600 1.75685300

C 4.00645800 -0.94867800 -0.56976900

C 4.14848100 -2.09416500 1.99006600

C 4.90932000 -1.97878400 -0.28862100

C 4.98641100 -2.54715900 0.97650900

H 4.20937100 -2.53558700 2.97963700

H 5.56001600 -2.33629200 -1.08039200

H 5.69534400 -3.34411800 1.17231000

C 2.32404100 -0.58631200 2.86418000

H 2.54335700 0.45015700 3.14018700

H 1.26881700 -0.61984800 2.57593300

H 2.44251000 -1.19535100 3.76098400

C 3.96064100 -0.34934000 -1.95467900

H 2.93974600 -0.16286300 -2.29148500

H 4.49823800 0.60354300 -2.00661900

H 4.43247200 -1.01601800 -2.67764500

C -2.26341300 -0.44651500 2.89002800

H -1.21747400 -0.54335900 2.58280600

H -2.41519200 0.60094200 3.17006300

H -2.40269100 -1.04845500 3.78862300

C -3.93930000 -0.13131800 -1.90977200

H -4.33403700 0.88920900 -1.95252900

H -2.91617700 -0.09742200 -2.28875200

H -4.53060700 -0.72688400 -2.60626500

C -0.04346600 -2.18167300 -0.10685400

H 0.80120500 -2.35115200 0.56467100

H -0.99106800 -2.34419200 0.41229600

C 0.05944100 -2.94493000 -1.34482500

H 1.04100100 -3.38932700 -1.52718900

H 0.09133700 -2.09680500 -2.30977300

C -1.08920400 -3.84492600 -1.76097500

H -1.12472600 -4.72352500 -1.10874100

H -2.05044800 -3.33258100 -1.66535200

H -0.98563700 -4.20187600 -2.78904000

Co 0.02521000 -0.07901200 -0.31664000

C 0.07495200 -1.08053200 -3.22050400

H 0.99555500 -1.36402900 -3.72745400

H -0.81715400 -1.42007000 -3.74435400

C 0.02984900 0.15670700 -2.51288800

H -0.89151100 0.72633400 -2.61764300

H 0.91360700 0.78522300 -2.60672700

**3/2Co(+)-7**

Atom x y z

C 1.24565000 2.60078600 0.09988700

C 1.31178700 3.99570800 0.12563900

C 0.12064000 4.71835900 0.14932900

C -1.09832200 4.04432600 0.17839800

C -1.08930500 2.64767000 0.15072700

N 0.06409400 1.97587300 0.07903800

H 0.14279400 5.80185200 0.16451000

H 2.26370300 4.51131700 0.13545200

H -2.02751400 4.59760900 0.22858100

C 2.41395300 1.67873500 0.16635900

C -2.28980600 1.77312900 0.26023000

N -2.05995200 0.50472600 0.22431500

N 2.13090200 0.42102800 0.15981200

C -3.63511600 2.41198500 0.45175600

H -3.62053600 3.09546500 1.30513100

H -3.90795400 3.00287100 -0.42813500

H -4.41128000 1.66913900 0.62003700

C 3.79173900 2.26339900 0.28611300

H 4.01820300 2.89127400 -0.58080400

H 3.86624400 2.90101100 1.17181300

H 4.55076100 1.48797400 0.35732900

C -3.11581700 -0.44980400 0.42569100

C -3.92045000 -0.86442300 -0.64983500

C -3.26213200 -0.99608300 1.71544400

C -4.87127200 -1.86117800 -0.40879900

C -4.22860100 -1.98593200 1.90592300

C -5.02520400 -2.42298300 0.85303100

H -5.50054000 -2.19466000 -1.22787800

H -4.35744600 -2.41382100 2.89503700

H -5.76780200 -3.19605000 1.01741400

C 3.15133900 -0.57324100 0.35433900

C 3.35959200 -1.04710900 1.66372500

C 3.86185300 -1.09226000 -0.74284300

C 4.28913400 -2.07247900 1.85288100

C 4.77984000 -2.11838100 -0.50127400

C 4.99172100 -2.61099500 0.78122500

H 4.46297600 -2.44763400 2.85639300

H 5.33816500 -2.53000600 -1.33602800

H 5.70683700 -3.40945900 0.94583000

C 2.63951700 -0.44185000 2.84506000

H 3.03199000 0.55086800 3.09127700

H 1.56854000 -0.31633100 2.66358600

H 2.75925000 -1.06315600 3.73338400

C 3.68053800 -0.54506100 -2.13702600

H 2.63074100 -0.48647800 -2.42765000

H 4.09092700 0.46622400 -2.23155200

H 4.19688800 -1.16833100 -2.86798700

C -2.43390500 -0.50040800 2.87593100

H -1.36819700 -0.45299700 2.63536900

H -2.73048800 0.50886800 3.18121400

H -2.55419400 -1.14812300 3.74515100

C -3.80408000 -0.24285000 -2.01974000

H -4.28188800 0.74252700 -2.05530400

H -2.76725900 -0.10568700 -2.32788800

H -4.29914600 -0.86138900 -2.76944800

C -0.01507200 -2.28524400 0.53561800

H 0.83309900 -1.99866200 1.14804500

H -0.98866400 -2.33014200 1.01280900

C 0.17023400 -2.78611500 -0.69923900

H 1.18181400 -2.80359100 -1.10246700

H 0.71877600 -1.21191800 -3.49314400

C -0.88980800 -3.43507400 -1.53087400

H -0.68817400 -4.51116300 -1.58563900

H -1.88677000 -3.29984200 -1.10855200

H -0.88214900 -3.06849400 -2.55871900

Co 0.00848500 -0.02204900 -0.47220600

C -0.07265800 -0.45810300 -3.55899800

H 0.01948500 -0.00012700 -4.55254100

H -1.02519100 -0.99553400 -3.55484400

C 0.00994400 0.58675600 -2.44429500

H -0.81373600 1.30473800 -2.54437200

H 0.92775800 1.17812300 -2.55427800

**3/2Co(+)-8**

Atom x y z

C 1.16999400 2.55564700 -0.09686800

C 1.20722100 3.93892200 -0.28239100

C 0.00002200 4.63098600 -0.35781600

C -1.20718300 3.93893300 -0.28242700

C -1.16997800 2.55565400 -0.09690500

N 0.00000500 1.92087300 0.03429000

H 0.00002900 5.70578800 -0.49882100

H 2.14734200 4.46688900 -0.37581200

H -2.14729700 4.46690800 -0.37587700

C 2.36123800 1.65136500 -0.09281200

C -2.36124000 1.65139700 -0.09288400

N -2.09229100 0.39194500 -0.08708100

N 2.09226600 0.39192000 -0.08699500

C -3.73101200 2.25913700 -0.15847900

H -3.91178800 2.91032100 0.70180900

H -3.82908500 2.87778400 -1.05570000

H -4.50429600 1.49544000 -0.18661500

C 3.73102600 2.25907000 -0.15837600

H 3.82916900 2.87763600 -1.05564600

H 3.91176300 2.91032500 0.70186500

H 4.50429500 1.49535100 -0.18639900

C -3.12113600 -0.60884700 -0.09995500

C -3.31499500 -1.32269200 -1.29604500

C -3.83476600 -0.90912600 1.07420600

C -4.27659700 -2.33394800 -1.30667900

C -4.77661500 -1.93972100 1.01481100

C -5.00360000 -2.64310900 -0.16222600

H -4.45011700 -2.88747800 -2.22379800

H -5.33433800 -2.19356600 1.91044100

H -5.74050300 -3.43834000 -0.18529200

C 3.12113600 -0.60885700 -0.09988000

C 3.83465700 -0.90923400 1.07431800

C 3.31513900 -1.32255400 -1.29603000

C 4.77654400 -1.93979400 1.01490700

C 4.27676200 -2.33379300 -1.30667200

C 5.00365700 -2.64305700 -0.16218000

H 5.33419100 -2.19371200 1.91056400

H 4.45038700 -2.88722100 -2.22383300

H 5.74058300 -3.43826700 -0.18525600

C 3.59763700 -0.17077600 2.36977900

H 4.00491500 0.84561500 2.35030200

H 2.53375200 -0.09069300 2.60892000

H 4.07970800 -0.68852000 3.19950200

C 2.52459200 -0.99387200 -2.53781300

H 1.44564900 -1.04391400 -2.35703100

H 2.73722600 0.01415600 -2.90809900

H 2.75591600 -1.69245700 -3.34238900

C -3.59791100 -0.17053700 2.36962500

H -2.53404500 -0.09014800 2.60874300

H -4.00547500 0.84573900 2.35010800

H -4.07982300 -0.68837300 3.19938300

C -2.52430700 -0.99415800 -2.53777800

H -2.73676100 0.01388900 -2.90810900

H -1.44538500 -1.04436400 -2.35690900

H -2.75566700 -1.69273700 -3.34234900

C -0.00013400 -1.89258100 1.34780700

H 0.87719400 -1.95186500 2.00392000

H -0.87772300 -1.95170800 2.00359400

C -0.00006000 -3.06367200 0.35477900

H 0.88415300 -3.05861300 -0.29081000

H -0.88397900 -3.05840300 -0.29121100

Co -0.00000400 -0.13265900 0.43452600

H -0.00029600 -4.03155100 0.87101200

**3/2Co(+)-TS-3/9**

Atom x y z

C -1.11049100 2.57971800 0.05199100

C -1.12612100 3.97258200 0.13135500

C 0.08642500 4.65528500 0.18363400

C 1.28113100 3.94089700 0.15746600

C 1.23156400 2.54859600 0.07718400

N 0.05202000 1.90725500 0.02292300

H 0.09997900 5.73717000 0.24727800

H -2.06056400 4.51777200 0.15520200

H 2.22887900 4.46142200 0.20122100

C -2.33198200 1.72661700 -0.00081500

C 2.43177600 1.66468600 0.04876600

N 2.19324700 0.40106800 0.00843600

N -2.13044700 0.45490300 -0.02252800

C 3.79534300 2.29368400 0.07571300

H 3.92971900 2.96914200 -0.77405900

H 3.92841300 2.88812800 0.98449700

H 4.57876200 1.54012600 0.04320800

C -3.67679400 2.39505600 -0.02056900

H -3.82112600 2.99842500 0.88058600

H -3.76156800 3.07000800 -0.87709600

H -4.48189400 1.66635200 -0.07537000

C 3.25496400 -0.56388500 -0.03983900

C 3.73081300 -1.11573300 1.16348300

C 3.73601100 -0.98082400 -1.29406600

C 4.70356400 -2.11539400 1.08222700

C 4.70642200 -1.98578700 -1.32085700

C 5.18600800 -2.55342300 -0.14618700

H 5.08582100 -2.55248400 1.99916900

H 5.08957800 -2.32204100 -2.27903100

H 5.93719500 -3.33448800 -0.18760800

C -3.22907500 -0.46929900 -0.07965900

C -3.67614400 -0.91417800 -1.33610300

C -3.77757600 -0.94970800 1.12240000

C -4.69170000 -1.87363600 -1.36556000

C -4.79395800 -1.90459400 1.03910000

C -5.24679000 -2.36878800 -0.19113000

H -5.05078000 -2.23090500 -2.32544800

H -5.23144700 -2.28835300 1.95522100

H -6.03326800 -3.11422300 -0.23431100

C -3.11277800 -0.35290200 -2.61912000

H -3.46356100 0.66892600 -2.80182400

H -2.02026800 -0.31681900 -2.61120900

H -3.42144300 -0.95416800 -3.47508600

C -3.29895400 -0.44779500 2.46238900

H -2.20893200 -0.47098700 2.54079000

H -3.61176800 0.58617800 2.64522500

H -3.70837700 -1.05314200 3.27188600

C 3.25937600 -0.34435600 -2.57780100

H 2.17323400 -0.22574700 -2.60796800

H 3.69105200 0.65283700 -2.71903500

H 3.55331200 -0.94339600 -3.44050300

C 3.23733500 -0.62919300 2.50414800

H 3.61290000 0.37454200 2.73244200

H 2.14651000 -0.57921800 2.54530200

H 3.57736800 -1.28720600 3.30475100

C 0.03886400 -2.01922600 -0.98169100

H -0.91725300 -2.18729500 -1.46698500

H 0.90631600 -1.96457600 -1.63094400

C 0.20505800 -2.39564700 0.35606400

H 0.10466000 -0.98140800 1.37920800

H 1.22665100 -2.54324500 0.69394500

C -0.83070900 -3.19281700 1.10873600

H -1.84693500 -2.92581600 0.81924900

H -0.68308900 -4.25018000 0.86213600

H -0.73153700 -3.08705600 2.18977100

Co 0.01815700 -0.12816600 0.01651900

**3/2Co(+)-9**

Atom x y z

C 1.12102400 2.61687400 -0.04985500

C 1.14208300 4.01314100 -0.07407100

C -0.07206300 4.69565400 -0.10324500

C -1.27026400 3.98453500 -0.09476600

C -1.21706000 2.58937500 -0.06980000

N -0.04017400 1.95617800 -0.06485000

H -0.08471100 5.77925900 -0.12509300

H 2.07598900 4.56028100 -0.06834400

H -2.21668700 4.50968300 -0.10517100

C 2.32912000 1.73886000 0.01203700

C -2.40591100 1.68368000 -0.02584600

N -2.15291000 0.42241400 0.02690600

N 2.10553300 0.47129800 0.05710100

C -3.77598600 2.29587900 -0.03450900

H -3.90402200 2.96921000 0.81811300

H -3.92367700 2.89204300 -0.93994800

H -4.55243100 1.53580300 0.00792700

C 3.68384900 2.38444700 0.02973000

H 3.77600400 3.06407100 0.88198500

H 4.47837300 1.64487100 0.09218700

H 3.83627900 2.98090700 -0.87475600

C -3.20713500 -0.55169700 0.10710800

C -3.74786600 -1.08221100 -1.07841700

C -3.61113200 -0.99802700 1.37802000

C -4.70818300 -2.09067800 -0.95987300

C -4.57347400 -2.00884200 1.44157200

C -5.11712700 -2.55576200 0.28507700

H -5.13935800 -2.51300900 -1.86187000

H -4.89889500 -2.36630200 2.41331700

H -5.86053500 -3.34234400 0.35366800

C 3.18505100 -0.47419100 0.14372100

C 3.56160500 -0.94090400 1.41580600

C 3.78033500 -0.95461900 -1.03586000

C 4.55615200 -1.91940500 1.48626400

C 4.77041300 -1.93348200 -0.91109500

C 5.15570200 -2.41663500 0.33442400

H 4.86264800 -2.29067900 2.45896700

H 5.24334200 -2.31846800 -1.80888600

H 5.92415700 -3.17836600 0.40760500

C 2.94293900 -0.38154600 2.67405200

H 3.26747100 0.64742300 2.86348600

H 1.85028100 -0.36303500 2.62686300

H 3.22884200 -0.97325700 3.54439500

C 3.38787500 -0.42741000 -2.39415800

H 2.30361500 -0.38180500 -2.51901800

H 3.77416200 0.58443100 -2.56184100

H 3.79522600 -1.05777700 -3.18554600

C -3.06461500 -0.38243500 2.64396300

H -1.97971200 -0.25059000 2.61256700

H -3.49567400 0.60750300 2.83042400

H -3.30037500 -1.00119400 3.51059200

C -3.33310200 -0.57184400 -2.43674400

H -3.73531600 0.42885500 -2.63152000

H -2.24722000 -0.50453600 -2.53750900

H -3.70863700 -1.22460000 -3.22573800

C 0.04304000 -2.20772600 0.81777100

H 1.05537200 -2.29030500 1.20086000

H -0.73680600 -1.95336300 1.52865100

C -0.26960800 -2.63631700 -0.42271600

H 0.00275900 -0.27075000 -1.89516800

H -1.31684400 -2.63047800 -0.71753900

C 0.68211100 -3.25890500 -1.39412100

H 1.72073600 -3.17229300 -1.07216200

H 0.44448600 -4.32447600 -1.49217400

H 0.57935200 -2.81929900 -2.38849500

Co -0.01155500 -0.08094400 -0.31043500

**3/2Co(+)-10**

Atom x y z

C 1.17034100 2.38208200 0.07115200

C 1.20830900 3.76193100 0.27779700

C 0.00000000 4.45155800 0.36575500

C -1.20830900 3.76193100 0.27779700

C -1.17034100 2.38208200 0.07115200

N 0.00000000 1.75153600 -0.06282900

H 0.00000000 5.52391300 0.52434200

H 2.14864500 4.28841700 0.37826300

H -2.14864500 4.28841700 0.37826200

C 2.35764100 1.46834500 0.04788500

C -2.35764100 1.46834500 0.04788500

N -2.07617200 0.21373900 0.01823900

N 2.07617200 0.21373900 0.01824000

C -3.73328700 2.06028200 0.10753200

H -4.49854700 1.28819300 0.08486000

H -3.85947000 2.64270300 1.02547100

H -3.89770300 2.74299800 -0.73141800

C 3.73328700 2.06028200 0.10753300

H 3.85947000 2.64270300 1.02547100

H 4.49854700 1.28819300 0.08486000

H 3.89770300 2.74299800 -0.73141800

C -3.09522100 -0.80135600 0.02687000

C -3.70264800 -1.18586600 -1.18003600

C -3.38200000 -1.43276800 1.24822800

C -4.64457100 -2.21601100 -1.13053900

C -4.33427200 -2.45354500 1.24543200

C -4.96403000 -2.84274700 0.06860100

H -5.12579100 -2.53289500 -2.05002400

H -4.57711000 -2.95075900 2.17893000

H -5.69702600 -3.64173700 0.08415800

C 3.09522100 -0.80135600 0.02687000

C 3.38200000 -1.43276900 1.24822800

C 3.70264800 -1.18586500 -1.18003600

C 4.33427200 -2.45354500 1.24543200

C 4.64457100 -2.21601100 -1.13053900

C 4.96403000 -2.84274700 0.06860100

H 4.57711000 -2.95075900 2.17893000

H 5.12579100 -2.53289500 -2.05002400

H 5.69702700 -3.64173700 0.08415800

C 2.68960100 -1.02213000 2.52406300

H 2.93684900 0.00295600 2.81954000

H 1.59986100 -1.07224400 2.42761100

H 2.97617200 -1.67483400 3.34901800

C 3.33815800 -0.53818500 -2.49311800

H 2.26763400 -0.63325400 -2.70150500

H 3.58474900 0.52843600 -2.51942100

H 3.87274200 -1.01045300 -3.31757000

C -2.68960100 -1.02212900 2.52406300

H -1.59986100 -1.07224400 2.42761100

H -2.93684900 0.00295700 2.81954000

H -2.97617200 -1.67483300 3.34901800

C -3.33815800 -0.53818500 -2.49311800

H -3.58474900 0.52843600 -2.51942200

H -2.26763400 -0.63325500 -2.70150500

H -3.87274200 -1.01045400 -3.31757000

H 0.00000000 -1.71284700 -1.17537700

Co 0.00000000 -0.29218300 -0.48819600

**1Fe(+)**

**1Fe(+)-1**

Atom x y z

C -1.17707400 2.47433000 -0.02646800

C -1.21051000 3.86594200 0.05524700

C -0.00003400 4.56059400 0.08501700

C 1.21049300 3.86591100 0.05517700

C 1.17703000 2.47435600 -0.02652400

N -0.00002200 1.82832500 -0.08520100

H -0.00001700 5.64234100 0.14860600

H -2.15102100 4.40035200 0.10525600

H 2.15099400 4.40034300 0.10510800

C -2.32447100 1.53791700 -0.00828900

C 2.32449700 1.53791000 -0.00844000

N 1.99844100 0.27920000 -0.01345700

N -1.99833400 0.27917400 -0.01334700

C 3.72070400 2.07567700 0.04415400

H 3.90632200 2.73916100 -0.80576200

H 3.86602400 2.67050400 0.95139800

H 4.46100900 1.27989700 0.03246000

C -3.72072000 2.07559900 0.04416500

H -3.86619800 2.67037600 0.95141800

H -3.90630800 2.73909800 -0.80574600

H -4.46097600 1.27977300 0.03235700

C 3.01615400 -0.74363200 0.02237200

C 3.42349700 -1.24365100 1.26885700

C 3.51583800 -1.24398900 -1.19041400

C 4.38068700 -2.26083500 1.27797000

C 4.47060900 -2.26154400 -1.12872900

C 4.90363200 -2.76547600 0.09269800

H 4.71315900 -2.66284300 2.22950400

H 4.87290500 -2.66390700 -2.05274400

H 5.64383800 -3.55749100 0.12050100

C -3.01604500 -0.74366800 0.02253500

C -3.51604400 -1.24375600 -1.19023500

C -3.42310900 -1.24394200 1.26900700

C -4.47078000 -2.26134200 -1.12853900

C -4.38027100 -2.26115600 1.27813200

C -4.90349100 -2.76555600 0.09288100

H -4.87329600 -2.66351100 -2.05254500

H -4.71248100 -2.66339400 2.22966000

H -5.64365500 -3.55761100 0.12068900

C -3.03484200 -0.71486200 -2.51854400

H -3.25654300 0.34899600 -2.65078100

H -1.95150500 -0.83417400 -2.63140500

H -3.50816800 -1.24848500 -3.34307700

C -2.85062900 -0.70892600 2.55796400

H -1.75720400 -0.74972500 2.56142400

H -3.13316200 0.33410100 2.73632100

H -3.20609700 -1.28871400 3.41013200

C 3.03420600 -0.71545900 -2.51870900

H 1.95085500 -0.83500900 -2.63122700

H 3.25566900 0.34840900 -2.65125800

H 3.50739400 -1.24918500 -3.34325400

C 2.85117900 -0.70844900 2.55780600

H 3.13283300 0.33491900 2.73551400

H 1.75778400 -0.75023900 2.56174100

H 3.20751900 -1.28750000 3.41011000

C -0.00014800 -2.09499500 -0.17042200

H -0.00159900 -2.41671700 0.88095000

H -0.89057500 -2.51825900 -0.64571300

H 0.89136400 -2.51848800 -0.64343900

Fe -0.00006200 -0.12891900 -0.19746800

**1Fe(+)-2**

Atom x y z

C 1.17611500 2.43845100 -0.35472700

C 1.20584600 3.79352800 -0.68245100

C -0.00010300 4.48134400 -0.81742900

C -1.20602900 3.79359700 -0.68194700

C -1.17622700 2.43851700 -0.35423700

N -0.00003500 1.81236700 -0.12785000

H -0.00012500 5.53546300 -1.06775300

H 2.14721000 4.30236100 -0.84818700

H -2.14744100 4.30247000 -0.84729400

C 2.32444100 1.51722500 -0.31443200

C -2.32455300 1.51733200 -0.31363300

N -2.01155900 0.26863200 -0.12176000

N 2.01146200 0.26853200 -0.12246500

C -3.70916700 2.03972200 -0.55686000

H -4.00145100 2.73768700 0.23371600

H -3.75161700 2.58903000 -1.50152000

H -4.44136100 1.23709700 -0.59557300

C 3.70904500 2.03956400 -0.55780400

H 3.75118100 2.58986800 -1.50188800

H 4.00189000 2.73659700 0.23339300

H 4.44103200 1.23680400 -0.59768700

C -3.02222200 -0.75985800 -0.14185200

C -3.12950700 -1.54153300 -1.30833800

C -3.82742300 -0.99775700 0.98494000

C -4.05239900 -2.58707400 -1.31621500

C -4.72831200 -2.06678200 0.93186100

C -4.84068400 -2.85860700 -0.20253600

H -4.15077100 -3.19637800 -2.20874800

H -5.35130000 -2.27164300 1.79689000

H -5.54403800 -3.68379700 -0.22219600

C 3.02210100 -0.75996400 -0.14224100

C 3.82764100 -0.99718800 0.98443100

C 3.12904200 -1.54236500 -1.30830600

C 4.72852200 -2.06626100 0.93173100

C 4.05192400 -2.58789000 -1.31583200

C 4.84055100 -2.85876300 -0.20220200

H 5.35177300 -2.27057300 1.79670500

H 4.15005900 -3.19771100 -2.20803700

H 5.54391100 -3.68395500 -0.22158900

C 3.79284600 -0.12442100 2.21656900

H 4.53746700 0.67704600 2.15445300

H 2.82488600 0.35036600 2.37395900

H 4.02939300 -0.70332700 3.11099200

C 2.30978200 -1.23780600 -2.53719800

H 1.24126200 -1.18662500 -2.31513100

H 2.58862800 -0.27683100 -2.98254900

H 2.45523600 -2.00321500 -3.30016500

C -3.79222200 -0.12559200 2.21747700

H -2.82260700 0.34483600 2.37790400

H -4.53306100 0.67925200 2.15368200

H -4.03381000 -0.70382700 3.11096000

C -2.31057800 -1.23628100 -2.53728300

H -2.58987600 -0.27527500 -2.98228900

H -1.24203100 -1.18475100 -2.31541000

H -2.45588600 -2.00149900 -3.30047000

C -0.00044200 -2.07873200 0.35790700

H -0.00124000 -2.41548200 -0.68528500

H 0.89150300 -2.48927400 0.83952600

H -0.89206000 -2.48869000 0.84064000

C 0.00142200 -0.36579900 2.79162000

H 0.91935900 -0.93309400 2.88922100

H -0.91567700 -0.93428100 2.89010900

C 0.00056500 0.97719200 2.72528500

H -0.91849800 1.55236700 2.74106600

H 0.91895600 1.55345600 2.74032700

Fe 0.00000600 -0.09361500 0.34788300

**1Fe(+)-TS-2/3**

Atom x y z

C 1.18179700 2.48086100 0.27614500

C 1.20567400 3.84628200 0.55598100

C -0.00011100 4.53996200 0.66056600

C -1.20556500 3.84757300 0.54275100

C -1.17946600 2.48270800 0.26192500

N 0.00183900 1.84528500 0.06045900

H -0.00063400 5.60200800 0.87406300

H 2.14616200 4.36109500 0.70782600

H -2.14736900 4.36263900 0.68565600

C 2.32877000 1.56557500 0.28522100

C -2.32761300 1.56905600 0.25793400

N -2.01559800 0.30811000 0.13042700

N 2.01479400 0.30481200 0.15903100

C -3.71226100 2.10510600 0.47753400

H -3.76017800 2.66233600 1.41752000

H -3.99320100 2.79841000 -0.32045000

H -4.45106000 1.30852600 0.51962900

C 3.71370200 2.09827800 0.50971400

H 4.03157900 2.72330500 -0.33014500

H 3.74288400 2.72434500 1.40538800

H 4.43723000 1.29600200 0.63357400

C -3.02229400 -0.71917000 0.18472000

C -3.84463100 -0.98544400 -0.92647500

C -3.10538600 -1.48343700 1.36416700

C -4.75367400 -2.04340500 -0.82950800

C -4.03604400 -2.52253200 1.41501300

C -4.85318000 -2.80708200 0.32678000

H -5.39303000 -2.26547700 -1.67786600

H -4.11745000 -3.11381200 2.32134400

H -5.56621300 -3.62243900 0.37994500

C 3.01449900 -0.72750300 0.21019400

C 3.04576400 -1.53658400 1.36443700

C 3.87666900 -0.96411600 -0.87692400

C 3.96255000 -2.58633700 1.41323400

C 4.76787900 -2.03902500 -0.78495000

C 4.81589800 -2.84373800 0.34492300

H 4.00495000 -3.20929400 2.30077600

H 5.43474000 -2.23948200 -1.61765900

H 5.51626200 -3.67022400 0.39477900

C 2.13390400 -1.26310200 2.53299900

H 2.29834400 -0.26870600 2.95886700

H 1.07974500 -1.31050900 2.24305000

H 2.29096700 -1.99234100 3.32845200

C 3.89705200 -0.09797000 -2.11381200

H 2.92288500 0.33016300 -2.34747600

H 4.59990900 0.73530200 -2.00676800

H 4.22441800 -0.67256300 -2.98189300

C -2.23352700 -1.17794300 2.55537600

H -1.17041100 -1.22027900 2.30020600

H -2.42098700 -0.17688600 2.95591900

H -2.40983700 -1.89191900 3.36055000

C -3.78525200 -0.16654500 -2.19365700

H -4.21870500 0.83002300 -2.06055500

H -2.76427100 -0.02472100 -2.55138000

H -4.34937800 -0.65212600 -2.99068500

C 0.03854300 -1.56273000 -2.14226900

H 0.96225200 -1.66923300 -2.69739200

H -0.85224600 -1.67917800 -2.74662000

C 0.00314800 -1.99768100 -0.79187600

H -0.92597700 -2.41942000 -0.41901900

H 0.91221000 -2.41983500 -0.37307000

Fe 0.00211900 -0.00362900 -0.42260900

C 0.03419600 0.53219900 -2.62738500

H 0.05333000 0.12734600 -3.63332300

H -0.86772100 1.13480500 -2.51882500

H 0.92221800 1.14951300 -2.49256400

**1Fe(+)-3**

Atom x y z

C 1.17763300 2.70403100 -0.05797300

C 1.20953700 4.09122800 -0.19182800

C 0.00004900 4.78581600 -0.25024600

C -1.20943300 4.09120900 -0.19175000

C -1.17751600 2.70401700 -0.05789700

N 0.00006800 2.05431300 0.02105800

H 0.00003300 5.86422000 -0.35526200

H 2.15049200 4.62309800 -0.25880200

H -2.15039100 4.62307600 -0.25870000

C 2.32574300 1.77718500 -0.02547200

C -2.32561300 1.77714800 -0.02534000

N -2.00641700 0.51608700 0.03986000

N 2.00651300 0.51613700 0.03980500

C -3.72119200 2.31729900 -0.09115000

H -3.89704600 3.02148300 0.72739100

H -3.87384300 2.86803500 -1.02448800

H -4.46480900 1.52654500 -0.03362300

C 3.72131900 2.31734500 -0.09135600

H 3.87395200 2.86795700 -1.02477100

H 3.89718000 3.02164200 0.72708400

H 4.46494800 1.52660900 -0.03372900

C -3.03230100 -0.49768100 0.05342000

C -3.48304600 -1.01838200 -1.17032600

C -3.50945500 -0.96310600 1.28998800

C -4.44270600 -2.03298600 -1.13079400

C -4.46945300 -1.97747400 1.27667500

C -4.93331800 -2.51067600 0.07907600

H -4.80552800 -2.45168700 -2.06392500

H -4.85399100 -2.35197900 2.21978400

H -5.67628500 -3.30056400 0.08905300

C 3.03230300 -0.49772700 0.05338700

C 3.50948200 -0.96309000 1.28997600

C 3.48290700 -1.01859800 -1.17032800

C 4.46936200 -1.97756200 1.27670100

C 4.44243000 -2.03333900 -1.13076000

C 4.93307300 -2.51095500 0.07912200

H 4.85393900 -2.35200300 2.21982000

H 4.80510800 -2.45220000 -2.06387400

H 5.67593500 -3.30094000 0.08913900

C 3.01765500 -0.38388100 2.59339300

H 3.26982000 0.67647600 2.69677200

H 1.93000400 -0.46506900 2.69268200

H 3.46139500 -0.90575500 3.44161800

C 2.97311700 -0.49192000 -2.48948100

H 1.88225500 -0.42027300 -2.51053900

H 3.36393800 0.50791300 -2.70798300

H 3.27883200 -1.14132300 -3.31034300

C -3.01752200 -0.38405500 2.59343300

H -1.92984700 -0.46509700 2.69256800

H -3.26982900 0.67625000 2.69701500

H -3.46107900 -0.90612800 3.44163100

C -2.97324000 -0.49164100 -2.48944900

H -3.36368300 0.50838400 -2.70772400

H -1.88234800 -0.42042600 -2.51062100

H -3.27930800 -1.14077700 -3.31039200

C 0.00003800 -1.85980300 0.50345900

H 0.88521000 -2.10098100 1.10775000

H -0.88507900 -2.10092600 1.10785800

Fe 0.00006000 0.10289700 0.24318100

C -0.00006900 -2.69008300 -0.78365000

H 0.87810300 -2.44377200 -1.39148900

H -0.87833700 -2.44374100 -1.39133700

C -0.00012300 -4.20407600 -0.51905700

