

Supporting Information

Mechanism of Cu-Catalyzed Aerobic C(CO)–CH₃ Bond Cleavage: A Combined Computational and Experimental Study

Yuan-Ye Jiang^{*,†}, Guoqing Li[†], Daoshan Yang^{*,†,‡}, Zhaoshun Zhang[†], Ling Zhu[†], Xia
Fan[†], Siwei Bi^{*,†}

[†]School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, People's Republic of China

[‡]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao 266042,
People's Republic of China

Corresponding Author

* Y.-Y. Jiang: qfnu_yuanyejiang@163.com

*D. Yang: yangdaoshan@tsinghua.org.cn

*S. Bi: siweibi@126.com

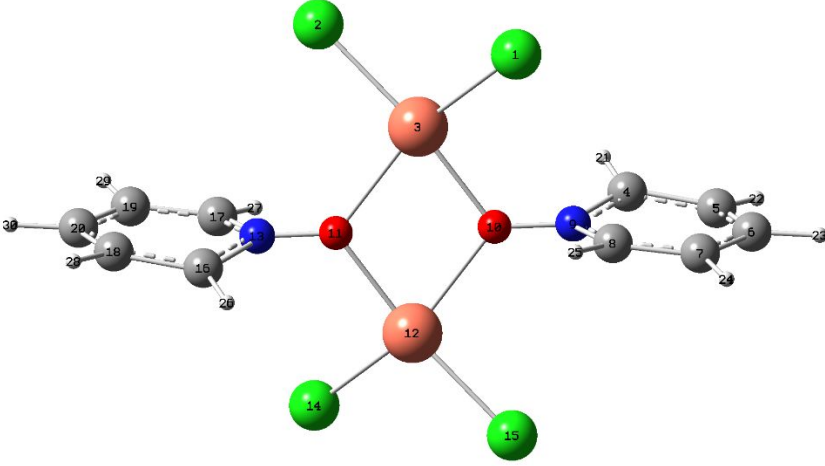
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Benchmark study for geometry optimization

Geometry optimization was performed in gas phase with Gaussian 09 program¹ by different DFT methods. The crystal structures were used as the input structures for geometry optimization. Cu, Br, I atoms were described by effective core potential LANL2DZ and the associated basis set plus extra polarization functions ($[\zeta(f) = 3.525]$ for Cu, $[\zeta(d) = 0.428]$ for Br and $[\zeta(d) = 0.289]$ for I).² Other atoms were described by basis set 6-31G(d). ‘Ultrafine’ grid was used to avoid possible integration grid errors.

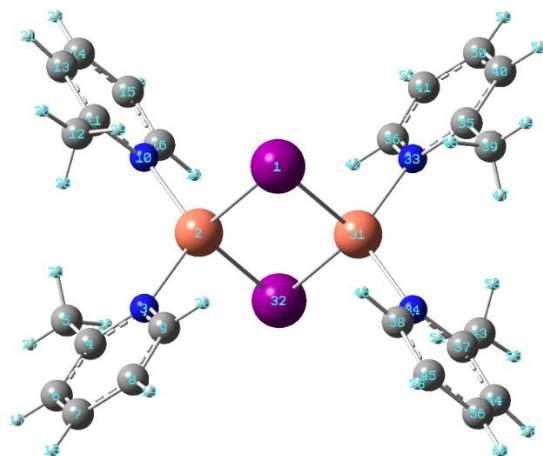
Table S1. Calculated bond lengths of Cu complexes by different methods (in angstrom).



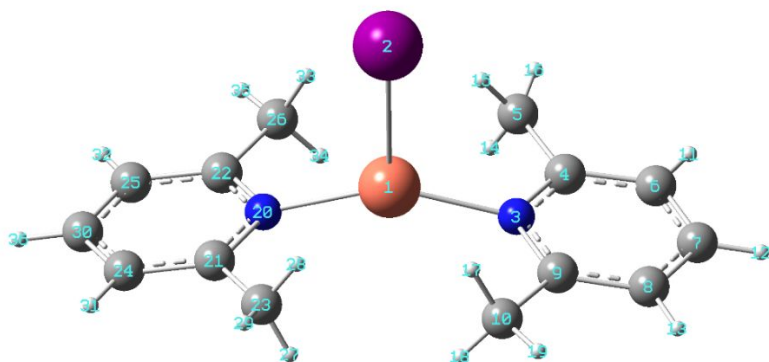
CSDrefcode: CUCPYO³

Bonds	Exp.	B3LYP	M06	M06-L	ω B97X-d	BP86	TPSS-h	BLYP
a1-a3	2.20953	2.24749	2.21618	2.22422	2.22676	2.24245	2.23514	2.26718
a2-a3	2.24306	2.24743	2.21608	2.22422	2.22691	2.24233	2.23479	2.26721
a3-a10	1.98505	2.06404	2.04123	2.04607	2.02766	2.06882	2.04571	2.09578
a3-a11	2.10025	2.0643	2.04168	2.04645	2.02748	2.06891	2.04602	2.09592
a10-a12	2.10025	2.0643	2.04168	2.04645	2.02748	2.06891	2.04602	2.09583
a11-a12	1.98505	2.06404	2.04123	2.04607	2.02766	2.06882	2.04571	2.09587
a12-a14	2.20953	2.24749	2.21618	2.22422	2.22676	2.24245	2.23514	2.26719
a12-a15	2.24306	2.24743	2.21608	2.22422	2.22691	2.24223	2.23479	2.2672

Table S1 continue

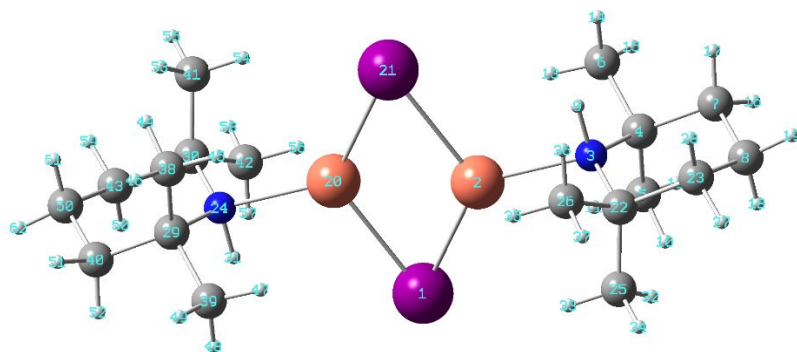
CSDrefcode: CENDEE⁴

Bonds	Exp.	B3LYP	M06	M06-L	ω B97X-d	BP86	TPSS-h	BLYP
a1-a2	2.71507	2.7855	2.6879	2.70662	2.71302	2.76545	2.74837	2.82836
a1-a31	2.66293	2.78452	2.70304	2.7474	2.71834	2.76503	2.74909	2.82692
a2-a3	2.04902	2.14881	2.15058	2.12406	2.15022	2.08905	2.11146	2.11788
a2-a10	2.06049	2.14904	2.13789	2.09832	2.14481	2.08855	2.11198	2.11803
a2-a32	2.66293	2.78452	2.70304	2.7474	2.71834	2.76503	2.74909	2.82692
a31-a32	2.71507	2.7855	2.6879	2.70662	2.71302	2.76545	2.74837	2.82836
a31-a33	2.04902	2.14881	2.15058	2.12406	2.15022	2.08905	2.11146	2.11788
a31-a34	2.06049	2.14904	2.13789	2.09832	2.14481	2.08855	2.11198	2.11803

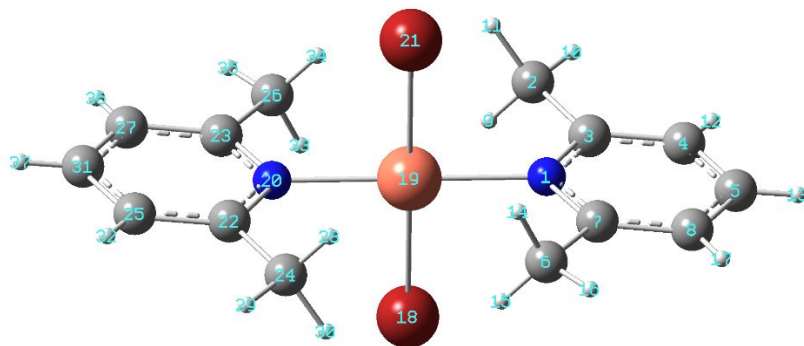
CSDrefcode: CENFAC⁴

Bonds	Exp.	B3LYP	M06	M06-L	ω B97X-d	BP86	TPSS-h	BLYP
a1-a2	2.6819	2.57489	2.52141	2.55654	2.52419	2.59036	2.58121	2.60963
a1-a3	1.98345	2.11569	2.08416	2.04569	2.10939	2.04748	2.06113	2.09223
a1-a20	1.98343	2.11568	2.08417	2.04568	2.10934	2.04748	2.06113	2.09223

Table S1 continue

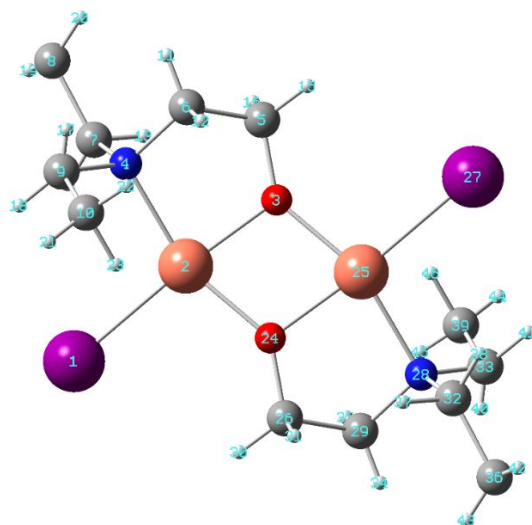
CSDrefcode: CERHAI⁵

Bonds	Exp.	B3LYP	M06	M06-L	ω B97X-d	BP86	TPSS-h	BLYP
a1-a2	2.50311	2.60987	2.56623	2.56777	2.57561	2.59066	2.59118	2.61815
a1-a20	2.65207	2.74832	2.70177	2.73652	2.7094	2.74291	2.73089	2.79519
a2-a3	2.10884	2.12202	2.0752	2.08153	2.08473	2.0915	2.09094	2.13135
a2-a20	2.53484	2.6313	2.49312	2.44248	2.5467	2.50754	2.52203	2.55375
a2-a21	2.65207	2.74832	2.70177	2.73652	2.7094	2.74291	2.73089	2.79519
a20-a21	2.50311	2.60897	2.56623	2.56777	2.57561	2.59066	2.59118	2.61815
a20-a24	2.10884	2.12202	2.0752	2.08153	2.08473	2.0915	2.09094	2.13135

CSDrefcode: BCULUT⁶

Bonds	Exp.	B3LYP	M06	M06-L	ω B97X-d	BP86	TPSS-h	BLYP
a1-a19	1.99689	2.06737	2.03522	2.03643	2.04087	2.05629	2.04899	2.08718
a19-a18	2.42464	2.49621	2.46278	2.47995	2.46172	2.49659	2.48135	2.53418
a19-a20	1.99689	2.06737	2.03522	2.03643	2.04087	2.05629	2.04899	2.08757
a19-a21	2.42464	2.49621	2.46278	2.47955	2.46172	2.49659	2.48135	2.53418

Table S1 continue

CSDrefcode: BITGEQ⁷

Bonds	Exp.	B3LYP	M06	M06-L	ω B97X-d	BP86	TPSS-h	BLYP
a1-a2	2.55407	2.5937	2.54778	2.55955	2.55688	2.584	2.58055	2.61513
a2-a3	1.91943	1.99126	1.99357	1.99005	1.97721	1.98992	1.97615	2.00846
a2-a4	2.04586	2.1187	2.07347	2.0923	2.09065	2.10272	2.08627	2.1454
a2-a24	1.90707	1.95216	1.93233	1.94184	1.93392	1.95742	1.94038	1.97766
a3-a25	1.90707	1.95214	1.9322	1.94179	1.93396	1.95744	1.94038	1.97767
a24-a25	1.91943	1.99126	1.99352	1.99002	1.97718	1.98993	1.97618	2.00845
a25-a27	2.55407	2.59371	2.54788	2.5596	2.55688	2.584	2.58048	2.61513
a25-a28	2.04586	2.11877	2.0734	2.09224	2.09061	2.10265	2.08634	2.1454

Table S2. Root-mean-square deviation (RMSD) of bond length calculation of different methods (in angstrom).^a

	B3LYP	M06	M06-L	ω B97X-d	BP86	TPSS-h	BLYP
RMSD	0.07924	0.05953	0.05735	0.06281	0.06055	0.05643	0.09164

^aRMSD were calculated based on the results in Table S1.

Benchmark study for energy calculation

First, the electronic energy change ΔE_1 of the isomerization of **P1** to **O1** was used for benchmark study (Eq. S1). Because no experimental result is available for this reaction, Holthausen et al. estimated ΔE_1 to be -5.7 kcal/mol with CCSD(T)-F12b/CBS(D/T) method and found that BLYP-D3/def2-TZVP(SDD) level of DFT calculation can well reproduce this value (Table S3 and S4).⁸ Because TPSS-h showed the best performance during our benchmark study for geometry optimization of Cu complexes, it was used for geometry optimization with BS1 (SDD for Cu and Def2-SVP for the other atoms). Based on the optimized structures, TPSS-h and BLYP, the method recommended by Holthausen et al., were used for energy calculation with BS2 (SDD for Cu and Def2-TZVP for the other atoms). Meanwhile, D3 version of Grimme's dispersion with the original D3 damping function was used for the energy calculation. Note that 'Ultrafine' grid was used for all of our geometry optimization and energy calculation.

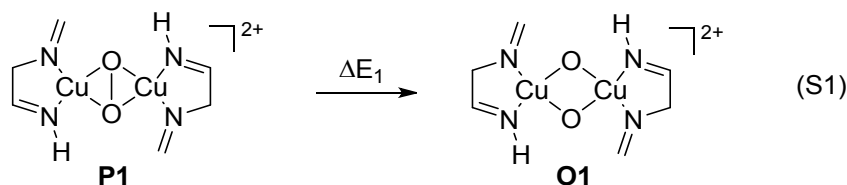


Table S3. Experimental measured and Calculated Gibbs free energies of the transformation of P1 to O1 (in kcal/mol).

Methods	ΔE_1
CCSD(T)-F12b/CBS(D/T) ^a	-5.7
BLYP-D3/def2-TZVP(SDD)	-5.8
BLYP-D3/BS2//TPSS-h/BS1	-5.9
TPSS-h-D3BJ/BS2//TPSS-h/BS1	-3.2
BP86-D3/BS2//TPSS-h/BS1	-5.6
M06-L-D3/BS2//TPSS-h/BS1	-5.5
BB95/BS2//TPSS-h/BS1	-0.6
B97D-D3/BS2//TPSS-h/BS1	3.8
M11L/BS2//TPSS-h/BS1	-9.8
PBE-D3/BS2//TPSS-h/BS1	-4.0
TPSS-D3/BS2//TPSS-h/BS1	-5.0
B3LYP-D3/BS2//TPSS-h/BS1	-2.2
CAM-B3LYP/BS2//TPSS-h/BS1	-1.7
M06/BS2//TPSS-h/BS1	3.7
TPSS-h/BS2//TPSS-h/BS1	-1.5
TPSS-h-D3/BS2//TPSS-h/BS1	-2.8
ω B97X-d/BS2//TPSS-h/BS1	2.9

^asee ref. 8 for details.

Table S4. Calculated electronic energies ΔE of P1 and O1 (in Hartree).

Methods	P1	O1
BLYP-D3/BS2//TPSS-h/BS1	-999.441545	-999.4509911
TPSS-h-D3BJ/BS2//TPSS-h/BS1	-999.5190244	-999.5240599
BP86-D3/BS2//TPSS-h/BS1	-999.9016857	-999.9105706
M06-L-D3/BS2//TPSS-h/BS1	-999.6155806	-999.6243641
BB95/BS2//TPSS-h/BS1	-999.7309704	-999.7319808
B97D-D3/BS2//TPSS-h/BS1	-1000.227742	-1000.221733
M11L/BS2//TPSS-h/BS1	-999.89625	-999.9119305
PBE-D3/BS2//TPSS-h/BS1	-998.9506498	-998.9569611
TPSS-D3/BS2//TPSS-h/BS1	-999.6383826	-999.6464082
B3LYP-D3/BS2//TPSS-h/BS1	-999.6702545	-999.673699
CAM-B3LYP/BS2//TPSS-h/BS1	-999.2069903	-999.2096675
M06/BS2//TPSS-h/BS1	-999.2725068	-999.2665999
TPSS-h/BS2//TPSS-h/BS1	-999.4865343	-999.4888848
TPSS-h-D3/BS2//TPSS-h/BS1	-999.5054221	-999.5098358
ω B97X-d/BS2//TPSS-h/BS1	-999.3983254	-999.3936458

Then the Gibbs free energy change of the reaction of **P2** into **O2** at 188 K was considered (Eq. S2). It was experimentally measured to be -0.05 ± 0.14 kcal/mol (Table S4).⁹ Both of the closed-shell singlet and the broken-symmetry singlet with the energy correction of Yamaguchi's method³ were calculated for **P2** as Holthausen did. Geometry optimization and calculation of thermodynamic correction were performed by using TPSS-h method, BS1 basis set at 188 K. The singlet-point energies were calculated by using BLYP-D3 method, BS2 basis set and SMD solvation model (solvent = THF). The BLYP-D3/BS2/SMD//TPSS-h/BS1 level of theory gives almost the same result with BLYP-D3/def2-TZVP(SDD) level of theory for the closed-shell singlet of P2 whereas the former gives a better result for the broken-symmetry singlet of **P2**.

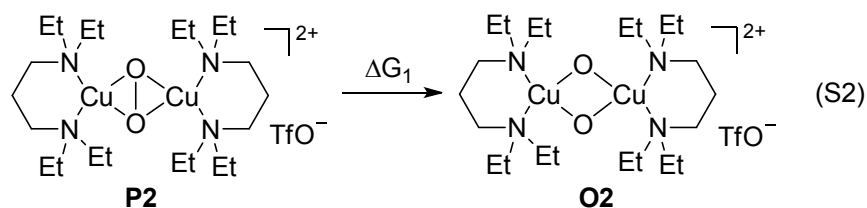


Table S5. Experimental measured and Calculated Gibbs free energies of the transformation of P2 to O2 (in kcal/mol).

Methods	ΔG_1
Exp.	-0.05 ± 0.14
BLYP-D3/def2-TZVP(SDD) ^a	-0.8
BLYP-D3/def2-TZVP(SDD) ^{a,b}	-4.7
BLYP-D3/BS2/SMD(THF)//TPSS-h/BS1	-0.8
BLYP-D3/BS2/SMD(THF)//TPSS-h/BS1 ^b	0.6
BP86-D3/BS2/SMD(THF)//TPSS-h/BS1	-1.5
M06-L-D3/BS2/SMD(THF)//TPSS-h/BS1	-1.7
BB95/BS2/SMD(THF)//TPSS-h/BS1	4.1
B97D-D3/BS2/SMD(THF)//TPSS-h/BS1	8.1
M11L /BS2/SMD(THF)//TPSS-h/BS1	0.8
PBE-D3/BS2/SMD(THF)//TPSS-h/BS1	1.6
TPSS-D3/BS2/SMD(THF)//TPSS-h/BS1	-1.6
B3LYP-D3/BS2/SMD(THF)//TPSS-h/BS1	5.6
CAM-B3LYP/BS2/SMD(THF)//TPSS-h/BS1	10.5
M06/BS2/SMD(THF)//TPSS-h/BS1	13.4
TPSS-h/BS2/SMD(THF)//TPSS-h/BS1	6.0
TPSS-h-D3/BS2/SMD(THF)//TPSS-h/BS1	2.0
ω B97X-d /BS2/SMD(THF)//TPSS-h/BS1	2.9

^aSee ref. 8 for details. ^bbroken symmetry calculation and energy correction by Yamaguchi's method were performed for **P2**.

Table S6. Calculated thermodynamic correction of Gibbs free energy ΔG_{cor188} , solution-phase single-point energies ΔE_{S} and Gibbs free energies at 188 K ΔG_{188} of **P2 and **O2** at the different levels (in Hartree).**

P2			
methods	ΔG_{cor188}	ΔE_{S}	ΔG_{188}
BLYP-D3/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2595.320506	-2594.586727
BP86-D3/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2596.335545	-2595.601766
M06-L-D3/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2595.749597	-2595.015818
BB95/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2595.563085	-2594.829306
B97D-D3/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2595.829502	-2595.095723
M11L /BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2595.843815	-2595.110036
PBE-D3/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2593.652119	-2592.91834
TPSS-D3/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2596.189068	-2595.45529
B3LYP-D3/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2596.090288	-2595.356509
CAM-B3LYP/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2594.945988	-2594.212209
M06/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2594.828861	-2594.095082
TPSS-h/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2595.80341	-2595.069631
TPSS-h-D3/BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2595.940655	-2595.206876
ω B97X-d /BS2/SMD(THF)//TPSS-h/BS1	0.730751	-2369.0586	-2368.324821
O2			
BLYP-D3/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2595.326186	-2594.587941
BP86-D3/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2596.342453	-2595.604208
M06-L-D3/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2595.756729	-2595.018484
BB95/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2595.56101	-2594.822765
B97D-D3/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2595.820985	-2595.08274
M11L /BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2595.84701	-2595.108765
PBE-D3/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2593.654079	-2592.915835
TPSS-D3/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2596.19604	-2595.457795
B3LYP-D3/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2596.085896	-2595.347651
CAM-B3LYP/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2594.933766	-2594.195521
M06/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2594.811993	-2594.073748
TPSS-h/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2595.798254	-2595.060009
TPSS-h-D3/BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2595.941991	-2595.203746
ω B97X-d /BS2/SMD(THF)//TPSS-h/BS1	0.735217	-2369.058484	-2368.32024

Finally, the Gibbs free energy barrier of the C–H activation on **P3** was examined at 263 K (Eq. S3). The

responding experimental result is 18.9 ± 1.5 kcal/mol.¹⁰ Geometry optimization and calculation of thermodynamic correction were performed by using TPSS-h method, BS1 basis set at 263 K. Single-point energy calculation was performed at the level of BLYP-D3/BS2/SMD with acetone as the solvent. BLYP-D3/BS2/SMD//TPSS-h/BS1 level of theory shows very similar performance with BLYP-D3/de2f-TZVP(SDD) level of theory (Table S7).

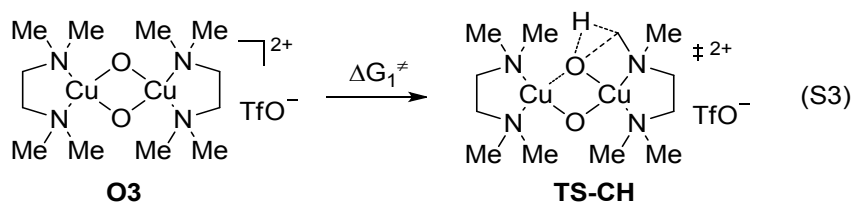


Table S7. Experimental measured and Calculated Gibbs free energies of the transformation of P2 to O2 (in kcal/mol).

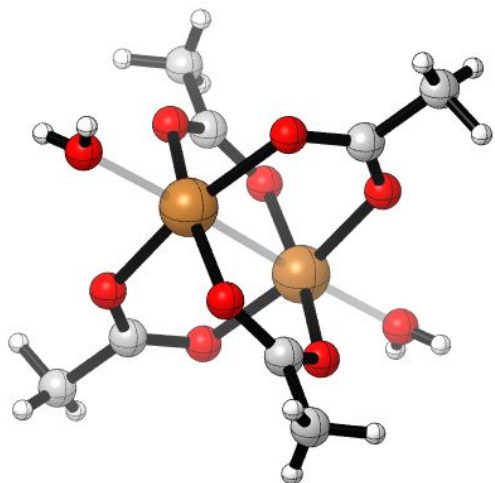
Methods	$\Delta G_1^\ddagger$
Exp.	18.9 ± 1.5
BLYP-D3/def2-TZVP(SDD) ^a	19.0
BLYP-D3/BS2//TPSS-h/BS1	19.2
BP86-D3/BS2/SMD(THF)//TPSS-h/BS1	17.5
M06-L-D3/BS2/SMD(THF)//TPSS-h/BS1	23.7
BB95/BS2/SMD(THF)//TPSS-h/BS1	15.8
B97D-D3/BS2/SMD(THF)//TPSS-h/BS1	15.6
M11L /BS2/SMD(THF)//TPSS-h/BS1	22.2
PBE-D3/BS2/SMD(THF)//TPSS-h/BS1	16.3
TPSS-D3/BS2/SMD(THF)//TPSS-h/BS1	20.8
B3LYP-D3/BS2/SMD(THF)//TPSS-h/BS1	24.0
CAM-B3LYP/BS2/SMD(THF)//TPSS-h/BS1	28.3
M06/BS2/SMD(THF)//TPSS-h/BS1	22.4
TPSS-h/BS2/SMD(THF)//TPSS-h/BS1	21.8
TPSS-h-D3/BS2/SMD(THF)//TPSS-h/BS1	23.1
ω B97X-d /BS2/SMD(THF)//TPSS-h/BS1	27.7

^aSee ref. 8 for details.

Table S8. Calculated thermodynamic correction of Gibbs free energy ΔG_{cor} , single-point energies ΔE_s and Gibbs free energies at 263 K ΔG_{263} of O3 and TS-CH at the level of BLYP-D3/BS2/SMD(acetone)//TPSS-h/BS1 (in Hartree).

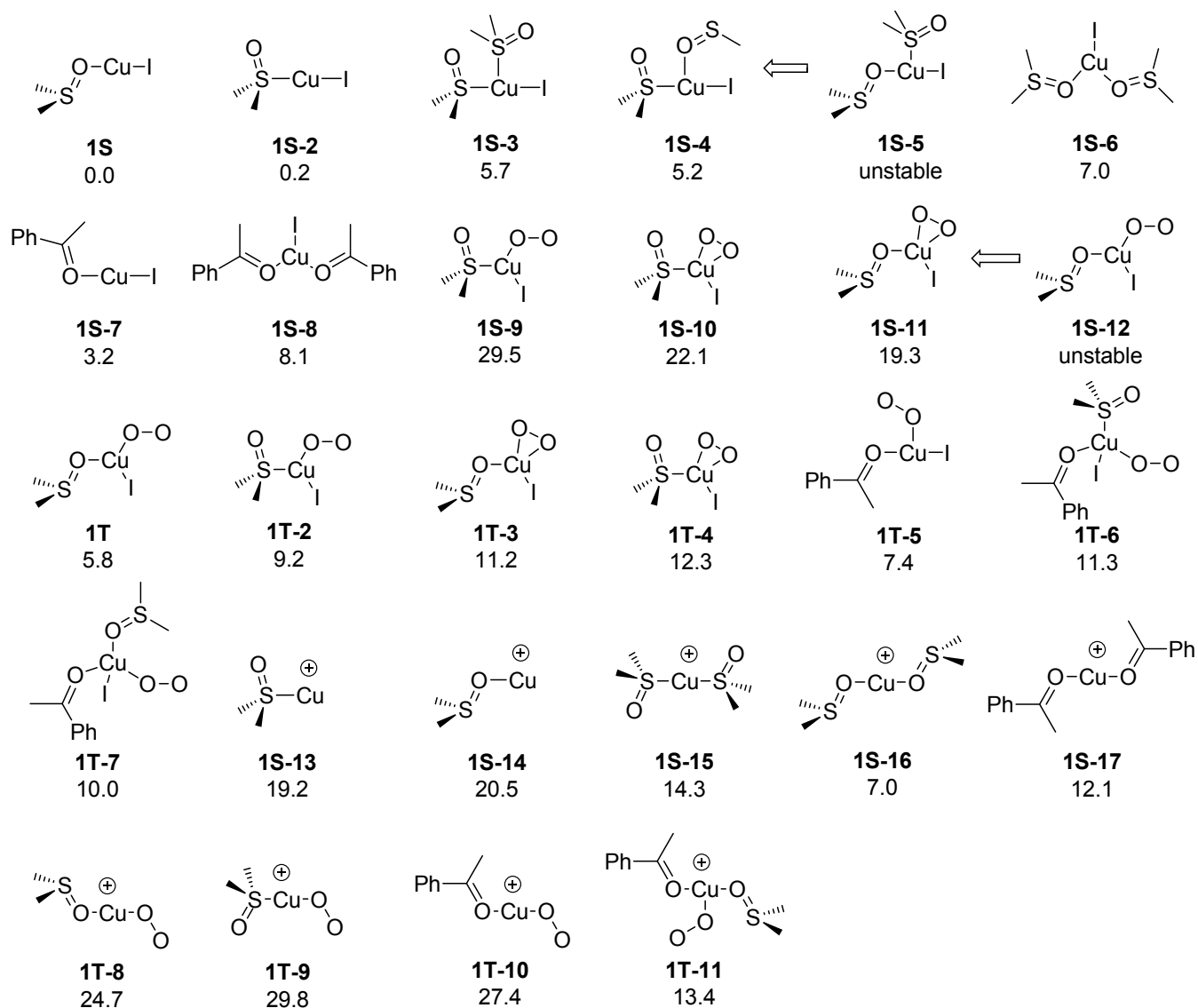
O3			
methods	$\Delta G_{\text{cor}263}$	E_s	ΔG_{263}
BLYP-D3/BS2//TPSS-h/BS1	0.436908	-2202.281833	-2201.841897
BP86-D3/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2203.05389	-2202.613954
M06-L-D3/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.538089	-2202.098153
BB95/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.558277	-2202.118341
B97D-D3/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.8289	-2202.388965
M11L /BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.682547	-2202.242611
PBE-D3/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2200.940906	-2200.50097
TPSS-D3/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.841593	-2202.401657
B3LYP-D3/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.784421	-2202.344485
CAM-B3LYP/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2201.940357	-2201.500421
M06/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2201.874653	-2201.434718
TPSS-h/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.528928	-2202.088992
TPSS-h-D3/BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.621	-2202.181064
ω B97X-d /BS2/SMD(THF)//TPSS-h/BS1	0.436908	-2202.218722	-2201.778786
TS-CH			
BLYP-D3/BS2//TPSS-h/BS1	0.430216	-2202.244499	-2201.811255
BP86-D3/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2203.019272	-2202.586028
M06-L-D3/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.493609	-2202.060365
BB95/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.526379	-2202.093135
B97D-D3/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.797417	-2202.364174
M11L /BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.640488	-2202.207244
PBE-D3/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2200.90826	-2200.475016
TPSS-D3/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.801689	-2202.368445
B3LYP-D3/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.739421	-2202.306177
CAM-B3LYP/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2201.888526	-2201.455282
M06/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2201.832255	-2201.399011
TPSS-h/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.487422	-2202.054178
TPSS-h-D3/BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.577466	-2202.144222
ω B97X-d /BS2/SMD(THF)//TPSS-h/BS1	0.430216	-2202.167836	-2201.734593

Table S9. Calculated electronic energies of open-shell singlet (OSS) and triplet (T) states of $[\text{Cu}(\text{OAc})_2]_2(\text{H}_2\text{O})_2$ based on the reported crystal structure.^a

CSDrefcode: CUAQAC04¹¹

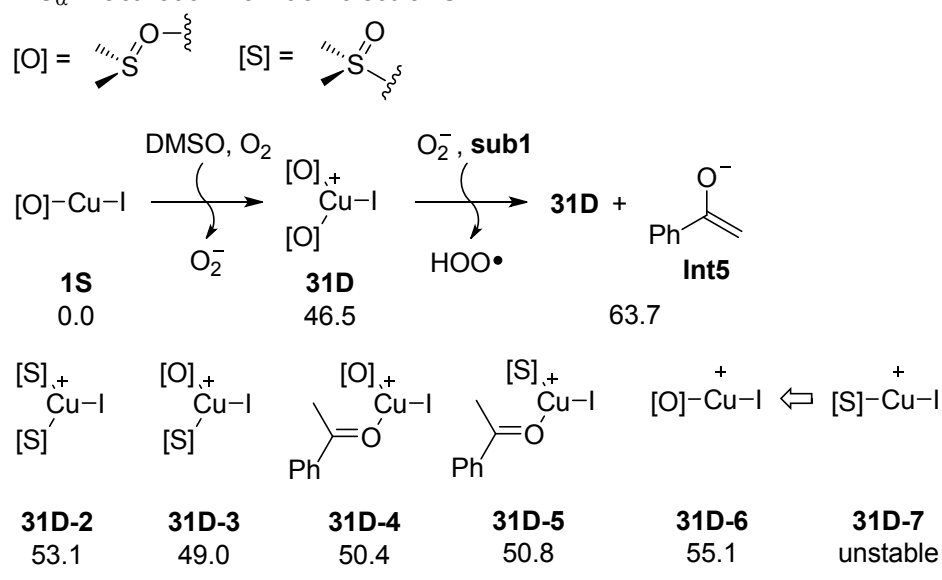
methods	OSS state (hartree)	T state (hartree)	E _{OSS} -E _T (kcal/mol)
BLYP-D3	-1460.792101	-1460.789573	-1.6
M06-L-D3	-1461.034714	-1461.032865	-1.2
B97D-D3	-1461.396563	-1461.393322	-2.0
B3LYP-D3	-1461.1631	-1461.162059	-0.7
TPSS-h	-1460.906348	-1460.904835	-0.9
TPSS-h-D3	-1460.941872	-1460.940359	-0.9

^aSDD for Cu and def2-TZVP basis set for the other atoms

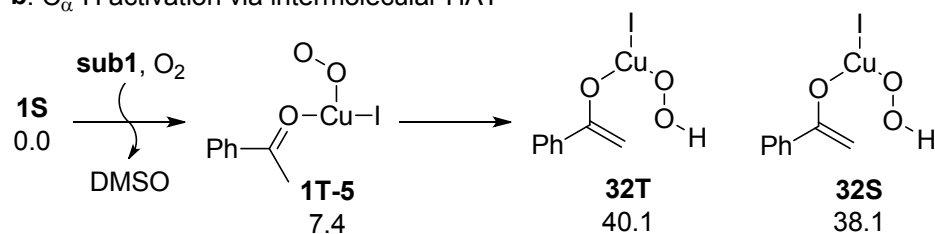


Scheme S1. Calculated relative solution-phase Gibbs free energies of possible resting states of monomeric Cu catalyst precursors (in kcal/mol). 1S-5, 1S-12 isomerized to 1S-4, 1S-11 respectively during geometry optimization.

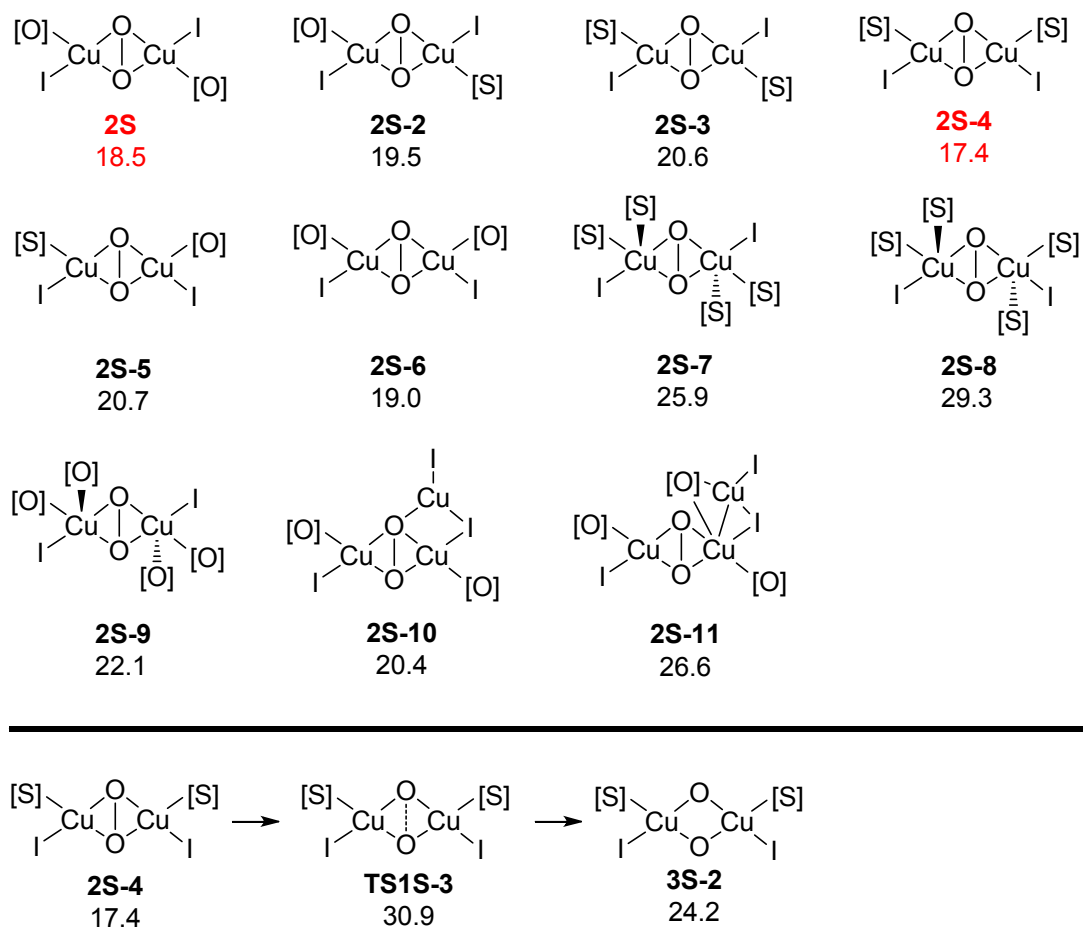
a. C_α-H activation via intramolecular SET



b. C_α-H activation via intermolecular HAT



Scheme S2. Calculated solution-phase Gibbs free energy changes of monomeric Cu-catalyzed C_α-H activation of sub (in kcal/mol). 31D-7 isomerized to 31D-6 during geometry optimization.



