# Supporting Information

## Effect of low spin excited states for magnetic anisotropy of transition metal mononuclear single molecule magnets

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**Table S1:** First three non-relativistic excitation energies for all models ($cm^{-1}$). Values were extracted from CASSCF(n,5) and NEVPT2 considering all roots of all multiplicities stemming from d configurations. Models without Jahn-Teller distortion are presented

| | Co(II) | | | | Fe(II) | | | |
|---|---|---|---|---|---|---|---|---|
| | JT | | noJT | | JT | | noJT | |
| | CASSCF | NEVPT2 | CASSCF | NEVPT2 | CASSCF | NEVPT2 | CASSCF | NEVPT2 |
| 2-L | 3.8 | 15.4 | 7.3 | 7.1 | 26.3 | 35.7 | 8.9 | 3.9 |
| | 1915.8 | 2082.3 | 1396.1 | 1430.3 | 2272.6 | 2056.9 | 2017.6 | 1893.6 |
| | 3247 | 3652 | 2210.1 | 2410.5 | 4694.3 | 5234.2 | 3237.8 | 3498.1 |
| 3-TP | 2217.8 | 2682.7 | 1408.2 | 1760.1 | 609 | 684.1 | 63.7 | 128.4 |
| | 2219.6 | 2685.2 | 1464.5 | 1857.3 | 1008 | 1311.3 | 70.7 | 134.6 |
| | 5741.3 | 7001.8 | 3706 | 4517.7 | 6366.5 | 6993 | 3132.4 | 3296.6 |
| 4-SP | 1195.9 | 1546.9 | 1000.5 | 1213.2 | 565.1 | 577.4 | 68.8 | 56.8 |
| | 1195.9 | 1546.9 | 1000.6 | 1213.3 | 1853.5 | 2329.7 | 402.4 | 495.2 |
| | 2947.2 | 3530.1 | 2475.9 | 2958.9 | 3429.6 | 3549.4 | 2879.8 | 2924.7 |
| 4-Td | 3016.5 | 3674.7 | 2268.5 | 2837.3 | 304.3 | 400.4 | 203.4 | 254.9 |
| | 3474 | 4195.7 | 2542 | 3130.9 | 3049.9 | 3526.1 | 2240.6 | 2653.1 |
| | 3700.8 | 4526.9 | 2687.2 | 3354.8 | 3901.3 | 4627.4 | 2925.8 | 3521 |
| 5-SPY | 1155.2 | 1518.9 | 664.5 | 850.2 | 970.9 | 1043.9 | 526.2 | 587.3 |
| | 1233.1 | 1670.8 | 824.2 | 1098.2 | 2171.3 | 2637.1 | 862.2 | 1055.6 |
| | 2779.7 | 3388.2 | 2306.5 | 2838.4 | 3729.4 | 4447.2 | 2704.4 | 3293.5 |
| 5-TBP | 2196.3 | 2885.2 | 588.4 | 827.2 | 913.8 | 1125.8 | 638 | 802 |
| | 2346.4 | 3070.6 | 679.4 | 975.5 | 3206.9 | 3867.7 | 2338.9 | 2914.6 |
| | 3427.8 | 4322.7 | 2500.9 | 3060.8 | 3452.6 | 4256.6 | 2697.2 | 3404.8 |
| 6-Oh | 394.7 | 536.3 | 4.2 | 0.2 | 461.6 | 560.9 | 299.3 | 375.7 |
| | 400 | 542.3 | 4.5 | 11.6 | 574 | 730.6 | 602.8 | 759.1 |
| | 5500.1 | 6911.3 | 5398.3 | 6632.4 | 6801 | 8142.6 | 7085.5 | 8457.8 |

**Table S2:** D ($cm^{-1}$) and E/D values obtained by effective Hamiltonian method. Presented results correspond to models without Jahn-Teller distortion,

| | | CASSCF | | NEVPT2 | |
|---|---|---|---|---|---|
| | | $D_{All}$ | $E/D_{All}$ | $D_{All}$ | $E/D_{All}$ |
| Fe(II) | 5-SPY | 18.0 | 0.31 | -16.3 | 0.32 |
| | 5-TBP | -10.1 | 0.15 | -8.1 | 0.20 |
| Co(II) | 3-TP | 79.1 | 0.02 | 73.1 | 0.03 |
| | 4-SP | 87.0 | 0.00 | 83.4 | 0.00 |
| | 4-Td | -14.6 | 0.24 | -12.4 | 0.27 |
| | 5-SPY | -117.9 | 0.21 | -107.3 | 0.20 |
| | 5-TBP | 62.7 | 0.15 | 58.3 | 0.01 |