H 0.88290700 -4.50414400 0.05205000

H -0.88314200 -4.50406500 0.05211400

H -0.00018300 -4.77036900 -1.45513200

**1Fe(+)-4**

Atom x y z

Fe -0.03928400 0.07460100 0.38534600

N -0.11123400 2.01772400 -0.03393400

C -1.31018100 2.62237900 -0.19276500

C -2.43570600 1.67470500 -0.19952700

N -2.09987300 0.42385200 -0.08362800

C -3.10066200 -0.60669600 -0.20601700

C -3.23964100 -1.23813200 -1.45496700

C -2.45415400 -0.78407600 -2.66017600

H -2.55358300 -1.49665700 -3.47973300

C -4.16288600 -2.27999600 -1.56551600

C -4.92338800 -2.68470600 -0.47496700

C -4.77792400 -2.03843100 0.74682100

C -3.87065800 -0.98762900 0.90667500

C -3.76404100 -0.28061300 2.23594400

H -2.73278400 -0.20796600 2.58650300

H -5.37871500 -2.34852900 1.59574100

H -4.28370000 -2.77720400 -2.52258300

C -3.83084100 2.18658000 -0.41454100

H -4.10761000 2.89424600 0.37239300

H -3.89962800 2.72283600 -1.36559400

H -4.55978800 1.38046600 -0.42702700

C -1.39252200 3.99471300 -0.42700900

C -0.21555800 4.73284900 -0.54174300

C 1.01293900 4.07652000 -0.48339900

C 1.03479600 2.70184000 -0.24833200

C 2.22182500 1.83321700 -0.29619500

N 1.97852900 0.56184800 -0.16577200

C 3.05007800 -0.39369900 -0.27859000

C 3.14892400 -1.11470900 -1.48554700

C 4.13901100 -2.09067800 -1.59056900

C 5.00377300 -2.35382000 -0.53220200

C 4.89863100 -1.62245600 0.64226600

C 3.93060700 -0.62306700 0.79246600

H 5.57973200 -1.82091200 1.46403900

H 4.23162700 -2.65075100 -2.51541200

C 3.57088100 2.43943000 -0.55369500

H 3.87102400 3.07951600 0.28178200

H 4.33497100 1.67911700 -0.69314200

H 3.54535800 3.06872800 -1.44725800

H 1.93339100 4.62589500 -0.63540800

H -0.25596600 5.80115200 -0.71751600

H -2.35429200 4.47978600 -0.53700500

H 5.76105400 -3.12426000 -0.62732800

C 3.90241400 0.17975600 2.07176600

H 4.66678300 0.96435800 2.05962700

H -5.63046500 -3.50054000 -0.57738600

C 2.24360400 -0.81593100 -2.65417600

H 2.40878800 -1.52639900 -3.46482200

C -0.14412400 -1.92603200 0.26434500

H -1.15623400 -2.16419900 0.61242000

H -0.16007400 -2.02149500 -0.83352100

H -1.38987400 -0.67143600 -2.44073400

H -2.80536100 0.18551800 -3.03026400

H -4.33354500 -0.80887400 3.00112800

H -4.15928400 0.73987500 2.19116900

H 4.11856800 -0.45363800 2.93446900

H 2.94501600 0.66844800 2.24941400

H 2.41941100 0.18673300 -3.05791100

H 1.18767400 -0.86459400 -2.37735600

C 0.61853600 -4.34966000 0.41086000

C 0.86391300 -2.90054400 0.86337200

H 1.33747100 -5.03308700 0.87176300

H 0.71648600 -4.44798200 -0.67424500

H -0.38534200 -4.68825400 0.68317000

H 1.88610200 -2.62032400 0.59647500

H 0.81281200 -2.87005100 1.95792800

C 0.14688100 -0.25918200 2.74156400

C -0.03314900 1.07641800 2.71030400

H -0.67482700 -0.94439600 2.91184600

H 1.13709400 -0.69781800 2.76914300

H -1.01509700 1.52485500 2.81228000

H 0.80394700 1.76412900 2.67861200

**1Fe(+)-TS-4/5**

Atom x y z

C 1.11935000 2.57026700 -0.30245300

C 1.12043600 3.93441000 -0.59067700

C -0.09017800 4.61276300 -0.69754000

C -1.27775600 3.89635900 -0.56711900

C -1.23147600 2.53264300 -0.28351000

N -0.04411000 1.89960000 -0.08851700

H -0.10920700 5.67419300 -0.91334200

H 2.05453100 4.45994000 -0.74214100

H -2.22949800 4.39426500 -0.70063500

C 2.32261700 1.72594400 -0.27679400

C -2.41287100 1.65144900 -0.26321300

N -2.16562800 0.39132600 -0.10240600

N 2.10980100 0.45957700 -0.09060800

C -3.77562900 2.24661800 -0.49489500

H -4.02197100 2.97296800 0.28494000

H -3.81217100 2.77584100 -1.45101400

H -4.54654600 1.47980400 -0.50550900

C 3.66886500 2.35257900 -0.51742600

H 3.69876100 2.84814000 -1.49191000

H 3.88421000 3.11469200 0.23691800

H 4.46390700 1.61109500 -0.49276900

C -3.21630200 -0.58316400 -0.19661100

C -3.37958800 -1.24813300 -1.42964900

C -4.01334800 -0.90531100 0.91703500

C -4.32853300 -2.26809500 -1.51348600

C -4.94420900 -1.94135300 0.78582100

C -5.10002200 -2.62503100 -0.41264400

H -4.46420500 -2.78496300 -2.45827700

H -5.56071100 -2.20389300 1.64000900

H -5.82656000 -3.42618200 -0.49269200

C 3.19668600 -0.47732300 -0.15713900

C 3.94372200 -0.78331500 0.99543600

C 3.45215400 -1.11073700 -1.38821700

C 4.93594500 -1.76316100 0.89804500

C 4.45736400 -2.07959200 -1.43682100

C 5.19078400 -2.41306300 -0.30372700

H 5.51985900 -2.01025600 1.77899000

H 4.66727300 -2.57348000 -2.38029500

H 5.96493000 -3.17045600 -0.35934900

C 3.72697800 -0.05334000 2.29864200

H 4.30981500 -0.50869500 3.10007400

H 4.03410100 0.99572200 2.23327300

H 2.67980400 -0.05462800 2.60832400

C 2.69768700 -0.73244500 -2.63957000

H 1.61498300 -0.74023700 -2.49106300

H 2.95930800 0.27479000 -2.98086200

H 2.92899200 -1.41850800 -3.45518800

C -3.94662500 -0.13265700 2.21258700

H -2.94366800 0.22339200 2.44427200

H -4.59531100 0.75010200 2.18006300

H -4.28880000 -0.74309700 3.05007000

C -2.59247100 -0.84065800 -2.65131900

H -2.93404600 0.12293400 -3.04506900

H -1.52606200 -0.73082800 -2.44229100

H -2.70741800 -1.57331800 -3.45121700

C 0.33621300 -1.94933700 1.24159100

H 1.42135900 -1.98784000 1.33434700

H -0.09580600 -2.68967700 1.90862700

C -0.13772200 -2.24785200 -0.17995000

H 0.05906900 -1.41467900 -0.88661600

H -1.21557800 -2.40828800 -0.19071500

C 0.57984600 -3.48479100 -0.75219800

H 1.66034300 -3.34021900 -0.79699700

H 0.37990600 -4.36238400 -0.13298200

H 0.22059000 -3.70053200 -1.76143200

C -0.19935900 -0.64334400 2.74644700

H 0.60760000 -1.08648600 3.31806000

H -1.16250900 -1.09547100 2.95066800

C -0.16597200 0.76396300 2.51742500

H -1.08373300 1.33757200 2.58772400

H 0.72839800 1.31612400 2.79024700

Fe 0.01331100 0.09204900 0.60761700

**1Fe(+)-5**

Atom x y z

C 1.35817100 -2.98782200 0.26969400

C 1.46482400 -4.35446700 0.51903000

C 0.29462600 -5.10875100 0.62963000

C -0.95024700 -4.49040900 0.50589200

C -0.99419100 -3.11907500 0.25710400

N 0.14687400 -2.41226200 0.13238800

H 0.35345500 -6.17297600 0.82427700

H 2.43285400 -4.82626700 0.63348400

H -1.86126300 -5.06658400 0.61001700

C 2.45374700 -2.00603600 0.15789600

C -2.18952900 -2.26520900 0.13728900

N -1.93867200 -0.99927500 -0.04509300

N 2.06751000 -0.77573600 -0.02562700

C -3.55472700 -2.87120300 0.25293400

H -3.69387000 -3.64568800 -0.50725700

H -3.67773900 -3.35419300 1.22714200

H -4.33933700 -2.12788700 0.13684300

C 3.87630900 -2.45953300 0.27969800

H 4.04646700 -2.92600800 1.25481800

H 4.10251300 -3.21471200 -0.47893900

H 4.57566200 -1.63512700 0.16632200

C -3.01827200 -0.04761400 -0.14248200

C -3.47477700 0.57254800 1.03199500

C -3.54304000 0.26157300 -1.40820600

C -4.48861100 1.52625100 0.91210700

C -4.55429700 1.22282700 -1.47598000

C -5.02455000 1.85214600 -0.32865300

H -4.85777200 2.01816500 1.80621700

H -4.97512400 1.47801800 -2.44312200

H -5.80901600 2.59736000 -0.40180900

C 3.03606300 0.28802200 -0.12956800

C 3.52731100 0.63944500 -1.39773400

C 3.41508000 0.96949500 1.03853000

C 4.42657900 1.70553300 -1.47460200

C 4.31717500 2.02822200 0.90942600

C 4.81886800 2.39690900 -0.33377300

H 4.82004100 1.99454200 -2.44374100

H 4.62605500 2.56866300 1.79836500

H 5.51558100 3.22409200 -0.41376300

C 3.11286100 -0.11036400 -2.63964300

H 3.43859400 -1.15545800 -2.61983600

H 2.02570100 -0.11648500 -2.77012200

H 3.54515800 0.34578500 -3.53056400

C 2.88692500 0.56699300 2.39346100

H 1.79489800 0.50613100 2.40670400

H 3.26479600 -0.41202400 2.70693400

H 3.18702100 1.28648200 3.15579300

C -3.05135900 -0.42835500 -2.65672600

H -1.96804400 -0.33080400 -2.78054100

H -3.27735900 -1.49971000 -2.65166500

H -3.52064100 -0.00388400 -3.54461400

C -2.91075600 0.21439700 2.38507600

H -3.21961700 -0.78645000 2.70596200

H -1.81727000 0.22763500 2.39126300

H -3.25470400 0.91547300 3.14611200

C -0.06183800 1.40863300 -0.80446100

H 0.83192500 1.62312200 -1.40557800

H -0.93270400 1.50044300 -1.46809400

C -0.17261400 2.40345600 0.35390100

H 0.69704400 2.31183200 1.01616800

H -1.05478000 2.17656500 0.96441600

C -0.27310800 3.86689900 -0.11459600

H 0.61074000 4.11180800 -0.71661500

H -1.13517300 3.96802700 -0.78577800

C -0.40259700 4.87023200 1.03663800

H 0.45802900 4.76540300 1.70927600

H -1.28639500 4.62046500 1.63701300

C -0.50339000 6.32163300 0.56179900

H -1.37487900 6.47085700 -0.08297200

H -0.59577500 7.01228300 1.40408800

H 0.38169600 6.61696900 -0.00985300

Fe 0.04190100 -0.49820000 -0.28585000

**1Fe(+)-6**

Atom x y z

C 1.03492700 2.70186500 0.24831600

C 1.01309800 4.07653800 0.48335600

C -0.21539400 4.73290800 0.54155700

C -1.39236600 3.99481700 0.42668700

C -1.31004300 2.62246200 0.19251900

N -0.11108900 2.01776200 0.03388100

H -0.25578700 5.80121300 0.71732300

H 1.93355400 4.62587100 0.63550800

H -2.35412800 4.47993200 0.53656900

C 2.22193900 1.83319800 0.29631700

C -2.43557300 1.67481100 0.19926200

N -2.09970300 0.42394500 0.08349700

N 1.97855700 0.56184700 0.16607400

C -3.83073200 2.18667900 0.41407700

H -3.89970900 2.72283400 1.36517300

H -4.10732300 2.89443200 -0.37284200

H -4.55970300 1.38058100 0.42631400

C 3.57092800 2.43946200 0.55400700

H 3.87018400 3.08145300 -0.28030600

H 3.54567900 3.06689000 1.44892300

H 4.33545800 1.67924100 0.69145200

C -3.10054400 -0.60655400 0.20605800

C -3.87053900 -0.98764300 -0.90658300

C -3.23959300 -1.23771200 1.45511800

C -4.77797000 -2.03825800 -0.74651100

C -4.16299400 -2.27943700 1.56587900

C -4.92356200 -2.68424300 0.47542700

H -5.37877800 -2.34847900 -1.59537700

H -4.28384900 -2.77643700 2.52304800

H -5.63077700 -3.49993800 0.57799800

C 3.04999900 -0.39382500 0.27880400

C 3.14864400 -1.11506800 1.48564400

C 3.93058200 -0.62310600 -0.79222500

C 4.13861100 -2.09115300 1.59059500

C 4.89850400 -1.62261900 -0.64208800

C 5.00345900 -2.35418800 0.53226200

H 4.23106500 -2.65143400 2.51532800

H 5.57967500 -1.82098100 -1.46382500

H 5.76064600 -3.12472900 0.62733200

C 2.24334700 -0.81624800 2.65427800

H 2.42119500 0.18541000 3.05965300

H 1.18745400 -0.86211000 2.37688100

H 2.40660600 -1.52831900 3.46391000

C 3.90264400 0.17995900 -2.07137700

H 2.94526600 0.66864700 -2.24919300

H 4.66692900 0.96463000 -2.05885800

H 4.11905300 -0.45324100 -2.93416100

C -2.45398800 -0.78359600 2.66023000

H -1.38959400 -0.67178100 2.44088600

H -2.80458200 0.18640100 3.02982800

H -2.55399200 -1.49574500 3.48009100

C -3.76368400 -0.28101700 -2.23603400

H -4.15976400 0.73917500 -2.19183200

H -2.73226900 -0.20769100 -2.58598700

H -4.33231100 -0.80999600 -3.00137900

C -0.14456600 -1.92611700 -0.26480800

H -0.16111700 -2.02148900 0.83306100

H -1.15649300 -2.16414100 -0.61348800

C 0.86382600 -2.90066600 -0.86315500

H 1.88577000 -2.62085500 -0.59492000

H 0.81405400 -2.86964600 -1.95776000

C 0.61750300 -4.34990600 -0.41157900

H 0.71406600 -4.44871300 0.67360700

H -0.38612000 -4.68815000 -0.68527400

H 1.33683700 -5.03333000 -0.87186600

C 0.14788500 -0.25924500 -2.74183900

H 1.13843500 -0.69713600 -2.76916200

H -0.67325600 -0.94505000 -2.91247300

C -0.03307200 1.07622000 -2.71043300

H -1.01530900 1.52398400 -2.81260700

H 0.80351500 1.76453500 -2.67845000

Fe -0.03933000 0.07459200 -0.38537800

**1Fe(+)-TS-6/7**

Atom x y z

C 1.17047500 2.70558000 -0.03193000

C 1.19449700 4.09789300 -0.09274500

C -0.01272800 4.79468200 -0.16185100

C -1.22106500 4.09532200 -0.13706700

C -1.19630100 2.70388500 -0.07564600

N -0.01244200 2.04057100 -0.06463400

H -0.01286200 5.87686400 -0.21034000

H 2.13497800 4.63499100 -0.07610500

H -2.16268600 4.63045400 -0.15358300

C 2.30239800 1.79899900 0.13109900

C -2.33253100 1.79492100 0.04722600

N -2.00449400 0.52842600 0.11643000

N 1.97306700 0.53143500 0.18467300

C -3.72822300 2.33797600 0.13656900

H -3.81319000 3.04248800 0.96880400

H -3.98682000 2.88619200 -0.77446900

H -4.46200600 1.54923600 0.28123400

C 3.69438100 2.33952700 0.27195000

H 4.03218700 2.78262800 -0.67028600

H 3.72747700 3.12779500 1.02813300

H 4.40195500 1.56367600 0.55463000

C -3.01624300 -0.46630700 0.37718100

C -3.77520100 -1.01502000 -0.67126500

C -3.18543100 -0.88446900 1.71024500

C -4.71175500 -2.00346900 -0.35408600

C -4.13317300 -1.87495200 1.97624500

C -4.89091500 -2.43523900 0.95457800

H -5.31053700 -2.43431800 -1.15015000

H -4.27744400 -2.20528100 2.99984000

H -5.62336100 -3.20312400 1.17828000

C 2.97107200 -0.47427400 0.44932400

C 3.04511100 -0.98643800 1.76071200

C 3.81347600 -0.94505500 -0.57329600

C 3.96033200 -2.00735700 2.02018800

C 4.70950300 -1.97445200 -0.26430200

C 4.78161000 -2.50839200 1.01534500

H 4.03063200 -2.40955000 3.02564000

H 5.36307800 -2.35263700 -1.04425300

H 5.48253000 -3.30678600 1.23324300

C 2.20517800 -0.41692800 2.87739900

H 2.50226300 0.60850600 3.12116400

H 1.14281900 -0.38173500 2.62340600

H 2.31265100 -1.01088800 3.78562700

C 3.82421400 -0.34997600 -1.96066200

H 4.55881200 0.45951200 -2.03502000

H 4.10892800 -1.09807600 -2.70285500

H 2.85929700 0.06235500 -2.25020000

C -2.38313200 -0.27529100 2.83286000

H -1.30730800 -0.35628800 2.65369600

H -2.60210700 0.78928300 2.96375400

H -2.60164800 -0.77112300 3.77914800

C -3.60442900 -0.57894100 -2.10554000

H -3.62611400 0.50761100 -2.22210100

H -2.65407600 -0.92569400 -2.51931500

H -4.40020500 -0.98810900 -2.72889700

C -0.04085900 -1.93472300 0.04343800

H 0.61360100 -1.93772700 0.91960000

H -1.06598800 -2.18371900 0.31721600

C 0.47818100 -2.78114300 -1.01412800

H 1.55821400 -2.93526300 -1.00542400

H 0.46525900 -2.00470300 -2.13211200

C -0.31222800 -3.97381500 -1.50048600

H -0.25736200 -4.77253200 -0.75206100

H -1.36915400 -3.72906200 -1.63254100

H 0.07730800 -4.37777700 -2.43821000

C 0.32816600 -1.13752300 -3.06535000

H 1.28541400 -1.27789900 -3.56574700

H -0.48407100 -1.62613200 -3.60449400

C 0.05942300 0.14615100 -2.46820100

H -0.93150200 0.55379900 -2.65493100

H 0.83641200 0.89670700 -2.60587900

Fe -0.00773500 0.14870300 -0.26640600

**1Fe(+)-7**

Atom x y z

C -1.25857400 2.56805300 -0.12196200

C -1.31212000 3.95474800 -0.25243600

C -0.12508100 4.68027000 -0.32872700

C 1.09267200 4.00305100 -0.31591800

C 1.10155100 2.61564600 -0.18289800

N -0.06179600 1.93254900 -0.02628800

H -0.14944900 5.75847100 -0.43010600

H -2.26775800 4.46083000 -0.31002500

H 2.02289900 4.54706000 -0.42179400

C -2.38716900 1.64348800 -0.16553400

C 2.26321900 1.73673000 -0.26733400

N 1.96757300 0.46298900 -0.25625300

N -2.03918900 0.38420000 -0.19064800

C 3.64091200 2.31336700 -0.41342700

H 3.67939700 3.00816600 -1.25674100

H 3.92246200 2.87754400 0.48070500

H 4.38589300 1.53890300 -0.57915400

C -3.79303700 2.16339700 -0.23889800

H -4.03681100 2.74834800 0.65270900

H -3.91512000 2.82523200 -1.10098600

H -4.51572000 1.35597600 -0.32907000

C 3.00191700 -0.52330400 -0.42716100

C 3.80819500 -0.92057600 0.65437100

C 3.14323400 -1.09842400 -1.70573200

C 4.75148400 -1.92932800 0.43270400

C 4.10275900 -2.09798600 -1.87774800

C 4.89892800 -2.51786100 -0.81736400

H 5.38026600 -2.25039600 1.25714400

H 4.22732200 -2.54712000 -2.85785000

H 5.63627400 -3.29893000 -0.96712400

C -3.03050900 -0.64565500 -0.36622000

C -3.20047800 -1.16172700 -1.66712500

C -3.76208500 -1.14586300 0.72641400

C -4.10245500 -2.21198500 -1.84868200

C -4.64793400 -2.20268300 0.49361700

C -4.81607600 -2.73776600 -0.77747200

H -4.24589500 -2.61793500 -2.84488600

H -5.21693000 -2.60331000 1.32657800

H -5.50701000 -3.55870900 -0.93485800

C -2.47081300 -0.57203500 -2.84993100

H -2.85280700 0.42274700 -3.10274900

H -1.39953000 -0.45388900 -2.66527400

H -2.59278700 -1.19926300 -3.73368600

C -3.65543300 -0.54728100 2.10758100

H -2.63334700 -0.28015600 2.37269300

H -4.25578300 0.36540400 2.19204700

H -4.02996700 -1.24136900 2.86141700

C 2.31722000 -0.62231900 -2.87521500

H 1.24983900 -0.58579900 -2.64065600

H 2.60233800 0.38869800 -3.18473900

H 2.45096400 -1.27548700 -3.73829600

C 3.70567100 -0.27288400 2.01324500

H 4.24775100 0.67859500 2.04458700

H 2.67468400 -0.06389600 2.29746800

H 4.14510300 -0.91120600 2.78107400

C 0.01022400 -2.13758300 -0.27222600

H -0.85524800 -1.96285600 -0.90028000

H 0.96034000 -2.30596400 -0.76725600

C -0.14252600 -2.44882400 1.03294000

H -1.13883300 -2.39087100 1.46586500

H -0.78996000 -0.93791100 3.51938600

C 0.92324900 -3.07117900 1.87840800

H 0.70895100 -4.14444800 1.95349500

H 1.91551800 -2.96300500 1.43872200

H 0.93236100 -2.68784000 2.89759900

Fe -0.01469700 0.10755900 0.34164700

C -0.00886400 -0.17325200 3.54166800

H -0.14938800 0.38375600 4.47748300

H 0.95015800 -0.68679900 3.63380800

C -0.05356800 0.77482400 2.34882300

H 0.77777800 1.48600600 2.41315900

H -0.96905000 1.37637000 2.38254600

**1Fe(+)-8**

Atom x y z

C 1.17757100 2.56068800 -0.00653600

C 1.20957600 3.95066400 -0.10763700

C -0.00000700 4.64636300 -0.14941400

C -1.20958900 3.95066100 -0.10763800

C -1.17758000 2.56068500 -0.00653600

N -0.00000400 1.90971100 0.05759700

H -0.00000800 5.72695200 -0.22890500

H 2.15049000 4.48401600 -0.16255600

H -2.15050400 4.48401100 -0.16255600

C 2.32553100 1.63265200 0.00137400

C -2.32553900 1.63264600 0.00137400

N -2.00588500 0.37056100 0.03612000

N 2.00587900 0.37056600 0.03611900

C -3.72120700 2.17347400 -0.05486800

H -3.89799200 2.86132400 0.77721200

H -3.87328800 2.74241100 -0.97736000

H -4.46448700 1.38135300 -0.01374300

C 3.72119800 2.17348000 -0.05486800

H 3.87328200 2.74240900 -0.97736400

H 3.89798000 2.86133800 0.77720700

H 4.46447900 1.38136000 -0.01373400

C -3.03057900 -0.64435200 0.02018900

C -3.47323800 -1.13707200 -1.21801300

C -3.51343800 -1.14006000 1.24270200

C -4.43050300 -2.15465800 -1.20785900

C -4.47060700 -2.15621100 1.19999500

C -4.92631900 -2.66217900 -0.01244700

H -4.78692000 -2.55221300 -2.15263800

H -4.85910100 -2.55422100 2.13178200

H -5.66678500 -3.45435300 -0.02525500

C 3.03057400 -0.64434600 0.02018800

C 3.51343700 -1.14004900 1.24270100

C 3.47323300 -1.13706700 -1.21801400

C 4.47060700 -2.15619900 1.19999500

C 4.43049800 -2.15465100 -1.20785900

C 4.92631700 -2.66217000 -0.01244600

H 4.85910400 -2.55420600 2.13178300

H 4.78691500 -2.55220900 -2.15263800

H 5.66678400 -3.45434400 -0.02525500

C 3.03039600 -0.59072800 2.56226200

H 3.28972300 0.46513800 2.69103100

H 1.94270200 -0.66745300 2.66433700

H 3.47441400 -1.13637800 3.39523900

C 2.95728600 -0.57859800 -2.52166400

H 1.86698100 -0.49687100 -2.53249700

H 3.35501900 0.42220800 -2.72270000

H 3.25079700 -1.21320000 -3.35842000

C -3.03038900 -0.59074700 2.56226300

H -1.94269600 -0.66749100 2.66433700

H -3.28969800 0.46512300 2.69103300

H -3.47441600 -1.13639100 3.39523900

C -2.95729400 -0.57860000 -2.52166200

H -3.35501900 0.42221100 -2.72269000

H -1.86698800 -0.49688200 -2.53250000

H -3.25081400 -1.21319400 -3.35842000

C 0.00001400 -2.01507600 0.44635400

H 0.88485400 -2.26869500 1.04395100

H -0.88484000 -2.26871800 1.04391800

C 0.00004700 -2.80513900 -0.86360100

H 0.88531500 -2.59865700 -1.47158300

H -0.88519600 -2.59866700 -1.47162200

H 0.00004900 -3.88526800 -0.67330600

Fe -0.00000200 -0.04718400 0.23268600

**1Fe(+)-TS-3/9**

Atom x y z

C -1.13922000 2.56650900 -0.08699000

C -1.15995000 3.95121700 -0.24155600

C 0.04606600 4.64950900 -0.24190600

C 1.24287000 3.94350000 -0.16362000

C 1.20772700 2.55541800 -0.01972800

N 0.02659700 1.90822100 0.11325600

H 0.05323200 5.72753800 -0.35012200

H -2.09656000 4.47743000 -0.37399300

H 2.18920900 4.46424600 -0.23373300

C -2.30255400 1.67058800 -0.20163900

C 2.37033100 1.65566600 -0.10554900

N 2.06620100 0.39700600 -0.18825300

N -2.01386000 0.40202900 -0.21927600

C 3.75550800 2.23168200 -0.16511600

H 3.82416800 2.98112700 -0.95812000

H 4.01451600 2.73023000 0.77363300

H 4.49836000 1.46271500 -0.36368000

C -3.67507000 2.25563800 -0.35792900

H -3.96688600 2.81318200 0.53680000

H -3.69240300 2.96001600 -1.19421300

H -4.42103200 1.48755500 -0.54610900

C 3.06606800 -0.62226300 -0.28379800

C 3.88799800 -0.94492100 0.81460800

C 3.13228200 -1.34627100 -1.49268400

C 4.77940200 -2.01413200 0.67126100

C 4.04950500 -2.39169500 -1.58943200

C 4.86647600 -2.73018300 -0.51484200

H 5.41453400 -2.28243300 1.50976000

H 4.12219000 -2.94679900 -2.51912900

H 5.56763100 -3.55284700 -0.60284600

C -3.04930100 -0.58970100 -0.29935700

C -3.14377300 -1.33759300 -1.48928100

C -3.87911600 -0.85069800 0.80750300

C -4.10343000 -2.34694600 -1.55920600

C -4.81384400 -1.88529800 0.69301300

C -4.93197900 -2.62513100 -0.47614500

H -4.19832600 -2.92311400 -2.47388900

H -5.45748600 -2.10726700 1.53841200

H -5.66611900 -3.42046800 -0.54378000

C -2.25002800 -1.04120500 -2.66605200

H -2.40701400 -0.03109900 -3.05658300

H -1.19180400 -1.11349600 -2.39591100

H -2.43365200 -1.74137400 -3.48165500

C -3.80507300 -0.05812300 2.09183300

H -2.79908800 0.30398400 2.31223300

H -4.46418700 0.81614400 2.06252500

H -4.13150100 -0.66523000 2.93772300

C 2.27033100 -0.97042100 -2.67160400

H 1.21066200 -0.91677800 -2.40431800

H 2.53978800 0.01079800 -3.07516700

H 2.37496800 -1.69666800 -3.47848400

C 3.85141300 -0.18890100 2.12261100

H 4.58739900 0.62212000 2.13613100

H 2.87601100 0.25329700 2.33068800

H 4.10221700 -0.84956600 2.95455500

C -0.12728400 -2.06404000 0.50015300

H -1.15147700 -2.40096000 0.37426200

H 0.58114200 -2.40518600 -0.25161100

C 0.34574600 -1.75269900 1.77794700

H 0.53218600 0.01096300 1.86950900

H 1.41681400 -1.81835600 1.93891100

C -0.49296300 -1.92428300 3.02036400

H -1.55343000 -1.76253900 2.82436200

H -0.37933100 -2.95635700 3.36955900

H -0.18063600 -1.26465600 3.83113800

Fe -0.00982700 0.00045100 0.37792000

**1Fe(+)-9**

Atom x y z

C 1.12850900 2.58646500 0.05678400

C 1.14041300 3.97670500 0.16639200

C -0.06763200 4.66888900 0.15744100

C -1.26324200 3.95635300 0.09863500

C -1.22200900 2.56720100 -0.00655800

N -0.03719800 1.91943600 -0.10892500

H -0.07892800 5.74937000 0.23599200

H 2.07634700 4.51052400 0.27086300

H -2.21221800 4.47474100 0.15046700

C 2.29018000 1.69728000 0.16319300

C -2.37259800 1.65762700 0.05439600

N -2.05136000 0.39949600 0.13936400

N 1.99300000 0.42975700 0.19597100

C -3.76727900 2.20876200 0.06667500

H -3.87684700 2.95558100 0.85769200

H -3.99632700 2.70679400 -0.88034300

H -4.50555700 1.42787400 0.23296200

C 3.66828700 2.27828900 0.27743800

H 3.70616500 3.01059500 1.08846400

H 4.41230200 1.51111800 0.47777700

H 3.94886000 2.80144200 -0.64158200

C -3.05682500 -0.62162600 0.21864500

C -3.78379000 -1.00587600 -0.92415500

C -3.23080400 -1.26456500 1.46072500

C -4.69282100 -2.06112500 -0.79332300

C -4.15867500 -2.30341000 1.54077400

C -4.88304300 -2.70472900 0.42274700

H -5.25842100 -2.37727900 -1.66416000

H -4.31332300 -2.80166000 2.49237800

H -5.59424200 -3.51977500 0.50024400

C 3.02398700 -0.56523100 0.28203300

C 3.14554200 -1.27301600 1.49441300

C 3.83187000 -0.85955300 -0.83277600

C 4.10172700 -2.28565600 1.57397500

C 4.76611400 -1.89328400 -0.70574100

C 4.90483900 -2.60013700 0.48184200

H 4.21607900 -2.83266800 2.50424200

H 5.39339800 -2.14090900 -1.55630800

H 5.63746100 -3.39617700 0.55763200

C 2.29469300 -0.92249700 2.68906200

H 2.52904300 0.07429700 3.07606100

H 1.22810600 -0.91981600 2.44437800

H 2.45011600 -1.63365400 3.50109500

C 3.73300300 -0.10013100 -2.13491900

H 2.72125400 0.25109500 -2.34269500

H 4.39116100 0.77558600 -2.13658300

H 4.04700900 -0.72706100 -2.97097000

C -2.47350300 -0.81516600 2.68585300

H -1.39739200 -0.74037000 2.50280900

H -2.80033600 0.17363000 3.02398700

H -2.62526600 -1.50866000 3.51373700

C -3.62881600 -0.31610300 -2.25973000

H -4.31011600 0.53710100 -2.34935700

H -2.61777700 0.05801700 -2.43018400

H -3.87586400 -0.99791000 -3.07528800