Scheme S3. Considered possible peroxide dicopper complexes and O-O activation processes

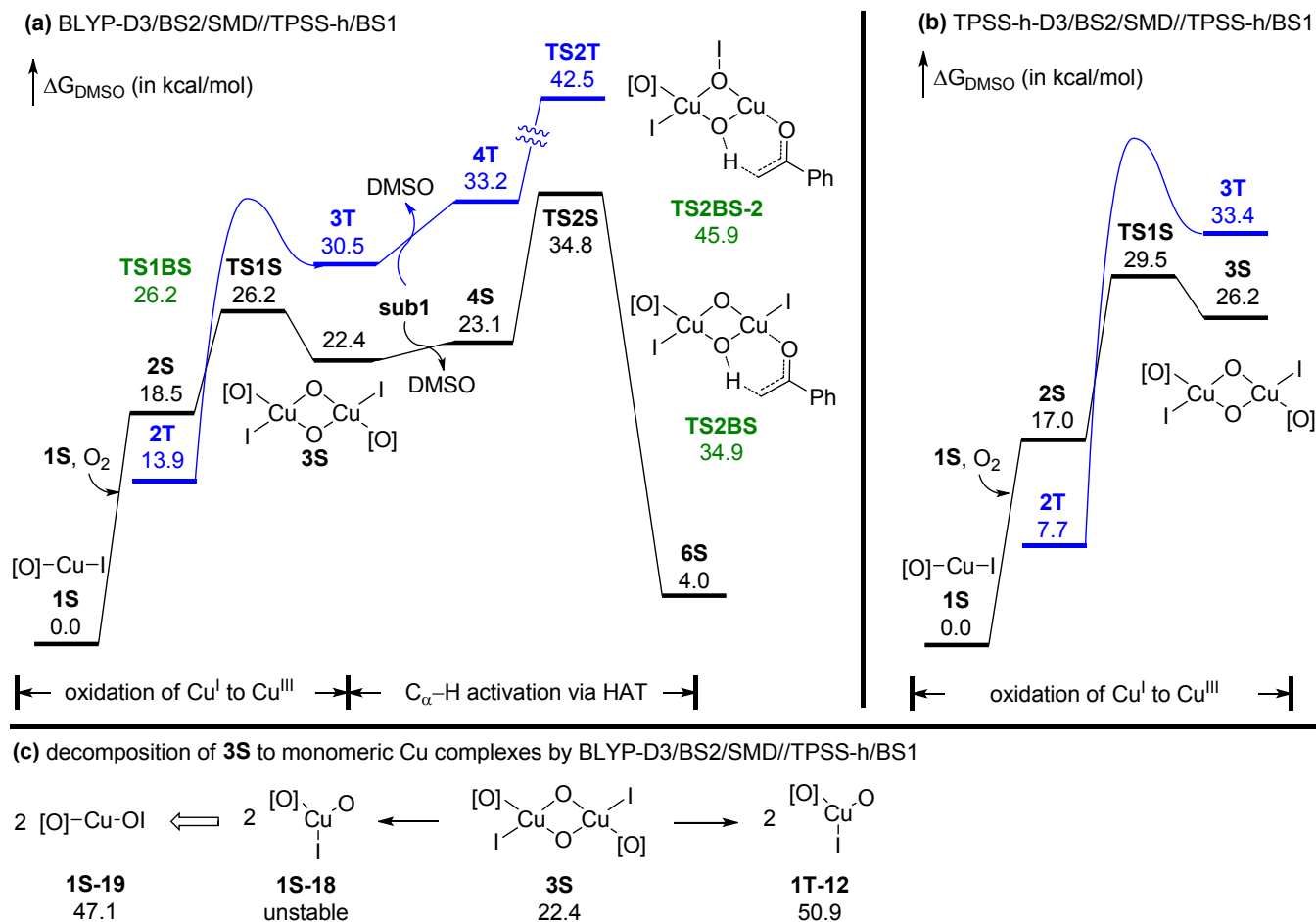


Figure S1. Calculated Gibbs free energy changes in the transformation of **sub1** to **int1** (in kcal/mol).

TS2BS was located by using the structure of **TS2S** as the starting point while **TS2BS-2** was located by using the structure of **TS2T** as the starting point. In view of the higher energy of **3T** relative to **TS1S**, we did not locate the O–O activation transition state in triplet state. Meanwhile, because the C_α–H and O–H activation of **int1** and **int2** catalyzed by **3S** are similar to the C_α–H activation of **sub** catalyzed by **3S**, we did not examined the relevant triplet states for the late-stage C_α–H and O–H activation.

Following reviewer's comments, TPSS-h-D3 was used instead of BLYP-D3 to recalculate the solution-phase single point energies. It predicts the same relative stabilities of **2S**, **2T**, **3S**, **TS1S** and **3T** (Figure S1b).

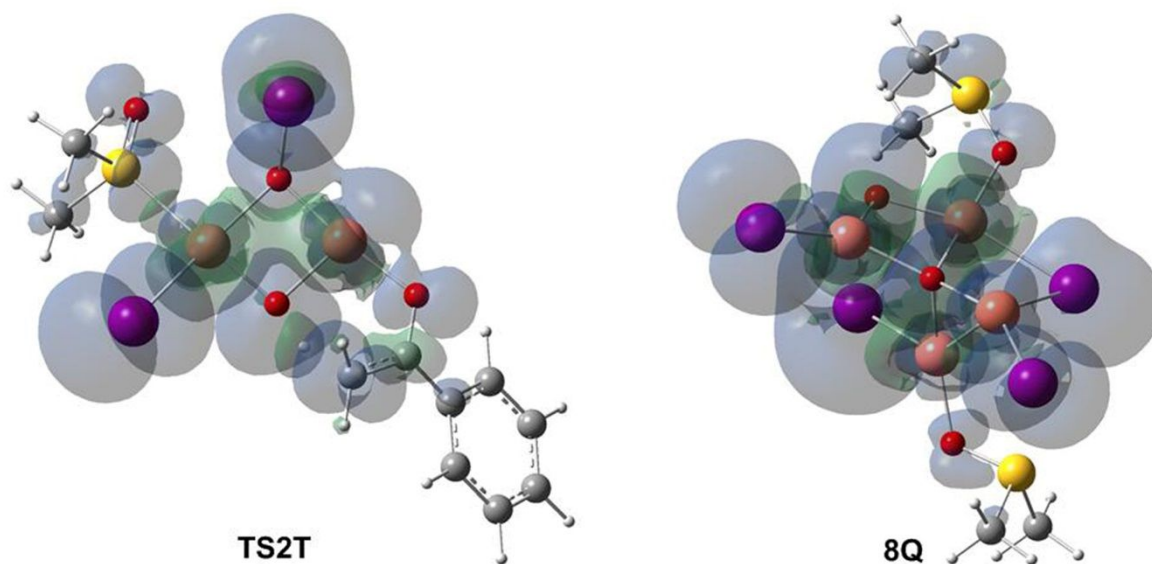
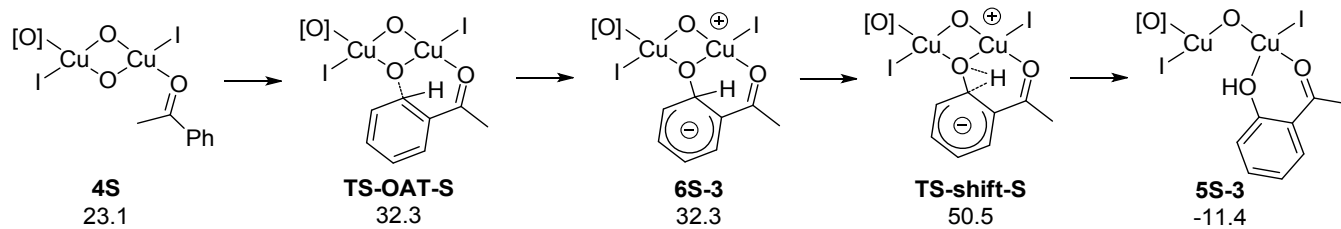
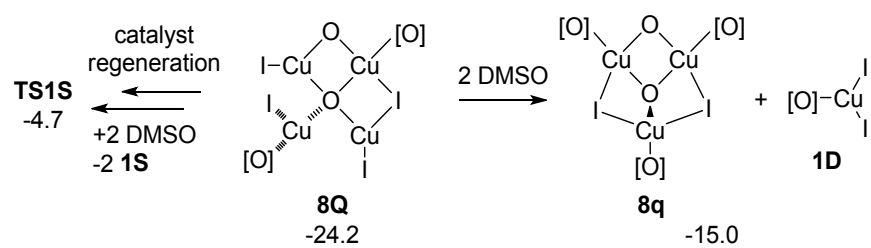


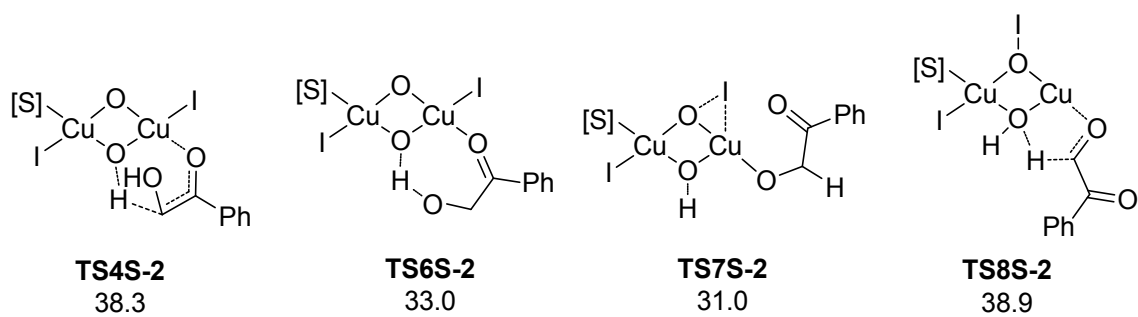
Figure S2. Spin density distribution of TS2T and 8Q (isoval = 0.0004).



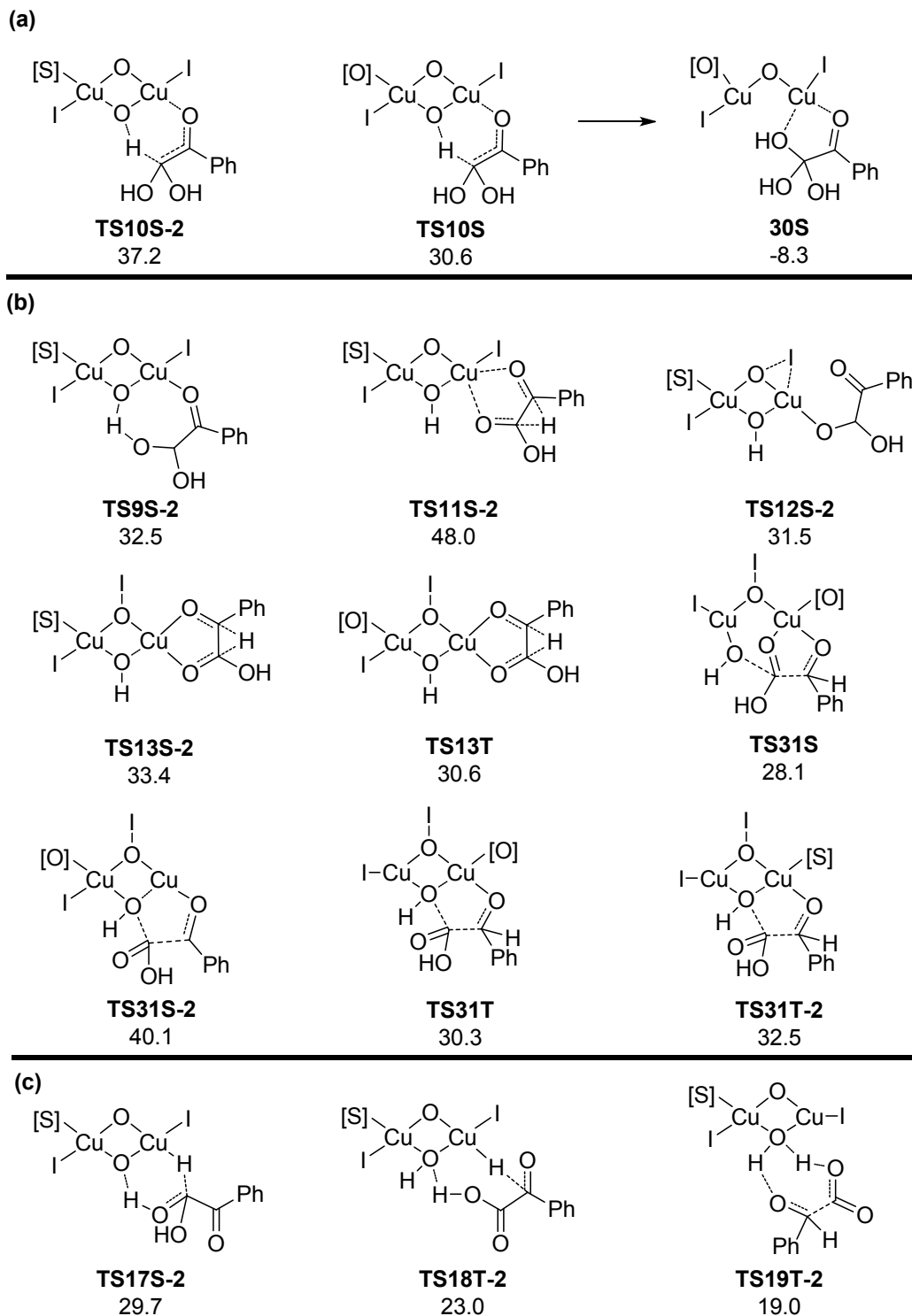
Scheme S4. *Ortho*-hydroxylation of sub1



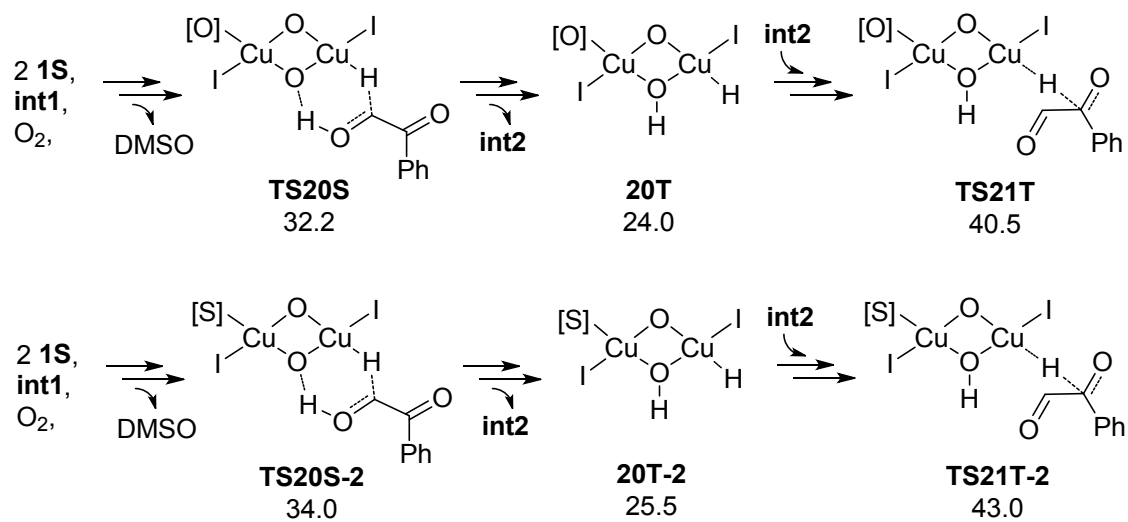
Scheme S5. Generation of Cu(II) complex from 8Q



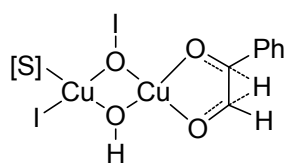
Scheme S6. Less favored transition states in the transformation of int1 to int2 and int3



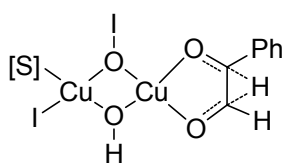
Scheme S7. Less favored transition states in the transformation of int3 to pro1 via (a) C $_{\alpha}$ -H activation, (b) O-H activation or (c) dehydrogenation



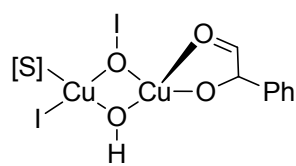
Scheme S8. Calculation results of the transformation of **int1** to **pro1** via dehydrogenation (in kcal/mol)



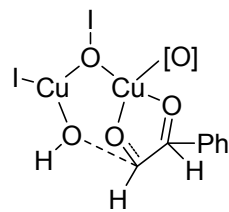
TS22S-2
36.2



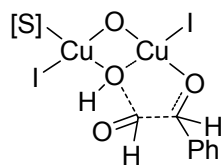
TS22T-2
35.7



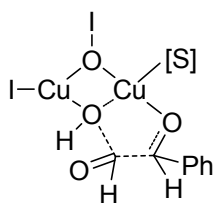
TS24S-2
29.4



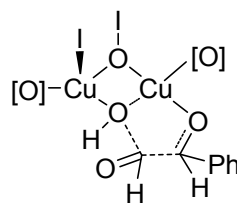
TS26S
40.7



TS26S-2
40.7



TS26T-2
45.9



TS26T-3
40.3

Scheme S9. Less favored transition states in the transformation of int1 to pro1 via O–H activation

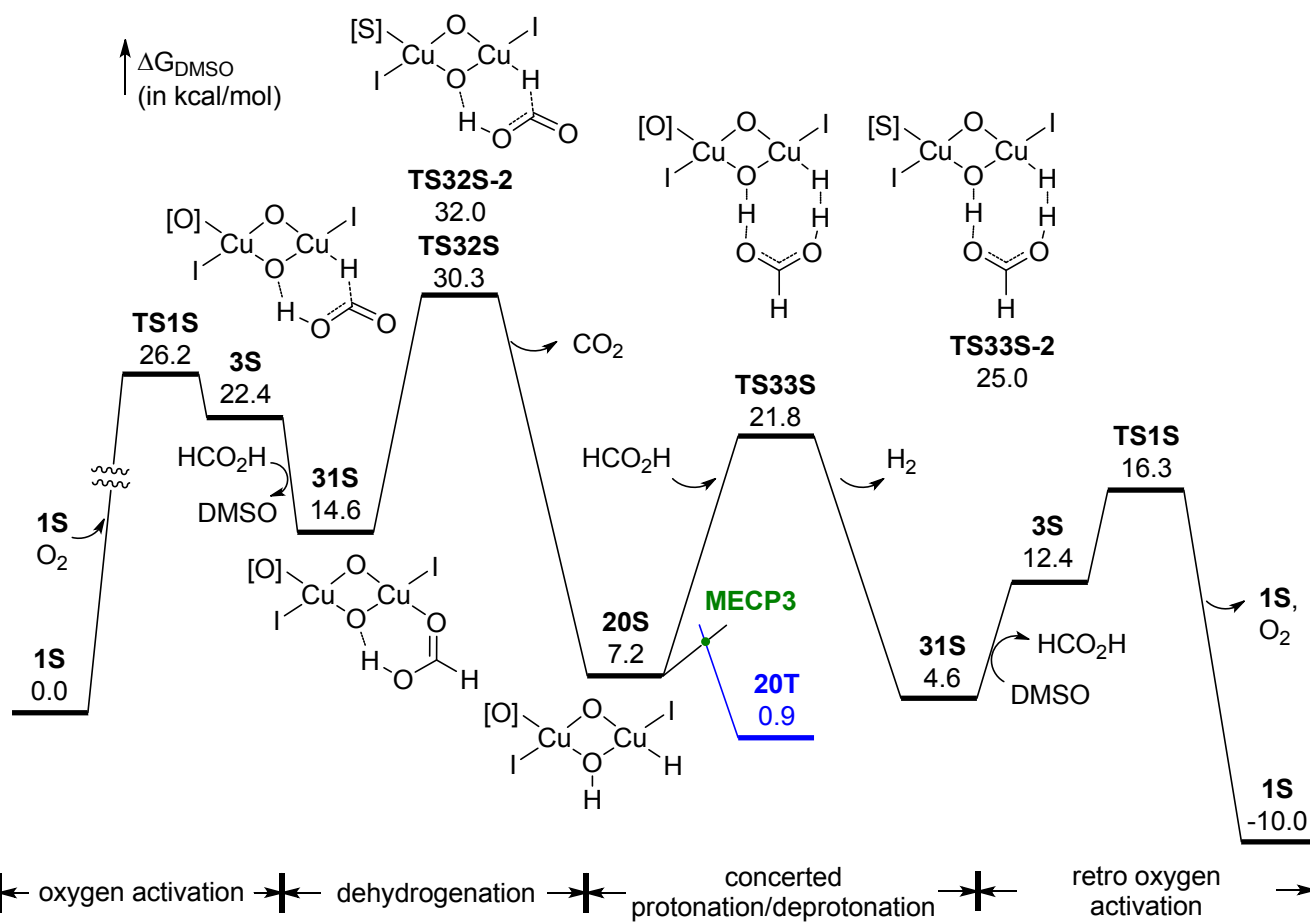


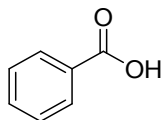
Figure S3. Calculated Gibbs free energy changes of Cu-catalyzed decomposition of formic acid.

Table S10. Calculated relative solution-phase Gibbs free energies of the key species in dimeric and monomeric Cu-catalyzed pathways (in kcal/mol).^a

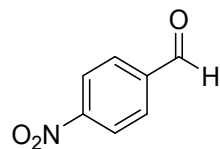
DFT methods used for solution-phase single-point energies	key transition states of dimeric Cu-catalyzed pathway				key intermediates of monomeric Cu-catalyzed pathway		
	TS2S	TS2T	TS6S	TS22S	31D + int5 + HOO·	32S	32T
<i>pure functionals</i>							
BLYP-D3	34.8	56.5	31.2	32.4	63.7	38.1	40.1
BP86-D3	25.4	34.5	22.6	23.7	61.0	34.9	38.1
M06-L-D3	32.7	38.1	28.3	24.0	66.4	45.1	43.2
BB95	41.1	49.6	38.5	34.0	66.9	41.0	44.1
B97D-D3	53.5	56.5	50.8	44.9	71.5	45.2	45.7
M11L	30.4	16.4	31.6	19.2	51.7	43.3	36.0
PBE-D3	30.2	39.1	28.1	27.4	62.1	37.1	39.5
TPSS-D3	25.8	34.1	22.4	22.3	61.6	37.7	38.3
<i>hybrid functionals</i>							
B3LYP-D3	59.7	47.4	58.1	52.9	64.4	53.5	46.1
CAM-B3LYP	84.7	57.9	83.4	74.0	67.8	68.4	52.5
M06	76.2	61.9	74.5	61.9	75.1	60.1	53.0
TPSS-h	50.5	48.6	49.6	43.8	65.1	49.9	44.8
TPSS-h-D3	41.7	40.1	39.5	36.0	63.2	46.8	42.7
ωB97X-d	90.3	63.5	88.3	78.1	71.0	68.8	55.3

^aThermodynamic corrections to Gibbs free energy were calculated by using methods for geometry optimization. Solution-phase single-point energies were calculated based on TPSS-h-optimized structures by different functionals and def2-TZVP basis set except that Cu and I atoms were described by SDD and the effective core potential.

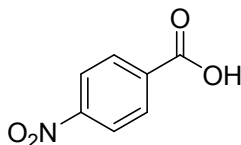
The energy barriers are significantly impacted by computational methods but this phenomenon is not surprising. Tables S3-S8 show that the pure functionals give better performances than hybrid functionals at reproducing the reference values. Interestingly, the methods having better performances in Tables S3-S8, such as pure functionals BLYP-D3, BP86-D3, M06-L-D3, TPSS-D3 and PBE-D3, also predict lower energy barriers for the dimeric Cu-catalyzed pathways in Table S10. The similar trend is found for the performances of hybrid functionals as well.



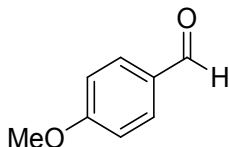
Benzoic acid (pro2).¹³ Eluent petroleum ether/ethyl acetate (5:1). White solid, 41.1 mg, 33.7% yield. ¹H NMR (DMSO-*d*₆, 500 MHz, ppm) δ 12.94 (s, 1H), 7.95 (d, 2H, *J* = 7.1 Hz), 7.61 (t, 1H, *J* = 7.4 Hz), 7.49 (t, 2H, *J* = 7.7 Hz). ¹³C NMR (DMSO-*d*₆, 125 MHz, ppm) δ 167.8, 133.3, 131.2, 129.7, 129.0.



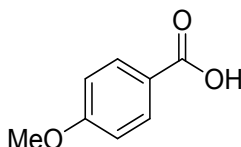
4-Nitrobenzaldehyde (pro1b).¹² Eluent petroleum ether/ethyl acetate (25:1). White solid, 56.3mg, 37.3% yield. ¹H NMR (DMSO-*d*₆, 500 MHz, ppm) δ 10.15 (s, 1H), 8.38 (d, 2H, *J* = 8.7 Hz), 8.14 (d, 2H, *J* = 8.7 Hz). ¹³C NMR (DMSO-*d*₆, 125 MHz, ppm) δ 192.7, 151.0, 140.5, 131.1, 124.7.



4-Nitrobenzoic acid (pro2b).¹³ Eluent petroleum ether/ethyl acetate (5:1). Yellow solid, 42.8mg, 25.6% yield. ¹H NMR (DMSO-*d*₆, 500 MHz, ppm) δ 8.27 (d, 2H, *J* = 8.8 Hz), 8.13 (d, 2H, *J* = 8.8 Hz). ¹³C NMR (DMSO-*d*₆, 125 MHz, ppm) δ 166.2, 150.4, 136.8, 131.1, 124.1.

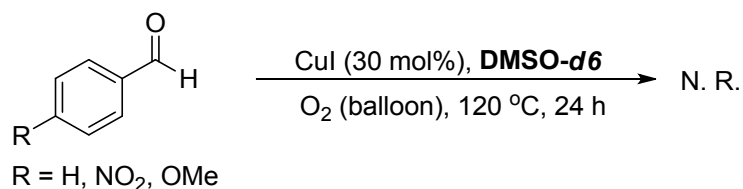


4-Methoxybenzaldehyde (pro1c).¹² Eluent petroleum ether/ethyl acetate (25:1). Yellow oil, 50.6 mg, 37.2% yield. ¹H NMR (CDCl₃, 500 MHz, ppm) δ 9.82 (s, 1H), 7.78 (d, 2H, *J* = 8.9 Hz), 6.95 (d, 2H, *J* = 8.9 Hz), 3.82 (s, 3H). ¹³C NMR (CDCl₃, 125 MHz, ppm) δ 190.8, 164.6, 131.9, 129.9, 114.3, 55.5.



4-Methoxybenzoic acid (pro2c).¹⁴ Eluent petroleum ether/ethyl acetate (5:1). White solid, 64.5 mg, 42.4% yield. ¹H NMR (CDCl₃, 500 MHz, ppm) δ 8.07 (d, 2H, *J* = 8.8 Hz), 6.95 (d, 2H, *J* = 8.8 Hz), 3.88 (s, 3H). ¹³C NMR (DMSO-*d*₆, 125 MHz, ppm) δ 167.5, 163.3, 131.8, 123.4, 114.3, 55.9.

III. General procedure of Cu-catalyzed oxidation of aldehydes



A solution of aldehydes (1.0 mmol) and CuI (0.3 mmol, 57 mg) in DMSO-*d*₆ (3.0 mL) under oxygen atmosphere (oxygen balloon) was prepared. The reaction mixture was heated to 120 °C for 24 h. Upon cooling to room temperature, the reaction mixture was then directly analyzed ¹H-NMR spectra, no other product was generated in the present conditions.

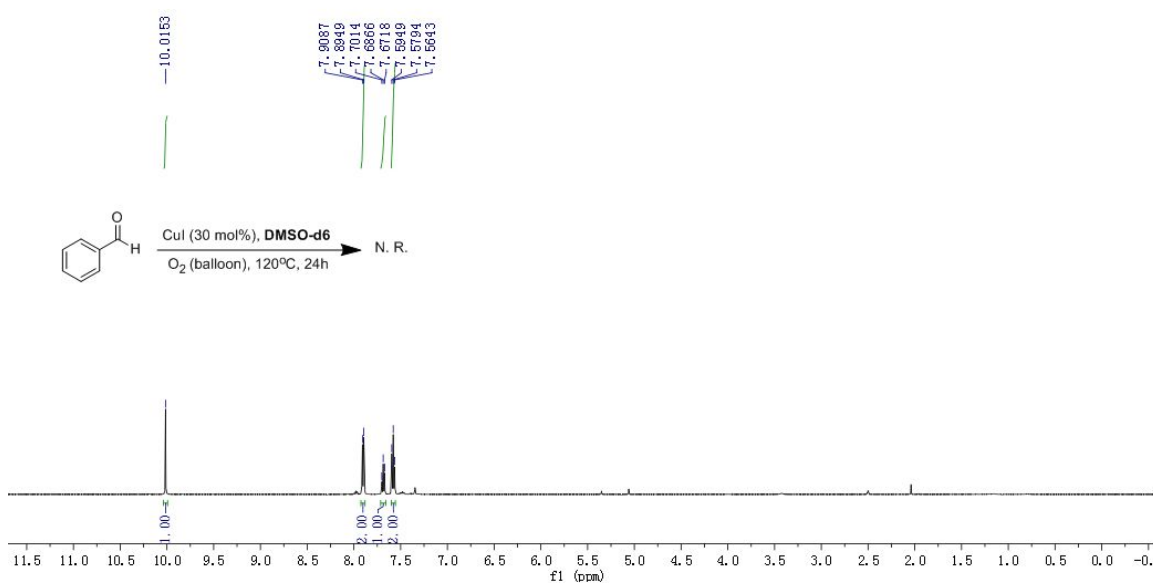


Figure S4. H-NMR spectra of the reaction mixture of compound **pro1**

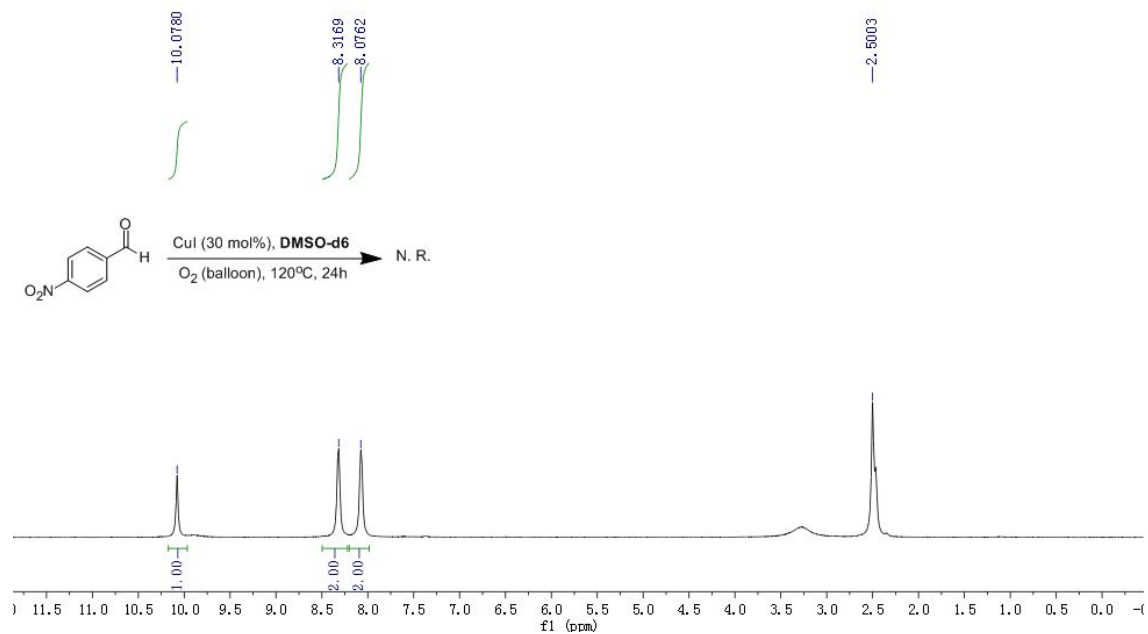


Figure S5. H-NMR spectra of the reaction mixture of compound **pro1b**

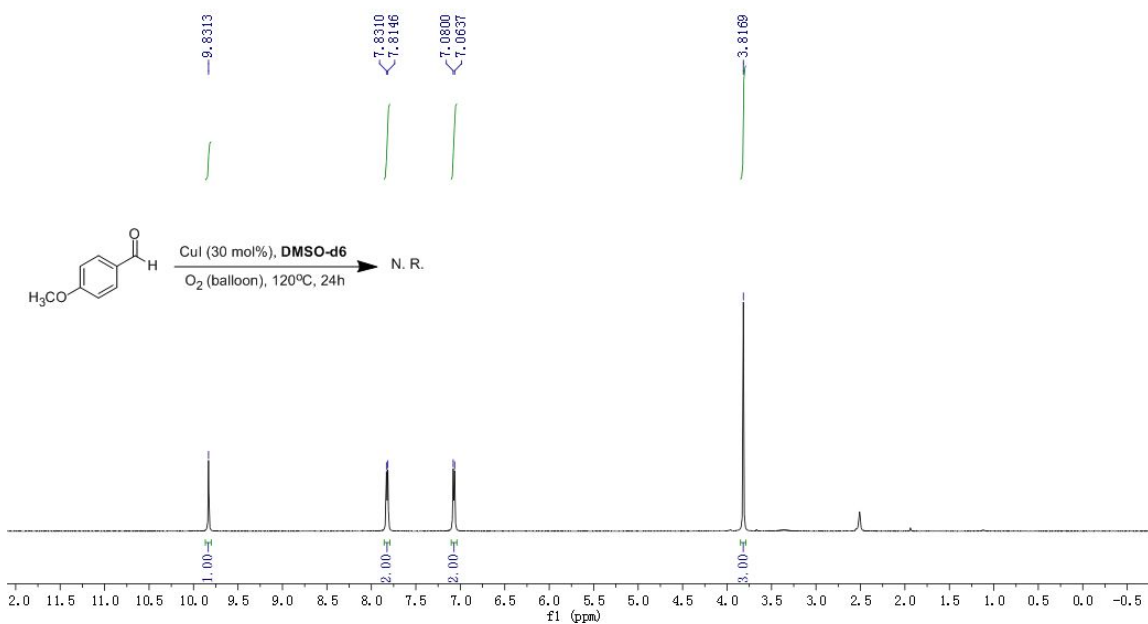
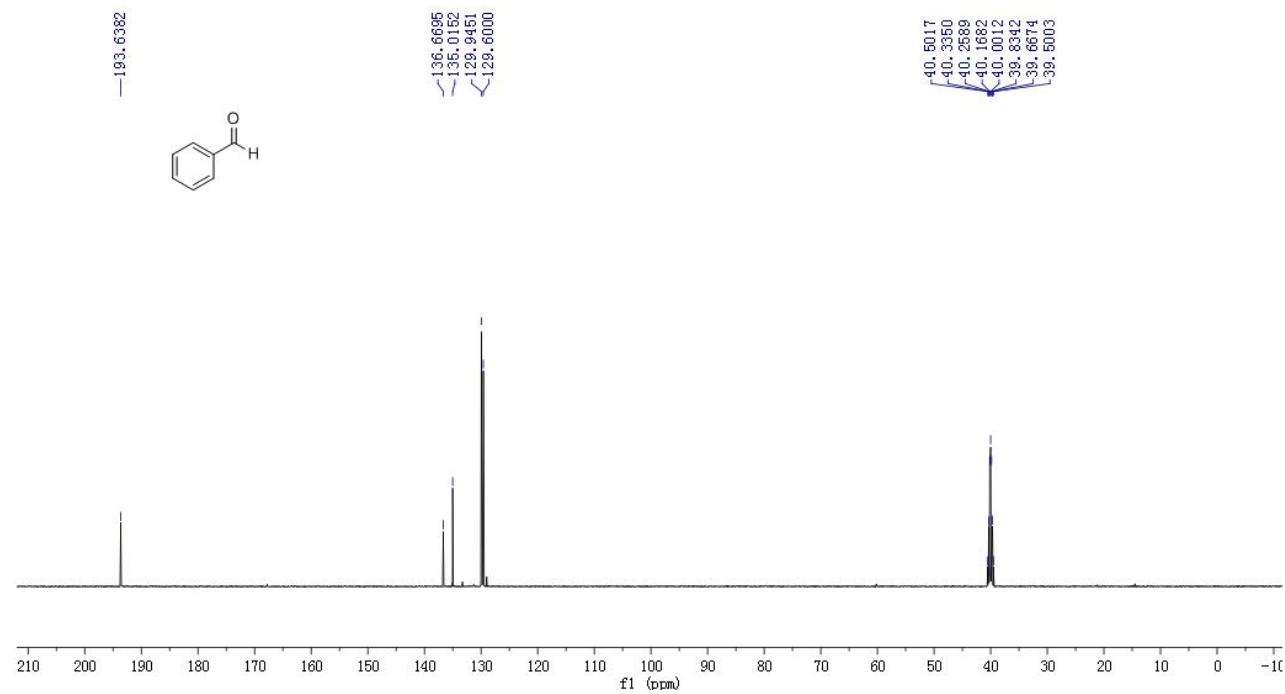
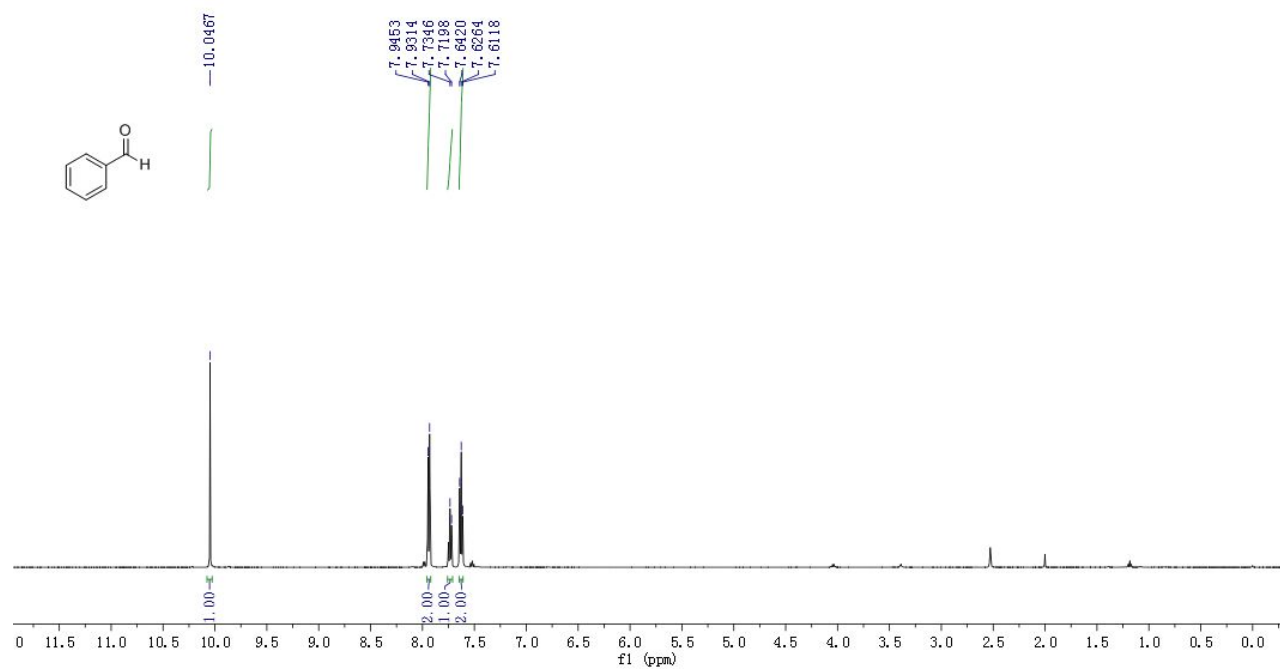
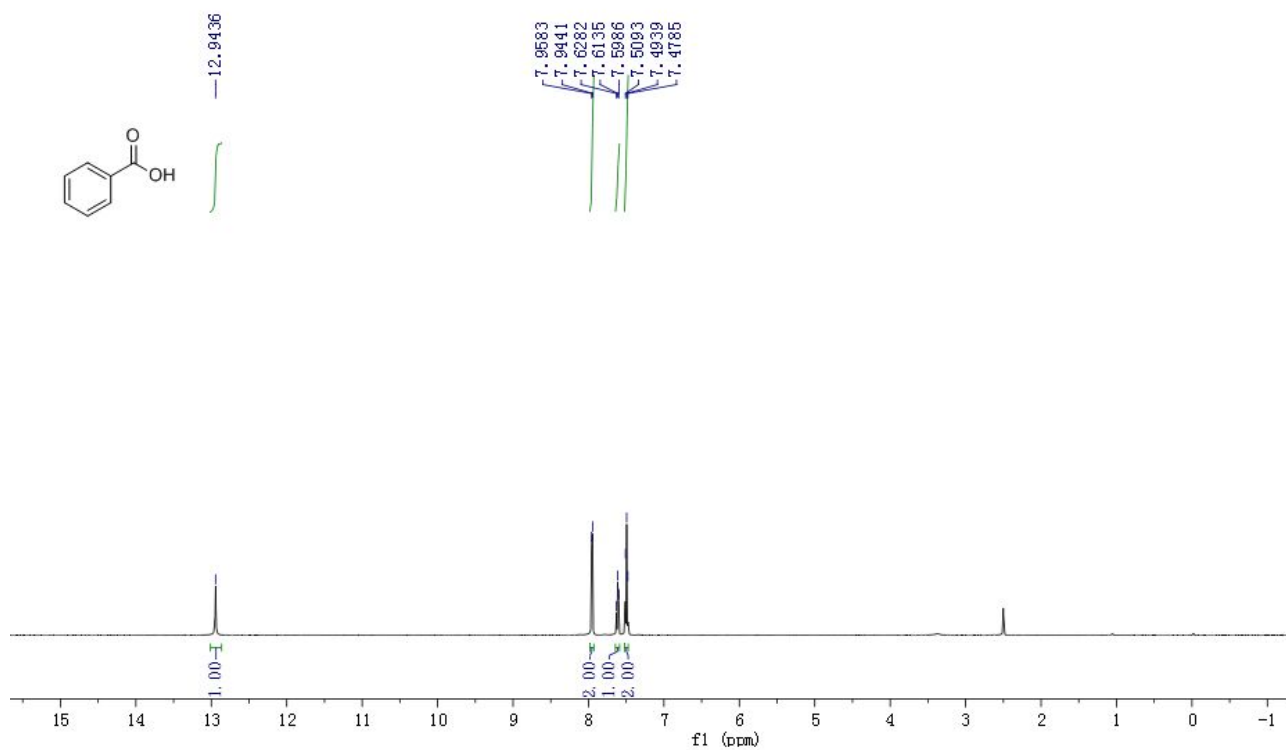
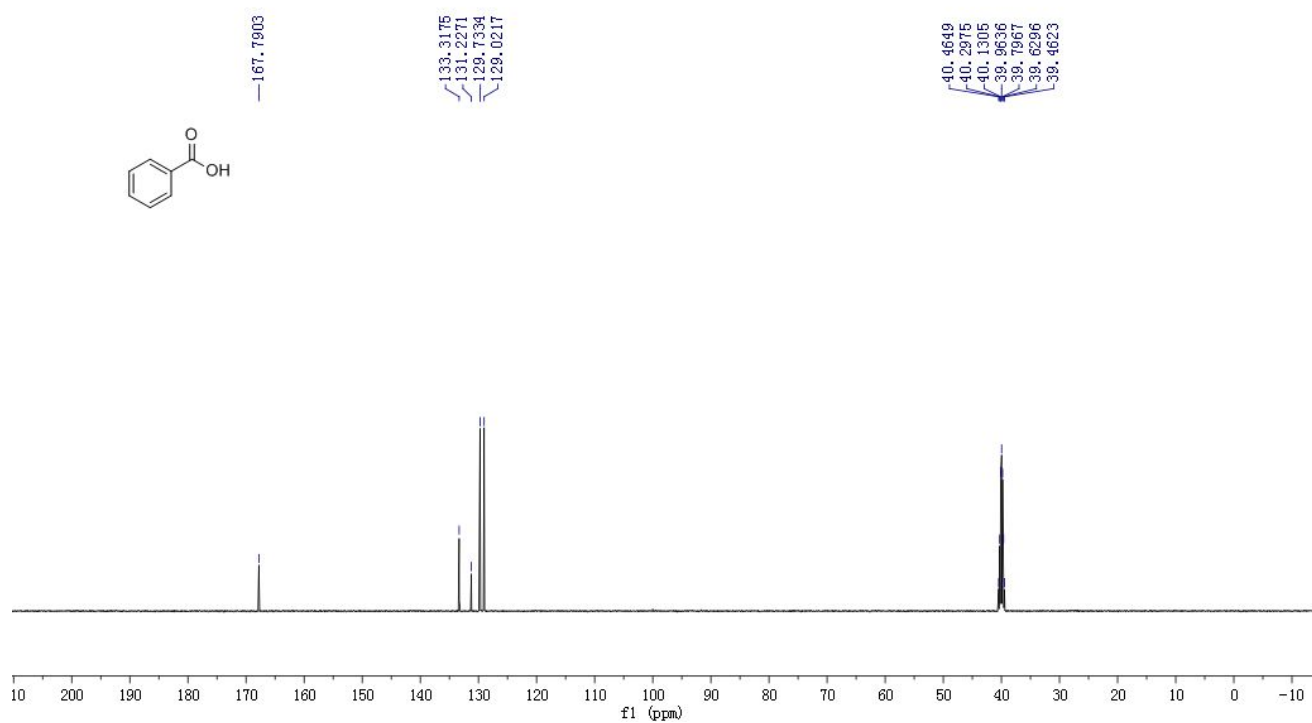


