

Supplementary Material

# Theoretical Perspectives on the Gas-phase Oxidation Mechanism and Kinetics of Carbazole Initiated by OH Radical in the Atmosphere

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**Table S1.** Comparison of the geometrical parameters of carbazole degradation by OH radical in M06-2X method with those of other 5 kinds of methods.

**Table S2.** Imaginary frequencies (in  $\text{cm}^{-1}$ ), zero-point energies (ZPE, in a.u.) and total energies (in a.u.) for the transition states involved in the oxidation reaction of carbazole initiated by OH radical.

**Table S3.** Cartesian coordinates for the transition states in the oxidation reaction of carbazole initiated by OH radical.

**Table S4.** Calculated bond lengths (angstrom) and bond energies ( $\text{kcal mol}^{-1}$ ) of C-H bonds and O-H bonds in the intermediates IM12-IM15 at M06-2X/6-311++G(3df,2p)//M06-2X/6-311+G(d,p) level.

**Table S5.** Comparison of the rate constants and lifetime of carbazole degradation by OH radical with those of other 5 kinds of NSO-HETs.

**Table S6.** RRKM calculated rate constants (in  $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for TS1, TS5 and TS14 involved in the OH-initiated oxidation degradation of carbazole at 298 K and 10–670 torr.

**Table S1** Comparison of the geometrical parameters of carbazole degradation by OH radical in M06-2X method with those of other 5 kinds of methods.

Parameter	HF/6-31G* (Lee and Boo, 1996)	MP2/6-31G* (Lee and Boo, 1996)	B3LYP/6-31G* (Lee and Boo, 1996)	M06-2X/6- 311G(d,p) (this paper)	X-ray (Batra et al., 1974)	Error rate 1 (%)	Error rate 2 (%)
Bond Length (angstrom)							
C1-C2	1.380	1.392	1.393	1.386	1.390	0.3%	0.4%
C2-C3	1.397	1.409	1.407	1.403	1.398	0.4%	0.4%
C3-C4	1.380	1.391	1.392	1.386	1.395	0.7%	0.4%
C4-C11	1.391	1.403	1.400	1.397	1.400	0.2%	0.4%
C11-C12	1.455	1.443	1.450	1.450	1.467	1.2%	0.5%
C1-C10	1.389	1.399	1.397	1.394	1.395	0.1%	0.4%
C10-C11	1.401	1.419	1.421	1.412	1.404	0.6%	0.5%
C10-N	1.378	1.383	1.387	1.382	1.414	2.3%	0.1%
C1-H	1.076	1.088	1.087	1.084	0.897	20.9%	0.4%
C2-H	1.076	1.088	1.087	1.084	0.981	10.5%	0.4%
C3-H	1.075	1.087	1.086	1.083	1.070	1.2%	0.4%
C4-H	1.076	1.089	1.087	1.084	0.983	10.3%	0.5%
N-H	0.992	1.012	1.008	1.007	0.964	4.5%	0.5%

**Continued Table S1**

Bond Angle (degree)							
C1-C2-C3	121.5	121.4	121.3	121.4	121.3	0.1%	0
C2-C3-C4	120.5	120.9	120.7	120.7	120.4	0.3%	0.2%
C3-C4-C11	119.2	118.8	119.2	119.4	119.5	0.1%	0.5%
C4-C11-C12	134.0	133.8	134.1	134.0	134.1	0.1%	0.2%
C1-C10-C11	121.8	122.0	121.9	121.8	122.3	0.4%	0.2%
C2-C1-C10	117.7	117.4	117.6	117.6	117.7	0.1%	0.2%
C4-C11-C10	119.5	119.4	119.2	119.4	118.8	0.5%	0
C10-C11-C12	106.5	106.8	106.7	106.6	107.1	0.5%	0.2%
C10-N-C13	109.4	109.7	109.7	109.5	108.2	1.2%	0.2%
C11-C10-N	108.8	108.4	108.4	108.6	108.8	0.2%	0.2%
C2-C1-H	121.0	121.1	120.1	121.1	118.4	2.3%	0
C3-C2-H	119.3	119.4	119.4	119.4	118.4	0.8%	0
C4-C3-H	120.0	119.7	119.8	119.9	120.8	0.8%	0.2%
C11-C4-H	121.5	120.6	120.4	120.4	120.3	0.1%	0.2%

Error rate 1 is the absolute value of error between M06-2X/6-311G(d,p) and X-ray method.

Error rate 2 is the absolute value of error between M06-2X/6-311G(d,p) and MP2/6-31G\* method.

**Table S2.** Imaginary frequencies (in  $\text{cm}^{-1}$ ), zero-point energies (ZPE, in a. u.) and total energies (in a.u.) for the transition states involved in the oxidation reaction of carbazole initiated by OH radical.

Transition	Imaginary	ZPE	Total energies
TS1	1371i	0.18348	−593.14130
TS2	1276i	0.18267	−593.13971
TS3	1288i	0.18279	−593.13965
TS4	1281i	0.18306	−593.14073
TS5	1035i	0.18530	−593.15057
TS6	521i	0.17033	−667.05646
TS7	1129i	0.16940	−666.98378
TS8	268i	0.16918	−666.98017
TS9	83i	0.17989	−796.98436
TS10	83i	0.16612	−591.85203
TS11	757i	0.19100	−668.46080
TS12	398i	0.18896	−593.15356
TS13	498i	0.18862	−593.14944
TS14	434i	0.18863	−593.15079
TS15	483i	0.18848	−593.15024
TS16	487i	0.18868	−593.14738
TS17	489i	0.18876	−593.14581
TS18	1553i	0.19337	−743.44381
TS19(a)	531i	0.19808	−743.49119
TS19(s)	433i	0.19804	−743.49058
TS20(a)	519i	0.19782	−743.49055
TS21(s)	525i	0.19787	−743.50174
TS22	1577i	0.19202	−743.48779
TS23(a)	573i	0.19766	−743.48887
TS23(s)	562i	0.19750	−743.48926
TS24(a)	480i	0.19767	−743.49861
TS24(s)	459i	0.19779	−743.50015
TS25(a)	631i	0.19703	−743.48864
TS25(s)	579i	0.19734	−743.49094
TS26	1082i	0.19335	−743.48894

**Continued Table S2**

TS27(a)	437i	0.19717	−743.49307
TS27(s)	475i	0.19738	−743.49115
TS28(a)	520i	0.19793	−743.48996
TS28(s)	495i	0.19670	−743.47754
TS29(a)	346i	0.19686	−743.48939
TS29(s)	442i	0.19664	−743.47702
TS30	1465i	0.19300	−743.48266
TS31(a)	627i	0.19740	−743.49104
TS31(s)	619i	0.19727	−743.49114
TS32(a)	507i	0.19812	−743.49703
TS32(s)	514i	0.19816	−743.50197
TS33(a)	522i	0.19738	−743.48555
TS33(s)	535i	0.19766	−743.49503
TS34	713i	0.20064	−743.49240
TS35	571i	0.20005	−743.47500
TS36	486i	0.20058	−743.51033
TS37	2157i	0.19631	−743.46723
TS38	1022i	0.19570	−819.90271
TS39	1684i	0.22094	−743.46547
TS40	2161i	0.22005	−819.90704
TS41	1301i	0.19559	−743.49661
TS42	1630i	0.22045	−819.92123
TS43	695i	0.19801	−743.54219
TS44	339i	0.19732	−743.48097
TS45	870i	0.19485	−743.51653
TS46	1437i	0.20019	−893.78557
TS47	528i	0.19267	−893.22582
TS48	1052i	0.17410	−742.34481
TS49	419i	0.20677	−873.38665
TS50	1397i	0.19643	−818.67565
TS51	774i	0.21833	−744.79591
TS52	315i	0.19391	−668.35732

TS53	215i	0.19902	−818.69550
TS54	914i	0.19818	−818.72835
TS55	171i	0.20967	−873.44264
<b>Continued Table S2</b>			
TS56	725i	0.20009	−743.45871
TS57	931i	0.20027	−743.47563
TS58	414i	0.20072	−743.47997
TS59	498i	0.20077	−743.48065
TS60	1174i	0.22109	−819.90330
TS61	1600i	0.19616	−743.46596
TS62	2135i	0.22038	−819.85751
TS63	599i	0.22121	−819.91128
TS64	627i	0.19790	−743.54210
TS65	1413i	0.20013	−893.78580
TS66	1090i	0.19112	−854.72656
TS67	970i	0.17425	−742.35123
TS68	225i	0.20712	−873.44264
TS69	1368i	0.19688	−744.07657
TS70	1414i	0.21660	−744.74879
TS71	688i	0.20703	−873.40113
TS72	934i	0.19837	−743.46121
TS73	561i	0.19879	−743.47196
TS74	601i	0.19974	−743.49479
TS75	2249i	0.19513	−743.41140
TS76	383i	0.22304	−819.89700
TS77	3975i	0.19464	−743.46640
TS78	1645i	0.19422	−743.47784
TS79	684i	0.19648	−743.46409
TS80	722i	0.20179	−893.83127
TS81	1904i	0.19866	−893.78688
TS82	266i	0.21735	−743.48169
TS83	1001i	0.19465	−743.50947
TS84	373i	0.20624	−873.36898
TS85	802i	0.21735	−744.77412

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TS86	569i	0.20703	−893.84263
TS87	521i	0.19973	−743.50854
TS88	141i	0.21690	−1023.72078
TS89	323i	0.20324	−818.70096
TS90	490i	0.20133	−818.71771

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**Table S3** Cartesian coordinates for the transition states in the oxidation reaction of carbazole initiated by OH radical.

TS1

0 2

C	−0.38291604	0.13991163	0.00000000
C	−1.09152004	1.35428163	−0.05874000
C	−0.39142004	2.53961463	−0.11048300
C	0.99373696	2.54180463	−0.07438800
C	1.71014596	1.32506263	−0.01331300
C	1.00425496	0.12093263	0.02337600
H	−0.93689104	−0.79029737	0.02578400
H	−2.17441504	1.35053363	−0.07692200
H	−0.91226204	3.63771763	−0.21681100
H	1.53491196	−0.82298837	0.07390200
C	3.16804796	3.10069963	−0.04778100
C	4.38125496	3.78755763	−0.04720500
C	5.54413396	3.03504863	0.00400300
C	5.50893696	1.63310463	0.05345800
C	4.30027696	0.95571963	0.05273100
C	3.11356996	1.68932163	0.00242000
H	4.41383296	4.86971163	−0.08651300
H	6.50153696	3.54228763	0.00507400
H	6.43809696	1.07836663	0.09226700
H	4.27483296	−0.12733037	0.09050100
O	−1.03024104	4.88025663	0.07292500
H	−1.30802304	4.79849463	0.99819500
N	1.87716996	3.59453063	−0.09354500
H	1.59440696	4.56190263	−0.12681200

TS2

0 2

C	−0.22091310	0.24300441	0.00000000
C	0.20654790	−1.08362559	−0.03164000
C	−0.63604710	−2.17486359	−0.00630700
C	−2.00265010	−1.88897259	0.02986700
C	−2.48426710	−0.56014659	0.05321100
C	−1.58448810	0.50642441	0.03818300
H	0.49986690	1.05047541	−0.01726700
H	1.39520990	−1.30252959	−0.10346700
H	−0.25500610	−3.18879859	−0.02399400
H	−1.94395010	1.52918241	0.05448200



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C	−4.25530010	−2.01951159	0.08259500
C	−5.57670910	−2.46229459	0.10825900
C	−6.57374610	−1.49972059	0.13910700
C	−6.26984310	−0.12989159	0.14540300
C	−4.95359510	0.30251541	0.11987900
C	−3.93067310	−0.64633859	0.08779700
H	−5.81676510	−3.51898559	0.10359800
H	−7.61063610	−1.81377459	0.15871700
H	−7.07539610	0.59322741	0.17050000
H	−4.72098210	1.36135841	0.12402000
O	2.61452190	−1.55995359	0.21250400
H	2.56182590	−1.42536959	1.17104000
N	−3.08110210	−2.75098959	0.04973100
H	−3.02226210	−3.75475559	0.02650100

TS3

02

C	0.48600882	0.05154639	0.00000000
C	0.38255682	1.44148639	0.05292200
C	1.53491782	2.21453239	0.10595600
C	2.76146982	1.55033839	0.11625000
C	2.85438882	0.14041739	0.07598600
C	1.68618982	−0.62617561	0.02479000
H	−0.53873918	−0.59272861	−0.08472000
H	−0.59189818	1.91418739	0.04202000
H	1.47904682	3.29631339	0.13780900
H	1.72189282	−1.70898061	−0.00663100
C	4.96098982	1.04059139	0.15697100
C	6.35362682	1.09402739	0.19417000
C	7.04108182	−0.10936261	0.17472600
C	6.36619082	−1.33824761	0.11955300
C	4.98184182	−1.38390661	0.08268000
C	4.26559782	−0.18583461	0.10170800
H	6.88028082	2.03998739	0.23737500
H	8.12409082	−0.09972261	0.20241900
H	6.93693382	−2.25834661	0.10524100
H	4.46184682	−2.33405561	0.03820500
O	−1.57658918	−1.27172461	0.23399300
H	−1.46335718	−1.29362361	1.19618600
N	4.03972482	2.07219339	0.16546900

H	4.26597982	3.05164839	0.19744900
TS4			
0 2			
C	0.05891016	−0.06627393	0.00000000
C	0.24806216	−1.45797293	0.06437700
C	−0.82504184	−2.33442193	0.12163000
C	−2.11198584	−1.79698593	0.10918200
C	−2.33550484	−0.40152193	0.04002100
C	−1.22689584	0.43015707	−0.02163000
H	0.91151316	0.59972507	−0.04080200
H	1.25720816	−1.85238493	0.07153200
H	−0.66569684	−3.40474093	0.17617400
H	−1.41287284	1.62441707	−0.10682900
C	−4.34979384	−1.48582693	0.12438000
C	−5.73214984	−1.66213893	0.15267900
C	−6.52192084	−0.52366793	0.10015500
C	−5.95795784	0.75904407	0.02017600
C	−4.58307684	0.93036807	−0.00764300
C	−3.76869984	−0.20275893	0.04760500
H	−6.17375984	−2.64975093	0.21348200
H	−7.60019384	−0.62906093	0.12009000
H	−6.60894584	1.62346907	−0.02160900
H	−4.13604084	1.91592107	−0.07396600
O	−1.68614584	2.84347407	0.21160300
H	−1.52983084	2.79477507	1.16739400
N	−3.33795784	−2.43063993	0.16102500
H	−3.47483984	−3.42603993	0.20619600
TS5			
0 2			
C	−0.16200294	−0.58173784	0.00000000
C	−0.55631594	0.73768316	−0.25160500
C	0.38019606	1.73897616	−0.47514200
C	1.72374306	1.37900516	−0.43058600
C	2.13793206	0.05857616	−0.15730100
C	1.18410506	−0.93183484	0.04740400
H	−0.91825794	−1.34016484	0.16194800
H	−1.61149194	0.98180316	−0.27494300

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H	0.08603906	2.76347316	−0.66813000
H	1.48000706	−1.95578384	0.24450900
C	3.97347206	1.41070316	−0.42911700
C	5.30648406	1.80810816	−0.47108000
C	6.27023206	0.83319616	−0.24624800
C	5.91247206	−0.49689584	0.00394500
C	4.57660206	−0.88439784	0.04919600
C	3.59586006	0.07909116	−0.15651500
H	5.57197206	2.84064316	−0.66287400
H	7.31820506	1.10698516	−0.26751100
H	6.68913606	−1.23415384	0.16683600
H	4.30925506	−1.91633784	0.24558400
O	2.81047306	4.26959716	0.52030400
H	2.80366006	3.90088916	1.41528200
N	2.83775506	2.17603716	−0.66379000
H	2.82259106	3.22558616	−0.51345300

TS6

0 2

C	−0.42709866	0.22827687	0.00000000
C	−0.80105866	1.51631587	−0.38190200
C	0.15947134	2.48289187	−0.68055700
C	1.49014734	2.11829687	−0.56823000
C	1.87818134	0.82831987	−0.16266600
C	0.91780034	−0.13178513	0.10935400
H	−1.19444566	−0.50708913	0.21039700
H	−1.85233866	1.76587087	−0.45757600
H	−0.11506666	3.48338187	−0.99145100
H	1.19699634	−1.13760113	0.40120900
C	3.72345634	2.14024887	−0.54132400
C	5.05259234	2.52455487	−0.62733400
C	6.02004734	1.57475687	−0.29301800
C	5.65523934	0.28491287	0.08578700
C	4.31224834	−0.10013413	0.15784900
C	3.34485834	0.84168787	−0.13964600
H	5.31998634	3.52131387	−0.95218600
H	7.06911234	1.83932787	−0.34372700
H	6.42814734	−0.43768613	0.31933200
H	4.04415034	−1.11177413	0.43982900
O	2.50011734	4.11580187	0.50507900

O	3.57862434	4.52352087	0.88511100
N	2.60994634	2.93936187	−0.83849500
TS7			
O 2			
C	−0.73631390	−1.06774667	−0.00963887
C	−0.27149890	−2.37193667	−0.36219187
C	−1.09222190	−3.45004667	−0.33492787
C	−2.46765590	−3.30821367	0.19328513
C	−2.95352290	−1.90239367	0.30365513
C	−2.08046790	−0.83800367	0.28941013
H	−0.04298290	−0.23661567	−0.03451087
H	0.76445610	−2.49172067	−0.65573987
H	−0.75081490	−4.45075167	−0.57054387
H	−2.44324590	0.17385133	0.42936813
C	−4.75544490	−3.25505367	−0.18455487
C	−6.06856090	−3.63290167	−0.38380987
C	−7.05321990	−2.67650367	−0.14609587
C	−6.71718690	−1.38051467	0.25816913
C	−5.39201390	−1.01180967	0.44761613
C	−4.39670690	−1.96642267	0.23290713
H	−6.31196490	−4.63708267	−0.70781087
H	−8.09518090	−2.93737667	−0.28588387
H	−7.50416390	−0.65550967	0.42646513
H	−5.13647690	−0.01060067	0.77404313
O	−3.51152890	−5.11759967	0.45297913
O	−2.55590990	−4.01469767	1.46744913
N	−3.59985290	−4.08157067	−0.39170587

TS8

O 2

C	−0.70692192	−0.83210603	0.00000000
C	−0.48230092	−1.90005403	−0.89843800
C	−1.38982392	−2.99420703	−0.96334200
C	−2.44098892	−2.99242903	−0.13697000
C	−2.80622992	−1.86145103	0.99878200
C	−1.76363592	−0.78056703	0.85679000
H	0.00989108	−0.01872103	0.01491100
H	0.38199008	−1.88877603	−1.54806500