C 0.01557200 -2.14435100 -0.15172200

H 0.99797800 -2.44091300 0.20087800

H -0.80877800 -2.24072300 0.54771600

C -0.22678900 -2.00147800 -1.48509800

H -0.04175800 0.40140800 -1.90200400

H -1.25776800 -1.88791600 -1.80814200

C 0.76603400 -2.28227900 -2.57290500

H 1.79082400 -2.29729400 -2.20147200

H 0.55028000 -3.27457200 -2.98695500

H 0.69041000 -1.56751700 -3.39304900

Fe -0.01710100 0.04541300 -0.36806600

**1Fe(+)-10**

Atom x y z

C -1.15317300 2.41713500 0.04565800

C -1.18407000 3.80681400 0.04008500

C 0.03528600 4.49699500 0.08233000

C 1.24161600 3.80407800 0.12018600

C 1.20297600 2.40477800 0.12178200

N 0.02216200 1.77471200 0.09276500

H 0.03721200 5.58077000 0.07834100

H -2.11965200 4.35040200 -0.00000300

H 2.18289900 4.33899900 0.14130700

C -2.31246200 1.47051500 -0.01487700

C 2.33991000 1.45376500 0.12256800

N 1.99425200 0.19817600 0.07768100

N -2.00027000 0.21429600 -0.02707900

C 3.74231600 1.97387200 0.17330600

H 3.96870700 2.56589800 -0.71910900

H 3.87011200 2.63424500 1.03625700

H 4.46770100 1.16708000 0.24345300

C -3.70100600 2.02305500 -0.06924700

H -3.81932300 2.66375000 -0.94876400

H -4.44727600 1.23381100 -0.11020300

H -3.89643900 2.64705200 0.80831300

C 2.98871300 -0.84620100 0.02230100

C 3.23919100 -1.58297500 1.19122300

C 3.61737400 -1.13561400 -1.19984000

C 4.18205600 -2.60945100 1.12337500

C 4.54482200 -2.18025100 -1.21822000

C 4.83343900 -2.90661500 -0.06881200

H 4.39871600 -3.18621800 2.01659800

H 5.03905400 -2.42836800 -2.15189500

H 5.55768500 -3.71293900 -0.10475700

C -3.01486800 -0.81094900 -0.08461000

C -3.38408900 -1.31738400 -1.33994000

C -3.54125700 -1.30954100 1.11677200

C -4.33969000 -2.33513700 -1.37120600

C -4.49175000 -2.32917400 1.03247400

C -4.89357000 -2.83593800 -0.19836300

H -4.64420800 -2.74223500 -2.32987900

H -4.91432900 -2.73226600 1.94707500

H -5.63178900 -3.62902100 -0.24297500

C -2.75961800 -0.79913000 -2.61071400

H -2.97602200 0.26047400 -2.78307500

H -1.66995200 -0.90779500 -2.59032400

H -3.12872600 -1.34881100 -3.47684800

C -3.08228600 -0.78769200 2.45537100

H -2.00047500 -0.90726700 2.58010700

H -3.30876500 0.27462800 2.59396600

H -3.56642100 -1.32843700 3.26887200

C 3.29449700 -0.37825600 -2.46519600

H 2.21584900 -0.29088100 -2.62386200

H 3.70640500 0.63663300 -2.46265800

H 3.71291100 -0.88715100 -3.33392500

C 2.50522000 -1.28712700 2.47359800

H 2.64736900 -0.25548800 2.81040000

H 1.42706000 -1.44760900 2.35207900

H 2.84287800 -1.94275200 3.27673100

H 0.02469600 -1.72980400 0.06468900

Fe 0.01744800 -0.17632400 0.10678800

**2Fe(+)**

**2Fe(+)-1**

Atom x y z

C 1.16956000 2.43390000 0.11743100

C 1.20659700 3.82339900 0.25057700

C 0.00097100 4.51904700 0.29785300

C -1.20435800 3.82415500 0.23379600

C -1.16597200 2.43468400 0.10149200

N 0.00215600 1.78943900 0.01873900

H 0.00064200 5.59847200 0.39725400

H 2.14703400 4.35433200 0.31940200

H -2.14543000 4.35551200 0.28972200

C 2.37579300 1.54560000 0.10796600

C -2.37236300 1.54685000 0.07752700

N -2.12978800 0.28471000 0.08248500

N 2.13179200 0.28362400 0.10013600

C -3.73295300 2.17759400 0.09316000

H -3.85291300 2.80149000 0.98404600

H -3.87124100 2.82765200 -0.77578100

H -4.51889900 1.42642300 0.09460200

C 3.73595800 2.17536200 0.15736900

H 3.89991300 2.82109500 -0.71033700

H 3.83118100 2.80342500 1.04825200

H 4.52050100 1.42319500 0.18482400

C -3.17789000 -0.69871200 0.06865400

C -3.81958300 -1.02161700 -1.13981900

C -3.45816100 -1.37177600 1.27025000

C -4.78565300 -2.03047200 -1.11029100

C -4.43867300 -2.36492500 1.24870800

C -5.10015500 -2.69324900 0.07052300

H -5.29111600 -2.30076000 -2.03168900

H -4.67872500 -2.88905100 2.16808900

H -5.85377100 -3.47298800 0.07046400

C 3.17437000 -0.70398600 0.08838200

C 3.39331300 -1.43073600 1.27211400

C 3.87000900 -0.98291900 -1.10156900

C 4.36780300 -2.42925500 1.25565900

C 4.82637600 -2.00099800 -1.06872200

C 5.08166400 -2.71407200 0.09665800

H 4.56167500 -2.99246700 2.16272900

H 5.37120800 -2.23881000 -1.97655200

H 5.82928900 -3.49956100 0.09893400

C 2.60955100 -1.13452800 2.52612100

H 2.78012900 -0.11711800 2.89206400

H 1.53095700 -1.23728000 2.36110800

H 2.88416700 -1.82053900 3.32784800

C 3.59185100 -0.24049800 -2.38610100

H 2.52109400 -0.17519600 -2.59662600

H 3.98517300 0.78152400 -2.37069100

H 4.06069200 -0.74702200 -3.23011500

C -2.73105700 -1.02936500 2.54661700

H -1.64663500 -1.13999300 2.43575000

H -2.91480900 0.00133800 2.86632100

H -3.04489300 -1.68364000 3.36038800

C -3.47171700 -0.33168900 -2.43630600

H -3.80695400 0.71071100 -2.45734900

H -2.39336000 -0.33152200 -2.61925700

H -3.94682900 -0.83507200 -3.27865600

C 0.02933400 -2.06618700 -1.35056500

H 0.39154900 -1.92213700 -2.37371800

H 0.69513500 -2.79148700 -0.86880300

H -0.96417800 -2.52158000 -1.41107600

Fe 0.00163900 -0.35027000 -0.28829100

**2Fe(+)-2**

Atom x y z

C 1.16911000 2.40603800 -0.27191200

C 1.21109400 3.79750900 -0.35879700

C 0.01388700 4.50794600 -0.31936200

C -1.18678600 3.81689500 -0.22053500

C -1.15929000 2.42042400 -0.13767300

N 0.00373800 1.75180400 -0.14563800

H 0.01903400 5.59035000 -0.37734000

H 2.15288200 4.32111400 -0.45574600

H -2.12603400 4.35378500 -0.21100400

C 2.38886900 1.53954300 -0.33300100

C -2.38885700 1.57562200 -0.09515600

N -2.20046900 0.31680800 0.07737600

N 2.19572900 0.28474500 -0.14803300

C -3.72197300 2.24351100 -0.29034700

H -3.91138500 2.96310300 0.51224800

H -3.75242400 2.79679800 -1.23312200

H -4.53056900 1.51683400 -0.29017200

C 3.71269200 2.18446600 -0.62857500

H 3.65359000 2.78654700 -1.53930400

H 4.00878000 2.85581400 0.18341400

H 4.49453300 1.43958600 -0.75650100

C -3.29814800 -0.61078500 -0.02611700

C -3.66551000 -1.06138100 -1.30875400

C -3.93317500 -1.08688500 1.13267300

C -4.67946700 -2.01610000 -1.40448600

C -4.94962500 -2.03452400 0.98265500

C -5.31901400 -2.50397900 -0.27112900

H -4.96955700 -2.37746700 -2.38582800

H -5.45611000 -2.40500100 1.86823400

H -6.10598000 -3.24406100 -0.36552400

C 3.27540900 -0.66386200 -0.18559500

C 4.11996100 -0.82277400 0.92804700

C 3.40857300 -1.46248900 -1.33835300

C 5.08902400 -1.83033000 0.87514400

C 4.40096900 -2.44254600 -1.34608400

C 5.23016800 -2.63663400 -0.24598500

H 5.74288700 -1.97418900 1.72954500

H 4.52092400 -3.06233800 -2.22866200

H 5.98763000 -3.41238800 -0.26601200

C 4.04811100 0.06927400 2.14560800

H 4.69673000 0.94541800 2.03555300

H 3.04225300 0.43951500 2.34699400

H 4.38865500 -0.46147700 3.03614300

C 2.53949900 -1.24018500 -2.55068900

H 1.47668100 -1.30977800 -2.30675600

H 2.70788700 -0.25386800 -2.99627100

H 2.75031700 -1.98377300 -3.31983700

C -3.55788000 -0.61100500 2.51492000

H -2.65222700 -1.10763700 2.87773500

H -3.38258800 0.46689100 2.55727000

H -4.35042100 -0.83940100 3.22865000

C -3.00598700 -0.52966000 -2.55797000

H -3.29807200 0.50520200 -2.76858100

H -1.91606500 -0.55070400 -2.48634000

H -3.29216600 -1.12335800 -3.42673300

C -0.30982000 -2.31865500 -0.49347400

H -0.59155100 -2.37667800 -1.55026900

H 0.60061300 -2.91539200 -0.36437900

H -1.10911800 -2.81149000 0.07096200

C 0.48223600 -1.16448700 2.43023600

H 1.52522200 -1.43198700 2.30572900

H -0.21539700 -1.99407200 2.47079100

C 0.08626100 0.10135600 2.66065600

H -0.93992700 0.34661300 2.89992000

H 0.79778300 0.91929600 2.70384600

Fe 0.00147000 -0.41704400 0.16537500

**2Fe(+)-TS-2/3**

Atom x y z

C 1.17218400 2.51798700 0.04555500

C 1.20765000 3.91337800 0.05886200

C 0.00571400 4.61514400 0.05434000

C -1.19751500 3.91571400 0.04820200

C -1.16474700 2.52016800 0.03521100

N 0.00315000 1.85614500 0.02722700

H 0.00673600 5.69903700 0.06070400

H 2.15024900 4.44468900 0.07276200

H -2.13912700 4.44891700 0.05391000

C 2.38635200 1.65257300 0.07356100

C -2.38079800 1.65723600 0.05501200

N -2.16298200 0.39231400 -0.01288700

N 2.16631800 0.38824800 0.00266300

C -3.72981300 2.30744000 0.16969900

H -3.78838900 2.92741000 1.06892500

H -3.91774000 2.96250400 -0.68634500

H -4.52386400 1.56547600 0.21162900

C 3.73608700 2.29944900 0.19713800

H 3.93752000 2.94210700 -0.66533400

H 3.78529000 2.93117500 1.08860200

H 4.52663000 1.55515000 0.25910100

C -3.23930300 -0.55881000 0.04738800

C -3.84729900 -0.99067200 -1.14488800

C -3.61115200 -1.07742800 1.30182600

C -4.81399000 -1.99617900 -1.05912300

C -4.58271100 -2.08084700 1.33368000

C -5.17401400 -2.54719400 0.16514400

H -5.29244900 -2.34385300 -1.96926400

H -4.87929400 -2.49570600 2.29178000

H -5.92169800 -3.33144800 0.20958700

C 3.24027200 -0.56600200 0.05872400

C 3.59020000 -1.11157800 1.30844100

C 3.86737600 -0.97427300 -1.13177600

C 4.55718600 -2.11902500 1.33560200

C 4.82760700 -1.98683700 -1.05079800

C 5.16491700 -2.56471200 0.16706900

H 4.83747200 -2.55378300 2.28977300

H 5.31902500 -2.31827700 -1.96016800

H 5.90802800 -3.35352800 0.20740400

C 2.99947500 -0.58818300 2.59585500

H 3.45465300 0.36695600 2.88122700

H 1.92291000 -0.41876300 2.52672000

H 3.17784400 -1.28341100 3.41729900

C 3.58339500 -0.30837300 -2.45700000

H 2.53962600 -0.01428500 -2.56811900

H 4.18846400 0.59735100 -2.57942500

H 3.83516900 -0.96944200 -3.28782700

C -3.03742100 -0.53288300 2.58822900

H -1.96082300 -0.35997600 2.52909100

H -3.49973600 0.42425800 2.85481400

H -3.22252300 -1.21689400 3.41755700

C -3.53155100 -0.35392100 -2.47676900

H -4.06106800 0.59835100 -2.59557400

H -2.46869700 -0.14624200 -2.60317600

H -3.84765200 -0.99600600 -3.30020800

C -0.06637800 -2.65822400 -0.35165100

H 0.81020400 -3.14406600 -0.75906000

H -1.00708700 -3.04213200 -0.72351900

C -0.01735100 -2.13584400 0.95925000

H -0.92647200 -2.15996600 1.54979400

H 0.91405000 -2.22290500 1.50774700

Fe 0.00318600 -0.28475700 -0.10899300

C 0.03449800 -1.32011200 -2.05851700

H -0.80885000 -1.78727000 -2.55824800

H -0.02083800 -0.23459200 -2.27388100

H 0.97099300 -1.69206100 -2.46308500

**2Fe(+)-3**

Atom x y z

C 1.10750400 2.71721900 0.07080500

C 1.12220300 4.11342800 0.05728200

C -0.09483000 4.79153700 0.06804500

C -1.29033700 4.07668900 0.05738700

C -1.23233000 2.68147000 0.07173000

N -0.05232700 2.05060900 0.12517600

H -0.11136000 5.87541500 0.06153400

H 2.05376400 4.66351100 0.03134000

H -2.23835600 4.59793700 0.03126300

C 2.32019200 1.84665000 -0.02877400

C -2.41642200 1.77380700 -0.02652500

N -2.13877600 0.52260400 -0.15942800

N 2.08270000 0.58897100 -0.17123700

C -3.79080900 2.37446200 -0.02761100

H -4.00349400 2.86963700 0.92463800

H -3.87277900 3.13400800 -0.81046200

H -4.55402400 1.62032700 -0.20405300

C 3.67419400 2.49278000 -0.02178300

H 3.73477800 3.25615500 -0.80293100

H 3.86555700 2.99302500 0.93235400

H 4.46323500 1.76519400 -0.19591000

C -3.14547400 -0.49175000 -0.25803700

C -3.24804500 -1.17390400 -1.48647800

C -3.91948100 -0.85453900 0.86019500

C -4.18176700 -2.20362800 -1.59235000

C -4.82821300 -1.90612800 0.70677800

C -4.96878700 -2.57004900 -0.50499500

H -4.28717200 -2.72709000 -2.53704700

H -5.42872500 -2.20806800 1.55887400

H -5.68270900 -3.38076400 -0.60007700

C 3.12503700 -0.38809100 -0.27265000

C 3.90228200 -0.73524900 0.84834300

C 3.26489000 -1.05110800 -1.50785100

C 4.84803300 -1.75341600 0.69301800

C 4.23371600 -2.04777500 -1.61495600

C 5.02204800 -2.39986600 -0.52380900

H 5.45150600 -2.04263600 1.54748200

H 4.36594800 -2.55656200 -2.56430100

H 5.76401600 -3.18483600 -0.62032300

C 3.73910100 -0.06729600 2.19286100

H 4.32126900 0.85772500 2.26365600

H 2.69904500 0.18242300 2.41165900

H 4.09221400 -0.72289300 2.98979500

C 2.41052100 -0.67696600 -2.69253300

H 1.34159400 -0.75501900 -2.46278000

H 2.58734200 0.35165700 -3.02170700

H 2.61088400 -1.33241900 -3.54058300

C -3.78625400 -0.17106600 2.20011200

H -2.75302300 0.09694000 2.43060200

H -4.38371600 0.74519100 2.25460100

H -4.13991200 -0.82485300 2.99820800

C -2.39157000 -0.78645300 -2.66580100

H -2.58216500 0.23839000 -2.99838000

H -1.32190400 -0.84824800 -2.43140600

H -2.57435200 -1.44692300 -3.51390300

C 0.03564400 -1.68811600 1.47908500

H 0.81272300 -1.53419000 2.23997700

H -0.91850800 -1.73640200 2.02072200

Fe -0.02718700 -0.08556400 0.24478900

C 0.28215400 -3.01126200 0.73228100

H 1.23681700 -2.96875300 0.19424500

H -0.49086600 -3.16047300 -0.03317500

C 0.29337800 -4.23711100 1.65732200

H 1.07916900 -4.15071700 2.41362200

H -0.66026700 -4.34257300 2.18288500

H 0.46966200 -5.16035500 1.09695300

**2Fe(+)-4**

Atom x y z

Fe -0.05268300 -0.18170800 0.22486200

N -0.17140800 1.97715700 -0.16930800

C -1.36812700 2.57146800 -0.30622900

C -2.54511200 1.64831700 -0.33364700

N -2.29323000 0.40888100 -0.11975300

C -3.32809600 -0.58889600 -0.15151600

C -3.46041000 -1.36249900 -1.32096400

C -2.65854600 -1.05467300 -2.56128400

H -2.80231200 -1.82702400 -3.31746100

C -4.39860500 -2.39506800 -1.32130200

C -5.17970100 -2.65854500 -0.20075400

C -5.04808900 -1.86852000 0.93328800

C -4.13103900 -0.81333100 0.98076500

C -4.08057500 0.07004600 2.20560200

H -3.09186000 0.49093500 2.39084800

H -5.66972900 -2.06292400 1.80168700

H -4.51523400 -2.99929900 -2.21510500

C -3.90153800 2.22230500 -0.63048000

H -4.20764900 2.91976700 0.15520800

H -3.88918000 2.78066600 -1.57051000

H -4.65348800 1.44018100 -0.70314300

C -1.47874400 3.95544900 -0.43955400

C -0.31826900 4.72516100 -0.43796100

C 0.91495300 4.09622700 -0.33070200

C 0.95665400 2.70355200 -0.19927000

C 2.22757300 1.92672600 -0.14324600

N 2.11179400 0.66451300 0.07228100

C 3.26543500 -0.19499600 -0.01387600

C 3.65470900 -0.65839900 -1.28546000

C 4.72425100 -1.55312900 -1.35962500

C 5.39924300 -1.96542600 -0.21692700

C 5.01143600 -1.47817400 1.02470600

C 3.93864000 -0.59183000 1.15386000

H 5.54699100 -1.78735900 1.91664200

H 5.03154200 -1.92486200 -2.33184000

C 3.52120500 2.65908000 -0.37388000

H 3.67379800 3.41935500 0.39836700

H 4.36963800 1.97996600 -0.35085100

H 3.51623800 3.17554900 -1.33774600

H 1.82728400 4.67713400 -0.35200300

H -0.37707500 5.80334900 -0.53258700

H -2.44611500 4.42847500 -0.54440500

H 6.22916900 -2.65902600 -0.29476500

C 3.54509300 -0.09144200 2.52211200

H 3.33845400 0.98186400 2.53407900

H -5.89475000 -3.47366400 -0.21563500

C 2.97057300 -0.19367000 -2.54854000

H 3.26468200 -0.81354900 -3.39616500

C 0.23407300 -2.07836100 -0.49827400

H -0.78360800 -2.46237400 -0.66012000

H 0.67225800 -1.96791300 -1.50088300

H -1.58770800 -0.98952300 -2.35597200

H -2.96096200 -0.10176800 -3.00950100

H -4.37779400 -0.48313000 3.09801400

H -4.77439500 0.91319900 2.11286500

H 4.34252900 -0.27604400 3.24286700

H 2.65353300 -0.60360000 2.89767800

H 3.23848600 0.83846800 -2.80090600

H 1.88222300 -0.23501200 -2.46918500

C 1.22705700 -4.44481400 -0.46725500

C 1.04006400 -3.12166200 0.28837700

H 1.78919200 -5.17131400 0.12777300

H 1.77312700 -4.28974700 -1.40263800

H 0.26269700 -4.89614700 -0.71955100

H 2.02834800 -2.72737600 0.54928600

H 0.53798000 -3.33850200 1.23950200

C -0.43297300 -0.78715000 2.50557800

C -0.12832400 0.51817000 2.65054600

H -1.45489300 -1.14165600 2.43694300

H 0.32679400 -1.55631000 2.58957600

H -0.89725700 1.28331600 2.66694000

H 0.88185300 0.85096800 2.84922500

**2Fe(+)-TS-4/5**

Atom x y z

C 1.14132100 2.60994100 -0.29078900

C 1.16055400 3.99897300 -0.42146300

C -0.04734400 4.68922400 -0.46286500

C -1.24286900 3.97890200 -0.39396900

C -1.19867400 2.59041600 -0.26628500

N -0.02243900 1.93682200 -0.20608200

H -0.05746000 5.76884600 -0.55692800

H 2.09730400 4.53593100 -0.49216900

H -2.18921800 4.50113900 -0.44353500

C 2.36560400 1.76619200 -0.25773300

C -2.40962200 1.72671500 -0.21908500

N -2.20746600 0.47723900 0.02020500

N 2.18585500 0.51843700 0.01010000

C -3.75109000 2.36160000 -0.46166100

H -3.96980000 3.10262800 0.31347100

H -3.77132200 2.88472500 -1.42151000

H -4.54806200 1.62228100 -0.45366600

C 3.69253300 2.41512400 -0.53856600

H 3.68275000 2.93065300 -1.50266700

H 3.92133300 3.16515500 0.22502100

H 4.49854100 1.68568000 -0.54388400

C -3.30167800 -0.45874400 -0.03530400

C -3.63606400 -1.01184500 -1.28879600

C -3.98398900 -0.83232800 1.13589500

C -4.62753600 -1.99351300 -1.33505800

C -4.97564200 -1.81381600 1.03420900

C -5.28821800 -2.40407700 -0.18276200

H -4.88945200 -2.43148900 -2.29298500

H -5.51452300 -2.10750400 1.92964600

H -6.05715200 -3.16681100 -0.23739800

C 3.29404500 -0.40011100 -0.02776300

C 3.98045200 -0.72669500 1.15476200

C 3.62811700 -0.99210500 -1.26192000

C 4.99654700 -1.68468200 1.08133600

C 4.64460700 -1.94923300 -1.28070300

C 5.32276500 -2.30158200 -0.11928300

H 5.54051100 -1.94191500 1.98477700

H 4.91121800 -2.41496600 -2.22410000

H 6.11149500 -3.04504700 -0.15317600

C 3.66465200 -0.07805600 2.48110600

H 4.52526700 -0.13384800 3.14924100

H 3.39290900 0.97464000 2.38272100

H 2.83538700 -0.57947800 2.98913800

C 2.94343600 -0.59063600 -2.54617900

H 1.85471700 -0.59957000 -2.45910500

H 3.22877000 0.41906500 -2.86094200

H 3.21709400 -1.26584900 -3.35758500

C -3.71543300 -0.19698400 2.47964200

H -2.94235300 -0.73085900 3.03985900

H -3.39736000 0.84370800 2.39820600

H -4.61670300 -0.21514600 3.09460700

C -2.99110100 -0.53388300 -2.56786800

H -3.38773100 0.43968100 -2.87713700

H -1.90936300 -0.42212700 -2.47776600

H -3.18860100 -1.22967200 -3.38430600

C 0.36575100 -2.30145600 0.47179700

H 1.45722800 -2.29758000 0.45988000

H 0.03915300 -3.19955800 0.99167200

C -0.23524200 -2.31662500 -0.93851600

H -0.01674700 -1.39329700 -1.49855600

H -1.32302000 -2.38943300 -0.87919600

C 0.30654300 -3.49694600 -1.76725400

H 1.39238500 -3.44354900 -1.87486900

H 0.06575000 -4.44776100 -1.28530500

H -0.13489700 -3.50718700 -2.76824600

C -0.08854300 -1.42123300 2.42936000

H 0.77027800 -2.00468100 2.73713400

H -1.02674400 -1.95849900 2.49639500

C -0.08666000 -0.02265600 2.64296200

H -1.01706400 0.47696200 2.88408200

H 0.81163200 0.44857800 3.02598600

Fe 0.01341800 -0.04079300 0.52654500

**2Fe(+)-5**

Atom x y z

C 1.13042600 -3.09187900 -0.23269200

C 1.15134000 -4.48546300 -0.31839200

C -0.06260800 -5.16658400 -0.37569800

C -1.26115700 -4.45938600 -0.31511300

C -1.20942500 -3.06644100 -0.22997700

N -0.03234300 -2.42772900 -0.23713400

H -0.07442800 -6.24831100 -0.44528500

H 2.08541600 -5.03175000 -0.33290500

H -2.20691600 -4.98528900 -0.32691800

C 2.33966500 -2.22541000 -0.07805800

C -2.39831000 -2.17374400 -0.07289600

N -2.12800000 -0.93494100 0.15536100

N 2.09769800 -0.98226100 0.15564800

C -3.76964800 -2.77908900 -0.12978900

H -3.96813700 -3.20947400 -1.11591100

H -3.85682100 -3.59068400 0.59845100

H -4.53920100 -2.04254700 0.08854100

C 3.69663000 -2.86220700 -0.14239000

H 3.76918000 -3.67590000 0.58515500

H 3.88011100 -3.29654700 -1.12970800

H 4.48407200 -2.14376800 0.07229600

C -3.14334800 0.06331600 0.31525400

C -3.27609300 0.64471200 1.59122100

C -3.89679100 0.50911600 -0.78699300

C -4.21841400 1.65868800 1.75812100

C -4.81616700 1.53988600 -0.57024300

C -4.98565200 2.10572900 0.68696900

H -4.34645700 2.10543100 2.73875100

H -5.40162500 1.90451300 -1.40815800

H -5.70712500 2.90245900 0.83085500

C 3.13727400 -0.00953400 0.31557600

C 3.89481100 0.42417000 -0.78876700

C 3.29340900 0.56001000 1.59417100

C 4.84049400 1.43089000 -0.57232400

C 4.26096100 1.55015900 1.76042300

C 5.03164000 1.98524400 0.68689300

H 5.42964700 1.78564300 -1.41190500

H 4.40652200 1.98736000 2.74292600

H 5.77333300 2.76322700 0.83064800

C 3.70606200 -0.14025100 -2.17667200

H 4.24582900 -1.08301600 -2.31494800

H 2.65566600 -0.32674900 -2.41083900

H 4.08886000 0.55372600 -2.92586200

C 2.45599700 0.09696100 2.75961800

H 1.38409600 0.21435400 2.56125400

H 2.61960000 -0.95941900 2.99341600

H 2.68513400 0.67200900 3.65724500

C -3.72904600 -0.06603400 -2.17310600

H -2.68505900 -0.28221400 -2.41029500

H -4.29537100 -0.99397500 -2.30526500

H -4.09558700 0.63522800 -2.92364700

C -2.44016100 0.16992200 2.75315800

H -2.62090900 -0.88254300 2.99151600

H -1.36701300 0.26811300 2.54954300

H -2.65306500 0.75208100 3.65016900

C 0.02969400 1.43233400 -1.24924300

H 0.90833200 1.43186200 -1.90702400

H -0.84922900 1.46378100 -1.90626900

C 0.05280700 2.67212200 -0.33773400

H 0.93465700 2.64416200 0.31601300

H -0.82060100 2.66850000 0.32849200

C 0.06435700 4.00323600 -1.11003900

H 0.93726200 4.02161900 -1.77499300

H -0.81519800 4.04247300 -1.76531500

C 0.08383800 5.23955700 -0.20463100

H 0.96284200 5.19544000 0.45060300

H -0.78879700 5.21579500 0.46012500

C 0.09492500 6.55720800 -0.98328300

H -0.79000900 6.65182400 -1.62009900

H 0.10950800 7.41924300 -0.31112600

H 0.97395300 6.63043600 -1.63099000

Fe -0.01380800 -0.28715400 -0.18560900

**2Fe(+)-6**

Atom x y z

C 0.95661300 2.70370600 0.19935900

C 0.91487800 4.09635300 0.33104300

C -0.31836700 4.72523100 0.43838600

C -1.47881900 3.95548100 0.43983400

C -1.36814300 2.57152200 0.30631800

N -0.17141600 1.97727200 0.16929200

H -0.37720700 5.80340600 0.53318100

H 1.82719900 4.67727600 0.35245700

H -2.44621400 4.42845800 0.54469800

C 2.22757700 1.92692500 0.14313500

C -2.54512300 1.64831900 0.33360900

N -2.29313700 0.40887700 0.11999400

N 2.11184900 0.66479100 -0.07276500

C -3.90164500 2.22229700 0.63004000

H -3.88945500 2.78110200 1.56980600

H -4.20776000 2.91932100 -0.15604000

H -4.65349600 1.44009300 0.70299800

C 3.52116800 2.65929100 0.37399900

H 3.67376000 3.41971500 -0.39810300

H 3.51611900 3.17556500 1.33797200

H 4.36963000 1.98020600 0.35086500

C -3.32795100 -0.58891400 0.15148900

C -4.13085500 -0.81316000 -0.98083800

C -3.46031100 -1.36274600 1.32080900

C -5.04790100 -1.86838200 -0.93358000

C -4.39847900 -2.39531600 1.32093900

C -5.17954700 -2.65860400 0.20030800

H -5.66949400 -2.06263300 -1.80205000

H -4.51512500 -2.99972200 2.21462500

H -5.89459100 -3.47373300 0.21502500

C 3.26542600 -0.19479100 0.01344900

C 3.65466700 -0.65809900 1.28508600

C 3.93852800 -0.59191500 -1.15424500

C 4.72397600 -1.55309800 1.35934000

C 5.01111900 -1.47849600 -1.02500000

C 5.39883300 -1.96571200 0.21667400

H 5.03121000 -1.92476300 2.33160100

H 5.54660100 -1.78789900 -1.91690900

H 6.22859800 -2.65950300 0.29457200

C 2.97059300 -0.19315200 2.54812300

H 3.23785300 0.83928500 2.79993300

H 1.88224100 -0.23529900 2.46905400

H 3.26534100 -0.81243100 3.39596700

C 3.54514000 -0.09170900 -2.52261600

H 2.65465300 -0.60519200 -2.89896700

H 3.33686200 0.98127100 -2.53440700

H 4.34336500 -0.27488200 -3.24287400

C -2.65864300 -1.05498200 2.56127300

H -1.58792900 -0.98822300 2.35587600

H -2.96230400 -0.10285800 3.01032500

H -2.80130200 -1.82816800 3.31681400

C -4.08036300 0.07034900 -2.20558900

H -4.77474000 0.91306900 -2.11309400

H -3.09181400 0.49184900 -2.39036400

H -4.37683900 -0.48295000 -3.09817900

C 0.23414500 -2.07793400 0.49880800

H 0.67195800 -1.96702500 1.50153700

H -0.78354000 -2.46201200 0.66048800

C 1.04054000 -3.12149700 -0.28706100

H 2.02893800 -2.72728200 -0.54763600

H 0.53896400 -3.33872100 -1.23837400

C 1.22717600 -4.44436500 0.46914100

H 1.77275900 -4.28896000 1.40475900

H 0.26269600 -4.89563900 0.72110800

H 1.78963600 -5.17106200 -0.12534300

C -0.43374500 -0.78829700 -2.50478900

H 0.32540900 -1.55809900 -2.58850600

H -1.45591300 -1.14204700 -2.43585600

C -0.12811200 0.51674100 -2.65058400

H -0.89648400 1.28245800 -2.66732100

H 0.88226100 0.84863900 -2.84972500

Fe -0.05258300 -0.18151700 -0.22525900

**2Fe(+)-TS-6/7**

Atom x y z

C 1.27987500 2.64778900 -0.07639800

C 1.35762500 4.04041700 -0.15188500

C 0.17793900 4.77671300 -0.20719800

C -1.04567200 4.11533200 -0.14632400

C -1.05401300 2.72121400 -0.06982600