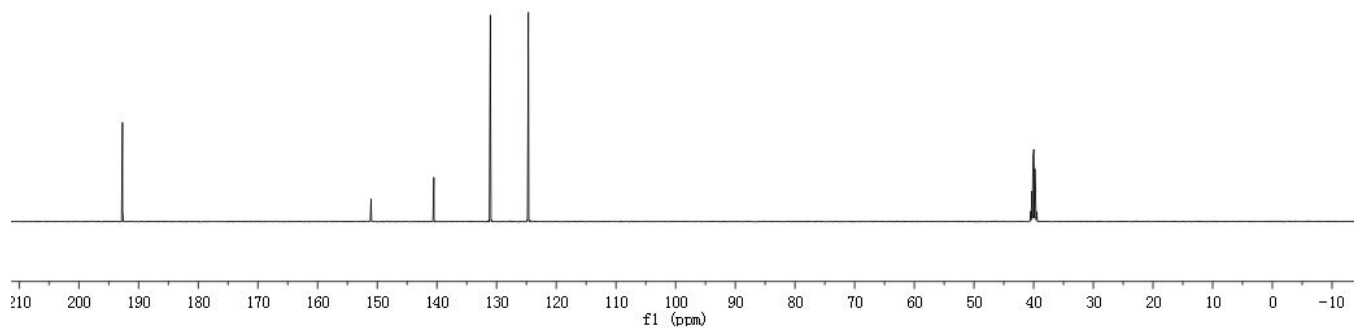
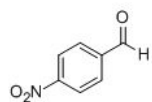
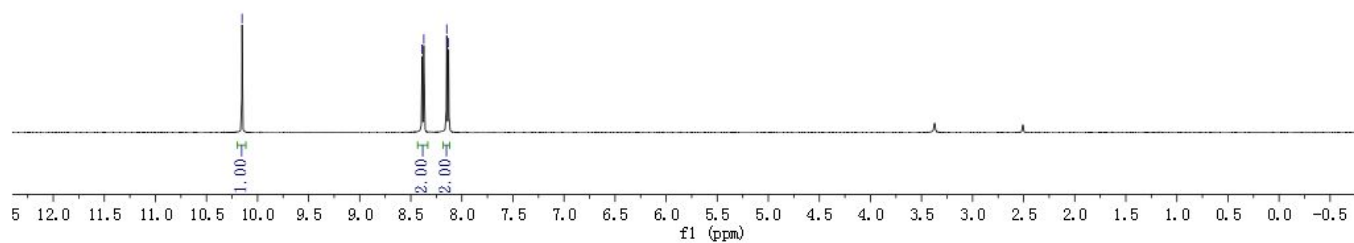
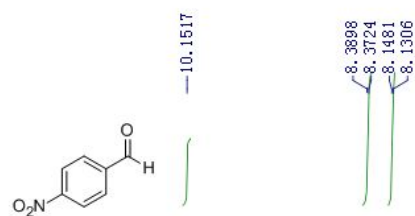
Figure S6. H-NMR spectra of the reaction mixture of compound **pro1c**

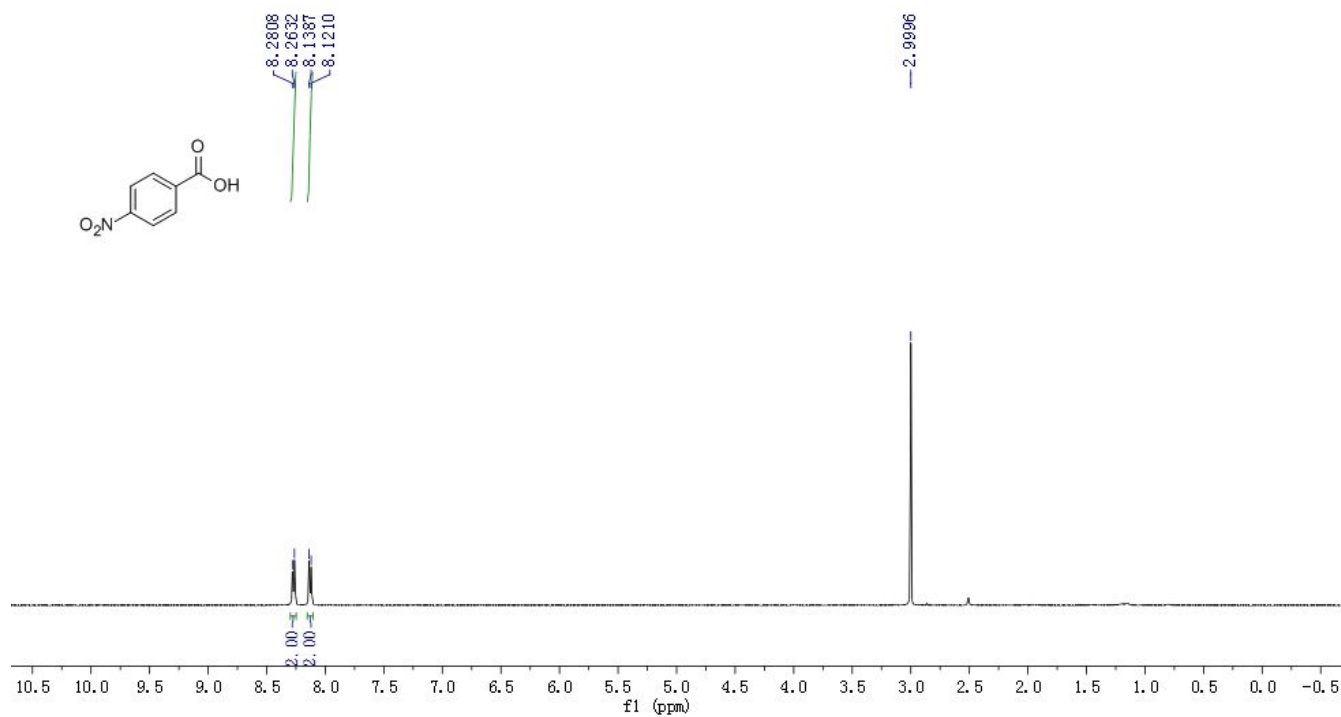
IV. ^1H - and ^{13}C -NMR Spectra Copies

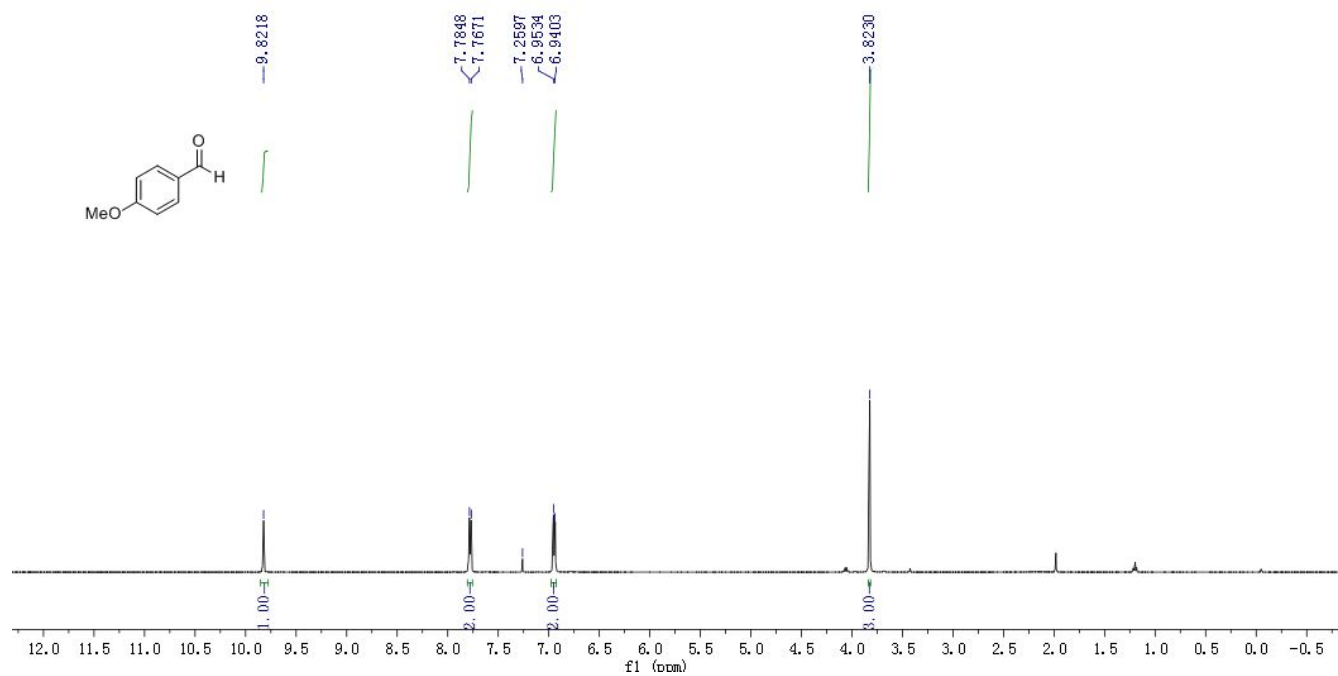
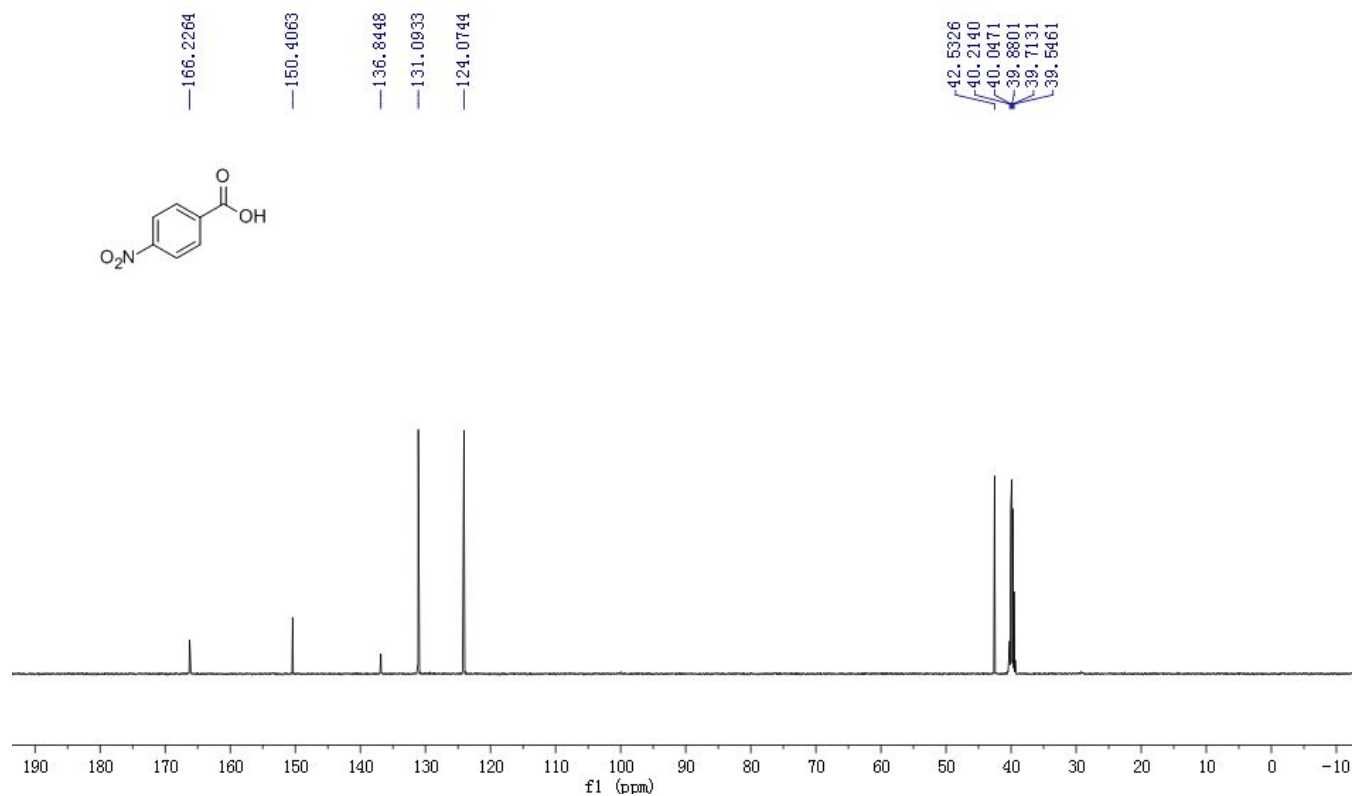


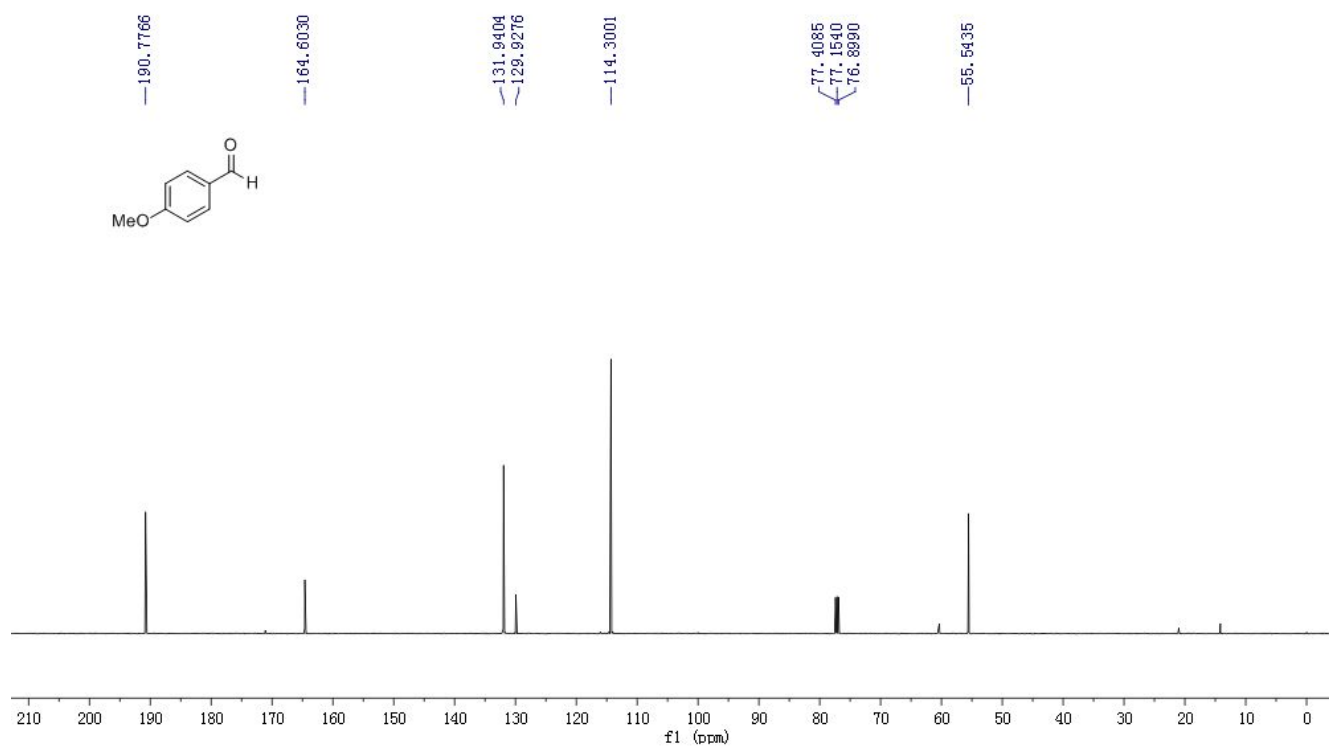












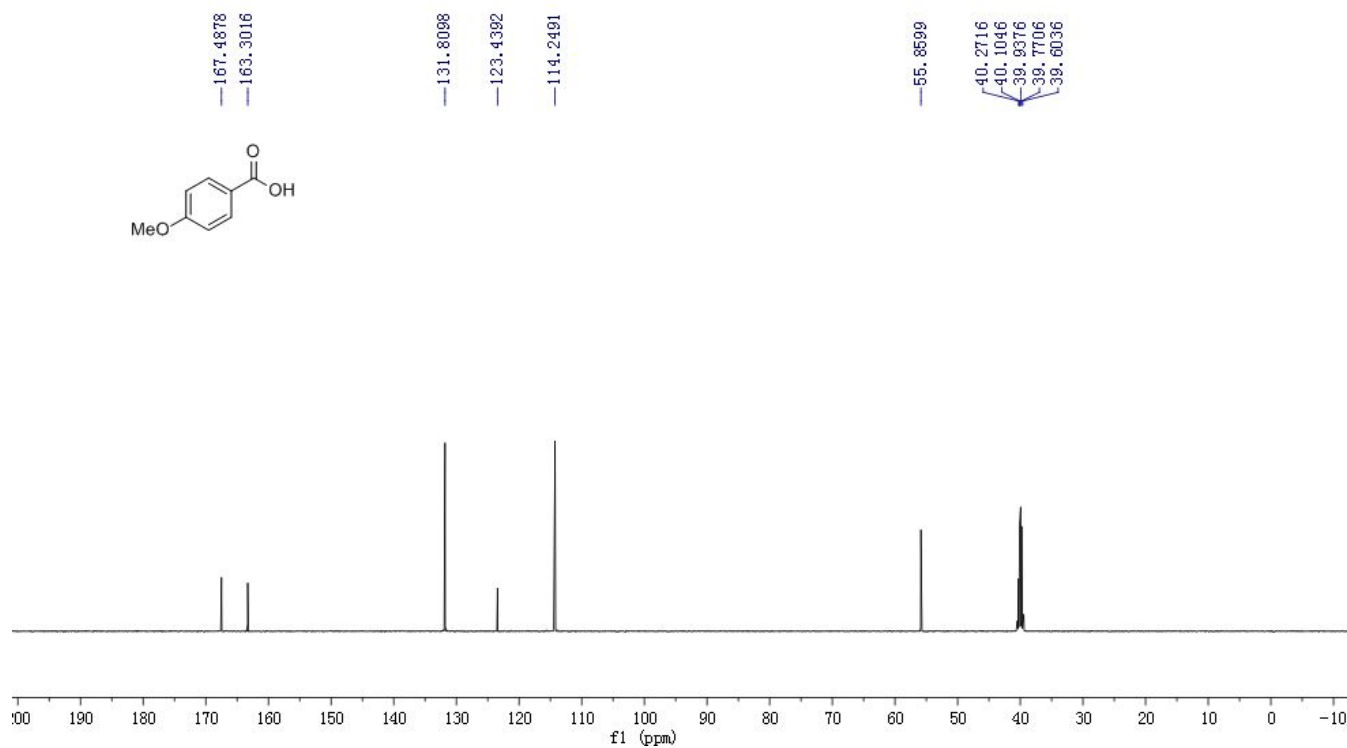
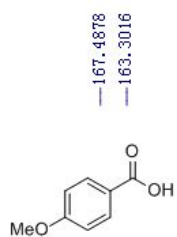
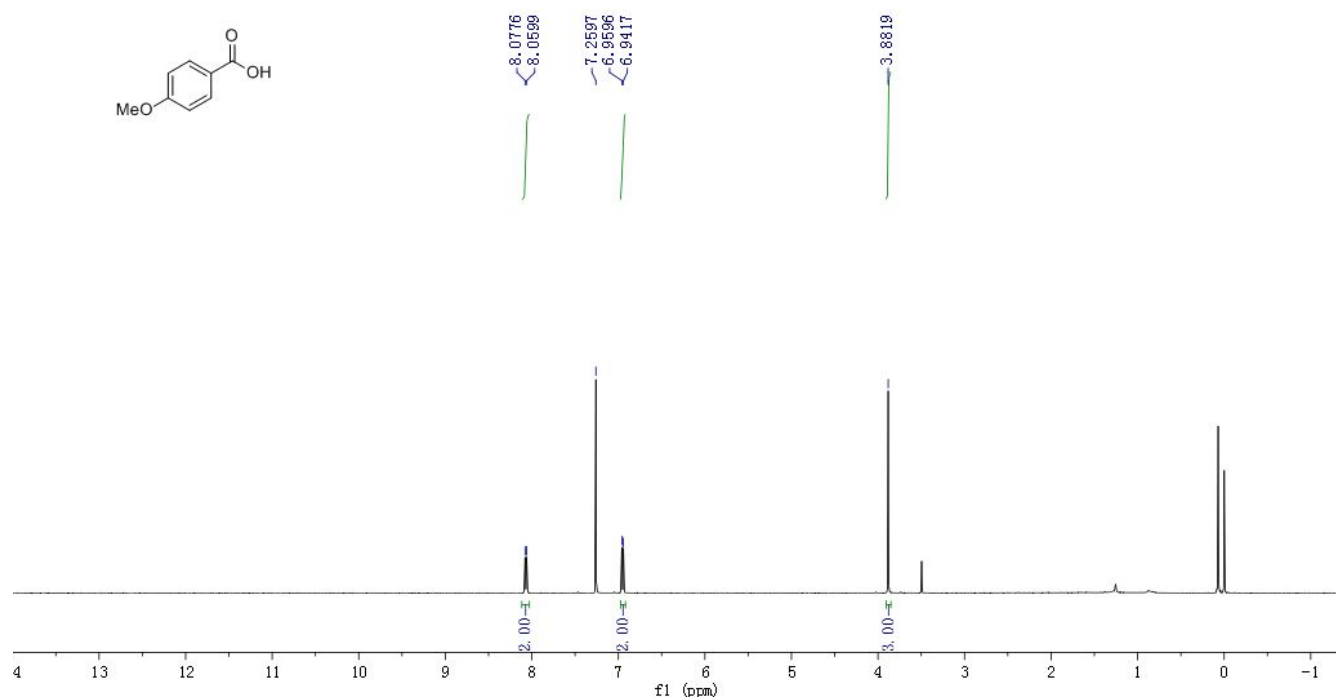
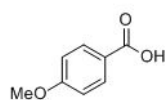


Table S11. Calculated thermodynamic corrections ΔG_{cor} , solution-phase single-point energies ΔE_{sol} and solution-phase Gibbs free energies ΔG_{sol} referring to 1 M at 298.15 K of located stationary points (in hartree)

	ΔG_{cor}	ΔE_{sol}	ΔG_{sol}
O ₂	-0.016266	-150.3989775	-150.4122156
DMSO	0.051532	-553.2445654	-553.1900055
CuI	-0.024739	-208.7729883	-208.7946994
sub1	0.105439	-384.9150532	-384.8065864
1S	0.042868	-762.0520824	-762.0061865
1S-2	0.043759	-762.0526538	-762.0058669
1S-3	0.115536	-1315.305678	-1315.187114
1S-4	0.114121	-1315.305096	-1315.187947
1S-6	0.112104	-1315.300225	-1315.185093
1S-7	0.097179	-593.7178449	-593.617638
1S-8	0.216571	-978.6359795	-978.4163806
1S-9	0.043582	-912.4179477	-912.3713379
1S-10	0.046081	-912.4322467	-912.3831378
1S-11	0.046311	-912.4369989	-912.3876601
1S-13	0.049147	-750.4466202	-750.3944454
1S-14	0.048176	-750.4435374	-750.3923336
1S-15	0.117192	-1303.71256	-1303.59234
1S-16	0.117128	-1303.724128	-1303.603972
1S-17	0.226444	-967.0584276	-966.8289557
1S-19	0.043103	-837.2208768	-837.1747459
1T	0.038981	-912.4512022	-912.4091933
1T-2	0.039247	-912.4460485	-912.4037736
1T-3	0.04251	-912.4461256	-912.4005878
1T-4	0.041499	-912.4432524	-912.3987255
1T-5	0.092745	-744.1189907	-744.0232179
1T-6	0.161802	-1297.371839	-1297.207009
1T-7	0.16272	-1297.374782	-1297.209034
1T-8	0.04581	-900.846664	-900.7978262
1T-9	0.045373	-900.8381538	-900.789753
1T-10	0.09856	-732.5117675	-732.4101797
1T-11	0.165299	-1285.790799	-1285.622472
1T-12	0.04221	-837.2139811	-837.1687432
2S	0.108755	-1674.506852	-1674.395069
2S-2	0.107525	-1674.504135	-1674.393582
2S-3	0.106188	-1674.500988	-1674.391772

2S-4	0.108046	-1674.507939	-1674.396865
2S-5	0.10831	-1674.50292	-1674.391582
2S-6	0.108894	-1674.506265	-1674.394343
2S-7	0.25191	-2781.018275	-2780.763337
2S-8	0.254582	-2781.015471	-2780.757861
2S-9	0.249692	-2781.022124	-2780.769404
2S-10	0.100751	-1883.312111	-1883.208332
2S-11	0.174217	-2436.571727	-2436.394482
2T	0.107625	-1674.513051	-1674.402398
TS1S	0.111646	-1674.497438	-1674.382764
TS1S-2	0.109717	-1674.489102	-1674.376357
TS1S-3	0.110715	-1674.489102	-1674.375359
TS1BS	0.111646	-1674.497438	-1674.382764
3S	0.111686	-1674.503608	-1674.388894
3S-2	0.112809	-1674.501915	-1674.386078
3T	0.107652	-1674.486664	-1674.375985
4S	0.165945	-1506.173346	-1506.004373
4T	0.161172	-1506.152419	-1505.988219
TS2S	0.16175	-1506.15042	-1505.985642
TS2S-2	0.161236	-1506.148129	-1505.983865
TS2T	0.159442	-1506.135909	-1505.973439
TS2BS	0.161762	-1506.15042	-1505.98563
TS2BS-2	0.159516	-1506.130519	-1505.967975
5S	0.164626	-1506.202519	-1506.034865
5S-2	0.163236	-1506.202203	-1506.035939
6S-2	0.164697	-1506.164624	-1505.996899
TS3S	0.166121	-1506.163536	-1505.994387
TS-OAT-S	0.168000	-1506.160721	-1505.989693
6S-3	0.169567	-1506.162219	-1505.989624
TS-Shift-S	0.162172	-1506.125844	-1505.960644
5S-3	0.166461	-1506.228984	-1506.059495
int1	0.108964	-460.1612751	-460.0492833
7S	0.036024	-1046.038696	-1045.999644
7S-2	0.037873	-1046.036123	-1045.995222
7T	0.033353	-1046.052167	-1046.015786
8Q	0.09462	-2092.143892	-2092.046245
8S	0.099617	-2092.142539	-2092.039894
9S	0.172852	-1581.423905	-1581.248026
TS4S	0.167862	-1581.399947	-1581.229058

TS4S-2	0.167201	-1581.393089	-1581.22286
10S	0.170243	-1581.431148	-1581.257877
TS5S	0.171075	-1581.428489	-1581.254386
int3	0.111986	-535.4157946	-535.3007807
TS6S	0.168811	-1581.40605	-1581.234212
TS6S-2	0.168098	-1581.402439	-1581.231313
11S	0.170836	-1581.425138	-1581.251274
TS7S	0.169114	-1581.413592	-1581.24145
TS7S-2	0.169745	-1581.407285	-1581.234512
12S	0.165229	-1581.433771	-1581.265514
TS8S	0.161939	-1581.38708	-1581.222113
TS8S-2	0.164868	-1581.38972	-1581.221824
int2	0.084214	-458.9492266	-458.8619847
H ₂ O	0.003356	-76.4530643	-76.44668046
13S	0.175711	-1656.676508	-1656.497769
TS9S	0.17225	-1656.662178	-1656.486901
TS9S-2	0.171135	-1656.657812	-1656.483649
TS10S	0.167092	-1656.656681	-1656.486561
TS10S-2	0.169249	-1656.648282	-1656.476006
30S	0.172678	-1656.724284	-1656.548578
14S	0.175689	-1656.681039	-1656.502322
TS11S	0.168071	-1656.636319	-1656.46522
TS11S-2	0.171189	-1656.633027	-1656.45881
TS12S	0.174385	-1656.668082	-1656.490669
TS12S-2	0.173945	-1656.662093	-1656.48512
15S	0.169835	-1656.69139	-1656.518527
TS13S	0.166364	-1656.657578	-1656.488186
TS13S-2	0.166531	-1656.651673	-1656.482114
TS13T	0.165891	-1656.655564	-1656.486645
16S	0.170555	-1656.705509	-1656.531926
TS14S	0.165845	-1656.665656	-1656.496783
17S	0.166929	-1656.707331	-1656.537374
pro1	0.079371	-345.6013055	-345.5189067
18S	0.067869	-1311.098096	-1311.027199
TS15S	0.068456	-1311.094645	-1311.023161
TS16S	0.129354	-1864.306819	-1864.174437
TS16S-2	0.058368	-1311.039912	-1310.978516
H ₂ CO ₃	0.012973	-265.0989299	-265.0829291
TS31S	0.172328	-1656.665935	-1656.49058

TS31S-2	0.172198	-1656.646619	-1656.471393
TS31T	0.172702	-1656.662734	-1656.487004
TS31T-2	0.172536	-1656.659119	-1656.483556
19S	0.176146	-1656.679905	-1656.500731
TS17S	0.165332	-1656.657597	-1656.489237
TS17S-2	0.165133	-1656.656168	-1656.488008
int4	0.090331	-534.2386182	-534.1452593
20S	0.057935	-1122.434703	-1122.37374
20T	0.052525	-1122.439247	-1122.383694
TS18T	0.16236	-1656.668455	-1656.503067
TS18T-2	0.161353	-1656.663059	-1656.498678
21T	0.166184	-1656.676925	-1656.507713
TS19T	0.165291	-1656.678135	-1656.509816
TS19T-2	0.165667	-1656.673804	-1656.505109
CO₂	-0.009206	-188.656552	-188.6627302
TS20S	0.162761	-1581.39832	-1581.232531
TS20S-2	0.161971	-1581.394756	-1581.229757
TS21T	0.156935	-1581.379324	-1581.219362
TS21T-2	0.156015	-1581.374421	-1581.215378
H₂	-0.001241	-1.16827612	-1.16648928
TS22S	0.163858	-1581.399094	-1581.232208
TS22S-2	0.164179	-1581.393341	-1581.226134
TS22T	0.163767	-1581.397809	-1581.231014
TS22T-2	0.163116	-1581.393052	-1581.226908
22S	0.166394	-1581.421428	-1581.252006
TS23S	0.161767	-1581.381294	-1581.216499
TS24S	0.166797	-1581.411448	-1581.241624
TS24S-2	0.166865	-1581.40693	-1581.237037
23S	0.165765	-1581.420738	-1581.251945
23T	0.166155	-1581.419327	-1581.250144
TS25S	0.163317	-1581.388908	-1581.222563
24T	0.164696	-1581.416397	-1581.248673
TS26S	0.169314	-1581.391318	-1581.218976
TS26S-2	0.165844	-1581.387954	-1581.219082
TS26T	0.164093	-1581.399532	-1581.232411
TS26T-2	0.166261	-1581.380009	-1581.21072
TS26T-3	0.235282	-2134.647999	-2134.409689
HCOOH	0.009662	-189.8259955	-189.8133056
31S	0.071664	-1311.099295	-1311.024603

TS32S	0.064584	-1311.067292	-1310.99968
TS32S-2	0.063381	-1311.063336	-1310.996927
TS33S	0.082438	-1312.249262	-1312.163796
TS33S-2	0.082909	-1312.244484	-1312.158547
int1b	0.106658	-664.7554698	-664.645784
TS4Sb	0.166095	-1785.992699	-1785.823577
TS6Sb	0.166145	-1785.999047	-1785.829875
TS22Sb	0.161465	-1785.996011	-1785.831518
TS26Tb	0.162082	-1785.996792	-1785.831682
TS29Tb	0.163906	-1785.99314	-1785.826206
int3b	0.109789	-740.0093466	-739.8965298
TS17Sb	0.163203	-1861.250469	-1861.084238
TS9Sb	0.169737	-1861.253836	-1861.081072
TS27Sb	0.16374	-1861.251579	-1861.084811
int1c	0.138507	-574.7104086	-574.5688737
TS4Sc	0.197189	-1695.950921	-1695.750704
TS6Sc	0.198771	-1695.95675	-1695.754951
TS22Sc	0.192931	-1695.945428	-1695.749469
TS26Tc	0.195118	-1695.939828	-1695.741683
TS29Tc	0.195014	-1695.943687	-1695.745645
int3c	0.141513	-649.9655471	-649.8210062
TS9Sc	0.20217	-1771.213594	-1771.008396
TS17Sc	0.195079	-1771.207979	-1771.009872
TS27Sc	0.195609	-1771.210284	-1771.011647
O₂⁻	-0.017123	-150.5028548	-150.51695
31D	0.110039	-1315.130416	-1315.017349
31D-2	0.113984	-1315.123923	-1315.006911
31D-3	0.112119	-1315.128539	-1315.013392
31D-4	0.16474	-1146.7955	-1146.627732
31D-5	0.167021	-1146.79706	-1146.627011
31D-6	0.042185	-761.8588412	-761.8136283
Int5	0.088973	-384.4011166	-384.3091157
HOO·	-0.008321	-150.981756	-150.9870491
32S	0.098591	-744.0758783	-743.9742595
32T	0.09336	-744.0674026	-743.9710147
1D	0.037764	-773.4613923	-773.4206005
8q	0.180659	-2425.174636	-2424.990949

Table S12. Calculated electronic energies ΔE for spin crossover processes (in hartree)^a

	ΔE
7S	-1043.434305
MECP1 in singlet state	-1043.413764
MECP1 in triplet state	-1043.413765
8Q	-2086.928096
MECP2 in quartet state	-2086.912957
MECP2 in singlet state	-2086.912951
20S	-1119.777018
MECP3 in singlet state	-1119.775842
MECP3 in triplet state	-1119.775842
23S	-1578.742154
MECP4 in singlet state	-1578.741164
MECP4 in triplet state	-1578.741191
12S	-1578.755428
MECP5 in singlet state	-1578.741168
MECP5 in triplet state	-1578.741193

^aMECPs were located with the method used for geometry optimization. The electronic barriers of spin crossover were calculated by using the energies of the MECPs in the same spin states with the **7S**, **8Q**, **20S**, **23S** and **12S**, respectively.