H	−1.24168292	−3.80458403	−1.66693400
H	−1.86610792	0.03967797	1.55784800
C	−4.70025692	−2.83889503	−0.00170000
C	−5.98186392	−3.08037803	−0.43572900
C	−6.85339692	−1.98824103	−0.40371700
C	−6.42555192	−0.74403103	0.05469000
C	−5.11832592	−0.54076603	0.50785400
C	−4.24514892	−1.61230203	0.48302600
H	−6.29359292	−4.05545203	−0.78737000
H	−7.87415392	−2.11139303	−0.74348700
H	−7.12543692	0.08314297	0.06406900
H	−4.80363092	0.42996897	0.87262500
O	−2.83021592	−2.47535603	2.15498100
O	−3.49570692	−4.36229403	1.21773700
N	−3.56957492	−3.77194603	0.12336500
TS9			
01			
C	0.87759121	−0.11456921	−0.02148093
C	−0.26021779	0.60428179	−0.39262193
C	−0.16459979	1.93092979	−0.80768293
C	1.10531121	2.46792479	−0.82488693
C	2.26448621	1.78009379	−0.45178793
C	2.14996821	0.46184779	−0.04364793
H	0.76956821	−1.14322121	0.30001307
H	−1.23107079	0.12737779	−0.34896293
H	−1.02532579	2.52552879	−1.08633193
H	3.01950021	−0.10937521	0.25796107
C	2.87701221	3.94095379	−1.01520293
C	3.62746421	5.07978479	−1.21918393
C	4.99224321	4.96486979	−0.96322893
C	5.54110121	3.75800379	−0.52593293
C	4.75150521	2.62323879	−0.32360193
C	3.39288721	2.71818779	−0.57268393
H	3.16399221	6.00299079	−1.54314893
H	5.63462121	5.82572779	−1.09797693
H	6.60532921	3.70275879	−0.33228793
H	5.19374921	1.69833279	0.02601707
O	0.71493821	4.65335379	−1.57343093
O	−0.28618579	6.17844879	2.18500707

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N	1.47471521	3.78840979	−1.20741893
N	−0.26533179	6.05007579	0.98230407
O	0.47467221	5.18045379	0.48086307

#### TS10

0 2

C	−0.11450381	−0.82061067	0.00000000
C	−0.64486381	0.43982333	−0.26971300
C	0.19922919	1.54943133	−0.36826200
C	1.54180219	1.31769533	−0.21331800
C	2.12598919	0.09782333	0.05908000
C	1.25398319	−0.99538767	0.16970200
H	−0.77665481	−1.67299867	0.09025200
H	−1.71427281	0.56315533	−0.39833700
H	−0.19338481	2.53974333	−0.56568900
H	1.64188819	−1.97837167	0.41279600
C	4.32296119	1.16718133	0.49301300
C	5.70939919	1.15295833	0.62525900
C	6.38873819	−0.04770967	0.50027200
C	5.67739619	−1.21815567	0.23260200
C	4.29633019	−1.19288267	0.09313500
C	3.58805119	0.00285833	0.23280500
H	6.22334219	2.08266433	0.83738900
H	7.46598719	−0.07730867	0.60782100
H	6.20731519	−2.15675467	0.12175700
H	3.76681919	−2.10572767	−0.15062000
O	4.16285219	3.40409533	0.51455500
N	3.57113219	2.37706533	0.70787200

#### TS11

0 2

C	−0.97328246	−0.76335877	0.00000000
C	−1.37050446	0.34992323	−0.74893600
C	−0.43479246	1.20115823	−1.32612700
C	0.90059154	0.88877923	−1.12098900
C	1.32829254	−0.23620777	−0.38982800
C	0.37400854	−1.06661877	0.18367500
H	−1.72838946	−1.40432577	0.43811800
H	−2.42620246	0.55136323	−0.88336100

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H	−0.71816646	2.06505123	−1.91370000
H	0.66854554	−1.93763177	0.75737900
C	3.17622254	0.87658623	−1.19984000
C	4.49713754	1.18421323	−1.48577000
C	5.46087754	0.32265823	−0.97566000
C	5.10542254	−0.79303977	−0.20882400
C	3.77127154	−1.08582977	0.06416000
C	2.78888154	−0.24458677	−0.44253600
H	4.74861954	2.05818723	−2.07217500
H	6.50748054	0.52108023	−1.17169700
H	5.88284554	−1.44073577	0.17717200
H	3.50739954	−1.95498677	0.65534700
O	1.99803954	2.54883123	−2.48215600
N	2.02824254	1.57464923	−1.55664300
H	2.03748754	3.34480923	−1.83630600
O	2.21859854	3.57659023	−0.34686000
H	1.50298054	3.81300923	0.25723700

TS12

02

C	−0.57314430	−0.50810014	−0.03756586
C	−0.80334830	−1.87101514	−0.27410786
C	0.23891670	−2.74254014	−0.55268286
C	1.52633370	−2.21326514	−0.58432286
C	1.77833770	−0.84614714	−0.34418086
C	0.71217470	0.01109086	−0.07091486
H	−1.41144330	0.14361486	0.17521714
H	−1.81683430	−2.25216314	−0.23955386
H	0.05702870	−3.79435314	−0.73818786
H	0.88638970	1.06487286	0.11437214
C	3.75225670	−1.93598914	−0.75367586
C	5.14056170	−2.15779414	−0.87075886
C	5.96720470	−1.02027214	−0.76418686
C	5.44698670	0.23258286	−0.45980786
C	4.07137170	0.42061086	−0.30270486
C	3.21503470	−0.66863614	−0.44717286
H	5.52270670	−3.07700414	−1.29174186
H	7.03517270	−1.14641214	−0.89182986
H	6.11747770	1.07638386	−0.35603386
H	3.67690970	1.40319886	−0.07000786

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O	5.42477670	−3.11278614	0.93146214
H	5.30362770	−2.34469914	1.50949814
N	2.73342470	−2.84491714	−0.84696086
H	2.87084270	−3.84178614	−0.89138486

### TS13

0 2

C	−0.17673048	−0.50810014	0.00000000
C	−0.53146748	−1.86752914	−0.00645100
C	0.41944052	−2.86511914	−0.14914200
C	1.75009552	−2.47168114	−0.28815700
C	2.12654952	−1.10834814	−0.28499600
C	1.14515852	−0.12264414	−0.13856000
H	−0.94889748	0.24214286	0.11583000
H	−1.57336048	−2.14337914	0.10426900
H	0.13848952	−3.91165914	−0.15236200
H	1.41819552	0.92652286	−0.13271300
C	3.99146852	−2.41811314	−0.54227100
C	5.32383052	−2.74952214	−0.71850400
C	6.26749152	−1.70261014	−0.73096600
C	5.82839752	−0.34534514	−0.70074700
C	4.49904652	−0.03219614	−0.53939600
C	3.55827252	−1.07252614	−0.45045500
H	5.65336752	−3.77845714	−0.79086700
H	7.27659952	−1.91602114	−1.05381500
H	6.57320252	0.43751386	−0.76392800
H	4.17681752	1.00141986	−0.48962200
O	7.00909852	−1.88022114	1.13997400
H	6.21842152	−1.59434814	1.62162000
N	2.88340952	−3.24295514	−0.44298000
H	2.90560952	−4.24823914	−0.46462300

### TS14

0 2

C	0.53000975	−0.09572901	0.01387879
C	1.04410175	1.18246499	0.27217579
C	0.21495075	2.29165999	0.35805179
C	−1.14977725	2.08674099	0.17581179
C	−1.68545625	0.80938599	−0.08638921



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C	−0.83163825	−0.29016101	−0.16529321
H	1.20657275	−0.93920801	−0.04362121
H	2.11136275	1.30874999	0.40945279
H	0.61632875	3.27791099	0.55885879
H	−1.22728325	−1.28013701	−0.36114821
C	−3.38315625	2.35831199	−0.02292921
C	−4.68060225	2.88709299	−0.09373721
C	−5.71233425	2.01325199	−0.34643021
C	−5.49120525	0.61170799	−0.48408521
C	−4.17209425	0.11432599	−0.48365421
C	−3.12217825	0.97902899	−0.21466721
H	−4.86157925	3.94695599	0.03959479
H	−6.72915825	2.38089699	−0.40057521
H	−6.28788325	−0.00556101	−0.87285921
H	−3.99885825	−0.94279701	−0.64501921
O	−6.10174525	−0.03659801	1.33316279
H	−5.41457425	0.39186499	1.86433279
N	−2.19272925	3.00232299	0.21153379
H	−2.09115625	3.98947799	0.37866579

TS15

0 2

C	0.55964652	0.22827687	0.00000000
C	0.04726952	−1.04406913	0.30547300
C	0.87824752	−2.13797913	0.48349000
C	2.25037652	−1.93087513	0.34293400
C	2.78220452	−0.66148513	0.02226800
C	1.92163952	0.42807687	−0.14046100
H	−0.12370748	1.05954787	−0.11988400
H	−1.02365248	−1.17271413	0.40966900
H	0.47692552	−3.11461513	0.72658100
H	2.32181652	1.41087687	−0.36018000
C	4.49060352	−2.16441813	0.25336900
C	5.79556352	−2.65987413	0.27850600
C	6.83253052	−1.77358813	−0.00596600
C	6.58371152	−0.43722813	−0.30997900
C	5.27229952	0.08491787	−0.28350600
C	4.21144352	−0.81775113	−0.04364300
H	5.99810952	−3.70021613	0.50477300
H	7.85301352	−2.13656913	−0.00153800

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H	7.40662452	0.23043987	−0.52932900
H	5.07059452	1.06045687	−0.70406600
O	5.43055352	1.09409987	1.48283400
H	5.61333752	0.33550587	2.05743400
N	3.29608052	−2.82304713	0.47985900
H	3.20292752	−3.79899513	0.70422200

#### TS16

0 2

C	0.70692192	−0.27245950	0.00000000
C	0.37360892	−1.61747750	−0.21835800
C	1.34738392	−2.58410650	−0.42703200
C	2.67731092	−2.17512150	−0.40564300
C	3.02906592	−0.83038250	−0.16580800
C	2.03247992	0.12858950	0.02683600
H	−0.08112708	0.45407450	0.15350500
H	−0.67011908	−1.90926750	−0.22812100
H	2.29317892	1.16550750	0.20559100
C	4.92469492	−2.12644650	−0.33261800
C	6.29271592	−2.38839150	−0.62463200
C	7.17992192	−1.34105850	−0.55291600
C	6.74008992	−0.02563950	−0.28370800
C	5.39340492	0.26522850	−0.11481200
C	4.46883792	−0.77184350	−0.18321400
H	6.61691292	−3.39982850	−0.83493500
H	8.23480092	−1.52224950	−0.71865200
H	7.46943192	0.77408150	−0.23797300
H	5.06522292	1.28668650	0.03678100
N	3.82468392	−2.92678950	−0.63902900
H	3.85069392	−3.90445750	−0.38693500
H	1.08162592	−3.61922850	−0.60430400
O	5.02498592	−2.64711450	1.56563500
H	5.71302692	−2.06624350	1.92125600

#### TS17

0 2

C	0.20618556	−0.21354933	0.00000000
C	−0.18528944	1.12545967	0.08909700
C	0.74997056	2.14805967	0.20305200

C	2.09077956	1.78611667	0.21684600
C	2.49955156	0.44643167	0.12603800
C	1.55274956	−0.56209433	0.02771500
H	−0.54845144	−0.98555633	−0.08454900
H	−1.23983144	1.37382967	0.07136100
H	0.44161756	3.18386667	0.27914500
H	1.85769756	−1.60101633	−0.01812000
H	3.20855056	3.60135367	0.35119000
C	4.35148056	1.83152067	0.22723900
C	5.68556656	2.21659567	0.11849300
C	6.62152456	1.22218167	−0.11735100
C	6.24618856	−0.13262133	−0.27546700
C	4.93474456	−0.52210133	−0.14578000
C	3.96197456	0.44392267	0.23984400
H	5.97601056	3.25867767	0.17449700
H	7.66549056	1.49376667	−0.21824400
H	7.00728356	−0.86573433	−0.51159800
H	4.63899656	−1.55718333	−0.26480200
O	3.97570256	0.19326667	2.15678300
H	4.92936956	0.22843167	2.32221700
N	3.22220656	2.59646167	0.30029800

TS18

02

C	−0.04282656	−0.05353319	0.00000000
C	−0.20527656	−1.44437719	−0.05738700
C	0.88721944	−2.29821119	−0.11383100
C	2.15032644	−1.71752519	−0.11890000
C	2.33534144	−0.32127019	−0.06203500
C	1.22184644	0.51570381	0.00063500
H	−0.91854956	0.58229681	0.04053900
H	−1.20456556	−1.86251519	−0.06004400
H	0.75901444	−3.37292319	−0.15894400
H	1.34348944	1.59192081	0.04136100
C	4.36184444	−1.36932019	−0.18201900
C	5.79227444	−1.57411819	−0.30310100
C	6.57016444	−0.37829419	0.01463700
C	5.98588044	0.85538681	0.11528100
C	4.57898144	1.02445581	0.06303400
C	3.76948744	−0.08999419	−0.07843300

H	5.88582744	−1.67974719	−1.51579300
H	7.64650944	−0.49574619	0.07284800
H	6.61210144	1.72644881	0.26505900
H	4.14870044	2.01344481	0.16424500
O	6.27660744	−2.82632219	0.13269400
H	6.38427944	−2.78869719	1.08820500
N	3.40325844	−2.32618019	−0.15749700
H	3.58756744	−3.30929119	−0.28579400
O	4.28861444	−1.16566819	−2.78038100
O	5.40184444	−1.69889319	−2.90789100
TS19a			
O 2			
C	0.85353878	−0.15463917	0.03353562
C	1.04511178	−1.53854417	0.18750162
C	−0.01599122	−2.42428917	0.11223562
C	−1.28136122	−1.88861417	−0.12411838
C	−1.49634922	−0.50115217	−0.28246638
C	−0.40537322	0.37085783	−0.19894938
H	1.70757878	0.50822483	0.09908862
H	2.04249778	−1.91989917	0.36955562
H	0.13208178	−3.49086517	0.23336662
H	−0.54404822	1.43989583	−0.31307538
C	−3.47497922	−1.59009117	−0.47253838
C	−4.91323122	−1.88466017	−0.72001938
C	−5.69624122	−0.60165217	−0.78086238
C	−5.07941722	0.65700383	−0.96707538
C	−3.72637422	0.80981383	−0.79640038
C	−2.91265422	−0.32993317	−0.50923938
H	−5.32970522	−2.49046817	0.09917462
H	−6.73623422	−0.72799917	−1.06107038
H	−5.69960222	1.51535983	−1.19222638
H	−3.26765622	1.78657983	−0.89978638
O	−5.10041722	−2.69856217	−1.87860338
H	−4.74757422	−2.22118417	−2.63664438
N	−2.50629822	−2.52291617	−0.24482438
H	−2.66105622	−3.51859317	−0.22389438
O	−6.13601522	−0.51463117	1.22507062
O	−6.32880222	−1.61110917	1.73797362

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TS19s

0 2

C	−0.97050509	−0.55882352	0.01270461
C	−1.09432909	−1.95501952	−0.07910039
C	−0.01088909	−2.75178152	−0.41060739
C	1.20146991	−2.11168252	−0.65511639
C	1.35084891	−0.70890652	−0.56363339
C	0.23987891	0.07036148	−0.22397139
H	−1.83916109	0.03237348	0.27592061
H	−2.05471009	−2.41787352	0.11250261
H	−0.10424009	−3.82911452	−0.47993539
H	0.32541291	1.14799448	−0.14448639
C	3.33757691	−1.64400852	−1.10917439
C	4.74770991	−1.78855652	−1.57842539
C	5.52567591	−0.57243752	−1.15415839
C	4.88988091	0.68072548	−1.07394839
C	3.52368491	0.76435948	−0.90607339
C	2.73714891	−0.42476952	−0.85892139
H	4.71496091	−1.76503752	−2.68280239
H	6.60133491	−0.63665352	−1.27306239
H	5.49533091	1.57617148	−1.01606439
H	3.05236591	1.73054448	−0.76592339
O	5.33206991	−3.02740452	−1.25515439
H	5.56045091	−3.02323452	−0.31532239
N	2.43430691	−2.64746552	−1.00575239
H	2.66305691	−3.62504052	−1.10448139
O	5.77158591	−2.08365552	1.35049461
O	5.50927291	−0.94559152	0.94365061

## TS20a

0 2

C	0.00000000	−0.05882353	0.00000000
C	0.50741600	−1.27682053	0.48399000
C	−0.33362600	−2.32199053	0.82755700
C	−1.70355400	−2.11714553	0.67196200
C	−2.23295800	−0.90428553	0.17853400
C	−1.36152100	0.13720847	−0.15453700
H	0.68870600	0.73802347	−0.25221300
H	1.57808000	−1.39962953	0.59434000

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H	0.05816400	-3.25872853	1.20620700
H	-1.74672900	1.08146047	-0.52229600
C	-3.93320100	-2.33587953	0.61840700
C	-5.28827600	-2.94420453	0.75601200
C	-6.32925800	-2.02154953	0.17812200
C	-6.06094400	-0.79007853	-0.29564000
C	-4.73182000	-0.21636153	-0.26840200
C	-3.66747800	-1.06922253	0.14085300
H	-5.51010300	-3.10996153	1.81801500
H	-7.34166100	-2.41008453	0.16956900
H	-6.86708700	-0.17770953	-0.68357300
H	-4.52539400	0.65641547	-0.87458500
O	-5.33841300	-4.25257553	0.19007600
H	-5.23546400	-4.16250053	-0.76354500
N	-2.76727000	-2.96521053	0.93828200
H	-2.70224200	-3.92716553	1.23286700
O	-4.97111300	1.03642647	1.34539300
O	-5.46200400	2.11977747	1.05245700

TS20s

O 2

C	-0.26509572	-0.84683357	0.00000000
C	0.04201028	0.49150643	0.29435400
C	-0.93868072	1.46991343	0.30198300
C	-2.24007072	1.07111143	0.00706000
C	-2.57007772	-0.26788357	-0.29425700
C	-1.56150572	-1.23494457	-0.29492300
H	0.52755128	-1.58482657	0.00747500
H	1.06552328	0.76400443	0.52179700
H	-0.70253672	2.50243443	0.53101200
H	-1.79015472	-2.27092357	-0.51746400
C	-4.45029272	1.00149443	-0.35640600
C	-5.86916172	1.44856743	-0.46697800
C	-6.75322572	0.27818743	-0.81027300
C	-6.30839672	-0.98159157	-0.96531300
C	-4.93428172	-1.33960757	-0.69550100
C	-3.99577772	-0.29157157	-0.53798900
H	-5.95624072	2.20576743	-1.25683600
H	-7.80539672	0.51124943	-0.93230200
H	-7.00855172	-1.77595757	-1.19559600

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H	−4.60095672	−2.35143057	−0.88717200
O	−6.29624472	2.11710043	0.71174600
H	−6.26872572	1.45747243	1.41767200
N	−3.40801372	1.81932843	−0.05091900
H	−3.50563472	2.78563543	0.21978600
O	−5.57483572	−0.65033657	1.86692500
O	−5.27035472	−1.71367957	1.33308200

#### TS21a

0 2

C	−0.73637700	−0.50810014	0.00000000
C	−0.60035400	−1.86420914	−0.30712700
C	−1.71159600	−2.67334914	−0.52664000
C	−2.95994600	−2.08022114	−0.42647900
C	−3.11786200	−0.71869714	−0.10829600
C	−1.99568300	0.07406186	0.10075300
H	0.14901600	0.09247086	0.16662500
H	0.39004600	−2.29790414	−0.37595000
H	−1.60300100	−3.72456514	−0.76366700
H	−2.09992600	1.12454286	0.34625600
C	−5.18153400	−1.74730614	−0.28318600
C	−6.63086200	−1.91223614	−0.62978900
C	−7.38540700	−0.68031914	−0.20804800
C	−6.77649300	0.46997086	0.13939800
C	−5.33326600	0.61913186	0.18486400
C	−4.55379100	−0.46338414	−0.06809100
H	−7.01133400	−2.80210114	−0.11655800
H	−8.46622200	−0.73777714	−0.26495900
H	−7.38179600	1.33443786	0.38793300
H	−4.90255700	1.58580786	0.41600800
O	−6.82404000	−2.19543014	−2.01364700
H	−6.61849800	−1.39848814	−2.51370700
N	−4.22745700	−2.64467914	−0.62544800
H	−4.41136800	−3.63256814	−0.71940000
O	−5.38070200	−3.39940914	1.77609900
O	−5.46145400	−2.16729714	1.67828400