**Table S3:** D ($cm^{-1}$) and E/D values with differently optimized orbitals. Subindex 'All' indicates orbitals optimized from a CASSCF(n,5) calculation including all roots of all multiplicities while 'HSorbs' corresponds to orbitals from an analogous calculation including only highest multiplicity roots. Presented results correspond to models without Jahn-Teller distortion,

| | | CASSCF | | | | NEVPT2 | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | $D_{All}$ | $E/D_{All}$ | $D_{HSorbs}$ | $E/D_{HSorbs}$ | $D_{All}$ | $E/D_{All}$ | $D_{HSorbs}$ | $E/D_{HSorbs}$ |
| Fe(II) | 5-SPY | -22.1 | 0.28 | -22.2 | 0.28 | -19.9 | 0.25 | -19.9 | 0.25 |
| | 5-TBP | -11.1 | 0.24 | -11.1 | 0.24 | -8.8 | 0.27 | -8.8 | 0.27 |
| Co(II) | 3-TP | 133.8 | 0.02 | 134.6 | 0.02 | 108.3 | 0.03 | 111.8 | 0.03 |
| | 4-SP | 160.2 | 0.00 | 162.6 | 0.00 | 135.5 | 0.00 | 139.4 | 0.00 |
| | 4-Td | -18.6 | 0.25 | -18.6 | 0.24 | -14.8 | 0.27 | -15.0 | 0.27 |
| | 5-SPY | -185.3 | 0.17 | -185.2 | 0.17 | -147.7 | 0.17 | -152.7 | 0.17 |
| | 5-TBP | 83.7 | 0.02 | 84.1 | 0.02 | 69.4 | 0.01 | 71.5 | 0.02 |