N 0.09211500 2.02103200 -0.08044700

H 0.21152700 5.85794800 -0.27331200

H 2.31572200 4.54370400 -0.16073600

H -1.97044800 4.67756500 -0.15087300

C 2.45603600 1.74954200 0.08327300

C -2.28327800 1.89791900 0.10288600

N -2.09368900 0.62714400 0.19126600

N 2.18718500 0.49296200 0.17213900

C -3.60903500 2.59352900 0.22803200

H -3.58641300 3.31871200 1.04638600

H -3.84620700 3.14728800 -0.68527800

H -4.41253500 1.88671700 0.42074500

C 3.82484000 2.35961700 0.19214500

H 4.08739100 2.89377800 -0.72591400

H 3.85816400 3.08718400 1.00798600

H 4.58332200 1.60314000 0.37879200

C -3.17050100 -0.28623600 0.45549400

C -4.02419100 -0.71440800 -0.57718300

C -3.28411900 -0.78622000 1.76624700

C -5.00517000 -1.65988600 -0.26395400

C -4.28448200 -1.72371200 2.02970900

C -5.13905400 -2.16250600 1.02484700

H -5.67307000 -2.00244000 -1.04780800

H -4.39043300 -2.11223700 3.03747400

H -5.90761200 -2.89511700 1.24536800

C 3.20922500 -0.48633300 0.41666600

C 3.31566200 -0.99579200 1.72465900

C 4.01560200 -0.96433500 -0.63185000

C 4.25794200 -1.99671300 1.96740500

C 4.93837600 -1.97284300 -0.33921600

C 5.06287600 -2.48750100 0.94551100

H 4.35775000 -2.39398100 2.97240000

H 5.56770200 -2.35563300 -1.13631900

H 5.78556000 -3.26977100 1.15006500

C 2.46116200 -0.45779300 2.84539600

H 2.69842000 0.58608900 3.07559100

H 1.39556800 -0.49180700 2.59941600

H 2.61018000 -1.03429700 3.75897700

C 3.91636700 -0.41668400 -2.03481800

H 4.30828300 0.60325700 -2.10852000

H 4.49397900 -1.02861600 -2.72850200

H 2.88605300 -0.39065700 -2.39404900

C -2.37275900 -0.30583000 2.86816100

H -1.31716400 -0.42153900 2.60408700

H -2.52721400 0.75418400 3.09466300

H -2.54783400 -0.86412600 3.78837900

C -3.90785400 -0.18637500 -1.98631600

H -4.15345900 0.87825300 -2.05367600

H -2.89922600 -0.30837100 -2.38667500

H -4.59239900 -0.71319800 -2.65182300

C -0.00658300 -2.19616300 0.12023600

H 0.87627400 -2.29311300 0.75573400

H -0.92404500 -2.30432200 0.70436300

C 0.03183400 -3.04598500 -1.05915900

H 0.99723100 -3.52121000 -1.24797000

H 0.04575600 -2.27413500 -2.10888500

C -1.15109700 -3.94619300 -1.36393000

H -1.17766500 -4.77693400 -0.65135900

H -2.09748100 -3.40687700 -1.26802300

H -1.09653400 -4.37512500 -2.36785800

C 0.02681700 -1.35771500 -3.11580500

H 0.93261200 -1.70253000 -3.61175100

H -0.87933300 -1.72589000 -3.59468100

C 0.01530100 -0.05342900 -2.53954600

H -0.89606500 0.52619800 -2.67787900

H 0.90975200 0.54819800 -2.69347900

Fe 0.02371500 -0.09364500 -0.31305000

**2Fe(+)-7**

Atom x y z

C -1.25857400 2.56805300 -0.12196200

C -1.31212000 3.95474800 -0.25243600

C -0.12508100 4.68027000 -0.32872700

C 1.09267200 4.00305100 -0.31591800

C 1.10155100 2.61564600 -0.18289800

N -0.06179600 1.93254900 -0.02628800

H -0.14944900 5.75847100 -0.43010600

H -2.26775800 4.46083000 -0.31002500

H 2.02289900 4.54706000 -0.42179400

C -2.38716900 1.64348800 -0.16553400

C 2.26321900 1.73673000 -0.26733400

N 1.96757300 0.46298900 -0.25625300

N -2.03918900 0.38420000 -0.19064800

C 3.64091200 2.31336700 -0.41342700

H 3.67939700 3.00816600 -1.25674100

H 3.92246200 2.87754400 0.48070500

H 4.38589300 1.53890300 -0.57915400

C -3.79303700 2.16339700 -0.23889800

H -4.03681100 2.74834800 0.65270900

H -3.91512000 2.82523200 -1.10098600

H -4.51572000 1.35597600 -0.32907000

C 3.00191700 -0.52330400 -0.42716100

C 3.80819500 -0.92057600 0.65437100

C 3.14323400 -1.09842400 -1.70573200

C 4.75148400 -1.92932800 0.43270400

C 4.10275900 -2.09798600 -1.87774800

C 4.89892800 -2.51786100 -0.81736400

H 5.38026600 -2.25039600 1.25714400

H 4.22732200 -2.54712000 -2.85785000

H 5.63627400 -3.29893000 -0.96712400

C -3.03050900 -0.64565500 -0.36622000

C -3.20047800 -1.16172700 -1.66712500

C -3.76208500 -1.14586300 0.72641400

C -4.10245500 -2.21198500 -1.84868200

C -4.64793400 -2.20268300 0.49361700

C -4.81607600 -2.73776600 -0.77747200

H -4.24589500 -2.61793500 -2.84488600

H -5.21693000 -2.60331000 1.32657800

H -5.50701000 -3.55870900 -0.93485800

C -2.47081300 -0.57203500 -2.84993100

H -2.85280700 0.42274700 -3.10274900

H -1.39953000 -0.45388900 -2.66527400

H -2.59278700 -1.19926300 -3.73368600

C -3.65543300 -0.54728100 2.10758100

H -2.63334700 -0.28015600 2.37269300

H -4.25578300 0.36540400 2.19204700

H -4.02996700 -1.24136900 2.86141700

C 2.31722000 -0.62231900 -2.87521500

H 1.24983900 -0.58579900 -2.64065600

H 2.60233800 0.38869800 -3.18473900

H 2.45096400 -1.27548700 -3.73829600

C 3.70567100 -0.27288400 2.01324500

H 4.24775100 0.67859500 2.04458700

H 2.67468400 -0.06389600 2.29746800

H 4.14510300 -0.91120600 2.78107400

C 0.01022400 -2.13758300 -0.27222600

H -0.85524800 -1.96285600 -0.90028000

H 0.96034000 -2.30596400 -0.76725600

C -0.14252600 -2.44882400 1.03294000

H -1.13883300 -2.39087100 1.46586500

H -0.78996000 -0.93791100 3.51938600

C 0.92324900 -3.07117900 1.87840800

H 0.70895100 -4.14444800 1.95349500

H 1.91551800 -2.96300500 1.43872200

H 0.93236100 -2.68784000 2.89759900

Fe -0.01469700 0.10755900 0.34164700

C -0.00886400 -0.17325200 3.54166800

H -0.14938800 0.38375600 4.47748300

H 0.95015800 -0.68679900 3.63380800

C -0.05356800 0.77482400 2.34882300

H 0.77777800 1.48600600 2.41315900

H -0.96905000 1.37637000 2.38254600

**2Fe(+)-8**

Atom x y z

C 1.18333000 2.52179500 -0.01730800

C 1.22643700 3.91765200 -0.02874800

C 0.02713900 4.62362000 -0.02351500

C -1.17859000 3.92858400 -0.00100800

C -1.14814700 2.53258800 0.00897100

N 0.01451400 1.86632800 -0.00990800

H 0.03195800 5.70743200 -0.03228500

H 2.17097300 4.44575800 -0.03987700

H -2.11812600 4.46550700 0.00969200

C 2.39391100 1.64566900 0.00277200

C -2.36645600 1.66744000 0.05296800

N -2.14589700 0.40268100 0.10810500

N 2.16327700 0.38356200 0.07303500

C -3.71787700 2.31922400 0.05630100

H -3.80986200 3.00036900 0.90748800

H -3.86647000 2.91445100 -0.84944900

H -4.51396800 1.58154500 0.12028400

C 3.75186000 2.28275700 -0.03840600

H 3.87304100 2.88212900 -0.94549000

H 3.88443100 2.95697300 0.81299800

H 4.54086900 1.53524900 -0.00932700

C -3.21039200 -0.56174900 0.14083100

C -3.85764800 -0.92600200 -1.05239600

C -3.50451400 -1.17594600 1.37020000

C -4.83985900 -1.91716100 -0.98160300

C -4.50065000 -2.15320700 1.39010700

C -5.16559400 -2.52307000 0.22605000

H -5.34955500 -2.21816500 -1.89113200

H -4.75045900 -2.63261300 2.33101700

H -5.93119700 -3.29032400 0.25872700

C 3.22522100 -0.58518500 0.10220300

C 3.59234700 -1.12771000 1.34483000

C 3.79479600 -1.02301500 -1.10507100

C 4.58414800 -2.11012200 1.36001500

C 4.77746600 -2.01354800 -1.03790100

C 5.17521800 -2.55072800 0.18101000

H 4.88876200 -2.53716700 2.30998400

H 5.22992300 -2.36912800 -1.95793100

H 5.93928100 -3.31961000 0.21136100

C 2.93950000 -0.66593300 2.62387400

H 3.12160900 0.39454800 2.82559500

H 1.85294900 -0.80442300 2.59542100

H 3.31644500 -1.22868100 3.47824800

C 3.35911200 -0.46192500 -2.43677400

H 2.27314300 -0.51043200 -2.56385900

H 3.65318900 0.58521400 -2.56570500

H 3.80790800 -1.02260900 -3.25705200

C -2.77479500 -0.78863600 2.63202800

H -1.69411200 -0.94456100 2.53718800

H -2.92528000 0.26335500 2.89416300

H -3.11483700 -1.38721600 3.47753100

C -3.50872600 -0.28954100 -2.37614600

H -3.87535800 0.73980200 -2.45252000

H -2.42876700 -0.26176700 -2.54726500

H -3.95471200 -0.84678200 -3.20034900

C -0.00128200 -2.33563600 -0.23390500

H 0.95919100 -2.70111400 0.15454600

H -0.75845300 -2.73501200 0.45509100

C -0.23818900 -2.92110300 -1.63761600

H 0.52278500 -2.59680700 -2.35584100

H -1.21128400 -2.62830400 -2.04542000

H -0.21839800 -4.01753100 -1.63659200

Fe 0.00478900 -0.30164500 -0.05224800

**2Fe(+)-3/9**

Atom x y z

C -1.10261900 2.60071700 0.05342700

C -1.11721300 3.99489400 0.12477500

C 0.09407300 4.67871200 0.17395600

C 1.28895400 3.96287900 0.14809200

C 1.23719000 2.57140000 0.07592000

N 0.05921300 1.92473100 0.03145400

H 0.10770300 5.76083100 0.23191000

H -2.05218600 4.53959700 0.14272100

H 2.23764300 4.48256300 0.18476800

C -2.32068000 1.75166900 -0.00490500

C 2.43042600 1.68415400 0.04209400

N 2.17836600 0.42127100 0.00301700

N -2.11474700 0.47883100 -0.02236600

C 3.79993100 2.29771500 0.05840700

H 3.93492400 2.96899700 -0.79457700

H 3.94377900 2.89464200 0.96388100

H 4.57590100 1.53664100 0.02376500

C -3.66825000 2.41329500 -0.03944600

H -3.82538400 3.01623600 0.85985500

H -3.74774100 3.08727400 -0.89719400

H -4.46921500 1.68064500 -0.10236700

C 3.23236700 -0.55519200 -0.04390000

C 3.71168300 -1.09732200 1.16224800

C 3.70287600 -0.98620100 -1.29698500

C 4.68071300 -2.10094200 1.08530200

C 4.67028900 -1.99413100 -1.31945600

C 5.15500300 -2.55138900 -0.14182300

H 5.06622700 -2.53134600 2.00398900

H 5.04653000 -2.34153100 -2.27634100

H 5.90362500 -3.33508200 -0.17999500

C -3.20897400 -0.45236700 -0.08564500

C -3.63362300 -0.91257400 -1.34471600

C -3.77540000 -0.92119700 1.11287400

C -4.64670400 -1.87400000 -1.38044100

C -4.78811600 -1.87972800 1.02272500

C -5.21977100 -2.35767800 -0.20962400

H -4.98958400 -2.24229500 -2.34203500

H -5.23977100 -2.25478800 1.93552300

H -6.00412300 -3.10508500 -0.25760200

C -3.04655700 -0.36651400 -2.62331600

H -3.36212300 0.66669800 -2.80532500

H -1.95331400 -0.36731600 -2.60856200

H -3.36974900 -0.95607600 -3.48198500

C -3.32242400 -0.40420200 2.45613000

H -2.23425900 -0.42777700 2.55593700

H -3.63817900 0.63181500 2.62113600

H -3.74840200 -1.00034300 3.26389300

C 3.21629000 -0.36332800 -2.58336200

H 2.12925800 -0.25188600 -2.60741600

H 3.64186300 0.63488300 -2.73540100

H 3.50877400 -0.96842400 -3.44228500

C 3.22513400 -0.59905100 2.50144800

H 3.59701400 0.40867700 2.71728800

H 2.13425000 -0.55468600 2.55293900

H 3.57405100 -1.24749400 3.30593600

C 0.04860500 -2.08288400 -0.94981500

H -0.88933900 -2.30515100 -1.44927200

H 0.92845600 -2.06076900 -1.58417000

C 0.19654500 -2.43076800 0.41140900

H -0.01591400 -1.08321700 1.41901000

H 1.21524800 -2.57540000 0.76110000

C -0.83756200 -3.26427200 1.13464500

H -1.85409900 -2.99152500 0.84944600

H -0.68423700 -4.31130800 0.85168700

H -0.74587400 -3.19136300 2.21926100

Fe 0.01558900 -0.17502500 0.02983300

**2Fe(+)-9**

Atom x y z

C 1.18824300 2.58062200 -0.03904100

C 1.23391600 3.97648400 -0.02958200

C 0.03602900 4.68491000 -0.01821900

C -1.17280000 3.99536600 -0.01090700

C -1.14649600 2.59934300 -0.02433800

N 0.01525600 1.93394700 -0.04451800

H 0.04471400 5.76884800 -0.01096100

H 2.17890700 4.50347800 -0.02962800

H -2.10989300 4.53613400 0.00563200

C 2.40264400 1.70531200 -0.02766500

C -2.36885600 1.73809800 -0.00484800

N -2.16103700 0.47081400 0.00570000

N 2.18378600 0.44081600 -0.00884100

C -3.71512500 2.40332400 0.00456700

H -3.82309800 3.05023800 0.88008600

H -3.83769100 3.03534500 -0.87995800

H -4.51934000 1.67157700 0.01703700

C 3.75541400 2.35804400 -0.02960900

H 3.87592200 3.00801900 0.84197500

H 4.55162100 1.61754900 -0.01804400

H 3.87958900 2.98372900 -0.91844400

C -3.25612500 -0.46063200 0.05251000

C -3.77790500 -0.96937600 -1.15053900

C -3.71715900 -0.89329700 1.30882100

C -4.77608900 -1.94374300 -1.06491700

C -4.71540100 -1.87049400 1.33967100

C -5.24004900 -2.39723400 0.16498500

H -5.19333500 -2.34866100 -1.98127800

H -5.08386400 -2.21726500 2.29986300

H -6.01231300 -3.15741500 0.20775700

C 3.26720500 -0.50348000 0.04766200

C 3.71627000 -0.92940200 1.31133300

C 3.79774700 -1.02314400 -1.14693500

C 4.70534500 -1.91517000 1.35822900

C 4.78635400 -2.00601100 -1.04439000

C 5.23461900 -2.45597300 0.19227500

H 5.06372700 -2.25625500 2.32428800

H 5.20972900 -2.41933500 -1.95417000

H 5.99946400 -3.22287100 0.24713000

C 3.18334800 -0.32158500 2.58669600

H 3.56605800 0.69317300 2.74251600

H 2.09255400 -0.25181800 2.59176500

H 3.48403800 -0.91172700 3.45320800

C 3.35279300 -0.52343900 -2.49955800

H 2.26621700 -0.54140500 -2.60741300

H 3.67882500 0.50801700 -2.67541200

H 3.78182600 -1.13354700 -3.29531400

C -3.18239800 -0.30694400 2.59327000

H -2.09156200 -0.23633900 2.59719400

H -3.56409800 0.70531800 2.76668000

H -3.48050300 -0.91138100 3.45064500

C -3.30244100 -0.47199400 -2.49366800

H -3.60637100 0.56581200 -2.67068600

H -2.21403200 -0.50762000 -2.58401600

H -3.72806900 -1.07112600 -3.29949700

C 0.22607600 -2.08276100 1.13832200

H 1.30007200 -2.23408000 1.15886500

H -0.21337700 -1.56294500 1.98562100

C -0.55192300 -2.70062100 0.22693600

H 0.07643200 -0.62665600 -1.98331800

H -1.63178000 -2.60520300 0.31230000

C -0.05388100 -3.60385900 -0.85630200

H 1.03571500 -3.62622700 -0.90837000

H -0.41087500 -4.62267800 -0.66781200

H -0.44477700 -3.30708300 -1.83234800

Fe 0.00605400 -0.18341200 -0.40541600

**2Fe(+)-10**

Atom x y z

C -1.16931800 2.37214300 -0.13257400

C -1.20761400 3.75477100 -0.32190000

C -0.00008700 4.44580500 -0.40475200

C 1.20747200 3.75474300 -0.32254400

C 1.16921900 2.37213300 -0.13312900

N -0.00003000 1.73759600 -0.01424700

H -0.00011300 5.52029300 -0.54776300

H -2.14804000 4.28363800 -0.40725100

H 2.14786900 4.28357300 -0.40844000

C -2.36338800 1.46812000 -0.08622100

C 2.36328800 1.46811700 -0.08698200

N 2.09849700 0.20965300 -0.04453500

N -2.09856700 0.20965500 -0.04444400

C 3.73346300 2.07283500 -0.13471200

H 3.85432600 2.67088100 -1.04306200

H 3.89103000 2.74371100 0.71508200

H 4.50597900 1.30785000 -0.12276400

C -3.73355400 2.07293300 -0.13323100

H -3.85480800 2.67107300 -1.04147200

H -4.50612100 1.30800800 -0.12102400

H -3.89067600 2.74373800 0.71670000

C 3.12768900 -0.79526100 -0.00683400

C 3.76464800 -1.09924000 1.20897700

C 3.39392700 -1.50047700 -1.19318500

C 4.71508600 -2.12316800 1.20047000

C 4.35806400 -2.50866100 -1.14970200

C 5.01659800 -2.81850000 0.03511200

H 5.21768600 -2.38012800 2.12712500

H 4.58786400 -3.05852800 -2.05656200

H 5.75793300 -3.60973600 0.05254600

C -3.12770000 -0.79528600 -0.00698000

C -3.39374400 -1.50027600 -1.19351700

C -3.76483600 -1.09955500 1.20866500

C -4.35786800 -2.50848100 -1.15039600

C -4.71527200 -2.12349000 1.19979500

C -5.01659000 -2.81858100 0.03425000

H -4.58752300 -3.05815700 -2.05740800

H -5.21800300 -2.38065000 2.12632300

H -5.75791800 -3.60983100 0.05140100

C -2.67012700 -1.17580300 -2.47682000

H -2.86711100 -0.15493100 -2.81935800

H -1.58405300 -1.27001400 -2.36462500

H -2.97467300 -1.85179500 -3.27616600

C -3.42436500 -0.37875100 2.48978200

H -2.35002800 -0.40835300 2.69291600

H -3.72791800 0.67336800 2.47184200

H -3.93151700 -0.84171900 3.33654700

C 2.67048900 -1.17628400 -2.47666500

H 1.58440900 -1.27061500 -2.36465100

H 2.86741600 -0.15544400 -2.81932900

H 2.97525200 -1.85236100 -3.27585600

C 3.42397700 -0.37813600 2.48987300

H 3.72734900 0.67403000 2.47165100

H 2.34963600 -0.40784800 2.69299100

H 3.93115900 -0.84078100 3.33679600

H -0.00142600 -1.46076300 1.59134100

Fe 0.00023000 -0.35602800 0.39709100

**1/2Fe(0)**

**1/2Fe(0)-1**

C -1.20038500 2.47476700 -0.00726300

C -1.21535600 3.86892200 -0.00597700

C 0.00013900 4.56144000 -0.00496600

C 1.21556600 3.86887800 -0.00594700

C 1.20056100 2.47469800 -0.00722700

N 0.00011100 1.81608700 -0.00722000

H 0.00016500 5.64582600 -0.00391400

H -2.14917800 4.41790500 -0.00557200

H 2.14942400 4.41780000 -0.00554500

C -2.31147000 1.54773600 -0.00674900

C 2.31136200 1.54751500 -0.00663500

N 1.95920200 0.26336800 -0.01140200

N -1.95974600 0.26345800 -0.01145200

C 3.74336900 2.00434800 0.00236100

H 4.29334700 1.60528300 -0.85445300

H 3.82027200 3.09044200 -0.02576600

H 4.26817900 1.65344900 0.89573200

C -3.74338200 2.00485600 0.00212600

H -3.82012400 3.09092400 -0.02731000

H -4.29366700 1.60481100 -0.85402600

H -4.26797800 1.65515000 0.89610400

C 2.98691900 -0.73317400 0.00314500

C 3.45431200 -1.22393800 1.23488100

C 3.46692900 -1.24581100 -1.21477100

C 4.43945500 -2.21407600 1.22605900

C 4.45234400 -2.23521900 -1.17831300

C 4.94328000 -2.71499200 0.03083000

H 4.80794300 -2.60045700 2.17200000

H 4.83077500 -2.63797700 -2.11342100

H 5.70718200 -3.48592700 0.04171300

C -2.98737500 -0.73315300 0.00301000

C -3.46677000 -1.24624800 -1.21495100

C -3.45501600 -1.22377800 1.23470800

C -4.45209900 -2.23574100 -1.17860000

C -4.44006100 -2.21401000 1.22578000

C -4.94346200 -2.71521800 0.03049000

H -4.83010500 -2.63881800 -2.11374200

H -4.80877500 -2.60026400 2.17168400

H -5.70731200 -3.48620600 0.04129300

C -2.90790500 -0.76400300 -2.52999400

H -3.04174600 0.31261500 -2.67291000

H -1.83229200 -0.95712200 -2.59004700

H -3.38865200 -1.27255400 -3.36792800

C -2.88742700 -0.71622000 2.53688400

H -1.80823600 -0.88897100 2.58777200

H -3.03868600 0.35945700 2.66962900

H -3.34912000 -1.22279600 3.38660000

C 2.90875200 -0.76311200 -2.52994500

H 1.83316500 -0.95610200 -2.59066300

H 3.04274600 0.31354100 -2.67244700

H 3.38991900 -1.27141500 -3.36779000

C 2.88666800 -0.71635600 2.53702700

H 3.03864300 0.35919300 2.67005000

H 1.80736000 -0.88834000 2.58764200

H 3.34782800 -1.22342300 3.38674000

Fe -0.00065000 -0.09731900 -0.02753600

C 0.00247800 -2.10815200 -0.05484700

H 0.00582300 -2.45461000 0.99214600

H -0.88562300 -2.55749500 -0.51469900

H 0.89011100 -2.55377000 -0.51910600

**1/2Fe(0)-2**

C -1.19110600 2.46133800 -0.18117800

C -1.21238600 3.83412000 -0.38899200

C -0.00277700 4.53595500 -0.47481600

C 1.20384700 3.84431100 -0.37969000

C 1.19986100 2.46344300 -0.17331900

N 0.00197100 1.80316600 -0.02909800

H -0.00479000 5.60704500 -0.64077400

H -2.15576700 4.35671600 -0.49896500

H 2.13994100 4.38011300 -0.48312400

C -2.31899900 1.56485900 -0.16227700

C 2.31371500 1.56375600 -0.14406200

N 1.96941500 0.28128500 -0.01914200

N -1.99271900 0.28785800 -0.04411000

C 3.73811000 2.02160700 -0.29714500

H 3.81615300 3.10811900 -0.29200300

H 4.37024400 1.63824800 0.50727900

H 4.17420600 1.66002900 -1.23396400

C -3.72616800 2.08275600 -0.30291800

H -3.98132800 2.75487500 0.52210400

H -3.84519600 2.65196200 -1.22956500

H -4.45187900 1.27189000 -0.31396300

C 2.99548500 -0.71251900 -0.12118800

C 3.68797300 -1.16657300 1.01788200

C 3.27046100 -1.24959400 -1.39590100

C 4.64657400 -2.17150100 0.85675000

C 4.23809900 -2.25033700 -1.50923700

C 4.92295900 -2.71457200 -0.39224100

H 5.18330300 -2.52930500 1.73062700

H 4.45094900 -2.67040100 -2.48804500

H 5.66808000 -3.49715200 -0.49443700

C -3.00443300 -0.72032700 -0.14412400

C -3.23867100 -1.29628800 -1.40948300

C -3.71422100 -1.15403000 0.99127200

C -4.17542300 -2.32680800 -1.51333800

C -4.64008100 -2.19069600 0.84013800

C -4.86967100 -2.78001900 -0.39726100

H -4.35760400 -2.77814900 -2.48429300

H -5.18832800 -2.53539600 1.71209900

H -5.58846200 -3.58767300 -0.49213000

C -2.51039700 -0.79834700 -2.63314000

H -2.82458700 0.21505000 -2.90498200

H -1.43119600 -0.75312400 -2.46911900

H -2.70401100 -1.44415400 -3.49178400

C -3.52692500 -0.49922600 2.33724100

H -2.47537600 -0.37050600 2.58971700

H -3.98004100 0.49845600 2.36206600

H -4.00146000 -1.08892400 3.12413100

C 2.53858400 -0.75395000 -2.61864800

H 1.45543100 -0.78846300 -2.47782800

H 2.78468700 0.28791300 -2.84861100

H 2.79318900 -1.35386400 -3.49458200

C 3.43920600 -0.57800100 2.38495600

H 3.77521900 0.46267500 2.44791000

H 2.38121500 -0.57379000 2.64474400

H 3.97876100 -1.13975700 3.15007100

C -0.02057800 -1.95603900 1.31348400

H -0.94790000 -2.07650300 1.86051600

H 0.87985400 -2.08694900 1.90075800

C 0.00986200 -2.05660400 -0.06253000

H 0.93765900 -2.27267000 -0.57829700

H -0.89714700 -2.26366800 -0.61782700

Fe 0.00371600 0.01097300 0.46912600

C -0.02438300 0.61570000 2.46040700

H -0.05978400 -0.15327900 3.23615400

H 0.87347500 1.22424800 2.60872600

H -0.88591100 1.28044300 2.58271400

**1/2Fe(0)-TS2/3**

C 1.18235100 2.49005100 0.13091500

C 1.21889200 3.85642400 0.36010700

C 0.00546400 4.56417700 0.44513800

C -1.19924300 3.87926600 0.35654900

C -1.20657000 2.49382000 0.13872100

N -0.00474400 1.83988900 -0.04868500

H 0.01148500 5.63459300 0.61663600

H 2.16277800 4.37250300 0.48861900

H -2.13159000 4.41906100 0.47317900

C 2.32767700 1.58736700 0.15254200

C -2.32190200 1.59757300 0.15942900

N -1.99984800 0.30194400 0.03618100

N 2.04002800 0.31463700 0.03100300

C -3.73281000 2.06666100 0.39124200

H -3.80459000 3.15372000 0.38773600

H -4.41780500 1.68665300 -0.37051800

H -4.11444800 1.71082400 1.35436000

C 3.71276900 2.13524700 0.38144400

H 3.97450100 2.86721600 -0.38773000

H 3.76994600 2.64913200 1.34549400

H 4.46340700 1.34802000 0.37493600

C -3.03576900 -0.67637600 0.14910800

C -3.80626000 -1.04612900 -0.97090100

C -3.24418400 -1.29424100 1.39855100

C -4.78355900 -2.03341000 -0.81490000

C -4.22835900 -2.27880000 1.50879100

C -4.99781400 -2.65011400 0.41201500

H -5.38314700 -2.32008300 -1.67434900

H -4.39004300 -2.75810900 2.47015900

H -5.76015700 -3.41622800 0.51265300

C 3.05412600 -0.68438500 0.17941600

C 3.15740800 -1.32980900 1.42838500

C 3.88544000 -1.05232700 -0.89593400

C 4.09913400 -2.34916300 1.58030800

C 4.81499500 -2.07742000 -0.69582100

C 4.92429800 -2.72713800 0.52743400

H 4.18247900 -2.85016100 2.54027600

H 5.46244100 -2.36552500 -1.51893700

H 5.65054300 -3.52259000 0.66019900

C 2.27703100 -0.92273400 2.58243300

H 2.47853500 0.10291800 2.90828400

H 1.21993400 -0.96082500 2.30637400

H 2.43207000 -1.57903200 3.44088400

C 3.79626000 -0.38213400 -2.24563600

H 2.90745000 -0.70221200 -2.79470200

H 3.74360100 0.70635500 -2.17134800

H 4.66731400 -0.63026300 -2.85530700

C -2.41044200 -0.90850500 2.59368800

H -1.34740900 -1.07078900 2.39513700

H -2.52014600 0.15026200 2.84785500

H -2.69111800 -1.49416800 3.47158500

C -3.59034100 -0.41737000 -2.32666600

H -3.49705100 0.66952700 -2.27543700

H -2.67430600 -0.78471800 -2.79666200

H -4.42052600 -0.65102800 -2.99665900

C 0.06338800 -1.85285900 -1.71534300

H 1.00096400 -2.13195100 -2.18673800

H -0.79224300 -2.12306300 -2.32573000

C -0.05898300 -2.05521700 -0.30050300

H -0.99849400 -2.45889900 0.06542900

H 0.81935700 -2.43458300 0.21820200

Fe -0.03870000 -0.02821400 -0.37412200

C 0.14749300 0.00248900 -2.60749700

H 0.13130500 -0.55588100 -3.54238800

H -0.72973300 0.65431600 -2.60581100

H 1.04990900 0.61360300 -2.59608200

**1/2Fe(0)- 3**

C -1.24781500 2.69031100 0.09812500

C -1.25820100 4.09303000 0.18150700

C -0.05869700 4.79132500 0.21575300

C 1.17014700 4.10373900 0.16531200

C 1.14155100 2.71899400 0.08490900

N -0.03456800 2.04565600 0.05676500

H -0.06765400 5.87375100 0.28089400

H -2.19578400 4.63501300 0.22043100

H 2.10718800 4.64666200 0.18952300

C -2.34337100 1.77021200 0.04386600

C 2.28420400 1.81004800 0.02068800

N 1.97622600 0.53532400 -0.04805100

N -1.98621100 0.47537900 -0.04283800

C 3.68437200 2.35691400 0.03300500

H 3.82452300 3.06900800 -0.78545300

H 3.87809300 2.89994300 0.96321900

H 4.42918900 1.57022500 -0.06505600

C -3.77900500 2.21416900 0.06685200

H -3.86362300 3.29858300 0.13278000

H -4.31132100 1.89223500 -0.83357400

H -4.32187800 1.78568300 0.91452700

C 3.01512900 -0.45192500 -0.10166600

C 3.55418200 -0.94934000 1.09721800

C 3.43312800 -0.93720800 -1.35284000

C 4.52889800 -1.94723100 1.02007900

C 4.41198400 -1.93293600 -1.38228200

C 4.95811500 -2.43848900 -0.20755900

H 4.95010200 -2.34454300 1.93884100

H 4.74337800 -2.31786300 -2.34213900

H 5.71263800 -3.21739300 -0.24879100

C -3.01219300 -0.51829300 -0.07937200

C -3.48278800 -0.98254600 -1.32147400

C -3.50291100 -1.05312800 1.12644300

C -4.46519500 -1.97551300 -1.33600500

C -4.48369100 -2.04617200 1.06723900

C -4.96806600 -2.50517000 -0.15272900

H -4.83374700 -2.33996300 -2.29072300