#### TS21s

0 2

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C	−0.27982326	−0.06627393	0.00000000
C	−0.38924926	−1.40950993	−0.37139000
C	0.73163074	−2.16358493	−0.70483100
C	1.96227874	−1.52868793	−0.65490600
C	2.09434974	−0.18308793	−0.27022400
C	0.96176174	0.55584807	0.05436600
H	−1.17264526	0.49139007	0.25371600
H	−1.36666126	−1.87579793	−0.40025600
H	0.64486874	−3.20468593	−0.99019300
H	1.04659574	1.59438407	0.35237600
C	4.17103574	−1.12615093	−0.63201900
C	5.60254074	−1.19406293	−1.05046500
C	6.34788974	−0.00998093	−0.49027100
C	5.72371874	1.09487507	−0.04600800
C	4.27550574	1.20739707	0.00884300
C	3.51952574	0.12341307	−0.29902100
H	5.63176174	−1.12230393	−2.14931600
H	7.42976974	−0.06907593	−0.53014300
H	6.31270874	1.93887507	0.29399600
H	3.82325474	2.13668307	0.33331000
O	6.19290774	−2.44418993	−0.76270000
H	6.17497274	−2.55598393	0.19519700
N	3.23327974	−2.03526393	−0.97587100
H	3.44505174	−3.02194593	−1.03487600
O	3.84177274	−2.75151193	1.49898600
O	4.47391274	−1.69033093	1.34207100

TS22

0 2

C	0.74946473	−0.07494647	0.00000000
C	0.40941673	−1.42750747	0.15836900
C	1.37104973	−2.42681247	0.13324700
C	2.69549373	−2.04020547	−0.05722800
C	3.05745273	−0.68251547	−0.22050900
C	2.06732973	0.30435753	−0.19023100
H	−0.03037727	0.67565853	0.02616000
H	−0.62944627	−1.69861147	0.30372500
H	1.10094973	−3.46858247	0.25690400
H	2.32903373	1.34833853	−0.31802600
C	4.94048873	−2.00420547	−0.33301800



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C	6.26439073	−2.33470047	−0.43153500
C	7.20643673	−1.27978447	−0.78725300
C	6.74262973	0.10176553	−0.67801300
C	5.40924773	0.39591353	−0.53619600
C	4.48503873	−0.64879147	−0.39399100
H	7.27027973	−1.35866447	−2.00382300
H	7.48848073	0.88236953	−0.76011400
H	5.07567373	1.42688753	−0.51260500
N	3.83613873	−2.81613547	−0.12141000
H	3.85768973	−3.82073647	−0.08060300
H	6.63062673	−3.35213747	−0.36224000
O	8.55353973	−1.51372147	−0.43965000
H	8.63417373	−1.41417547	0.51343800
O	7.35820373	−0.90427747	−3.40948800
O	7.03863773	0.28253953	−3.35639300

TS23a

0 2

C	−0.01449275	−0.27536232	0.00000000
C	−0.37019675	−1.62661332	−0.05945900
C	0.57573025	−2.62836532	−0.25158500
C	1.90436625	−2.24088132	−0.37221900
C	2.28156925	−0.88510032	−0.29047000
C	1.31541325	0.10342168	−0.12881500
H	−0.78202075	0.47554568	0.13664400
H	−1.41343375	−1.90346632	0.03825400
H	0.28312625	−3.66945732	−0.31233700
H	1.59857525	1.14964268	−0.10162000
C	4.16991825	−2.22046932	−0.55259000
C	5.46800425	−2.54855332	−0.52522500
C	6.51926025	−1.47624032	−0.45076600
C	5.96884925	−0.09129832	−0.21926500
C	4.66505825	0.20808068	−0.23908000
C	3.70020825	−0.82787232	−0.55423400
H	7.08730325	−1.46001732	−1.38929200
H	6.71439125	0.66968868	−0.01402000
H	4.31350625	1.21864068	−0.06598700
N	3.03102725	−3.02199832	−0.58762200
H	3.04929425	−4.02293632	−0.48877100
H	5.81271825	−3.57609532	−0.54897000

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O	7.50157525	−1.79089632	0.53402500
H	7.05290725	−1.84379332	1.38407500
O	3.68218525	−0.60920932	−2.48875700
O	2.56882925	−0.71061532	−3.00786900

#### TS23s

0 2

C	−0.98550723	−0.05797101	0.00000000
C	−1.34764823	−1.40714601	0.07271300
C	−0.39892723	−2.42354201	0.10436100
C	0.93932377	−2.05356301	0.04777400
C	1.31941377	−0.69941101	−0.05060200
C	0.35424477	0.30318599	−0.05027800
H	−1.75428023	0.70379399	−0.00864600
H	−2.39831723	−1.67039901	0.11309100
H	−0.69521423	−3.46283701	0.17579300
H	0.64593077	1.34656899	−0.09180900
C	3.20887177	−2.06162201	−0.08730800
C	4.49344277	−2.39748601	−0.25880600
C	5.53795077	−1.32515301	−0.40075800
C	4.97756577	0.06514199	−0.57996500
C	3.68743577	0.37484199	−0.41005200
C	2.76127677	−0.66344601	0.00035500
H	6.17233077	−1.55643201	−1.26281700
H	5.70536777	0.83417699	−0.81579100
H	3.32847477	1.39301999	−0.50653100
N	2.07285177	−2.85127301	0.07634500
H	2.06444977	−3.85202201	−0.02340200
H	4.82774377	−3.42860601	−0.26778000
O	6.44633277	−1.33745101	0.70246800
H	5.92671877	−1.16757901	1.49725400
O	3.05724677	−0.50359401	1.91586000
O	2.04256677	−0.59213001	2.61174000

#### TS24a

0 2

C	−0.95619394	−0.15942029	−0.02503882
C	−1.29261094	−1.49725929	0.26344218
C	−0.32309394	−2.46929029	0.42805618

C	1.01084106	−2.07674029	0.29492218
C	1.37064206	−0.73449329	0.00678918
C	0.36199606	0.22851071	−0.15408082
H	−1.74719094	0.56992271	−0.14784282
H	−2.33676994	−1.77044729	0.35746318
H	−0.58809294	−3.49663729	0.64803918
H	0.61650606	1.25819371	−0.37760782
C	3.25470306	−1.98726029	0.21531418
C	4.59921506	−2.33071929	0.07301018
C	5.62585806	−1.22475929	0.10439118
C	5.06060406	0.12438971	−0.26268382
C	3.74198506	0.36593171	−0.31902382
C	2.79713206	−0.69757929	−0.05550682
H	6.42543506	−1.48806529	−0.59396682
H	5.78245606	0.91687471	−0.42263682
H	3.36972806	1.35622971	−0.55641082
N	2.16234506	−2.81790929	0.40136018
H	2.20768206	−3.80401429	0.59649218
H	4.95767206	−3.32716629	0.30573818
O	6.27590906	−1.17203229	1.37708818
H	5.64555506	−0.81666129	2.01251418
O	4.65632106	−2.55161329	−1.97680782
O	3.64603206	−2.13013229	−2.51981882

#### TS24s

0 2

C	−0.43478260	−0.15942029	0.00000000
C	−0.80434660	−1.51519229	−0.10389800
C	0.14003340	−2.51674729	−0.23297800
C	1.48343740	−2.13477029	−0.25341900
C	1.87635440	−0.77570229	−0.15405700
C	0.89261740	0.21734971	−0.02454300
H	−1.20724460	0.59261171	0.10233900
H	−1.85500060	−1.77909929	−0.08057800
H	−0.15099260	−3.55753129	−0.30899600
H	1.17370240	1.26096671	0.05581700
C	3.72703840	−2.07994329	−0.35973700
C	5.06892740	−2.43557429	−0.23532500
C	6.09975940	−1.35934229	−0.44702700
C	5.58311640	0.02574971	−0.14549100

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C	4.27414440	0.30498271	−0.06336600
C	3.30365740	−0.75717729	−0.20330400
H	6.37694640	−1.37714629	−1.51380300
H	6.33888740	0.79655271	−0.04571400
H	3.93137640	1.31512271	0.12949600
N	2.61623440	−2.90458229	−0.35889700
H	2.63645940	−3.90707929	−0.44340200
H	5.40765040	−3.46062129	−0.33248500
O	7.30560040	−1.64954729	0.23240600
H	7.09895040	−1.70727329	1.17159400
O	5.14086240	−2.44276929	1.85992100
O	4.14552340	−1.90139229	2.33666300

TS25a

0 2

C	−0.11594203	0.10144927	0.00000000
C	−0.41781503	−1.26396473	0.06428300
C	0.57747597	−2.23504473	0.05656000
C	1.89721097	−1.80381373	−0.01699400
C	2.21871797	−0.43031373	−0.07980000
C	1.20380797	0.52435227	−0.07431400
H	−0.91867703	0.82752727	0.00703900
H	−1.45430403	−1.57538873	0.12009100
H	0.33110997	−3.28887973	0.10341700
H	1.44401197	1.58010927	−0.12707300
C	4.17033397	−1.70418573	−0.10109900
C	5.48345197	−1.99724373	−0.06636900
C	6.48935997	−0.88821573	−0.09490800
C	5.89866997	0.46470527	−0.39731800
C	4.52377597	0.72811127	−0.24660700
C	3.66018697	−0.33390673	−0.15280100
H	7.24098097	−1.08515973	−0.87302800
H	6.60568597	1.28279627	−0.31172500
H	4.15615097	1.74687727	−0.27245100
N	3.06373997	−2.54780373	−0.04768100
H	3.11207897	−3.54830873	0.03851300
H	5.85236397	−3.01093173	0.03735400
O	7.25768997	−0.84693573	1.11089900
H	6.64164197	−0.77669473	1.84692200
O	7.10707297	−0.12405673	−2.77762500

O	6.05628097	0.38380527	−2.39727500
TS25s			
0 2			
C	−0.50724637	−0.51449276	0.00000000
C	−1.00170137	−1.77735776	0.34505800
C	−0.16686137	−2.88223476	0.47125600
C	1.19093463	−2.69247776	0.23903500
C	1.70522563	−1.42532076	−0.10822800
C	0.85029763	−0.33256876	−0.22656900
H	−1.18893937	0.32171224	−0.08712300
H	−2.06408937	−1.90024976	0.52034600
H	−0.56193137	−3.85403576	0.74080900
H	1.24159263	0.64348324	−0.48949200
C	3.43378263	−2.99235376	−0.01703700
C	4.66974163	−3.50457376	−0.12417700
C	5.79889563	−2.59969176	−0.53958100
C	5.46000163	−1.13772076	−0.39977100
C	4.14106263	−0.68506076	−0.54742000
C	3.13745763	−1.57381176	−0.25731500
H	6.00045663	−2.77242776	−1.60982000
H	6.28958363	−0.46212476	−0.57534800
H	3.93254463	0.37182924	−0.66029800
N	2.22527563	−3.61017776	0.29040100
H	2.12406563	−4.58113676	0.52981600
H	4.89000363	−4.55762076	0.00439000
O	7.02008663	−2.92344476	0.09645300
H	6.92183963	−2.71286676	1.03128200
O	4.50719263	−1.14862176	2.17266300
O	5.60638563	−1.07811976	1.61236000
TS26			
0 2			
C	−2.08015257	0.26717557	0.00000000
C	−2.27015757	1.68619057	0.32572300
C	−1.20459857	2.52515757	0.56144300
C	0.07653043	1.97327257	0.56111300
C	0.30670443	0.56243357	0.42482000
C	−0.74665657	−0.28448843	0.24154900

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H	−2.16340157	0.30500657	−1.19850000
H	−3.28826457	2.04758857	0.38528100
H	−0.62349857	−1.35979943	0.17192000
C	2.30654743	1.64377857	0.77441800
C	3.67348243	1.82694257	0.94886500
C	4.47849143	0.69512157	0.91637600
C	3.93793243	−0.58015843	0.71459400
C	2.57073443	−0.75038243	0.53914200
C	1.74490643	0.36911857	0.57202100
H	4.09705743	2.81209057	1.10389000
H	5.54814343	0.80466857	1.04933000
H	4.59499743	−1.44041943	0.69278100
H	2.15309843	−1.73766943	0.37796900
N	1.28451743	2.58845157	0.76184700
H	1.41410443	3.58023157	0.87532900
H	−1.36007757	3.57836557	0.76226800
O	−3.16122657	−0.58324643	0.32597600
H	−3.19138957	−0.67276843	1.28275300
O	−2.55170057	0.97547657	−2.51300600
O	−2.78872257	2.12648557	−2.13143000

TS27a

0 2

C	−0.44927536	−0.15942029	0.00000000
C	−0.57884936	1.30277071	0.35012600
C	0.46584464	2.13086371	0.47200700
C	1.79018164	1.59997371	0.25961500
C	1.99699264	0.15943271	0.17828200
C	0.95647464	−0.68007529	0.07265300
H	−0.79409636	−0.28294829	−1.04089000
H	−1.59014936	1.67246771	0.48665600
H	1.07737864	−1.75595829	0.02060500
C	4.00408464	1.24454771	0.48338300
C	5.37169264	1.43715171	0.59547500
C	6.18669164	0.31441271	0.48227300
C	5.64927764	−0.95727329	0.27054200
C	4.27393964	−1.13483129	0.15734100
C	3.44788564	−0.02369829	0.25881400
H	5.79174664	2.42191771	0.76025600
H	7.26095364	0.43234871	0.55992000

H	6.31156664	−1.80996729	0.18913600
H	3.85531464	−2.11960129	−0.01565800
N	2.96971864	2.19154671	0.60311800
H	3.13614564	3.17006771	0.40636300
H	0.33954764	3.18171571	0.70492300
O	−1.25314036	−0.97666729	0.84723500
H	−2.17638536	−0.85867829	0.60976000
O	1.89351564	1.98574071	−1.79415300
O	2.84064164	2.75662171	−1.98607000
TS27s			
O 2			
C	0.08695652	−0.66666666	0.00000000
C	−0.05601148	0.83395334	0.06491400
C	0.96768952	1.67942134	0.23219200
C	2.28741252	1.13045534	0.43753000
C	2.51932852	−0.30292266	0.29403100
C	1.49945252	−1.15646266	0.12927100
H	−0.29136948	−0.99672366	−0.98168400
H	−1.06525748	1.22100134	−0.04196900
H	1.65068052	−2.22813266	0.06418300
C	4.51855052	0.83444934	0.38074500
C	5.88470852	1.05491934	0.44420900
C	6.71275552	−0.06419366	0.47630000
C	6.18890252	−1.35798966	0.43882500
C	4.81401052	−1.56394066	0.37677200
C	3.97528352	−0.45825666	0.35596100
H	6.29335052	2.05755434	0.47258400
H	7.78580752	0.07473634	0.53162200
H	6.85990152	−2.20740166	0.46414600
H	4.40548652	−2.56762366	0.35728300
N	3.47814752	1.78262834	0.29161000
H	3.59989652	2.70874434	0.68313300
H	0.82217252	2.75279734	0.27516400
O	−0.67924548	−1.31254766	1.01633500
H	−1.60805848	−1.10077066	0.88639100
O	2.21602052	1.16663634	2.49304400
O	3.09092952	1.94401634	2.89224000

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**TS28a**
**0 2**

C	−0.44927536	−0.33333333	0.00000000
C	−0.93964936	−1.59220233	−0.38663000
C	−0.08298136	−2.63902033	−0.68303200
C	1.28514864	−2.39335833	−0.58038100
C	1.79808264	−1.13843733	−0.18498200
C	0.91073564	−0.09667333	0.10234500
H	−1.15048536	0.46310367	0.21680200
H	−2.00948836	−1.74628333	−0.45805700
H	−0.46142436	−3.60760333	−0.98743700
H	1.28234564	0.87865367	0.39473200
C	3.52007964	−2.55761533	−0.57858500
C	4.88533064	−3.14341133	−0.71557600
C	5.91960064	−2.15903833	−0.23594300
C	5.63469464	−0.90422533	0.16009100
C	4.29123564	−0.36451233	0.13665200
C	3.23684564	−1.26776033	−0.17935600
H	5.08052764	−3.37711433	−1.77000800
H	6.94138664	−2.52234633	−0.23316300
H	6.43670864	−0.24788133	0.47858200
H	4.08203664	0.54307667	0.68815200
O	4.98457764	−4.40759333	−0.06280100
H	4.91313364	−4.25296233	0.88533100
N	2.36142464	−3.23339033	−0.82026600
H	2.31185064	−4.21359533	−1.05070500
O	4.45102764	0.77668567	−1.56631400
O	4.93529764	1.88438067	−1.36874100

**TS28s**
**0 2**

C	0.68115941	−0.14492753	0.00000000
C	0.52655941	1.31186247	0.37329100
C	1.57692941	2.13495647	0.50970200
C	2.89891141	1.57488147	0.38969900
C	3.12716141	0.20446547	0.27348300
C	2.04319741	−0.69322553	0.30504500
H	0.55875341	−0.20493453	−1.10049200
H	−0.48771759	1.68320547	0.47432300
H	2.17865241	−1.75688253	0.14932400



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C	5.13110441	1.30942647	0.40713400
C	6.50947041	1.50932647	0.44657500
C	7.31689841	0.38502947	0.38736300
C	6.76823041	−0.90466653	0.28943300
C	5.39764241	−1.09541953	0.24469400
C	4.55972541	0.02183647	0.30239900
H	6.93426941	2.50303947	0.52687800
H	8.39317241	0.50368247	0.41988800
H	7.43120341	−1.76015953	0.25063600
H	4.97925241	−2.09262553	0.17139800
N	4.09861641	2.23179347	0.46005500
H	4.21292741	3.22728647	0.55663300
H	1.44612041	3.18715147	0.73612300
O	−0.29415159	−0.97282253	0.60997000
H	−1.14475359	−0.80803353	0.19620600
O	1.85634341	−0.99438553	2.37301300
O	1.62398541	−2.15291753	2.68148000

TS29a

0 2

C	−0.10144927	−0.05797101	0.00000000
C	−0.25449027	1.41709399	0.17183400
C	0.85191473	2.26467599	0.26875700
C	2.10745273	1.70146299	0.19070400
C	2.32497873	0.26217699	0.17067300
C	1.27484573	−0.58223301	0.17553600
H	−0.33512927	−0.22876801	−1.09227600
H	−1.21945427	1.76118199	0.52018900
H	1.38813473	−1.65919101	0.22934600
C	4.35334373	1.35001999	0.25843000
C	5.72755673	1.53451999	0.30751800
C	6.52616973	0.39411499	0.31505200
C	5.96846773	−0.88553101	0.27288400
C	4.58814373	−1.05520101	0.22226800
C	3.77472473	0.06997999	0.21886100
H	6.16450473	2.52526999	0.33932500
H	7.60318873	0.50527499	0.35259200
H	6.61747873	−1.75214401	0.27764900
H	4.15533173	−2.04824501	0.18491700
N	3.33515373	2.30581299	0.23594300

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H	3.48160473	3.30129699	0.26457700
H	0.72051273	3.32647599	0.43628300
O	−1.03438027	−0.81272301	0.75855200
H	−1.83016027	−0.92571701	0.23210200
O	−1.06607327	1.79509299	−1.76513800
O	−1.20683727	0.72722499	−2.37769500