**Table S4:** D-tensors ($cm^{-1}$) for S→S and S→S-1 contributions for CASSCF(n,5) calculations.

| | | Fe(II) | | | | | | Co(II) | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | S→S | | | S→S-1 | | | S→S | | | S→S-1 | | |
| 2-L | x | -5 | 0 | -83 | 4 | 0 | 0 | -26 | 0 | -18 | 11 | 0 | 0 |
| noJT | y | 0 | -5 | 3 | 0 | 4 | 0 | 0 | -7 | 0 | 0 | 14 | 0 |
| | z | -83 | 3 | -4800 | 0 | 0 | 2 | -18 | 0 | -36469 | 0 | 0 | 4 |
| 3-TP | x | -450 | 0 | 0 | 3 | 0 | 0 | -124 | 3 | 1 | 6 | 0 | 0 |
| noJT | y | 0 | -498 | 0 | 0 | 3 | 0 | 3 | -124 | 18 | 0 | 6 | 1 |
| | z | 0 | 0 | 0 | 0 | 0 | 5 | 1 | 18 | -2 | 0 | 1 | 14 |
| 4-Td | x | -17 | 0 | 0 | 2 | 0 | 0 | -62 | 0 | 0 | 8 | 0 | 0 |
| noJT | y | 0 | -7 | 0 | 0 | 4 | 0 | 0 | -40 | 0 | 0 | 9 | 0 |
| | z | 0 | 0 | -11 | 0 | 0 | 5 | 0 | 0 | -48 | 0 | 0 | 9 |
| 4-SP | x | -26 | 0 | -97 | 4 | 0 | 0 | -150 | 0 | 0 | 6 | 0 | 0 |
| noJT | y | 0 | -26 | 0 | 0 | 5 | 0 | 0 | 0 | 0 | 0 | 16 | 0 |
| | z | -97 | 0 | -429 | 0 | 0 | 2 | 0 | 0 | -150 | 0 | 0 | 6 |
| 5-SPY | x | -15 | -11 | -6 | 3 | -1 | -1 | -207 | 0 | 0 | 5 | 0 | 0 |
| noJT | y | -11 | -16 | -1 | -1 | 4 | 0 | 0 | 0 | 0 | 0 | 14 | 0 |
| | z | -6 | -1 | -14 | -1 | 0 | 5 | 0 | 0 | -54 | 0 | 0 | 7 |
| 5-TBP | x | -7 | -2 | -2 | 3 | -1 | 0 | -75 | 0 | 0 | 6 | 0 | 0 |
| noJT | y | -2 | -5 | -1 | -1 | 4 | 0 | 0 | -78 | 2 | 0 | 6 | 0 |
| | z | -2 | -1 | -17 | 0 | 0 | 4 | 0 | 2 | 0 | 0 | 0 | 14 |
| 6-Oh | x | -25 | 0 | -19 | 4 | 0 | -1 | -14858 | -10 | -276 | 6 | 0 | 0 |
| noJT | y | 0 | -17 | 0 | 0 | 5 | 0 | -10 | -13 | -451 | 0 | 15 | 0 |
| | z | -19 | 0 | -17 | -1 | 0 | 3 | -276 | -451 | -15461 | 0 | 0 | 6 |
| 2-L | x | -5 | 0 | 0 | 4 | 0 | 0 | -15 | 0 | -5 | 9 | 0 | 0 |
| JT | y | 0 | -2 | 0 | 0 | 4 | 0 | 0 | -12 | 0 | 0 | 13 | 0 |
| | z | 0 | 0 | -1604 | 0 | 0 | 2 | -5 | 0 | -64336 | 0 | 0 | 5 |
| 3-TP | x | -14 | -22 | 1 | 4 | -1 | 0 | -78 | 0 | 1 | 6 | 0 | 0 |
| JT | y | -22 | -40 | 0 | -1 | 3 | 0 | 0 | -76 | 11 | 0 | 6 | 1 |
| | z | 1 | 0 | -10 | 0 | 0 | 4 | 1 | 11 | -2 | 0 | 1 | 14 |
| 4-Td | x | -13 | 0 | 0 | 2 | 0 | 0 | -46 | 0 | 0 | 7 | 0 | 0 |
| JT | y | 0 | -5 | 0 | 0 | 4 | 0 | 0 | -29 | 0 | 0 | 9 | 0 |
| | z | 0 | 0 | -7 | 0 | 0 | 5 | 0 | 0 | -35 | 0 | 0 | 8 |
| 4-SP | x | -3 | 0 | 0 | 4 | 0 | 0 | -123 | 0 | 0 | 6 | 0 | 0 |
| JT | y | 0 | -6 | 0 | 0 | 5 | 0 | 0 | 0 | 0 | 0 | 17 | 0 |
| | z | 0 | 0 | -56 | 0 | 0 | 2 | 0 | 0 | -123 | 0 | 0 | 6 |
| 5-SPY | x | -10 | -2 | 0 | 2 | 0 | 0 | -111 | -12 | 0 | 7 | 0 | 0 |
| JT | y | -2 | -11 | 0 | 0 | 4 | 0 | -12 | -17 | 0 | 0 | 13 | 0 |
| | z | 0 | 0 | -5 | 0 | 0 | 5 | 0 | 0 | -52 | 0 | 0 | 7 |
| 5-TBP | x | -7 | -2 | -2 | 3 | -1 | 0 | -49 | 0 | 0 | 6 | 0 | 0 |
| JT | y | -2 | -4 | -1 | -1 | 4 | 0 | 0 | -51 | 1 | 0 | 6 | 0 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | z | -2 | -1 | -12 | 0 | 0 | 4 | 0 | 1 | -6 | 0 | 0 | 13 |
| 6-Oh | x | -17 | 0 | -13 | 4 | 0 | -1 | -128 | 48 | -49 | 9 | -1 | 1 |
| JT | y | 0 | -18 | 0 | 0 | 5 | 0 | 48 | -125 | -51 | -1 | 9 | 1 |
| | z | -13 | 0 | -12 | -1 | 0 | 3 | -49 | -51 | -126 | 1 | 1 | 9 |

Cartesian coordinates for all models

Calculations with fixed M-L distances:

Co(II)-2-L

| | | | |
|---|---|---|---|
| Co | -0.004588 | -0.000000 | -0.000009 |
| O | -0.006228 | -0.000000 | -2.112747 |
| H | 0.004067 | 0.814203 | -2.669994 |
| H | 0.004115 | -0.814203 | -2.669995 |
| O | -0.002949 | 0.000000 | 2.112729 |
| H | 0.002815 | 0.814222 | 2.670008 |
| H | 0.002767 | -0.814222 | 2.670008 |