Cartesian coordinates of all located stationary points and MECPs (in angstrom)

O₂				C	1.96482900	-1.14117700	-0.00022200
O	0.00000000	0.00000000	0.60910500	H	3.67843900	0.17345800	-0.00006500
O	0.00000000	0.00000000	-0.60910500	H	2.31351500	2.25015200	0.00033000
DMSO				H	-0.15402700	2.11325500	0.00041900
S	-0.25766800	0.43295500	0.00000000	H	0.06083200	-2.17746300	-0.00034900
O	1.09301000	1.11434800	0.00000000	H	2.56156300	-2.04924000	-0.00039500
C	-0.25766800	-0.80495900	-1.35651500	C	-1.69692100	-0.20185600	0.00006400
H	-0.21215800	-0.24900400	-2.29590600	O	-2.21182200	-1.31479100	0.00045400
H	0.62481200	-1.44522900	-1.26531400	C	-2.56148700	1.04953200	-0.00041300
H	-1.17733800	-1.39704800	-1.31891500	H	-2.35947200	1.66713700	0.88325900
C	-0.25766800	-0.80495900	1.35651500	H	-2.35963400	1.66638100	-0.88464900
H	-1.17733800	-1.39704800	1.31891500	H	-3.61035800	0.74862900	-0.00019300
H	0.62481200	-1.44522900	1.26531400	1S-2			
H	-0.21215800	-0.24900400	2.29590600	I	2.27480300	-0.00014100	-0.05781300
CuI				Cu	-0.12641100	0.00080300	0.22639400
Cu	0.00000000	0.00000000	-1.55209600	S	-2.39628800	0.00025500	0.17016700
I	0.00000000	0.00000000	0.84926000	C	-2.89636000	-1.37787100	-0.90810100
1S				H	-3.97361100	-1.31355700	-1.08556500
I	2.35438700	0.14516600	-0.05590000	H	-2.33331200	-1.32413100	-1.84412600
Cu	0.03032700	-0.50036000	0.15823400	H	-2.65876100	-2.30299800	-0.37905700
S	-2.79662400	0.09585400	-0.50536100	C	-2.89808700	1.37427500	-0.91249000
C	-4.45195000	-0.45325800	0.00665100	H	-3.97522300	1.30789600	-1.08988900
H	-4.50490400	-0.45040200	1.09824800	H	-2.66189300	2.30136900	-0.38626200
H	-5.20143500	0.21187200	-0.43129000	H	-2.33485500	1.31847000	-1.84828100
H	-4.58185900	-1.46797900	-0.37465100	O	-3.23171300	0.00182800	1.41658900
C	-2.78656400	1.71206300	0.33521200	1S-3			
H	-2.98586200	1.56691600	1.40023300	Cu	0.04379000	-0.57893200	0.00002200
H	-1.78896700	2.13453000	0.19272000	I	-2.42634900	-0.72563100	-0.00040700
H	-3.53845600	2.35859000	-0.12693600	S	2.28593700	-1.22495600	0.00041000
O	-1.86043100	-0.82791800	0.33127100	O	2.71465400	-2.66536500	0.00050100
sub1				C	3.09609600	-0.33395200	1.36661300
C	2.59353600	0.11011600	-0.00003600	C	3.09655500	-0.33398900	-1.36554600
C	1.82659000	1.27885500	0.00018900	H	2.67215400	-0.70923800	2.30049100
C	0.43241800	1.19884900	0.00023800	H	4.16748300	-0.55195300	1.33028200
C	-0.20615400	-0.05225200	0.00004200	H	2.90510000	0.73765400	1.24355000
C	0.57447400	-1.22106300	-0.00019300	H	2.90551700	0.73762000	-1.24257700
				H	4.16792900	-0.55198900	-1.32885000
				H	2.67292600	-0.70930200	-2.29955600

S	0.46813500	1.97208600	0.00005400
O	1.86218400	2.58380600	0.00028600
C	-0.49774500	2.68147900	1.37202200
C	-0.49726500	2.68142700	-1.37227900
H	-0.00261300	2.38611500	2.29946300
H	-0.50932700	3.77083500	1.27997700
H	-1.50403600	2.25478200	1.33233000
H	-1.50357200	2.25473700	-1.33292100
H	-0.50887200	3.77078700	-1.28028300
H	-0.00181100	2.38602200	-2.29953700

1S-4

Cu	0.26730300	-0.53184200	0.00064000
I	-2.09217700	-1.30795700	-0.06446500
S	2.57554000	-0.86671500	0.07083700
O	3.32567700	-2.16608200	0.17879700
C	3.16131800	0.27830700	1.36343800
C	3.19483600	0.07123200	-1.36481200
H	2.89976500	-0.16751000	2.32563800
H	4.24702200	0.38584300	1.28545600
H	2.64312400	1.23177500	1.23125400
H	2.68551300	1.03813700	-1.38231900
H	4.28002100	0.18090500	-1.28271200
H	2.94494400	-0.50740300	-2.25677500
O	0.59904700	1.59907300	-0.04485900
S	-0.68392300	2.40485100	-0.39277000
C	-1.67568100	2.46584300	1.13091200
C	-0.11703200	4.13723200	-0.38047000
H	-2.05529200	1.45219600	1.28708900
H	-1.03956900	2.78020300	1.96301300
H	-2.50657800	3.16168100	0.98029800
H	-0.97913700	4.79876500	-0.50652400
H	0.40056100	4.34245100	0.56032900
H	0.56891300	4.25830300	-1.22162400

1S-6

Cu	0.00002600	-0.47215400	0.01115100
I	-0.00073100	2.04552500	-0.14441900
O	1.65295100	-1.68227700	0.10750300
S	2.94119200	-0.96401000	-0.36565100
C	3.42932300	0.16953400	0.97385400

C	4.24620000	-2.21264700	-0.10723400
H	2.67426500	0.96107200	0.99436500
H	3.44315000	-0.37666800	1.92128400
H	4.41334300	0.58802200	0.74108100
H	5.22307500	-1.76360500	-0.30963500
H	4.18674000	-2.58352100	0.91941900
H	4.05472300	-3.02577000	-0.81048700
O	-1.65185400	-1.68251000	0.10659200
S	-2.94053000	-0.96433900	-0.36560300
C	-4.24483000	-2.21390000	-0.10793700
C	-3.42868900	0.16758200	0.97524800
H	-4.05319800	-3.02627700	-0.81200800
H	-4.18470000	-2.58565800	0.91835800
H	-5.22202800	-1.76519300	-0.30950700
H	-4.41309600	0.58571300	0.74350500
H	-3.44156400	-0.37958700	1.92213400
H	-2.67411800	0.95957300	0.99605900

1S-7

I	-3.47370100	-0.05307300	-0.00008600
Cu	-1.06376800	-0.23408500	0.00014500
O	0.84504500	-0.32303500	-0.00105600
C	1.72181900	0.57052300	0.00016100
C	3.13982100	0.17063400	0.00021200
C	1.32905200	2.02661800	0.00104400
C	4.17511500	1.12566400	-0.00040800
C	3.46390000	-1.20133600	0.00059600
H	1.73472100	2.53646300	0.88272300
H	1.72610300	2.53389800	-0.88615700
H	0.23951900	2.11386100	0.00587200
C	5.50700100	0.71523300	-0.00069600
H	3.94323500	2.18626300	-0.00089600
C	4.79490300	-1.60575700	0.00046200
H	2.65788600	-1.92738800	0.00100600
C	5.81775300	-0.64872300	-0.00019700
H	6.30130600	1.45551300	-0.00129100
H	5.03953600	-2.66369700	0.00084000
H	6.85656600	-0.96644100	-0.00031500

1S-8

I	0.00039300	-3.44797400	-0.27171300
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Cu	-0.00017000	-0.96535400	-0.12082500
O	-1.51171000	0.43573700	-0.02967400
C	-2.70311000	0.32752400	0.31084100
C	-3.60425300	1.49588500	0.14667700
C	-3.22868400	-0.96351400	0.88847800
C	-4.95011800	1.45974900	0.55418100
C	-3.09045400	2.67341200	-0.42883400
H	-3.51784700	-0.81835900	1.93724500
H	-4.11842100	-1.30132200	0.34519800
H	-2.45473400	-1.73383100	0.82738200
C	-5.76504800	2.57984100	0.38899300
H	-5.36198200	0.56046900	1.00187200
C	-3.90680600	3.78831500	-0.59565600
H	-2.05015900	2.68597200	-0.73724000
C	-5.24548100	3.74350100	-0.18647600
H	-6.80306200	2.54530600	0.70679000
H	-3.50525900	4.69290900	-1.04341500
H	-5.88220800	4.61426500	-0.31665400
O	1.51160400	0.43580500	-0.02998900
C	2.70286200	0.32784100	0.31105800
C	3.60402000	1.49616900	0.14665400
C	3.22826300	-0.96286100	0.88961300
C	4.94964700	1.46041100	0.55497400
C	3.09045800	2.67328100	-0.42991100
H	4.11857100	-1.30066100	0.34727300
H	3.51643500	-0.81723100	1.93859000
H	2.45453800	-1.73337500	0.82814700
C	5.76457300	2.58047200	0.38955600
H	5.36132500	0.56145600	1.00348600
C	3.90681300	3.78814700	-0.59697700
H	2.05034500	2.68555200	-0.73893900
C	5.24524800	3.74371500	-0.18697200
H	6.80240100	2.54623400	0.70799600
H	3.50545400	4.69241200	-1.04556800
H	5.88197800	4.61444900	-0.31733800

1S-9

I	1.68239300	-0.91151800	0.02461800
Cu	-0.03867700	0.92385800	-0.14928600
S	-2.10812600	-0.27195400	0.00581400
C	-1.99887500	-1.27661000	1.51685300

H	-2.84110700	-1.97353300	1.53412500
H	-1.03601700	-1.79467700	1.51610500
H	-2.06111200	-0.59047300	2.36409200
C	-2.03200300	-1.60816400	-1.22417700
H	-2.87261600	-2.28634800	-1.05452700
H	-2.11682800	-1.14361900	-2.20878200
H	-1.06799300	-2.11404300	-1.12353800
O	-3.44061100	0.42172100	-0.06304800
O	0.47227900	2.71046600	-0.43859100
O	0.70155500	3.50295700	0.52013300

1S-10

I	-1.82331000	-0.58793000	0.00014000
Cu	0.14208100	0.97657500	-0.00128200
S	1.96293200	-0.55109500	-0.00072600
C	1.67392200	-1.68913000	-1.38547700
H	2.39692400	-2.50608600	-1.31458400
H	0.64170000	-2.04467800	-1.33172800
H	1.83596500	-1.12104400	-2.30388200
C	1.67727000	-1.67942900	1.39268100
H	2.39979800	-2.49714000	1.32574000
H	1.84175800	-1.10501600	2.30671000
H	0.64481300	-2.03506700	1.34392400
O	3.38174800	-0.07046300	-0.00431900
O	-0.40851700	2.77906400	0.00084300
O	0.93177600	2.68859200	-0.00002800

1S-11

I	-1.25849300	-1.29876500	-0.09863000
Cu	-0.48983900	1.11765200	0.05462800
S	2.18106100	-0.29155400	-0.33945700
C	3.85866500	0.36248700	-0.57902800
H	4.16384900	0.90804500	0.31698300
H	4.53692300	-0.46905300	-0.79018700
H	3.81538300	1.03787600	-1.43562700
C	2.47602300	-1.24160300	1.18089700
H	2.87738500	-0.57374100	1.94735800
H	1.50713300	-1.64555500	1.48190800
H	3.17184800	-2.05502700	0.95473400
O	1.43649600	1.00752600	0.12687100
O	-2.01269900	2.16777500	0.09657800

O	-0.93281800	2.96965400	0.15006600
1S-13			
Cu	-1.56815800	0.00002000	-0.08088000
S	0.67641800	0.00001900	0.18499000
C	1.41211500	1.39869100	-0.70504200
H	2.49772700	1.34014500	-0.58347400
H	1.12758100	1.34417900	-1.75979000
H	1.03534600	2.31487000	-0.24565500
C	1.41194500	-1.39888300	-0.70482800
H	2.49756700	-1.34045700	-0.58329000
H	1.03507100	-2.31494700	-0.24529700
H	1.12740000	-1.34449500	-1.75957900
O	1.04860400	0.00012200	1.62774800

1S-14			
Cu	1.93339500	0.00001400	-0.01739700
S	-1.12931300	0.00000200	-0.45715800
C	-2.11068600	-1.38543600	0.17630300
H	-2.20932100	-1.28817300	1.26014400
H	-3.08712000	-1.36796200	-0.31639600
H	-1.58136700	-2.30460100	-0.08262300
C	-2.10982600	1.38600700	0.17644100
H	-2.20849100	1.28847200	1.26025300
H	-1.57997400	2.30491900	-0.08226700
H	-3.08632000	1.36929100	-0.31619400
O	0.13452600	-0.00072800	0.49746000

1S-15			
Cu	0.00000100	-0.14792200	0.00004300
S	-2.24751400	0.06984800	0.14694600
O	-2.49251400	0.84130700	1.40851100
C	-3.17993300	-1.48770000	0.12897800
C	-2.98191600	0.89677200	-1.29285300
H	-2.82962800	-2.08705600	0.97163200
H	-4.24012600	-1.25073300	0.25501900
H	-3.00019000	-2.00629800	-0.81700800
H	-2.80942700	0.28880500	-2.18548900
H	-4.05081800	1.02778400	-1.10230500
H	-2.49782800	1.87052800	-1.39118700
S	2.24750800	0.06989100	-0.14693000

O	2.49250000	0.84152500	-1.40838900
C	3.17971200	-1.48778600	-0.12930700
C	2.98215200	0.89648500	1.29292600
H	2.82928000	-2.08691400	-0.97207200
H	4.23994000	-1.25097200	-0.25534300
H	2.99992500	-2.00655700	0.81657600
H	2.80974300	0.28836100	2.18547100
H	4.05103900	1.02744300	1.10224700
H	2.49816100	1.87026200	1.39151600

1S-16			
Cu	-0.00003200	-0.24565200	0.00001600
O	1.80307500	-0.31644400	0.48300100
S	2.97015600	0.34035700	-0.34158900
C	3.95847300	1.16165300	0.93833900
C	4.07056400	-1.05575300	-0.70476100
H	3.37212200	2.00599400	1.30602500
H	4.15573200	0.45227700	1.74584900
H	4.88762000	1.52071500	0.48701700
H	4.99708200	-0.66758100	-1.13723500
H	4.26270200	-1.60886200	0.21793500
H	3.55853000	-1.69011000	-1.43112100
O	-1.80311500	-0.31666300	-0.48306000
S	-2.97008600	0.34032400	0.34157700
C	-3.95831100	1.16171100	-0.93839200
C	-4.07070700	-1.05558200	0.70483000
H	-3.37189200	2.00602600	-1.30602400
H	-4.15550300	0.45232700	-1.74591100
H	-4.88748600	1.52078800	-0.48714600
H	-4.99708200	-0.66719500	1.13742300
H	-4.26310000	-1.60866800	-0.21782600
H	-3.55872600	-1.69004200	1.43114000

1S-17			
Cu	-0.00000100	-0.00018400	0.08685200
O	-1.85737700	-0.12040700	0.13266000
C	-2.79639300	0.61142700	-0.28620900
C	-4.17426600	0.19433500	-0.03803100
C	-2.48961400	1.88858700	-1.02422400
C	-5.26510300	0.97141000	-0.48537200
C	-4.41780600	-1.00736000	0.66414000

H	-2.93591600	1.87542100	-2.02487400
H	-2.90446700	2.75102300	-0.49012600
H	-1.40815500	2.01705100	-1.11901300
C	-6.56858400	0.55318700	-0.23487000
H	-5.09811600	1.89778000	-1.02571200
C	-5.72192600	-1.41868600	0.91061800
H	-3.57446700	-1.59760500	1.00554100
C	-6.79733700	-0.63963600	0.46172400
H	-7.40529100	1.15212200	-0.57952200
H	-5.90733200	-2.34169700	1.45061100
H	-7.81567900	-0.96299900	0.65573200
O	1.85736400	0.12033400	0.13256500
C	2.79643700	-0.61147500	-0.28622600
C	4.17426800	-0.19427800	-0.03802300
C	2.48976900	-1.88869500	-1.02418700
C	5.26517400	-0.97130100	-0.48528700
C	4.41769800	1.00747900	0.66408000
H	2.93592800	-1.87542600	-2.02490200
H	2.90484000	-2.75107700	-0.49017300
H	1.40831800	-2.01733500	-1.11883500
C	6.56861600	-0.55296300	-0.23478100
H	5.09826800	-1.89771500	-1.02557700
C	5.72178000	1.41891600	0.91056900
H	3.57430500	1.59768200	1.00542300
C	6.79726000	0.63992100	0.46174700
H	7.40537700	-1.15185500	-0.57937400
H	5.90710300	2.34197400	1.45050900
H	7.81557300	0.96337400	0.65576000

1S-19

Cu	-0.36855400	1.12525100	0.07292500
O	1.38362400	1.33521300	-0.29131600
I	2.29676200	-0.45448800	0.01566500
O	-2.21112700	0.85552300	0.42745300
S	-2.78776400	-0.28267700	-0.48141400
C	-2.10453300	-1.84125300	0.16938100
C	-4.48128500	-0.44945300	0.16030500
H	-1.03352000	-1.83567800	-0.05291400
H	-2.26405600	-1.88134600	1.25007700
H	-2.59209500	-2.67959600	-0.33743900
H	-4.96199200	-1.30748900	-0.31749500

H	-4.43879900	-0.56893800	1.24574800
H	-5.01069100	0.46981600	-0.09766300

1T

I	-2.05352400	-0.74302100	-0.07244500
Cu	-0.10651700	0.76476700	0.11940200
S	2.45895200	-0.74267300	-0.49316100
C	4.21504300	-0.66868600	-0.02984500
H	4.29075200	-0.48573800	1.04495300
H	4.69906300	-1.60898800	-0.30864400
H	4.65749800	0.16052200	-0.58540200
C	1.94827700	-2.08546600	0.62453800
H	2.22772400	-1.83035200	1.65031600
H	0.86064300	-2.16857200	0.53575700
H	2.42745200	-3.01403300	0.30006800
O	1.88454100	0.57154800	0.11088800
O	-0.13518400	2.75950600	0.52827800
O	0.30557900	3.48853600	-0.38137800

1T-2

I	2.17934200	-0.17728900	0.00002300
Cu	-0.09348300	0.77472200	-0.00006500
S	-1.91935600	-0.81767700	0.00000000
C	-1.52122900	-1.94196000	1.37518900
H	-2.14091500	-2.83925700	1.29580300
H	-0.45417400	-2.17787400	1.32611100
H	-1.74733300	-1.40997000	2.30166800
C	-1.52129500	-1.94198100	-1.37519100
H	-2.14101500	-2.83925100	-1.29577400
H	-1.74741500	-1.40999100	-2.30166600
H	-0.45424800	-2.17794000	-1.32615100
O	-3.38852900	-0.49097600	0.00001700
O	-1.12991900	2.49659700	-0.00019700
O	-2.37457400	2.51565200	0.00026600

1T-3

I	-1.34766300	-1.29738200	-0.09191400
Cu	-0.45143900	1.07569500	0.03197600
S	2.23720900	-0.32995300	-0.34930600
C	3.96370100	0.21526800	-0.51314300
H	4.26015700	0.74872300	0.39327200

H	4.59955900	-0.65764000	-0.68643800
H	4.00502300	0.88502000	-1.37436200
C	2.41269400	-1.28837100	1.18571400
H	2.81691300	-0.64117700	1.96856400
H	1.40962600	-1.63636500	1.44323600
H	3.07083100	-2.14093300	0.99318000
O	1.53120700	1.00137300	0.06168500
O	-1.93589300	2.48381600	0.12987400
O	-0.80756000	3.10560400	0.15346100

1T-4

I	-1.89244100	-0.58473400	-0.00001000
Cu	0.09250500	0.92282200	0.00007800
S	2.03752900	-0.57272300	0.00008200
C	1.73012000	-1.71900500	-1.37852700
H	2.42717800	-2.55766100	-1.29978800
H	0.68742900	-2.04508600	-1.32729100
H	1.91051100	-1.16616200	-2.30285800
C	1.72987300	-1.71985100	1.37792300
H	2.42691400	-2.55848100	1.29875500
H	1.91015500	-1.16759100	2.30262100
H	0.68718100	-2.04587100	1.32633300
O	3.47572800	-0.13463900	0.00035700
O	-0.20351400	3.12105100	0.00003600
O	1.00365500	2.70941200	-0.00004000

1T-5

I	3.37047900	-0.55627200	0.06627900
Cu	1.05919400	0.13754000	-0.31498600
C	-1.31339000	0.22651600	1.95100600
H	-1.65486600	1.21879800	2.26992200
H	-1.74090900	-0.511173700	2.63733600
O	-0.89883400	-0.08677600	-0.38859700
O	0.84956000	2.25092000	-0.75457900
O	0.07452700	2.85743300	0.00314500
C	-1.74449300	-0.03506500	0.52901900
C	-3.16926300	-0.22285100	0.19501600
C	-3.52498000	-0.49414000	-1.14134600
C	-4.17687100	-0.13033700	1.17420900
C	-4.86059700	-0.67209900	-1.48754800
H	-2.73924700	-0.56157200	-1.88624900

C	-5.51400400	-0.30553900	0.82178600
H	-3.92097200	0.08264900	2.20748300
C	-5.85625400	-0.57775500	-0.50691500
H	-5.12983900	-0.88336300	-2.51804300
H	-6.28762400	-0.23112400	1.57999700
H	-6.89884300	-0.71630700	-0.77880400
H	-0.22262300	0.19142000	2.01902700

1T-6

I	-2.98593800	-1.22158600	-0.47656800
Cu	-0.86242300	-0.29993300	0.43938000
C	1.68933100	-2.65102900	0.01631100
H	0.60549200	-2.77532900	0.07905900
H	2.05009800	-3.06347400	-0.93212400
H	2.16302500	-3.22035200	0.82577500
O	1.15657700	-0.35215100	0.41986400
O	-0.96276300	-0.01455100	2.56027800
O	-0.49901300	1.08385800	2.91050300
C	2.03642900	-1.18711500	0.13888500
C	3.41893500	-0.71016300	-0.06747000
C	3.65607200	0.67991600	-0.08331900
C	4.49196100	-1.60344700	-0.24687700
C	4.94881700	1.15967300	-0.27516200
H	2.81899200	1.36132200	0.04052800
C	5.78462800	-1.11535400	-0.43009900
H	4.32074900	-2.67584600	-0.23529300
C	6.01280200	0.26505300	-0.44518500
H	5.12897200	2.23034000	-0.29396100
H	6.61160400	-1.80674800	-0.56211100
H	7.02054900	0.64368800	-0.59247100
S	-0.66058100	2.20616200	-0.37193900
O	0.56855400	3.08845100	-0.30488000
C	-2.07867800	3.09705300	0.35227200
C	-1.26943900	2.18443700	-2.09155100
H	-1.86434300	3.22857000	1.41485300
H	-2.18554300	4.07030600	-0.13474200
H	-2.97410800	2.48193900	0.22293300
H	-2.17790800	1.57677500	-2.13273400
H	-1.44744200	3.21024700	-2.42619100
H	-0.48789200	1.72308000	-2.69936000

1T-7

I	-2.11493600	-1.99193400	0.07858000
Cu	-0.62028300	0.05380400	0.38524000
C	1.87758000	-1.68140300	-1.24987700
H	0.80651400	-1.86308100	-1.12693100
H	2.09846500	-1.50885100	-2.31086600
H	2.43415600	-2.57240900	-0.93827000
O	1.43844000	0.21256900	0.15304500
O	-0.46329000	0.69291500	2.37034800
O	0.22765200	1.72152400	2.49859400
C	2.28655800	-0.48032500	-0.43309700
C	3.71714200	-0.10061300	-0.32004700
C	4.06214600	0.99678300	0.49159400
C	4.72880200	-0.80079500	-1.00155900
C	5.39344600	1.38264500	0.61925300
H	3.26950000	1.52467800	1.01201100
C	6.06145700	-0.40889500	-0.87433100
H	4.47836200	-1.64820800	-1.63254600
C	6.39461400	0.68109100	-0.06404800
H	5.65488900	2.22777700	1.24949000
H	6.83848800	-0.95231500	-1.40403300
H	7.43348400	0.98341700	0.03599200
O	-1.38116900	1.84481900	-0.38921100
S	-2.73664000	1.75880200	-1.13058600
C	-4.01891600	1.56342100	0.14875800
C	-3.08931400	3.49604400	-1.55453000
H	-3.89777900	0.55407400	0.55091900
H	-3.86525000	2.31397700	0.92917400
H	-5.00306100	1.66903500	-0.31791900
H	-4.09019300	3.56780000	-1.99034700
H	-3.00576400	4.10809700	-0.65268600
H	-2.33990900	3.80503600	-2.28622000

1T-8

Cu	-2.25043700	-0.02132000	-0.00976500
C	0.27462600	2.15085300	0.00507000
H	0.70914800	2.62677300	0.89126200
H	0.71234700	2.63340100	-0.87595700
O	-0.39689900	-0.15906100	-0.00535200
O	-4.14353400	0.02381000	-0.01455700
O	-4.85958700	-0.97943200	0.03924900

C	0.56184800	0.67321900	-0.00000600
C	1.92300800	0.16512700	0.00102800
C	2.14414300	-1.23289000	-0.00404200
C	3.02972500	1.04627700	0.00696100
C	3.43962800	-1.73217100	-0.00317200
H	1.29152600	-1.90280700	-0.00858600
C	4.32355900	0.53763100	0.00780200
H	2.88057900	2.12120000	0.01089100
C	4.52872700	-0.84847900	0.00274600
H	3.60917200	-2.80392400	-0.00706200
H	5.17192700	1.21392600	0.01236900
H	5.54088300	-1.24167600	0.00342600
H	-0.80431700	2.33144200	0.00381200

1T-9

Cu	0.84090100	0.00031200	-0.20723500
S	-1.37882700	-0.00001900	0.20525700
C	-2.22175300	-1.39556200	-0.59106700
H	-3.28467400	-1.33422600	-0.34034500
H	-2.06631900	-1.34291200	-1.67247400
H	-1.79563700	-2.31331600	-0.18057700
C	-2.22279000	1.39502600	-0.59081400
H	-3.28563800	1.33284900	-0.33999300
H	-1.79731000	2.31303300	-0.18023100
H	-2.06741100	1.34264300	-1.67224100
O	-1.57628500	-0.00020100	1.68578200
O	2.79248900	0.00012700	-0.41027700
O	3.61371600	-0.00037500	0.49985200

1T-10

Cu	-2.25043700	-0.02132000	-0.00976500
C	0.27462600	2.15085300	0.00507000
H	0.70914800	2.62677300	0.89126200
H	0.71234700	2.63340100	-0.87595700
O	-0.39689900	-0.15906100	-0.00535200
O	-4.14353400	0.02381000	-0.01455700
O	-4.85958700	-0.97943200	0.03924900
C	0.56184800	0.67321900	-0.00000600
C	1.92300800	0.16512700	0.00102800
C	2.14414300	-1.23289000	-0.00404200
C	3.02972500	1.04627700	0.00696100

C	3.43962800	-1.73217100	-0.00317200
H	1.29152600	-1.90280700	-0.00858600
C	4.32355900	0.53763100	0.00780200
H	2.88057900	2.12120000	0.01089100
C	4.52872700	-0.84847900	0.00274600
H	3.60917200	-2.80392400	-0.00706200
H	5.17192700	1.21392600	0.01236900
H	5.54088300	-1.24167600	0.00342600
H	-0.80431700	2.33144200	0.00381200

1T-11

Cu	-0.98755400	-0.29375400	-0.00010800
C	1.56913700	-2.38192300	0.00058600
H	0.49143300	-2.56709800	0.00078100
H	2.01123800	-2.85575400	-0.88312400
H	2.01149600	-2.85536200	0.88437500
O	0.88076600	-0.08045300	0.00001000
O	-1.24755600	2.11754300	0.00098800
O	-0.25241900	2.83160400	-0.00017400
C	1.83927800	-0.89947900	0.00020300
C	3.20629100	-0.38049900	0.00004200
C	3.41514200	1.01656100	-0.00029700
C	4.31872500	-1.24963500	0.00020800
C	4.70717400	1.52823500	-0.00046300
H	2.55475400	1.67680400	-0.00042200
C	5.60999100	-0.73005100	0.00003500
H	4.17820900	-2.32589800	0.00046700
C	5.80464300	0.65634400	-0.00029800
H	4.86594700	2.60192400	-0.00071900
H	6.46346400	-1.40031400	0.00016100
H	6.81335900	1.05853000	-0.00042900
O	-2.80781400	-0.76368300	-0.00044900
S	-4.01926000	0.23697500	-0.00034900
C	-5.04076000	-0.34433300	-1.38179600
C	-5.03985000	-0.34326600	1.38223000
H	-4.49792500	-0.11699100	-2.30145200
H	-5.19589800	-1.42161600	-1.28449000
H	-5.99035500	0.19800000	-1.36653700
H	-5.98944000	0.19908400	1.36719800
H	-5.19509200	-1.42061800	1.28585200
H	-4.49640200	-0.11523800	2.30135500

1T-12

Cu	0.41440400	1.37727600	0.08946000
O	1.65590600	2.63171800	0.18547700
I	1.44975800	-0.98301800	-0.10744700
O	-1.51131500	1.02237000	0.10243300
S	-2.11061400	-0.35103100	-0.34317500
C	-2.27195100	-1.32587400	1.18262700
C	-3.86170100	0.08518200	-0.56010500
H	-1.25767800	-1.60618400	1.47479200
H	-2.74537100	-0.71077900	1.95228100
H	-2.86409100	-2.21988800	0.96563000
H	-4.43381700	-0.82518900	-0.76046700
H	-4.22196400	0.59116600	0.33882700
H	-3.91696800	0.75776200	-1.41835400

2S

Cu	1.79996500	0.00350200	-0.04163100
O	0.03748500	-0.72391900	-0.06236800
O	-0.03757100	0.72408100	-0.06267200
Cu	-1.80009500	-0.00332500	-0.04087800
I	-3.46649700	1.94463800	0.00677300
I	3.46633900	-1.94459200	0.00682800
O	2.92276400	1.61313300	-0.07699400
S	4.40824400	1.54409300	0.40160200
C	5.39569200	1.31742400	-1.10814600
C	4.76191100	3.30529000	0.68262500
H	5.22178400	0.28952200	-1.43367600
H	5.05987100	2.03043600	-1.86569500
H	6.45157900	1.46390100	-0.86139200
H	5.82463800	3.42444900	0.91250900
H	4.48052800	3.87533100	-0.20608200
H	4.15607400	3.61692800	1.53570000
O	-2.92231100	-1.61338700	-0.07500400
S	-4.40848300	-1.54416200	0.40139600
C	-5.39373100	-1.31808600	-1.10986400
C	-4.76252900	-3.30524000	0.68262200
H	-5.21933700	-0.29031300	-1.43555600
H	-5.05680400	-2.03139200	-1.86664800
H	-6.44998900	-1.46443600	-0.86463400
H	-5.82556700	-3.42428300	0.91112500

H	-4.47996300	-3.87564900	-0.20547300
H	-4.15785200	-3.61654900	1.53664000

2S-2

Cu	-1.62708400	-0.29581200	-0.07815900
O	0.13732300	0.39145700	-0.15056400
O	0.19613000	-1.05896400	-0.16428000
Cu	1.98172500	-0.23279800	-0.15823300
I	3.98207300	-1.72272700	0.07207000
S	2.83293100	2.03355500	-0.22163600
O	3.13443700	2.69917500	-1.53323200
C	4.28659400	2.11296500	0.86121600
C	1.68367900	3.06115400	0.74390900
H	5.04852500	1.47170400	0.41406300
H	4.62482000	3.15156300	0.91206100
H	4.01596900	1.72630400	1.84723800
H	1.52929300	2.59610500	1.72127400
H	2.10432200	4.06575300	0.83985700
H	0.73990800	3.08959400	0.19585600
I	-3.10455400	1.78441900	0.14889900
O	-2.85028800	-1.80955600	-0.15130500
S	-4.32915700	-1.65943900	0.33914500
C	-5.29442300	-1.27660400	-1.15234500
C	-4.80541900	-3.40243300	0.52805300
H	-5.04234300	-0.24951600	-1.42503600
H	-5.01573200	-1.97223200	-1.94813600
H	-6.35839000	-1.35285700	-0.90904400
H	-5.87379200	-3.45647400	0.75581100
H	-4.56610400	-3.94225800	-0.39122900
H	-4.22333700	-3.80091800	1.36124100

2S-3

Cu	1.80485800	-0.05357300	-0.08742300
O	0.01558200	0.72871000	0.02981600
O	-0.01532300	-0.72708100	-0.02930100
Cu	-1.80464500	0.05479000	0.08763500
I	-3.66212400	-1.62421200	-0.01565300
S	-2.85807200	2.20229800	0.19573800
O	-3.16486900	2.81865700	1.52804500
C	-4.35120100	2.15019600	-0.83175400
C	-1.83802500	3.33389900	-0.79695700

H	-5.03433700	1.44144700	-0.35986600
H	-4.78413500	3.15373100	-0.86395800
H	-4.08209700	1.79288500	-1.82923000
H	-1.67435700	2.89001900	-1.78267800
H	-2.34879600	4.29765900	-0.87094900
H	-0.88510300	3.44360800	-0.27572900
I	3.66398200	1.62348400	0.01578200
S	2.85609000	-2.20229100	-0.19619100
O	3.16322100	-2.81868000	-1.52840100
C	1.83406300	-3.33302800	0.79543300
C	4.34846600	-2.15208100	0.83249200
H	0.88145300	-3.44164800	0.27340400
H	2.34378700	-4.29733100	0.86960200
H	1.67000800	-2.88919900	1.78110600
H	4.07889900	-1.79465900	1.82980700
H	4.78028200	-3.15609000	0.86489900
H	5.03277800	-1.44399800	0.36131300

2S-4

Cu	1.77856600	0.39771400	0.36780200
O	-0.01822600	-0.18054900	0.65323400
O	-0.04343800	1.24788000	0.44159800
Cu	-1.81704600	0.35085500	0.24436100
I	-3.96821200	1.56152700	-0.05040200
S	-2.23365700	-2.01025800	-0.31297400
O	-1.48964700	-2.49458800	-1.53185200
C	-4.00297200	-2.36190100	-0.49474100
C	-1.83476900	-3.07464800	1.10366200
H	-4.36960200	-1.73957400	-1.31295000
H	-4.12397700	-3.42392300	-0.72396100
H	-4.51145600	-2.08381600	0.43171700
H	-2.38588100	-2.71753000	1.97828900
H	-2.10754000	-4.10442100	0.85689400
H	-0.75537900	-2.99595900	1.26343100
I	3.85759100	1.62758400	-0.23458300
S	2.36993300	-1.98967700	0.21194300
O	1.62506400	-3.03386100	1.00635100
C	4.15579800	-2.27392700	0.35663000
C	2.13957200	-2.28784000	-1.56445900
H	4.41102300	-2.16152400	1.41212900
H	4.37697600	-3.28833800	0.01500100

H	4.67297100	-1.51428600	-0.23489900
H	2.70357600	-1.52967200	-2.11568300
H	2.48457500	-3.29759300	-1.80304900
H	1.06733700	-2.19693100	-1.76015700

2S-5

Cu	1.69434100	0.10142300	0.00652000
O	-0.12578900	0.83291600	0.02535700
O	-0.05876600	-0.61800000	0.00120300
Cu	-1.90962300	0.09896800	0.01107100
I	-3.74200500	-1.62809100	-0.00843300
S	-3.21526100	2.16608900	0.03109600
O	-2.60366200	3.53990400	0.04099200
C	-4.38466200	1.99963200	1.41386000
C	-4.39285100	2.02411500	-1.34744900
H	-3.80581500	2.09942200	2.33447900
H	-5.12480700	2.80141700	1.34450900
H	-4.84314500	1.00855600	1.35838400
H	-4.85131900	1.03232700	-1.30698900
H	-5.13217300	2.82482700	-1.25943400
H	-3.81941000	2.14006600	-2.26955000
I	3.28764300	-1.88877800	-0.06389900
O	2.86999900	1.65554800	0.09239100
S	4.37196600	1.54369700	-0.33513200
C	4.78353700	3.29659900	-0.58215000
C	5.29237200	1.26927400	1.20781800
H	4.21869800	3.63420600	-1.45322900
H	4.48697600	3.86499400	0.30257400
H	5.85687100	3.38645200	-0.77241000
H	6.36092400	1.38276100	1.00185700
H	4.95232000	1.98573500	1.96009300
H	5.07335700	0.24467000	1.51577900

2S-6

Cu	1.79739100	0.23085100	-0.01436800
O	-0.00000200	1.00735200	0.00033800
O	-0.00015400	-0.44483200	0.00014700
Cu	-1.79754700	0.23114500	0.01524400
I	-3.39164300	-1.76491600	0.05501100
I	3.39193800	-1.76480700	-0.05526200
O	2.98828600	1.80335200	0.03889600

S	4.49278500	1.65429100	-0.35478700
C	4.95845100	3.39501700	-0.60345400
C	5.38196100	1.37261300	1.20635200
H	4.42083300	3.74301800	-1.48765600
H	4.66015900	3.97736700	0.27172100
H	6.03743100	3.45600600	-0.77248400
H	6.45621000	1.46151400	1.01836700
H	5.04452500	2.10208200	1.94739700
H	5.13503400	0.35518400	1.51727600
O	-2.98838700	1.80361600	-0.03676000
S	-4.49353900	1.65368800	0.35420800
C	-4.96028300	3.39407400	0.60317600
C	-5.37989700	1.37264900	-1.20863900
H	-4.42421400	3.74172300	1.48845800
H	-4.66081900	3.97708800	-0.27115400
H	-6.03955500	3.45453800	0.77052700
H	-6.45451300	1.46103300	-1.02251000
H	-5.04141600	2.10270000	-1.94863300
H	-5.13206800	0.35549500	-1.51975300

2S-7

Cu	-1.83923700	0.03693900	0.01608700
O	0.02119100	-0.54887700	-0.46187100
O	-0.00665300	0.50499200	0.52098200
Cu	1.85322900	-0.06104800	-0.00751600
S	-3.37098000	-1.04120000	-1.49966800
O	-2.94576800	-2.31902900	-2.17508200
C	-3.98713500	0.14303500	-2.73499400
C	-4.88852000	-1.32120200	-0.54624000
H	-3.16330200	0.34994900	-3.42121300
H	-4.82104700	-0.31476600	-3.27365800
H	-4.29091800	1.05311700	-2.21072500
H	-5.22351000	-0.36115900	-0.14523600
H	-5.62966400	-1.77162800	-1.21264100
H	-4.62014000	-2.00376000	0.26778200
S	3.45255100	0.97066600	1.47406600
O	3.04905100	2.20756600	2.23479200
C	4.90848600	1.32097900	0.45007100
C	4.15789100	-0.25816500	2.61444400
H	4.58523400	2.03512000	-0.31556400
H	5.67996600	1.75284800	1.09397000

H	5.23394100	0.38592000	-0.01308000
H	4.44349200	-1.13786900	2.03152700
H	5.01494300	0.18990800	3.12417600
H	3.37936800	-0.51103400	3.33717100
I	3.26964100	-1.96434100	-0.93612200
S	1.80492300	2.37650200	-1.24337500
O	3.08982600	3.05484500	-1.68375300
C	0.86323600	3.53504800	-0.20142000
C	0.65955700	2.31238300	-2.66039700
H	1.42821200	3.64088400	0.72732000
H	0.79163800	4.49349400	-0.72325900
H	-0.12206200	3.10975300	0.00634000
H	-0.29593200	1.90929900	-2.31466100
H	0.54149400	3.31983800	-3.06864900
H	1.10429800	1.64913900	-3.40503900
I	-3.27546100	1.97997500	0.82411300
S	-1.88823700	-2.31251800	1.37651500
O	-3.20136200	-2.97722500	1.74761000
C	-0.86549100	-2.15498700	2.87691700
C	-0.86045800	-3.51596500	0.47683600
H	-1.38829900	-1.47194500	3.54953000
H	-0.75531900	-3.13834700	3.34205100
H	0.10303100	-1.73499600	2.59354500
H	0.12737300	-3.08284300	0.30056400
H	-0.80571000	-4.43846800	1.06157500
H	-1.36221200	-3.69199500	-0.47723700