#### TS29s

0 2

C	−0.05797101	−0.08695652	0.00000000
C	−0.18597301	1.35601148	0.40063300
C	0.90915399	2.21690048	0.33031800
C	2.16279099	1.63883048	0.33524900
C	2.36326099	0.19142948	0.37668400
C	1.31271999	−0.64347852	0.28671300
H	−0.16524901	−0.10922452	−1.10169500
H	−1.19521201	1.74945648	0.40892600
H	1.41535999	−1.72288752	0.31361400
C	4.39745399	1.26443848	0.52441800
C	5.76823199	1.43938548	0.64116800
C	6.55129899	0.29356748	0.75294200
C	5.98194299	−0.98125152	0.74424300
C	4.60444599	−1.14083652	0.62483300
C	3.80681399	−0.01002952	0.51882900
H	6.21444299	2.42643748	0.64670800
H	7.62568799	0.39673348	0.84755300
H	6.61943899	−1.85197352	0.83108700
H	4.16175999	−2.13013552	0.61991600
N	3.39442799	2.22964048	0.39348000
H	3.54645399	3.22279348	0.45979300
H	0.78409499	3.28722948	0.43786900
O	−1.10524801	−0.89497752	0.47783600
H	−1.14819701	−0.80279852	1.43983900
O	−0.08811101	1.05565248	2.52986900
O	−0.75125401	0.14940748	3.06336600

#### TS30

0 2

C	−1.27862589	0.03816794	0.00000000
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C	-1.06912389	-1.30679606	0.16488500
C	-2.13800089	-2.22755206	0.24143000
C	-3.43212189	-1.73042606	0.16499600
C	-3.70038189	-0.35509406	-0.00319700
C	-2.61323289	0.56795394	-0.25597000
H	-0.45159889	0.73700394	-0.04270300
H	-0.05629689	-1.67777506	0.26658800
H	-2.64716589	0.57166494	-1.48815600
C	-5.67157389	-1.47297406	0.24614700
C	-7.04649489	-1.67289106	0.34582100
C	-7.86204489	-0.55591106	0.24805900
C	-7.33200789	0.73084494	0.05439300
C	-5.96603689	0.92916494	-0.04191500
C	-5.11983689	-0.18228606	0.05996600
H	-7.46462989	-2.66225306	0.48830900
H	-8.93606789	-0.68061506	0.31978900
H	-8.00610789	1.57467594	-0.02321200
H	-5.54591889	1.91475694	-0.20050400
N	-4.63954789	-2.38917906	0.29492000
H	-4.74707289	-3.37874906	0.43950100
H	-1.94742089	-3.28337106	0.38798700
O	-2.84016589	1.92708194	0.03467800
H	-2.85308889	2.02602794	0.99173400
O	-3.09650589	0.22374494	-2.83520200
O	-3.84779489	-0.73321206	-2.64150400

TS31a

02

C	0.17391304	-0.53623188	0.00000000
C	0.38948004	-1.85645588	0.14933000
C	-0.67875596	-2.82373788	0.32207500
C	-1.95748196	-2.37774188	0.24798200
C	-2.25305396	-1.00152088	-0.09877700
C	-1.20294896	0.06654912	0.00230000
H	1.00412804	0.15636712	-0.07278900
H	1.40771004	-2.22825488	0.16949400
H	-1.33125696	0.72719412	-0.86586700
C	-4.20807996	-2.11789388	0.34658900
C	-5.57410396	-2.31085688	0.50513500
C	-6.39497296	-1.19241788	0.38836400

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C	−5.88033596	0.08129012	0.12296500
C	−4.51288396	0.26818712	−0.03634900
C	−3.67581396	−0.83835288	0.07830900
H	−5.98904096	−3.29048688	0.70897900
H	−7.46494496	−1.31505188	0.51062100
H	−6.55549196	0.92377612	0.04537300
H	−4.09343396	1.24772512	−0.23188400
N	−3.16850596	−3.03481888	0.41239700
H	−3.26417496	−3.98809988	0.71826600
H	−0.44276396	−3.86093088	0.52496600
O	−1.40437596	0.92622312	1.12091200
H	−1.21740796	0.42425912	1.92050800
O	−2.11099696	−1.24186288	−2.03791200
O	−2.33645296	−0.19445988	−2.64334400

TS31s

02

C	−0.14492753	−0.24637681	0.00000000
C	0.05831547	−1.55133781	0.24276100
C	−1.03129353	−2.50926981	0.34996900
C	−2.30138253	−2.03704281	0.32886200
C	−2.57746153	−0.60908381	0.27702900
C	−1.52214053	0.31148219	−0.25315200
H	0.68018247	0.44901519	−0.10092400
H	1.06909147	−1.92422381	0.36133000
H	−1.66274353	0.35411419	−1.34599500
C	−4.55395553	−1.76356381	0.35172100
C	−5.92674853	−1.96191981	0.40503200
C	−6.73885253	−0.83577181	0.29468700
C	−6.21017653	0.45026519	0.14556300
C	−4.83482053	0.64458019	0.10132900
C	−4.00566753	−0.47161481	0.18657000
H	−6.35353753	−2.94951381	0.53102500
H	−7.81458453	−0.96355581	0.33100800
H	−6.87988953	1.29777019	0.07648000
H	−4.40054753	1.63186919	0.00213300
N	−3.52121253	−2.68463381	0.44154000
H	−3.63874953	−3.67446781	0.57373600
H	−0.81606253	−3.56378081	0.46852600
O	−1.68622753	1.64797919	0.17306300

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H	−1.62066853	1.66560019	1.13409100
O	−2.28518653	−0.28771481	2.20456800
O	−3.11326553	0.49838919	2.68700000

#### TS32a

0 2

C	−0.36231884	−0.04347826	0.00000000
C	−0.17770184	−1.36098426	0.45872400
C	−1.25440184	−2.20270626	0.54370000
C	−2.56556984	−1.65238626	0.37388600
C	−2.80828884	−0.31259126	0.17824900
C	−1.69568084	0.67298174	0.09281900
H	0.50612616	0.60119774	−0.09375500
H	0.82553716	−1.74827226	0.58205200
H	−1.81374384	1.28898574	−0.80911200
C	−4.79439584	−1.42998026	0.26425300
C	−6.17553584	−1.63547826	0.23699300
C	−6.98069284	−0.52444226	0.06691100
C	−6.43335684	0.76677774	−0.07197700
C	−5.06786284	0.96866574	−0.04659300
C	−4.22351284	−0.14019126	0.11791900
H	−6.60049584	−2.62629526	0.34757800
H	−8.05664284	−0.64878926	0.04314700
H	−7.10075184	1.61061074	−0.19671900
H	−4.64849584	1.96342574	−0.14126800
N	−3.76596884	−2.33056826	0.42375200
H	−3.86975684	−3.32705426	0.51733100
H	−1.12794184	−3.25329726	0.77879300
O	−1.74757484	1.52011874	1.24444000
H	−1.16938684	2.27410874	1.09687500
O	−0.57955684	−0.41973726	−1.99339400
O	−0.86784284	−1.57900726	−2.24932500

#### TS32s

0 2

C	0.89855071	0.13043478	0.00000000
C	1.10479471	−1.26022422	0.07961000
C	0.03702271	−2.09063422	0.30345300
C	−1.28341429	−1.54005622	0.25141800

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C	−1.54047529	−0.22418922	−0.06126300
C	−0.42979529	0.71155278	−0.42043700
H	1.74692671	0.79605678	−0.11324800
H	2.11326271	−1.64477722	0.16342000
H	−0.39694529	0.82338478	−1.51592400
C	−3.51064429	−1.29934622	0.33530300
C	−4.88739529	−1.48394022	0.48225000
C	−5.70249629	−0.39033922	0.25693100
C	−5.17038629	0.86369378	−0.10526800
C	−3.80983629	1.04904278	−0.24574200
C	−2.95511729	−0.04467422	−0.02578400
H	−5.30043729	−2.44588922	0.76203800
H	−6.77535529	−0.49943922	0.36206500
H	−5.84630629	1.69355978	−0.27114700
H	−3.39457329	2.01309978	−0.51363300
N	−2.47554729	−2.19327822	0.48718300
H	−2.56776029	−3.14917822	0.78791000
H	0.18345071	−3.14625522	0.50179000
O	−0.61892129	2.02932778	0.05702600
H	−0.64300929	1.98760378	1.01919700
O	0.64478671	0.49277978	2.01151300
O	0.35248271	−0.51028722	2.65663900

TS33a

0 2

C	0.52173912	0.17391304	0.00000000
C	0.72886812	−1.14606796	0.14913100
C	−0.36391888	−2.09106096	0.20518700
C	−1.66980188	−1.53400396	0.22471000
C	−1.92870488	−0.18536896	0.08946400
C	−0.84168188	0.81039604	−0.11698600
H	1.36976112	0.85108704	−0.04340500
H	1.73896812	−1.53149796	0.22148200
H	−0.93320788	1.21409804	−1.13953200
C	−3.89702988	−1.31839296	0.29142300
C	−5.27695488	−1.52844196	0.35772700
C	−6.09356888	−0.41625396	0.28096500
C	−5.56136488	0.88323104	0.14792900
C	−4.19930788	1.09204404	0.08290000
C	−3.34345788	−0.02057996	0.14218900

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H	−5.69014788	−2.52397196	0.46853000
H	−7.16825888	−0.54488096	0.32989600
H	−6.23866688	1.72720704	0.10243800
H	−3.78402588	2.08883304	−0.00238200
N	−2.86051488	−2.21916896	0.36034100
H	−2.94749388	−3.22025796	0.28391900
H	−0.19041588	−3.08473296	0.59733100
O	−1.01260388	1.88249704	0.80931300
H	−0.43285188	2.60562604	0.55434400
O	−0.34410288	−2.93702696	−1.67645000
O	−1.30260088	−3.69211896	−1.80568500

TS33s

0 2

C	−0.27536231	−0.20289855	0.00000000
C	−0.05790031	−1.52321855	0.12667700
C	−1.14366331	−2.47555755	0.21689800
C	−2.45511531	−1.93641655	0.12219900
C	−2.72261931	−0.58859855	0.00435600
C	−1.64077231	0.42325545	−0.14988700
H	0.56858569	0.48057045	−0.02616000
H	0.95484669	−1.90151755	0.20220900
H	−1.70133431	0.85660045	−1.16257600
C	−4.68463431	−1.74093155	0.14702900
C	−6.06290631	−1.96086755	0.21352600
C	−6.88759931	−0.85485455	0.13250700
C	−6.36509431	0.44756445	−0.00874200
C	−5.00428431	0.66671945	−0.06716800
C	−4.14012631	−0.43815955	0.01052900
H	−6.46896931	−2.95933255	0.32395000
H	−7.96135031	−0.99111255	0.18117900
H	−7.04869931	1.28598945	−0.06197600
H	−4.59668531	1.66688845	−0.14992000
N	−3.64248231	−2.63822855	0.18439000
H	−3.70932031	−3.60085955	0.47645600
H	−0.96210431	−3.52039555	0.00076600
O	−1.85741831	1.46585845	0.79987800
H	−1.24755731	2.18500845	0.61255400
O	−1.10099231	−3.00358955	2.20121500
O	−2.00431431	−3.79772055	2.44452500

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TS34

0 2

C	−0.38291604	−0.55223543	−0.00722916
C	−0.11789804	0.82509757	0.05965284
C	−1.11967204	1.76101257	−0.14326916
C	−2.39511004	1.27836757	−0.42142216
C	−2.68511804	−0.10224543	−0.49174116
C	−1.65646204	−1.02449143	−0.27754116
H	0.42411096	−1.25501443	0.15942684
H	0.88809596	1.16309157	0.27609084
H	−0.91696404	2.82392457	−0.08899416
H	−1.85308204	−2.08946143	−0.31758316
C	−4.57814904	1.08293857	−0.86965716
C	−5.97573904	1.44744657	−1.25892816
C	−6.89757304	0.30236757	−0.84703116
C	−6.33717204	−1.11321443	−1.02145416
C	−4.97378204	−1.31612243	−0.98058716
C	−4.09889804	−0.21267143	−0.77427016
H	−6.02184504	1.59231957	−2.34458416
H	−7.88552604	0.42077157	−1.30212016
H	−6.99676404	−1.89314843	−1.37415016
H	−4.57711804	−2.32174443	−1.05771316
O	−6.38649004	2.66773057	−0.67872616
H	−6.55071004	2.49775057	0.25805484
N	−3.57538704	1.96969957	−0.66846816
H	−3.70367504	2.97033857	−0.65202816
O	−7.00183504	−1.04368143	0.82007384
O	−6.98366504	0.34745857	0.56957484

## TS35

0 2

C	−0.19145802	0.27245950	0.00000000
C	0.08466398	1.65063350	−0.02460500
C	−0.90807402	2.57721950	−0.29329300
C	−2.18993102	2.08835150	−0.53832000
C	−2.49015602	0.70661350	−0.51759200
C	−1.46593002	−0.20734950	−0.24343400
H	0.61019598	−0.42301250	0.21636200



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H	1.09295298	1.99427550	0.17141400
H	-0.69680102	3.63983050	-0.31160800
H	-1.66892302	-1.27156050	-0.21471900
C	-4.37262902	1.87253650	-0.97857000
C	-5.80625002	2.22715450	-1.24978600
C	-6.63052802	0.99048550	-0.87032200
C	-6.07598902	-0.29647050	-1.42729300
C	-4.79002502	-0.53097550	-0.94705300
C	-3.89659202	0.59408750	-0.80591200
H	-5.95730602	2.49008950	-2.30252100
H	-7.69019902	1.14400850	-1.08111800
H	-6.73187502	-1.09623150	-1.73822800
H	-4.38897202	-1.53844150	-0.94219500
O	-6.21013702	3.35284850	-0.49898800
H	-6.20739902	3.08158450	0.42884900
N	-3.36199402	2.76923650	-0.83022400
H	-3.49142702	3.76925150	-0.81888500
O	-5.88704902	-0.43229350	0.78028200
O	-6.43669202	0.85103150	0.55327600

TS36

02

C	-1.68893132	-0.57251908	0.00000000
C	-1.47106132	0.80221492	0.17176600
C	-2.50796532	1.72017092	0.05578600
C	-3.76879532	1.22283692	-0.24093400
C	-4.01375832	-0.16097708	-0.41149800
C	-2.95213732	-1.06336308	-0.28778700
H	-0.85686632	-1.25823608	0.10003400
H	-0.47402032	1.15736092	0.40207600
H	-2.33620632	2.78110992	0.19138800
H	-3.11777632	-2.12751808	-0.40850200
C	-5.96948732	1.00356792	-0.61816600
C	-7.32827932	1.30542292	-1.17692500
C	-8.17783832	0.14302792	-0.67486600
C	-7.60939732	-1.19737008	-1.06194200
C	-6.27187032	-1.39663208	-0.99784600
C	-5.41567032	-0.29846408	-0.68317200
H	-7.28815332	1.29347592	-2.27025300
H	-9.22476632	0.26536592	-0.95079100

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H	−8.29016532	−2.01678208	−1.25367700
H	−5.84776732	−2.38104008	−1.16231600
O	−7.80766432	2.55738192	−0.77390600
H	−7.85595732	2.52109692	0.19193000
N	−4.96992632	1.90151892	−0.43582900
H	−5.12242832	2.89196492	−0.32581300
O	−6.94071332	0.83451792	1.14854000
O	−8.12240632	0.20539292	0.77181900

TS37

0 2

C	−1.39312969	−0.22900763	0.00000000
C	−1.15567169	1.11309837	0.35441500
C	−2.19696769	1.99127837	0.58794500
C	−3.49585969	1.49276537	0.46559100
C	−3.75765769	0.15115837	0.10023300
C	−2.67942669	−0.71533363	−0.13079600
H	−0.55036269	−0.88613663	−0.17582900
H	−0.13513969	1.46437237	0.44622500
H	−2.01227169	3.02358137	0.86064200
H	−2.85409569	−1.74742363	−0.41221800
C	−5.71364769	1.23994537	0.37540000
C	−7.15967269	1.34819537	0.62579300
C	−7.87150869	0.33603737	−0.30331800
C	−7.36562469	−1.06320363	−0.15586600
C	−6.03260569	−1.18406263	−0.06555300
C	−5.18779869	0.00381037	0.05230200
H	−8.03738669	2.21163237	0.16197200
H	−7.66204669	0.68697337	−1.32487100
H	−8.04036869	−1.90587163	−0.23250400
H	−5.56079269	−2.15967263	−0.04774800
O	−7.44125669	1.25876037	1.96741500
H	−8.39389869	1.11650137	2.06646700
N	−4.70803169	2.12555937	0.64757600
H	−4.83846869	3.08661237	0.91798100
O	−9.29119169	1.97948137	−0.22299600
O	−9.22256969	0.59788137	−0.00774500

TS38

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0 2

C	0.71564888	−0.30534351	0.00000000
C	0.89860988	1.08818349	0.04770400
C	−0.15673912	1.95779849	−0.16581300
C	−1.40533512	1.39893949	−0.43562300
C	−1.61377612	−0.00160651	−0.48507300
C	−0.52599212	−0.85599351	−0.26140000
H	1.56406388	−0.95590851	0.17421700
H	1.88349288	1.48854549	0.25534500
H	−0.01660012	3.03175549	−0.12858400
H	−0.65680512	−1.93168051	−0.28901100
C	−3.56628012	1.05112049	−0.87036200
C	−4.98343412	1.29004849	−1.28247600
C	−5.84586312	0.10866649	−0.82019900
C	−5.18894712	−1.23636351	−1.03068300
C	−3.85634512	−1.36517651	−0.95489300
C	−3.01274312	−0.19590151	−0.76422600
H	−5.02110212	1.30202449	−2.37877800
H	−6.82273512	0.17265349	−1.31158300
H	−5.83303412	−2.09777651	−1.14695700
H	−3.39721412	−2.34486451	−1.03530900
O	−5.48503912	2.53619749	−0.85400700
H	−5.73787912	2.44047249	0.07135800
N	−2.61897612	2.01374849	−0.68803900
H	−2.80609512	3.00399649	−0.69710800
O	−7.00250012	−0.53711251	1.07041400
O	−6.06120112	0.36237349	0.58356100
O	−9.00423212	0.71828149	0.70771800
H	−8.91269612	1.29062849	1.48682000
H	−7.88965912	−0.19324851	0.70688800

TS39

0 2

C	−0.08838605	−0.33134883	0.00318073
C	−0.34518505	−1.70287583	−0.17438627
C	0.68471095	−2.62337883	−0.25110927
C	1.98718695	−2.13627483	−0.14127627
C	2.26799295	−0.76297383	0.03858173
C	1.20519995	0.14625717	0.10780673
H	−0.92111005	0.35905117	0.05727873

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H	−1.36974805	−2.04521383	−0.25350227
H	0.48675995	−3.67958683	−0.39002927
H	1.39303495	1.20537817	0.24145973
C	4.21177295	−1.91440783	−0.03554027
C	5.66000195	−2.25596183	0.06930873
C	6.47100595	−0.96836483	−0.10146727
C	5.91903495	0.31030217	0.32257973
C	4.57550795	0.47473217	0.36575173
C	3.70259195	−0.64405283	0.11025773
H	5.96570695	−2.96178183	−0.71252127
H	6.73508795	−0.90724883	−1.34323427
H	6.61629395	1.11255917	0.52657773
H	4.14834495	1.43702117	0.62413373
O	5.89221895	−2.82514283	1.34645773
H	6.84625795	−2.93475683	1.44044273
N	3.19479595	−2.81022983	−0.18634927
H	3.30791495	−3.81041183	−0.23252027
O	8.08148695	−1.24961183	−1.28979827
O	7.82376195	−1.18531383	0.13845573