Co(II)-3-TP

| | | | |
|---|---|---|---|
| Co | -0.041408 | 0.073935 | -0.000863 |
| O | -1.092835 | 1.888242 | -0.258660 |
| H | -1.374225 | 2.495942 | 0.464115 |
| H | -1.385463 | 2.260725 | -1.122617 |
| O | -1.102764 | -1.734427 | 0.258006 |
| H | -1.103351 | -2.193880 | 1.130175 |
| H | -1.111247 | -2.414482 | -0.455544 |
| O | 2.071142 | 0.064361 | -0.027398 |
| H | 2.581404 | -0.106348 | 0.798670 |
| H | 2.558748 | -0.334068 | -0.785886 |

Co(II)-4-SP

| | | | |
|---|---|---|---|
| Co | 0.000015 | -0.019102 | -0.000001 |
| O | -0.000130 | -0.001516 | -2.112666 |
| H | 0.000196 | 0.809472 | -2.658866 |
| H | 0.000187 | -0.802947 | -2.672947 |
| O | -2.112652 | -0.001706 | 0.000143 |
| H | -2.658773 | 0.809334 | 0.000099 |
| H | -2.673018 | -0.803077 | 0.000128 |
| O | 0.000160 | -0.001520 | 2.112664 |
| H | -0.000266 | 0.809466 | 2.658866 |
| H | -0.000252 | -0.802952 | 2.672943 |
| O | 2.112682 | -0.001706 | -0.000146 |
| H | 2.658804 | 0.809333 | -0.000119 |
| H | 2.673048 | -0.803078 | -0.000097 |

Co(II)-4-Td

| | | | |
|---|---|---|---|
| Co | -0.000000 | -0.000000 | 0.033946 |
| O | 1.725044 | -0.000000 | 1.253736 |
| H | 2.257223 | 0.789601 | 1.476832 |
| H | 2.257225 | -0.789601 | 1.476829 |
| O | -1.725044 | 0.000000 | 1.253736 |
| H | -2.257225 | 0.789601 | 1.476829 |
| H | -2.257223 | -0.789601 | 1.476831 |
| O | -0.000000 | 1.725044 | -1.185844 |
| H | 0.000001 | 2.652135 | -0.875336 |
| H | 0.000000 | 1.741678 | -2.163190 |
| O | -0.000000 | -1.725044 | -1.185844 |
| H | -0.000000 | -1.741678 | -2.163190 |

| | | | |
|---|---|---|---|
| H | -0.000000 | -2.652135 | -0.875336 |

Co(II)-5-TBP

| | | | |
|---|---|---|---|
| Co | 0.097018 | -0.002032 | 0.000263 |
| O | -0.945485 | 1.834586 | -0.060465 |
| H | -0.487269 | 2.696586 | -0.087363 |
| H | -1.906086 | 2.008302 | -0.066440 |
| O | 0.099545 | -0.070419 | -2.111366 |
| H | -0.318158 | 0.704612 | -2.541029 |
| H | -0.318656 | -0.870871 | -2.491031 |
| O | -0.973156 | -1.822763 | 0.057948 |
| H | -1.936216 | -1.982422 | 0.060661 |
| H | -0.527626 | -2.691395 | 0.085526 |
| O | 0.094490 | 0.066356 | 2.111893 |
| H | -0.323720 | 0.867738 | 2.489557 |
| H | -0.325159 | -0.707727 | 2.541382 |
| O | 2.209694 | -0.017918 | 0.003307 |
| H | 2.779501 | 0.019043 | 0.795630 |
| H | 2.781285 | -0.031678 | -0.788473 |

Co(II)-5-SPY

| | | | |
|---|---|---|---|
| Co | 0.000008 | -0.000000 | -0.090340 |
| O | 0.000029 | 0.000000 | 2.022398 |
| H | -0.000017 | 0.781493 | 2.605138 |
| H | -0.000078 | -0.781493 | 2.605138 |
| O | 0.000023 | 2.045650 | -0.618524 |
| H | 0.000034 | 2.848386 | -0.064042 |
| H | -0.000073 | 2.318269 | -1.556270 |
| O | -2.045648 | 0.000021 | -0.618504 |
| H | -2.569372 | 0.785892 | -0.356864 |
| H | -2.569367 | -0.785878 | -0.356933 |
| O | -0.000018 | -2.045650 | -0.618524 |
| H | 0.000022 | -2.318269 | -1.556270 |
| H | 0.000056 | -2.848386 | -0.064042 |
| O | 2.045652 | -0.000021 | -0.618545 |
| H | 2.569372 | 0.785866 | -0.356942 |
| H | 2.569377 | -0.785881 | -0.356873 |