2S-8

Cu	-1.49663900	-0.09614500	-0.15857600
O	0.15751700	0.34411300	0.74860100
O	0.17340400	-1.07344300	0.57118900
Cu	2.02346200	-0.18005400	0.46747000
I	-3.44571700	-1.53821200	-0.97680400
I	4.13900700	-1.53560000	0.45216100
S	-2.27982000	-0.25081000	2.62184300
O	-3.11729200	0.86928700	3.22232600
C	-0.82270800	-0.49570900	3.69309700
C	-3.10436500	-1.83336700	2.99537800
H	-0.24158100	0.42627600	3.64138100
H	-1.15225200	-0.68296100	4.71874400
H	-0.23402100	-1.32573100	3.29499200

H	-2.45031700	-2.65481800	2.69047800
H	-3.32906500	-1.87432700	4.06504400
H	-4.02206200	-1.86156800	2.40507700
S	-2.40914300	2.13127200	-0.35428600
O	-1.54815700	3.30454800	0.05557000
C	-4.03015400	2.25210500	0.44771300
C	-2.88935400	2.31391500	-2.09347200
H	-3.86913600	2.07387800	1.51619400
H	-4.43601900	3.24958500	0.25726700
H	-4.66525800	1.46721900	0.02744400
H	-3.57187400	1.49674800	-2.34129500
H	-3.35373500	3.29482700	-2.22640900
H	-1.97244700	2.22073800	-2.67647300
S	2.70111200	2.15269600	0.13981200
O	2.75243500	2.54565400	-1.31731000
C	4.30981200	2.49750200	0.90751800
C	1.65560500	3.33305300	1.03901300
H	5.02107300	1.79124800	0.47460300
H	4.59017300	3.52991600	0.68239700
H	4.23176800	2.32866200	1.98488600
H	1.69541500	3.09293000	2.10547300
H	2.02880100	4.34307600	0.84770100
H	0.63280400	3.22452400	0.66215300
S	0.99880800	-0.20318700	-2.16607100
O	-0.44627400	0.33329500	-2.14899000
C	0.89622200	-1.93786200	-2.69517800
C	1.77460300	0.50231200	-3.64764200
H	0.33977200	-2.45865400	-1.91361700
H	0.36283300	-1.99928600	-3.64721200
H	1.90924200	-2.34324600	-2.76861300
H	2.74850100	0.02553700	-3.79011400
H	1.11860600	0.33279100	-4.50558100
H	1.91021700	1.56559600	-3.44683600

2S-9

Cu	-1.71799300	-0.32617300	-0.02144100
O	0.17240200	-0.52295400	0.67693900
O	-0.25337200	0.83434100	0.61651000
Cu	1.80170400	0.48477600	0.47840600
I	3.52890400	-1.41225600	0.82784900
I	-3.15137000	1.29795900	-1.43737400

O	1.72962300	0.76214700	-1.74238300
S	1.42428800	-0.54520900	-2.49550600
C	0.29213200	-0.06480800	-3.83946400
C	2.90294100	-0.87122900	-3.51102000
H	-0.64783700	0.23685900	-3.36806300
H	0.72449900	0.77178000	-4.39571600
H	0.12285600	-0.92596000	-4.49327100
H	2.70825100	-1.71406800	-4.18140500
H	3.15988700	0.02970300	-4.07520800
H	3.70296300	-1.12157900	-2.81047900
O	-2.72254400	-0.94145100	1.84966300
S	-2.79180600	-0.13790100	3.15975400
C	-1.07542300	0.14830200	3.71163600
C	-3.16720500	1.58666400	2.70026900
H	-0.64638900	-0.82708800	3.94954600
H	-0.51670600	0.61652300	2.89735300
H	-1.09873700	0.77660000	4.60771600
H	-3.15766200	2.20340000	3.60446400
H	-2.43171800	1.93086000	1.96877100
H	-4.16021100	1.58992700	2.24652700
O	2.53385900	2.33331700	0.81650600
S	1.53132400	3.52235100	0.79272500
C	2.63356200	4.95822700	0.61217300
C	0.76933200	3.58051400	-0.85861700
H	3.23576800	5.01644300	1.52099400
H	3.27802300	4.79812000	-0.25586900
H	2.03144000	5.86427000	0.49854400
H	0.21001000	4.51800900	-0.93876900
H	1.55039600	3.50311800	-1.61824800
H	0.09335500	2.72570600	-0.93270100
O	-1.89867000	-2.20641200	-0.76115700
S	-1.43895200	-3.31663400	0.22753900
C	-2.48676300	-4.72729500	-0.24044300
C	0.14189500	-3.92740600	-0.43305100
H	-3.50827400	-4.46340900	0.04055500
H	-2.42141300	-4.87942200	-1.32093500
H	-2.16235100	-5.61743500	0.30637800
H	0.43301500	-4.82235000	0.12536800
H	0.03059600	-4.14483900	-1.49892500
H	0.88241500	-3.13832400	-0.27347400

2S-10

Cu	1.86768500	-1.00336700	-0.43861800
O	0.06755100	-0.35604600	-0.90243500
O	-0.02543000	-1.60938500	-0.14039900
Cu	-1.78602600	-1.07748800	-0.58273400
I	-3.32533700	-2.87097900	0.37686500
I	3.17269000	1.20188600	-1.00629000
O	3.07139900	-2.31564700	0.36814600
S	4.60505200	-2.01799900	0.43256200
C	4.85585500	-1.11850900	1.99237400
C	5.26641400	-3.63179900	0.93639100
H	4.43122900	-0.12228200	1.84894300
H	4.33990600	-1.64631300	2.79862600
H	5.92985900	-1.04299100	2.18642100
H	6.33623900	-3.53030200	1.13945400
H	4.72354100	-3.98033800	1.81823800
H	5.10586500	-4.31475800	0.09995900
O	-2.88727100	0.31604800	-1.31983300
S	-4.30342900	0.72073800	-0.77977800
C	-4.13588700	0.98927600	1.01081800
C	-4.35977800	2.46321900	-1.28905000
H	-4.03934200	0.00320000	1.47153200
H	-3.25041900	1.60652000	1.20038000
H	-5.04906900	1.48001900	1.36231500
H	-5.27746600	2.91501400	-0.90187700
H	-3.46877300	2.96561600	-0.90141200
H	-4.36528500	2.47517400	-2.38062900
Cu	0.67219100	1.48650800	-0.08657500
I	-0.67138200	3.19156100	1.15765700

2S-11

Cu	1.55051900	0.96317500	0.79007200
O	-0.24507100	0.33617000	1.19498800
O	-0.33582900	1.71518700	0.77251500
Cu	-2.08860300	0.93573500	0.81678700
I	-3.62450500	2.73541100	-0.12917300
I	2.97317800	-1.20618000	1.28879900
O	2.81232300	2.46084500	0.50793400
S	4.32517500	2.11906600	0.33553800
C	4.50308500	1.50840700	-1.36903100
C	5.05162500	3.76865800	0.10333500

H	3.95632500	0.56433400	-1.41799300
H	4.06880500	2.23308600	-2.06209400
H	5.56571300	1.34478700	-1.57185800
H	6.10867100	3.65910000	-0.15561100
H	4.50260000	4.29508900	-0.68121400
H	4.95125000	4.29732300	1.05328400
O	-3.22501100	-0.57233600	1.30335800
S	-2.54880600	-1.94176800	1.67108200
C	-3.11823200	-2.23262800	3.37453700
C	-3.60000100	-3.14962300	0.82357400
H	-2.61351100	-1.49931900	4.00697900
H	-4.20126000	-2.09382900	3.42277200
H	-2.83158600	-3.24422700	3.67613000
H	-3.31795500	-4.15224300	1.15649400
H	-4.64621400	-2.92498200	1.04645500
H	-3.38428300	-3.04779700	-0.24157400
Cu	1.07443100	-1.50573900	-0.49806500
I	-0.49848100	-3.17956100	-1.56035100
O	1.15405300	0.45519200	-1.48908500
S	-0.28833600	0.82794900	-1.98413800
C	-0.19825500	2.60562800	-2.34189100
C	-0.34219500	0.21588100	-3.69438900
H	-0.05697800	3.10568600	-1.38300900
H	0.63973900	2.79720700	-3.01753200
H	-1.15060900	2.91920200	-2.77738700
H	-1.26968000	0.56532300	-4.15779100
H	0.53453800	0.57973500	-4.23666700
H	-0.33822000	-0.87527000	-3.63023700

TS1S

Cu	-1.52559500	0.01211400	0.10854100
O	-0.02536600	-0.99953300	0.12042000
O	0.02536400	0.99953200	0.12044700
Cu	1.52559300	-0.01211600	0.10856200
I	3.26291000	1.90639300	0.01706700
I	-3.26291000	-1.90639400	0.01697100
O	-2.73833300	1.52915200	0.17293700
S	-4.15863800	1.48682000	-0.48250400
C	-5.31840300	1.30844900	0.90586000
C	-4.41979000	3.25425300	-0.81968500
H	-5.21375400	0.28100600	1.26012200

H	-5.04797000	2.02092500	1.68945900
H	-6.33395100	1.48413400	0.53835900
H	-5.44382700	3.40279100	-1.17419900
H	-4.22575700	3.82713600	0.09021000
H	-3.70740500	3.53424200	-1.59809100
O	2.73833100	-1.52915700	0.17293500
S	4.15864400	-1.48680800	-0.48248500
C	5.31839000	-1.30847400	0.90589900
C	4.41979900	-3.25423200	-0.81971000
H	5.21373700	-0.28104100	1.26018600
H	5.04794600	-2.02097100	1.68947600
H	6.33394300	-1.48415100	0.53840700
H	5.44384100	-3.40276100	-1.17421400
H	4.22575400	-3.82713900	0.09016700
H	3.70742400	-3.53420000	-1.59813300

TS1S-2

Cu	1.56709200	-0.08540700	-0.06999200
O	0.04966900	0.96154900	0.02173600
O	-0.04966900	-0.96154500	-0.02172900
Cu	-1.56709200	0.08541000	0.07000000
I	-3.44343600	-1.62366200	-0.00653200
S	-2.82238400	2.09138600	0.19011700
O	-3.34026700	2.57111300	1.51108300
C	-4.15423700	2.05118900	-1.03851800
C	-1.73130200	3.33948000	-0.54908200
H	-4.86019400	1.28616500	-0.70998600
H	-4.62655500	3.03672800	-1.07067000
H	-3.73080000	1.77413300	-2.00756300
H	-1.45817300	3.02017300	-1.55784800
H	-2.25705400	4.29791200	-0.55471400
H	-0.83585100	3.38923700	0.07394700
I	3.44343900	1.62366100	0.00655000
S	2.82237700	-2.09138600	-0.19013900
O	3.34021700	-2.57111000	-1.51112400
C	1.73131000	-3.33947700	0.54908700
C	4.15426700	-2.05120200	1.03845500
H	0.83583700	-3.38922100	-0.07391200
H	2.25705500	-4.29791400	0.55469100
H	1.45821900	-3.02017800	1.55786500
H	3.73086200	-1.77414700	2.00751400

H	4.62658000	-3.03674400	1.07058900
H	4.86021900	-1.28618100	0.70990500

TS1S-3

Cu	1.50551600	-0.07242600	-0.02527500
O	-0.03948600	0.90540800	-0.00420900
O	-0.07079700	-1.04123000	-0.00095800
Cu	-1.60856100	-0.03529100	0.05954400
I	-3.44670500	-1.76150200	-0.03547900
S	-2.88571400	1.97539400	0.20867700
O	-3.16459500	2.54084200	1.56853000
C	-4.41365700	1.88711600	-0.76211900
C	-1.93321200	3.16226200	-0.78189400
H	-5.06228600	1.16630600	-0.26118300
H	-4.86955700	2.88064900	-0.78143900
H	-4.17351800	1.53023600	-1.76677400
H	-1.89029300	2.80500500	-1.81422500
H	-2.42599700	4.13583900	-0.71473400
H	-0.92465500	3.20180200	-0.36254800
I	3.41780200	-1.73623400	0.01704000
S	2.81966900	1.94893000	-0.04967000
O	2.03702900	3.22701500	-0.17719500
C	4.11890200	1.87755900	-1.31564500
C	3.84553900	1.97600000	1.44812500
H	3.61668200	1.89139600	-2.28503500
H	4.76397600	2.75353000	-1.20841800
H	4.66747500	0.94089300	-1.18712200
H	4.40080300	1.03519000	1.49352300
H	4.50853000	2.84434000	1.41036500
H	3.16306300	2.05553200	2.29683800

2T

Cu	-1.37424100	-0.06120300	1.22608500
O	-0.00905300	-0.69968200	2.55455100
O	0.00899900	0.69962700	2.55456700
Cu	1.37421500	0.06117600	1.22611500
I	1.95549700	2.01562900	-0.34438800
I	-1.95548900	-2.01562200	-0.34447200
O	-2.33824600	1.49934600	0.51052300
S	-2.19991000	1.73369200	-1.02928600
C	-3.90663500	1.60703400	-1.63908000

C	-1.98327600	3.53196500	-1.13452100
H	-4.18105300	0.55330200	-1.55421400
H	-4.55919400	2.22612600	-1.01808800
H	-3.93612600	1.92229000	-2.68625900
H	-2.03464900	3.83516800	-2.18430100
H	-2.75608300	4.02347800	-0.53825000
H	-0.98959600	3.74080800	-0.73163900
O	2.33823500	-1.49935700	0.51054100
S	2.19993200	-1.73366900	-1.02927600
C	3.90666900	-1.60699600	-1.63903600
C	1.98329600	-3.53193900	-1.13456100
H	4.18109700	-0.55327000	-1.55411300
H	4.55920900	-2.22612500	-1.01806200
H	3.93617600	-1.92220100	-2.68623000
H	2.03466400	-3.83511400	-2.18434900
H	2.75610700	-4.02346700	-0.53830700
H	0.98961900	-3.74079500	-0.73167900

3S

Cu	-1.43279800	0.00829700	0.16799000
O	-0.02650600	-1.10887100	0.17900200
O	0.02650300	1.10886600	0.17903200
Cu	1.43279600	-0.00830200	0.16801100
I	3.18657100	1.89517600	0.02598300
I	-3.18657200	-1.89517600	0.02588700
O	-2.67464500	1.49256800	0.25946700
S	-4.01725300	1.49666100	-0.54555200
C	-5.31758100	1.32555500	0.71251800
C	-4.19797700	3.27429100	-0.87999900
H	-5.27262400	0.29062800	1.05724300
H	-5.11165300	2.01825500	1.53254500
H	-6.28569100	1.53287000	0.24669300
H	-5.17464600	3.45436300	-1.33834000
H	-4.08712500	3.82942800	0.05448300
H	-3.39957100	3.54509900	-1.57355300
O	2.67464200	-1.49257500	0.25946700
S	4.01726100	-1.49664700	-0.54553400
C	5.31757100	-1.32557400	0.71255800
C	4.19798900	-3.27426800	-0.88002500
H	5.27260900	-0.29065600	1.05731000
H	5.11163300	-2.01829600	1.53256400

H	6.28568800	-1.53287700	0.24674100
H	5.17466400	-3.45432800	-1.33835700
H	4.08712400	-3.82943000	0.05444100
H	3.39959200	-3.54505800	-1.57359700

3S-2

Cu	1.32046100	0.02943000	-0.07759600
O	-0.03540800	1.23849700	-0.10287100
O	-0.06439000	-1.14601400	-0.06907800
Cu	-1.41788700	0.05459100	-0.00096300
I	-3.15004000	-1.78526600	-0.00611200
S	-2.85089900	1.92244900	0.20511900
O	-3.16525400	2.38604000	1.59406500
C	-4.37729100	1.75348100	-0.75948100
C	-2.00691000	3.23058100	-0.72229200
H	-4.96731300	0.97069800	-0.27983500
H	-4.90510100	2.71078100	-0.74178600
H	-4.11891100	1.45208700	-1.77777600
H	-1.97294100	2.94915300	-1.77762400
H	-2.56202000	4.15969900	-0.56789000
H	-0.99007700	3.29135600	-0.32661600
I	3.12680400	-1.75375700	0.02362400
S	2.79112400	1.91881800	-0.03391600
O	2.13070100	3.25327800	-0.21317900
C	4.17080300	1.74985000	-1.20130800
C	3.68662400	1.86192900	1.54420900
H	3.74027500	1.79753100	-2.20355100
H	4.86387500	2.58046200	-1.04435600
H	4.64307600	0.77824900	-1.03721300
H	4.17039900	0.88496800	1.62540600
H	4.40763700	2.68311900	1.57226700
H	2.93983100	1.98381900	2.33157400

3T

Cu	-1.44705800	-0.02942800	0.45992600
O	-0.00391300	1.04521700	0.96614500
O	0.12037500	-1.11065900	0.99609300
Cu	1.45037300	-0.00696300	0.48167400
I	2.96170600	-1.96917500	-0.23876400
I	-2.94541900	1.99466500	-0.22484100
O	-2.67299600	-1.53462300	0.14261500

S	-4.22078900	-1.33959800	0.09897500
C	-4.64681000	-1.25384800	-1.66717600
C	-4.78852300	-3.03761900	0.41906800
H	-4.29363100	-0.28177400	-2.01756100
H	-4.14141800	-2.06657600	-2.19554600
H	-5.73374200	-1.32368200	-1.77174100
H	-5.87425700	-3.08273600	0.29392900
H	-4.27966500	-3.72196200	-0.26405800
H	-4.51943800	-3.27012500	1.45129100
O	2.62769100	1.47846400	0.08630700
S	4.18759200	1.34145200	0.09674100
C	4.66517500	1.30423000	-1.65639300
C	4.66212500	3.05558100	0.46988000
H	4.36189500	0.32587000	-2.03422500
H	4.14101100	2.10484400	-2.18454400
H	5.75071700	1.42038800	-1.72814900
H	5.74789900	3.15294100	0.38077400
H	4.14231900	3.72889000	-0.21573600
H	4.34907600	3.25135500	1.49722200

TS1BS

Cu	-1.52559500	0.01211400	0.10854100
O	-0.02536600	-0.99953300	0.12042000
O	0.02536400	0.99953200	0.12044700
Cu	1.52559300	-0.01211600	0.10856200
I	3.26291000	1.90639300	0.01706700
I	-3.26291000	-1.90639400	0.01697100
O	-2.73833300	1.52915200	0.17293700
S	-4.15863800	1.48682000	-0.48250400
C	-5.31840300	1.30844900	0.90586000
C	-4.41979000	3.25425300	-0.81968500
H	-5.21375400	0.28100600	1.26012200
H	-5.04797000	2.02092500	1.68945900
H	-6.33395100	1.48413400	0.53835900
H	-5.44382700	3.40279100	-1.17419900
H	-4.22575700	3.82713600	0.09021000
H	-3.70740500	3.53424200	-1.59809100
O	2.73833100	-1.52915700	0.17293500
S	4.15864400	-1.48680800	-0.48248500
C	5.31839000	-1.30847400	0.90589900
C	4.41979900	-3.25423200	-0.81971000

H	5.21373700	-0.28104100	1.26018600
H	5.04794600	-2.02097100	1.68947600
H	6.33394300	-1.48415100	0.53840700
H	5.44384100	-3.40276100	-1.17421400
H	4.22575400	-3.82713900	0.09016700
H	3.70742400	-3.53420000	-1.59813300

4S

Cu	-0.53288700	0.71158200	-0.19852300
O	1.22926600	1.08451600	-0.11762500
O	0.14413500	-1.00117200	-0.27082000
Cu	1.89809500	-0.62100700	-0.14685400
I	2.43534800	-3.11748400	-0.08368200
S	3.77995900	1.53901900	0.40348600
O	3.69722800	0.03334800	-0.07157600
C	3.62415500	2.54195200	-1.10202500
C	5.57611900	1.65983400	0.63971900
H	2.57813100	2.44719300	-1.39916400
H	4.29798000	2.15056800	-1.86872900
H	3.86115100	3.58070100	-0.85307200
H	5.83334100	2.69974800	0.86033500
H	6.08073000	1.30728200	-0.26278000
H	5.83003500	1.02053500	1.48724500
I	-1.20948500	3.18579700	0.12711500
O	-2.36167400	0.10564100	-0.38320300
C	-2.95351000	-0.58269600	0.48335800
C	-4.32368000	-1.03009900	0.17821200
C	-2.24439600	-0.88694700	1.77227500
C	-5.05827600	-1.85493400	1.05188800
C	-4.91154000	-0.61198600	-1.03461700
H	-2.78761400	-1.55010700	2.44435200
H	-2.06005700	0.06775000	2.28412800
H	-1.26748600	-1.31946800	1.51743000
C	-6.35128900	-2.25388500	0.71717700
H	-4.62719500	-2.19286300	1.98774900
C	-6.20299000	-1.01013700	-1.36132500
H	-4.33825200	0.02573300	-1.69849600
C	-6.92448300	-1.83244200	-0.48644900
H	-6.91067100	-2.89269700	1.39385700
H	-6.65047300	-0.68246800	-2.29479500
H	-7.93300600	-2.14410000	-0.74338600

4T

Cu	-0.33772700	0.78866100	-0.51590800
O	1.50827300	0.90113300	-0.71977700
O	0.14552100	-1.05583400	-1.16736800
Cu	1.83334400	-0.90946700	-0.54387400
I	1.15853700	-3.31399300	0.15336200
S	3.88381600	0.89529700	0.44694900
O	3.63443800	-0.60324200	-0.00021200
C	4.27607000	1.81073300	-1.07129400
C	5.57496400	0.70353000	1.08814000
H	3.32997400	1.88410900	-1.61001300
H	5.02876100	1.26031100	-1.64189000
H	4.63728300	2.80395100	-0.78810400
H	5.96717300	1.69119600	1.34731700
H	6.19731300	0.21547000	0.33439100
H	5.50866100	0.08058000	1.98215400
I	-0.10821700	3.22671300	0.38002500
O	-2.29858000	0.52402500	-0.48773500
C	-2.91724100	-0.17768100	0.34210000
C	-4.37680800	-0.32751500	0.17758700
C	-2.14373300	-0.82855900	1.45700300
C	-5.14286300	-1.19279500	0.98156800
C	-5.01549500	0.42056700	-0.83310300
H	-2.75738700	-1.33068500	2.20476400
H	-1.54532100	-0.05245900	1.95077600
H	-1.44279100	-1.54955900	1.01441800
C	-6.51719800	-1.30801700	0.77636600
H	-4.67304600	-1.78732800	1.75761500
C	-6.38793700	0.30858100	-1.02812300
H	-4.41505500	1.08388900	-1.44623700
C	-7.14084900	-0.55688400	-0.22435600
H	-7.10060900	-1.98209100	1.39633000
H	-6.87391200	0.89201600	-1.80443300
H	-8.21263800	-0.64534100	-0.37869300

TS2S

Cu	0.72645500	0.75642400	0.63731900
O	-0.96195000	1.16718200	0.12416800
O	-0.07244800	-0.92098600	0.74977600
Cu	-1.75118300	-0.50737200	0.11848500

I	-2.58763700	-2.93513500	0.09734500
S	-3.19339400	1.72647400	-1.11795000
O	-3.38518000	0.28891300	-0.48116200
C	-3.35674800	2.89999300	0.25717400
C	-4.84430500	1.91986200	-1.85093500
H	-2.44166400	2.78271600	0.84009700
H	-4.24469700	2.64901000	0.84320800
H	-3.42301200	3.91074100	-0.15648600
H	-4.93802300	2.93620400	-2.24413600
H	-5.60121100	1.71561300	-1.09014700
H	-4.91973200	1.19326100	-2.66199000
I	1.41537600	3.17449500	0.23441700
O	2.47713000	0.11130900	1.14484200
C	2.72948300	-1.13350300	0.93045300
C	3.81635500	-1.45141700	-0.02010700
C	1.91107300	-2.13522000	1.55847700
C	4.32684900	-2.75493500	-0.17137600
C	4.36518200	-0.40209500	-0.78382000
H	1.57334100	-1.89390200	2.56473300
H	2.10671300	-3.18696800	1.36992800
H	0.71944800	-1.77158200	0.96185900
C	5.35560200	-3.00435900	-1.07764800
H	3.93496600	-3.57119400	0.42708900
C	5.39249600	-0.65681600	-1.68846400
H	3.96947100	0.59976600	-0.65169800
C	5.88774800	-1.95748400	-1.83837300
H	5.74565000	-4.01187400	-1.18823200
H	5.80723200	0.15562000	-2.27791600
H	6.68991000	-2.15507700	-2.54410600

TS2S-2

Cu	-0.84008700	0.74875800	-0.55036500
O	0.79287700	1.30903600	-0.00171600
O	0.06215400	-0.87211800	-0.61440200
Cu	1.73555800	-0.28581900	-0.05028200
I	2.97369800	-2.50122100	-0.07768800
S	3.50860100	1.12077900	0.64890300
O	4.91714400	0.70197700	0.92110800
C	3.45621800	2.46073700	-0.57255300
C	2.78544800	1.94849500	2.09176000
H	3.90576100	2.06923900	-1.48754500

H	4.03979200	3.30324700	-0.19226000
H	2.40226800	2.70721200	-0.72623700
H	1.75776300	2.20934600	1.82471400
H	3.39558600	2.82177000	2.33687500
H	2.80788400	1.22668000	2.91094800
I	-1.69271000	3.10991700	-0.14452300
O	-2.52576300	-0.00178200	-1.12901200
C	-2.69540200	-1.26841500	-0.97741400
C	-3.79525000	-1.70883200	-0.09606400
C	-1.77563300	-2.17786300	-1.61258400
C	-4.20459400	-3.05427200	-0.01837100
C	-4.46402700	-0.73768500	0.67611200
H	-1.42724300	-1.86849100	-2.59678500
H	-1.89711900	-3.24860000	-1.47602400
H	-0.64324500	-1.75443400	-0.96567900
C	-5.25179100	-3.42064700	0.82451700
H	-3.71961800	-3.81259500	-0.62470300
C	-5.50928600	-1.10932600	1.51700600
H	-4.14590500	0.29700500	0.60044400
C	-5.90329800	-2.45051900	1.59419600
H	-5.56339800	-4.45949700	0.87878900
H	-6.01708600	-0.35700300	2.11323200
H	-6.71965700	-2.73940800	2.25031800

TS2T

Cu	-1.20151300	1.29342100	0.14863300
O	0.56931500	1.65928500	0.68175400
O	-0.83951400	-0.50754300	0.68554100
Cu	1.02007300	-0.40939300	0.55560500
I	1.33594700	-2.79419200	-0.53993200
S	4.10693400	-0.69262400	0.21232000
O	2.91312400	-0.03793700	0.97368600
C	4.70179300	-2.02691800	1.29587800
C	5.43026500	0.51175500	0.54096600
H	3.94922800	-2.81664400	1.24900600
H	4.80093900	-1.64205900	2.31427400
H	5.65968400	-2.38978300	0.91092400
H	6.37454700	0.12281500	0.14910300
H	5.49227400	0.69671500	1.61615600
H	5.15425200	1.42973700	0.01852900
I	1.52581700	2.95439300	-0.53869600

O	-3.00182000	1.13650800	-0.40044600
C	-3.49494600	-0.05151400	-0.57095700
C	-4.89449300	-0.24451900	-0.12168000
C	-2.66948000	-1.11198200	-1.04182000
C	-5.65354900	-1.35729500	-0.52683400
C	-5.48919500	0.72194000	0.71071100
H	-1.99006000	-0.84143900	-1.85362400
H	-3.10723600	-2.10057300	-1.14725500
H	-1.70418700	-1.04781500	-0.09587300
C	-6.97199300	-1.50586000	-0.09765400
H	-5.21935000	-2.09507900	-1.19404500
C	-6.80573000	0.57043900	1.13995900
H	-4.89919800	1.58047400	1.01299600
C	-7.54960600	-0.54485600	0.73827800
H	-7.55059100	-2.36719100	-0.41928700
H	-7.25318500	1.31821800	1.78883500
H	-8.57701000	-0.66253800	1.07217000

TS2BS

Cu	-0.72641200	0.75616800	-0.63786200
O	0.96192300	1.16725400	-0.12470600
O	0.07283600	-0.92108600	-0.75046100
Cu	1.75131300	-0.50720600	-0.11861700
I	2.58798100	-2.93488500	-0.09723600
S	3.19273100	1.72706300	1.11809600
O	3.38505400	0.28957400	0.48131700
C	3.35656700	2.90067400	-0.25688900
C	4.84326600	1.92069800	1.85189000
H	2.44176600	2.78332600	-0.84023700
H	4.24480500	2.64981800	-0.84254100
H	3.42253600	3.91140900	0.15684600
H	4.93676000	2.93716600	2.24481900
H	5.60055800	1.71622900	1.09154500
H	4.91829800	1.19435000	2.66320500
I	-1.41584300	3.17401500	-0.23449700
O	-2.47699100	0.11074000	-1.14529300
C	-2.72924200	-1.13401500	-0.93044400
C	-3.81604000	-1.45167100	0.02028400
C	-1.91077600	-2.13588200	-1.55816500
C	-4.32643200	-2.75517400	0.17203500
C	-4.36489600	-0.40212000	0.78366300

H	-1.57324100	-1.89492700	-2.56457400
H	-2.10628300	-3.18757800	-1.36918300
H	-0.71908700	-1.77190600	-0.96191000
C	-5.35511600	-3.00435400	1.07845100
H	-3.93452700	-3.57161000	-0.42617500
C	-5.39214300	-0.65660000	1.68845000
H	-3.96925700	0.59972100	0.65117500
C	-5.88729400	-1.95725100	1.83883900
H	-5.74508900	-4.01185700	1.18940700
H	-5.80690500	0.15601200	2.27764200
H	-6.68940600	-2.15465400	2.54468400

TS2BS-2

Cu	-1.26375400	1.24187100	-0.87188200
O	0.57471600	1.48555300	-0.36804700
O	-0.57019500	-0.55558500	-0.87032700
Cu	1.11947300	-0.42156800	-0.17800100
I	1.22865300	-2.99177700	-0.27606900
S	4.09236200	-0.91296400	0.43414600
O	2.85253500	0.01601500	0.62483800
C	4.26486900	-1.80536600	2.00880900
C	5.45553800	0.27062600	0.64826800
H	3.44110700	-2.52128700	2.04420500
H	4.19419000	-1.09094200	2.83314700
H	5.22528700	-2.32952100	2.01478200
H	6.40408300	-0.27401100	0.65703000
H	5.30583500	0.82720100	1.57641700
H	5.41801600	0.95008300	-0.20533700
I	1.59811800	3.20167100	0.08394600
O	-3.18838600	1.16540000	-0.84028800
C	-3.64447800	-0.03257000	-0.73370700
C	-4.86995500	-0.19242000	0.09071000
C	-2.96290100	-1.13977200	-1.34917000
C	-5.63074200	-1.37599600	0.08804100
C	-5.29185700	0.88735600	0.89003500
H	-2.66358600	-0.92701100	-2.37875400
H	-3.39368500	-2.13162000	-1.22914200
H	-1.65414800	-1.11772700	-0.88399600
C	-6.77923100	-1.47866400	0.87237600
H	-5.33692800	-2.21030900	-0.54032700
C	-6.44009300	0.78314700	1.67143200

H	-4.70034700	1.79653600	0.88421800
C	-7.18562700	-0.40121600	1.66596700
H	-7.36033500	-2.39643200	0.86032800
H	-6.75360900	1.62115800	2.28776600
H	-8.08085000	-0.48366100	2.27646300

5S

Cu	-0.20882800	0.88862300	-0.00038000
O	1.66225700	0.74029600	-0.02367000
O	-1.48858900	0.36306800	1.96606900
Cu	1.32340400	-1.30754700	-0.37226500
I	-0.42945300	-2.69559500	0.77581000
S	3.70588900	-0.03388300	-1.74110100
O	2.68061800	-1.20315900	-1.82596200
C	3.00130900	1.33600300	-2.70842500
C	4.95962800	-0.56329500	-2.95336000
H	2.17959100	1.71539200	-2.09871100
H	2.64414400	0.95414200	-3.66883700
H	3.76790500	2.10438600	-2.84671300
H	5.69722900	0.23380300	-3.08635700
H	4.46766100	-0.80814100	-3.89833700
H	5.44182900	-1.45305800	-2.54317600
I	2.46304000	1.86235800	1.51425600
O	-2.05916000	1.08289900	-0.55233300
C	-3.03972700	0.72997100	0.12982700
C	-4.39501400	0.80804200	-0.44359200
C	-2.82994500	0.22291400	1.55434100
C	-5.53187200	0.41476500	0.28868200
C	-4.54956900	1.27824300	-1.76245600
H	-3.15500700	-0.82595600	1.59824000
H	-3.46546400	0.80470700	2.23322800
H	-1.06748500	-0.53329100	1.91795900
C	-6.79798400	0.49359500	-0.28911400
H	-5.43422600	0.04371300	1.30436000
C	-5.81567800	1.35638200	-2.33406500
H	-3.66454400	1.57245500	-2.31669000
C	-6.94108800	0.96475700	-1.59825800
H	-7.67123300	0.18742600	0.27891900
H	-5.92976000	1.71881500	-3.35138900
H	-7.92908400	1.02501000	-2.04597200

5S-2

Cu	-0.62874600	1.14353900	-0.57882500
O	1.20543300	1.33283700	-0.87935500
O	-1.72428600	-0.31854600	-2.08950100
Cu	1.53697400	-0.43493500	-0.11160800
I	0.22754800	-2.62591200	-0.38363700
S	3.63091400	-1.07310500	0.98134300
O	4.73316900	-0.16786900	1.47036400
C	4.33566600	-2.29357200	-0.17832000
C	3.20014200	-2.24190000	2.31494600
H	4.68183300	-1.73865600	-1.05307200
H	5.17869000	-2.79639800	0.30430400
H	3.55188600	-3.00001300	-0.46584000
H	2.45522600	-2.94936000	1.94098100
H	4.11110000	-2.74759100	2.64769000
H	2.78122600	-1.65092000	3.13231100
I	2.10186000	2.99003600	-0.07202300
O	-2.46317000	1.10065400	0.03717400
C	-3.31868200	0.29065800	-0.36983300
C	-4.64805600	0.24865500	0.25993600
C	-2.97632900	-0.64745100	-1.52486200
C	-5.63411600	-0.66759900	-0.15553700
C	-4.93141700	1.14235200	1.31191800
H	-3.74970100	-0.55629500	-2.29754000
H	-2.98750000	-1.68072300	-1.15132800
C	-6.87915300	-0.68651200	0.47050300
H	-5.43456300	-1.36813100	-0.96081900
C	-6.17692600	1.12079200	1.93144400
H	-4.16188700	1.84058800	1.62394900
C	-7.15183100	0.20699000	1.51171500
H	-7.63547800	-1.39571600	0.14822800
H	-6.39139000	1.81199500	2.74098700
H	-8.12365900	0.19081300	1.99687300
H	-1.09255200	-1.04908700	-1.87659300

6S-2

Cu	-0.99161900	0.40029800	-0.65991500
O	0.43062300	1.21684300	0.14530800
O	0.07800000	-1.21328900	-0.40927400
Cu	1.62818100	-0.17527500	0.05874100
I	3.38119400	-2.03455600	-0.21612000

S	3.11371200	1.53254500	0.65942700	H	3.51333000	0.53141300	2.83026400
O	3.88471400	2.15683600	-0.45742400	H	1.54946200	2.29798100	2.45016500
C	4.24376600	0.93274700	1.94638700	H	2.75086200	3.57698600	1.99585300
C	2.20261600	2.79908000	1.58001100	H	1.33605000	3.19832000	0.92682900
H	4.85745900	0.15533400	1.48858400	I	-2.04772300	2.64210300	-0.32504100
H	4.85360800	1.77537900	2.28360500	O	-2.43162700	-0.48520100	-1.58971200
H	3.65091300	0.51149400	2.76260100	C	-2.56359300	-1.68666700	-1.07055600
H	1.72060700	2.33044200	2.44039300	C	-3.54429900	-1.86375300	0.02844200
H	2.92342000	3.56537400	1.87920400	C	-1.81037400	-2.73033500	-1.59190800
H	1.44336600	3.18807300	0.90225000	C	-3.61640100	-3.03859400	0.80226300
I	-1.96732000	2.70377600	-0.34146100	C	-4.43201200	-0.80759600	0.30637900
O	-2.39499500	-0.43663700	-1.57450100	H	-1.21654100	-2.55585300	-2.48157100
C	-2.62035000	-1.66087300	-1.13395300	H	-1.89538500	-3.75091500	-1.23850700
C	-3.57938000	-1.82828700	-0.01297500	C	-4.55537000	-3.15175400	1.82539300
C	-2.01611000	-2.72535700	-1.77597300	H	-2.92621600	-3.85780000	0.62464200
C	-3.66320600	-3.01850400	0.73351900	C	-5.37404400	-0.92769300	1.32690100
C	-4.42396500	-0.75312100	0.31689200	H	-4.36833700	0.09558800	-0.29129700
H	-1.37120100	-2.53344100	-2.62751500	C	-5.43928600	-2.09890300	2.08852700
H	-2.25893700	-3.75663600	-1.54793700	H	-4.59572700	-4.05921500	2.42117500
C	-4.57737600	-3.13115900	1.77949000	H	-6.05676900	-0.10723000	1.52863100
H	-2.99454800	-3.84671100	0.51763500	H	-6.17269800	-2.19173400	2.88477500
C	-5.34108600	-0.87170700	1.36079700	H	0.45304900	-1.53793500	-1.53735600
H	-4.35106900	0.16339400	-0.25951500				
C	-5.42158700	-2.06005000	2.09361100				
H	-4.62666600	-4.05110700	2.35524400				
H	-5.99273400	-0.03679000	1.60247400				
H	-6.13472300	-2.15121300	2.90830800				
H	0.25879400	-1.71528100	-1.23001800				

TS3S

Cu	-0.98473600	0.39907700	-0.76075700
O	0.43663700	1.20971800	0.04081200
O	0.15666600	-1.21409800	-0.66190800
Cu	1.65617100	-0.16002000	-0.00852200
I	3.45039300	-1.98386800	-0.19391000
S	3.05498600	1.58772200	0.72450300
O	3.86878900	2.26447100	-0.33088100
C	4.13484100	0.98141600	2.05158000
C	2.06656200	2.80478300	1.63285300
H	4.78453000	0.22543300	1.60754300
H	4.71163800	1.82777800	2.43453900

int1

C	3.02653300	-0.22696800	0.00030100
C	2.19163000	-1.34891300	0.00007100
C	0.80578900	-1.18677700	-0.00015200
C	0.24580600	0.10246300	-0.00020200
C	1.09280800	1.22459600	0.00001100
C	2.47569100	1.06032400	0.00027900
H	4.10550200	-0.35545700	0.00050300
H	2.62003700	-2.34705700	0.00008200
H	0.16627800	-2.06496700	-0.00031300
H	0.64006100	2.21112400	-0.00004300
H	3.12623300	1.93030500	0.00046200
C	-1.22243000	0.32578500	-0.00050600
O	-1.70733400	1.45749000	-0.00035600
C	-2.19154900	-0.85783600	-0.00071100
H	-1.99349000	-1.48224000	-0.88743300
H	-1.99215300	-1.48474000	0.88380000
O	-3.51621700	-0.40031800	0.00141900

H	-3.42973500	0.57961000	-0.00010000
7S			
Cu	-0.35470800	1.46361900	0.41056700
O	-1.58958700	0.14493500	0.87649300
Cu	-0.23457600	-1.11286600	0.39326900
I	1.83552300	-2.32801300	-0.06582800
S	2.48759100	2.19586300	0.20108800
O	1.00958900	2.70578100	0.02368000
C	3.41787900	3.74002500	-0.00952600
C	2.92166500	1.38974200	-1.36629500
H	3.17806300	4.37583800	0.84488600
H	3.10501500	4.22001400	-0.94004900
H	4.48683700	3.51037400	-0.01957000
H	4.00372800	1.22895300	-1.38162600
H	2.59906800	2.02504600	-2.19539800
H	2.41132800	0.42154900	-1.37659500
I	-3.26747600	0.16439500	-0.31920600