TS40

02

C	−0.12847967	−0.35331905	0.00000000
C	0.22653733	0.97904495	−0.28008600
C	−0.72385267	1.98325395	−0.31937300
C	−2.04793467	1.62338595	−0.06454900
C	−2.42710367	0.29005095	0.21684800
C	−1.44268567	−0.70611605	0.24506600
H	0.64403333	−1.11219805	0.02169300
H	1.26492833	1.22262395	−0.46967200
H	−0.45042467	3.00901595	−0.53746800
H	−1.70688767	−1.73627905	0.45514800
C	−4.26561367	1.60317295	0.24724400
C	−5.65253167	2.08580595	0.54160800
C	−6.57234167	0.89169495	0.35639200
C	−6.12108067	−0.43113305	0.81706200
C	−4.80303667	−0.72264905	0.80219000
C	−3.85372467	0.30218195	0.41931800
H	−5.96106767	2.88795495	−0.13284500
H	−6.88547867	−1.15730505	1.06271100

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H	−4.45196867	−1.70533005	1.09316800
O	−5.72352167	2.66537495	1.83890200
H	−5.46061367	1.99535495	2.47983200
N	−3.18982767	2.40042095	−0.03923100
H	−3.21988267	3.40332595	−0.12762000
O	−8.74899667	0.24704995	0.23638400
O	−7.87776567	1.24341295	0.56503400
O	−7.50141767	−0.06826905	−1.81106900
H	−6.73214367	0.51147695	−0.95396300
H	−8.24190167	−0.07901005	−1.02280900
H	−7.79562367	0.53358695	−2.50350100

TS41

02

C	−0.85419732	−0.21354933	0.00000000
C	−0.97658832	−1.61403233	−0.04498100
C	0.11357968	−2.42292333	−0.31456100
C	1.33673068	−1.79431733	−0.54212200
C	1.48220268	−0.38583633	−0.50728000
C	0.36091368	0.40633867	−0.22569000
H	−1.72952932	0.38572867	0.21891600
H	−1.94281032	−2.06876833	0.13673100
H	0.02032068	−3.50196133	−0.34490500
H	0.44524368	1.48615467	−0.18325900
C	3.47757868	−1.33328433	−0.96472100
C	4.91207068	−1.51441633	−1.31434100
C	5.73901268	−0.28269133	−0.59998500
C	5.01741668	1.02174467	−0.73806300
C	3.67545968	1.08684667	−0.77617300
C	2.87018668	−0.11505133	−0.77108100
H	5.07617368	−1.25413733	−2.37678300
H	6.73122768	−0.31087733	−1.05450700
H	5.62409668	1.91801367	−0.77275000
H	3.18723768	2.05483367	−0.82053200
O	5.45281768	−2.68696133	−0.97575200
H	6.16271768	−2.42133533	0.07702300
N	2.57786268	−2.33964933	−0.82505300
H	2.81778268	−3.31848733	−0.87120500
O	6.61884068	−1.77085433	0.84830300
O	5.83578168	−0.64645933	0.74260600

TS42

0 2

C	-1.32165603	-0.28662419	0.00000000
C	-1.18030803	1.10692081	0.12458800
C	-2.26975403	1.95248181	0.00518100
C	-3.51098403	1.36976181	-0.24511500
C	-3.67651503	-0.03229219	-0.37600600
C	-2.55513103	-0.86206519	-0.24595400
H	-0.44671603	-0.91744219	0.09946800
H	-0.20065203	1.52679381	0.31798100
H	-2.16214303	3.02629181	0.10346000
H	-2.65260903	-1.93808219	-0.33512400
C	-5.67222603	0.98458681	-0.62498100
C	-7.11383203	1.22341381	-0.89974900
C	-7.93597203	-0.06108619	-0.30939800
C	-7.24964203	-1.35372219	-0.64864700
C	-5.91094403	-1.43084919	-0.74671300
C	-5.07909103	-0.25358619	-0.61171800
H	-7.29946203	1.01893981	-1.97616200
H	-8.94701903	0.03047981	-0.71131900
H	-7.87026103	-2.23461119	-0.75262800
H	-5.44541103	-2.39372519	-0.93089500
O	-7.56939703	2.40554181	-0.48836700
H	-8.87950503	2.45030281	-0.49823100
N	-4.75343203	1.95773281	-0.40829700
H	-4.99178203	2.93436481	-0.32209000
O	-8.69130603	1.07640781	1.56474800
O	-7.98620303	0.03648881	1.09573900
O	-9.91484703	2.15947481	-0.21358200
H	-9.37275303	1.52391581	0.78736900
H	-10.45706703	2.92012181	0.00811800

TS43

0 2

C	-2.30303030	0.01010101	0.00000000
C	-2.11040330	1.39419301	-0.14058600
C	-3.18456130	2.26242401	-0.24730300
C	-4.46129830	1.70714201	-0.20765100

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C	−4.67801130	0.31918401	−0.06340400
C	−3.57574330	−0.53455599	0.03950900
H	−1.43951130	−0.63910499	0.07774700
H	−1.10267230	1.79040201	−0.16695300
H	−3.03621830	3.33017101	−0.35692600
H	−3.71471030	−1.60405299	0.14882400
C	−6.67669130	1.38064301	−0.19862000
C	−8.13649730	1.67619801	−0.21263600
C	−8.91097530	0.38643801	−0.05121300
C	−8.31912230	−0.85321899	0.16679600
C	−6.93889230	−1.01307699	0.13906000
C	−6.11157230	0.12611201	−0.05042000
H	−8.42416130	2.10867301	−1.18526200
H	−8.97932130	−1.70069399	0.30443200
H	−6.50020130	−1.99349899	0.27726000
O	−8.39775430	2.63720601	0.80649800
H	−9.32245730	2.53358501	1.06997700
N	−5.70126730	2.32245601	−0.29825000
H	−5.87111930	3.31625101	−0.28986300
O	−10.82880430	1.29578301	0.99342100
O	−10.21993130	0.45473301	−0.20854900
H	−11.67182730	1.51790001	0.57631000

TS44

0 2

C	−0.98550723	−0.61594203	0.00000000
C	−0.73191423	0.75509397	0.18306000
C	−1.70384323	1.70803397	−0.07175600
C	−2.94197623	1.25308697	−0.51898100
C	−3.21781723	−0.12130903	−0.71643200
C	−2.21778123	−1.06312703	−0.44109200
H	−0.19985823	−1.33103303	0.21100100
H	0.24282977	1.07264097	0.53256200
H	−1.51049623	2.76378997	0.07509700
H	−2.40639723	−2.12233803	−0.57274800
C	−5.05074323	1.10080697	−1.23846700
C	−6.38266223	1.58010397	−1.72254300
C	−7.37183723	0.12081097	−0.76714300
C	−6.81574123	−1.11526003	−1.32760700
C	−5.47633523	−1.30308503	−1.41817900

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C	−4.58515423	−0.20420003	−1.15513000
H	−6.67318623	1.14036597	−2.69507600
H	−8.41341123	0.35397097	−0.97670500
H	−7.50487123	−1.85463603	−1.72436600
H	−5.07595623	−2.25832803	−1.74281300
O	−6.79704623	2.69635497	−1.38050400
N	−4.08681023	1.96095097	−0.84845500
H	−4.23421123	2.95911897	−0.79447700
O	−7.89320023	−0.24350403	1.40436400
O	−7.00285223	0.46218697	0.52481300
H	−7.32650323	−0.96740603	1.70303100

TS45

02

C	−0.63768115	−0.24637682	0.00000000
C	−0.25651515	1.08315318	0.27510600
C	−1.12260115	2.13951618	0.07554600
C	−2.39402515	1.83708618	−0.42241100
C	−2.79413615	0.51249018	−0.70913300
C	−1.89728015	−0.54222682	−0.47979200
H	0.07176085	−1.04505482	0.17756400
H	0.73816485	1.27785018	0.65756300
H	−0.83173415	3.15945118	0.29570100
H	−2.19071515	−1.56802982	−0.67097300
C	−4.50388815	1.91297018	−1.17671800
C	−5.68283015	2.61467518	−1.70228800
C	−7.22964415	−0.18544182	−0.70621000
C	−6.25559015	−0.85683482	−1.48004100
C	−4.91949915	−0.57993582	−1.61689900
C	−4.15827515	0.56753918	−1.17872200
H	−6.45385315	1.99093418	−2.17611200
H	−8.23090015	−0.61139082	−0.64210200
H	−6.61212215	−1.76502882	−1.95526200
H	−4.32360515	−1.34595582	−2.10689600
O	−5.76768315	3.81833218	−1.64998400
N	−3.45197015	2.65880418	−0.71598600
H	−3.48301515	3.66786318	−0.67839900
O	−6.10416315	0.47301518	1.30267600
O	−7.00833115	0.87118918	0.01318700
H	−5.28441815	0.91046418	1.02429500



TS46

0 2

C	-1.41221367	-0.19083969	0.00000000
C	-1.10947567	1.15788631	0.26774200
C	-2.08969767	2.13370431	0.26251600
C	-3.39401467	1.72973231	-0.02298800
C	-3.72210167	0.37599431	-0.28740500
C	-2.70572767	-0.58957969	-0.27551400
H	-0.61484667	-0.92346269	0.01505400
H	-0.08514167	1.43704131	0.48349400
H	-1.85393367	3.17075231	0.46942800
H	-2.93307167	-1.63045069	-0.47475100
C	-5.59334767	1.63127031	-0.36741900
C	-6.97790867	2.02483731	-0.65654700
C	-7.96914067	0.84731731	-0.49501400
C	-7.38909167	-0.49438869	-0.88241100
C	-6.06934767	-0.72873469	-0.84936800
C	-5.13857967	0.33574831	-0.51960100
H	-6.84857867	1.96360531	-1.90902400
H	-8.87316267	1.07799431	-1.06642700
H	-8.09092367	-1.28600869	-1.11229400
H	-5.68029767	-1.71548469	-1.07537000
O	-7.39138167	3.22348231	-0.46056300
N	-4.55584467	2.47316631	-0.10113000
H	-4.66570367	3.45696131	0.09180700
O	-9.36853067	-0.03794869	1.08357100
O	-8.29551867	0.87803631	0.89458900
H	-10.06793367	0.55674531	1.38197700
O	-6.38828567	1.67302931	-3.27384200
O	-5.26124567	1.23970731	-3.25070600

TS47

0 1

C	0.21413278	-1.59528906	0.00000000
C	0.51708078	-0.23087906	0.18257800
C	-0.47521022	0.71217894	0.36471300
C	-1.79703722	0.25834294	0.36227900
C	-2.12195922	-1.10799706	0.17935700

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C	-1.09162422	-2.04152906	-0.00339900
H	1.02304678	-2.30063806	-0.14381100
H	1.55324678	0.08534794	0.17770100
H	-0.24022122	1.76039294	0.50360500
H	-1.31795722	-3.09061606	-0.15321200
C	-4.01647122	0.08954894	0.42958400
C	-5.42943122	0.44655094	0.57549900
C	-6.32680822	-0.71791406	0.18279600
C	-5.82827622	-2.05967806	0.35194200
C	-4.47734122	-2.29654806	0.15267400
C	-3.55370522	-1.19551206	0.23904700
H	-6.15912222	-0.63182106	-1.01249200
H	-6.54303622	-2.86943606	0.42048500
H	-4.10331822	-3.31245906	0.15693300
O	-5.82581822	1.54165194	0.88112800
N	-2.97302922	0.95949694	0.52007000
H	-3.07812822	1.95437494	0.65074000
O	-8.47045522	-1.39966606	-0.16006100
O	-7.65641822	-0.44871006	0.51097400
H	-8.88617722	-0.85383906	-0.84055400
O	-5.29398622	-1.07038106	-2.16966100
O	-5.03001722	-2.24286606	-1.81203100

TS48

0 2

C	-0.24809159	-0.32442748	0.00000000
C	0.01627741	1.04383052	0.20746000
C	-1.00439559	1.96500052	0.34175300
C	-2.31416559	1.48469852	0.26382000
C	-2.60110459	0.11323252	0.05434800
C	-1.54324759	-0.79673048	-0.07744200
H	0.58154541	-1.01311348	-0.09979700
H	1.04426541	1.38078152	0.26288000
H	-0.79870959	3.01635452	0.50199800
H	-1.73895359	-1.85053248	-0.23791100
C	-4.53386159	1.27428552	0.21956700
C	-5.95270359	1.57884152	0.27001700
C	-6.83819959	0.37631352	0.06738100
C	-6.28234659	-0.92752948	-0.07635400
C	-4.92597159	-1.11430448	-0.12039900

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C	−4.03516259	−0.00465848	0.02996800
H	−6.97780359	−1.74947348	−0.18658900
H	−4.51856559	−2.10906748	−0.26046800
O	−6.40625459	2.69412752	0.46219500
N	−3.51053159	2.16289152	0.36171100
H	−3.63969159	3.15233752	0.51140000
O	−8.63337659	1.12055552	1.55430000
O	−8.09124159	0.57582852	−0.00720000
H	−8.50370459	2.05888352	1.34112600

TS49

0 1

C	−0.40404040	−0.67676767	0.00000000
C	−0.17074340	0.63847133	0.43628000
C	−1.16782240	1.60097533	0.40350500
C	−2.40931940	1.21357133	−0.08690800
C	−2.67086840	−0.10748567	−0.52067300
C	−1.64504340	−1.05987267	−0.47489200
H	0.40134760	−1.39918867	0.04462000
H	0.81061460	0.90663833	0.80820600
H	−0.98673440	2.61197433	0.74712400
H	−1.82254740	−2.07785367	−0.80137900
C	−4.56371540	1.13865833	−0.66445100
C	−5.92516540	1.55865133	−1.09173600
C	−6.89341940	0.33966333	−1.00778900
C	−6.27152840	−0.98223267	−1.36344000
C	−4.93490240	−1.18538767	−1.33923500
C	−4.05670740	−0.14696967	−0.89505200
H	−5.85160540	1.86532633	−2.14525600
H	−7.66000540	0.48791333	−1.80581400
H	−6.95684240	−1.79143067	−1.58389000
H	−4.53089740	−2.16783567	−1.55911200
O	−6.40250740	2.64592233	−0.35026200
H	−7.05660740	2.28058133	0.26624400
N	−3.57503940	1.95595833	−0.24149900
H	−3.74037440	2.89062333	0.10256300
O	−6.41261440	−0.26667567	1.56089800
O	−7.64641040	0.36469233	0.12418800
O	−4.54633840	0.48574433	2.31089000
N	−5.42142340	0.41268133	1.48581000

TS50

0 2

C	-0.01908397	-0.15267175	0.00000000
C	0.34600103	1.20403025	0.07156900
C	-0.57593497	2.20951525	-0.15795000
C	-1.88211797	1.82340425	-0.45971600
C	-2.27201597	0.46643925	-0.53205100
C	-1.31503597	-0.52999875	-0.30021100
H	0.73187503	-0.91175375	0.18207100
H	1.36991503	1.46604425	0.30930000
H	-0.29436897	3.25463825	-0.10571500
H	-1.58519997	-1.57835875	-0.35468200
C	-4.06127397	1.77537725	-0.96971500
C	-5.45050397	2.22834125	-1.25989900
C	-6.30017797	1.03483725	-1.78105800
C	-5.90725397	-0.34052575	-1.37172100
C	-4.63852697	-0.60772075	-0.99867000
C	-3.67627697	0.46161025	-0.85361000
H	-5.45243397	2.99692425	-2.04507700
H	-5.79460097	0.91842025	-2.92232100
H	-6.66010797	-1.11112675	-1.48439700
H	-4.34188097	-1.62323975	-0.75852900
O	-6.02163697	2.75261025	-0.07714700
H	-6.95943697	2.89029825	-0.25883200
N	-2.99417697	2.59558725	-0.74056000
H	-3.04225397	3.60032625	-0.68162300
O	-7.53117597	1.32078425	-2.02165700
O	-4.24697597	-0.37103775	-3.89596000
O	-4.81571597	0.68276325	-4.03174300

TS51

0 2

C	-0.62977095	-0.49618320	0.00000000
C	-0.54542895	0.74092880	0.64846800
C	-1.60133895	1.65054980	0.62366300
C	-2.73632895	1.27817380	-0.07167200
C	-2.84643495	0.03464780	-0.73397200
C	-1.77594695	-0.86073220	-0.69257500

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H	0.21015505	−1.17775520	0.04555400
H	0.35905305	0.99871180	1.18576600
H	−1.53204495	2.60501680	1.13084700
H	−1.84338395	−1.82321020	−1.18554000
C	−4.80037895	1.21733880	−0.93752200
C	−6.06805395	1.67834780	−1.57282800
C	−7.00138595	0.46170980	−1.84621400
C	−6.21954495	−0.76053120	−2.28846400
C	−4.90110595	−0.98490020	−2.01299600
C	−4.15877395	−0.01004620	−1.31284700
H	−5.77329795	2.13239280	−2.52985500
H	−7.67683095	0.75691980	−2.66177800
H	−6.80519095	−1.54576520	−2.75407700
H	−4.43558395	−1.92838020	−2.27475900
O	−6.72415395	2.63718080	−0.79531600
H	−7.41735695	2.12493080	−0.33846900
N	−3.93206595	1.98490580	−0.27790500
H	−4.18368495	2.87901580	0.11943400
O	−7.72051095	0.16803480	−0.70737500
O	−5.82961995	0.09085780	0.75245200
H	−6.82042995	0.04292980	0.16138600
H	−5.96363895	0.61771280	1.54474700

TS52

0 2

C	−0.21739130	−0.61594203	0.00000000
C	0.06575270	0.75270397	0.17054700
C	−0.88457130	1.72339497	−0.08949500
C	−2.13646630	1.29270997	−0.53039900
C	−2.43696930	−0.07739003	−0.72639400
C	−1.45678230	−1.03879703	−0.43993300
H	0.55246170	−1.34559603	0.21908600
H	1.04757970	1.05187697	0.51671300
H	−0.66784730	2.77560397	0.05144400
H	−1.66824830	−2.09425103	−0.56587300
C	−4.23846930	1.16051697	−1.28126300
C	−5.57848630	1.55149697	−1.69155500
C	−6.70978030	0.23553997	−0.83284800
C	−6.04407830	−1.07053403	−1.22453100
C	−4.72079430	−1.24752903	−1.34413400

C	−3.79452330	−0.13911603	−1.18864100
H	−5.84532030	1.32827897	−2.72320500
H	−7.57648630	0.50611597	−1.46345800
H	−6.71972530	−1.90970203	−1.36375600
H	−4.32353630	−2.23805703	−1.54197400
O	−6.03317730	2.76509197	−1.27708400
N	−3.26528130	2.02244697	−0.84633700
H	−3.32923330	3.02676397	−0.90348800
O	−6.71387930	0.62974197	0.36152900
H	−6.18259330	2.70449997	−0.31984200
TS53			
O 2			
C	−0.23188405	−0.28985508	0.00000000
C	0.23586095	1.01404492	0.24686100
C	−0.59296105	2.11425092	0.11552300
C	−1.90934705	1.87977592	−0.28314100
C	−2.39887205	0.58014092	−0.54044000
C	−1.54090005	−0.51718608	−0.38190100
H	0.44604195	−1.12559808	0.12116100
H	1.26520195	1.15893492	0.55157600
H	−0.23456105	3.11729092	0.31300800
H	−1.89901405	−1.52680408	−0.54765400
C	−4.07273405	2.07508592	−0.88299800
C	−5.19485205	2.78247892	−1.33818400
C	−6.88747305	−0.01580208	−0.32944700
C	−5.90557405	−0.71266908	−1.16239200
C	−4.58805005	−0.42567108	−1.30654200
C	−3.78967605	0.69881292	−0.89831900
H	−6.11241805	2.29008492	−1.61474900
H	−7.83710905	−0.56938108	−0.19792400
H	−6.25777905	−1.64836608	−1.58407200
H	−3.99897205	−1.20485608	−1.78930200
O	−5.17531205	4.10803492	−1.17928200
H	−5.77245505	4.53777992	−1.80760900
N	−2.94029805	2.76023392	−0.49706300
H	−2.89400605	3.76618292	−0.45548200
O	−6.73180905	1.04697792	0.23314500
O	−4.79665605	2.94990992	−3.61399400
O	−5.13283505	4.09144992	−3.86120400