Co(II)-6-Oh

| | | | |
|---|---|---|---|
| Co | -0.000003 | 0.000023 | -0.000005 |
| O | -0.000005 | -2.112715 | -0.000041 |
| H | 0.784775 | -2.690739 | 0.000648 |
| H | -0.784779 | -2.690748 | -0.000460 |
| O | 0.000452 | 0.000058 | -2.112743 |
| H | 0.000368 | 0.789716 | -2.686025 |
| H | 0.000806 | -0.789456 | -2.686224 |
| O | -2.112741 | 0.000025 | -0.000462 |
| H | -2.688677 | -0.000308 | -0.786790 |
| H | -2.688767 | 0.000069 | 0.785801 |
| O | -0.000001 | 2.112762 | 0.000030 |
| H | -0.784799 | 2.690752 | 0.000023 |
| H | 0.784842 | 2.690690 | -0.000132 |
| O | -0.000458 | -0.000013 | 2.112733 |
| H | -0.000368 | 0.789608 | 2.686066 |

| | | | |
|---|---|---|---|
| H | -0.000802 | -0.789566 | 2.686156 |
| O | 2.112735 | 0.000021 | 0.000450 |
| H | 2.688662 | -0.000005 | 0.786784 |
| H | 2.688760 | -0.000175 | -0.785812 |

Fe(II)-2-L

| | | | |
|---|---|---|---|
| Fe | 0.000001 | -0.000000 | -0.000000 |
| O | 0.041605 | -0.000599 | 2.150576 |
| H | -0.016054 | 0.799258 | 2.725848 |
| H | -0.016810 | -0.799241 | 2.727510 |
| O | -0.041602 | 0.000599 | -2.150576 |
| H | 0.016807 | 0.799243 | -2.727508 |
| H | 0.016053 | -0.799259 | -2.725849 |

Fe(II)-3-TP

| | | | |
|---|---|---|---|
| Fe | -0.000002 | -0.000000 | -0.001528 |
| O | -1.075491 | 1.862801 | 0.000063 |
| H | -0.649651 | 2.747356 | 0.001163 |
| H | -2.054455 | 1.936318 | -0.001526 |
| O | -1.075492 | -1.862802 | -0.001121 |
| H | -2.054452 | -1.936315 | 0.001903 |
| H | -0.649649 | -2.747355 | 0.000741 |
| O | 2.150975 | -0.000001 | -0.000094 |
| H | 2.704107 | 0.811052 | 0.002218 |
| H | 2.704109 | -0.811054 | -0.001820 |

Fe(II)-4-SP

| | | | |
|---|---|---|---|
| Fe | -0.000048 | -0.010472 | 0.000069 |
| O | -2.145911 | -0.007887 | 0.148311 |
| H | -2.652442 | 0.815553 | 0.303702 |
| H | -2.661331 | -0.555187 | -0.479914 |
| O | 0.147503 | -0.211463 | 2.136548 |
| H | 0.570301 | 0.473037 | 2.695052 |
| H | -0.660778 | -0.506471 | 2.606628 |
| O | 2.145815 | -0.008783 | -0.148172 |
| H | 2.652691 | 0.814292 | -0.304259 |
| H | 2.661319 | -0.556214 | 0.479846 |
| O | -0.147681 | -0.211830 | -2.136368 |
| H | -0.569976 | 0.472742 | -2.695174 |
| H | 0.660538 | -0.507319 | -2.606268 |