H -4.86654900 -2.46632400 1.99302200

H -5.72861100 -3.27913500 -0.18125300

C -2.92524200 -0.43370100 -2.61038700

H -3.08823100 0.64411800 -2.70710600

H -1.84415200 -0.59165400 -2.66766900

H -3.38626400 -0.91907800 -3.47305000

C -2.97722200 -0.57389100 2.45678800

H -1.88731500 -0.64653800 2.50249900

H -3.22661500 0.47484300 2.64805300

H -3.39166700 -1.16589600 3.27529000

C 2.84931100 -0.39113800 -2.63161400

H 1.75975400 -0.48141700 -2.64393000

H 3.08037000 0.67053400 -2.76719500

H 3.24118500 -0.92709200 -3.49791400

C 3.10412200 -0.41675000 2.43540500

H 3.45996100 0.60465400 2.60930400

H 2.01471400 -0.38919000 2.51449600

H 3.48586200 -1.03722100 3.24811800

C -0.01810400 -1.88433200 -0.35623300

H -0.95145900 -2.21021000 -0.83384600

H 0.78749400 -2.12037200 -1.07114700

C 0.19513500 -2.73081700 0.90940700

H -0.61428200 -2.53854000 1.62560100

H 1.12240100 -2.43696500 1.41695800

C 0.25412700 -4.24293700 0.64307600

H -0.67067300 -4.59229700 0.17282300

H 1.07944400 -4.48881200 -0.03298800

H 0.39697500 -4.81743600 1.56612400

Fe -0.03396100 0.11710900 -0.08972600

**1/2Fe(0)- 4**

C 1.19748800 2.61239300 -0.30122500

C 1.20174000 3.97721900 -0.62829000

C 0.00302100 4.64857000 -0.81648100

C -1.21153800 3.94800100 -0.69387700

C -1.17905000 2.60367400 -0.35751000

N -0.00132000 1.95721800 -0.13598200

H 0.00037700 5.70153800 -1.07431200

H 2.14197700 4.50327100 -0.74816800

H -2.15335400 4.45232700 -0.87302100

C 2.32504200 1.73992300 -0.17921800

C -2.33513300 1.71399500 -0.26698800

N -2.06802800 0.47511500 0.04929200

N 2.02248200 0.46735200 0.09944000

C -3.70966800 2.24275900 -0.58458200

H -3.93504000 3.11848300 0.02996500

H -3.77264800 2.56091200 -1.62954200

H -4.47964900 1.49394300 -0.41159400

C 3.72260200 2.24105100 -0.43652800

H 3.93304500 2.32266200 -1.50932200

H 3.87090500 3.23344800 -0.00430400

H 4.47170000 1.57566800 -0.01015800

C -3.10569000 -0.51278200 -0.01938300

C -3.36430800 -1.12611200 -1.26040600

C -3.82755200 -0.87614600 1.13229200

C -4.31414400 -2.14905500 -1.31387500

C -4.77430200 -1.89816500 1.02938300

C -5.01065600 -2.54409800 -0.17858100

H -4.50787800 -2.63705600 -2.26459800

H -5.33432200 -2.18618000 1.91423200

H -5.74129700 -3.34442100 -0.23612600

C 3.05970300 -0.51466200 -0.01916700

C 3.81203700 -0.93053900 1.09366900

C 3.31159800 -1.06553500 -1.29606900

C 4.76229800 -1.94390500 0.92373700

C 4.26450300 -2.07644700 -1.41887200

C 4.98211300 -2.52739200 -0.31538400

H 5.34157100 -2.26847500 1.78428500

H 4.44755300 -2.51222400 -2.39696800

H 5.71692600 -3.31852500 -0.42637300

C 3.68176400 -0.28570700 2.45421700

H 4.65669100 0.06791500 2.80443200

H 3.00550300 0.56679500 2.44498100

H 3.31945600 -0.99659200 3.20325000

C 2.60206500 -0.55186800 -2.52615100

H 1.54029100 -0.37941100 -2.34606300

H 3.02598400 0.40089300 -2.86315200

H 2.69798400 -1.25828900 -3.35321300

C -3.63733200 -0.15587900 2.44382500

H -2.62903100 -0.27979900 2.84036900

H -3.80812600 0.92081400 2.34511500

H -4.33577500 -0.53047600 3.19434200

C -2.67901600 -0.66706500 -2.52496200

H -3.14191100 0.24513400 -2.91942300

H -1.62299200 -0.44542600 -2.36701500

H -2.75208000 -1.42754400 -3.30456100

C 0.03133200 -1.92601400 0.49410800

H 0.88666700 -2.30105000 1.07331800

H -0.86584100 -2.27265400 1.02979500

C 0.05196900 -2.64023000 -0.86656600

H 0.95700700 -2.37673900 -1.42199100

H -0.79174500 -2.31947000 -1.48719800

C -0.00355000 -4.17221600 -0.74826500

H 0.84728300 -4.55021600 -0.17215800

H -0.91603300 -4.49372600 -0.23548800

H 0.01640100 -4.66044900 -1.73034000

C 0.12687200 -0.25942500 2.64599400

H 1.11278800 -0.66443900 2.81493900

H -0.68701200 -0.94204700 2.85039700

C -0.08426800 1.08347700 2.50214500

H -1.07323800 1.51984200 2.57581900

H 0.73927100 1.78884200 2.51261700

Fe 0.02873100 0.13338500 0.47984700

**1/2Fe(0)-TS4/5**

C 1.23140700 2.55638000 -0.30320000

C 1.26945600 3.92495400 -0.53384900

C 0.07525800 4.64983800 -0.62545400

C -1.13717200 3.97983600 -0.47991900

C -1.15971200 2.60353900 -0.25184800

N 0.02854100 1.89188100 -0.16777100

H 0.09384600 5.71831000 -0.80667500

H 2.22210000 4.42992600 -0.64565300

H -2.06739100 4.53130400 -0.55036500

C 2.36396900 1.67920700 -0.21497100

C -2.30396900 1.76401700 -0.11948800

N -2.01870900 0.47702600 0.09710000

N 2.06732100 0.41009000 0.01928900

C -3.70674500 2.28763100 -0.28187300

H -3.76201500 3.35522900 -0.06849200

H -4.07832300 2.13957300 -1.30219500

H -4.40481400 1.77816900 0.38399500

C 3.76028800 2.20872300 -0.42600800

H 3.89388000 2.56685600 -1.45191100

H 3.96432800 3.05437400 0.23637900

H 4.51476100 1.44710300 -0.23999600

C -3.10365500 -0.45722600 0.04704700

C -3.49764900 -0.98160200 -1.20246100

C -3.76365600 -0.86382700 1.22609500

C -4.50336700 -1.95206200 -1.24274200

C -4.77020400 -1.82875100 1.13780600

C -5.13399900 -2.38435900 -0.08342300

H -4.79723000 -2.36506300 -2.20392200

H -5.28000900 -2.14059100 2.04505600

H -5.91314700 -3.13851000 -0.13144400

C 3.12609800 -0.55689000 -0.00791600

C 3.83026000 -0.90333200 1.16464600

C 3.45963800 -1.16027100 -1.24013300

C 4.78226000 -1.92573300 1.09717800

C 4.41304000 -2.18123900 -1.25841600

C 5.05986200 -2.58141600 -0.09578300

H 5.32369000 -2.19704700 1.99913100

H 4.65571400 -2.65753600 -2.20420300

H 5.79577600 -3.37866900 -0.12399400

C 3.65088800 -0.15849300 2.46756100

H 4.53899600 -0.27590800 3.09234800

H 3.49421700 0.90985900 2.31002500

H 2.79886300 -0.51745000 3.04842100

C 2.86343600 -0.67909600 -2.54220000

H 1.84033400 -0.32530700 -2.42597300

H 3.44509800 0.15656900 -2.94853500

H 2.87306700 -1.47091600 -3.29468800

C -3.43575900 -0.25815900 2.56924400

H -2.52482700 -0.68035300 2.99936000

H -3.27980800 0.82042000 2.50573100

H -4.24554600 -0.44067900 3.27909300

C -2.89651400 -0.49240700 -2.49925000

H -3.49000100 0.32651900 -2.92201400

H -1.88373100 -0.11400400 -2.36948600

H -2.87591400 -1.28851100 -3.24717000

C -0.27957600 -2.07218400 0.52507000

H 0.21230600 -2.90971900 1.01926500

H -1.35297400 -2.20665100 0.64789400

C 0.10531000 -2.15398200 -0.95996900

H 1.18700500 -2.24035600 -1.05319500

H -0.18672100 -1.25560600 -1.52474700

C -0.55455300 -3.36831100 -1.63682100

H -0.24776800 -4.29741500 -1.14693100

H -1.64420700 -3.31063900 -1.58670700

H -0.26525600 -3.43666700 -2.69063100

C 0.18324200 -1.04746800 2.20488800

H 1.15386000 -1.50620200 2.34978300

H -0.60158800 -1.62896100 2.67946000

C 0.11235600 0.38527100 2.31029900

H -0.79109600 0.82724000 2.71842900

H 1.01657000 0.92715400 2.56765400

Fe -0.00436700 0.12098600 0.34430400

**1/2Fe(0)-5**

C -1.59245500 2.86757200 0.36872700

C -1.76197500 4.23649900 0.62943100

C -0.64693500 5.05680600 0.74612400

C 0.64950500 4.52303300 0.60290100

C 0.77576200 3.16466600 0.34712100

N -0.31825800 2.37188700 0.23826500

H -0.77381700 6.11469100 0.94805800

H -2.75753700 4.65211800 0.73928600

H 1.52042600 5.16113600 0.69189100

C -2.58732000 1.85340400 0.20485800

C 2.00889100 2.40285800 0.16349100

N 1.83841800 1.12023900 -0.06365400

N -2.10014400 0.62525300 -0.05296500

C 3.34215700 3.09300800 0.23962500

H 3.37909700 3.93264800 -0.46026100

H 3.50646700 3.50563400 1.24003900

H 4.16392700 2.41797800 0.01038700

C -4.05195600 2.18325100 0.30176700

H -4.29184100 2.65741400 1.25932700

H -4.35357100 2.88454100 -0.48447100

H -4.67172000 1.29361000 0.20564400

C 2.97584000 0.26581300 -0.24171400

C 3.58871800 -0.30835700 0.88533100

C 3.41853800 -0.01987700 -1.54481000

C 4.66461600 -1.17634400 0.68253800

C 4.49939100 -0.89067700 -1.70007200

C 5.12054000 -1.46811700 -0.59801900

H 5.14460400 -1.63086000 1.54419400

H 4.85152900 -1.12035700 -2.70136100

H 5.95486600 -2.14800000 -0.73728000

C -2.99877800 -0.47298600 -0.21461400

C -3.40413600 -0.85008000 -1.50826300

C -3.42877600 -1.19181200 0.91656400

C -4.24910300 -1.95322800 -1.64989800

C -4.27192700 -2.29014800 0.73068600

C -4.68296100 -2.67240100 -0.54153300

H -4.56594200 -2.25124500 -2.64533200

H -4.60609600 -2.85227400 1.59819900

H -5.33572100 -3.53025600 -0.66901200

C -2.92986100 -0.08413800 -2.71682400

H -3.23707600 0.96561100 -2.68375900

H -1.83768200 -0.08891700 -2.78095300

H -3.32674500 -0.51980900 -3.63605300

C -2.99504100 -0.78369100 2.30225700

H -1.90869900 -0.68034000 2.36621400

H -3.41857000 0.18262600 2.59542800

H -3.31163600 -1.52063600 3.04311600

C 2.75211000 0.60459100 -2.74486100

H 1.67812800 0.39980900 -2.75653100

H 2.86686900 1.69347300 -2.75729100

H 3.17865400 0.21743900 -3.67195200

C 3.10769100 0.00535800 2.28073300

H 3.35120400 1.03154600 2.57704000

H 2.02365100 -0.09989200 2.36815500

H 3.57088600 -0.66208100 3.00958500

C 0.11660500 -1.45234100 -0.64560400

H -0.77331900 -1.81767800 -1.17414900

H 0.94809100 -1.51828900 -1.36615200

C 0.40841700 -2.40743600 0.52359100

H -0.42171400 -2.37889700 1.24280300

H 1.29812000 -2.07863800 1.07732700

C 0.62670600 -3.87041300 0.10109200

H -0.25356600 -4.21325200 -0.45848300

H 1.46787600 -3.91577500 -0.60328400

C 0.88995400 -4.82700500 1.26934100

H 1.76737300 -4.48104700 1.83106300

H 0.04763800 -4.78115000 1.97168300

C 1.10724800 -6.27823600 0.83270100

H 1.28898700 -6.93644100 1.68805800

H 0.23449700 -6.66674400 0.29786900

H 1.96692100 -6.36672600 0.16047700

Fe -0.11590200 0.49115100 -0.14873300

**1/2Fe(0)-6**

C -1.05787400 2.68836000 -0.23919500

C -1.01229400 4.07392500 -0.44785200

C 0.21138000 4.71764600 -0.55496600

C 1.39611800 3.96321500 -0.47561800

C 1.31355400 2.59684300 -0.25882300

N 0.10984000 1.97307100 -0.11032600

H 0.25645000 5.78848800 -0.71731200

H -1.93429900 4.63807600 -0.53224500

H 2.35835800 4.44664300 -0.59359900

C -2.22596200 1.86276400 -0.19167600

C 2.44607500 1.67345600 -0.22079600

N 2.14478600 0.41983600 -0.02017500

N -1.98697600 0.56537100 0.00082100

C 3.84032300 2.19871300 -0.44952400

H 3.91196300 2.69631300 -1.42078900

H 4.10274000 2.94101300 0.30987400

H 4.58098200 1.40288500 -0.41934700

C -3.59231600 2.46334000 -0.40591700

H -3.82184700 3.21025800 0.36111500

H -3.65551300 2.97086400 -1.37393600

H -4.37390300 1.70676500 -0.37752900

C 3.17523100 -0.57664900 -0.07438100

C 3.90386300 -0.92509800 1.07807800

C 3.41432700 -1.21973400 -1.30476600

C 4.84844600 -1.95141300 0.98193800

C 4.36700200 -2.23928200 -1.35237200

C 5.07669100 -2.61392100 -0.21765300

H 5.41420700 -2.22756600 1.86694600

H 4.55078800 -2.74328600 -2.29654600

H 5.81001700 -3.41218900 -0.26980300

C -3.08751500 -0.34886900 -0.06680600

C -3.39431400 -0.94898900 -1.30435400

C -3.84406400 -0.64939100 1.08290900

C -4.41128700 -1.90499700 -1.35395800

C -4.85418400 -1.61066800 0.98701700

C -5.13049300 -2.24974200 -0.21572600

H -4.64074600 -2.38104700 -2.30294500

H -5.43429400 -1.85371000 1.87266400

H -5.91200600 -3.00102500 -0.26865800

C -2.68224800 -0.53869300 -2.56975200

H -2.99393800 0.46034300 -2.89532900

H -1.60089000 -0.50305000 -2.43765500

H -2.90524000 -1.23107400 -3.38404700

C -3.62816400 0.07897100 2.38743000

H -2.61157100 -0.02796100 2.76597100

H -3.81231200 1.15317900 2.28411300

H -4.30891300 -0.29604500 3.15423900

C 2.67980300 -0.80565300 -2.55523200

H 1.59791300 -0.85463000 -2.42011700

H 2.91970100 0.22250300 -2.84665900

H 2.94511300 -1.45403900 -3.39227700

C 3.71237800 -0.21093100 2.39418300

H 3.76410200 0.87596700 2.28658100

H 2.74622700 -0.43868200 2.84880200

H 4.48579200 -0.50652300 3.10557500

C 0.01005700 -1.86708100 -0.26111300

H -0.24501700 -1.74354400 -1.33036300

H 1.05940300 -2.19018200 -0.24441000

C -0.83665600 -3.01418200 0.29612200

H -1.88817100 -2.72209900 0.37516900

H -0.51349600 -3.24812600 1.31861500

C -0.74901600 -4.30408000 -0.53360700

H -1.11624400 -4.14361700 -1.55289200

H 0.28561500 -4.65520600 -0.61167200

H -1.34307200 -5.11314100 -0.09290500

C -0.01305800 -0.74477400 2.24263900

H -0.96836500 -1.23313500 2.37714000

H 0.84225400 -1.40688500 2.31221200

C 0.13137100 0.62114300 2.38274100

H 1.09728800 1.07983000 2.55352800

H -0.72184200 1.26155100 2.57660000

Fe 0.00600700 0.09764400 0.29407100

**1/2Fe(0)-TS6/7**

C -1.07185100 2.72080800 -0.13729800

C -1.06297200 4.10860800 -0.24037600

C 0.15084700 4.79573400 -0.29691700

C 1.33989000 4.06626200 -0.25065200

C 1.30011000 2.67957800 -0.14728000

N 0.10058200 1.99823000 -0.08798500

H 0.16943400 5.87644200 -0.37660800

H -1.99870000 4.65453000 -0.27691700

H 2.29499800 4.57735100 -0.29519200

C -2.23964400 1.88241200 -0.07533200

C 2.43227300 1.79561800 -0.09104000

N 2.11629700 0.51834600 0.00172600

N -1.99385700 0.58946800 0.01816100

C 3.83598400 2.33965100 -0.13852200

H 4.00570100 2.90535800 -1.05984100

H 4.01924600 3.02371900 0.69587500

H 4.57820100 1.54563600 -0.09029300

C -3.61312700 2.50362500 -0.12618100

H -4.40165500 1.75631600 -0.07688500

H -3.75716800 3.20137600 0.70435200

H -3.74785400 3.07515000 -1.04951800

C 3.16996200 -0.45083200 0.07125000

C 3.68795700 -0.82583800 1.32715900

C 3.66811100 -1.02630200 -1.11416700

C 4.64231000 -1.84509700 1.37934200

C 4.62352800 -2.04147500 -1.01388700

C 5.09860400 -2.46452500 0.22167700

H 5.03520400 -2.14825500 2.34579600

H 5.00129700 -2.49921600 -1.92392400

H 5.83235700 -3.26220600 0.28133700

C -3.12255700 -0.29623800 0.07314700

C -3.67305400 -0.79860900 -1.12147900

C -3.68186200 -0.63784600 1.31991800

C -4.73186900 -1.70774800 -1.04235700

C -4.74079300 -1.54877500 1.35317900

C -5.25683700 -2.09641900 0.18412500

H -5.15075500 -2.10835000 -1.96120200

H -5.16762600 -1.82417400 2.31334500

H -6.07436800 -2.80897400 0.22833700

C -3.19050600 -0.32459600 -2.47051000

H -3.63558200 0.64398800 -2.72671300

H -2.11014000 -0.19165000 -2.49904800

H -3.47337400 -1.02703800 -3.25729800

C -3.20378500 0.00658100 2.59774900

H -3.60379100 -0.51388100 3.47020600

H -2.11716200 0.01745400 2.67457300

H -3.53356200 1.04964400 2.66175200

C 3.26076000 -0.51862000 -2.47736100

H 3.93122500 0.28482300 -2.80588400

H 3.32092500 -1.31219300 -3.22547800

H 2.24847300 -0.11903200 -2.48735100

C 3.30332500 -0.09801500 2.59390400

H 3.95448400 0.77017100 2.75218400

H 2.27887100 0.26920800 2.56975800

H 3.41336300 -0.74530600 3.46671600

C 0.12953900 -1.52264100 -1.27099200

H -0.19430400 -0.89627800 -2.11302000

H 1.17542200 -1.80187700 -1.38557600

C -0.72599500 -2.67439800 -1.04878100

H -1.75682300 -2.57890600 -1.38812900

H -0.94054400 -2.66366000 0.25956000

C -0.16654200 -4.07296000 -1.23478900

H -0.02439600 -4.29155600 -2.29983600

H 0.80989800 -4.17474000 -0.75174600

H -0.83175100 -4.84112200 -0.82694600

C -0.71071700 -2.45429700 1.56151100

H -1.73167100 -2.36966500 1.92506500

H -0.27744900 -3.43391300 1.77032900

C 0.14943400 -1.30154500 1.61845800

H 1.19737500 -1.54716300 1.76089300

H -0.17903400 -0.52024900 2.31528200

Fe 0.08757400 0.12051200 0.04376000

**1/2Fe(0)- 7**

C -1.25796700 2.52191400 -0.11554800

C -1.30736500 3.90526500 -0.23263900

C -0.11549600 4.63567000 -0.31209600

C 1.10179100 3.95660600 -0.31194400

C 1.12169200 2.56650800 -0.19406200

N -0.05329600 1.87151000 -0.03627900

H -0.14043300 5.71512800 -0.40627800

H -2.26289200 4.41464800 -0.28235500

H 2.02926600 4.50761500 -0.41447100

C -2.38369100 1.62056200 -0.15327500

C 2.26292900 1.70372100 -0.28334600

N 1.97079400 0.40692500 -0.23753500

N -2.05870000 0.34203300 -0.15401700

C 3.65520100 2.25660900 -0.43773900

H 4.32983200 1.52346500 -0.87815100

H 3.66203500 3.14343400 -1.07400100

H 4.07728800 2.54877500 0.53030200

C -3.79163900 2.15099600 -0.24309000

H -4.00967500 2.82887400 0.58690600

H -3.94012400 2.71652700 -1.16832800

H -4.52400600 1.34655700 -0.22577700

C 3.02383900 -0.54313800 -0.42236400

C 3.84774900 -0.93193000 0.65085900

C 3.20268600 -1.09592300 -1.70746400

C 4.83122400 -1.89857500 0.42116000

C 4.19711200 -2.05933700 -1.89102100

C 5.00597400 -2.46595000 -0.83539300

H 5.46487400 -2.20969500 1.24687700

H 4.33740400 -2.49150300 -2.87764900

H 5.77050400 -3.22023300 -0.99244800

C -3.07413000 -0.64709300 -0.34820900

C -3.31584800 -1.09805300 -1.66228000

C -3.78433900 -1.18577200 0.74171300

C -4.25507300 -2.11254400 -1.86086200

C -4.71328500 -2.20072100 0.49590600

C -4.94724700 -2.66921100 -0.79155700

H -4.44192000 -2.46786400 -2.87010700

H -5.26119700 -2.62438300 1.33262100

H -5.66820600 -3.46253600 -0.96127100

C -2.59906800 -0.48142400 -2.83834200

H -2.93503500 0.54492300 -3.02159300

H -1.52028500 -0.42772600 -2.67521700

H -2.78235900 -1.05395700 -3.74965100

C -3.59080000 -0.65744500 2.14041900

H -4.04029400 0.33513700 2.25858400

H -4.06053200 -1.31555300 2.87403600

H -2.53752900 -0.55342000 2.39540200

C 2.37155900 -0.62553000 -2.87521400

H 1.30915500 -0.58869300 -2.62713800

H 2.65252300 0.38806300 -3.18202200

H 2.50597200 -1.27956900 -3.73920600

C 3.70253900 -0.31521400 2.01985800

H 4.23404300 0.64104500 2.08386900

H 2.66033100 -0.12017700 2.26907600

H 4.12431200 -0.96806500 2.78691200

C -0.05009000 -1.95708000 -0.39134600

H -0.95156700 -1.95942700 -0.99027800

H 0.86715000 -2.19677200 -0.91921300

C -0.10221300 -2.11143900 0.97776700

H -1.07933800 -2.15305900 1.45043300

H -0.74248200 -1.09780300 3.64947700

C 1.00958100 -2.77943400 1.74676200

H 0.77513300 -3.84703000 1.85376300

H 1.96265500 -2.71306500 1.22145800

H 1.13993700 -2.38413400 2.75229400

C -0.04780200 -0.25144500 3.67379100

H -0.31624600 0.34459900 4.55851500

H 0.94405500 -0.66425400 3.87820400

C -0.07366500 0.59600700 2.40233300

H 0.73297700 1.33918200 2.45743300

H -0.99837100 1.18741800 2.38464600

Fe 0.00294200 0.03733200 0.35778800

**1/2Fe(0)- 8**

C -1.17222700 2.56372500 0.01841700

C -1.21328700 3.95004900 0.05848600

C 0.00951300 4.64957300 0.08592900

C 1.21526400 3.96131000 0.07148400

C 1.21743200 2.55663700 0.02945400

N 0.00981600 1.90072400 0.00604900

H 0.00898300 5.73350600 0.11923100

H -2.15517600 4.48507400 0.07014700

H 2.14781600 4.51283500 0.09531100

C -2.30640300 1.64268100 -0.01262500

C 2.32078300 1.64457300 0.00717700

N 1.97529800 0.34406600 -0.03670100

N -1.98646000 0.36900900 -0.04172500

C 3.75245800 2.10143700 0.02213700

H 3.82760800 3.18851800 0.03183300

H 4.28889400 1.72283400 0.89739000

H 4.29766300 1.73695600 -0.85371900

C -3.71161000 2.17627100 -0.00963600

H -3.90884100 2.73612700 0.90990500

H -3.85999000 2.87004300 -0.84214900

H -4.44880000 1.38043500 -0.08998500

C 3.01005400 -0.64089000 -0.03909400

C 3.49774900 -1.13664500 1.18444100

C 3.49122800 -1.13794400 -1.26447500

C 4.48785900 -2.12179900 1.16000300

C 4.48264500 -2.12184100 -1.24430200

C 4.98367400 -2.61157300 -0.04320800

H 4.86843500 -2.51173400 2.09985700

H 4.85942500 -2.51134600 -2.18584400

H 5.75133500 -3.37902500 -0.04484800

C -3.01609800 -0.62861300 -0.06148100

C -3.43153800 -1.15722100 -1.29587900

C -3.54941900 -1.09180700 1.15340900

C -4.40222500 -2.16114400 -1.29202500

C -4.51583000 -2.09977300 1.10979600

C -4.94260500 -2.63331100 -0.10078500

H -4.73146400 -2.57949400 -2.23855200

H -4.93231000 -2.47109800 2.04153000

H -5.69054500 -3.41949900 -0.11596200

C -2.85341400 -0.64681700 -2.59184700

H -3.10002000 0.40608100 -2.76412100

H -1.76260500 -0.72066300 -2.59890500

H -3.23540800 -1.21791600 -3.43992600

C -3.10308000 -0.51235600 2.47331000

H -2.01497000 -0.43766400 2.53556800

H -3.49965800 0.49686000 2.63084700

H -3.44783400 -1.12994100 3.30461500

C 2.93449700 -0.63463900 -2.57226100

H 1.85630800 -0.81075500 -2.63219100

H 3.08136300 0.44230400 -2.69938000

H 3.40870500 -1.13764700 -3.41755100

C 2.95677700 -0.62591300 2.49682300

H 3.20273500 0.42747400 2.66602100

H 1.86647100 -0.69879900 2.53109500

H 3.36236100 -1.19752100 3.33408700

C 0.03049100 -2.04052000 -0.26652500

H -0.76044700 -2.30962100 -0.98445800

H 0.97345300 -2.37656500 -0.71410200

C -0.19891400 -2.83189400 1.03271100

H -1.14592100 -2.57520000 1.51889600

H 0.59979100 -2.65545700 1.76170700

H -0.22696100 -3.91725600 0.86118300

Fe 0.02640000 -0.03260700 -0.07451900

**1/2Fe(0)- TS3/9**

C 1.14556200 2.57139800 0.00522100

C 1.14749500 3.96442600 0.00843600

C -0.06356900 4.65774900 -0.03115500

C -1.26483600 3.94119100 -0.04224200

C -1.23424900 2.55092100 -0.04365100

N -0.03802900 1.87540300 -0.05956800

H -0.07360400 5.74171900 -0.03210000

H 2.08506500 4.50734600 0.04545200

H -2.21312300 4.46640600 -0.04231000

C 2.28214900 1.69477700 0.08963100

C -2.36216200 1.65359900 0.00616300

N -2.03498600 0.37476900 0.04819300

N 1.97463600 0.40530600 0.09166500

C -3.77053400 2.18435900 0.02013200

H -3.88799400 2.96317100 0.77855200

H -4.03070000 2.63440000 -0.94400300

H -4.49480200 1.39876100 0.22762900

C 3.67790600 2.25054400 0.18755300

H 4.00111900 2.68494900 -0.76497600

H 3.72910700 3.04633900 0.93537100

H 4.39940200 1.48343800 0.46322400

C -3.06814700 -0.61175600 0.11143500

C -3.69126400 -1.05783400 -1.06955600

C -3.41445700 -1.15394900 1.36464000

C -4.65017900 -2.07084800 -0.97461300

C -4.38169000 -2.15994000 1.41265200

C -4.99448800 -2.62344200 0.25309600

H -5.13089300 -2.42696100 -1.88138100

H -4.65462400 -2.58375800 2.37476500

H -5.73829900 -3.41202600 0.30715900

C 3.03340600 -0.55270400 0.16739400

C 3.31776100 -1.15683900 1.40797800

C 3.75647300 -0.89951200 -0.98944900

C 4.31860100 -2.12907100 1.46410200

C 4.74848100 -1.87941300 -0.88753500

C 5.02884500 -2.49636000 0.32575400

H 4.54272000 -2.60078100 2.41652000

H 5.30463900 -2.15961100 -1.77774700

H 5.79943400 -3.25843900 0.38549600

C 2.58436500 -0.73776100 2.65726800

H 2.80010700 0.30323300 2.91982900

H 1.50178200 -0.80960300 2.52808300

H 2.87254200 -1.36039200 3.50673700

C 3.49052300 -0.22509900 -2.31370400

H 2.43018000 -0.01176100 -2.45413100

H 4.02377500 0.72922200 -2.38963000

H 3.83041800 -0.84931800 -3.14292600

C -2.78417300 -0.63373000 2.63270900

H -1.69363900 -0.62711100 2.56768000

H -3.09059900 0.39694600 2.84095700

H -3.07342200 -1.24356900 3.49090100

C -3.36422700 -0.44564500 -2.41057700

H -3.91795200 0.48709600 -2.56840500

H -2.30429400 -0.20414900 -2.50157800

H -3.63713800 -1.12194900 -3.22358300

C -0.01469800 -2.02019400 0.39832400

H 0.93855700 -2.39054400 0.76548700

H -0.86741100 -2.23815800 1.03455200

C -0.21657300 -1.95772400 -0.99750500

H -0.06690900 -0.41816500 -1.55162900

H -1.24745700 -2.03364100 -1.33046100

C 0.75655000 -2.57948200 -1.97765300

H 1.78956900 -2.48143000 -1.64599900

H 0.53823800 -3.65116000 -2.05357800

H 0.67076000 -2.15046900 -2.97984800

Fe -0.02012000 0.00521800 -0.05827800

**1/2Fe(0)-9**

C 1.14655800 2.57287200 -0.02507900

C 1.15212200 3.96407300 -0.06984400

C -0.06055000 4.65663200 -0.12341000

C -1.26042100 3.94108200 -0.11955800

C -1.23034400 2.55008800 -0.07279700

N -0.03490700 1.87836800 -0.03862500

H -0.07008700 5.73999900 -0.16112300

H 2.09060200 4.50642200 -0.06495500

H -2.20902600 4.46492700 -0.15061900

C 2.28810900 1.69620000 0.04660200

C -2.35823500 1.65496900 -0.03051500

N -2.03266600 0.37457400 0.02441400

N 1.98357700 0.41006500 0.07135500

C -3.76489800 2.19059900 -0.04325100

H -3.92146300 2.90577400 0.76999100

H -3.97369200 2.72000100 -0.97882600

H -4.50041200 1.39547200 0.06148000

C 3.68510500 2.25571500 0.08431200

H 3.76744000 3.05399800 0.82684900

H 4.42065900 1.49109100 0.32694900

H 3.96184100 2.68851100 -0.88340200

C -3.07546600 -0.60274200 0.09100900

C -3.62414100 -1.11718500 -1.10026000

C -3.50749300 -1.06646300 1.34813900

C -4.59257100 -2.12015800 -1.00861600

C -4.47718100 -2.07182700 1.39211600

C -5.01576900 -2.60191700 0.22530800

H -5.01675300 -2.52714000 -1.92209500

H -4.81270300 -2.43918100 2.35778600

H -5.76359100 -3.38687600 0.27722900

C 3.04891400 -0.54303500 0.13276800