7S-2

Cu	0.00937400	-1.23708600	0.34146500
O	1.50118900	-0.14762500	0.84257200
Cu	0.37105000	1.27643200	0.36889700
I	-2.30296100	-1.85772300	-0.13914200
S	-1.29729100	2.68528200	-0.08394600
O	-1.09396600	4.17200400	-0.09963200
C	-2.65055500	2.22443600	1.03496600
C	-2.02612300	2.11342400	-1.64487700
H	-2.35063200	2.51001700	2.04527800
H	-3.54725900	2.77579700	0.73842900
H	-2.80074600	1.14134900	0.96499800
H	-2.21107000	1.03650100	-1.56353000
H	-2.95130400	2.66994500	-1.81917500
H	-1.30568800	2.32422300	-2.43782300
I	3.24057100	-0.30804200	-0.22820900

7T

Cu	1.54690200	-0.51868700	-0.49151800
O	0.26730600	-1.63001100	-1.14046100
Cu	-1.33549600	-1.10879500	-0.53280300
I	-0.54500000	1.43837600	-0.23902400

S	-3.85592200	-0.11271800	0.85332900
O	-3.18820800	-1.25845900	0.02439500
C	-4.63089400	0.97802400	-0.37695700
C	-5.35246800	-0.93079500	1.47438800
H	-3.81599400	1.48548300	-0.89797900
H	-5.22009200	0.37552400	-1.07317500
H	-5.25450700	1.70949300	0.14530900
H	-5.97842800	-0.18980800	1.97950500
H	-5.88089800	-1.39566800	0.63852900
H	-5.02553000	-1.69201100	2.18541100
I	3.75267500	-0.08871800	0.52993700

8Q

Cu	-1.16151200	-1.23004000	-0.81778900
O	-2.67358200	-0.29202700	-0.05079200
Cu	-1.83397500	1.42056400	0.05046700
I	-2.52335300	3.79506200	0.14679400
I	1.29985400	-2.27514300	-1.24858900
S	-3.66198400	-2.92508100	-1.81704400
O	-2.12093700	-2.71282800	-1.70614300
C	-4.32345700	-2.92341500	-0.12372000
C	-4.37641600	-1.35212200	-2.38596200
H	-3.90212400	-3.79487200	0.38179900
H	-4.01452500	-1.99548200	0.36568100
H	-5.41226900	-3.01499700	-0.18427600
H	-5.46449400	-1.46188700	-2.42265000
H	-4.07336000	-0.56205200	-1.69171300
H	-3.98690300	-1.17003500	-3.39003100
O	-0.19658300	0.40729800	-0.30894700
Cu	0.70755100	-0.30788800	1.20656600
Cu	1.51447000	0.55521800	-1.16163000
I	-1.62355400	-0.87756900	2.40048600
I	3.67913700	1.72065800	-1.48342800
S	3.60821800	-0.88416700	1.84966400
O	2.18779100	-0.56458300	2.43792300
C	4.61577700	0.54053200	2.34684100
C	4.24744400	-2.11057200	3.02657300
H	4.30054500	1.37755100	1.71960600
H	4.44228000	0.74897500	3.40567400
H	5.66641800	0.30998300	2.14842600
H	5.29838500	-2.30756900	2.79669400

H	4.12598000	-1.73020400	4.04390700
H	3.65682100	-3.01804800	2.88643700
8S			
Cu	-1.49384200	-1.38317400	-0.32353000
O	-2.28638700	-0.31406600	-1.58838500
Cu	-1.30905200	1.20780100	-1.39088700
I	-0.03447700	3.38880100	-1.25204700
I	0.13124100	-2.69002000	1.26127200
S	-4.32581100	-2.63949100	-0.78283800
O	-2.90039400	-2.70126400	-0.13469700
C	-4.99339900	-0.98825300	-0.43245800
C	-4.06523100	-2.50198500	-2.57630600
H	-5.13702600	-0.92936900	0.64838600
H	-4.25445500	-0.25586100	-0.77375600
H	-5.95407100	-0.89499400	-0.94819200
H	-5.03560400	-2.33611100	-3.05367800
H	-3.36821400	-1.67489600	-2.74764000
H	-3.64420200	-3.45477900	-2.90486700
O	-0.12425200	-0.09231000	-0.39936500
Cu	0.07786200	1.43437500	0.96365800
Cu	1.56350600	-0.94951800	-0.17884000
I	-2.32362700	1.55381000	1.78934600
I	3.80065400	-1.85623500	-0.95169300
S	3.19913800	1.99461700	1.16967100
O	2.01719000	0.95661100	1.11280800
C	4.54356000	1.01572200	1.89482400
C	3.82669700	2.14542800	-0.52774000
H	4.25061100	0.79016400	2.92207600
H	4.66109600	0.09665200	1.31260900
H	5.45560800	1.61971000	1.88564100
H	4.71669600	2.78169900	-0.49701200
H	4.05310600	1.15027600	-0.92151800
H	3.03752300	2.62638000	-1.11033700

9S

Cu	-0.47326600	0.69957000	0.06311300
O	1.28155000	1.12568300	0.09565600
O	0.26534900	-1.00798000	0.16152000
Cu	2.02088200	-0.55646100	0.15646600
I	2.53273100	-3.07040700	0.16059700

S	4.39716400	1.45012500	0.07490200
O	3.86732000	-0.02217000	0.15890700
C	3.60627900	2.38909400	1.41682600
C	3.60959300	2.22834800	-1.36769000
H	3.99106200	1.97468200	2.35143200
H	2.52197100	2.26382500	1.33777100
H	3.90906200	3.43597500	1.31919200
H	3.91611100	3.27836800	-1.39297500
H	2.52472800	2.11667600	-1.27414000
H	3.99289600	1.70625900	-2.24733600
I	-1.09008200	3.20385200	-0.07670700
O	-2.31605800	0.09463700	0.28328000
C	-2.96955700	-0.68718600	-0.43379600
C	-4.34160200	-1.03948100	-0.02407200
C	-2.37682600	-1.27015700	-1.71717900
C	-5.11713900	-1.96017200	-0.75560600
C	-4.88411100	-0.43288200	1.12612800
H	-2.38809700	-2.36774700	-1.61780300
C	-6.41092900	-2.26836000	-0.33981000
H	-4.71660900	-2.44086400	-1.64269100
C	-6.17784400	-0.74255500	1.53428300
H	-4.27741200	0.27781700	1.67710900
C	-6.94155700	-1.66052200	0.80309400
H	-7.00463600	-2.98066700	-0.90456100
H	-6.59350200	-0.27100400	2.41962000
H	-7.95097700	-1.90220000	1.12376300
O	-1.11027300	-0.77625200	-2.03550600
H	-0.45018300	-1.15178500	-1.38312300
H	-3.05126700	-1.01217400	-2.54259800

TS4S

Cu	-0.46157300	0.97115600	-0.00436500
O	1.25539100	1.05420300	0.56982300
O	-0.16627700	-0.77739500	0.56162200
Cu	1.67392300	-0.75847300	0.49917800
I	1.70632800	-3.24672300	-0.30374500
S	4.41142400	0.74355300	0.62477900
O	3.59575500	-0.59254600	0.59145500
C	3.74674100	1.74072000	1.99097100
C	3.85216000	1.74593600	-0.78387600
H	4.00808300	1.22012900	2.91505400

H	2.66057700	1.81515900	1.86381200
H	4.22991800	2.72206600	1.96410600
H	4.37775800	2.70476200	-0.74660100
H	2.76637400	1.86758400	-0.70835200
H	4.13482000	1.19919900	-1.68625300
I	-0.32596500	3.46662200	-0.53111700
O	-2.30852700	0.65709900	-0.56530400
C	-2.78991200	-0.51769700	-0.50415000
C	-4.13193300	-0.70338400	0.07219700
C	-1.94612700	-1.65767600	-0.88493500
C	-4.87632900	-1.88179800	-0.13103300
C	-4.69080900	0.34811400	0.82635700
H	-1.12017900	-1.53416200	0.07527200
C	-6.14792200	-2.00990100	0.42540200
H	-4.47861500	-2.68463100	-0.74373800
C	-5.95912100	0.21307000	1.38177500
H	-4.11118800	1.25482100	0.96437900
C	-6.68801700	-0.96667700	1.18452700
H	-6.72026400	-2.91794400	0.26109900
H	-6.38233100	1.02288900	1.96859600
H	-7.67905000	-1.07009400	1.61751500
O	-1.13427400	-1.40662100	-1.97845100
H	-0.35442800	-2.00191600	-1.90581800
H	-2.38059000	-2.65929300	-0.83397700

10S

Cu	-0.80550100	0.45250500	-0.54778100
O	0.65031100	1.23816600	0.24605900
O	0.14927700	-1.18073900	-0.01957300
Cu	1.76703700	-0.23809600	0.34264000
I	3.16343800	-2.39412400	-0.17674800
S	3.41183100	2.28801100	1.21165200
O	3.29596200	0.74559400	0.95671200
C	2.87542100	3.12583200	-0.30763900
C	2.05854800	2.75770200	2.32856100
H	3.60550100	2.86825100	-1.07818900
H	1.87412800	2.75567800	-0.55187800
H	2.88983200	4.20387600	-0.12152600
H	2.06649100	3.84711900	2.43051700
H	1.12529700	2.38640200	1.89067500
H	2.27271200	2.28982500	3.29212200

I	-1.59692600	2.85810000	-0.72233200
O	-2.22645600	-0.46416900	-1.39715000
C	-2.49695900	-1.60130000	-0.81254500
C	-3.53397400	-1.65000500	0.24222500
C	-1.86094300	-2.76561500	-1.24784800
C	-3.68408400	-2.73453200	1.12896900
C	-4.39628800	-0.54422300	0.36597000
H	-2.13288900	-3.75250000	-0.88873700
C	-4.68397700	-2.71860900	2.09965300
H	-3.00039800	-3.57819700	1.09039300
C	-5.39469800	-0.53368000	1.33856900
H	-4.26675900	0.29356100	-0.31156900
C	-5.54542500	-1.62100500	2.20540900
H	-4.78309900	-3.55733400	2.78299200
H	-6.05604000	0.32426200	1.42035500
H	-6.32300000	-1.61121300	2.96410600
H	0.34555100	-1.74642000	-0.79552600
O	-0.93723000	-2.69423900	-2.22741100
H	-0.59691500	-3.58436100	-2.42690800

TS5S

Cu	-0.88691500	0.44913900	-0.72633600
O	0.48931500	1.27186600	0.15195800
O	0.21737300	-1.17567500	-0.35331900
Cu	1.72065400	-0.11076900	0.32389000
I	3.31706300	-2.10882400	-0.27463200
S	3.01472900	2.46934900	1.58890700
O	3.05471600	0.94068000	1.25340700
C	2.63277900	3.33350800	0.03915500
C	1.46679300	2.77749000	2.48621600
H	3.48412800	3.17569600	-0.62669100
H	1.71259300	2.88642100	-0.35686900
H	2.51853000	4.39909800	0.25926200
H	1.36647700	3.85671700	2.63637200
H	0.65443800	2.36288900	1.87548300
H	1.55435300	2.27106800	3.45014200
I	-1.92248300	2.74743200	-0.85834700
O	-2.29707600	-0.66568900	-1.48747900
C	-2.26059300	-1.76213600	-0.80597600
C	-3.13959200	-1.94010300	0.36609600
C	-1.31469600	-2.76600700	-1.15982200

C	-3.30343000	-3.17161000	1.03345400	I	-2.17382400	-2.86495600	0.32628500
C	-3.86446700	-0.81839100	0.81679500	S	-3.78590200	0.46042000	-0.53599400
H	-1.12742100	-3.63528700	-0.53934800	O	-5.09376500	-0.26043900	-0.63045000
C	-4.15034600	-3.26910000	2.13519700	C	-3.67620300	1.42745100	0.99429200
H	-2.78942300	-4.06424400	0.68861000	C	-3.70294300	1.78868100	-1.77019200
C	-4.70961100	-0.92218900	1.91879000	H	-3.69891600	0.71467800	1.82133500
H	-3.74995300	0.12407700	0.28995900	H	-4.53738600	2.09900700	1.04539100
C	-4.85296600	-2.14516000	2.58370100	H	-2.72496700	1.96524100	0.96512400
H	-4.26840000	-4.22347300	2.64009800	H	-2.71567900	2.25073700	-1.68342500
H	-5.25783900	-0.04866800	2.25946700	H	-4.51739400	2.49257000	-1.57985900
H	-5.51393300	-2.22527000	3.44210400	H	-3.82905200	1.31760000	-2.74721500
H	0.63647100	-1.48186500	-1.18734700	I	0.65237600	3.44287500	0.48671500
O	-0.76973600	-2.74493500	-2.38297800	O	2.44423000	0.51129900	0.45472000
H	-0.12681300	-3.47349000	-2.46927200	C	2.81000000	-0.70712700	0.47677500
int3				C	4.14790300	-1.05139400	-0.02868000
O	3.26126400	0.16228800	0.47794400	C	1.84106800	-1.73404500	0.87272100
O	1.34091700	1.73530800	-0.20612400	C	4.76644000	-2.27950400	0.27709100
C	0.94750600	0.59406700	0.02761300	C	4.83372000	-0.10700200	-0.81903900
C	-0.48569700	0.23069400	0.02570600	H	1.07606600	-1.57943400	-0.13137700
C	2.03420400	-0.46805000	0.32773400	C	6.03980900	-2.56166000	-0.21436500
C	-0.91650400	-1.10121600	0.15891500	H	4.26999600	-3.00040500	0.91894800
C	-1.43539400	1.26127500	-0.10046400	C	6.10313200	-0.39593700	-1.30926300
H	1.82602400	-1.01586200	1.25742200	H	4.34999000	0.83916700	-1.03755200
H	3.14633300	1.03679400	0.03832700	C	6.70649600	-1.62411300	-1.01000400
C	-2.28081300	-1.39325400	0.16791400	H	6.51520200	-3.50712900	0.02874300
H	-0.18611100	-1.90151300	0.21697500	H	6.62448600	0.33125000	-1.92452200
C	-2.79529600	0.96542200	-0.08483300	H	7.69856300	-1.84763600	-1.39218500
H	-1.08011900	2.28162500	-0.20535100	O	1.00553600	-1.33043700	1.90657900
C	-3.21897400	-0.36287500	0.05094900	H	0.17147600	-1.84363600	1.83103500
H	-2.61276500	-2.42319100	0.26245400	H	2.17858800	-2.77217900	0.91250000
H	-3.52673800	1.76317400	-0.17793300	TS6S			
H	-4.28080600	-0.59386900	0.06253100	Cu	-0.51273900	0.58231400	-0.09097700
O	1.99604300	-1.35417200	-0.78942000	O	1.20802600	1.11591800	-0.39291200
H	2.83419000	-1.85091700	-0.75483000	O	0.27826400	-1.15298400	-0.24178500
TS4S-2				Cu	2.02578200	-0.53138500	-0.23700100
Cu	0.63239200	0.96088500	-0.09504000	I	2.85309300	-2.95113400	0.03343000
O	-1.06734200	1.24036400	-0.65838400	S	4.24264500	1.65928200	-0.20815400
O	0.20973000	-0.75455100	-0.69303700	O	3.81835500	0.14885300	-0.24039600
Cu	-1.62733800	-0.52082400	-0.57363100	C	3.47719300	2.47569600	-1.64228700
				C	3.34439200	2.46009400	1.15449500

H	3.94674300	2.04260400	-2.52835000
H	2.40112900	2.28211900	-1.62224500
H	3.70713000	3.54366100	-1.58081700
H	3.60383900	3.52300900	1.14351800
H	2.27312500	2.29144400	1.01045200
H	3.70710900	1.99722100	2.07507700
I	-1.13059500	3.02862600	0.29891800
O	-2.42569900	0.03552200	-0.54485300
C	-3.06564900	-0.68669600	0.23872500
C	-4.45953700	-1.05167600	-0.08316000
C	-2.38740100	-1.17589400	1.52989500
C	-5.20781100	-1.90019100	0.75435400
C	-5.04925000	-0.53146600	-1.25120600
H	-3.01425000	-0.81227300	2.36583800
C	-6.52376400	-2.22138700	0.42610900
H	-4.76779300	-2.31127800	1.65759600
C	-6.36404800	-0.85541900	-1.57392800
H	-4.46140600	0.12389500	-1.88525300
C	-7.10196400	-1.70046800	-0.73649400
H	-7.09769300	-2.87694900	1.07413700
H	-6.81589600	-0.45148900	-2.47504800
H	-8.12780100	-1.95325000	-0.98970400
O	-1.09406100	-0.74855900	1.64787400
H	-0.17842600	-1.31762800	0.73319400
H	-2.48081500	-2.27916200	1.52655400

TS6S-2

Cu	-0.63767100	0.58754600	-0.12660300
O	1.05011600	1.22897000	-0.40593000
O	0.20791000	-1.11656400	-0.27483400
Cu	1.92830900	-0.38214400	-0.25253100
I	3.17601500	-2.57066800	0.02729300
S	3.81764300	1.02396300	-0.19060800
O	5.24943000	0.60241600	-0.14837200
C	3.40340700	2.07710200	1.22704200
C	3.52001300	2.15324100	-1.57805700
H	3.56995800	1.47551000	2.12309100
H	4.07065900	2.94295500	1.21925600
H	2.35031600	2.34955000	1.12281100
H	2.44936700	2.37454400	-1.59104800
H	4.13404900	3.04597000	-1.43408700

H	3.82600400	1.62038200	-2.48075100
I	-1.36780400	2.99414500	0.26846300
O	-2.51272600	-0.04311800	-0.53435200
C	-3.11372400	-0.79608500	0.25247000
C	-4.49229500	-1.21723400	-0.06138500
C	-2.40728700	-1.26334400	1.53774600
C	-5.19784200	-2.10070800	0.77749700
C	-5.11252800	-0.71524200	-1.22198800
H	-3.04000100	-0.92180300	2.37791200
C	-6.50194300	-2.47392900	0.45787300
H	-4.73416300	-2.49849800	1.67475700
C	-6.41529400	-1.09161700	-1.53584100
H	-4.55821500	-0.03251400	-1.85727200
C	-7.11057000	-1.97095600	-0.69717400
H	-7.04301000	-3.15608400	1.10660700
H	-6.89088000	-0.70186300	-2.43088200
H	-8.12709600	-2.26456300	-0.94357300
O	-1.12863600	-0.79215300	1.64912300
H	-0.25034200	-1.29286300	0.71720100
H	-2.46303400	-2.36884600	1.53130500

11S

Cu	0.47708900	0.31442800	-0.62542300
O	-0.88125100	0.92653100	0.41710600
O	-0.55388900	-1.35771000	-0.42372300
Cu	-2.05830900	-0.48573400	0.25125800
I	-3.61248900	-2.41692100	-0.49775400
S	-3.50408500	1.83706300	1.74708000
O	-3.49692100	0.37985400	1.16327100
C	-2.07539500	1.99425600	2.86047400
C	-3.02622600	2.96845500	0.40720700
H	-2.27967200	1.34550900	3.71520600
H	-1.18012700	1.67980700	2.31583500
H	-2.01965100	3.03713000	3.18696900
H	-2.97931800	3.97820000	0.82587800
H	-2.06481700	2.63813000	0.00438100
H	-3.82146800	2.91029900	-0.33938800
I	1.24674800	2.70328500	-0.85843800
O	2.25902000	-0.49884800	0.72364800
C	3.18240300	-0.74960400	-0.05489300
C	4.50755500	-1.19858300	0.44581600

C	2.95424800	-0.54847600	-1.55584400
C	5.58295700	-1.47252300	-0.41783100
C	4.68141600	-1.34792500	1.83339600
H	3.60170500	0.28863400	-1.87658000
C	6.81025400	-1.88761900	0.09964800
H	5.47020300	-1.36024900	-1.49224700
C	5.90627000	-1.76613000	2.34695800
H	3.84054000	-1.13133200	2.48439800
C	6.97246500	-2.03613700	1.48063100
H	7.63785200	-2.09629000	-0.57211300
H	6.03396200	-1.88230000	3.41946400
H	7.92842100	-2.36206300	1.88136600
O	1.62631000	-0.34169000	-1.89094700
H	-0.76368400	-1.79954600	-1.27208300
H	3.29919500	-1.44772300	-2.09361600

TS7S

Cu	0.54193200	0.56545500	-1.00800000
O	-0.96819200	1.02891600	-0.02642700
O	-0.06529500	-1.20554900	-0.76961300
Cu	-1.71995800	-0.71791300	0.19696500
I	-2.53933300	-3.15021000	-0.45675000
S	-3.32811300	1.06833000	2.27838700
O	-3.02792400	-0.28393400	1.56658100
C	-1.73983000	1.73938800	2.85318200
C	-3.71499900	2.27035400	0.97291200
H	-1.39982900	1.08764800	3.66118800
H	-1.04025200	1.72568400	2.01088000
H	-1.90914200	2.75075700	3.23443300
H	-3.84814200	3.25335500	1.43412900
H	-2.90125600	2.27252100	0.24313900
H	-4.65101300	1.94233200	0.51537700
I	-0.16243400	3.15364800	-0.80790200
O	2.39734100	0.47715300	0.41591300
C	3.24303000	-0.15945300	-0.22426600
C	4.48913100	-0.63677600	0.42398800
C	2.94787900	-0.48269400	-1.69146100
C	5.46112100	-1.37295400	-0.27714200
C	4.69361500	-0.34396000	1.78466100
H	3.83541700	-0.26265500	-2.30772200
C	6.61577000	-1.80830200	0.37336100

H	5.31986000	-1.61293300	-1.32683800
C	5.84909300	-0.77562600	2.43016600
H	3.93193100	0.22280800	2.31030900
C	6.81143200	-1.50889200	1.72522100
H	7.36173400	-2.37876300	-0.17223200
H	6.00279100	-0.54520400	3.48053200
H	7.71242600	-1.84727200	2.22948900
O	1.88964400	0.25710300	-2.19422500
H	-0.32821200	-1.60359400	-1.62641200
H	2.77784300	-1.57493000	-1.75549000

TS7S-2

Cu	0.69228300	0.48839900	-0.79377900
O	-0.67100800	1.05589700	0.33672900
O	0.15746400	-1.32289800	-0.52015200
Cu	-1.57041700	-0.64180000	0.22436800
I	-3.34538200	-2.10763500	-0.92076500
S	-2.76774100	0.10663300	2.12769300
O	-3.63909300	-0.74693200	2.99711400
C	-3.72217200	1.45777500	1.38301600
C	-1.62066400	1.05925500	3.16811400
H	-4.44486100	0.99315300	0.70882800
H	-4.23111400	2.01209700	2.17633800
H	-3.02514900	2.08603300	0.82308300
H	-0.96239200	1.62268200	2.50391500
H	-2.20224400	1.69888100	3.83743700
H	-1.04890500	0.32932700	3.74487900
I	0.05519600	3.00993000	-0.69375200
O	2.66669400	0.36746400	0.45064000
C	3.42201100	-0.31027500	-0.25668800
C	4.69633200	-0.84524700	0.27833000
C	2.97794500	-0.62350800	-1.68922800
C	5.56819400	-1.62179300	-0.50630600
C	5.03325500	-0.56641600	1.61568800
H	3.81235800	-0.45578300	-2.38954100
C	6.75524700	-2.11043800	0.03927000
H	5.32421300	-1.85157600	-1.53935500
C	6.22086200	-1.05164300	2.15596400
H	4.34775800	0.03205600	2.20694100
C	7.08293900	-1.82466900	1.36839400
H	7.42381300	-2.71140500	-0.57004700

H	6.47748200	-0.83200000	3.18829500
H	8.00903200	-2.20463900	1.79080500
O	1.92487300	0.18070900	-2.09984200
H	-0.08217400	-1.74726700	-1.36934800
H	2.73666600	-1.70286100	-1.72824800

12S

Cu	1.22541900	-1.02551200	0.04816900
O	0.02380200	0.51723300	0.05665900
O	-0.51351500	-1.73197800	-0.05270600
Cu	-1.80203600	-0.35453500	0.02111800
I	-3.79311100	-2.05570100	-0.08499000
S	-4.19803300	1.51808200	-0.37759700
O	-2.74804500	1.36334200	0.17739700
C	-5.28593400	1.39806900	1.07477100
C	-4.29051000	3.31852300	-0.62114300
H	-5.26946500	0.34987500	1.38053800
H	-4.89535900	2.04200700	1.86716500
H	-6.29810200	1.69300500	0.78181800
H	-5.31259500	3.59045500	-0.90038200
H	-3.98103900	3.82225500	0.29773900
H	-3.60108600	3.56215100	-1.43177900
I	0.55099700	2.46055700	0.05141500
O	2.99462300	-0.12824000	0.04604200
C	3.93154400	-0.96443700	0.02276900
C	5.32517600	-0.48631600	-0.01053400
C	3.54884200	-2.42981000	0.00591600
C	6.40795000	-1.38607700	-0.03391400
C	5.57386000	0.89962000	-0.02151800
H	3.95800500	-2.84092300	-0.94295400
C	7.71549700	-0.90527100	-0.06935800
H	6.23030500	-2.45731300	-0.02496900
C	6.88224800	1.37456800	-0.05495000
H	4.72848400	1.57978100	-0.00356000
C	7.95356800	0.47362100	-0.07926100
H	8.54802000	-1.60233900	-0.08788700
H	7.07056600	2.44420000	-0.06272300
H	8.97408400	0.84560500	-0.10551700
O	2.19201300	-2.63146900	0.13605400
H	-0.70790800	-2.68306200	0.04665800
H	4.11413200	-2.93702800	0.81333300

TS8S

Cu	-0.45760300	-1.84576600	0.36433500
O	1.02432100	-0.96517000	1.12853000
O	-0.73204300	-0.37272400	-1.36157900
Cu	0.38984700	0.66632300	-0.17867700
I	1.98497200	1.53450700	-2.08427500
S	1.87139900	2.69950100	1.58849500
O	0.52422900	1.97242400	1.30835200
C	1.69138600	3.14315300	3.34407900
C	3.13333900	1.40185100	1.79454500
H	0.87299600	3.86306000	3.40775500
H	1.44705100	2.24347300	3.91409300
H	2.62059700	3.59947800	3.69728900
H	4.01535700	1.84582700	2.26636800
H	2.70550400	0.59318600	2.39216300
H	3.37805300	1.04255200	0.79203500
I	2.40900200	-2.28538100	0.42482100
O	-2.34965100	-0.45294800	1.08967700
C	-3.19060600	-0.74449700	0.22976000
C	-4.48016900	-0.02273700	0.12973400
C	-2.77315300	-1.81079300	-0.77910800
C	-5.54640800	-0.48495300	-0.66288200
C	-4.63514600	1.16109800	0.87632600
H	-3.50574200	-2.17835200	-1.50698000
C	-6.74302300	0.23074600	-0.71252700
H	-5.45468500	-1.40822600	-1.22564100
C	-5.82887800	1.87438000	0.81971000
H	-3.80346000	1.50023300	1.48553900
C	-6.88427700	1.41022800	0.02457500
H	-7.56500800	-0.13295000	-1.32213000
H	-5.94058400	2.79134500	1.39115900
H	-7.81627300	1.96707000	-0.01863300
O	-1.96575700	-2.74166600	-0.27484900
H	-0.30048000	-0.37502200	-2.24326400
H	-1.97861100	-1.01374900	-1.38501900

TS8S-2

Cu	0.29642300	-2.07903100	0.02737200
O	1.48080400	-0.93507500	0.94355000
O	-0.28146200	-0.55527100	-1.59834900

Cu	0.31068700	0.54347000	-0.12442700
I	1.34343500	2.48500800	-1.48328900
S	-0.20204800	1.53655200	1.99327800
O	-1.44847000	2.35637200	2.21330400
C	1.25849100	2.51868000	2.43578500
C	-0.08211700	0.25342300	3.27408500
H	1.33139500	3.32707600	1.70599100
H	1.12474000	2.91031900	3.44789800
H	2.13749600	1.87276800	2.36293700
H	0.81906600	-0.33233200	3.07466600
H	-0.06363100	0.73389900	4.25600600
H	-0.96763500	-0.37314300	3.16169800
I	3.23460800	-1.52590800	0.10352700
O	-1.72466500	-0.98017100	0.82296900
C	-2.54953400	-1.34583000	-0.03447800
C	-3.87675900	-0.71670300	-0.15508200
C	-2.03641900	-2.36265200	-1.05424600
C	-4.93276700	-1.33632100	-0.85083100
C	-4.08449700	0.53499000	0.46058700
H	-2.75916200	-2.83664100	-1.72815800
C	-6.17631700	-0.71140400	-0.93231800
H	-4.79468700	-2.31286300	-1.30422400
C	-5.32632900	1.15706500	0.36369000
H	-3.26580500	1.01448100	0.98998100
C	-6.37206000	0.53576900	-0.33000800
H	-6.99141300	-1.19589200	-1.46172700
H	-5.47864100	2.12780200	0.82583100
H	-7.34018200	1.02384200	-0.40129500
O	-1.07219300	-3.17241300	-0.60908000
H	0.11380300	-0.23946800	-2.43704600
H	-1.43730600	-1.47535000	-1.68524500

int2

O	-3.47074700	-0.62469700	-0.12828800
O	-1.75265400	1.55765700	-0.11537300
C	-1.30818300	0.42519900	0.01385400
C	0.14915900	0.12860500	0.01745900
C	-2.31668000	-0.72668000	0.22438900
C	0.66176300	-1.17976700	-0.05882600
C	1.04040500	1.21683000	0.06485900
H	-1.95329900	-1.63284600	0.75256900

C	2.04135600	-1.39185900	-0.08107800
H	-0.00448200	-2.03497100	-0.12042500
C	2.41492100	1.00154600	0.05291700
H	0.62460100	2.21856200	0.11072500
C	2.91728800	-0.30441700	-0.01913600
H	2.43164900	-2.40329400	-0.14667500
H	3.09794900	1.84509400	0.09627800
H	3.99061100	-0.47296000	-0.02980500

H₂O

O	0.00000000	0.00000000	0.12008500
H	0.00000000	-0.76324400	-0.48034000
H	0.00000000	0.76324400	-0.48034000

13S

Cu	-0.39266300	0.73482700	-0.15407800
O	1.35317300	1.18596700	-0.13424000
O	0.36589000	-0.95367700	-0.34518800
Cu	2.11361900	-0.48640600	-0.21110600
I	2.65277100	-2.99160300	-0.26291200
S	4.45962000	1.53859300	0.06122800
O	3.95016200	0.06393500	-0.08631500
C	3.73215900	2.50261500	-1.29861500
C	3.58916500	2.27534100	1.47777600
H	4.16971300	2.11380600	-2.22091400
H	2.64636600	2.36713500	-1.28087400
H	4.01933100	3.54933800	-1.16058400
H	3.88652200	3.32613700	1.54531900
H	2.51178000	2.15967500	1.32342000
H	3.92854100	1.73382500	2.36369500
I	-1.04811900	3.21438000	0.15605800
O	-2.22831200	0.12455900	-0.36167000
C	-2.91560100	-0.68129500	0.29498600
C	-4.31554400	-0.89391400	-0.09849400
C	-2.32899500	-1.37834900	1.54928400
C	-5.14026600	-1.83714400	0.54794200
C	-4.84617500	-0.09847200	-1.13666900
H	-2.94206300	-1.07378200	2.41136500
C	-6.47015900	-1.97836200	0.15662100
H	-4.72795500	-2.47247400	1.32307800
C	-6.17464700	-0.24557900	-1.51919400

H	-4.20294500	0.62980700	-1.61877200
C	-6.98802200	-1.18529200	-0.87265200
H	-7.10223600	-2.70981100	0.65109300
H	-6.58030400	0.37012600	-2.31627800
H	-8.02622700	-1.29887500	-1.17230600
O	-1.03748700	-0.99458900	1.85324200
H	-0.42182200	-1.25468100	1.09638900
O	-2.44944200	-2.76788800	1.28957200
H	-1.95024400	-3.21286200	2.00018000

TS9S

Cu	-0.45050300	0.65506700	-0.21205400
O	1.28418200	1.17850700	-0.32424100
O	0.33259200	-1.08136700	-0.44681200
Cu	2.08009000	-0.48425300	-0.26954600
I	2.86933000	-2.92851600	-0.16380100
S	4.30712800	1.66395700	0.09965400
O	3.87314000	0.16828200	-0.09335100
C	3.64509300	2.61703400	-1.30150200
C	3.33150400	2.35487600	1.46939000
H	4.16077100	2.25059900	-2.19197900
H	2.56662400	2.45012800	-1.36526100
H	3.89138300	3.66979700	-1.13343900
H	3.60443800	3.40956500	1.57110000
H	2.26960300	2.22013900	1.24517500
H	3.62822400	1.80499100	2.36539600
I	-1.03711100	3.11088500	0.20975900
O	-2.32558900	0.13924300	-0.55695800
C	-2.96658000	-0.62623800	0.18935600
C	-4.37718500	-0.90042600	-0.11734700
C	-2.25958100	-1.21075600	1.45810800
C	-5.14051200	-1.79446400	0.66022700
C	-4.97973300	-0.22446800	-1.19947100
H	-2.83903200	-0.85033700	2.33235500
C	-6.48387300	-2.00449900	0.35323500
H	-4.66935300	-2.33700800	1.47162500
C	-6.32057100	-0.44026700	-1.49756100
H	-4.38140200	0.46567700	-1.78482300
C	-7.07392300	-1.33014800	-0.72057100
H	-7.07026400	-2.69743300	0.94922500
H	-6.78242400	0.08245600	-2.32990600

H	-8.12202600	-1.49711600	-0.95379900
O	-0.97303100	-0.83899900	1.55649800
H	-0.13089200	-1.30936200	0.50789300
O	-2.43554000	-2.63332300	1.32095700
H	-1.69919200	-3.00716600	1.84067500

TS9S-2

Cu	-0.57229100	0.67591400	-0.23493700
O	1.12574400	1.30996400	-0.34236600
O	0.26374100	-1.02114000	-0.49747500
Cu	1.98466900	-0.31762900	-0.30242400
I	3.18762400	-2.54360100	-0.16106500
S	3.88416200	1.03990100	0.01311300
O	5.30641100	0.59337800	0.09346500
C	3.39579800	1.94649700	1.50636500
C	3.67853900	2.31153300	-1.26347900
H	3.50100800	1.25244600	2.34286500
H	4.07110300	2.79734400	1.62883700
H	2.35398800	2.24674000	1.36993300
H	2.61314700	2.55206200	-1.31462200
H	4.29237500	3.17439200	-0.99254800
H	4.03048800	1.87061700	-2.19844100
I	-1.27942100	3.08039600	0.24641600
O	-2.41570500	0.07390500	-0.54508300
C	-3.01131200	-0.74445900	0.18331600
C	-4.41099200	-1.07071000	-0.11818200
C	-2.26806100	-1.34011900	1.42674900
C	-5.12849400	-2.01720300	0.64133600
C	-5.05260500	-0.39074800	-1.17558800
H	-2.85021300	-1.02756200	2.31640800
C	-6.46492700	-2.27452000	0.34101000
H	-4.62767000	-2.56179800	1.43320300
C	-6.38610300	-0.65442400	-1.46708100
H	-4.49033500	0.34002100	-1.74711600
C	-7.09352900	-1.59621200	-0.70820500
H	-7.01579000	-3.00728600	0.92296800
H	-6.87792200	-0.12881400	-2.28012000
H	-8.13608800	-1.80047500	-0.93628000
O	-0.99468600	-0.91971400	1.52998000
H	-0.20342700	-1.28129600	0.48068700
O	-2.38686800	-2.76121000	1.24516300

H	-1.63998500	-3.12446500	1.75738000	O	1.01018400	1.40058500	0.00186600
				O	0.13556400	-0.78794400	-0.26187200
TS10S				Cu	1.88225900	-0.22723700	0.09034100
Cu	0.19560400	1.24862900	-0.17330700	I	2.97402200	-2.51995600	0.11192200
O	-1.62888200	1.11119200	-0.25008700	S	3.75565500	1.16532100	0.56660400
O	-0.15760100	-0.55657700	-0.46136800	O	5.15784400	0.71045000	0.82092400
Cu	-2.00205600	-0.73911600	-0.21832100	C	3.70579700	2.38594700	-0.77443600
I	-1.55554600	-3.33797600	0.17864100	C	3.14104900	2.17211300	1.94537200
S	-4.80807300	0.59046100	0.06585600	H	4.08745200	1.88851900	-1.66859400
O	-3.93605900	-0.70335400	-0.04100600	H	4.34732600	3.22953700	-0.50642200
C	-4.34388600	1.64314400	-1.33924400	H	2.65817000	2.67186400	-0.90211900
C	-4.08836300	1.58425900	1.40470500	H	2.11814100	2.46400300	1.69231300
H	-4.68260000	1.13320000	-2.24398400	H	3.80641500	3.02899300	2.07977000
H	-3.25077400	1.75576900	-1.32160500	H	3.15798000	1.53576600	2.83278200
H	-4.85570800	2.60475700	-1.23635500	I	-1.50554800	3.28663300	-0.25300800
H	-4.62130000	2.53853700	1.45338400	O	-2.38039100	0.04973700	-0.93704100
H	-3.02216000	1.71852400	1.17813300	C	-2.70212100	-1.13388700	-0.62908400
H	-4.23734400	1.02343900	2.33014500	C	-3.90785700	-1.35890400	0.17604000
I	0.32505800	3.75414100	0.14217500	C	-1.69657400	-2.18257900	-1.06146100
O	2.19497600	0.65176800	0.04539600	C	-4.42501100	-2.63454200	0.49304600
C	2.77426700	-0.44400900	-0.06066300	C	-4.58971900	-0.20291000	0.62527200
C	4.24211000	-0.51033500	-0.03502500	H	-0.76889200	-1.81038700	-0.31519300
C	1.93495700	-1.72979100	-0.17847100	C	-5.59530300	-2.74034500	1.24193200
C	4.93359900	-1.73086400	0.09757900	H	-3.91256900	-3.52624500	0.15916500
C	4.96094700	0.70274900	-0.08790600	C	-5.75495200	-0.32179700	1.37242500
H	0.77188800	-1.24959900	-0.56372200	H	-4.18494600	0.77164900	0.37289000
C	6.32475100	-1.73284600	0.17290200	C	-6.26026000	-1.59137700	1.68203100
H	4.38450300	-2.66374200	0.14925500	H	-5.98898600	-3.72292300	1.48410300
C	6.34963600	0.68940600	-0.02452200	H	-6.27021600	0.57009000	1.71590400
H	4.41048000	1.63343400	-0.17845800	H	-7.17108100	-1.68388100	2.26721500
C	7.03195100	-0.52761700	0.10649800	O	-2.06775600	-3.49222700	-0.88539400
H	6.85797700	-2.67224400	0.28228400	H	-1.43687500	-4.02248200	-1.41054800
H	6.90320400	1.62216700	-0.07381300	O	-1.15392200	-1.98802500	-2.32227200
H	8.11713900	-0.53532500	0.15864300	H	-0.38062700	-1.40105400	-2.18199200
O	2.38709700	-2.55302100	-1.18247200				
H	1.86093300	-3.37876600	-1.15257600	30S			
O	1.69071700	-2.29672500	1.03379800	Cu	-0.21635100	1.11219200	0.07474600
H	0.77412500	-2.70100700	1.02973200	O	1.54706600	0.82843400	0.08463600
TS10S-2				O	-0.87111000	-0.86051500	1.17379100
Cu	-0.67823600	0.89056800	-0.39944100	Cu	1.83041300	-0.97436500	0.09082900
				I	1.13724200	-3.46088800	-0.29954300