Fe(II)-4-Td

| | | | |
|---|---|---|---|
| Fe | -0.000000 | -0.000000 | 0.029735 |
| O | 0.000000 | -1.756267 | -1.212133 |
| H | 0.000002 | -1.778661 | -2.189835 |
| H | -0.000001 | -2.685013 | -0.905579 |
| O | 1.756266 | 0.000000 | 1.271603 |
| H | 2.287040 | 0.786185 | 1.510536 |
| H | 2.287037 | -0.786185 | 1.510540 |
| O | -0.000000 | 1.756266 | -1.212133 |
| H | 0.000001 | 2.685013 | -0.905579 |
| H | -0.000002 | 1.778661 | -2.189835 |
| O | -1.756267 | -0.000000 | 1.271603 |

| | | | |
|---|---|---|---|
| H | -2.287036 | 0.786186 | 1.510542 |
| H | -2.287041 | -0.786185 | 1.510535 |

Fe(II)-5-TBP

| | | | |
|---|---|---|---|
| Fe | 0.013894 | -0.025260 | -0.000013 |
| O | 0.188507 | 0.070099 | -2.141770 |
| H | -0.532780 | 0.465244 | -2.669929 |
| H | 0.536302 | -0.689267 | -2.649915 |
| O | -1.020694 | 1.860566 | -0.000396 |
| H | -0.788223 | 2.646845 | -0.530397 |
| H | -1.808905 | 2.087548 | 0.529112 |
| O | -1.094968 | -1.860338 | -0.172119 |
| H | -1.548227 | -2.278807 | 0.585479 |
| H | -1.541426 | -2.173657 | -0.981444 |
| O | 2.157345 | -0.076006 | 0.172478 |
| H | 2.753910 | 0.081587 | -0.585013 |
| H | 2.660953 | 0.133111 | 0.981890 |
| O | -0.160717 | -0.120617 | 2.141745 |
| H | -0.108162 | 0.700215 | 2.669766 |
| H | 0.293189 | -0.821264 | 2.650523 |

Fe(II)-5-SPY

| | | | |
|---|---|---|---|
| Fe | 0.017268 | -0.002338 | -0.060896 |
| O | 0.059478 | 0.016605 | 2.089585 |
| H | -0.582071 | 0.462677 | 2.674999 |
| H | 0.696998 | -0.443224 | 2.669151 |
| O | -0.070761 | 2.074093 | -0.615328 |
| H | -0.411536 | 2.814880 | -0.077495 |
| H | 0.576859 | 2.447566 | -1.244700 |
| O | -2.074118 | -0.084202 | -0.556994 |
| H | -2.537730 | 0.673956 | -0.962683 |
| H | -2.748279 | -0.672557 | -0.166407 |
| O | 0.084192 | -2.088240 | -0.581704 |
| H | -0.234347 | -2.357879 | -1.466553 |
| H | -0.160856 | -2.807555 | 0.033733 |
| O | 2.087548 | 0.070055 | -0.640039 |
| H | 2.749878 | 0.659377 | -0.228322 |
| H | 2.547475 | -0.763214 | -0.866345 |

Fe(II)-6-Oh

| | | | |
|---|---|---|---|
| Fe | -0.000000 | -0.000007 | 0.000000 |
| O | -2.150825 | -0.000009 | 0.025682 |
| H | -2.727644 | 0.784317 | -0.039039 |
| H | -2.727154 | -0.784619 | -0.040000 |
| O | -0.000001 | 2.150971 | -0.000001 |
| H | -0.217429 | 2.732706 | 0.751981 |
| H | 0.217430 | 2.732706 | -0.751982 |
| O | 0.025681 | -0.000006 | 2.150825 |
| H | 0.806337 | 0.001489 | 2.735253 |
| H | -0.762276 | -0.000946 | 2.725405 |
| O | 2.150825 | -0.000007 | -0.025681 |
| H | 2.727644 | 0.784319 | 0.039043 |
| H | 2.727154 | -0.784617 | 0.039995 |
| O | 0.000001 | -2.150986 | 0.000001 |

```
  H      0.216453   -2.732925   -0.752132
  H     -0.216454   -2.732925    0.752134
  O     -0.025682   -0.000009   -2.150825
  H     -0.806337    0.001498   -2.735252
  H      0.762276   -0.000952   -2.725405
```