C 3.44493200 -1.05071800 1.38511900

C 3.66678600 -0.97695600 -1.05505200

C 4.44780000 -2.02281500 1.42515500

C 4.66658200 -1.94965300 -0.96787900

C 5.05428800 -2.47682000 0.25896900

H 4.75582800 -2.42392400 2.38650200

H 5.14349800 -2.29674400 -1.88011600

H 5.82823900 -3.23632000 0.30663200

C 2.83298400 -0.52832200 2.66153500

H 3.15478300 0.49808800 2.86902700

H 1.74227300 -0.50675700 2.60936900

H 3.12533000 -1.14290000 3.51541000

C 3.27665200 -0.39717700 -2.39210900

H 2.19741200 -0.25669400 -2.46721100

H 3.73950200 0.58358800 -2.55154200

H 3.60460800 -1.04511600 -3.20782200

C -2.98094700 -0.46193000 2.62743000

H -1.90170500 -0.30234700 2.59424100

H -3.43418300 0.51684500 2.82151800

H -3.20800700 -1.10048900 3.48363500

C -3.19599800 -0.58436600 -2.44546100

H -3.65848300 0.38746200 -2.65349500

H -2.11578900 -0.43486600 -2.49348100

H -3.49529700 -1.26350700 -3.24665500

C 0.04749300 -1.98420700 0.72646400

H 1.04068800 -2.22726700 1.08919700

H -0.73664500 -1.94450000 1.47659400

C -0.26777800 -2.16576800 -0.59781600

H 0.00246100 -0.06158100 -1.58140700

H -1.31586100 -2.18461300 -0.87267900

C 0.65116100 -2.78500600 -1.61419800

H 1.69941800 -2.71961900 -1.32306000

H 0.40521500 -3.85039600 -1.71748200

H 0.53461800 -2.32973000 -2.60016400

Fe -0.01842000 0.00909100 -0.07118400

**1/2Fe(0)-10**

C -1.19400700 2.40081300 0.06691000

C -1.19496400 3.79911800 0.06931300

C 0.01259400 4.48737000 -0.04114600

C 1.22700900 3.78303600 -0.14191500

C 1.19397600 2.39696500 -0.12709400

N 0.00419400 1.74026900 -0.03352800

H 0.01676900 5.57142800 -0.04483100

H -2.12377400 4.35162900 0.15190800

H 2.16549000 4.31942800 -0.22067500

C -2.30304500 1.48351800 0.13747500

C 2.31921700 1.46932700 -0.16772600

N 1.98951200 0.19794800 -0.07800800

N -1.96248700 0.19514400 0.06922900

C 3.72785300 1.98056700 -0.28523500

H 3.81303000 2.68897700 -1.11344500

H 4.02750100 2.51278700 0.62353300

H 4.43558300 1.17051300 -0.45023300

C -3.72697100 1.95110800 0.24901900

H -4.24868000 1.88272600 -0.71186100

H -4.28911100 1.33504300 0.95354300

H -3.78404900 2.98720000 0.58323300

C 2.99145400 -0.82467000 -0.04376200

C 3.62286500 -1.13561600 1.17291900

C 3.26731000 -1.54488600 -1.21871500

C 4.56396000 -2.16789400 1.18460800

C 4.21913100 -2.56445500 -1.16238000

C 4.86884800 -2.87540400 0.02734300

H 5.05550200 -2.42220100 2.11918900

H 4.44301500 -3.12674700 -2.06416600

H 5.60173900 -3.67542900 0.05505900

C -2.97924900 -0.81018100 0.06272900

C -3.57151900 -1.18877000 -1.15525700

C -3.32599400 -1.44386300 1.26920000

C -4.54416500 -2.19107300 -1.13854000

C -4.30531300 -2.43887600 1.24141300

C -4.91800600 -2.80968400 0.04935100

H -5.00566300 -2.49418500 -2.07409100

H -4.58147800 -2.93359100 2.16822000

H -5.67505000 -3.58756200 0.04421500

C -3.13686800 -0.56284200 -2.45699900

H -3.35450100 0.50892200 -2.50233800

H -2.05740800 -0.66892300 -2.59913100

H -3.63957800 -1.03624600 -3.30271600

C -2.62960300 -1.08015300 2.55498500

H -1.55414600 -1.26984200 2.47498900

H -2.74566000 -0.02179500 2.80806500

H -3.01739600 -1.66772800 3.38961800

C 2.52897400 -1.24295700 -2.49654800

H 1.45337200 -1.40236600 -2.36362100

H 2.66093500 -0.20558100 -2.81900700

H 2.86891900 -1.89034200 -3.30714700

C 3.27485000 -0.39934000 2.44288900

H 3.62172700 0.63941300 2.43102700

H 2.19324100 -0.37083300 2.59994500

H 3.73059100 -0.88368400 3.30845800

H -0.00781700 -1.75509100 0.02271900

Fe -0.00583300 -0.16601500 -0.01620500

**3/2Fe(0)**

**3/2Fe(0)-1**

C -1.18882700 2.46786100 0.00001100

C -1.20111200 3.85871700 0.00001900

C 0.01540900 4.55588100 0.00001300

C 1.22939000 3.86289700 0.00000300

C 1.21099900 2.46745400 -0.00000400

N 0.01402600 1.81080000 -0.00000700

H 0.01287900 5.64001300 0.00001900

H -2.13398400 4.40960100 0.00003000

H 2.16409000 4.41043200 0.00000300

C -2.31038600 1.55250400 0.00001800

C 2.32184400 1.54714300 -0.00000500

N 1.97039500 0.26350200 -0.00000100

N -1.98869400 0.25968600 0.00001300

C 3.75475800 2.00129300 -0.00001300

H 4.29142600 1.62510500 -0.87565500

H 3.83308100 3.08755700 0.00001200

H 4.29145000 1.62506200 0.87559500

C -3.73554900 2.02890800 0.00001300

H -3.80255400 3.11571700 0.00017100

H -4.27600100 1.65690500 -0.87531200

H -4.27609500 1.65664100 0.87516400

C 2.99674700 -0.73636200 -0.00000300

C 3.47153400 -1.23534900 1.22542900

C 3.47152800 -1.23535200 -1.22543500

C 4.45474000 -2.22730200 1.20236700

C 4.45473300 -2.22730500 -1.20237700

C 4.94956400 -2.71978300 -0.00000600

H 4.82900500 -2.62135300 2.14278400

H 4.82899200 -2.62135800 -2.14279500

H 5.71113700 -3.49309400 -0.00000700

C -3.02464000 -0.72437600 0.00000300

C -3.50255600 -1.22398800 -1.22490200

C -3.50254400 -1.22402400 1.22489800

C -4.49731000 -2.20427300 -1.20237500

C -4.49729800 -2.20430800 1.20235200

C -5.00007000 -2.68921400 -0.00001600

H -4.87368000 -2.59626300 -2.14292600

H -4.87366000 -2.59632500 2.14289600

H -5.77146200 -3.45280000 -0.00002300

C -2.92955500 -0.73847500 -2.53249900

H -3.07223600 0.33662600 -2.67943000

H -1.85115800 -0.91942100 -2.57558300

H -3.39354500 -1.25274100 -3.37640700

C -2.92953400 -0.73854100 2.53250200

H -1.85113200 -0.91945800 2.57556200

H -3.07224500 0.33655000 2.67947200

H -3.39349700 -1.25285000 3.37640000

C 2.92030700 -0.72950600 -2.53530700

H 1.83862500 -0.88104300 -2.59267700

H 3.09344300 0.34218400 -2.67476100

H 3.37901300 -1.25102200 -3.37752500

C 2.92032200 -0.72950000 2.53530200

H 3.09345700 0.34219100 2.67475100

H 1.83863900 -0.88103800 2.59267900

H 3.37903200 -1.25101300 3.37751900

Fe 0.00987500 -0.12066000 -0.00000200

C 0.06699600 -2.12214400 0.00001300

H 0.61496400 -2.49440800 0.87787800

H -0.91675100 -2.60387600 0.00000100

H 0.61498900 -2.49441800 -0.87783200

**3/2Fe(0)-2**

C 1.18457800 2.37942500 -0.15159700

C 1.19938400 3.76926900 -0.21074700

C 0.00004600 4.48307700 -0.23287500

C -1.19936400 3.76927200 -0.21058900

C -1.18454300 2.37948200 -0.15141300

N -0.00001400 1.67527300 -0.11531200

H 0.00005300 5.56619400 -0.27064700

H 2.14340000 4.29995600 -0.23892000

H -2.14336700 4.29998200 -0.23868200

C 2.39629600 1.57131200 -0.15115000

C -2.39635800 1.57137000 -0.15082800

N -2.23387800 0.28754200 0.01444600

N 2.23375800 0.28741100 0.01411200

C -3.73675300 2.23523500 -0.36804700

H -3.95925400 2.94782000 0.43206500

H -3.75764800 2.79180300 -1.30911800

H -4.53907500 1.50028500 -0.39158600

C 3.73670800 2.23509000 -0.36853300

H 3.75760400 2.79144700 -1.30973400

H 3.95929200 2.94784500 0.43140400

H 4.53901200 1.50011500 -0.39195100

C -3.33333900 -0.61503600 -0.07669200

C -3.64856100 -1.17927200 -1.33042900

C -4.05448900 -0.98174600 1.07642000

C -4.66661200 -2.13188800 -1.40017900

C -5.06954700 -1.93527600 0.95800300

C -5.37299900 -2.51753500 -0.26644000

H -4.90719900 -2.57368500 -2.36282200

H -5.62960500 -2.21919100 1.84456600

H -6.16044000 -3.26093000 -0.33848000

C 3.33323900 -0.61515300 -0.07697500

C 4.05477900 -0.98135400 1.07606800

C 3.64815200 -1.17987900 -1.33057800

C 5.06984300 -1.93489600 0.95773800

C 4.66623100 -2.13246500 -1.40024400

C 5.37296400 -2.51763400 -0.26655300

H 5.63017900 -2.21841800 1.84425300

H 4.90657000 -2.57462500 -2.36278200

H 6.16041900 -3.26102200 -0.33852600

C 3.76489400 -0.36262500 2.42211700

H 3.65943400 0.72361400 2.36583000

H 2.83939500 -0.74997500 2.85721500

H 4.56898100 -0.58143500 3.12768900

C 2.91832400 -0.75135100 -2.57869700

H 1.83716600 -0.83669700 -2.45733800

H 3.13064700 0.29277200 -2.83366800

H 3.21574800 -1.36396100 -3.43199400

C -3.76407700 -0.36362800 2.42263000

H -2.83882500 -0.75182900 2.85752100

H -3.65779900 0.72254900 2.36669800

H -4.56826300 -0.58209400 3.12819100

C -2.91906800 -0.75023200 -2.57856700

H -3.13157300 0.29395200 -2.83314600

H -1.83787000 -0.83547600 -2.45746400

H -3.21660800 -1.36258300 -3.43200800

C -0.00103200 -2.25081200 -0.85604000

H -0.00051900 -2.24727600 -1.95330700

H 0.88071900 -2.82838000 -0.54944500

H -0.88392100 -2.82706300 -0.55024600

C 0.00107500 -1.44631800 2.38979500

H 0.92058400 -2.01085900 2.28091700

H -0.91781500 -2.01221900 2.28266700

C 0.00036900 -0.14219200 2.69218300

H -0.91982200 0.41254600 2.82842200

H 0.91994400 0.41402600 2.82652600

Fe 0.00002100 -0.37631600 0.00609600

**3/2Fe(0)-TS2/3**

C 1.19138900 2.48219600 0.02395700

C 1.20800600 3.87295100 0.05394700

C 0.00767100 4.58660900 0.05448000

C -1.19469200 3.87607900 0.03664800

C -1.18134000 2.48541800 0.00783200

N 0.00414700 1.78424600 -0.00722700

H 0.00897800 5.67027900 0.07384200

H 2.15243800 4.40371000 0.07854400

H -2.13785000 4.40949700 0.04779000

C 2.38593500 1.65826900 0.04866300

C -2.37874900 1.66464700 0.02095700

N -2.18426600 0.37205600 -0.03628100

N 2.18835800 0.36623800 -0.01650900

C -3.73895000 2.31225000 0.12328000

H -3.83464600 2.89260100 1.04585800

H -3.91328800 3.00018000 -0.70914200

H -4.53184600 1.56629500 0.11259600

C 3.74678500 2.30114100 0.16923300

H 3.94126900 2.97682900 -0.66890700

H 3.82677400 2.89345200 1.08555100

H 4.53604300 1.55143900 0.18448400

C -3.26616600 -0.54848800 0.04363100

C -3.88178800 -1.01222300 -1.13648900

C -3.66459800 -1.03805200 1.30452600

C -4.86232400 -2.00196300 -1.03547900

C -4.64813400 -2.02889500 1.35758000

C -5.23978700 -2.51928300 0.19900000

H -5.33697000 -2.36672100 -1.94206300

H -4.95266100 -2.41682600 2.32555500

H -5.99682000 -3.29479400 0.25802600

C 3.26742100 -0.55844700 0.05630600

C 3.64174200 -1.08430200 1.31010700

C 3.90521300 -0.98857100 -1.12465000

C 4.62015600 -2.08042000 1.35293500

C 4.87879800 -1.98639900 -1.03399200

C 5.23025300 -2.54128800 0.19153600

H 4.90629000 -2.49612100 2.31496800

H 5.36883600 -2.32709200 -1.94178900

H 5.98214200 -3.32239000 0.24217800

C 3.04342500 -0.54781500 2.58773000

H 3.46935800 0.42911600 2.84385600

H 1.96436900 -0.40816200 2.50783400

H 3.24387700 -1.21854800 3.42587300

C 3.59428100 -0.34767200 -2.45489400

H 2.52489100 -0.19588000 -2.59985600

H 4.06714700 0.63779200 -2.53900100

H 3.96889200 -0.95716700 -3.28005800

C -3.08441800 -0.47200700 2.57784600

H -2.00617600 -0.32212000 2.50573000

H -3.52311200 0.50462500 2.81280500

H -3.28581700 -1.12965700 3.42605900

C -3.53489200 -0.41650700 -2.47844100

H -3.94742800 0.59348800 -2.58357600

H -2.45815500 -0.33159700 -2.62439500

H -3.94416200 -1.01997200 -3.29141100

C -0.08299600 -2.64357200 -0.28860100

H 0.78021600 -3.16233500 -0.68527700

H -1.03071200 -3.03014400 -0.64085500

C -0.01952100 -2.10413400 1.01590600

H -0.92439400 -2.10816200 1.61296400

H 0.91396400 -2.19253400 1.56029700

Fe 0.00451400 -0.24718300 -0.10839300

C 0.03233500 -1.39620600 -2.05362100

H -0.80319800 -1.89244100 -2.54236600

H -0.02608000 -0.32463000 -2.31737200

H 0.97248300 -1.78293100 -2.44002900

**3/2Fe(0)-3**

C -1.18494000 2.67144900 -0.10532600

C -1.20427800 4.06261200 -0.08658400

C 0.00015300 4.77168500 -0.10776500

C 1.20454800 4.06254900 -0.08657900

C 1.18513700 2.67138800 -0.10532200

N 0.00008200 1.98586600 -0.20352800

H 0.00018100 5.85546800 -0.09168200

H -2.14605200 4.59630200 -0.03423100

H 2.14635000 4.59619000 -0.03422100

C -2.35770000 1.82230100 0.02571900

C 2.35785500 1.82217800 0.02571800

N 2.10968100 0.54051500 0.14163600

N -2.10959400 0.54062400 0.14164300

C 3.73745000 2.43146200 0.05077900

H 3.96696400 2.93882900 -0.89126200

H 3.81989000 3.17797300 0.84579900

H 4.50062000 1.67480900 0.22359900

C -3.73726300 2.43165600 0.05077800

H -3.81966200 3.17818100 0.84579100

H -3.96675500 2.93902500 -0.89126800

H -4.50047200 1.67504500 0.22360900

C 3.14747700 -0.42512500 0.25737300

C 3.35085100 -1.03398200 1.51209400

C 3.88553100 -0.83223800 -0.87186600

C 4.31933500 -2.03215800 1.62455500

C 4.83851900 -1.84235100 -0.71453000

C 5.06240900 -2.43824200 0.52085800

H 4.48635800 -2.49956300 2.59073100

H 5.40730500 -2.16733200 -1.58102400

H 5.80589600 -3.22237500 0.62181500

C -3.14744300 -0.42495800 0.25739400

C -3.88552400 -0.83204200 -0.87183800

C -3.35084700 -1.03379100 1.51212100

C -4.83856700 -1.84210100 -0.71448800

C -4.31938600 -2.03191100 1.62459700

C -5.06248600 -2.43796600 0.52090700

H -5.40737400 -2.16705900 -1.58097700

H -4.48643200 -2.49929700 2.59077800

H -5.80601700 -3.22205600 0.62187400

C -3.65813500 -0.20852200 -2.22705700

H -4.11587100 0.78377800 -2.30446300

H -2.59435300 -0.08909800 -2.44162400

H -4.09385500 -0.82654800 -3.01445600

C -2.53940900 -0.60996300 2.71062800

H -1.46824500 -0.76530700 2.54500600

H -2.66593300 0.45254600 2.93835600

H -2.82552500 -1.17932200 3.59712900

C 3.65817200 -0.20869100 -2.22707700

H 2.59439500 -0.08921700 -2.44164500

H 4.11595200 0.78359000 -2.30447100

H 4.09386500 -0.82672700 -3.01448300

C 2.53944400 -0.61011900 2.71060900

H 2.66603900 0.45237800 2.93835200

H 1.46826800 -0.76538800 2.54498600

H 2.82552400 -1.17951000 3.59710100

C 0.00000200 -1.78721400 -1.44262600

H -0.87454200 -1.80263600 -2.10944500

H 0.87493300 -1.80295700 -2.10892900

C -0.00048100 -3.06958500 -0.58906900

H -0.87643200 -3.07927400 0.07304300

H 0.87510700 -3.07960700 0.07352200

C -0.00050000 -4.36808800 -1.40956500

H -0.88282600 -4.42180400 -2.05589000

H 0.88215900 -4.42213800 -2.05540700

H -0.00084400 -5.25859300 -0.76993500

Fe 0.00002600 -0.04910500 -0.33734500

**3/2Fe(0)-4**

C 1.12095200 2.58900300 -0.40559200

C 1.10623700 3.95541000 -0.67357300

C -0.10353800 4.61866000 -0.87363100

C -1.28657600 3.87623100 -0.81431900

C -1.24280900 2.51522000 -0.53724700

N -0.04927500 1.86202900 -0.31996300

H -0.12618100 5.68255300 -1.07884000

H 2.03820200 4.50434600 -0.73205100

H -2.23855000 4.36484000 -0.98218300

C 2.34774800 1.82654800 -0.24478100

C -2.43987300 1.68374000 -0.47263500

N -2.26620800 0.45089500 -0.09197100

N 2.21007500 0.56448100 0.06628500

C -3.77461300 2.26656500 -0.87738900

H -4.07232100 3.07932100 -0.20809100

H -3.73507200 2.68066900 -1.88842800

H -4.55608900 1.50939800 -0.85207800

C 3.68134800 2.50135500 -0.47055000

H 3.76343200 2.89898900 -1.48629500

H 3.81536800 3.34312700 0.21521700

H 4.50490000 1.80783900 -0.31230400

C -3.34829100 -0.47361500 -0.04649300

C -3.53426500 -1.35284000 -1.13292500

C -4.17702300 -0.55213300 1.08998200

C -4.53447200 -2.32256200 -1.04811300

C -5.16264700 -1.54227000 1.13400700

C -5.34140200 -2.42906800 0.07948900

H -4.67774500 -3.00406800 -1.88164400

H -5.79937100 -1.61103600 2.01151800

H -6.10750200 -3.19586700 0.13353900

C 3.33277700 -0.31224400 0.08097200

C 3.97306200 -0.62381500 1.29516100

C 3.75322100 -0.90702000 -1.12625200

C 5.02481100 -1.54256800 1.28463800

C 4.80633600 -1.82375500 -1.09034700

C 5.44107800 -2.14628800 0.10364500

H 5.52211100 -1.78427000 2.21970000

H 5.12873700 -2.29067000 -2.01660100

H 6.25548500 -2.86353100 0.11366400

C 3.55157400 0.03576400 2.58339800

H 3.64459100 1.12539700 2.53449100

H 2.50752200 -0.18084600 2.81771800

H 4.16240200 -0.31168700 3.41886700

C 3.09163900 -0.55799300 -2.43644700

H 2.00332300 -0.61940100 -2.36749800

H 3.33227700 0.46167400 -2.75661700

H 3.41908500 -1.23415200 -3.22841300

C -4.04834800 0.42965600 2.22882700

H -3.01151300 0.57924000 2.53053100

H -4.44226600 1.41600500 1.95879800

H -4.60701700 0.08799500 3.10246500

C -2.69052300 -1.22909900 -2.37579700

H -2.87837100 -0.28574900 -2.90026000

H -1.62552700 -1.25210000 -2.13761700

H -2.90157200 -2.04183300 -3.07333700

C 0.01883600 -2.21576100 0.16885000

H 0.59041500 -2.52070500 1.06146400

H -1.01632700 -2.53025300 0.37679000

C 0.55233200 -3.02681300 -1.02313500

H 1.60797000 -2.78679000 -1.19147100

H 0.03310600 -2.74102000 -1.94768900

C 0.42304500 -4.54782200 -0.85278100

H 0.97077500 -4.88966500 0.03180600

H -0.62384100 -4.84113300 -0.72073900

H 0.81617800 -5.09447900 -1.71845600

C -0.35828600 -0.41677800 2.98013900

H 0.46844900 -1.08097000 3.20618400

H -1.32585400 -0.89197900 2.86428100

C -0.19458900 0.90372500 2.88128400

H -1.02232100 1.57270100 2.67515100

H 0.77349300 1.37253000 3.01793900

Fe 0.00850100 -0.14049400 0.19845000

**3/2Fe(0)-TS4/5**

C 1.20013800 2.58096200 -0.21928000

C 1.21921200 3.95985400 -0.42556300

C 0.02490900 4.66577900 -0.55008900

C -1.18085900 3.95764500 -0.49044700

C -1.17037500 2.58495000 -0.27818000

N 0.00799300 1.89686100 -0.10742200

H 0.02908600 5.73750800 -0.71128200

H 2.16498800 4.48320300 -0.50127600

H -2.12026400 4.48193100 -0.61740100

C 2.39100600 1.76291300 -0.14852000

C -2.37661400 1.77023900 -0.24652500

N -2.21431000 0.49825600 0.00267000

N 2.20785200 0.47848200 0.06330300

C -3.71746300 2.41506500 -0.51410900

H -3.93707100 3.18653600 0.22989100

H -3.73879400 2.89896400 -1.49448700

H -4.52137100 1.68241000 -0.48269100

C 3.74877500 2.40201200 -0.33129100

H 3.83296600 2.89638500 -1.30338600

H 3.92981400 3.16376400 0.43308300

H 4.54605900 1.66483100 -0.26033600

C -3.31887000 -0.39995200 -0.06274800

C -3.62216300 -1.01212300 -1.29687200

C -4.05492100 -0.71955100 1.09501200

C -4.64449800 -1.96199800 -1.34402600

C -5.07312100 -1.67215100 1.00025500

C -5.36652900 -2.29919500 -0.20473800

H -4.87682300 -2.43859200 -2.29211200

H -5.64399800 -1.92029600 1.89055100

H -6.15741400 -3.04051600 -0.25725700

C 3.30652200 -0.42664000 -0.03088300

C 3.99162600 -0.86227700 1.12054500

C 3.67104800 -0.91840100 -1.30477100

C 4.99974200 -1.82149400 0.98131000

C 4.67933800 -1.87931500 -1.39542500

C 5.33866800 -2.34074300 -0.26131700

H 5.53038800 -2.15595200 1.86848100

H 4.95214900 -2.26504900 -2.37363900

H 6.12041800 -3.08860200 -0.34806000

C 3.68837200 -0.30396600 2.48961700

H 4.56011900 -0.39440800 3.14173500

H 3.40461900 0.74878300 2.45159800

H 2.86702100 -0.83795900 2.97549500

C 3.00844400 -0.40118200 -2.55803000

H 1.92157100 -0.37797500 -2.46590300

H 3.32453700 0.62209100 -2.78848000

H 3.26648100 -1.02189000 -3.41848100

C -3.76852600 -0.05273700 2.41734300

H -2.81938400 -0.38992300 2.84063600

H -3.70248200 1.03448200 2.32707900

H -4.55226700 -0.28046100 3.14265000

C -2.87146000 -0.63891400 -2.55104900

H -3.07429400 0.39364300 -2.85438300

H -1.79075100 -0.71550300 -2.41453500

H -3.15637500 -1.28622200 -3.38269500

C -0.38424800 -2.32484000 0.45819900

H -0.15555300 -3.24969900 0.99002600

H -1.46964800 -2.27670400 0.34496700

C 0.33041800 -2.37402900 -0.89684200

H 1.41227600 -2.42662500 -0.74888400

H 0.14994200 -1.46313800 -1.48426700

C -0.11476400 -3.57847400 -1.74635200

H 0.09422900 -4.51769800 -1.22532300

H -1.18902500 -3.54580300 -1.94847800

H 0.41018000 -3.60580200 -2.70782300

C 0.00840600 -1.48060500 2.42636100

H 0.91911500 -2.06129800 2.52075400

H -0.88125500 -2.03994100 2.69370300

C 0.05643900 -0.09359800 2.71721800

H -0.82963800 0.39998800 3.10149700

H 0.99740500 0.36178700 2.99955800

Fe 0.00693800 0.01173600 0.58949200

**3/2Fe(0)-5**

C 1.18589700 -3.07220600 -0.14402400

C 1.20569700 -4.46301100 -0.11812700

C 0.00098400 -5.17251400 -0.13326900

C -1.20398800 -4.46346400 -0.11806900

C -1.18470800 -3.07265000 -0.14395900

N 0.00046700 -2.38976200 -0.24249700

H 0.00118600 -6.25609700 -0.11066800

H 2.14757100 -4.99664400 -0.06642000

H -2.14566800 -4.99744200 -0.06633500

C 2.35792300 -2.22123900 -0.02049400

C -2.35703000 -2.22212100 -0.02033500

N -2.11101200 -0.94012300 0.10584400

N 2.11144800 -0.93933000 0.10570500

C -3.73822400 -2.82744000 -0.01530400

H -3.95548900 -3.33139900 -0.96201400

H -3.83342000 -3.57562900 0.77657500

H -4.50116900 -2.06879200 0.14889400

C 3.73935100 -2.82601300 -0.01565500

H 3.83480000 -3.57461600 0.77579400

H 3.95689300 -3.32933500 -0.96264600

H 4.50196800 -2.06713600 0.14901000

C -3.15079300 0.02409500 0.23121400

C -3.38373200 0.58926700 1.50041100

C -3.86176500 0.46702800 -0.90144300

C -4.35646000 1.58269600 1.62217800

C -4.82192300 1.46827800 -0.73347500

C -5.07519300 2.02277700 0.51564800

H -4.54573100 2.01916600 2.59861700

H -5.37170900 1.82021000 -1.60163900

H -5.82295800 2.80172500 0.62513200

C 3.15089500 0.02524900 0.23112400

C 3.86160400 0.46859000 -0.90153100

C 3.38375900 0.59030900 1.50038800

C 4.82142900 1.47015300 -0.73351200

C 4.35616000 1.58405000 1.62220600

C 5.07462800 2.02455000 0.51566800

H 5.37100500 1.82240400 -1.60168000

H 4.54536700 2.02045300 2.59868900

H 5.82213300 2.80374100 0.62520000

C 3.59557500 -0.10744900 -2.27053100

H 3.99503600 -1.12199900 -2.37621800

H 2.52548700 -0.16214700 -2.48283300

H 4.06151400 0.50540600 -3.04445000

C 2.59863000 0.12756300 2.70182700

H 1.52229100 0.24458700 2.54325700

H 2.76652800 -0.93207800 2.91817600

H 2.87400900 0.69755200 3.59132100

C -3.59564600 -0.10908000 -2.27039600

H -2.52555800 -0.16331100 -2.48282000

H -3.99464700 -1.12382800 -2.37590900

H -4.06196200 0.50345800 -3.04433800

C -2.59827800 0.12702900 2.70183500

H -2.76500900 -0.93285400 2.91785000

H -1.52204100 0.24532000 2.54345900

H -2.87440600 0.69647000 3.59144900

C -0.00046900 1.52313800 -1.21356500

H 0.87296800 1.61662400 -1.87546800

H -0.87410500 1.61612400 -1.87527600

C -0.00070500 2.69942100 -0.21919300

H 0.87501500 2.63444200 0.44119200

H -0.87626500 2.63392600 0.44135400

C -0.00116100 4.08615700 -0.88366600

H 0.87504300 4.16568000 -1.54135300

H -0.87760300 4.16523100 -1.54108300

C -0.00128900 5.25612500 0.10620200

H -0.87685700 5.17446800 0.76302600

H 0.87447000 5.17480500 0.76281800

C -0.00163000 6.62898000 -0.57146600

H -0.00174100 7.44265500 0.16049500

H 0.88013300 6.75864300 -1.20749200

H -0.88354600 6.75828300 -1.20735400

Fe 0.00011300 -0.34819800 -0.35591600

**3/2Fe(0)-6**

C 1.05655900 2.62949200 0.29517900

C 1.02509900 4.01107400 0.46458300

C -0.19499800 4.68028600 0.55102500

C -1.37006000 3.92891500 0.48051500

C -1.30979000 2.55009200 0.31092600

N -0.10434000 1.88862400 0.21001300

H -0.23091500 5.75636700 0.67462400

H 1.95155000 4.56846700 0.52896100

H -2.33051300 4.42359200 0.55754300

C 2.29666000 1.87235800 0.22602800

C -2.50012000 1.71036100 0.25679500

N -2.30912500 0.45007000 -0.01383100

N 2.18734700 0.59773300 -0.03716800

C -3.85429200 2.32063700 0.54016800

H -3.87913100 2.79645900 1.52438200

H -4.10173200 3.09144600 -0.19595000

H -4.63861800 1.56693400 0.50870900

C 3.61133500 2.57286900 0.48533700

H 3.78587500 3.36749600 -0.24625300

H 3.62745900 3.03831600 1.47490300

H 4.44578000 1.87701800 0.42598400

C -3.38871400 -0.47979000 0.01939000

C -4.10763800 -0.78013700 -1.15418000

C -3.68716800 -1.13559700 1.23201600

C -5.10124900 -1.76144200 -1.09983800

C -4.68456800 -2.11265000 1.23793000

C -5.38665500 -2.43431500 0.08195800

H -5.65922400 -1.99482700 -2.00225400

H -4.91183400 -2.62511600 2.16823100

H -6.15692500 -3.19851700 0.10406200

C 3.33059900 -0.25358200 -0.00410800

C 3.69999900 -0.85552600 1.21672600

C 4.04523000 -0.53142800 -1.18557500

C 4.76586700 -1.75742000 1.22425800

C 5.10740600 -1.43764000 -1.13030500

C 5.46532400 -2.05735100 0.06087500

H 5.04789300 -2.22968600 2.16084700

H 5.66189100 -1.65381800 -2.03913200

H 6.28900800 -2.76359200 0.08412200

C 2.97331300 -0.52547900 2.49657700

H 3.14985300 0.50980200 2.80831400

H 1.89388300 -0.64409900 2.38669000

H 3.30663100 -1.17283200 3.30998300

C 3.70125700 0.14288700 -2.49106000

H 2.74787200 -0.20852800 -2.89381400

H 3.61977300 1.22820300 -2.38587300

H 4.46596400 -0.05981100 -3.24345400

C -2.96421700 -0.77833700 2.50652900

H -1.88116900 -0.82725800 2.38177900

H -3.20264400 0.23880500 2.83639700

H -3.24380200 -1.45788300 3.31387000

C -3.84235800 -0.05377100 -2.45044700

H -3.82790000 1.03173100 -2.32039200

H -2.88003700 -0.33332900 -2.88676800

H -4.61271600 -0.28774800 -3.18789100

C -0.06111800 -2.08313400 0.66049900