TS54

0 2

C	0.05797101	0.01449275	0.00000000
C	-0.24701099	-1.33285025	0.17996500
C	0.75584801	-2.28706025	0.35696900
C	2.06730201	-1.84534525	0.34941700
C	2.39303201	-0.49184925	0.17134600
C	1.38459201	0.44265375	-0.00659300
H	-0.73998499	0.73261375	-0.13950000
H	-1.28280199	-1.65073125	0.18118000
H	0.51482501	-3.33376525	0.49620200
H	1.62004601	1.49028375	-0.15705800
C	4.37412001	-1.78786725	0.39237500
C	6.80168801	-0.55791525	-1.44420900
C	7.00208101	0.35542975	-0.30917400
C	6.02270601	0.93066575	0.39491800
C	4.57540501	0.75484075	0.25326700
C	3.85496001	-0.37757025	0.21997300
H	5.77691901	-0.81871325	-1.71304000
H	8.03913801	0.59254275	-0.09490600
H	6.30797201	1.67294775	1.13688200
H	4.01032001	1.68625075	0.25760200
O	7.76176301	-1.29112625	-1.84263000
H	8.03644501	-0.76820625	-2.88254600
N	3.24524601	-2.57979125	0.50124000
H	3.30859001	-3.58096225	0.60043400
O	5.51230301	-2.18529325	0.43624100
O	6.93188301	0.73834575	-2.91723100
O	7.83866901	0.18389775	-3.60896200

TS55

0 1

C	-0.20700637	-0.19108279	0.00000000
C	-0.64131137	-1.49942279	0.28220400
C	0.25101963	-2.55325279	0.36571700
C	1.60072563	-2.26843679	0.15231000
C	2.05612963	-0.96060379	-0.13146900
C	1.13162963	0.08959121	-0.20109100

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H	−0.93639237	0.60794521	−0.05176000
H	−1.69677737	−1.68512479	0.44057300
H	−0.08524237	−3.55922979	0.58730100
H	1.46756263	1.10116821	−0.39624100
C	3.82746563	−2.35782279	−0.07872000
C	5.20200463	−2.92900079	−0.15317800
C	6.20301763	−1.82229079	−0.36965900
C	5.89614563	−0.54211479	−0.56144900
C	4.48670763	−0.00202279	−0.58854400
C	3.48408063	−1.05264879	−0.27205800
H	5.26872463	−3.63868979	−0.98528000
H	7.24196263	−2.13685479	−0.35315100
H	6.69296463	0.17838721	−0.70660300
H	4.26781663	0.47291321	−1.55002500
O	5.51505763	−3.70949979	0.99442400
H	5.49585563	−3.12673979	1.76147600
N	2.70174563	−3.10212279	0.16527200
H	2.70653563	−4.07952979	0.41007700
O	4.28286263	0.98083921	0.46047600
O	4.87634063	2.25850821	0.24904800
N	5.54515863	2.38646721	−0.95637500
O	5.95993963	3.47233521	−1.05619900

TS55

0 1

C	−0.20700637	−0.19108279	0.00000000
C	−0.64131137	−1.49942279	0.28220400
C	0.25101963	−2.55325279	0.36571700
C	1.60072563	−2.26843679	0.15231000
C	2.05612963	−0.96060379	−0.13146900
C	1.13162963	0.08959121	−0.20109100
H	−0.93639237	0.60794521	−0.05176000
H	−1.69677737	−1.68512479	0.44057300
H	−0.08524237	−3.55922979	0.58730100
H	1.46756263	1.10116821	−0.39624100
C	3.82746563	−2.35782279	−0.07872000
C	5.20200463	−2.92900079	−0.15317800
C	6.20301763	−1.82229079	−0.36965900
C	5.89614563	−0.54211479	−0.56144900
C	4.48670763	−0.00202279	−0.58854400



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C	3.48408063	−1.05264879	−0.27205800
H	5.26872463	−3.63868979	−0.98528000
H	7.24196263	−2.13685479	−0.35315100
H	6.69296463	0.17838721	−0.70660300
H	4.26781663	0.47291321	−1.55002500
O	5.51505763	−3.70949979	0.99442400
H	5.49585563	−3.12673979	1.76147600
N	2.70174563	−3.10212279	0.16527200
H	2.70653563	−4.07952979	0.41007700
O	4.28286263	0.98083921	0.46047600
O	4.87634063	2.25850821	0.24904800

TS56

0 2

C	−0.63768115	−0.36231884	0.00000000
C	−1.14049415	−1.67247584	0.10253200
C	−0.29932015	−2.77085084	0.08753100
C	1.06964585	−2.52796384	−0.03271500
C	1.59457185	−1.21967784	−0.14160900
C	0.71905485	−0.12608284	−0.12039600
H	−1.32819215	0.47173416	0.02193700
H	−2.20882415	−1.82464584	0.19806100
H	−0.68901815	−3.77862184	0.16982300
H	1.10177085	0.88605416	−0.18520800
C	3.29808985	−2.69631184	−0.19390300
C	4.65993485	−3.30511884	−0.18529600
C	5.67485085	−2.29458384	−0.64965200
C	5.46286485	−0.94417984	−0.54566700
C	4.08362885	−0.32626684	−0.32044000
C	3.02132885	−1.36056884	−0.24568300
H	4.69463185	−4.19880484	−0.81423400
H	6.66892985	−2.66995884	−0.86506300
H	6.24793785	−0.25932984	−0.84452200
H	3.84672785	0.46395516	−1.03762800
O	5.02593085	−3.75352584	1.11667900
H	5.03755985	−2.96994684	1.68506400
N	2.13192585	−3.40923484	−0.07641600
H	2.07609785	−4.40537484	0.06103000
O	4.34916285	0.30342616	0.93952800
O	5.40062785	−0.57604284	1.33631000

TS57

0 2

C	-0.11594203	-0.33333333	0.00000000
C	-0.63399703	-1.64001733	0.05356500
C	0.19783297	-2.74557033	0.02751000
C	1.57106997	-2.51409133	-0.05432300
C	2.11294497	-1.20748533	-0.11010300
C	1.24562897	-0.10744833	-0.08081300
H	-0.79856003	0.50713867	0.02566400
H	-1.70571503	-1.78406533	0.11753100
H	-0.20222503	-3.75169033	0.07101700
H	1.63575297	0.90328267	-0.11540800
C	3.79790097	-2.70789133	-0.16662600
C	5.16072597	-3.32198933	-0.19649200
C	6.19412997	-2.21600033	-0.36123900
C	5.86069797	-0.97920633	-0.87136300
C	4.66815497	-0.40105333	-0.13825600
C	3.53890797	-1.36622833	-0.18166400
H	5.25500897	-3.98422233	-1.06546500
H	7.22133397	-2.56531233	-0.40904700
H	6.58365997	-0.32153333	-1.33628300
H	4.39941897	0.61301167	-0.42933400
O	5.41213697	-4.14219133	0.92109500
H	5.38252097	-3.56135433	1.69284800
N	2.62397297	-3.40844633	-0.09818600
H	2.55758197	-4.40719733	0.01668200
O	5.23118697	-0.27100433	1.19464200
O	5.80137997	-1.49416633	1.48001500

TS58

0 2

C	-0.36231884	-0.39130436	0.00000000
C	-0.88650184	-1.68347436	-0.12859900
C	-0.05992684	-2.79628636	-0.23212600
C	1.30946716	-2.56949236	-0.20523900
C	1.85308816	-1.27891436	-0.08129300
C	1.01020116	-0.17893736	0.03245200
H	-1.03943684	0.44936164	0.08504500

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H	-1.96078284	-1.82174436	-0.14521400
H	-0.47018484	-3.79446736	-0.32707200
H	1.42218616	0.81570764	0.15767400
C	3.54637416	-2.79988936	-0.26090500
C	4.91326216	-3.38747436	-0.20549200
C	5.92210416	-2.35666736	-0.66311200
C	5.68295616	-1.04880936	-0.72052200
C	4.37947816	-0.40163236	-0.32441400
C	3.30386116	-1.42949536	-0.03734000
H	4.98050016	-4.28679836	-0.82333900
H	6.91565816	-2.73894136	-0.87324500
H	6.48444416	-0.36588936	-0.98328300
H	4.07929716	0.37969964	-1.02855100
O	5.20718716	-3.81613636	1.11999100
H	5.11361916	-3.03372936	1.68458100
N	2.37030016	-3.47451836	-0.30031700
H	2.28140516	-4.47855536	-0.32099100
O	4.48098216	0.14501164	0.98392000
O	3.91073016	-1.00833536	1.63775200

TS59

0 2

C	-0.79710144	-0.05797102	0.00000000
C	-1.32099644	-1.36383402	0.03348500
C	-0.49812144	-2.48058402	0.04978000
C	0.87476356	-2.26383202	0.01636600
C	1.42654256	-0.95218302	-0.02796200
C	0.56598256	0.15848898	-0.02406500
H	-1.47717944	0.78447298	-0.00078100
H	-2.39540744	-1.50118802	0.05427200
H	-0.91038944	-3.48129402	0.09314200
H	0.97025756	1.16348698	-0.04377800
C	3.10737556	-2.49042402	0.07476400
C	4.41762156	-3.11129902	-0.32870600
C	5.48267556	-2.04089302	-0.39512800
C	5.28149056	-0.77239902	-0.04463400
C	3.96669356	-0.31787402	0.55214600
C	2.83396456	-1.10842502	-0.02732100
H	4.29248156	-3.55908202	-1.32111800
H	6.45824856	-2.37904202	-0.72973500

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H	6.09235756	−0.05420402	−0.08663500
H	3.83837356	0.76335398	0.52988500
O	4.77551256	−4.17891202	0.52117400
H	4.86227156	−3.78681502	1.40178200
N	1.91905456	−3.17055602	0.04182200
H	1.83679956	−4.17117302	0.12840400
O	3.90890156	−0.68964202	1.94041600
O	3.76193956	−2.09259202	1.92937800

TS60

0 2

C	−0.15267175	−0.64885495	0.00000000
C	−0.76229775	−1.91532995	0.06616700
C	−0.01125075	−3.07736095	0.08747200
C	1.37731325	−2.94458995	0.03989900
C	2.00846325	−1.68039195	−0.01580500
C	1.22351125	−0.51990895	−0.03768500
H	−0.77666175	0.23650205	−0.01929100
H	−1.84308975	−1.98219995	0.09889500
H	−0.48363275	−4.05139595	0.13647200
H	1.69515825	0.45493105	−0.08844200
C	3.59079325	−3.28679595	−0.00458200
C	4.89114725	−4.01591995	−0.04802300
C	6.03327325	−3.03097095	−0.00811400
C	5.89478625	−1.70849895	−0.02968100
C	4.56864325	−0.99377195	−0.09154700
C	3.42242325	−1.93438495	−0.03454900
H	4.95570325	−4.60734995	−0.96813900
H	7.02002825	−3.47846095	0.06051300
H	6.76569525	−1.06365295	0.02493100
H	4.51891125	−0.35195895	−0.98171000
O	4.98972425	−4.98238795	0.99247300
H	4.97861925	−4.51153395	1.83286500
N	2.36715725	−3.90712895	0.03121200
H	2.23411925	−4.90067095	0.13173300
O	4.44180725	−0.12018095	1.05224700
O	5.31140725	0.95715405	0.89139100
O	3.72726725	2.52849805	0.10401200
H	3.24997525	2.52114605	0.95031900
H	4.79005525	1.60061005	0.28892900

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TS61

0 2

C	−0.15942029	−0.69565220	0.00000000
C	−0.65939229	−2.01020020	0.02097700
C	0.18197271	−3.10593920	−0.06890800
C	1.54877871	−2.85208420	−0.18057600
C	2.06784071	−1.53823920	−0.19260500
C	1.19699371	−0.44578320	−0.10493700
H	−0.85321029	0.13312980	0.06941900
H	−1.72750129	−2.16966020	0.10682100
H	−0.20648129	−4.11728920	−0.05675800
H	1.59047671	0.56336880	−0.11967800
C	3.77698871	−3.01351420	−0.36178200
C	5.13899771	−3.61896320	−0.46185900
C	6.19613271	−2.55414820	−0.28643100
C	5.94260171	−1.24493020	−0.22466400
C	4.57116671	−0.69304620	−0.35886000
C	3.49512171	−1.67359020	−0.29909700
H	5.26580171	−4.08656820	−1.44568100
H	7.21223871	−2.92460520	−0.19905500
H	6.73403971	−0.51643020	−0.08806000
H	4.53559871	−0.08678220	−1.46888800
O	5.30416471	−4.69301920	0.45553300
H	5.27437871	−4.32812520	1.34661500
N	2.61471971	−3.72994120	−0.29713900
H	2.57058571	−4.73439520	−0.22387600
O	4.31875671	1.20922680	−0.99750200
O	4.35099071	0.52281880	0.28351100

## TS62

0 2

C	−0.34351143	−0.95419846	0.00000000
C	−0.79265043	−2.27891546	−0.14363500
C	0.09243657	−3.32335746	−0.34769300
C	1.44954057	−3.00772946	−0.41029600
C	1.92029957	−1.68305646	−0.26177300
C	1.00369057	−0.64463146	−0.05293000
H	−1.06865343	−0.16551246	0.15881200

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H	-1.85455643	-2.48692646	-0.09239900
H	-0.25628843	-4.34327446	-0.45769200
H	1.35271657	0.37318354	0.07100200
C	3.68387357	-3.06833346	-0.56848000
C	5.06318057	-3.61681946	-0.73675800
C	6.07969057	-2.53919446	-0.44605400
C	5.78122357	-1.25309346	-0.24074400
C	4.39447557	-0.73460846	-0.35396600
C	3.35473257	-1.75303646	-0.36168000
H	5.19854357	-3.99066246	-1.75871800
H	7.10714657	-2.88119846	-0.37616200
H	6.54440257	-0.51953046	-0.00749100
H	4.46011657	-0.09562846	-1.52190200
O	5.26854557	-4.76836446	0.07575300
H	5.21463257	-4.49070846	0.99689300
N	2.54595357	-3.82715146	-0.61043000
H	2.53631757	-4.83329646	-0.66767800
O	4.08174757	0.38096854	0.38467600
O	4.96889957	1.40584554	0.17802000
O	4.68740857	1.02933254	-2.18822000
H	5.51811057	0.92984054	-2.66474200
H	4.90292357	1.44339354	-1.20973200

TS63

0 2

C	-3.05343493	1.10687021	0.00000000
C	-3.63359993	-0.11266779	-0.36258900
C	-2.86210493	-1.24399479	-0.65884400
C	-1.49646793	-1.09884079	-0.57793600
C	-0.88240893	0.12712721	-0.22419000
C	-1.67444793	1.24223221	0.07932300
H	-3.69160793	1.94942321	0.23325100
H	-4.71316793	-0.19091379	-0.41008900
H	-3.32668593	-2.18415579	-0.92820900
H	-1.21007393	2.17054621	0.38897100
C	0.71095707	-1.47765579	-0.57132300
C	2.00662707	-2.23000679	-0.45891800
C	3.11146307	-1.24016779	-0.13171900
C	2.96260207	0.05148521	0.15174900
C	0.51456107	-0.10331579	-0.22033800

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H	2.22629107	−2.69271779	−1.43642100
H	4.09521507	−1.69197079	−0.05877100
H	3.81535207	0.64916621	0.45406100
O	1.83330207	−3.18306779	0.51769400
H	1.32947107	−2.51060379	1.46065100
N	−0.47033193	−2.03621479	−0.79977800
H	−0.58343193	−3.03950579	−0.87617400
O	1.36972107	1.43863021	1.38905900
O	1.84097007	0.66176021	2.48152100
O	0.79537507	−1.69984579	2.09769200
H	0.25156307	−2.09836279	2.77912800
H	1.37061607	−0.22277179	2.40390000
C	1.65010407	0.79272721	0.15012700
H	1.68733907	1.62716421	−0.56345700

TS64

02

C	−1.01449274	−0.18840580	0.00000000
C	−1.51276274	−1.50070980	−0.06612000
C	−0.66505474	−2.59179080	−0.16726000
C	0.70341526	−2.33160280	−0.20803400
C	1.22041726	−1.01972980	−0.14717500
C	0.34632426	0.06533520	−0.03570400
H	−1.71152874	0.63609220	0.08655600
H	−2.58322674	−1.66418980	−0.03383400
H	−1.05097974	−3.60315880	−0.21348800
H	0.74211526	1.07086720	0.03675100
C	2.93941026	−2.49937680	−0.28713700
C	4.30411026	−3.09891280	−0.37085600
C	5.35244026	−2.02579980	−0.22538200
C	5.06781926	−0.70775580	−0.12852100
C	3.72074426	−0.21042080	−0.16771000
C	2.65731026	−1.14791780	−0.20300600
H	4.42823526	−3.59592080	−1.34226600
H	6.37860526	−2.37532180	−0.20888500
H	5.86028726	0.02595320	−0.03102900
H	3.51450026	2.28605020	1.41172300
O	4.47334326	−4.15824480	0.57065900
H	4.46323326	−3.76819580	1.45159000
N	1.77573826	−3.20896280	−0.30158800

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H	1.72266826	−4.21544880	−0.28305500
O	3.49311726	1.08880420	−0.12278800
O	3.02511726	1.45642120	1.33515500

#### TS65

0 2

C	−1.15151515	−1.02020200	0.00000000
C	−1.69901615	−2.31396300	0.09753200
C	−0.90702215	−3.44472900	0.00964900
C	0.46268285	−3.25556300	−0.18141700
C	1.03288385	−1.96082700	−0.28310100
C	0.20457785	−0.83150100	−0.18670200
H	−1.80855915	−0.16241300	0.07367700
H	−2.76624915	−2.42672300	0.24584200
H	−1.33310015	−4.43774100	0.08897200
H	0.62925685	0.16328700	−0.25825800
C	2.66577285	−3.49973000	−0.42263900
C	3.99179485	−4.13647400	−0.56611800
C	5.11094985	−3.14153200	−0.42345400
C	4.90950585	−1.82324000	−0.41808300
C	3.55741785	−1.15788000	−0.52266200
C	2.44544485	−2.15034700	−0.44868000
H	4.02412485	−4.25401100	−1.81365400
H	6.10375885	−3.57006100	−0.34279700
H	5.74780885	−1.14362600	−0.30198900
H	3.51080985	−0.57779700	−1.45268700
O	4.15422285	−5.37575800	−0.23773400
H	2.53271185	−0.91297000	1.91654300
N	1.48384985	−4.17604900	−0.29362500
H	1.41938685	−5.17640300	−0.18290200
O	3.46287885	−0.70619800	1.74443100
O	3.41156785	−0.12435200	0.45269300
O	3.91158285	−3.78360800	−3.23781200
O	3.63689585	−2.61135300	−3.26956000