Calculations allowing Jahn-Teller distortions:

```
Co(II)-2-L (JT)
Co -0.000048 -0.000000 0.000004
O 0.000171 -0.000005 1.878821
O -0.000269 0.000005 -1.878826
H -0.000069 -0.801145 2.459100
H -0.000072 0.801144 2.459086
H 0.000144 0.801149 -2.459100
H 0.000142 -0.801148 -2.459086

Co(II)-3-TP (JT)
Co 0.000142 0.001628 0.008344
O -0.962811 1.662417 -0.226764
O -0.971117 -1.654362 0.244160
O 1.934236 -0.006587 -0.015662
H -1.132371 -2.112827 1.098681
H -1.392110 -2.187379 -0.466317
H -1.371505 2.202443 0.485595
H -1.131627 2.115527 -1.082614
H 2.502725 -0.268012 -0.773844
H 2.524440 0.247152 0.728420

Co(II)-4-SP (JT)
Co 0.000001 -0.018709 0.000001
O -0.000121 -0.001776 -2.027174
O 0.000123 -0.001898 2.027177
O -2.027176 -0.002010 0.000122
O 2.027175 -0.002024 -0.000120
H -0.000059 -0.783882 -2.615271
H 0.000164 0.790842 -2.600937
H 0.000143 -0.784032 2.615235
H -0.000246 0.790692 2.600978
H -2.600991 0.790571 -0.000552
H 2.600994 0.790553 -0.000148
H -2.615222 -0.784154 0.000449
H 2.615216 -0.784173 0.000241

Co(II)-4-Td (JT)
Co 0.000000 -0.000000 0.022526
O 0.000002 1.640536 -1.137508
O -0.000002 -1.640536 -1.137508
O 1.628019 -0.000002 1.173709
O -1.628020 0.000002 1.173709
H -0.000022 1.663248 -2.115453
H 0.000020 -1.663248 -2.115453
H -0.000019 -2.569570 -0.830718
```

H 0.000022 2.569570 -0.830718
H -2.138222 -0.788259 1.449375
H 2.138221 0.788259 1.449377
H 2.138252 -0.788259 1.449331
H -2.138251 0.788259 1.449331

Co(II)-5-SPY (JT)
Co -0.000000 -0.000000 0.004930
O 0.030084 -2.067414 -0.528930
O -0.030087 2.067413 -0.528929
O 0.000004 -0.000000 2.019766
O -1.967135 -0.028626 -0.503031
O 1.967132 0.028626 -0.503040
H 0.596453 0.514913 2.598126
H -0.181104 -2.421479 -1.414075
H -0.247172 2.833948 0.035641
H 0.247161 -2.833950 0.035642
H 0.181111 2.421479 -1.414072
H -0.596448 -0.514910 2.598128
H -2.533602 -0.814564 -0.626503
H 2.533604 0.814563 -0.626496
H -2.534322 0.763427 -0.573580
H 2.534320 -0.763428 -0.573577

Co(II)-5-TBP (JT)
Co 0.007617 0.000206 -0.000027
O 0.004629 0.033738 2.126864
O 0.010604 -0.033325 -2.126861
O -0.993955 1.758840 -0.029160
O -1.014925 -1.746595 0.026076
O 2.024326 -0.011754 0.002995
H -0.493807 0.556618 -2.718545
H 0.360347 -0.749860 -2.690215
H 0.359775 0.747029 2.690951
H -0.502800 -0.553865 2.718277
H -0.854050 2.524949 -0.619841
H -0.885990 -2.514684 0.616690
H -1.601276 2.046472 0.680889
H -1.622682 -2.027038 -0.686461
H 2.599853 0.044846 0.790400
H 2.602337 -0.075577 -0.782031

Co(II)-6-Oh (JT)
Co -0.000000 -0.000002 0.000001
O 0.012082 2.114491 0.011695
O -0.012082 -2.114495 -0.011695
O -0.012326 0.011756 -2.113213
O 0.012326 -0.011761 2.113213
O 2.112390 -0.012003 -0.012387
O -2.112391 0.012000 0.012386
H -0.128936 0.751722 2.703209
H -0.137820 0.796993 -2.677528
H 0.137809 -0.796985 2.677547

H 0.128940 -0.751711 -2.703227
H 0.753143 -2.701937 0.130532
H -0.794807 -2.681201 -0.141566
H -0.753139 2.701942 -0.130521
H 0.794811 2.681196 0.141551
H 2.700528 0.135259 0.751392
H -2.700529 -0.135260 -0.751392
H 2.678124 -0.144766 -0.795378
H -2.678123 0.144760 0.795379

Fe(II)-2-L (JT)
Fe -0.000003 0.000000 0.000000
O 0.000285 0.000035 -1.922866
O -0.000290 -0.000034 1.922866
H 0.000057 -0.796801 -2.507453
H -0.000038 0.796802 2.507453
H 0.000789 0.796735 -2.507636
H -0.000801 -0.796735 2.507637