S	4.70802900	0.35094700	0.38629600
O	3.79550900	-0.91337000	0.41422400
C	4.02825400	1.50569500	1.61049800
C	4.26533500	1.27156600	-1.11375600
H	4.17422000	1.05254400	2.59368900
H	2.96357600	1.62695900	1.36741400
H	4.57934300	2.44865100	1.54493200
H	4.82199200	2.21343700	-1.12263300
H	3.17878300	1.43228200	-1.07716300
H	4.55790100	0.65392400	-1.96592800
I	0.46837900	3.52753000	-0.31440000
O	-2.26282700	1.12402900	0.12642000
C	-2.85922100	0.02943500	0.15955700
C	-4.32153500	-0.02661400	0.13064900
C	-1.88136300	-1.17938800	0.19927600
C	-5.04879000	-1.22653800	-0.01830600
C	-5.01318100	1.20258200	0.22697900
H	-1.22127000	-1.04818400	2.06636200
C	-6.44146300	-1.18755100	-0.06507600
H	-4.52313500	-2.16846900	-0.10410500
C	-6.40150500	1.22766200	0.18847800
H	-4.43913700	2.11722900	0.33120700
C	-7.11761800	0.03159000	0.04191700
H	-6.99994500	-2.11072300	-0.18660600
H	-6.92921500	2.17325800	0.26804800
H	-8.20342200	0.05255700	0.00850200
O	-2.46439200	-2.38946100	0.52140300
H	-1.74362300	-3.05940200	0.46164900
O	-1.26380600	-1.11514300	-1.03698100
H	-0.54726800	-1.81067500	-1.05809000

14S

Cu	-0.18389100	1.03503900	0.39525200
O	1.37617300	0.85810700	-0.53575500
O	-0.32128000	-0.83801300	-0.05274400
Cu	1.52176500	-0.97842200	-0.28535600
I	1.56574000	-3.43460300	0.54639600
S	4.27057300	0.10312200	-1.28063500
O	3.35593100	-1.07882900	-0.79917400
C	3.40745600	0.95767800	-2.63379900
C	4.25070700	1.38236500	0.00959700

H	3.37947200	0.25641600	-3.47080600
H	2.40250800	1.22286100	-2.29266500
H	3.99934000	1.83772600	-2.90287800
H	4.86092900	2.21837000	-0.34527400
H	3.21310600	1.67249900	0.19596700
H	4.71147800	0.93269100	0.89203600
I	0.51982100	3.45713400	0.51661500
O	-2.35922400	1.03744300	-0.86575400
C	-3.06702000	0.42549600	-0.07126600
C	-4.35955200	-0.17750500	-0.47487200
C	-2.60365400	0.35617700	1.42024900
C	-5.13853900	-0.95386600	0.40170900
C	-4.81560000	0.05753700	-1.78571200
H	-3.43676800	0.70492600	2.05508100
C	-6.35660200	-1.48065900	-0.02873100
H	-4.77523400	-1.17121000	1.40024200
C	-6.03280900	-0.46764100	-2.20930400
H	-4.19891600	0.65689600	-2.44777300
C	-6.80588900	-1.23632100	-1.33003800
H	-6.95267700	-2.08566800	0.64840400
H	-6.38236900	-0.28092000	-3.22074700
H	-7.75597100	-1.64706200	-1.66102400
O	-1.52488700	1.12982900	1.67491500
H	-0.73214000	-1.34148900	0.69211000
O	-2.37416700	-1.05367500	1.70326300
H	-2.08637000	-1.08043300	2.63592200

TS11S

Cu	-0.40578800	0.77473800	-0.67468900
O	1.33271300	1.25150500	-0.65089900
O	0.38574100	-0.82383000	-1.57745900
Cu	1.90184700	-0.50899800	-0.51664800
I	2.41411000	-3.04445000	-0.35034800
S	3.81895600	1.22869200	1.21825700
O	3.49364000	-0.09999400	0.44878300
C	3.86599900	2.58437100	0.00697800
C	2.35191800	1.68863500	2.18173700
H	4.69486500	2.36430400	-0.66938700
H	2.91314800	2.62019200	-0.52562800
H	4.06784100	3.50882700	0.55678300
H	2.58485700	2.61755500	2.71102700

H	1.50638000	1.79891400	1.49881000
H	2.18141000	0.87936500	2.89432300
I	-0.78996500	3.25653300	-0.21510500
O	-2.22517100	0.28953400	-0.70741900
C	-2.61843900	-0.44788900	0.29462400
C	-4.02176200	-0.93543000	0.24415000
C	-1.64292000	-0.70036600	1.35687700
C	-4.44702500	-2.10806000	0.89235600
C	-4.92777900	-0.21463700	-0.55604600
H	-2.47697100	0.31741600	1.58089500
C	-5.76687700	-2.53819500	0.74819700
H	-3.75286100	-2.67127000	1.50356300
C	-6.24369900	-0.65084900	-0.69157500
H	-4.58291500	0.67974200	-1.06403800
C	-6.66691500	-1.81350900	-0.03855300
H	-6.09072700	-3.44555900	1.25018200
H	-6.93872100	-0.08546500	-1.30582700
H	-7.69313200	-2.15457100	-0.14477400
O	-0.41741200	-0.33306300	1.23643600
H	-0.00541100	-1.66592300	-1.26377600
O	-1.95759500	-1.64452900	2.31148500
H	-1.16682200	-1.67084700	2.88363100

TS11S-2

Cu	-0.49843000	0.96164600	-0.72301000
O	1.24304300	1.46296900	-0.72610900
O	0.24237700	-0.56588600	-1.77642100
Cu	1.71043400	-0.32904800	-0.58508900
I	2.46244400	-2.75079600	-0.41400000
S	3.28454000	0.59192900	0.86120500
O	4.35450500	-0.18155800	1.55779400
C	2.24306800	1.46685000	2.05857400
C	4.00494500	1.94791700	-0.10398200
H	1.60668200	0.71709700	2.53010300
H	2.91389500	1.93999600	2.78075000
H	1.62996300	2.17748000	1.50177400
H	3.19030100	2.43126500	-0.64838000
H	4.50680300	2.62870100	0.58852600
H	4.72754400	1.49208500	-0.78377500
I	-0.90264200	3.37042500	-0.02466900
O	-2.28696200	0.38203100	-0.61891900

C	-2.51078700	-0.53338000	0.28481900
C	-3.85984900	-1.16278500	0.25689400
C	-1.43306400	-0.84628700	1.22804400
C	-4.10046100	-2.47744600	0.69119100
C	-4.90789400	-0.41271800	-0.30816600
H	-2.34878700	0.03595900	1.64554000
C	-5.38028100	-3.02165800	0.57139800
H	-3.29716400	-3.06333800	1.12019000
C	-6.18262600	-0.96311700	-0.41897700
H	-4.70534800	0.59465000	-0.65631300
C	-6.42205200	-2.26926700	0.02150500
H	-5.56133500	-4.03887100	0.90684600
H	-6.98830600	-0.37516300	-0.84918300
H	-7.41588500	-2.69959800	-0.06618700
O	-0.26088800	-0.32858300	1.11261200
H	-0.16944600	-1.42853200	-1.56590800
O	-1.59210500	-1.94964100	2.03382200
H	-0.76495600	-1.99160900	2.55105500

TS12S

Cu	-0.34867800	-0.83006200	-0.36801300
O	1.20928400	-1.18689000	0.63098800
O	-0.62055000	0.71695400	0.76155500
Cu	1.26734300	0.81759200	0.86175200
I	1.65407900	2.96511900	-0.67531600
S	4.24729300	0.08765500	1.48213500
O	2.95776000	0.89816500	1.80151400
C	3.94956200	-1.60372100	2.08429900
C	4.22605900	-0.23374200	-0.30560200
H	3.94123800	-1.55274300	3.17528300
H	2.98042300	-1.93752300	1.70412600
H	4.77019800	-2.24385200	1.74630400
H	5.12160900	-0.80647200	-0.56452500
H	3.30994900	-0.77986200	-0.54855400
H	4.23233100	0.74124200	-0.79886100
I	1.06628100	-2.91949000	-0.81028900
O	-2.66503600	-1.37718100	0.44478800
C	-3.29327200	-0.48792500	-0.12442200
C	-4.64460200	-0.07387400	0.31949200
C	-2.65253900	0.15464700	-1.40072800
C	-5.33820200	0.99356200	-0.27871900

C	-5.24711000	-0.79319800	1.36887700
H	-3.37791000	0.06601000	-2.22947900
C	-6.61722600	1.32959100	0.16610300
H	-4.86362200	1.57576200	-1.06135200
C	-6.52430800	-0.45581400	1.80666400
H	-4.69398500	-1.61109900	1.81944100
C	-7.21172700	0.60543200	1.20390500
H	-7.14791600	2.15884200	-0.29275100
H	-6.98703900	-1.01512200	2.61486200
H	-8.20876500	0.86921700	1.54639900
O	-1.51234200	-0.46955500	-1.76387400
H	-1.04302700	1.41087100	0.19669200
O	-2.46196200	1.56092800	-1.09894900
H	-1.94759700	1.91641600	-1.85046900

TS12S-2

Cu	0.53211800	0.84060400	-0.48000800
O	-1.02431200	1.24572200	0.50372400
O	0.55948200	-0.86423200	0.38140200
Cu	-1.38849700	-0.69531500	0.45068300
I	-2.45348000	-2.57101700	-0.96257800
S	-3.22882700	-0.20141400	1.86720600
O	-4.03839600	-1.20425900	2.63098600
C	-4.27800500	0.74484900	0.73051400
C	-2.69034900	1.12572400	2.98852400
H	-4.63314500	0.03955600	-0.02395400
H	-5.11402400	1.17157900	1.29145000
H	-3.65543200	1.51560300	0.26959900
H	-2.03842800	1.79470100	2.42239000
H	-3.57304700	1.63149400	3.38895100
H	-2.13411400	0.64084900	3.79344300
I	-0.72199400	3.06550100	-0.78494700
O	2.77070000	1.06832600	0.55696100
C	3.38972300	0.21939300	-0.08111600
C	4.66454300	-0.35332700	0.40607700
C	2.82758100	-0.18480600	-1.48526300
C	5.35299700	-1.36303600	-0.29068900
C	5.20144300	0.15374000	1.60493100
H	3.62304800	-0.00498700	-2.23127900
C	6.56195200	-1.85148100	0.20529900
H	4.92612700	-1.78383100	-1.19457700

C	6.40851200	-0.33593200	2.09424300
H	4.65452800	0.93083600	2.12910500
C	7.09121900	-1.33835800	1.39341800
H	7.08832800	-2.63547900	-0.33130700
H	6.82048200	0.05934400	3.01834900
H	8.03352600	-1.72105900	1.77603600
O	1.75262700	0.55698500	-1.83615700
H	0.92605000	-1.52323300	-0.25277000
O	2.54715800	-1.60200500	-1.43154200
H	2.15668800	-1.81864300	-2.30015100

15S

Cu	1.14689400	-0.89119100	-0.13035500
O	-0.10247900	0.60028300	0.02730200
O	-0.55762400	-1.67774600	0.05192300
Cu	-1.88929200	-0.33524300	0.06674600
I	-3.81477000	-2.10273500	-0.10542300
S	-4.33598000	1.45970100	-0.38453500
O	-2.89733000	1.34413800	0.21006200
C	-5.45977900	1.29401800	1.03552400
C	-4.47476000	3.25828800	-0.61682300
H	-5.42202000	0.24412500	1.33325500
H	-5.11079000	1.94162700	1.84411700
H	-6.47133800	1.56245800	0.71618100
H	-5.49606400	3.50180600	-0.92365100
H	-4.20744200	3.76288100	0.31470300
H	-3.76972900	3.52917400	-1.40504600
I	0.35657900	2.55626900	0.16429600
H	-0.73922700	-2.59066300	-0.24268000
O	2.89251500	0.06978000	-0.18647800
C	3.84993600	-0.73796000	-0.16712500
C	5.23013900	-0.24422500	-0.13408700
C	3.49647900	-2.23783000	-0.16393100
C	6.30711500	-1.13131200	0.05761000
C	5.47622100	1.13335100	-0.29956100
C	7.61201900	-0.64131500	0.08146600
H	6.11317600	-2.18565600	0.22450300
C	6.78182400	1.61321100	-0.28388500
H	4.63220200	1.80088700	-0.44064800
C	7.84975200	0.72588500	-0.09460800
H	8.44284300	-1.32258900	0.23924500

H	6.97292800	2.67412600	-0.41647700
H	8.86890500	1.10276400	-0.08161600
O	2.18550500	-2.44102000	-0.44397400
H	4.12638600	-2.79253400	-0.88345400
O	3.86363400	-2.64115000	1.17930700
H	3.16204400	-3.28132900	1.40588800

TS13S

Cu	-1.13464600	-0.94899900	-0.04380100
O	0.09970700	0.56374700	-0.08552800
O	0.59814800	-1.69726100	-0.17758000
Cu	1.89938900	-0.33119100	-0.10123400
I	3.86390300	-2.06388200	0.05139400
S	4.29356100	1.48538900	0.49622400
O	2.87345800	1.36675100	-0.14446100
C	5.45699300	1.41020600	-0.89885500
C	4.38137100	3.27367500	0.81465800
H	5.44993700	0.37488900	-1.24588900
H	5.11520800	2.08796000	-1.68547700
H	6.45365000	1.68402100	-0.53977500
H	5.38807100	3.52593600	1.16016200
H	4.12633800	3.81493100	-0.09953300
H	3.64969400	3.49068700	1.59521900
I	-0.39146900	2.50935000	-0.13730600
H	0.81872500	-2.63261400	-0.00971000
O	-2.80636600	0.00666200	0.12636600
C	-3.81767300	-0.81266100	0.15732400
C	-5.19403800	-0.23615900	0.12241000
C	-3.46704700	-2.22240000	0.10991500
C	-6.37282900	-1.00244100	0.13985200
C	-5.28275600	1.16368200	0.04491900
C	-7.61437000	-0.36915600	0.07760700
H	-6.32113200	-2.08258500	0.20393500
C	-6.52834800	1.78791400	-0.02032300
H	-4.36494400	1.74109900	0.03166200
C	-7.69846700	1.02427000	-0.00356300
H	-8.52002400	-0.96939100	0.09161900
H	-6.58370700	2.87120500	-0.08390400
H	-8.66936300	1.50979000	-0.05377500
O	-2.22240200	-2.56901300	0.02171300
H	-3.78079800	-1.66030900	1.34008200

O	-4.40792600	-3.18077100	-0.12835600
H	-3.92908200	-4.02863600	-0.04576900

TS13S-2

Cu	0.99027000	-0.97246900	0.04488300
O	-0.17556400	0.59123500	0.04750900
O	-0.74750100	-1.66376300	0.17618500
Cu	-2.02338500	-0.24881200	0.05066100
I	-4.00435800	-1.94638300	-0.01610100
S	-3.35195500	1.76863500	-0.08956000
O	-2.79804600	3.16769300	-0.08629200
C	-4.60826500	1.63545300	1.21802600
C	-4.41081800	1.55917300	-1.55264400
H	-4.08765300	1.77359700	2.16795800
H	-5.33843000	2.43525700	1.06795400
H	-5.06383400	0.64345400	1.17140600
H	-4.86618900	0.56642700	-1.51874200
H	-5.15712500	2.35813600	-1.54903300
H	-3.76137200	1.65370900	-2.42544700
I	0.50708700	2.47184700	0.12798900
H	-0.97013100	-2.60266700	0.03298500
O	2.68282600	-0.07604000	-0.12441400
C	3.67548000	-0.92358900	-0.14234200
C	5.06453800	-0.38158800	-0.11920200
C	3.27976800	-2.31913800	-0.08251900
C	6.21383800	-1.17483700	0.04333600
C	5.19731200	1.01230700	-0.23696600
C	7.47215700	-0.57297300	0.08335500
H	6.12728400	-2.25042900	0.13626600
C	6.45876100	1.60458600	-0.19440300
H	4.30119900	1.61194300	-0.35303500
C	7.60050000	0.81401900	-0.03540700
H	8.35541900	-1.19261600	0.21113300
H	6.54945800	2.68344300	-0.28487400
H	8.58387700	1.27505000	-0.00189900
O	2.02127700	-2.61980700	0.01262300
H	3.60547100	-1.77562700	-1.31316500
O	4.18346600	-3.31036200	0.15371600
H	3.67775000	-4.14239500	0.06859900

TS13T

Cu	-1.05952000	-0.81608200	-0.36557100
O	0.14771000	0.67670800	0.05854900
O	0.57022000	-1.55483900	-1.08247600
Cu	1.84089300	-0.32187800	-0.36030500
I	3.63791200	-2.12753000	0.33883200
S	4.06829200	1.41679300	0.86323700
O	3.00739100	1.26101500	-0.27137600
C	5.67529300	1.24138900	0.03265400
C	4.08397300	3.21970200	1.09842900
H	5.76546100	0.18662500	-0.23493900
H	5.68608400	1.87191900	-0.86017100
H	6.46546600	1.52684300	0.73358900
H	4.87969100	3.48075800	1.80205500
H	4.23058500	3.70902500	0.13251900
H	3.11018500	3.49004500	1.51141200
I	-0.26934900	2.53186900	-0.56940800
H	0.75547400	-2.48042800	-0.84001100
O	-2.72170300	0.03464000	0.15161700
C	-3.71996600	-0.80068400	0.17719400
C	-5.09074700	-0.25847000	0.40599000
C	-3.36484500	-2.17487100	-0.13122500
C	-6.26355000	-1.03250100	0.36059300
C	-5.18338900	1.12149700	0.65281800
C	-7.50407000	-0.42593100	0.56091900
H	-6.20758900	-2.09786800	0.17278300
C	-6.42777200	1.71939000	0.84978100
H	-4.27001500	1.70563800	0.67958400
C	-7.59230100	0.94785400	0.80559600
H	-8.40567500	-1.03120200	0.52325600
H	-6.48714400	2.78792700	1.03770700
H	-8.56240200	1.41288000	0.95908000
O	-2.13561000	-2.45601700	-0.42269300
H	-3.52988400	-1.81848100	1.19858100
O	-4.31468600	-3.11586800	-0.39926700
H	-3.81888800	-3.95090000	-0.50762200

16S

Cu	-1.33114100	-0.72487700	0.80775600
O	-0.00539400	0.66481500	0.47211500
O	0.30217000	-1.64290500	0.51361100
Cu	1.65360100	-0.39294000	0.06475700

I	3.43504800	-2.28453700	-0.37556700
S	4.24604800	1.21589600	-0.16534000
O	2.69430500	1.21373600	-0.34954500
C	4.92764600	1.04201400	-1.84182100
C	4.56478700	2.99185200	0.06363500
H	4.73719200	0.00931800	-2.14136200
H	4.41806600	1.74282000	-2.50829500
H	6.00399500	1.23535300	-1.80498500
H	5.64523700	3.16111400	0.08562800
H	4.09025300	3.55035100	-0.74670400
H	4.12025100	3.27035700	1.02100900
I	-0.30406900	2.63881800	0.64938000
H	0.41754000	-2.59136600	0.32129500
O	-2.80867700	0.38267500	1.16037000
C	-4.01313700	-0.26907300	0.98682900
C	-4.66156700	-0.03767400	-0.39765200
C	-3.78300200	-1.76860700	1.13426100
C	-5.95766100	-0.48445300	-0.69077400
C	-3.93304000	0.65675800	-1.36819100
C	-6.51309200	-0.24842500	-1.95025400
H	-6.53466400	-1.01532800	0.06280200
C	-4.49106800	0.89046300	-2.62878000
H	-2.94563500	1.02631100	-1.10968200
C	-5.77888200	0.43647000	-2.92430100
H	-7.51962300	-0.59539000	-2.16960900
H	-3.91992000	1.43378900	-3.37717000
H	-6.21244000	0.62058200	-3.90375300
O	-2.64957800	-2.26512900	1.01272500
H	-4.74046000	0.03221900	1.76131700
O	-4.83654700	-2.53840900	1.39398700
H	-4.52594900	-3.46887800	1.41612000

TS14S

Cu	1.39408500	-0.17704100	-0.26829600
O	-0.05763900	-1.38180800	-0.34303900
O	-0.17609400	0.97942800	-0.11926400
Cu	-1.65728000	-0.36638800	-0.06075800
I	-3.13953700	-2.54185900	0.05389000
S	-4.52142600	0.75799100	-0.07543300
O	-3.01186500	1.02295300	0.22940000
C	-5.28170800	0.39382200	1.53574600

C	-5.13336200	2.45996500	-0.27104800
H	-4.93618600	-0.60299300	1.81737600
H	-4.95268400	1.14148700	2.26217000
H	-6.36973400	0.39999100	1.41989400
H	-6.22237300	2.43901000	-0.37158200
H	-4.82392400	3.05485900	0.59152800
H	-4.67879200	2.85545900	-1.18136600
O	2.89085900	0.99701700	-0.41479900
C	3.70537200	0.04882900	-0.79983900
C	5.04493800	-0.07222700	-0.16244300
C	2.95071200	-1.72569600	-0.13187100
C	5.28361500	0.54461000	1.07502200
C	6.07058000	-0.78762600	-0.79985100
H	3.70104000	-0.22624800	-1.87218000
C	6.54326200	0.44879300	1.66311900
H	4.47781400	1.09700800	1.54707900
C	7.32921200	-0.88269000	-0.20735400
H	5.88219700	-1.26534100	-1.75956800
C	7.56531100	-0.26596100	1.02616300
H	6.73190100	0.92958100	2.61886400
H	8.12345000	-1.43262300	-0.70405900
H	8.54518600	-0.34053800	1.48966500
O	2.85160400	-1.95718800	1.04878600
O	3.07102000	-2.70933400	-1.05509100
H	3.05432100	-2.30916700	-1.94441500
H	-0.02800000	-2.28060900	0.03518300
I	-0.21026400	2.98699600	-0.15828400

17S

Cu	1.13096800	-1.24700800	-0.19188600
O	-0.68843800	-1.84474500	-0.14792900
O	0.12011000	0.43731300	-0.05500300
Cu	-1.80481100	-0.21392000	-0.06028400
I	-3.90662900	-1.67208000	0.57499900
S	-4.10195700	1.81008100	-0.50577200
O	-2.57415900	1.61989800	-0.27998400
C	-4.81102900	2.12103500	1.14141900
C	-4.16875700	3.51899500	-1.13029400
H	-4.77934000	1.16619200	1.67071400
H	-4.20501200	2.87245400	1.65478000
H	-5.84641400	2.45475200	1.02304300

H	-5.21392200	3.82900000	-1.22144500
H	-3.61780000	4.17205800	-0.44908600
H	-3.69136200	3.51543200	-2.11218700
O	2.90966500	-0.39868900	0.01009200
C	4.01855400	-0.96519700	0.03500600
C	5.25675700	-0.23274300	0.25586200
C	1.66537800	-3.10324800	-0.78026600
C	5.25037800	1.16254200	0.45698900
C	6.46941800	-0.94757100	0.26519500
H	4.06334000	-2.05397100	-0.11985000
C	6.45282900	1.82883000	0.66477400
H	4.30128900	1.69043700	0.44434700
C	7.67035500	-0.27261300	0.47421700
H	6.45950500	-2.02332600	0.10768200
C	7.65920600	1.11257200	0.67345300
H	6.45980000	2.90341800	0.82073900
H	8.60921300	-0.81770700	0.48224900
H	8.59538200	1.63931000	0.83682200
O	2.78205200	-3.57407000	-0.69653500
O	0.66868300	-3.74558400	-1.41015500
H	-0.13343300	-3.17811900	-1.25625600
H	-0.92813800	-2.44132800	0.59194700
I	0.82319200	2.32091800	-0.17443800

pro1

O	2.84762900	-0.39763800	0.00000100
C	1.99188000	0.47278400	-0.00000100
C	0.53432600	0.21751800	-0.00000100
C	0.04877500	-1.10109700	-0.00000100
C	-0.36380600	1.29516600	-0.00000100
C	-1.32360000	-1.33453300	0.00000000
H	0.76644000	-1.91621100	-0.00000100
C	-1.73951400	1.06015600	0.00000000
H	0.02075500	2.31334800	-0.00000100
C	-2.21737000	-0.25434700	0.00000100
H	-1.70366800	-2.35232000	0.00000000
H	-2.43651100	1.89336800	0.00000100
H	-3.28822600	-0.43941700	0.00000100
H	2.27603600	1.54845300	0.00000400

18S

Cu	-1.18624500	0.93843200	0.31624300
O	0.49248400	1.82277000	0.51151700
O	0.02485100	-0.58541100	0.31551300
Cu	1.80380000	0.26037500	0.11739600
I	4.23081500	0.36076700	-0.22932500
S	-4.04748600	0.24874000	-0.62756700
O	-2.81922200	-0.08591600	0.28738100
C	-4.60408100	-1.41813300	-1.08610500
C	-5.37635300	0.68481900	0.52767300
H	-3.81833500	-1.85041900	-1.70854300
H	-4.73669300	-2.01584900	-0.18145500
H	-5.53626300	-1.33609800	-1.65236300
H	-6.31995600	0.72786200	-0.02410400
H	-5.41535100	-0.06241900	1.32429600
H	-5.12145200	1.66932700	0.92094900
C	-2.00116000	2.75642800	-0.02722000
O	-3.19932400	2.93383300	-0.03933000
O	-1.09510400	3.67524600	-0.33048300
H	-0.21177700	3.21739000	-0.17247700
H	0.63008700	2.09632800	1.44093300
I	-0.41873000	-2.53839400	0.13640800

TS15S

Cu	-0.19621200	0.67361600	1.04054200
O	0.22856000	-0.78450300	2.06117000
O	-1.20332700	-0.33240100	-0.41760700
Cu	0.54893300	-1.12239500	-0.64051800
I	3.00275100	-0.82376500	-0.70100300
C	1.05293200	1.51301600	2.28475300
O	0.57594100	2.15968100	3.16529700
O	2.32114300	1.38224300	1.95083500
H	2.45836000	0.77804400	1.15994700
H	1.18495100	-0.95084700	2.16033300
I	-2.74215500	-1.54372000	0.11964600
O	-0.58729100	2.33859100	0.15895200
S	-0.90678100	2.20155000	-1.38047800
C	-2.71598500	2.24766800	-1.48969600
C	-0.55149300	3.89802700	-1.92219500
H	-3.06788500	1.28122800	-1.12555400
H	-3.09243900	3.06490500	-0.86927200
H	-2.99708200	2.38211200	-2.53842900

H	-0.85791300	4.00867800	-2.96624500
H	-1.08037700	4.60227700	-1.27546700
H	0.52742100	4.03896500	-1.83277200

TS16S

Cu	-1.74405500	1.07886200	0.18158400
O	-0.64376800	-0.62239700	0.12366800
O	0.00404100	1.71321900	0.08254900
Cu	1.13184900	0.24636700	0.08375200
I	3.14691400	1.84326500	-0.27028800
S	3.52021100	-1.68596300	-0.34827900
O	2.12616000	-1.45758700	0.30692000
C	4.72726000	-1.50113500	1.00060900
C	3.56085500	-3.50191600	-0.47353800
H	4.75924200	-0.43504000	1.23423000
H	4.38728100	-2.07898500	1.86415800
H	5.70501500	-1.84483500	0.64935000
H	4.54959000	-3.81617400	-0.82060900
H	3.32412000	-3.93662300	0.50059400
H	2.79780200	-3.78271200	-1.20200600
I	-1.00012300	-2.63056100	0.07172100
H	-0.43618600	2.80082000	0.28362500
C	-1.54626700	3.58315400	0.44028500
O	-1.90658600	4.07892100	1.48501100
O	-2.04059500	3.96720000	-0.77494500
H	-2.68128500	4.69218400	-0.59107100
O	-3.64659700	0.70721700	0.28865700
S	-4.26880200	-0.45863300	-0.53570400
C	-4.90204200	-1.60898100	0.72013800
C	-5.85898100	0.23967200	-1.07760300
H	-4.02746500	-2.07452400	1.17964700
H	-5.47768000	-1.04602700	1.45953800
H	-5.51608000	-2.36899800	0.22817900
H	-6.45290400	-0.54534200	-1.55436600
H	-6.37744800	0.66171300	-0.21287300
H	-5.62870400	1.02576100	-1.79962500

TS16S-2

Cu	1.46247200	-0.17145800	0.06009400
O	-0.05054900	-1.31596800	0.10359600
O	-0.14043100	1.11894800	0.01851200

Cu	-1.53939700	-0.16150800	0.09036200
I	-3.68511600	-1.36922000	0.06723000
S	4.47730600	-0.30692900	-0.29790200
O	3.24782500	0.54423300	0.15571200
C	5.80037400	0.93560300	-0.34846400
C	5.00853900	-1.22033200	1.18121300
H	5.56071700	1.62147800	-1.16330100
H	5.81982000	1.47134400	0.60387200
H	6.75255400	0.43497900	-0.54463700
H	5.98148000	-1.67739400	0.97749700
H	5.06177400	-0.52973600	2.02698800
H	4.26201200	-1.99923900	1.35314500
C	1.63927700	-2.95435500	-0.15255100
O	2.61349800	-3.43637600	0.36733200
O	1.27857000	-3.10371600	-1.43112600
H	0.46673400	-2.54628000	-1.51376000
H	0.63548300	-2.28051400	0.40131300
I	-0.73426300	3.04940400	-0.05838700

H₂CO₃

O	-0.43722000	1.17849100	-0.00010900
H	-1.41281900	1.18222800	0.00030800
C	-0.06498200	-0.13425000	-0.00004400
O	1.27533900	-0.23496100	-0.00020200
O	-0.81951400	-1.07363700	0.00009900
H	1.65387300	0.66412100	0.00165800

TS31S

Cu	-0.43724800	1.06809400	0.60998600
O	1.33134800	0.43021900	0.37026000
O	-0.99905300	-1.94337100	0.38153500
Cu	0.75143500	-1.36395200	0.07452000
I	2.90874500	-2.50545200	-0.54796200
S	-1.56683100	3.70960900	-0.20429300
O	-0.24793800	2.85741300	-0.19059100
C	-0.90377700	5.32993100	-0.69297100
C	-2.41291300	3.27929800	-1.75184900
H	-0.29206900	5.68807400	0.13726500
H	-0.28979900	5.20936300	-1.58862800
H	-1.73675300	6.01637600	-0.87053300
H	-3.24571300	3.97318000	-1.90082800

H	-1.70020900	3.32841400	-2.57933700
H	-2.77862100	2.26294300	-1.59591900
I	2.99511300	1.51895600	0.06504300
O	-2.30682400	1.02415900	0.28236800
C	-2.95223200	-0.00091000	0.97302300
C	-3.78128700	-0.89219500	0.05925800
C	-1.90121700	-0.76146300	1.81101700
C	-3.46468100	-0.99551800	-1.30294100
C	-4.87047900	-1.61480200	0.56391700
H	-3.62792400	0.41597100	1.74484600
C	-4.21364600	-1.82571900	-2.14250800
H	-2.63370600	-0.41416300	-1.69084100
C	-5.61626300	-2.44691900	-0.27382300
H	-5.12671900	-1.53490600	1.61751100
C	-5.28968500	-2.55577400	-1.62951200
H	-3.95844100	-1.89956400	-3.19654900
H	-6.45396300	-3.00855500	0.13102600
H	-5.87329000	-3.20011200	-2.28134200
O	-0.84006500	-0.15220100	2.14460400
H	-1.55081500	-2.24488000	-0.36144400
O	-2.38711600	-1.73124800	2.59032000
H	-1.64430500	-2.05706500	3.13784900

30T

Cu	-0.60545400	-1.17801400	-0.55105800
O	1.09675500	-1.34176000	0.49665200
O	0.29063500	0.25709800	-1.59423400
Cu	1.60838100	0.53118800	0.35125300
I	3.11617600	2.52892100	0.38009100
I	2.61159200	-2.49228800	-0.13375200
H	0.19410800	0.28428100	-2.56569900
O	-2.28089900	-0.36568800	-0.97404800
C	-2.13454000	1.01223700	-1.15404800
C	-3.21313000	1.78581700	-0.40672100
C	-0.72756900	1.47283900	-0.67443900
C	-3.94204700	2.79031400	-1.05402200
C	-3.48742400	1.49786400	0.93817300
C	-4.93325400	3.50095100	-0.37054800
H	-3.73166500	3.01794000	-2.09675800
C	-4.47466200	2.20865400	1.62202000
H	-2.91589900	0.72314300	1.43912600

C	-5.20166600	3.21093600	0.96928200
H	-5.49367800	4.27765600	-0.88432300
H	-4.67543300	1.98530300	2.66684900
H	-5.97112900	3.76236200	1.50328200
O	-0.31947100	1.11436900	0.49887600
H	-2.18180100	1.29368100	-2.21949000
O	-0.37397500	2.66275900	-1.19050100
H	0.44277600	2.95692600	-0.72570200
S	-2.97714100	-2.51481100	0.66385500
O	-1.52004100	-2.78113000	0.15812700
C	-4.05758200	-2.76620500	-0.77385600
H	-3.83834100	-1.92202200	-1.43068500
H	-3.81624900	-3.72187500	-1.24712300
H	-5.09888200	-2.73863300	-0.43882800
C	-3.31979000	-4.07054900	1.53931800
H	-4.36656800	-4.07847500	1.85674300
H	-3.10046000	-4.91258800	0.87821900
H	-2.66314200	-4.09665300	2.41114600

TS31S-2

Cu	0.42446900	-1.78285700	0.43437300
O	-1.37758400	-1.24156300	0.15351300
O	1.11095700	0.48664800	0.64862800
Cu	-0.80927300	0.75371400	0.60425800
I	-0.83648400	2.82522800	-0.98119500
S	-3.85018400	0.64610000	1.64203700
O	-2.37140000	1.08485600	1.79076900
C	-4.20791200	0.59385100	-0.14080700
C	-3.89049400	-1.14224800	1.97763000
H	-4.05498100	1.60523200	-0.52363800
H	-3.51585600	-0.09871000	-0.62584700
H	-5.24840400	0.28276600	-0.27471300
H	-4.88826900	-1.52356200	1.73942400
H	-3.10890400	-1.61743500	1.37530300
H	-3.68660200	-1.26951500	3.04310700
I	-1.21396800	-2.13573600	-1.69677500
O	2.22321100	-2.16841100	0.33951400
C	2.93749700	-1.25900200	1.12221600
C	3.88682700	-0.38175300	0.32016500
C	1.86662100	-0.45895700	1.93098100
C	3.71885400	-0.22990700	-1.06285100

C	4.93934800	0.28771200	0.96082900
H	3.50728300	-1.79496900	1.90035200
C	4.57933000	0.59789500	-1.79112900
H	2.92424800	-0.77961700	-1.55701300
C	5.79642100	1.11532300	0.23276400
H	5.07922500	0.16888300	2.03243700
C	5.61729700	1.27461500	-1.14558700
H	4.44072500	0.70830100	-2.86339100
H	6.60475100	1.63468800	0.74077800
H	6.28682700	1.91640700	-1.71182000
O	0.83564600	-1.15462900	2.29941900
H	1.69909200	1.07939500	0.13783800
O	2.36467300	0.44715000	2.80052200
H	1.65029600	0.63504600	3.44250400

TS31T

Cu	-0.60545400	-1.17801400	-0.55105800
O	1.09675500	-1.34176000	0.49665200
O	0.29063500	0.25709800	-1.59423400
Cu	1.60838100	0.53118800	0.35125300
I	3.11617600	2.52892100	0.38009100
I	2.61159200	-2.49228800	-0.13375200
H	0.19410800	0.28428100	-2.56569900
O	-2.28089900	-0.36568800	-0.97404800
C	-2.13454000	1.01223700	-1.15404800
C	-3.21313000	1.78581700	-0.40672100
C	-0.72756900	1.47283900	-0.67443900
C	-3.94204700	2.79031400	-1.05402200
C	-3.48742400	1.49786400	0.93817300
C	-4.93325400	3.50095100	-0.37054800
H	-3.73166500	3.01794000	-2.09675800
C	-4.47466200	2.20865400	1.62202000
H	-2.91589900	0.72314300	1.43912600
C	-5.20166600	3.21093600	0.96928200
H	-5.49367800	4.27765600	-0.88432300
H	-4.67543300	1.98530300	2.66684900
H	-5.97112900	3.76236200	1.50328200
O	-0.31947100	1.11436900	0.49887600
H	-2.18180100	1.29368100	-2.21949000
O	-0.37397500	2.66275900	-1.19050100
H	0.44277600	2.95692600	-0.72570200

S	-2.97714100	-2.51481100	0.66385500
O	-1.52004100	-2.78113000	0.15812700
C	-4.05758200	-2.76620500	-0.77385600
H	-3.83834100	-1.92202200	-1.43068500
H	-3.81624900	-3.72187500	-1.24712300
H	-5.09888200	-2.73863300	-0.43882800
C	-3.31979000	-4.07054900	1.53931800
H	-4.36656800	-4.07847500	1.85674300
H	-3.10046000	-4.91258800	0.87821900
H	-2.66314200	-4.09665300	2.41114600

TS31T-2

Cu	-0.42001100	-1.25962500	-0.77012900
O	1.25394700	-1.15616500	0.31587500
O	0.15181100	0.40598000	-1.71158900
Cu	1.25748100	0.82015600	0.31399900
I	2.21330200	3.10000300	0.63859400
I	2.99704300	-1.77512500	-0.48812900
H	0.08988400	0.47100000	-2.68429200
O	-2.17703700	-0.92310900	-1.33818500
C	-2.41971100	0.44646300	-1.37908900
C	-3.71315300	0.80832700	-0.64410600
C	-1.21117100	1.22582200	-0.76897900
C	-4.22104500	2.11563400	-0.67871400
C	-4.42200900	-0.18661600	0.04042500
C	-5.40864000	2.42713800	-0.01374700
H	-3.68385400	2.89065800	-1.21849600
C	-5.61402000	0.12760500	0.70019400
H	-4.04529900	-1.20430200	0.02226400
C	-6.10760900	1.43460900	0.68085300
H	-5.79003700	3.44455000	-0.04182100
H	-6.16107200	-0.65352400	1.22202100
H	-7.03431700	1.67755800	1.19401900
O	-0.76627600	0.88327900	0.39780400
H	-2.49129900	0.81772200	-2.41631100
O	-1.15444700	2.50677400	-1.16685300
H	-0.47507300	2.96092200	-0.61787300
S	-1.22419000	-2.98653800	0.76397500
O	-2.43323000	-3.84352700	0.52199500
C	-1.48506700	-1.93262300	2.22182500
H	-2.26819500	-1.21779700	1.96318100

H	-1.79202900	-2.56326700	3.06082300
H	-0.55216900	-1.40257700	2.42949700
C	0.13475900	-4.01185100	1.40891100
H	0.97867500	-3.35508100	1.63097700
H	-0.21609800	-4.54041900	2.29924300
H	0.40084100	-4.72768000	0.62850300