H 0.13922300 -2.02588700 1.74288900

H -1.10491800 -2.42324700 0.58554800

C 0.84984600 -3.16459900 0.05688600

H 1.89713100 -2.84264700 0.08454900

H 0.61253100 -3.30158100 -1.00675500

C 0.74209300 -4.53128500 0.74976600

H 1.01945800 -4.45688900 1.80677400

H -0.28344300 -4.91362800 0.70969300

H 1.39656600 -5.27972300 0.28727100

C -0.05768600 -0.88913300 -2.60037000

H 0.87385600 -1.44394100 -2.59575400

H -0.96292800 -1.48461500 -2.55268700

C -0.08801500 0.44342200 -2.72354000

H -1.02008700 0.99381800 -2.76317200

H 0.81937400 1.02971700 -2.80301300

Fe -0.02584000 -0.14933200 -0.09012700

**3/2Fe(0)-TS6/7**

C 1.04611100 2.71242300 0.15053500

C 1.02706900 4.09998600 0.25716700

C -0.18675500 4.78508600 0.31112200

C -1.36756000 4.04337200 0.25222600

C -1.31887200 2.65795100 0.14634000

N -0.11940200 1.97671800 0.09973100

H -0.21219400 5.86538300 0.39384500

H 1.95825300 4.65132100 0.29774500

H -2.32474900 4.54914200 0.28846600

C 2.28460200 1.95168200 0.08487900

C -2.51538500 1.83271700 0.07708600

N -2.31653400 0.55002600 -0.02528900

N 2.16963200 0.65703200 -0.01856100

C -3.88140600 2.47654000 0.12585600

H -4.02456600 3.03386500 1.05618100

H -4.01675100 3.18349400 -0.69774200

H -4.66834900 1.72738800 0.05818000

C 3.60912400 2.68009500 0.13762400

H 4.44311100 1.98418800 0.07036000

H 3.70089900 3.39620900 -0.68393200

H 3.71494600 3.24359500 1.06910600

C -3.39337000 -0.37387600 -0.09568800

C -3.87915000 -0.77819900 -1.35540000

C -3.91250900 -0.92978200 1.09073300

C -4.85882400 -1.77240900 -1.40659300

C -4.89158600 -1.92124100 0.99168100

C -5.35941700 -2.35082100 -0.24526400

H -5.23305600 -2.09317200 -2.37475600

H -5.29106600 -2.35907700 1.90219400

H -6.11432000 -3.12848200 -0.30380400

C 3.32025400 -0.17635300 -0.08774100

C 3.88105200 -0.69376600 1.09733500

C 3.85615500 -0.52045000 -1.34547400

C 4.94964900 -1.58864600 0.99908800

C 4.92580100 -1.41730900 -1.39672500

C 5.46740200 -1.96006200 -0.23654300

H 5.38124000 -1.99470200 1.90968100

H 5.33880100 -1.68881300 -2.36413100

H 6.29398100 -2.66097600 -0.29486200

C 3.37624000 -0.25721500 2.45038700

H 3.70612300 0.76012000 2.69009000

H 2.28670300 -0.25089300 2.49776100

H 3.75051900 -0.91340300 3.23880300

C 3.31885800 0.09792100 -2.61224000

H 3.73884100 -0.38985300 -3.49410600

H 2.23139100 0.03079900 -2.67061300

H 3.56939900 1.16254400 -2.67657700

C -3.46069600 -0.43524600 2.44304400

H -3.91502800 0.53278300 2.68441600

H -3.74908100 -1.13370400 3.23135300

H -2.37983000 -0.29605600 2.48819500

C -3.39104300 -0.11917100 -2.62198800

H -3.82326200 0.88105800 -2.74195900

H -2.30725900 0.00432400 -2.62756600

H -3.67353400 -0.70250700 -3.50077300

C -0.07611700 -1.71552300 1.43866300

H 0.28885700 -1.04464600 2.22258000

H -1.12323800 -1.97709900 1.58874000

C 0.78363200 -2.83550300 1.15271200

H 1.82239400 -2.72585900 1.46848200

H 0.98702000 -2.80600100 -0.16800300

C 0.25456700 -4.25141400 1.29713900

H 0.14886900 -4.51276600 2.35606400

H -0.73438200 -4.34911800 0.83927500

H 0.91812500 -4.99034200 0.83697800

C 0.79929400 -2.67800000 -1.48629200

H 1.83523400 -2.58468800 -1.80769000

H 0.40393200 -3.68402000 -1.63592500

C -0.07511100 -1.56362300 -1.68751100

H -1.12084900 -1.80834100 -1.85454300

H 0.28995500 -0.79213900 -2.37044700

Fe -0.08557700 -0.09234500 -0.03343100

**3/2Fe(0)-7**

C -1.10914400 2.76080000 0.09209300

C -1.09542100 4.15354100 0.02593800

C 0.12429400 4.83098700 0.00490300

C 1.31558100 4.09303200 -0.00136400

C 1.26141200 2.70614300 0.06977800

N 0.06375600 2.05783300 0.19211200

H 0.15021200 5.91329100 -0.04932500

H -2.02452900 4.70911700 -0.03221000

H 2.26779400 4.60419100 -0.08339100

C -2.29278500 1.92962700 -0.01803800

C 2.41257700 1.81840100 -0.05467100

N 2.15030400 0.53679700 -0.05161900

N -2.08231000 0.63138500 -0.01878100

C 3.79473300 2.40395000 -0.21698100

H 3.86840700 2.99851300 -1.13254700

H 4.03930200 3.06724800 0.61756200

H 4.55224300 1.62390900 -0.26385800

C -3.65337900 2.56771400 -0.16101600

H -3.85608800 3.25195100 0.66799500

H -3.72572200 3.15100600 -1.08429900

H -4.44230000 1.81778600 -0.17945000

C 3.16837700 -0.41935200 -0.33697900

C 3.92807100 -1.00362300 0.69537400

C 3.35025500 -0.81611400 -1.67814800

C 4.84991400 -2.00018000 0.36331800

C 4.28213800 -1.81646900 -1.96323600

C 5.02744100 -2.41291400 -0.95234500

H 5.43783900 -2.45505000 1.15534900

H 4.42187300 -2.12801800 -2.99448600

H 5.74524600 -3.19184200 -1.18887200

C -3.13463600 -0.28104800 -0.31622000

C -3.36232600 -0.62535100 -1.66510900

C -3.88486700 -0.88242100 0.71440100

C -4.32292100 -1.59589500 -1.95959100

C -4.83853700 -1.84492600 0.37333100

C -5.05648100 -2.20997900 -0.95103100

H -4.49495900 -1.86939100 -2.99680600

H -5.41947800 -2.31117800 1.16397200

H -5.79731700 -2.96461100 -1.19530600

C -2.60753400 0.05735700 -2.77987200

H -2.99955200 1.06231500 -2.97349200

H -1.54894300 0.18174200 -2.54283200

H -2.68893600 -0.50753700 -3.71068800

C -3.68498000 -0.48447100 2.15443600

H -3.87973700 0.58131800 2.31096100

H -4.35725300 -1.04304200 2.80877200

H -2.66108400 -0.66366800 2.48483100

C 2.56578300 -0.16491400 -2.79038300

H 1.49518900 -0.14550600 -2.57389600

H 2.86862700 0.87612100 -2.94605800

H 2.71464700 -0.69355200 -3.73395000

C 3.76938600 -0.56068900 2.12747400

H 3.97508300 0.50744900 2.24955700

H 2.75359200 -0.72490300 2.48922700

H 4.45457800 -1.10545400 2.77992100

C 0.03947800 -2.37790600 -0.93536000

H -0.38381900 -1.54898300 -1.49440500

H 1.11540900 -2.51049300 -0.99111700

C -0.74757400 -3.23737300 -0.28594300

H -1.82166100 -3.06093300 -0.28272900

H -0.86692300 -2.34839800 2.86989000

C -0.27358200 -4.46181000 0.43555000

H -0.70927400 -5.36381300 -0.00957300

H 0.81407200 -4.55735400 0.40377000

H -0.58546300 -4.44917400 1.48440300

C 0.03949000 -1.82800100 3.19761600

H 0.08899600 -1.94231200 4.29032800

H 0.88340800 -2.39047100 2.78366500

C 0.04734500 -0.36094500 2.74720200

H 0.93173300 0.14709300 3.15678200

H -0.80223100 0.16878700 3.20092600

Fe 0.00354300 0.11956600 0.73379400

**3/2Fe(0)-8**

C 1.19777200 2.55559300 -0.00029000

C 1.21179600 3.94130200 -0.13607300

C -0.00002600 4.63847100 -0.18918400

C -1.21182900 3.94128600 -0.13606400

C -1.19778800 2.55556900 -0.00028300

N 0.00000100 1.89489400 0.10903200

H -0.00003600 5.71645600 -0.30313100

H 2.14667700 4.48218900 -0.22187000

H -2.14671300 4.48217000 -0.22183700

C 2.31514900 1.64731300 0.00054800

C -2.31511600 1.64724600 0.00055500

N -1.97910700 0.35874400 0.02487000

N 1.97918700 0.35880800 0.02484800

C -3.74358700 2.11439900 -0.02751900

H -3.81441100 3.20051800 -0.06055200

H -4.27749400 1.71405400 -0.89377400

H -4.28888400 1.76965300 0.85591300

C 3.74356000 2.11467800 -0.02764600

H 4.27730500 1.71487900 -0.89425600

H 3.81416700 3.20083200 -0.06015900

H 4.28916700 1.76963000 0.85546700

C -3.01381100 -0.62898400 0.00813200

C -3.46464700 -1.12474900 -1.22897600

C -3.53006400 -1.12027100 1.22132100

C -4.45422900 -2.11086300 -1.23077200

C -4.51810300 -2.10648000 1.17305100

C -4.98219000 -2.59985400 -0.04131800

H -4.80752900 -2.50238500 -2.18036500

H -4.92242900 -2.49426900 2.10360800

H -5.74745900 -3.36929800 -0.06013800

C 3.01382200 -0.62898500 0.00812700

C 3.53001100 -1.12026700 1.22134900

C 3.46464500 -1.12483500 -1.22895000

C 4.51795000 -2.10657600 1.17314400

C 4.45412000 -2.11105900 -1.23067900

C 4.98200400 -2.60005800 -0.04119600

H 4.92222600 -2.49435800 2.10372500

H 4.80740100 -2.50265200 -2.18025000

H 5.74718900 -3.36958600 -0.05996900

C 3.02435500 -0.60646200 2.54652800

H 3.18715700 0.46915300 2.66595700

H 1.94845800 -0.77388200 2.65258800

H 3.52535400 -1.11047900 3.37528400

C 2.89463700 -0.60660100 -2.52629200

H 1.80222300 -0.62901100 -2.51988300

H 3.18290300 0.43241200 -2.71870900

H 3.24310400 -1.20484200 -3.37040400

C -3.02435500 -0.60661000 2.54653600

H -1.94849000 -0.77421300 2.65261300

H -3.18697500 0.46902700 2.66601300

H -3.52545700 -1.11057900 3.37525800

C -2.89446400 -0.60658200 -2.52626700

H -3.18206300 0.43265900 -2.71844200

H -1.80206000 -0.62968300 -2.51995900

H -3.24337200 -1.20443600 -3.37047200

C 0.00004900 -2.03071100 0.51255300

H 0.87766000 -2.31320100 1.11171800

H -0.87755500 -2.31324000 1.11171000

C 0.00007300 -2.85757700 -0.78201200

H 0.88278100 -2.65505800 -1.39766400

H -0.88269200 -2.65517400 -1.39762000

H 0.00014700 -3.93949700 -0.58821800

Fe 0.00002800 -0.03249600 0.25948600

**3/2Fe(0)-TS3/9**

C -1.12235600 2.56572800 0.07201000

C -1.12254500 3.95415500 0.11202400

C 0.08964000 4.65275900 0.15015200

C 1.28057000 3.92797100 0.14744300

C 1.25098500 2.53601800 0.10433300

N 0.05431900 1.85347500 0.06545500

H 0.10146100 5.73595200 0.18203800

H -2.05954000 4.49833100 0.11488800

H 2.23067000 4.44880300 0.17792000

C -2.32796700 1.75570000 0.03503400

C 2.42479000 1.69359100 0.08835500

N 2.19413200 0.40135300 0.03967200

N -2.14969100 0.46042300 0.01611400

C 3.80426000 2.30461100 0.12878800

H 3.93736100 2.92006100 1.02328800

H 4.57529500 1.53612800 0.13381600

H 3.97931000 2.95147000 -0.73611900

C -3.68410800 2.41856400 0.02167900

H -3.79887100 3.06690000 -0.85167300

H -4.48391600 1.68066300 0.00129100

H -3.82452300 3.04368300 0.90803500

C 3.25739700 -0.54228500 -0.01758300

C 3.71558400 -1.14365300 1.17215600

C 3.78607100 -0.91768600 -1.26871300

C 4.69928100 -2.13137500 1.08422600

C 4.76564000 -1.91317800 -1.30897900

C 5.22074500 -2.52181600 -0.14487000

H 5.05804400 -2.59969100 1.99636600

H 5.17409600 -2.21184400 -2.27027100

H 5.97893700 -3.29688700 -0.19459700

C -3.24682300 -0.44488200 -0.04289900

C -3.74451000 -0.84844200 -1.29746400

C -3.76517300 -0.98152700 1.15223200

C -4.76177700 -1.80547100 -1.33415400

C -4.78499000 -1.93210700 1.06702000

C -5.28095400 -2.34842500 -0.16413900

H -5.14886800 -2.12601500 -2.29719300

H -5.19086400 -2.35210200 1.98287300

H -6.06868800 -3.09359800 -0.21112700

C -3.20862000 -0.24669300 -2.57289900

H -3.55797500 0.78279000 -2.71101400

H -2.11711000 -0.21093200 -2.57313800

H -3.53581200 -0.82014100 -3.44257200

C -3.23855100 -0.53316900 2.49250400

H -2.14989800 -0.61581300 2.54168500

H -3.48344800 0.51537300 2.69364400

H -3.66735300 -1.13121600 3.29910600

C 3.32827500 -0.24300600 -2.53879000

H 2.24224100 -0.13582300 -2.57433600

H 3.74512800 0.76636200 -2.63041300

H 3.64796300 -0.80710000 -3.41735100

C 3.17103800 -0.71720600 2.51289600

H 3.46136200 0.31040300 2.75750700

H 2.07894900 -0.74597600 2.53009700

H 3.54696100 -1.36300500 3.30918900

C 0.00960700 -1.92970000 -1.17075900

H -0.95087200 -2.11072700 -1.64333400

H 0.85293000 -1.81727700 -1.84286200

C 0.23273600 -2.41809000 0.13922800

H 0.02248400 -1.25454800 1.33805900

H 1.26904500 -2.59637700 0.41262000

C -0.74648400 -3.37519100 0.79019200

H -1.78111800 -3.07416600 0.61808300

H -0.61395000 -4.36962500 0.34781400

H -0.58871400 -3.45609400 1.86807500

Fe 0.01605400 -0.15253500 0.07141500

**3/2Fe(0)-9**

C 1.14035000 2.58346600 0.05731700

C 1.15358500 4.00993400 0.11342500

C -0.06363100 4.68111900 0.09344700

C -1.27115100 3.98943400 0.05467900

C -1.22990400 2.56528200 0.00107100

N -0.03769400 1.93003800 -0.06618600

H -0.07332500 5.76661600 0.12808100

H 2.08927300 4.55009200 0.17114700

H -2.21733000 4.51387200 0.07185200

C 2.25484700 1.69591800 0.16266300

C -2.33502900 1.65788900 0.06157000

N -2.01438600 0.35901800 0.13649400

N 1.95845000 0.38681000 0.19149400

C -3.73889100 2.19133800 0.09418300

H -3.85477700 2.91388600 0.90912000

H -3.98308800 2.72282000 -0.83252400

H -4.47399500 1.40142600 0.23761900

C 3.64166000 2.25817500 0.30006800

H 3.68183300 2.97308500 1.12889600

H 4.38188000 1.48259200 0.48797300

H 3.94222300 2.80633700 -0.59996900

C -3.03577700 -0.63195600 0.17942600

C -3.72724900 -1.01676900 -0.98860500

C -3.30829100 -1.25854600 1.41451200

C -4.66876000 -2.04710200 -0.89959800

C -4.25951000 -2.27943500 1.45762800

C -4.93436300 -2.67958100 0.30876900

H -5.19881200 -2.35416700 -1.79689100

H -4.47416900 -2.76283400 2.40637800

H -5.66615400 -3.47977000 0.35650000

C 3.00635700 -0.57523000 0.23795700

C 3.22815500 -1.26990400 1.44635300

C 3.78060300 -0.86273500 -0.90620300

C 4.21281300 -2.25895700 1.48615500

C 4.75404000 -1.86322600 -0.82197600

C 4.97126200 -2.56168200 0.35980000

H 4.38759200 -2.79420200 2.41509300

H 5.34718100 -2.09514100 -1.70221500

H 5.72957500 -3.33699500 0.40425200

C 2.43801300 -0.92670400 2.68453500

H 2.59796200 0.11218800 2.98797700

H 1.36189600 -1.03624100 2.52440500

H 2.72413600 -1.56809600 3.52073300

C 3.58789600 -0.10964100 -2.20047800

H 2.53983300 0.13323900 -2.38017200

H 4.14044300 0.83643800 -2.19804900

H 3.95731300 -0.69280000 -3.04695600

C -2.61886600 -0.80237800 2.67702400

H -1.53036200 -0.80622600 2.57731100

H -2.89630900 0.22436800 2.93570700

H -2.88633200 -1.44181300 3.52076200

C -3.49208500 -0.32731000 -2.31154800

H -4.10305300 0.57810600 -2.40068100

H -2.45274700 -0.02141600 -2.43884200

H -3.76603100 -0.97986900 -3.14366900

C 0.01283800 -2.09758100 0.09549900

H 0.99681600 -2.38312800 0.45081900

H -0.80441700 -2.17732500 0.80328500

C -0.23820100 -2.00551100 -1.24574800

H -0.02124000 0.33155400 -1.84796100

H -1.27254000 -1.93245000 -1.56552000

C 0.74129200 -2.37929800 -2.32242000

H 1.77144600 -2.35349200 -1.96691600

H 0.53136800 -3.40597100 -2.64933900

H 0.65340100 -1.73280200 -3.19674500

Fe -0.01985000 0.04627000 -0.29388900

**3/2Fe(0)-10**

C -1.18586700 2.34958400 -0.02325400

C -1.20672900 3.72261500 -0.24610300

C -0.00008900 4.42497900 -0.33302500

C 1.20660800 3.72261500 -0.24682200

C 1.18588500 2.34960200 -0.02390600

N 0.00006000 1.69367700 0.16701000

H -0.00013900 5.49414800 -0.51078100

H -2.14858800 4.24361900 -0.37388200

H 2.14839200 4.24361400 -0.37518400

C -2.34818400 1.47547600 -0.03284800

C 2.34821500 1.47551200 -0.03383700

N 2.08234000 0.19115100 0.00686900

N -2.08231100 0.19109900 0.00741900

C 3.73783800 2.05424600 -0.11047900

H 3.87801800 2.61582900 -1.03920000

H 3.92373500 2.74662000 0.71559700

H 4.49367600 1.27187700 -0.07683500

C -3.73784800 2.05423800 -0.10872300

H -3.87863000 2.61562900 -1.03746900

H -4.49369600 1.27191000 -0.07442300

H -3.92316400 2.74678100 0.71734000

C 3.11255400 -0.79439400 -0.03714600

C 3.72729500 -1.23060700 1.15169200

C 3.43612700 -1.37105800 -1.27969600

C 4.68771700 -2.24165400 1.06753500

C 4.40325200 -2.37745200 -1.31638200

C 5.02943500 -2.81237900 -0.15347000

H 5.16770700 -2.58745600 1.97836700

H 4.66099200 -2.82727200 -2.27089200

H 5.77540000 -3.59952600 -0.19739500

C -3.11257000 -0.79438000 -0.03690400

C -3.43672400 -1.37005700 -1.27976800

C -3.72679400 -1.23149900 1.15186000

C -4.40388300 -2.37640200 -1.31680100

C -4.68728300 -2.24245900 1.06734800

C -5.02955900 -2.81222200 -0.15394700

H -4.66205200 -2.82549100 -2.27154000

H -5.16688900 -2.58893500 1.97812600

H -5.77556800 -3.59931200 -0.19816200

C -2.75039200 -0.91221800 -2.54256500

H -2.97626100 0.13289200 -2.77824500

H -1.66232600 -0.98162900 -2.45243700

H -3.06005700 -1.51784800 -3.39646700

C -3.35056900 -0.63692800 2.48558900

H -2.27830700 -0.74150400 2.67278700

H -3.58483700 0.43127100 2.54243600

H -3.88633000 -1.13439500 3.29633600

C 2.74922200 -0.91419500 -2.54253400

H 1.66121500 -0.98421700 -2.45210200

H 2.97441100 0.13093700 -2.77874200

H 3.05901400 -1.52004700 -3.39623200

C 3.35160000 -0.63509000 2.48515100

H 3.58596800 0.43312600 2.54120200

H 2.27939900 -0.73947700 2.67280200

H 3.88761300 -1.13205100 3.29604100

H 0.00059600 -1.57186100 1.62716200

Fe 0.00017400 -0.30053700 0.57026600

(ArPDI)Co+ (Singlet)1

**0Co(+)B**

C 1.18510600 2.45417000 0.00014600

C 1.21200400 3.84735300 0.00025100

C -0.00002600 4.54114600 0.00030900

C -1.21206000 3.84735700 0.00026100

C -1.18516600 2.45417500 0.00017600

N -0.00003100 1.80712400 0.00013600

H -0.00002500 5.62460700 0.00042200

H 2.15353400 4.38255300 0.00026800

H -2.15358800 4.38256100 0.00027400

C 2.30554400 1.49208500 0.00005900

C -2.30560500 1.49208900 0.00016300

N -1.91081300 0.25097500 0.00017300

N 1.91075300 0.25097000 0.00005500

C -3.72355800 1.96354000 0.00009900

H -3.92056400 2.58591400 0.87873000

H -3.92105900 2.58409300 -0.87972400

H -4.42533200 1.13221200 0.00112500

C 3.72349600 1.96353500 0.00004700

H 3.92076400 2.58492800 -0.87922700

H 3.92073600 2.58506800 0.87922800

H 4.42527100 1.13220600 0.00012700

C -2.83247600 -0.85592100 0.00003100

C -3.23231600 -1.40252900 -1.23207500

C -3.23167900 -1.40331200 1.23196700

C -4.06872100 -2.52062000 -1.20497500

C -4.06812300 -2.52139600 1.20459800

C -4.48576000 -3.07608300 -0.00025100

H -4.39336700 -2.95923500 -2.14297200

H -4.39228400 -2.96058400 2.14249400

H -5.13320200 -3.94609200 -0.00038100

C 2.83244300 -0.85590900 -0.00009600

C 3.23195100 -1.40309600 1.23183800

C 3.23205900 -1.40266800 -1.23220300

C 4.06849900 -2.52109400 1.20444600

C 4.06859200 -2.52067300 -1.20512500

C 4.48595200 -3.07590700 -0.00041600

H 4.39288900 -2.96013300 2.14233300

H 4.39306200 -2.95939400 -2.14313300

H 5.13347900 -3.94585300 -0.00054600

C 2.79122900 -0.80027000 2.54344800

H 3.27456700 0.16436900 2.73185700

H 1.71187600 -0.62384500 2.57373300

H 3.04585600 -1.45602300 3.37655100

C 2.79134700 -0.79946700 -2.54364600

H 1.71189200 -0.62369700 -2.57412600

H 3.27414500 0.16554800 -2.73149200

H 3.04658900 -1.45468600 -3.37697900

C -2.79075800 -0.80059400 2.54355800

H -1.71133900 -0.62453600 2.57383500

H -3.27374900 0.16422300 2.73193200

H -3.04560100 -1.45623400 3.37668200

C -2.79179800 -0.79915800 -2.54350200

H -3.27370100 0.16643000 -2.73066100

H -1.71217100 -0.62448000 -2.57451400

H -3.04816000 -1.45375700 -3.37697700

Co -0.00003500 0.01666000 0.00014600

**0Co(+)B-1B**

Atom x y z

C -1.17381700 2.51243100 0.01705200

C -1.20890000 3.90623500 0.02644000

C 0.00001700 4.60245400 0.02992900

C 1.20892200 3.90620700 0.02545900

C 1.17379900 2.51240800 0.01620700

N -0.00001800 1.85912200 0.01074300

H 0.00003000 5.68613100 0.03688900

H -2.15142400 4.43904500 0.03121200

H 2.15145900 4.43900000 0.02941000

C -2.31690400 1.57367800 0.01409600

C 2.31687100 1.57363600 0.01331400

N 1.97261200 0.32134900 0.00263700

N -1.97261700 0.32139900 0.00285700

C 3.71469900 2.10776700 0.02543900

H 3.88890100 2.74007600 -0.85091700

H 3.87455200 2.73635400 0.90714100

H 4.45521600 1.31196300 0.02979400

C -3.71472800 2.10781900 0.02653300

H -3.87460500 2.73576900 0.90869300

H -3.88888300 2.74076800 -0.84936500

H -4.45526900 1.31203300 0.03028700

C 2.99321900 -0.69842500 0.00176400

C 3.42848500 -1.21888300 1.23280100

C 3.48828800 -1.16709600 -1.22710900

C 4.37304400 -2.24798400 1.20804700

C 4.43081000 -2.19863400 -1.19848300

C 4.86873700 -2.73881100 0.00519700

H 4.72177400 -2.66610000 2.14687500

H 4.82420700 -2.57873600 -2.13584600

H 5.59773600 -3.54167700 0.00610200

C -2.99320100 -0.69840700 0.00146300

C -3.48756600 -1.16707400 -1.22768100

C -3.42911200 -1.21888700 1.23225400

C -4.43011100 -2.19861000 -1.19958200

C -4.37369100 -2.24795500 1.20698600

C -4.86872900 -2.73876900 0.00385400

H -4.82300600 -2.57868700 -2.13716600

H -4.72296500 -2.66604900 2.14562000

H -5.59774600 -3.54161900 0.00435800

C -3.05721900 -0.55936300 -2.54139800

H -3.56493800 0.39364300 -2.72796600

H -1.98391600 -0.35849000 -2.57722200

H -3.30468800 -1.21923600 -3.37391900

C -2.93151400 -0.66409900 2.54523600

H -1.84934800 -0.50994100 2.54809800

H -3.38975500 0.30517400 2.77102400

H -3.17915300 -1.33415600 3.36940300

C 3.05861400 -0.55946900 -2.54108500

H 1.98535200 -0.35847700 -2.57743100

H 3.56653100 0.39344900 -2.72755200

H 3.30638100 -1.21947400 -3.37341300

C 2.93044500 -0.66395100 2.54556400

H 3.38931900 0.30494100 2.77172000

H 1.84841400 -0.50896100 2.54785400

H 3.17713000 -1.33429400 3.36978800

Co -0.00002700 -0.01639000 -0.00207200

C -0.00093600 -2.07488000 0.56966100

H -0.92255200 -2.24061300 1.11557100

H 0.91980800 -2.23983900 1.11731900

C 0.00049100 -1.99476700 -0.79480400

H 0.92107700 -2.09570600 -1.35749400

H -0.91883200 -2.09627600 -1.35949700

**0Co(+)B-2B**

Atom x y z

C -1.19448200 0.74604700 2.22531600

C -1.20697000 1.57230900 3.34557400

C 0.00034300 1.97799500 3.91861400

C 1.20741200 1.57134800 3.34573800

C 1.19440600 0.74511700 2.22547700

N -0.00017800 0.31163600 1.70092000

H 0.00054200 2.62118300 4.79084500

H -2.14870800 1.90046700 3.77002100

H 2.14937300 1.89875000 3.77028200

C -2.31092000 0.22696500 1.48811300

C 2.31053300 0.22519000 1.48842500

N 1.95884800 -0.47100100 0.41534000

N -1.95963900 -0.46952300 0.41509200

C 3.72763100 0.43246000 1.94844500

H 3.87532600 1.45372800 2.30610200

H 3.98063600 -0.23978300 2.77581300

H 4.44255400 0.24953200 1.14792100

C -3.72793500 0.43518900 1.94794700

H -3.98209300 -0.23815800 2.77406900

H -3.87454600 1.45601700 2.30725100

H -4.44278500 0.25443400 1.14685600

C 2.97321400 -1.20128600 -0.29115300

C 3.32538500 -2.48152200 0.18421800

C 3.59075100 -0.65866700 -1.43458100

C 4.27436000 -3.22126900 -0.52607000

C 4.53956200 -1.43340300 -2.10798200

C 4.87619000 -2.70821000 -1.66833700

H 4.54236900 -4.21249200 -0.17197200

H 5.02343800 -1.02170100 -2.98866900

H 5.61045400 -3.29592700 -2.20990300

C -2.97453900 -1.19896800 -0.29150100

C -3.59160400 -0.65576000 -1.43491400

C -3.32779700 -2.47894400 0.18375600

C -4.54103600 -1.42965500 -2.10840500

C -4.27738200 -3.21783800 -0.52660100

C -4.87875400 -2.70420300 -1.66885200

H -5.02452500 -1.01748100 -2.98908300

H -4.54622600 -4.20886100 -0.17257800

H -5.61348300 -3.29127800 -2.21048300

C -3.28580700 0.74097300 -1.91415100

H -3.39834400 1.47907800 -1.11569300

H -2.26200500 0.83560600 -2.27867300

H -3.95800000 1.02499900 -2.72584900

C -2.72072800 -3.04653900 1.44437800

H -1.65813800 -2.81175600 1.52596300

H -3.20448500 -2.64020700 2.33955800

H -2.84128200 -4.13123100 1.47842400

C 3.28605700 0.73824300 -1.91404100

H 2.26296400 0.83307700 -2.28056600

H 3.39717400 1.47616300 -1.11524200

H 3.95980000 1.02231300 -2.72444000

C 2.71783300 -3.04848300 1.44488900

H 3.20191700 -2.64244200 2.34002600

H 1.65543700 -2.81281400 1.52644400

H 2.83749500 -4.13327000 1.47905500

Co -0.00033400 -0.44591200 0.03977500

C -0.00101900 -2.34434600 -0.96221500

H -0.91824500 -2.85830200 -0.70801800

H 0.91575400 -2.85898200 -0.70775200

C -0.00048800 -1.32245000 -1.88709600

H 0.91590600 -1.02610300 -2.38235000

H -0.91655800 -1.02530300 -2.38247700

Al 0.00302600 4.14627400 -1.36807400

C -1.69350800 4.61714000 -0.45284800

H -2.57615600 4.13853500 -0.89194500

H -1.68612700 4.36997000 0.61490600

H -1.87330100 5.69967500 -0.51240000

C 1.69887700 4.61480200 -0.45037900

H 1.69028100 4.36552700 0.61688400

H 2.58189200 4.13686700 -0.88945800

H 1.87896500 5.69741900 -0.50752600

C 0.00049100 1.40182100 -0.82343000

H 0.90259000 1.88649800 -0.44516700

H -0.90128100 1.88735000 -0.44549600

H 0.00067500 1.37066300 -1.91226400

C 0.00402900 3.96005700 -3.34105900

H 0.00405100 4.94981300 -3.81893200

H 0.88612600 3.43714000 -3.72743200

H -0.87761700 3.43688400 -3.72812300

**0Co(+)B-TS2B/3B**

Atom x y z

C 3.61831600 1.23949300 -0.33137400

C 5.00210100 1.28744500 -0.47608900

C 5.72227000 0.09366000 -0.55478500

C 5.04608300 -1.12532500 -0.47346600

C 3.66138600 -1.12720800 -0.32904700

N 2.96329600 0.04390000 -0.27937800

H 6.79981700 0.11321400 -0.66793900

H 5.51408700 2.24138900 -0.52408500

H 5.59204600 -2.06033400 -0.51911800

C 2.68909800 2.34794300 -0.19928700

C 2.77310500 -2.26851000 -0.19593000

N 1.51818800 -1.93812100 -0.00272300