Fe(II)-3-TP (JT)
Fe -0.009576 -0.017051 -0.000544
O -1.001931 1.697354 -0.114494
O -0.990704 -1.724106 0.002813
O 1.970622 -0.011076 0.113143
H -0.598435 -2.621147 0.093464
H -1.201851 2.200450 -0.934122
H -1.963309 -1.835037 -0.090419
H -1.308304 2.243472 0.642279
H 2.506953 0.073431 0.931739
H 2.596533 -0.006291 -0.643859

Fe(II)-4-SP (JT)
Fe 0.000021 0.097136 -0.000010
O -0.010827 -0.092369 2.019671
O 0.010787 -0.092812 -2.019651
O 2.084800 0.098768 0.011145
O -2.084758 0.099647 -0.011165
H -0.777517 -0.129445 -2.599151
H 0.777464 -0.129213 2.599177
H 0.801839 -0.124914 -2.595672
H -0.801891 -0.123976 2.595703
H -2.669663 0.885233 -0.016794
H 2.670030 0.884114 0.016564
H 2.669508 -0.686645 0.012689
H -2.669792 -0.685524 -0.012506

Fe(II)-4-Td (JT)
Fe 0.000000 -0.000000 0.017869
O -0.000124 1.659013 -1.155231
O 0.000123 -1.659014 -1.155230
O 1.670539 0.000124 1.199118
O -1.670538 -0.000124 1.199118
H 0.000574 2.589937 -0.851803

H -0.000575 -2.589939 -0.851801
H 0.001308 -1.688316 -2.133874
H -0.001308 1.688314 -2.133876
H -2.190518 0.784483 1.467586
H 2.190529 -0.784480 1.467571
H 2.192034 0.784508 1.465284
H -2.192045 -0.784506 1.465268

Fe(II)-5-TBP (JT)
Fe 0.018250 -0.033105 0.000363
O -0.072592 -0.081223 2.119960
O 0.109132 0.015036 -2.120119
O -1.002350 1.820489 -0.001296
O -1.047632 -1.797826 -0.085382
O 2.077808 -0.075887 0.087662
H -0.323832 0.667334 2.695485
H 0.227232 -0.793423 2.718423
H -0.344828 0.660461 -2.696179
H 0.514937 -0.642328 -2.718793
H -0.765928 2.621609 -0.507124
H -1.410073 -2.205942 -0.895814
H -1.471845 -2.245607 0.672236
H -1.807927 2.043793 0.503569
H 2.618605 -0.000689 0.898023
H 2.681042 0.047306 -0.671018

Fe(II)-5-SPY (JT)
Fe 0.000130 0.000673 -0.004297
O 0.001000 0.001074 2.064695
O -0.010082 2.086339 -0.543247
O 0.009896 -2.086685 -0.542828
O -2.002565 -0.009013 -0.520496
O 2.002846 0.010161 -0.522303
H 0.017414 -2.888527 0.015557
H -0.090902 -2.398084 -1.463614
H -0.049464 2.890440 0.010565
H 0.113847 2.395577 -1.461946
H -0.264736 0.736915 2.649375
H 0.268653 -0.732268 2.651656
H -2.535715 0.784925 -0.719243
H 2.534665 -0.787317 -0.710488
H -2.614046 -0.768362 -0.459602
H 2.619056 0.764151 -0.443780

Fe(II)-6-Oh (JT)
Fe 0.000000 -0.000006 -0.000000
O -0.000003 2.169120 -0.000003
O 0.000003 -2.169166 0.000003
O 0.026397 -0.000003 2.158027
O -0.026398 -0.000010 -2.158027
O 2.124872 -0.000004 -0.025992
O -2.124872 -0.000010 0.025993
H 0.221336 -2.751243 -0.750515

H -0.221338 -2.751242 0.750520
H -0.221546 2.751242 0.750424
H 0.221548 2.751241 -0.750429
H -0.760977 -0.000102 2.733382
H 0.760976 -0.000123 -2.733383
H 0.807399 0.000256 2.741992
H -0.807400 0.000288 -2.741992
H 2.701315 -0.784799 0.039590
H -2.701313 -0.784804 -0.039606
H -2.701471 0.784678 -0.039477
H 2.701470 0.784683 0.039494