#### TS66

0 1

C	−0.49872000	−0.64469600	0.13231500
C	−1.05218200	−1.92249600	−0.05728400



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C	−0.25805500	−3.03194900	−0.29591200
C	1.11907800	−2.83076700	−0.34603100
C	1.69278700	−1.55096400	−0.16235100
C	0.86941900	−0.44728800	0.08520400
H	−1.15720900	0.19388800	0.32076900
H	−2.12779900	−2.04440700	−0.01346300
H	−0.69036100	−4.01463500	−0.43936700
H	1.30406700	0.53238000	0.23979200
C	3.32393900	−3.08606700	−0.55712200
C	4.65061200	−3.73976000	−0.59452000
C	5.77810200	−2.79379700	−0.44745600
C	5.58202900	−1.47604900	−0.31007900
C	4.22911700	−0.86151400	−0.43020200
C	3.11523000	−1.73359400	−0.27409600
H	6.76928700	−3.22906700	−0.41868300
H	6.40939600	−0.78537800	−0.19781500
H	4.18502200	−0.77226100	−1.69794000
O	4.76370000	−4.94066000	−0.69345300
H	4.52627000	1.77450200	−1.08435100
N	2.14183000	−3.74285500	−0.55565500
H	2.05596100	−4.72961400	−0.74865100
O	5.03056300	1.27280800	−0.42932600
O	4.03947300	0.40945900	0.10752800
O	3.65558400	−2.50558700	−2.69033000
O	4.16936300	−1.36875500	−2.88560700

TS67

02

C	−0.26717556	−1.14503815	0.00000000
C	−0.85440456	−2.41648215	−0.13529300
C	−0.08702156	−3.55184915	−0.32541400
C	1.29600144	−3.38051215	−0.38325600
C	1.90246644	−2.10920515	−0.25502700
C	1.10466444	−0.97789015	−0.05434900
H	−0.90611456	−0.28464015	0.15613700
H	−1.93263456	−2.50970315	−0.08512300
H	−0.53983556	−4.53091315	−0.42510600
H	1.56773644	−0.00768815	0.07236200
C	3.50018644	−3.69622615	−0.55178900
C	4.79924644	−4.34499115	−0.72216600

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C	5.94314644	−3.41872015	−0.67547100
C	5.77454444	−2.08974315	−0.48637300
C	4.46131544	−1.48617915	−0.36895700
C	3.32155944	−2.33032715	−0.37196900
H	6.92482144	−3.86316115	−0.78683800
H	6.61952944	−1.41232615	−0.44318000
O	4.90607544	−5.55164215	−0.88542100
H	4.20800444	1.07673385	1.25188000
N	2.29763944	−4.32139015	−0.56071800
H	2.18619744	−5.31710415	−0.68486100
O	3.83478144	0.18404885	1.26459500
O	4.37319844	−0.20081315	−0.27994000

TS68

0 1

C	−0.20700637	−0.19108279	0.00000000
C	−0.64131137	−1.49942279	0.28220400
C	0.25101963	−2.55325279	0.36571700
C	1.60072563	−2.26843679	0.15231000
C	2.05612963	−0.96060379	−0.13146900
C	1.13162963	0.08959121	−0.20109100
H	−0.93639237	0.60794521	−0.05176000
H	−1.69677737	−1.68512479	0.44057300
H	−0.08524237	−3.55922979	0.58730100
H	1.46756263	1.10116821	−0.39624100
C	3.82746563	−2.35782279	−0.07872000
C	5.20200463	−2.92900079	−0.15317800
C	6.20301763	−1.82229079	−0.36965900
C	5.89614563	−0.54211479	−0.56144900
C	4.48670763	−0.00202279	−0.58854400
C	3.48408063	−1.05264879	−0.27205800
H	5.26872463	−3.63868979	−0.98528000
H	7.24196263	−2.13685479	−0.35315100
H	6.69296463	0.17838721	−0.70660300
H	4.26781663	0.47291321	−1.55002500
O	5.51505763	−3.70949979	0.99442400
H	5.49585563	−3.12673979	1.76147600
N	2.70174563	−3.10212279	0.16527200
H	2.70653563	−4.07952979	0.41007700
O	4.28286263	0.98083921	0.46047600

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O	4.87634063	2.25850821	0.24904800
N	5.54515863	2.38646721	−0.95637500
O	5.95993963	3.47233521	−1.05619900

# TS69

0 1

C	0.38216560	−0.50955412	0.00000000
C	−0.10068640	−1.79960912	0.28773300
C	0.74964960	−2.88847812	0.36857000
C	2.10915560	−2.65790512	0.15194600
C	2.61231060	−1.36579212	−0.12981400
C	1.72995160	−0.28058312	−0.20896000
H	−0.31780040	0.31518888	−0.05583500
H	−1.16218340	−1.94470612	0.44913900
H	0.37353860	−3.88072312	0.58832500
H	2.11118960	0.70954288	−0.42734100
C	4.33124860	−2.83070912	−0.08647000
C	5.69124060	−3.44728112	−0.12076600
C	6.74679060	−2.37284112	−0.24056600
C	6.49516660	−1.07629212	−0.42394200
C	5.10660560	−0.53372112	−0.55724500
C	4.03385760	−1.51046512	−0.26782200
H	5.77416260	−4.13468812	−0.97048300
H	7.76978560	−2.72428312	−0.15197400
H	7.29492060	−0.34690512	−0.49397200
H	4.98675960	−0.27774212	−1.79858800
O	5.91354260	−4.28167412	1.01321000
H	5.90262560	−3.72020312	1.79608100
N	3.17640160	−3.53418012	0.15825200
H	3.15085660	−4.50274012	0.43488800
O	4.92246960	0.73390288	−0.26402400
O	4.69677960	1.13542988	−2.01199000
H	4.45978960	1.95028388	−2.49989800

# TS70

0 2

C	1.87022891	−0.49618320	0.00000000
C	1.38607491	−1.80585120	0.17492600
C	2.23924591	−2.89507120	0.18522300

C	3.60137291	-2.64530020	0.00895400
C	4.10665191	-1.33562420	-0.16871400
C	3.22042791	-0.24996620	-0.16747200
H	1.17049591	0.33052380	0.00461900
H	0.32269291	-1.96511920	0.30785200
H	1.86344591	-3.90209720	0.32314600
H	3.59719691	0.75938980	-0.28059000
C	5.82734191	-2.79269520	-0.19689000
C	7.18587491	-3.40652420	-0.25941000
C	8.23703191	-2.32372820	-0.28270600
C	7.98321691	-1.02211420	-0.38536100
C	6.59251891	-0.43290120	-0.50356300
C	5.53232191	-1.46614720	-0.29615500
H	7.28201291	-4.02276520	-1.16037200
H	9.25967191	-2.67777820	-0.19624400
H	8.79036691	-0.29681620	-0.37920200
H	6.49979891	-0.00952220	-1.53102000
O	7.39725991	-4.32301020	0.80965600
H	7.36027191	-3.82638420	1.63432900
N	4.67128791	-3.51631820	-0.02700400
H	4.64342091	-4.50412820	0.16895600
O	6.43890991	0.70709680	0.25213200
O	5.71362274	2.96243175	-0.12186920
H	6.06591817	1.63489287	0.01202799
H	5.84671732	3.37424135	0.73504310

TS71

01

C	-0.46464646	-0.83838383	0.00000000
C	-0.93300546	-2.16500183	-0.03054200
C	-0.07027946	-3.23148383	-0.20882600
C	1.28636454	-2.94063083	-0.36299700
C	1.77555654	-1.61305783	-0.33385400
C	0.87953754	-0.55095483	-0.14638600
H	-1.17295746	-0.03228883	0.14658100
H	-1.99257946	-2.35529583	0.09065100
H	-0.43421846	-4.25188183	-0.23022800
H	1.24026654	0.47004117	-0.10219100
C	3.50956854	-3.02970183	-0.62843500
C	4.87565354	-3.60659083	-0.80425900

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C	5.91719754	−2.52176083	−0.65603300
C	5.65784054	−1.22210083	−0.53877100
C	4.25494454	−0.66178783	−0.56948100
C	3.19807354	−1.70858483	−0.50182300
H	4.97080454	−4.06666983	−1.79408300
H	6.94398254	−2.87315383	−0.63322500
H	6.45126454	−0.49263583	−0.41858600
H	4.18402054	−0.17864083	−1.62678500
O	5.10812754	−4.68328483	0.09750400
H	5.07894654	−4.32882983	0.99280500
N	2.36237354	−3.78291783	−0.55710900
H	2.34560754	−4.78963983	−0.51952100
O	4.09429354	0.40202017	0.23087900
O	3.54195754	1.77249917	−0.71754700
N	3.67105454	1.44250717	−1.89493100
O	3.39195254	2.17608817	−2.79821500

TS72

0 2

C	0.17389814	−0.21739130	−0.00227645
C	0.06310114	−1.46301330	−0.61835545
C	1.18780214	−2.20640830	−0.97024945
C	2.43665914	−1.66896330	−0.68739745
C	2.55429014	−0.42582930	−0.05863345
C	1.43319814	0.30874070	0.28272255
H	−0.71849786	0.33466670	0.26387355
H	−0.92064486	−1.86576930	−0.82987745
H	1.08893414	−3.17126030	−1.45321745
H	1.53256214	1.26568470	0.78390755
C	4.69301314	−1.44162630	−0.29384545
C	6.04291514	−1.32016030	−1.01712245
C	6.62513214	0.06897070	−0.95105145
C	5.94702214	1.19968070	−0.60925745
C	4.60626014	1.15651170	−0.17176445
C	4.01101614	−0.14380730	0.15438255
H	5.88200514	−1.54893330	−2.07638845
H	7.66170914	0.13375770	−1.26589145
H	6.44584914	2.15977870	−0.67516345
H	4.04108814	2.05876770	0.02722155
O	6.95451214	−2.28200330	−0.53844445

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H	6.84273914	−2.30645830	0.42201055
N	3.69811514	−2.19058830	−1.01659245
H	3.81257914	−3.19567130	−1.04163145
O	4.88388314	−1.90478630	1.04689555
O	4.50071014	−0.17801630	1.47877755

### TS73

0 2

C	0.60869564	−0.26086957	0.00000000
C	0.58127564	−1.65037757	−0.14011600
C	1.74954164	−2.39788157	−0.26186400
C	2.95992764	−1.71699957	−0.23815300
C	3.00001864	−0.31748757	−0.08767500
C	1.82454664	0.41339243	0.02904600
H	−0.31944636	0.28877743	0.08969900
H	−0.37338736	−2.16308157	−0.15669100
H	1.71453164	−3.47452357	−0.37523000
H	1.85737264	1.49064543	0.14551400
C	5.19941364	−1.21256757	−0.10495000
C	6.42632664	−1.14580157	−1.02108600
C	7.20537664	0.05912143	−0.58354700
C	6.56584064	0.95906243	0.27021300
C	5.11771664	1.16685143	0.18793000
C	4.40303364	0.06079343	−0.05963800
H	6.08076464	−1.08044557	−2.05767300
H	8.28314064	0.04043943	−0.67925900
H	7.15989864	1.73173943	0.74561300
H	4.68720064	2.13251343	0.42043600
O	7.18891064	−2.32596557	−0.91744700
H	7.43268264	−2.41834657	0.01273300
N	4.24678364	−2.22590257	−0.39860400
H	4.47347264	−3.18950857	−0.20550300
O	5.71126464	−1.43200857	1.25429500
O	6.60456564	−0.41671257	1.63480300

### TS74

0 2

C	−0.20289855	−0.37681161	0.00000000
C	−0.76625255	−1.64783261	−0.13526700

C	0.00622945	−2.76150861	−0.45920100
C	1.36867645	−2.57290861	−0.64252100
C	1.95081545	−1.29654061	−0.50106100
C	1.16364045	−0.19586661	−0.18138600
H	−0.83276655	0.46650539	0.25261100
H	−1.83216855	−1.77455361	0.01433600
H	−0.44369655	−3.74084261	−0.56810300
H	1.61111045	0.78506739	−0.06764200
C	3.63044245	−2.94164561	−0.85889200
C	4.68965445	−3.24906861	−1.89500400
C	5.88732345	−2.44772461	−1.43589100
C	5.73254845	−1.13353661	−1.06311100
C	4.42373245	−0.60094661	−0.82024300
C	3.37003045	−1.45132561	−0.74348300
H	4.33736845	−2.88038561	−2.86390900
H	6.86806145	−2.84990861	−1.66314400
H	6.60231745	−0.50717261	−0.91083800
H	4.29505345	0.46392539	−0.66192000
O	4.94517245	−4.61867761	−2.02416300
H	5.35960545	−4.88769261	−1.19339800
N	2.33370445	−3.50641861	−1.02307600
H	2.21225145	−4.49184161	−0.84349900
O	5.56718645	−3.45944561	0.32864100
O	4.20015845	−3.33036961	0.43690300

TS75

0 2

C	−0.57251909	0.45801526	0.00000000
C	−0.57420709	−0.60673074	−0.89563200
C	0.60754991	−1.25880274	−1.25603600
C	1.78978191	−0.82702674	−0.68180400
C	1.79454391	0.24803426	0.22854100
C	0.62541891	0.90338126	0.56390000
H	−1.50455309	0.94103326	0.26486700
H	−1.51190009	−0.94297674	−1.32218900
H	0.59776791	−2.08089474	−1.96184100
H	0.63784891	1.73086426	1.26346600
C	3.86236491	−0.87784074	0.24722800
C	5.40355291	−0.79795374	0.17280800
C	5.90693391	0.29800126	−0.69512600

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C	5.24514391	1.45935626	−0.55461400
C	3.92884391	1.55879226	0.09796000
C	3.23081391	0.47245026	0.47720800
H	5.37254291	−2.12400074	0.09958900
H	6.82367991	0.21093026	−1.26545200
H	5.61751591	2.35627226	−1.03805700
H	3.41248991	2.50977126	0.02024400
O	5.90474691	−0.65056174	1.46078600
H	6.68201591	−0.08603874	1.42218900
N	3.10841191	−1.29565974	−0.92720300
H	3.18208291	−2.29413174	−1.09336800
O	4.48354791	−2.91329974	0.68195100
O	3.74534991	−1.87220774	1.25704200

TS75

0 2

C	−0.57251909	0.45801526	0.00000000
C	−0.57420709	−0.60673074	−0.89563200
C	0.60754991	−1.25880274	−1.25603600
C	1.78978191	−0.82702674	−0.68180400
C	1.79454391	0.24803426	0.22854100
C	0.62541891	0.90338126	0.56390000
H	−1.50455309	0.94103326	0.26486700
H	−1.51190009	−0.94297674	−1.32218900
H	0.59776791	−2.08089474	−1.96184100
H	0.63784891	1.73086426	1.26346600
C	3.86236491	−0.87784074	0.24722800
C	5.40355291	−0.79795374	0.17280800
C	5.90693391	0.29800126	−0.69512600
C	5.24514391	1.45935626	−0.55461400
C	3.92884391	1.55879226	0.09796000
C	3.23081391	0.47245026	0.47720800
H	5.37254291	−2.12400074	0.09958900
H	6.82367991	0.21093026	−1.26545200
H	5.61751591	2.35627226	−1.03805700
H	3.41248991	2.50977126	0.02024400
O	5.90474691	−0.65056174	1.46078600
H	6.68201591	−0.08603874	1.42218900
N	3.10841191	−1.29565974	−0.92720300
H	3.18208291	−2.29413174	−1.09336800



O	4.48354791	-2.91329974	0.68195100
O	3.74534991	-1.87220774	1.25704200
TS76			
O 2			
C	-0.45801524	-0.38167938	0.00000000
C	-0.50829624	-1.74327338	-0.30990400
C	0.64613376	-2.46010338	-0.59257300
C	1.86659976	-1.75111738	-0.57157800
C	1.92138276	-0.35952538	-0.23284900
C	0.75534676	0.32035162	0.04306200
H	-1.37931124	0.14412262	0.21990400
H	-1.46472124	-2.25037938	-0.32237800
H	0.63118476	-3.50718138	-0.85563900
H	0.77218376	1.37050262	0.30883800
C	4.08783576	-1.29818038	-0.30735700
C	5.39314276	-1.19617538	-1.07477400
C	6.11711276	0.06134662	-0.64644200
C	5.45530476	1.16424662	-0.27279800
C	3.99367176	1.17230762	-0.19424500
C	3.32373376	0.01184362	-0.24937300
H	5.13452076	-1.07730838	-2.13709100
H	7.19871076	0.03820262	-0.71689300
H	5.99024776	2.07599062	-0.03623200
H	3.46953376	2.11674362	-0.09516500
O	6.18047176	-2.35583638	-0.97496500
H	6.05905276	-2.73654038	-0.09363100
N	3.10066776	-2.21247238	-0.86694500
H	3.27030376	-3.21265638	-0.80801100
O	4.57534276	-2.98680238	1.23422300
O	4.30888376	-1.60150638	1.07339800
O	2.16470976	-3.69754238	1.06885400
H	3.61047176	-3.34737938	1.31227300
H	1.75667676	-4.16644738	1.80469800
TS77			
O 2			
C	-0.66273930	-0.33136966	0.00000000
C	-0.72107730	-1.70038266	-0.33650600

C	0.42427970	-2.44740766	-0.50932700
C	1.66353870	-1.80838466	-0.32207700
C	1.72276270	-0.43128066	0.03841700
C	0.55127170	0.31051834	0.17955600
H	-1.58644030	0.22083034	0.12208800
H	-1.68960030	-2.16835166	-0.46657500
H	0.38923770	-3.49513466	-0.78047700
H	0.58899970	1.36121434	0.44208600
C	3.86492970	-1.38544966	-0.03166600
C	5.11228570	-1.22015566	-0.92115300
C	5.86650470	0.01437934	-0.47970900
C	5.24055970	1.08777134	0.02060600
C	3.78869870	1.08310734	0.19048700
C	3.12124570	-0.08071066	0.12040200
H	4.74723370	-1.04369666	-1.94268000
H	6.93981870	-0.00788966	-0.62999000
H	5.79361970	1.98443834	0.27292400
H	3.26446270	2.02173234	0.33470100
O	5.91168170	-2.36531566	-0.95606800
H	5.85138770	-2.82130566	-0.10416200
N	2.89797370	-2.37113966	-0.47627100
H	3.32653070	-3.23523466	0.20288200
O	4.26301070	-3.25179266	1.15801200
O	4.28150870	-1.86164466	1.26408800

TS78

02

C	0.38291604	-0.00736377	0.00000000
C	0.33316704	-1.36287677	-0.33832800
C	1.49129304	-2.10669877	-0.54098800
C	2.71094504	-1.46224077	-0.37811100
C	2.77330004	-0.10224277	-0.02556200
C	1.60642204	0.63321623	0.15184700
H	-0.53800996	0.54165923	0.14917100
H	-0.63004296	-1.84665477	-0.45033700
H	1.44466404	-3.15306477	-0.81700600
H	1.65181104	1.68223223	0.42143200
C	4.93769204	-1.04015377	-0.07628100
C	6.26416904	-0.86766477	-0.98614600
C	6.95493104	0.41171423	-0.59132400

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C	6.28482804	1.47220523	−0.12039100
C	4.83709404	1.43015023	0.06287400
C	4.18083504	0.25963023	0.03122600
H	5.82118604	−0.76404277	−1.99355500
H	8.02838804	0.43510723	−0.74052700
H	6.80609304	2.39671323	0.09800700
H	4.29192304	2.36129823	0.17328200
O	7.00397404	−1.98565877	−0.88427300
H	6.69521804	−2.49611777	0.21206600
N	3.99509904	−1.98076277	−0.58420500
H	4.18730604	−2.95290477	−0.37761700
O	6.00151704	−2.65069777	1.10275600
O	5.45192504	−1.38880777	1.19588000