N 1.44715000 1.97260900 -0.00452700

C 3.30501700 -3.66955600 -0.27861800

H 3.81431200 -3.83276200 -1.23338900

H 4.04096100 -3.85192400 0.51094000

H 2.51329700 -4.40920300 -0.18222200

C 3.16970400 3.76724200 -0.28474800

H 3.91033300 3.97337300 0.49439300

H 3.65872200 3.95103600 -1.24643400

H 2.35375800 4.47809300 -0.17471600

C 0.52435900 -2.96680800 0.13412900

C 0.23978500 -3.48158300 1.41114800

C -0.17496100 -3.39524700 -1.00780200

C -0.78290100 -4.42628400 1.52709600

C -1.19056700 -4.34041700 -0.84282900

C -1.49927400 -4.84995600 0.41331100

H -1.02312400 -4.82544400 2.50781100

H -1.74987500 -4.67140000 -1.71233800

H -2.30101100 -5.57220800 0.52433300

C 0.41750600 2.96506100 0.13588600

C -0.30075200 3.36916500 -1.00314400

C 0.11833400 3.46732400 1.41465100

C -1.35026700 4.27569300 -0.83335700

C -0.93795200 4.37362400 1.53529600

C -1.67349400 4.77167600 0.42451200

H -1.92506200 4.58640800 -1.70023600

H -1.18941900 4.76236800 2.51736900

H -2.50167200 5.46281000 0.53917500

C 0.06332200 2.86544100 -2.37894600

H 0.96738000 3.35500200 -2.75865200

H 0.26364600 1.79149200 -2.38321400

H -0.73847600 3.06641300 -3.09132900

C 0.92704500 3.06341600 2.62300600

H 1.09814700 1.98520300 2.65695300

H 1.91357000 3.54065700 2.62427700

H 0.42302900 3.35914000 3.54465200

C 0.17384700 -2.87556700 -2.38162700

H 0.32732300 -1.79393100 -2.38453800

H 1.10022900 -3.32486000 -2.75725600

H -0.61501900 -3.11075200 -3.09798500

C 1.02970800 -3.05014600 2.62234500

H 2.03116600 -3.49518700 2.62812600

H 1.16555600 -1.96694600 2.65526400

H 0.53182300 -3.36096900 3.54235300

Co 1.17199000 0.01143400 0.07977300

C -0.63410100 -0.01987900 1.07537800

H -0.74120800 0.88888300 1.66038300

H -0.71197600 -0.93047100 1.66230500

C -1.21518100 -0.03073800 -0.20304100

H -1.26794600 -0.94731300 -0.77270500

H -1.29487200 0.88132900 -0.77674600

Al -5.81010200 -0.05583200 -0.23110500

C -6.24878100 -1.70730100 -1.28914900

H -5.86709200 -1.67322100 -2.31850100

H -5.85091700 -2.62515600 -0.83600600

H -7.33467500 -1.85561100 -1.37273700

C -6.31392600 -0.13288700 1.71082900

H -5.95950900 -1.04425500 2.21039500

H -5.92542900 0.71466100 2.29090000

H -7.40508800 -0.11764200 1.84309200

C -3.57715700 -0.05883000 -0.20734300

H -3.42463300 -0.99249500 0.31668900

H -3.45423500 -0.04850400 -1.28328300

H -3.43537600 0.86663800 0.33371700

C -6.23456900 1.67903000 -1.15325800

H -7.31868400 1.83067200 -1.25169500

H -5.85270200 2.55508300 -0.61203900

H -5.82665500 1.73528000 -2.17157700

**0Co(+)B-3B**

Atom x y z

C -1.19022100 2.69903200 0.09065500

C -1.20735300 4.08769000 0.00535300

C 0.00000000 4.79119800 -0.02662900

C 1.20735400 4.08769000 0.00535100

C 1.19022200 2.69903200 0.09065400

N 0.00000000 2.01600700 0.16461300

H 0.00000000 5.87291900 -0.09399800

H -2.15153800 4.61892900 -0.04276000

H 2.15153900 4.61892800 -0.04276300

C -2.30446000 1.78299600 0.08871100

C 2.30446000 1.78299600 0.08871000

N 1.94226600 0.51438700 0.05862700

N -1.94226700 0.51438800 0.05862800

C 3.72183800 2.28156300 0.12352900

H 3.96964000 2.82413600 -0.79484800

H 3.86562700 2.97785800 0.95474200

H 4.43392700 1.46611300 0.23464300

C -3.72183800 2.28156400 0.12353100

H -3.86562600 2.97785800 0.95474500

H -3.96963900 2.82413900 -0.79484500

H -4.43392700 1.46611500 0.23464300

C 2.93470200 -0.51700000 0.06980300

C 3.20928900 -1.17556200 1.28220100

C 3.57632800 -0.88764200 -1.12540900

C 4.14833000 -2.20879500 1.27967500

C 4.50493000 -1.93131000 -1.08214900

C 4.79362400 -2.58913000 0.10766500

H 4.36988500 -2.72251000 2.21060900

H 5.00217300 -2.23128900 -2.00003600

H 5.51507200 -3.39987800 0.12111200

C -2.93470300 -0.51699900 0.06980300

C -3.57632800 -0.88764100 -1.12540900

C -3.20928900 -1.17556300 1.28220100

C -4.50492900 -1.93131000 -1.08215000

C -4.14833000 -2.20879700 1.27967400

C -4.79362300 -2.58913100 0.10766300

H -5.00217200 -2.23128800 -2.00003700

H -4.36988400 -2.72251200 2.21060800

H -5.51507100 -3.39987900 0.12111000

C -3.28783500 -0.17559600 -2.42416800

H -3.78451900 0.80004800 -2.47138300

H -2.21902700 0.00185900 -2.55616400

H -3.64496800 -0.76086800 -3.27382200

C -2.51468600 -0.76865000 2.55763000

H -1.42689000 -0.81983900 2.45470800

H -2.75036600 0.26212600 2.84046600

H -2.80881900 -1.41710400 3.38517900

C 3.28783400 -0.17559800 -2.42416800

H 2.21902600 0.00185800 -2.55616400

H 3.78451900 0.80004600 -2.47138500

H 3.64496600 -0.76087100 -3.27382300

C 2.51468600 -0.76864800 2.55763000

H 2.75036500 0.26212800 2.84046400

H 1.42689000 -0.81983800 2.45470800

H 2.80882000 -1.41710100 3.38518000

C -0.00000100 -1.52365300 -0.97712000

H -0.87897400 -1.60105400 -1.62855400

H 0.87897200 -1.60105400 -1.62855500

C 0.00000000 -2.72839400 -0.01594600

H -0.87712800 -2.69397500 0.64142400

H 0.87712800 -2.69397500 0.64142400

C 0.00000000 -4.08374500 -0.74323900

H -0.88312800 -4.18430000 -1.38210000

H 0.88312900 -4.18429900 -1.38210000

H 0.00000100 -4.92387500 -0.03852200

Co 0.00000000 0.20716300 -0.01227000

**0Co(+)B-1C**

C -1.03156700 3.20945500 0.05767100

C -0.99338300 4.60093800 0.10180400

C 0.24332900 5.24880000 0.12674000

C 1.41743100 4.49326700 0.10596100

C 1.33178900 3.10384800 0.06163100

N 0.11985900 2.47835700 0.03862600

H 0.29169800 6.33096000 0.16139000

H -1.91375900 5.17308800 0.11680500

H 2.38484300 4.98169500 0.12456700

C -2.19247800 2.33764100 0.02110700

C 2.41026900 2.13182800 0.02859000

N 1.99762600 0.88649200 -0.00624100

N -1.89151500 1.06094200 -0.01341900

C 3.84310300 2.58095500 0.03023400

H 4.03509600 3.25686400 -0.80878500

H 4.07134400 3.13634600 0.94571100

H 4.53267300 1.74301000 -0.04060000

C -3.58006400 2.91116300 0.01812600

H -3.75459100 3.50256400 0.92267700

H -3.71688200 3.58408500 -0.83414300

H -4.33992200 2.13483800 -0.03380300

C 2.96935300 -0.16994600 -0.05346200

C 3.46499500 -0.70116200 1.14814800

C 3.37667400 -0.66364900 -1.30386800

C 4.40695400 -1.72943300 1.07433700

C 4.32061600 -1.69309100 -1.32956800

C 4.83835000 -2.22112600 -0.15220800

H 4.79422100 -2.15692800 1.99410300

H 4.64385300 -2.08808500 -2.28805800

H 5.56247600 -3.02819400 -0.18992500

C -2.95049300 0.09225800 -0.06140300

C -3.37893100 -0.38365200 -1.31187500

C -3.49906500 -0.38620400 1.13931900

C -4.39444700 -1.34216600 -1.33910500

C -4.51404100 -1.34304700 1.06416700

C -4.96411600 -1.81718400 -0.16279500

H -4.73321100 -1.72409400 -2.29737900

H -4.94277000 -1.72955300 1.98361000

H -5.74604600 -2.56844000 -0.20168800

C -2.75530000 0.12217100 -2.58805700

H -2.98552800 1.17808300 -2.76710100

H -1.66551300 0.03878800 -2.55484700

H -3.11547800 -0.44436100 -3.44841100

C -3.00411100 0.11137600 2.47443000

H -1.91292900 0.08395800 2.52940400

H -3.30553100 1.14759200 2.66441700

H -3.40113700 -0.49939100 3.28684100

C 2.81336000 -0.09750100 -2.58323100

H 1.72036800 -0.07889000 -2.56104000

H 3.14260300 0.93280800 -2.75712700

H 3.12794500 -0.69192100 -3.44284100

C 2.99740500 -0.17617000 2.48284500

H 3.37988900 0.83055700 2.68466600

H 1.90718300 -0.11443700 2.52762200

H 3.33613700 -0.82285700 3.29408700

Co 0.04025400 0.65305800 -0.00031300

Al -0.24771600 -3.91962400 0.14614500

C -0.77778800 -4.25881400 -1.74172100

H -1.74561900 -3.81596200 -2.00518100

H -0.04539600 -3.88285500 -2.46653300

H -0.87062100 -5.33651900 -1.93525200

C 1.59326200 -4.44059000 0.68302200

H 2.36670600 -4.13938200 -0.03143500

H 1.88873200 -4.03564600 1.65818100

H 1.66399400 -5.53409100 0.77332700

C -0.03876400 -1.35060300 0.01007100

H 0.77785800 -1.75649800 -0.59300800

H -1.01807200 -1.68072400 -0.34391000

H 0.10476400 -1.60595900 1.06937400

C -1.64588800 -4.09196600 1.55005400

H -1.88220100 -5.15093700 1.72640300

H -1.33353200 -3.68721300 2.52075400

H -2.59069900 -3.60467400 1.28714900

**1Co(+)B**

Atom x y z

C 1.17456000 2.41075600 -0.07718100

C 1.21197800 3.80692300 -0.08130600

C -0.00000300 4.49725600 -0.00001700

C -1.21198300 3.80692200 0.08128500

C -1.17456100 2.41075500 0.07719400

N 0.00000100 1.78262600 0.00002000

H -0.00000400 5.58114700 -0.00003100

H 2.14731200 4.34928000 -0.14229800

H -2.14731800 4.34927800 0.14225600

C 2.32828200 1.45960400 -0.14324300

C -2.32828100 1.45960200 0.14325500

N -2.02224500 0.19992800 0.08650200

N 2.02224600 0.19992900 -0.08652300

C -3.71258900 2.01467900 0.28200600

H -3.76892000 2.67732900 1.15086300

H -3.97812500 2.61573400 -0.59341700

H -4.45494000 1.22839400 0.39779900

C 3.71259200 2.01468600 -0.28196000

H 3.76893800 2.67734300 -1.15081100

H 3.97811000 2.61573400 0.59347300

H 4.45494600 1.22840400 -0.39774800

C -3.02828400 -0.82693400 0.10611500

C -3.76703800 -1.11070800 -1.05594700

C -3.16358100 -1.58861900 1.28094000

C -4.67776200 -2.16968100 -1.00430900

C -4.09418000 -2.62814500 1.28563200

C -4.84935700 -2.91813700 0.15405400

H -5.25539600 -2.40933000 -1.89131700

H -4.22209200 -3.21867500 2.18708500

H -5.56371900 -3.73376400 0.17234700

C 3.02828500 -0.82693300 -0.10611900

C 3.76702900 -1.11069900 1.05595100

C 3.16359000 -1.58862800 -1.28093700

C 4.67775100 -2.16967500 1.00432900

C 4.09418800 -2.62815500 -1.28561300

C 4.84935500 -2.91814000 -0.15402600

H 5.25537600 -2.40931900 1.89134500

H 4.22210700 -3.21869300 -2.18706100

H 5.56371500 -3.73376800 -0.17230600

C 3.58348000 -0.32602200 2.33270700

H 4.06987700 0.65425800 2.29053700

H 2.52823200 -0.15250300 2.56105200

H 4.02017900 -0.85945900 3.17761700

C 2.33063900 -1.28985400 -2.50213300

H 1.25567400 -1.36738600 -2.28928800

H 2.50373600 -0.28120700 -2.88901500

H 2.54941100 -1.99276200 -3.30643000

C -2.33061700 -1.28983600 2.50212600

H -1.25565400 -1.36737400 2.28927100

H -2.50370700 -0.28118600 2.88900200

H -2.54938300 -1.99273800 3.30643100

C -3.58349600 -0.32603900 -2.33270900

H -4.06984900 0.65426200 -2.29052500

H -2.52824700 -0.15256500 -2.56108300

H -4.02024200 -0.85945800 -3.17760500

Co -0.00000100 -0.18030400 -0.00002600

**1Co(+)B-1B**

Atom x y z

C 1.16360000 2.43085300 -0.08676600

C 1.19967200 3.82539000 -0.15475400

C -0.00000800 4.52783300 -0.18076800

C -1.19968200 3.82538500 -0.15456400

C -1.16360300 2.43084800 -0.08662300

N 0.00000500 1.76412200 -0.03729600

H -0.00001600 5.61064600 -0.22925200

H 2.14248600 4.35504000 -0.18811000

H -2.14250200 4.35503600 -0.18774200

C 2.38581500 1.57450300 -0.08843700

C -2.38583100 1.57448000 -0.08829100

N -2.18006100 0.30888100 -0.03236800

N 2.18001400 0.30889700 -0.03242200

C -3.72905400 2.24205300 -0.18332700

H -3.89510300 2.90692600 0.66943100

H -3.79011500 2.85671700 -1.08615600

H -4.53475900 1.51268300 -0.21182700

C 3.72905300 2.24203400 -0.18363000

H 3.79014300 2.85644300 -1.08663200

H 3.89510200 2.90713700 0.66894400

H 4.53473700 1.51263600 -0.21192500

C -3.27717600 -0.61506300 -0.03976400

C -3.60043100 -1.25527000 -1.24901500

C -3.93725600 -0.92105400 1.16290600

C -4.62071600 -2.20865400 -1.23501800

C -4.94644200 -1.88720600 1.12743800

C -5.29050000 -2.52603600 -0.05822200

H -4.88889700 -2.70770300 -2.16078800

H -5.46597200 -2.13929200 2.04646100

H -6.07666000 -3.27290500 -0.06472900

C 3.27712500 -0.61507100 -0.03976100

C 3.93713900 -0.92098100 1.16297700

C 3.60044300 -1.25534400 -1.24894500

C 4.94627400 -1.88718600 1.12764400

C 4.62068800 -2.20877600 -1.23481400

C 5.29037200 -2.52611800 -0.05795400

H 5.46575200 -2.13921900 2.04671000

H 4.88890700 -2.70789900 -2.16053300

H 6.07650100 -3.27302100 -0.06436300

C 3.58019000 -0.23339900 2.45864600

H 3.93275900 0.80325400 2.48485900

H 2.49958800 -0.20446000 2.62687800

H 4.03471500 -0.74542200 3.30750200

C 2.87865800 -0.91422000 -2.52906100

H 1.79250700 -1.01056300 -2.42377200

H 3.07233700 0.11446300 -2.85006500

H 3.19164800 -1.57181400 -3.34072400

C -3.58037400 -0.23361300 2.45867400

H -2.49974300 -0.20377800 2.62650000

H -3.93387200 0.80271400 2.48537800

H -4.03412600 -0.74631700 3.30753800

C -2.87845600 -0.91417400 -2.52903200

H -3.07107800 0.11487900 -2.84946000

H -1.79238600 -1.01171800 -2.42390700

H -3.19219600 -1.57101400 -3.34101200

Co 0.00009500 -0.30915300 0.17041700

C 0.68508400 -2.28105900 0.63572000

H 1.24678800 -2.20441800 1.56140900

H 1.25331400 -2.62761800 -0.22081200

C -0.68496300 -2.28106800 0.63542600

H -1.25279400 -2.62757100 -0.22140700

H -1.24708400 -2.20453600 1.56086000

**1Co(+)B-2B**

Atom x y z

C 1.12467500 0.63400200 -2.18520400

C 1.20650000 1.40812500 -3.34423600

C 0.03486200 1.88880600 -3.91871700

C -1.18855600 1.57010100 -3.33791900

C -1.20358800 0.80041400 -2.17323800

N -0.06055700 0.37408500 -1.60475200

H 0.07456300 2.50134500 -4.81207800

H 2.16558900 1.63947700 -3.78850500

H -2.11102500 1.92040100 -3.78302300

C 2.29998300 0.00054200 -1.53449500

C -2.44665200 0.35891200 -1.49269800

N -2.28367500 -0.36590000 -0.44063300

N 2.04699300 -0.72172200 -0.49875500

C -3.77703900 0.75422000 -2.07786200

H -3.88336600 1.84302000 -2.09335300

H -3.87214800 0.40507900 -3.11012800

H -4.59991100 0.33883600 -1.49997500

C 3.66456800 0.21667900 -2.13348600

H 3.69499000 -0.11208500 -3.17631100

H 3.92257900 1.27994800 -2.11988200

H 4.42737000 -0.32813400 -1.58131800

C -3.39129500 -0.94748300 0.24837700

C -3.77705000 -2.25396400 -0.10920400

C -4.01628500 -0.26067700 1.30629500

C -4.79989400 -2.86653000 0.61794400

C -5.03476000 -0.91627200 2.00333100

C -5.42582400 -2.20805400 1.67001900

H -5.10437500 -3.87432500 0.35151500

H -5.52522700 -0.39827400 2.82193200

H -6.21527300 -2.69959600 2.22903100

C 3.06086700 -1.49879300 0.14119100

C 3.82584000 -0.96846900 1.19707300

C 3.20636400 -2.83940800 -0.26866600

C 4.73839000 -1.81395400 1.83524400

C 4.12942300 -3.64388400 0.40218100

C 4.89113300 -3.14061000 1.45047800

H 5.33654400 -1.41581300 2.64920000

H 4.24822800 -4.67845900 0.09398100

H 5.60238000 -3.77901800 1.96418500

C 3.68245100 0.46396100 1.64795700

H 3.72777600 1.17447400 0.81907600

H 2.73143000 0.64038400 2.15632400

H 4.47632600 0.72917700 2.34758900

C 2.39994300 -3.39222800 -1.41841500

H 1.33562900 -3.16749300 -1.31238300

H 2.71591100 -2.96820400 -2.37810800

H 2.51558500 -4.47527800 -1.48833100

C -3.62060400 1.14686400 1.67688700

H -2.55499400 1.23117300 1.89690300

H -3.82796800 1.85922500 0.87190400

H -4.17099000 1.48495200 2.55607600

C -3.12239600 -2.96968700 -1.26560900

H -3.42358100 -2.54351800 -2.22928900

H -2.03275200 -2.90296700 -1.22056100

H -3.40045000 -4.02507500 -1.27776200

Co -0.10789000 -0.37805700 0.33282900

C -0.23155700 -2.27198200 1.29470200

H 0.64669300 -2.84195000 1.01233700

H -1.18942600 -2.71730100 1.04867500

C -0.14479200 -1.27881800 2.24951600

H -1.03126900 -0.91783100 2.76152100

H 0.79912800 -1.04575900 2.73189300

Al 0.69442500 3.91423100 1.27478500

C 1.60729000 4.27721000 -0.49577000

H 2.53187400 3.69440800 -0.62822500

H 0.97168500 4.05908100 -1.36640100

H 1.90315700 5.33038500 -0.59754800

C -1.05066200 4.90057000 1.47944300

H -1.73283200 4.74825200 0.63012500

H -1.60660500 4.60547900 2.38028500

H -0.90675400 5.98709800 1.55763200

C 0.15740800 1.84302800 1.16607900

H -0.67333500 1.90005600 0.46611300

H 1.09333900 1.44282900 0.77498000

H -0.10019800 1.51932600 2.17000600

C 1.93675200 4.08695300 2.84905600

H 2.27620900 5.12262900 2.98995100

H 1.46906200 3.79150200 3.79839600

H 2.84967300 3.48238500 2.75243100

**1Co(+)B-TS2B/3B**

Atom x y z

C -1.09017700 -0.82058000 2.45619800

C -1.10467500 -0.85065700 3.84637600

C 0.09060000 -0.73108000 4.55901100

C 1.28734000 -0.61523500 3.84854100

C 1.27238500 -0.59531900 2.45762100

N 0.08730000 -0.67011200 1.76157200

H 0.09073400 -0.74146300 5.64262300

H -2.04150200 -0.96573400 4.37824200

H 2.22736900 -0.54688700 4.38292800

C -2.27752600 -0.97527700 1.62739300

C 2.47266100 -0.56277900 1.63291200

N 2.28563500 -0.52323000 0.34134500

N -2.10042600 -0.85847200 0.33868800

C 3.83115000 -0.62784600 2.28987600

H 3.97456300 0.20968400 2.97858200

H 3.94816400 -1.54692600 2.87142900

H 4.62815800 -0.59419600 1.54943800

C -3.60634100 -1.28472500 2.27358800

H -3.54116900 -2.16870500 2.91338200

H -3.93795100 -0.45329600 2.90311500

H -4.37525700 -1.46396100 1.52442200

C 3.37131800 -0.64010100 -0.57167400

C 3.74074800 -1.92204500 -1.02826200

C 4.01362800 0.51313300 -1.06249800

C 4.74381800 -2.02418800 -1.99485600

C 5.01231500 0.36308600 -2.02797200

C 5.37600700 -0.89328200 -2.49943900

H 5.02949900 -3.00863200 -2.35435300

H 5.51050500 1.24914100 -2.41094400

H 6.14965700 -0.99064900 -3.25432800

C -3.16156400 -1.07745100 -0.58631300

C -4.02726300 -0.02797900 -0.94803100

C -3.28306300 -2.35099700 -1.18392700

C -4.97744700 -0.25851000 -1.94792800

C -4.24976500 -2.53621400 -2.17317700

C -5.08735100 -1.49703900 -2.56640500

H -5.64166500 0.55114600 -2.23727500

H -4.34498900 -3.51256400 -2.63960300

H -5.82610800 -1.65575900 -3.34544700

C -3.99437400 1.30676700 -0.24451000

H -4.68862200 1.32001200 0.60412300

H -3.00847700 1.54434900 0.15229000

H -4.29618000 2.11377300 -0.91565700

C -2.42284600 -3.50538100 -0.73198300

H -1.36664300 -3.23345700 -0.68850900

H -2.70290400 -3.84329500 0.27223000

H -2.53074000 -4.35825200 -1.40508400

C 3.65971900 1.88128900 -0.53686800

H 2.58552100 2.06580900 -0.57041200

H 3.96594400 2.00605100 0.50766200

H 4.15387600 2.66381800 -1.11547500

C 3.08629600 -3.16138800 -0.46972400

H 3.38627800 -3.34399300 0.56819200

H 1.99750700 -3.07606600 -0.47139700

H 3.36433300 -4.04387200 -1.04937900

Co 0.06960500 -0.49764800 -0.18862000

C 0.20278900 -1.21747300 -2.13692400

H -0.68423400 -1.79121200 -2.38824900

H 1.14578700 -1.73048400 -2.29484000

C 0.17161000 0.17777600 -2.44405600

H 1.10322000 0.62553100 -2.76986900

H -0.69481900 0.57452400 -2.96269800

Al -0.59009100 4.46041300 -0.05611300

C -1.19393700 3.95159200 1.75906400

H -1.36838100 4.85162700 2.36545500

H -2.13500900 3.39165700 1.76867300

H -0.45761000 3.35574100 2.30930400

C 1.27436200 5.07739200 -0.30263200

H 1.99215400 4.58814500 0.36418700

H 1.64522200 4.95620200 -1.32636000

H 1.34252400 6.15275000 -0.08507300

C -0.13897800 1.64754400 -1.01631000

H 0.32309600 1.76078200 -0.02669200

H -1.21326800 1.80561400 -0.96705300

H 0.33156600 2.34762100 -1.70179300

C -1.91878400 4.88449500 -1.45944500

H -2.84404400 4.30479600 -1.37668600

H -2.21420300 5.94128100 -1.39939000

H -1.53353500 4.73800700 -2.47462100

**1Co(+)B-3B**

Atom x y z

C 1.18583200 2.67571500 0.10616600

C 1.20677500 4.06507000 0.03196000

C 0.00009800 4.77249000 0.03276400

C -1.20661600 4.06512200 0.03195700

C -1.18572700 2.67577300 0.10617000

N 0.00002700 2.00769300 0.25831300

H 0.00011800 5.85468700 -0.02788900

H 2.14657300 4.59810200 -0.05356500

H -2.14638800 4.59819900 -0.05356500

C 2.33869100 1.79857900 -0.03424000

C -2.33863600 1.79868500 -0.03424700

N -2.05967300 0.52199100 -0.15754700

N 2.05967500 0.52188100 -0.15758000

C -3.73055200 2.37676500 -0.05949200

H -3.99218600 2.82686700 0.90323900

H -3.80972000 3.16383000 -0.81412600

H -4.47265300 1.61497600 -0.29141600

C 3.73064800 2.37654900 -0.05941500

H 3.80990700 3.16361100 -0.81404500

H 3.99229200 2.82661600 0.90332500

H 4.47268900 1.61470000 -0.29133600

C -3.07620400 -0.46536400 -0.29120600

C -3.21970600 -1.09301600 -1.54538200

C -3.84885400 -0.87263800 0.81430800

C -4.16372200 -2.11081300 -1.68210500

C -4.77505500 -1.90403300 0.63291200

C -4.94028100 -2.51858300 -0.60207400

H -4.28437700 -2.59294100 -2.64792300

H -5.36918100 -2.23072500 1.48160900

H -5.66318700 -3.31932700 -0.72086900

C 3.07621000 -0.46549600 -0.29117000

C 3.84876300 -0.87277300 0.81441300

C 3.21984800 -1.09310100 -1.54534300

C 4.77497400 -1.90417000 0.63309100

C 4.16387300 -2.11091000 -1.68199300

C 4.94030600 -2.51871300 -0.60188900

H 5.36900600 -2.23089500 1.48184100

H 4.28462400 -2.59301500 -2.64781000

H 5.66321100 -3.31946800 -0.72062100

C 3.69351600 -0.23103100 2.17159700

H 4.24269300 0.71447700 2.24066500

H 2.64878200 -0.01641300 2.40142300

H 4.08234800 -0.88584500 2.95384600

C 2.37357200 -0.66452000 -2.71722000

H 1.30655000 -0.74220500 -2.48831900

H 2.55477500 0.37878400 -2.99361100

H 2.57777100 -1.28294500 -3.59348300

C -3.69364100 -0.23092400 2.17150900

H -2.64886800 -0.01661600 2.40146900

H -4.24253300 0.71474800 2.24053400

H -4.08276300 -0.88562700 2.95370300

C -2.37327200 -0.66448400 -2.71716200

H -2.55424100 0.37887400 -2.99347000

H -1.30628000 -0.74241400 -2.48817900

H -2.57751000 -1.28280800 -3.59348800

C -0.00008100 -1.59217100 1.58988000

H 0.87493800 -1.59032100 2.25564500

H -0.87489800 -1.59010100 2.25590000

C -0.00039300 -2.89071600 0.76399600

H 0.87524500 -2.91651000 0.10201300

H -0.87623800 -2.91625300 0.10227700

C -0.00041100 -4.17018800 1.61519300

H 0.88218500 -4.20890700 2.26221300

H -0.88284900 -4.20870900 2.26244000

H -0.00058800 -5.07527900 0.99641500

Co 0.00003100 0.05375100 0.42648100

**1Co(+)B-1C**

C -1.16670100 3.00936200 -0.70197100

C -1.18002300 4.35652600 -1.04931900

C 0.03006600 5.02138500 -1.27144700

C 1.23277400 4.33780400 -1.06733700

C 1.20366100 2.99123500 -0.71834200

N 0.01357300 2.31927600 -0.64818900

H 0.03623500 6.07073900 -1.54223500

H -2.11673300 4.89607600 -1.12455500

H 2.17644500 4.86287000 -1.15672000

C -2.32569300 2.22073400 -0.30155700

C 2.35482600 2.18718200 -0.32609900

N 2.06954900 1.01220800 0.17886400

N -2.05355200 1.03938900 0.19516400

C 3.74844100 2.73860700 -0.47807300

H 4.00502400 2.88214200 -1.53214800

H 3.83417600 3.71334700 0.00953500

H 4.48831200 2.07550600 -0.03403700

C -3.71194900 2.79462300 -0.43801400

H -3.78018800 3.76223500 0.06650600

H -3.97163600 2.95994500 -1.48804100

H -4.45931000 2.13547300 -0.00083900

C 3.08180100 0.10351700 0.60514100

C 3.23220800 -0.10712100 1.99041500

C 3.83865400 -0.63058900 -0.32829700

C 4.17189200 -1.04132000 2.42635500

C 4.76010400 -1.56468800 0.15501200

C 4.93432300 -1.76882100 1.51802400

H 4.29898800 -1.20451100 3.49252300

H 5.34006400 -2.14510900 -0.55620100

H 5.65218000 -2.50158700 1.87189200

C -3.07586000 0.13839900 0.61255700

C -3.84761000 -0.56978400 -0.32921500

C -3.22097600 -0.09461200 1.99465200

C -4.78004800 -1.49832800 0.14361000

C -4.17180700 -1.02229100 2.42007300

C -4.95024200 -1.72261400 1.50400400

H -5.37249300 -2.05822100 -0.57384200

H -4.29486800 -1.20232600 3.48397100

H -5.67713200 -2.45040600 1.84956300

C -3.68453500 -0.35966800 -1.81522700

H -4.22887100 0.52444800 -2.16541000

H -2.63860100 -0.22639600 -2.09739700

H -4.07178700 -1.21617900 -2.36950800

C -2.36765400 0.64725300 2.99226800

H -1.30200700 0.46837600 2.81735900

H -2.51354500 1.73016300 2.93440300

H -2.59743400 0.33300200 4.01205000

C 3.67315300 -0.44058000 -1.81647900

H 2.63044200 -0.27804900 -2.09413300

H 4.24332800 0.42005700 -2.18386900

H 4.02910900 -1.31850700 -2.35799700

C 2.39765500 0.66603600 2.98030800

H 2.56494900 1.74488400 2.90576100

H 1.32784200 0.50652800 2.81275100

H 2.62596200 0.36264000 4.00371000

Co 0.00571800 0.41938800 -0.19728400

Al -0.03503000 -4.12657200 -1.14575300

C -1.60657400 -4.21877100 -2.36178600

H -2.54781100 -3.94424500 -1.87081500

H -1.50630800 -3.58047900 -3.24808500

H -1.74657600 -5.24110700 -2.73949700

C 1.76549400 -4.31522500 -1.96939800

H 1.86177800 -3.79020600 -2.92764600

H 2.57192100 -3.95453400 -1.31998600

H 1.99022500 -5.37052000 -2.17740800

C -0.01746200 -1.55323500 -0.69124000

H 0.78693700 -1.75722800 -1.40144200

H -0.99924000 -1.80242900 -1.09895800

H 0.15917700 -2.05622200 0.26654000

C -0.27279700 -4.77730100 0.71635500

H -0.37922900 -5.87083700 0.73523500

H 0.57581600 -4.54320100 1.37019600

H -1.17184000 -4.37656700 1.19950200