TS79

0 2

C	0.01915426	−0.83962437	−0.01074115
C	−0.00240574	−2.23144237	−0.12864215
C	1.13159126	−3.00023037	0.12113785
C	2.29369526	−2.34485937	0.51011985
C	2.31813426	−0.93553737	0.62717785
C	1.18938326	−0.17720937	0.35541185
H	−0.88138474	−0.27178137	−0.20894715
H	−0.92238874	−2.72337437	−0.42201215
H	1.12089026	−4.07852037	0.02346385
H	1.20860426	0.90391863	0.43669785
C	4.35422026	−1.94852837	1.04999185
C	5.62464026	−1.63960737	−0.62026715
C	6.40145226	−0.52126037	−0.07931915
C	5.83909626	0.53095363	0.54735985
C	4.38838726	0.55609363	0.73891685
C	3.71164026	−0.59075037	0.90881285
H	4.84175726	−1.42040037	−1.34216715
H	7.48356226	−0.59438637	−0.16038915
H	6.44441226	1.36496463	0.88124885
H	3.85044126	1.49445163	0.63532985
O	6.26723726	−2.79984537	−0.90087915
H	6.72948626	−3.10870137	−0.10995515
N	3.51445826	−2.93663537	0.85202985
O	5.82378926	−3.46620637	1.89658785

O	5.37460426	−2.11985837	1.95838485
H	4.98266826	−3.95605137	1.79460885
TS80			
0 2			
C	−1.85114507	−1.12595418	0.00000000
C	−2.03160607	−2.49666518	0.17177800
C	−0.94922307	−3.34506818	0.41547300
C	0.30842093	−2.77711418	0.48275300
C	0.49964893	−1.39572918	0.31258200
C	−0.57659507	−0.56004418	0.06758300
H	−2.70847907	−0.49250918	−0.19132100
H	−3.03020707	−2.91278718	0.11226700
H	−1.08102307	−4.41166318	0.54726500
H	−0.44162907	0.50700782	−0.07161200
C	2.44057993	−2.54370618	0.69045300
C	4.92854093	−1.48378618	−1.15070300
C	5.06679893	−0.41480718	−0.13172100
C	4.06341193	0.21300382	0.48586300
C	2.62072493	−0.01283318	0.35121000
C	1.94776093	−1.16645418	0.43768700
H	5.59628893	−2.34304318	−1.01747400
H	6.08936193	−0.14774518	0.11610400
H	4.32721393	1.02131182	1.16421400
H	2.02479093	0.88991882	0.22787500
O	3.88351493	−1.61645018	−1.85582700
N	1.53491493	−3.44923118	0.71987100
O	3.94998693	−4.19128318	1.12400500
O	3.73178593	−2.80861218	0.89807400
H	3.04574693	−4.56371518	1.04821300
H	4.29979793	−1.16571018	−2.93769700
O	6.03428593	−0.68783518	−2.52100300
O	5.21250793	−0.68101518	−3.48759800
TS81			
0 2			
C	−0.47709921	−0.09541985	0.00000000
C	−0.52112221	−1.44605585	−0.35708100
C	0.63608779	−2.16316085	−0.64702600

C	1.85134179	−1.49665085	−0.56264800
C	1.90764479	−0.14212085	−0.18899200
C	0.74180479	0.56604315	0.08212400
H	−1.39639421	0.43264515	0.21868500
H	−1.47951021	−1.94886885	−0.41362100
H	0.59027879	−3.20632785	−0.93533600
H	0.78653279	1.61039115	0.36973600
C	4.08688579	−1.04210285	−0.36308000
C	5.36494779	−0.87377985	−1.21101700
C	6.04960779	0.43202815	−0.99429500
C	5.36696379	1.49888615	−0.53819800
C	3.93918079	1.43404115	−0.24851400
C	3.30673679	0.25015515	−0.22169800
H	4.72362779	−0.58566185	−2.30022900
H	7.09478779	0.48559415	−1.27535500
H	5.87053779	2.45207915	−0.42221600
H	3.38768879	2.35912315	−0.12406300
O	6.02616579	−1.92628185	−1.50144300
N	3.12834479	−1.98115785	−0.88018400
H	3.34168979	−2.95255985	−0.69138000
O	4.97366579	−2.71043685	0.97983400
O	4.51456979	−1.37129285	0.97173500
H	5.85297579	−2.65532785	0.57073300
O	2.78401279	−0.28271985	−3.35735400
O	3.96487979	−0.03517485	−3.35145900

TS82

02

C	−0.59420289	−0.10869565	0.00000000
C	−0.68618889	−1.48214865	−0.24623800
C	0.43657411	−2.30257865	−0.22818100
C	1.65861511	−1.71212265	0.07051000
C	1.76579811	−0.33287865	0.32520800
C	0.63575711	0.47606935	0.27590200
H	−1.48839389	0.50107035	−0.02585600
H	−1.65407389	−1.91943365	−0.46084700
H	0.36103411	−3.36332865	−0.43261500
H	0.71116711	1.54127435	0.46192300
C	3.87396011	−1.34953465	0.47257200
C	5.19786011	−1.02415465	−0.96526000

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C	5.89460711	0.18502635	−0.37846900
C	5.28487311	1.17073535	0.29289400
C	3.84712711	1.13570535	0.53086100
C	3.18130811	−0.03850465	0.52703400
H	4.43585011	−0.78778565	−1.73233900
H	6.96442211	0.21077035	−0.55791100
H	5.84842911	2.03775735	0.61965400
H	3.30024011	2.06996135	0.60250100
O	5.83499711	−2.10461465	−1.04746500
N	2.91644911	−2.29729665	0.13755600
H	3.10228811	−3.28187065	0.25217200
O	5.17843811	−2.99567165	1.33405700
O	4.73241511	−1.65932065	1.50598500
H	5.78977511	−2.89510565	0.56917800

TS83

02

C	0.46376811	−0.15942029	0.00000000
C	0.21871211	−1.52412229	0.20176100
C	1.25418311	−2.41619629	0.44293100
C	2.54390711	−1.89844329	0.48742400
C	2.81198511	−0.53121429	0.28664800
C	1.75658911	0.34312771	0.03552600
H	−0.36701089	0.50766771	−0.19288700
H	−0.79932289	−1.89256029	0.16574600
H	1.06431411	−3.47167229	0.59502700
H	1.94079411	1.39723571	−0.13769900
C	4.78575111	−1.65251729	0.62265200
C	7.36613111	−0.59994529	−1.08882700
C	7.38722111	0.48135071	−0.08865700
C	6.31985311	1.14596071	0.42892900
C	4.91638111	0.86460671	0.36699600
C	4.25536611	−0.34349529	0.37373100
H	8.36211511	−1.02210329	−1.32205700
H	8.37646411	0.87131571	0.13451000
H	6.55434611	2.07341171	0.94920200
H	4.27819411	1.74339071	0.41709600
O	6.38817611	−0.98994729	−1.67997000
N	3.74789411	−2.54249929	0.71360700
H	3.88545211	−3.52552429	0.88944400

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O	6.37122411	−1.63424829	2.38696200
O	5.99749711	−2.02282129	0.85509900
H	6.96313411	−0.89962329	2.16339500

TS84

0 1

C	0.25036818	−0.21354933	0.00000000
C	0.19835518	−1.37748033	−0.79663600
C	1.33222518	−1.91842233	−1.36547200
C	2.55056618	−1.26244333	−1.13537000
C	2.62229318	−0.13561433	−0.27207400
C	1.44993918	0.41876067	0.25467800
H	−0.66439182	0.16984667	0.43417900
H	−0.75907182	−1.85669033	−0.96304300
H	1.28634618	−2.80261833	−1.98937400
H	1.49376518	1.29275067	0.89340600
C	4.79023018	−0.92950033	−0.78251000
C	6.07548018	−0.45956233	−1.46916900
C	6.78808418	0.50826067	−0.55940300
C	6.11918918	1.34570667	0.24716500
C	4.66446118	1.28895467	0.34723800
C	4.01189118	0.24515067	−0.18196500
H	5.79835318	0.06455067	−2.39201100
H	7.87028518	0.52463867	−0.62721700
H	6.65104518	2.07791267	0.84284300
H	4.13230918	2.06661467	0.88530400
O	6.87540418	−1.55415033	−1.84185700
H	6.91452118	−2.13292233	−1.06871300
N	3.77579718	−1.51988833	−1.68381200
H	3.98365918	−2.45379433	−2.02345800
O	2.65138518	−1.42995233	2.92176000
O	5.02990418	−1.93566433	0.10680100
N	3.37906218	−1.52237733	1.96566300
O	4.58340318	−1.47962633	2.00192500

TS85

0 2

C	−0.89935767	−1.18843681	0.00000000
C	−1.00141167	−2.56962581	−0.32172800

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C	0.10431233	−3.35243181	−0.51624800
C	1.37233133	−2.73952881	−0.37974200
C	1.48164633	−1.34766981	−0.03152500
C	0.32674133	−0.57662281	0.13913500
H	−1.80835067	−0.61720081	0.14213000
H	−1.98714467	−3.01052581	−0.41125000
H	0.02558533	−4.40491581	−0.75590800
H	0.40124833	0.47390719	0.39285800
C	3.63438533	−2.36848981	−0.04680400
C	4.90364533	−2.27565381	−0.88779700
C	5.64434733	−1.00634881	−0.52665500
C	5.00918833	0.10925319	−0.13813700
C	3.55790633	0.12712319	−0.00153400
C	2.88180933	−1.03772981	−0.01512500
H	4.63168333	−2.22682081	−1.94986500
H	6.72215733	−1.03460581	−0.64494200
H	5.56217733	1.02059019	0.05567800
H	3.04038033	1.07649619	0.09026700
O	5.68838833	−3.42793881	−0.70868600
H	5.63037033	−3.62930581	0.23714900
N	2.58591833	−3.25854681	−0.62244900
H	2.74132633	−4.25825681	−0.57352400
O	3.97593633	−2.81786181	1.20666200
H	3.01966833	−2.86753581	1.74746700
O	1.71595633	−2.91582381	2.05373600
H	1.43969433	−2.26720381	2.70770000

TS86

0 2

C	0.33333333	0.26086957	0.00000000
C	−0.18929767	−1.03271443	−0.09143900
C	0.61702333	−2.13006643	−0.38297600
C	1.97316933	−1.90345143	−0.57438200
C	2.51500133	−0.60469043	−0.47922000
C	1.69064733	0.48128457	−0.19369100
H	−0.32348467	1.09024057	0.22882800
H	−1.24988767	−1.18864143	0.06741900
H	0.19880633	−3.12620343	−0.45999600
H	2.10698933	1.47879957	−0.11194200
C	4.24235333	−2.19408843	−0.83896500



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C	5.29050533	-2.47092843	-1.92470300
C	6.44559933	-1.77872843	-1.19243200
C	6.24643633	-0.28280643	-1.16721800
C	4.93236833	0.18982457	-0.92054100
C	3.93285233	-0.71408143	-0.72190400
H	5.02947733	-2.01908043	-2.87886300
H	7.43123733	-2.06935043	-1.55492100
H	6.94214133	0.33157957	-1.72490800
H	4.73265033	1.25534257	-0.91568000
O	5.50726933	-3.83655843	-2.11445800
H	5.81113533	-4.20791543	-1.27700000
N	2.96370733	-2.81791243	-0.92672700
H	2.88442233	-3.79927843	-0.70756700
O	6.32819833	-2.36372643	0.11994200
O	4.93060133	-2.67384543	0.33312700
O	7.36986433	0.14852757	0.49369300
O	8.49469633	-0.30850543	0.37289200

TS87

02

C	-0.97101448	0.10144928	0.00000000
C	-0.72973548	1.48358328	0.16452600
C	-1.74332848	2.42048228	0.16997600
C	-3.05913448	1.96048128	0.00939600
C	-3.31494248	0.56995628	-0.14119500
C	-2.25956848	-0.35743972	-0.15202200
H	-0.13770148	-0.58861172	0.00008100
H	0.29281452	1.82165328	0.28993900
H	-1.53323448	3.47541828	0.29284900
H	-2.46562748	-1.41507472	-0.26996100
C	-5.35873448	1.77186228	-0.01060900
C	-6.47654448	2.09066928	-1.01802700
C	-7.46383248	0.95022528	-0.78359300
C	-6.88817848	-0.41032372	-0.74773500
C	-5.54443148	-0.66272072	-0.50280200
C	-4.71766648	0.42061628	-0.27336000
H	-6.11025548	2.14898328	-2.04523200
H	-8.35154148	1.06425428	-1.41570300
H	-7.58488248	-1.23541772	-0.84839000
H	-5.17516448	-1.68029672	-0.46898500

O	-7.06654548	3.31292628	-0.68763900
H	-7.34640848	3.21663028	0.23547100
N	-4.20998448	2.68213028	-0.06693900
H	-4.30571248	3.58750528	0.37030000
O	-5.91703848	1.77979228	1.24169900
O	-7.77697148	0.88210228	0.56763300
TS88			
01			
C	-1.45038161	0.38167938	0.00000000
C	-1.83290761	-0.95930962	-0.01666100
C	-0.90420761	-1.98032962	-0.21175300
C	0.42474239	-1.62190762	-0.38408500
C	0.82355339	-0.27539062	-0.36555500
C	-0.11301361	0.72981238	-0.17465700
H	-2.19538661	1.15226438	0.15242800
H	-2.87615361	-1.21665262	0.12386500
H	-1.21230561	-3.01881262	-0.23119800
H	0.19473939	1.76930338	-0.15430700
C	2.72179039	-1.70224462	-0.54449600
C	3.86436139	-1.96571962	-1.51982300
C	4.89979339	-1.11952762	-0.79147000
C	4.62967639	0.40200738	-0.95021600
C	3.16317839	0.72332038	-0.75843100
C	2.27194639	-0.24925962	-0.57168800
H	3.63671239	-1.62351762	-2.52741100
H	5.93235839	-1.35428462	-1.05180900
H	4.92162239	0.63291338	-1.99998100
H	2.88460539	1.77227638	-0.76064200
O	4.21754139	-3.32034062	-1.57897800
H	4.45844139	-3.60125562	-0.68809300
N	1.51726739	-2.45511062	-0.65365800
H	1.52499339	-3.41774662	-0.35135700
O	4.72337039	-1.51803262	0.57457200
O	3.36627939	-2.00661462	0.71302200
O	5.46719539	1.11735538	-0.15571700
O	7.37066739	2.60374038	2.32346200
O	6.02931539	0.95517538	1.79670000
N	6.65845139	1.91990438	1.67472300

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TS89

0 2

C	0.51391867	−0.48179871	0.00000000
C	−0.01869633	−1.76463571	−0.12097200
C	0.77420367	−2.85178171	−0.48770800
C	2.11927067	−2.61595471	−0.72313600
C	2.66830467	−1.33140871	−0.60324300
C	1.86740567	−0.25876471	−0.24269200
H	−0.12621333	0.34203029	0.28854300
H	−1.07264533	−1.92464471	0.07333300
H	0.35110167	−3.84409871	−0.58670000
H	2.29019967	0.73435729	−0.14074000
C	4.37841467	−2.92050571	−1.02617400
C	5.47862567	−3.30586171	−2.00686200
C	6.62748267	−2.76516071	−1.20112000
C	6.46097767	−0.70493871	−1.48960700
C	5.01745667	−0.48415971	−1.10574000
C	4.09403767	−1.42900971	−0.93259100
H	5.35499267	−2.83739271	−2.98044300
H	7.67454767	−2.90230371	−1.45002100
H	6.63543367	−0.89994471	−2.56757200
H	4.75753167	0.55981829	−0.94897400
O	5.55554267	−4.69816671	−2.20904400
H	5.73010567	−5.12236971	−1.36095700
N	3.10075067	−3.52230871	−1.15512000
H	3.01121467	−4.51231071	−0.98231000
O	6.37324467	−3.02303371	0.10807900
O	4.98386367	−3.36868371	0.22909200
O	7.36714867	−0.21042871	−0.81259200

## TS90

0 2



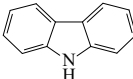
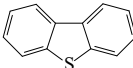
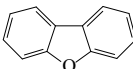
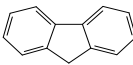
C	−1.06870224	−0.26717557	0.00000000
C	−1.52713224	−1.55873957	0.27971700
C	−0.65227424	−2.63037557	0.41531800
C	0.70666276	−2.38107357	0.25444300
C	1.17584676	−1.09496857	−0.04135200
C	0.28997276	−0.02796557	−0.15692600
H	−1.77776124	0.54462743	−0.09896700

H	-2.59082924	-1.73013657	0.39696100
H	-1.01463624	-3.62475257	0.64541600
H	0.65269876	0.96872043	-0.38125800
C	2.96190476	-2.65551157	-0.12364400
C	3.31669876	-3.16853457	-1.57640100
C	4.79117776	-3.06618757	-1.51896200
C	4.94788676	-0.15500157	-0.17321600
C	3.47642076	-0.11889357	-0.19440400
C	2.63238376	-1.16181557	-0.12562800
H	2.83981976	-2.55528057	-2.33851300
H	5.45747776	-2.50817857	-2.16701300
H	5.43675476	-1.10456657	0.09047100
H	3.06323676	0.88496643	-0.24604400
O	2.86700076	-4.49932157	-1.74644100
H	3.54757576	-5.10178057	-1.42674600
N	1.76321176	-3.28179957	0.39123100
H	1.61075076	-4.22254757	0.04883300
O	5.20587576	-3.39673757	-0.31792300
O	4.07824676	-3.01322157	0.66951500
O	5.60835076	0.83264643	-0.40037900

**Table S4.** Calculated bond lengths (angstrom) and bond energies (kcal/mol) of C-H bonds and O-H bonds in the intermediates IM12-IM15 at M06-2X/6-311++G(3df,2p)//M06-2X/6-311+G(d,p) level.

Intermediates	Bonds	Bond length (angstrom)	Bond energy (kcal/mol)
IM12	O-H	0.964	61.19
	C-H	1.099	20.89
IM13	O-H	0.963	58.30
	C-H	1.098	17.40
IM14	O-H	0.962	59.67
	C-H	1.102	14.54
IM15	O-H	0.962	57.58
	C-H	1.104	16.80

**Table S5** Comparison of the rate constants and lifetime of carbazole degradation by OH radical with those of other 5 kinds of NSO-HETs.

Compound	Structure	T(K)	P(Torr)	Rate constant (cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> )	Lifetime (h)	Method	Ref.
Pyrrole		298 ± 2	25-100	$(1.03 \pm 0.06) \times 10^{-10}$	2.7	Exp.	(Wallington, 1986)
Indole		297 ± 2	1 atm	$(1.54 \pm 0.35) \times 10^{-10}$	2	Exp.	(Atkinson et al., 1995)
Carbazole		298	1 atm	$6.52 \times 10^{-12}$	37.70	M06-2X/6-311++G(3df,2p)//6-311+G(d,p)	This paper
Dibenzothiophene		297 ± 2	1 atm	$(8.1 \pm 2.6) \times 10^{-12}$	36	Exp.	(Kwok et al., 1999)
Dibenzofuran		298.15	1 atm	$2.7 \times 10^{-11}$	10.8	B3LYP/6-311++G(3df,2p)//6-31g(d)	(Altarawneh et al., 2008)
Fluorene		298	1 atm	$2.29 \times 10^{-11}$	12.51	M06-2X/6-311++G(3df,2p)//6-311+G(d,p)	(Ding et al., 2019)

**Table S6.** RRKM calculated rate constants (in  $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) for TS1, TS5 and TS14 involved in the OH-initiated oxidation degradation of carbazole at 298 K and 10–670 torr.

Pressure (Torr)	TS1	TS5	TS14
10	5.76E-18	3.14E-12	8.42E-14
260	6.62E-17	3.66E-12	9.60E-14
510	1.03E-16	3.68E-12	9.64E-14
760	1.31E-16	3.70E-12	9.65E-14