19S

Cu	-0.15915200	1.11353900	0.43697200
O	-1.89161600	0.84626400	0.01750300
O	-0.24122700	-0.73251500	0.62966700
Cu	-1.94710100	-0.99127700	0.08920500
I	-1.47068100	-3.50128400	0.27765300
S	-4.77047100	-0.07399200	-0.82746400
O	-3.76778600	-1.22260400	-0.46115800
C	-4.79232300	1.09014000	0.56914900
C	-3.97227800	0.95699800	-2.09464500
H	-5.23220600	0.55263800	1.41223700
H	-3.76448300	1.39964900	0.78221300
H	-5.42835100	1.93626200	0.29233300
H	-4.63285800	1.80349000	-2.30476100
H	-2.99621700	1.27824100	-1.71787900
H	-3.87351500	0.33109000	-2.98442700
I	-0.39006600	3.65171100	0.07072100
O	4.01292500	1.86113100	0.14280800
C	3.92260500	0.63261200	0.15209400
C	5.05515400	-0.25941700	-0.14832100
C	2.54015000	0.04174100	0.51035600
C	4.90770200	-1.65691200	-0.22515100
C	6.32190600	0.32341200	-0.34542700
H	2.57228100	-0.60853300	1.39052500
C	6.01844400	-2.45701900	-0.49123000
H	3.92806200	-2.10797700	-0.10953400
C	7.42601800	-0.48109400	-0.60799400
H	6.41209100	1.40321000	-0.28344800
C	7.27482000	-1.87212600	-0.67947400
H	5.90366300	-3.53481600	-0.55671700
H	8.40321800	-0.03111800	-0.75674400
H	8.13767900	-2.49975400	-0.88489800
O	2.03102900	-0.58614800	-0.61001000
H	1.14058300	-0.95719900	-0.33213100

O	1.73227500	1.18431500	0.92123300
H	2.24048200	1.98689900	0.61321700

TS17S

Cu	0.32167400	0.85472600	0.07739800
O	-1.42676000	1.24220600	0.46882500
O	-0.31223600	-0.87493000	0.18577700
Cu	-2.09727900	-0.46198300	0.19791600
I	-2.64648300	-2.92391100	-0.26004100
S	-4.52984800	1.45374500	0.48191400
O	-3.94255300	0.01044800	0.27925400
C	-3.77367000	2.13207800	1.98758100
C	-3.77756400	2.52401000	-0.77773400
H	-4.15454100	1.53756200	2.82096000
H	-2.68625400	2.04247500	1.88925100
H	-4.09720100	3.17221200	2.09014300
H	-4.12254100	3.54706300	-0.60044300
H	-2.68979900	2.42801800	-0.69256500
H	-4.14200100	2.16856100	-1.74413200
I	1.30049400	3.15509300	-0.04715800
O	4.17414900	0.00739900	-2.09892800
C	3.63096900	-0.60424800	-1.18595000
C	4.35086700	-1.15453700	-0.02488100
C	2.06518100	-0.71275200	-1.31537000
C	3.71098800	-1.81472600	1.04204900
C	5.74861500	-0.97076900	0.00266400
H	1.79652300	0.19982600	-0.46876000
C	4.46672500	-2.27490500	2.12025200
H	2.64031200	-1.97488000	1.01381400
C	6.49399100	-1.43912900	1.07899500
H	6.22187000	-0.45578300	-0.82703000
C	5.85262800	-2.09084100	2.14036200
H	3.97258000	-2.78298400	2.94293900
H	7.57042900	-1.29600300	1.09709000
H	6.43481800	-2.45511500	2.98243700
O	1.50394400	-1.83276600	-0.92786000
H	0.41608300	-1.54373700	-0.50494600
O	1.64515800	-0.22276500	-2.52577000
H	2.40121800	0.30885300	-2.87013200

TS17S-2

Cu	-0.52094900	0.83807600	0.02954000
O	1.14474500	1.37180700	-0.52369000
O	0.24655600	-0.82912700	0.04588600
Cu	1.97832100	-0.23467500	-0.17526800
I	3.14214500	-2.40783500	0.38119400
S	3.89022900	1.03777700	-0.60520600
O	5.28865200	0.51812100	-0.61532900
C	3.70138800	2.39699700	0.57796800
C	3.48583100	1.85140000	-2.17304700
H	3.94737200	1.99240300	1.56202700
H	4.40147100	3.19123700	0.30612900
H	2.65578500	2.71098300	0.52826800
H	2.43832300	2.15800400	-2.10869900
H	4.17041900	2.69194300	-2.31292000
H	3.63225800	1.10544200	-2.95698800
I	-1.70961300	3.03566000	0.04263500
O	-4.44794000	-0.35785100	2.00875600
C	-3.71711500	-0.88155600	1.17606200
C	-4.19303400	-1.48465400	-0.07933800
C	-2.18163000	-0.82115200	1.52109300
C	-3.32760900	-1.97370800	-1.07745200
C	-5.58795700	-1.52731500	-0.27862800
H	-1.89108600	0.09643400	0.69789900
C	-3.86053200	-2.49130300	-2.25764900
H	-2.25502900	-1.95611300	-0.92660700
C	-6.10974200	-2.05462800	-1.45481100
H	-6.23691800	-1.13936100	0.49982000
C	-5.24542600	-2.53606900	-2.44647100
H	-3.19310000	-2.86547800	-3.02804900
H	-7.18484400	-2.08866800	-1.60443000
H	-5.65284300	-2.94577900	-3.36665300
O	-1.46832200	-1.89006300	1.23491600
H	-0.45692400	-1.54134400	0.80350200
O	-1.98310800	-0.28810500	2.76259600
H	-2.83622700	0.14618700	3.00174500

int4

O	-2.00889900	-1.69269900	-0.00019800
O	-1.39381400	1.74563700	0.00018200
C	-1.00845700	0.57121400	0.00001300
C	0.41771700	0.20615900	-0.00004000

C	-2.14921400	-0.48780200	-0.00006000
C	0.87862200	-1.12626800	0.00012900
C	1.34919800	1.26644000	-0.00013600
C	2.24995800	-1.38186300	0.00014700
H	0.16186100	-1.93792300	0.00014600
C	2.71353100	1.00118100	-0.00011400
H	0.97471800	2.28498400	-0.00019800
C	3.16569100	-0.32546900	0.00001200
H	2.60419700	-2.40849200	0.00025500
H	3.42677500	1.82028300	-0.00023700
H	4.23235300	-0.53315700	0.00001900
O	-3.34329800	0.11554500	0.00003300
H	-3.13410200	1.08488400	0.00017800

20S

Cu	1.53801700	-0.41536400	0.34754900
O	0.35608500	1.06291600	0.32128900
O	-0.11183200	-1.33929800	0.90600200
Cu	-1.16527100	0.06069800	0.26593100
I	-3.12786800	-1.60366600	-0.22015300
S	-1.92372500	3.04059200	-0.19414700
O	-2.32412600	1.52366100	-0.12715000
C	-1.01112200	3.43176200	1.32881800
C	-0.61230000	3.19088700	-1.44386100
H	-1.73925300	3.38344300	2.14175600
H	-0.22308700	2.67840400	1.43284500
H	-0.62082000	4.44989100	1.23662600
H	-0.24209700	4.22032300	-1.42584500
H	0.15299600	2.45252500	-1.18588800
H	-1.08331800	2.97848300	-2.40622200
I	4.03103400	-0.36845300	-0.22124800
H	2.66406100	-1.55001800	0.30913300
H	-0.42677000	-2.16903100	0.49640800

20T

Cu	1.64505200	-0.20137700	0.22989100
O	0.30114000	1.10002600	-0.12180100
O	0.23863200	-1.27075200	1.03219000
Cu	-1.13907700	0.03243100	0.60785700
I	-2.85399000	-1.75919300	-0.27991100
S	-2.66916000	2.71267000	0.04319700

O	-2.45452600	1.47771800	0.96241600
C	-1.18315500	3.75321400	0.20284700
C	-2.39664600	2.14265100	-1.66305900
H	-1.16359400	4.12691300	1.22888700
H	-0.30681200	3.13206800	-0.00935900
H	-1.27124600	4.58895300	-0.49835700
H	-2.54917200	2.98998500	-2.33847700
H	-1.38046000	1.74378500	-1.73419600
H	-3.13346700	1.35948800	-1.85526500
I	4.20720500	-0.10657900	-0.22797900
H	2.92414800	-1.26297300	0.28386200
H	-0.00966400	-2.12670700	0.63408000

TS18T

Cu	0.49220800	0.53488800	0.07988500
O	-1.23438800	1.24943400	-0.23069400
O	-0.46158600	-1.00181300	0.83187000
Cu	-2.23150300	-0.20989000	0.49316800
I	-3.29871700	-2.30151900	-0.64311100
S	-4.46459900	1.99178800	0.26071200
O	-3.89551700	0.72317800	0.96699700
C	-3.31300900	3.35739300	0.60406700
C	-4.13177200	1.78839400	-1.51513300
H	-3.35660100	3.54753100	1.67859500
H	-2.30680900	3.05805100	0.29674100
H	-3.65913800	4.23820200	0.05456600
H	-4.52563700	2.66500600	-2.03803700
H	-3.05302200	1.68150700	-1.66021500
H	-4.65913300	0.88611500	-1.83240900
I	2.05317500	2.40965400	-0.45431900
C	2.59611100	-1.43475500	0.62146200
C	3.90849300	-1.27490300	-0.07640600
C	2.55121100	-1.11438500	2.22445500
C	4.79727800	-0.22613800	0.21923900
C	4.22542900	-2.19675700	-1.08826500
H	1.97779900	-0.25395800	0.38437700
C	5.99484400	-0.11485300	-0.48485900
H	4.55819300	0.48744500	0.99921200
C	5.42513700	-2.08230800	-1.78609400
H	3.52297800	-2.99548900	-1.30372700
C	6.31134500	-1.04049100	-1.48531700

H	6.68206900	0.69340500	-0.25313600
H	5.67146200	-2.80079500	-2.56262200
H	7.24679800	-0.94992300	-2.03067700
H	-0.28588900	-1.82499500	0.32837700
O	1.34441300	-1.09702200	2.74632100
H	0.61878700	-1.20201700	2.04634600
O	3.58448300	-1.00160400	2.83357000
O	1.82067100	-2.39992700	0.33538300

TS18T-2

Cu	0.59849900	0.54016900	0.00121300
O	-1.11719600	1.32142800	-0.35669600
O	-0.39853500	-1.01482200	0.63027500
Cu	-2.15118300	-0.17354900	0.12076900
I	-3.64274600	-2.10519500	-0.56019200
S	-3.95763700	1.53340400	0.37743900
O	-5.30511700	1.35639300	1.01289200
C	-4.12339200	1.99395600	-1.37011800
C	-3.17506400	3.04305000	1.02483700
H	-4.58099300	1.14164500	-1.87689700
H	-4.76203100	2.87807500	-1.44550400
H	-3.11816300	2.18017300	-1.75686000
H	-2.21476500	3.16857500	0.51900700
H	-3.84959000	3.88480700	0.84731800
H	-3.03299700	2.89413400	2.09713500
I	2.23251400	2.37345900	-0.42892300
C	2.63149500	-1.50633300	0.56680900
C	3.98741600	-1.35476100	-0.03930100
C	2.49288300	-1.23277000	2.18841500
C	4.87036200	-0.32673900	0.33726100
C	4.35663600	-2.26128200	-1.04798600
H	2.05040200	-0.31102500	0.34601300
C	6.11322600	-0.22074200	-0.28355200
H	4.59088000	0.37463300	1.11501100
C	5.60121900	-2.15198600	-1.66239900
H	3.65855500	-3.04412000	-1.32651500
C	6.48090500	-1.13096500	-1.28100200
H	6.79586800	0.57091000	0.01022700
H	5.88799200	-2.85803700	-2.43630400
H	7.45160000	-1.04448700	-1.76140500
H	-0.15516000	-1.83059300	0.14303700

O	1.26147900	-1.18667500	2.63550000
H	0.56624200	-1.23810000	1.89030600
O	3.49697300	-1.18281600	2.85053400
O	1.86118800	-2.45095600	0.21302600

21T

Cu	-0.44022000	1.81657800	0.02003800
O	-2.22673600	1.34032000	-0.05574500
O	-0.32517900	-0.16317700	0.23681800
Cu	-2.14298000	-0.51127000	-0.02761500
I	-1.68795400	-3.05628100	-0.01966800
S	-5.15415200	0.23574800	-0.33982600
O	-4.01452700	-0.84004800	-0.23452000
C	-4.97388100	1.34740600	1.08523800
C	-4.70948700	1.35315500	-1.70080900
H	-5.21449100	0.75538300	1.97104800
H	-3.93879400	1.70237200	1.10601300
H	-5.69389200	2.16350300	0.97357100
H	-5.43750100	2.16948800	-1.72299900
H	-3.68870300	1.70523600	-1.52255500
H	-4.77912200	0.76490500	-2.61848200
I	1.31862800	3.54972300	-0.02365700
C	2.78361500	-0.69538900	0.09980100
C	4.19898000	-1.00700600	-0.30638900
C	2.51973100	-1.17847600	1.71642900
C	5.24607800	-0.17559300	0.11135700
C	4.46905700	-2.11251400	-1.12109200
H	2.63325300	0.39361200	0.27270300
C	6.55639900	-0.44663500	-0.28521500
H	5.03658400	0.68317900	0.74548900
C	5.78014800	-2.38372700	-1.51463600
H	3.64610300	-2.74153100	-1.44605800
C	6.82532600	-1.55266700	-1.09739200
H	7.36464300	0.20333300	0.03812100
H	5.98715800	-3.24149100	-2.14873900
H	7.84546900	-1.76499500	-1.40568700
H	0.34303200	-0.63614600	-0.36687900
O	1.29401100	-1.02576100	2.15427300
H	0.63550800	-0.71673900	1.45362800
O	3.45836500	-1.56623100	2.35564700
O	1.81887800	-1.25882400	-0.61894000

TS19T

Cu	-0.51790200	1.83283700	0.00869800
O	-2.26637600	1.23618700	-0.10284400
O	-0.26728700	-0.13625100	0.22289800
Cu	-2.06165500	-0.60286400	-0.02807400
I	-1.46564600	-3.11707000	0.09389300
S	-5.11005400	-0.05347800	-0.40549600
O	-3.90859400	-1.05241600	-0.24807000
C	-5.02749100	1.10765800	0.98905100
C	-4.70995600	1.05133600	-1.79058400
H	-5.24808800	0.52698300	1.88749400
H	-4.01697500	1.52698500	1.01751100
H	-5.79468100	1.87331900	0.84039400
H	-5.48701600	1.81923300	-1.84923700
H	-3.71677000	1.47181000	-1.60488800
H	-4.72504000	0.43441000	-2.69180600
I	1.06634400	3.72728500	-0.00521900
C	2.78946200	-0.50551800	-0.16807400
C	4.18749500	-0.92003800	-0.44696600
C	2.53082300	-0.94725000	1.78592700
C	5.25523300	-0.11362600	-0.02549700
C	4.44258400	-2.10409100	-1.15553300
H	2.66583300	0.56351500	0.09299600
C	6.56807600	-0.48397900	-0.31539000
H	5.05478200	0.80110200	0.52766600
C	5.75568000	-2.47271200	-1.44203900
H	3.60326400	-2.71196800	-1.47867800
C	6.81937700	-1.66457700	-1.02250300
H	7.39287500	0.14407200	0.00897700
H	5.95317600	-3.38776500	-1.99349200
H	7.84231600	-1.95431000	-1.24716600
H	0.44179400	-0.55298000	-0.41055500
O	1.29366000	-0.84390000	2.16401400
H	0.63045700	-0.60048400	1.41888100
O	3.51495300	-1.20693900	2.40711400
O	1.81707000	-1.09569600	-0.77038500

CO₂

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.17291500

O	0.00000000	0.00000000	-1.17291500
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TS19T-2

Cu	-0.35644300	1.95650000	0.04093800
O	-2.15184800	1.46789100	0.03078500
O	-0.15092300	-0.01579400	0.26646000
Cu	-1.99007200	-0.35333400	0.02250500
I	-1.89161500	-2.88468000	-0.09249000
S	-4.30933300	-0.20536100	-0.20636700
O	-5.23459600	-1.37139600	-0.28979300
C	-4.48950600	0.86852400	-1.65472900
C	-4.77252300	0.88965000	1.16168100
H	-4.26593400	0.25016000	-2.52662000
H	-5.52346000	1.22104800	-1.69208900
H	-3.76280200	1.67489500	-1.53963700
H	-4.02308900	1.68291100	1.19916700
H	-5.78376100	1.26031600	0.97547600
H	-4.75133300	0.27716300	2.06553600
I	1.13885900	3.90849600	-0.11333500
C	2.89347400	-0.82160700	0.12862800
C	4.28269700	-1.24910000	-0.26008200
C	2.54804100	-1.34720600	1.72666700
C	5.39230000	-0.53540700	0.21049700
C	4.46828200	-2.34536700	-1.11013000
H	2.84175900	0.26712300	0.34839300
C	6.68101000	-0.91371200	-0.16858100
H	5.24876400	0.31545500	0.87330900
C	5.75755500	-2.72398200	-1.48653100
H	3.59846100	-2.88253600	-1.47523100
C	6.86519000	-2.01016800	-1.01657300
H	7.53825300	-0.35489800	0.19618300
H	5.89916300	-3.57405700	-2.14828300
H	7.86822200	-2.30620600	-1.31152600
H	0.48647600	-0.50391900	-0.35546900
O	1.34279100	-1.06994100	2.15483700
H	0.73104600	-0.65853800	1.45744800
O	3.42726100	-1.87047000	2.35311200
O	1.89648800	-1.26616000	-0.62552500

TS20S

Cu	0.45889200	0.87655600	-0.18034600
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O	-1.24696100	1.25484600	0.39821200
O	-0.19857500	-0.85386000	-0.10115800
Cu	-1.97983700	-0.42570700	0.12522900
I	-2.65219000	-2.84285000	-0.41351900
S	-4.31948000	1.50606900	0.82672200
O	-3.79003100	0.07523300	0.44817700
C	-3.36371400	2.06385600	2.26572400
C	-3.70961700	2.65621800	-0.43848800
H	-3.64371200	1.41310300	3.09706500
H	-2.30043400	1.97075300	2.01638600
H	-3.65036000	3.09680800	2.48452000
H	-4.00493600	3.66825800	-0.14592100
H	-2.62204400	2.53792400	-0.49808900
H	-4.20076900	2.37864900	-1.37376500
I	1.43740600	3.16071800	-0.31793300
O	4.46106900	-0.57290200	-2.22905800
C	3.73017600	-0.87447400	-1.30001000
C	4.21116900	-1.31663000	0.02676800
C	2.19590900	-0.77993100	-1.58723500
C	3.33413000	-1.62200800	1.08382900
C	5.60258700	-1.39036900	0.22471800
H	2.04638500	-0.34377800	-2.59016800
H	1.93504500	0.14821900	-0.85640200
C	3.85305200	-1.98797800	2.32584100
H	2.26120400	-1.59790600	0.92743900
C	6.11188000	-1.76048900	1.46579900
H	6.25960100	-1.14808300	-0.60472300
C	5.23669800	-2.05805800	2.51785200
H	3.17692000	-2.22576200	3.14176900
H	7.18596800	-1.81534200	1.61796000
H	5.63423300	-2.34641100	3.48719500
O	1.51686900	-1.88153300	-1.29998500
H	0.37296900	-1.51024000	-0.80376600

TS21T

Cu	0.49782900	0.61855700	0.28091300
O	-1.21605000	1.28490500	-0.15081700
O	-0.46123800	-0.80985200	1.15549700
Cu	-2.20743700	-0.17513000	0.61151800
I	-3.06103600	-2.39113600	-0.48314300
S	-4.52622100	1.84875800	-0.03206400

O	-3.96193000	0.69309300	0.84763600
C	-3.49658200	3.31391800	0.29157000
C	-3.98963900	1.51398100	-1.73715200
H	-3.66685500	3.59904300	1.33196500
H	-2.44825600	3.05219200	0.12084000
H	-3.82780900	4.11636500	-0.37471700
H	-4.37307800	2.31340900	-2.37829800
H	-2.89679000	1.46675500	-1.75788400
H	-4.42544900	0.55370300	-2.02153000
I	2.10722000	2.42563700	-0.36149100
C	2.53739700	-1.45534800	0.67602600
C	3.85409000	-1.34564600	-0.01429600
C	2.44659000	-1.13778900	2.24943600
C	4.77594300	-0.32966000	0.29453200
C	4.15618300	-2.28743700	-1.01262900
H	1.96727600	-0.21776600	0.52514500
C	5.99147900	-0.26878900	-0.38528200
H	4.54540100	0.40449600	1.05824000
C	5.37285300	-2.22196000	-1.68670800
H	3.42769200	-3.05988400	-1.23715900
C	6.29203800	-1.21275000	-1.37308300
H	6.70335600	0.51567000	-0.14634600
H	5.60702200	-2.95276500	-2.45544700
H	7.24102600	-1.16142700	-1.89983200
H	-0.17004300	-1.67420100	0.78510000
O	3.40680200	-0.97632600	2.94980300
O	1.71114800	-2.37426300	0.37932100
H	1.39495200	-1.17520800	2.58206700

TS20S-2

Cu	0.60812000	0.88432700	-0.17929400
O	-1.05875100	1.36733100	0.43789400
O	-0.14167100	-0.80012700	-0.20966500
Cu	-1.88640400	-0.24694300	0.10691500
I	-3.06869700	-2.41057500	-0.44283000
S	-3.77367400	1.00614100	0.68231600
O	-5.15986300	0.46084600	0.75855600
C	-3.67839700	2.39977100	-0.47116400
C	-3.29139400	1.78047700	2.24769500
H	-3.97244000	2.01659800	-1.45057800
H	-4.37752600	3.17121500	-0.13801600

H	-2.63791200	2.73356700	-0.47176000
H	-2.25858100	2.11762600	2.12638300
H	-3.98821400	2.59587000	2.45844900
H	-3.36704700	1.00641400	3.01421000
I	1.74457100	3.09604700	-0.18920100
O	4.55049700	-0.77058700	-2.24423800
C	3.78024800	-1.04551300	-1.33899900
C	4.19670800	-1.56659900	-0.01986100
C	2.26575500	-0.82190400	-1.65020800
C	3.27666300	-1.82666300	1.01263200
C	5.57284100	-1.76570300	0.19815700
H	2.16820300	-0.34308700	-2.63892200
H	2.04686400	0.08176900	-0.89046800
C	3.73873900	-2.27284100	2.25075200
H	2.21252800	-1.70397700	0.84187800
C	6.02478900	-2.21562400	1.43499300
H	6.26394500	-1.55617400	-0.61225500
C	5.10746400	-2.46794100	2.46269500
H	3.02965000	-2.47520200	3.04799000
H	7.08706500	-2.36758900	1.60284300
H	5.46034000	-2.81837000	3.42880900
O	1.50453800	-1.89137900	-1.42453000
H	0.44228800	-1.48450800	-0.94322400

TS21T-2

Cu	0.61357000	0.63637600	0.23866400
O	-1.08817600	1.37943700	-0.23862100
O	-0.40092900	-0.81086700	0.98009000
Cu	-2.10194800	-0.13819600	0.25194300
I	-3.42468600	-2.22091800	-0.35799300
S	-4.03186000	1.45708200	0.10511600
O	-5.44041600	1.26012200	0.58402300
C	-3.99645500	1.73364500	-1.68927200
C	-3.42346500	3.07782100	0.66827200
H	-4.33689500	0.80695200	-2.15626900
H	-4.66773200	2.56046000	-1.93646800
H	-2.96206100	1.94966800	-1.96955500
H	-2.41381300	3.21578800	0.27400100
H	-4.11375600	3.84888100	0.31602600
H	-3.41322000	3.05297200	1.75985900
I	2.30613900	2.39177900	-0.31248700

C	2.58017100	-1.52526100	0.61717400
C	3.92566800	-1.44569800	-0.01524200
C	2.43928900	-1.24165700	2.20470600
C	4.85826300	-0.45491300	0.34162000
C	4.24705600	-2.38852500	-1.00734500
H	2.05104400	-0.29021000	0.48069100
C	6.10286500	-0.41971900	-0.28458000
H	4.61306400	0.27962300	1.10051400
C	5.49263500	-2.34842000	-1.62767300
H	3.51073800	-3.14152300	-1.26909300
C	6.42184700	-1.36418100	-1.26642000
H	6.82312500	0.34465100	-0.00901600
H	5.74219100	-3.07937600	-2.39124500
H	7.39352200	-1.33286400	-1.75153700
H	-0.07275800	-1.67385100	0.63777700
O	3.37786300	-1.13558600	2.94018400
O	1.74432600	-2.42432600	0.28446200
H	1.37365800	-1.24615900	2.49170300

TS22S

Cu	1.23247200	-1.03334800	-0.04274600
O	0.02739100	0.50618300	0.00387400
O	-0.51018000	-1.74277300	0.14421800
Cu	-1.78681100	-0.35381900	0.09829000
I	-3.79206500	-2.04506700	0.05539300
S	-4.16117300	1.50021600	-0.45445100
O	-2.72650100	1.36330600	0.14880900
C	-5.28578400	1.47966400	0.97395500
C	-4.21957100	3.28312800	-0.80827900
H	-5.29156000	0.45165100	1.34209500
H	-4.90666700	2.16524000	1.73632200
H	-6.28597900	1.76880400	0.63740900
H	-5.22985300	3.55030800	-1.13141200
H	-3.92762500	3.83753900	0.08678400
H	-3.50533400	3.46772600	-1.61296300
I	0.55216800	2.44395800	0.00009800
H	-0.75000800	-2.68024600	0.02035000
O	2.92239800	-0.11829500	-0.24086300
C	3.89620200	-0.98871600	-0.26150600
C	5.30203300	-0.50256400	-0.09908900
C	3.51707600	-2.38482000	-0.16473700

C	6.42332400	-1.28037500	-0.43016400
C	5.48424600	0.78026200	0.43460300
C	7.70844700	-0.78752100	-0.20681900
H	6.29929700	-2.26149400	-0.88326200
C	6.77352800	1.27020900	0.65426600
H	4.60785700	1.37465300	0.66979700
C	7.88743300	0.48862000	0.33855800
H	8.57022900	-1.39509900	-0.46862900
H	6.90595900	2.26489100	1.07087700
H	8.88995100	0.87188900	0.50734100
O	2.26939000	-2.70018300	-0.10442700
H	3.93720300	-1.77684800	-1.37732200
H	4.27409800	-3.16910200	-0.07559800

TS22T

Cu	1.14058400	-0.93146800	0.59806000
O	-0.00256700	0.64597100	0.87600700
O	-0.50802600	-1.77144700	1.14096700
Cu	-1.70819400	-0.39529400	0.57029700
I	-3.41811900	-2.03895000	-0.60057500
S	-3.95758500	1.48991900	-0.45172300
O	-2.85407900	1.20036200	0.61453900
C	-5.53281100	1.11589300	0.37543600
C	-4.04618400	3.30444500	-0.37650100
H	-5.58295500	0.02862500	0.46169500
H	-5.53732900	1.58593600	1.36230200
H	-6.35185200	1.48722500	-0.24793000
H	-4.86890300	3.64855100	-1.00982700
H	-4.18482000	3.61683900	0.66134000
H	-3.09297900	3.67769600	-0.75555700
I	0.37157500	2.38680200	-0.03431400
H	-0.67951500	-2.62740600	0.70630200
O	2.79652900	-0.05272400	0.13377800
C	3.72937700	-0.92792700	-0.14927300
C	5.14288500	-0.45056400	-0.26273700
C	3.33344400	-2.31923600	-0.09108700
C	6.24575500	-1.29491900	-0.06126500
C	5.35387500	0.90438300	-0.55703000
C	7.54274000	-0.79068800	-0.17314300
H	6.10077500	-2.33875300	0.20243300
C	6.65150200	1.40456400	-0.66412300

H	4.49040300	1.54854400	-0.68727300
C	7.74884100	0.55797800	-0.47761200
H	8.39122300	-1.44926800	-0.00980000
H	6.80688000	2.45557400	-0.89151700
H	8.75946700	0.94847800	-0.55928200
O	2.12238100	-2.60847400	0.23204400
H	3.50326900	-1.58709000	-1.30710900
H	4.04479500	-3.12677100	-0.28611700

TS22S-2

Cu	-1.07652100	-1.06431700	0.02655500
O	0.05116300	0.52882300	-0.01936300
O	0.67413500	-1.71413800	-0.13242700
Cu	1.91740100	-0.26745800	-0.05211900
I	3.94256000	-1.91374300	-0.02884800
S	3.20085300	1.78260800	0.05899800
O	2.61668300	3.16926800	0.06861600
C	4.43315700	1.67881100	-1.27392600
C	4.29385300	1.59682700	1.50011800
H	3.89018100	1.80494700	-2.21294900
H	5.14712100	2.49561900	-1.13810400
H	4.91282700	0.69782900	-1.23732500
H	4.77104900	0.61478400	1.45641500
H	5.02131200	2.41280500	1.48178600
H	3.66022300	1.67642200	2.38594400
I	-0.67455500	2.39300800	-0.11369700
H	0.91991000	-2.64606300	0.01858100
O	-2.78708000	-0.21164300	0.19033100
C	-3.73617800	-1.11756700	0.25581500
C	-5.15597700	-0.67026800	0.10958900
C	-3.30439300	-2.49766100	0.22311800
C	-6.15844400	-1.50709600	-0.40444600
C	-5.47309200	0.64493000	0.47979200
C	-7.46731700	-1.03645500	-0.52613600
H	-5.92064000	-2.51572800	-0.73052800
C	-6.78120700	1.11147800	0.35306400
H	-4.68250400	1.28728900	0.85384800
C	-7.78204000	0.27091800	-0.14498500
H	-8.23712800	-1.68762000	-0.93051300
H	-7.02000700	2.13121900	0.64169600
H	-8.80051300	0.63570400	-0.24495800

O	-2.04670600	-2.76212300	0.13232300
H	-3.71914700	-1.81073600	1.40794200
H	-4.02184500	-3.32273600	0.25259500

TS22T-2

Cu	1.07674600	-0.93845700	0.49314500
O	-0.08305000	0.70132900	0.48736200
O	-0.58040600	-1.78318000	0.96188900
Cu	-1.78425500	-0.37590000	0.43367500
I	-3.66912700	-1.65649800	-0.74518700
S	-3.18595600	1.46546000	1.29187800
O	-4.08242900	1.12586000	2.44845900
C	-4.15272000	2.21035600	-0.05212900
C	-2.15857900	2.89607200	1.75148300
H	-4.80981000	1.42577500	-0.43257700
H	-4.73115200	3.04592600	0.35144300
H	-3.46457900	2.53644700	-0.83696900
H	-1.61410700	3.25288900	0.87410500
H	-2.81911800	3.66674300	2.15805800
H	-1.45553500	2.55273700	2.51192300
I	0.11715900	1.78496200	-1.19891200
H	-0.74481700	-2.64757400	0.54362900
O	2.74633200	-0.02377100	0.20412000
C	3.72842600	-0.88015800	0.04862100
C	5.13329400	-0.36991600	0.09007600
C	3.36125400	-2.27855400	0.09067400
C	6.21220500	-1.17087100	0.49493700
C	5.35848800	0.96798400	-0.26571100
C	7.50382600	-0.64162300	0.52302700
H	6.04881000	-2.19781600	0.80934200
C	6.64997800	1.49325900	-0.23254900
H	4.51109200	1.58084000	-0.55545000
C	7.72591200	0.68886700	0.15674500
H	8.33344000	-1.26545900	0.84339600
H	6.81750100	2.53038100	-0.50923700
H	8.73147600	1.09924700	0.18400900
O	2.12623700	-2.59252700	0.27739500
H	3.65090000	-1.56191800	-1.11088100
H	4.10724300	-3.07198700	-0.00618900

22S

Cu	1.33329900	-0.87797000	-0.52700500
O	0.06571500	0.58098400	-0.25116300
O	-0.31917900	-1.70702300	-0.09850200
Cu	-1.66180100	-0.38375900	0.07627000
I	-3.58581100	-2.17242400	0.24949500
S	-4.16896800	1.36037400	-0.11466900
O	-2.66713700	1.27852500	0.30977100
C	-5.11273000	1.24987400	1.43538200
C	-4.34900000	3.14684700	-0.40389700
H	-5.03100800	0.21324500	1.76862000
H	-4.67467000	1.93183600	2.16884900
H	-6.15720600	1.50192600	1.22842300
H	-5.40136900	3.37289700	-0.59855000
H	-3.97889800	3.69192500	0.46768900
H	-3.74354100	3.38606800	-1.28020000
I	0.49973300	2.53547300	-0.29415300
H	-0.55480200	-2.64514800	-0.21939700
O	2.84880700	0.15134500	-0.93671800
C	3.98445800	-0.59978400	-1.13287400
C	5.09645600	-0.35652100	-0.08826300
C	3.69464200	-2.07663700	-1.04622300
C	6.41047800	-0.79087500	-0.31091900
C	4.77360700	0.29240900	1.10791100
C	7.39421400	-0.58130600	0.65842800
H	6.67341400	-1.27695900	-1.24954300
C	5.76013800	0.50392100	2.07458000
H	3.75752000	0.64798200	1.24520400
C	7.06921700	0.06444500	1.85553200
H	8.41249900	-0.91479500	0.47650500
H	5.50692400	1.01784600	2.99822900
H	7.83470400	0.23167400	2.60847600
O	2.55863100	-2.48445400	-0.76052300
H	4.43075300	-0.42949300	-2.13635100
H	4.49432300	-2.81570700	-1.20591100

TS23S

Cu	1.46717400	-0.26865100	-0.10884900
O	-0.08190500	0.91895500	0.01849400
O	0.03118900	-1.44786500	0.25159700
Cu	-1.57631200	-0.40703900	0.17503600
I	-3.08320400	-2.56739800	-0.12848900

S	-4.34625400	0.81120200	-0.34128900
O	-2.95715900	0.98074600	0.34978100
C	-5.49115600	0.33651600	0.98933000
C	-4.86280100	2.54599000	-0.52286300
H	-5.24074800	-0.69297500	1.25374500
H	-5.34414200	1.00526000	1.84149800
H	-6.51525300	0.39337800	0.60813200
H	-5.89030500	2.57644900	-0.89682600
H	-4.77498900	3.05076200	0.44220500
H	-4.18383500	3.00138300	-1.24631900
I	-0.08330500	2.92896700	-0.01399900
O	2.93751200	0.78541200	-0.74370800
C	3.62792700	-0.31214800	-0.91944800
C	5.04549700	-0.39387600	-0.47331100
C	3.09741500	-1.68281400	0.47297100
C	5.55015800	0.54644600	0.44220800
C	5.87892300	-1.41553200	-0.96174400
H	3.41378200	-0.92897200	-1.81071400
C	6.87738100	0.46566200	0.85209400
H	4.88960300	1.32802100	0.80355300
C	7.20719000	-1.49594900	-0.54000300
H	5.49023300	-2.13039300	-1.68456100
C	7.70616900	-0.55689000	0.36725800
H	7.27305800	1.19702900	1.55120700
H	7.85171400	-2.28202500	-0.92293900
H	8.74046300	-0.61650800	0.69448900
O	3.03521900	-1.43805500	1.64819400
H	-0.04945000	-2.37579300	-0.03551300
H	3.33085000	-2.69094700	0.06130600

TS24S

Cu	1.19445800	-0.89028800	-0.45787900
O	-0.01129400	0.65562900	-0.25639300
O	-0.59693800	-1.57843300	-0.53624900
Cu	-1.81297600	-0.17386800	-0.23128100
I	-3.84470600	-1.81786800	-0.20296100
S	-4.20909300	1.74597200	-0.27170200
O	-2.70383700	1.52937500	0.09802200
C	-5.10841000	1.60746900	1.30173100
C	-4.25921200	3.55452200	-0.44917000
H	-5.09377700	0.54910600	1.56978000

H	-4.59775800	2.20848500	2.05854700
H	-6.13744200	1.94621900	1.14852300
H	-5.29718100	3.86939200	-0.58996200
H	-3.81911700	4.01552300	0.43815700
H	-3.66782800	3.80069400	-1.33309800
I	0.53698600	2.58491000	-0.20831300
H	-0.85903700	-2.48547800	-0.29116000
O	2.92778500	-1.29931500	-0.91922300
C	3.86161500	-1.71222000	-0.00032000
C	5.09500000	-0.80001500	0.06877400
C	3.30388400	-1.80966700	1.42167400
C	6.30213700	-1.27088800	0.60381000
C	5.00704800	0.52630400	-0.37045700
C	7.40805000	-0.42337500	0.70548400
H	6.38491500	-2.30698100	0.92825000
C	6.11577000	1.37049900	-0.27368700
H	4.07463500	0.87606000	-0.80153800
C	7.31648600	0.90103500	0.26744400
H	8.34103500	-0.79969900	1.11688300
H	6.04214200	2.39688700	-0.62385700
H	8.17762600	1.55985700	0.34047000
O	2.14782400	-1.52950300	1.69927800
H	4.22666300	-2.73098800	-0.24728300
H	4.00420000	-2.14253700	2.21180600

TS24S-2

Cu	1.12343800	-0.98390000	-0.61566500
O	-0.02957200	0.57703500	-0.27007900
O	-0.65762900	-1.64955000	-0.65855200
Cu	-1.84643700	-0.24533100	-0.15552900
I	-3.84459100	-1.90230500	0.00292700
S	-3.07317700	1.73558400	0.47310600
O	-2.45584300	3.10577600	0.53573100
C	-3.83904200	1.35338600	2.07607400
C	-4.55419400	1.80939300	-0.57752800
H	-3.02991100	1.31483600	2.80837400
H	-4.53467900	2.15998400	2.32235600
H	-4.33789400	0.38392600	2.00344300
H	-5.04274800	0.83242200	-0.57020900
H	-5.20183400	2.60095400	-0.19130600
H	-4.21188100	2.05893800	-1.58396900

I	0.71191600	2.43988200	-0.28799500
H	-0.86917700	-2.55649400	-0.36668000
O	2.84251200	-1.36414200	-1.13728500
C	3.77144400	-1.91084000	-0.28407300
C	4.97273400	-0.99316000	-0.01144100
C	3.18568400	-2.27736300	1.08066900
C	6.17992900	-1.52528500	0.46259100
C	4.85393000	0.38898900	-0.19944900
C	7.25571400	-0.68315300	0.75373200
H	6.28690200	-2.60117400	0.59051100
C	5.93350400	1.22828700	0.08599600
H	3.92314100	0.79121500	-0.58606000
C	7.13389100	0.69694000	0.56695800
H	8.18920600	-1.10539300	1.11616300
H	5.83709800	2.29960600	-0.06955200
H	7.97186600	1.35252800	0.78758500
O	2.02347600	-2.05173200	1.38305900
H	4.17404100	-2.85272800	-0.70888000
H	3.87034300	-2.75407100	1.80755500

TS25S

Cu	-1.13545900	-0.70396300	-0.51822800
O	0.10859300	0.78652300	-0.36773400
O	0.56224300	-1.53893400	-0.68821100
Cu	1.88733700	-0.23075200	-0.33483000
I	3.74455600	-2.08413700	-0.30320300
S	3.19816500	1.87317100	1.59152000
O	2.94706600	1.36833700	0.14783000
C	1.56717100	2.18892000	2.34023400
C	3.66035100	0.43631000	2.60948100
H	1.18812000	3.12001700	1.91552500
H	0.89177300	1.36775700	2.08170100
H	1.69047400	2.28755100	3.42271200
H	3.85194800	0.79435500	3.62591800
H	2.86401000	-0.31263000	2.59363600
H	4.56460100	0.00937300	2.17204300
I	-0.37997500	2.67599900	-0.93375400
O	-2.58508100	-1.90716600	-0.90179300
C	-3.40489600	-0.88787700	-0.85160700
C	-4.69252900	-0.98926600	-0.11087200
C	-2.73994300	0.46620700	0.49818200

C	-4.89214700	-2.02722400	0.81626900
C	-5.70874700	-0.04389800	-0.33614900
H	-3.45066900	-0.21047600	-1.72223400
C	-6.10091800	-2.11866300	1.49939400
H	-4.09603600	-2.74831000	0.97090300
C	-6.91588800	-0.13648000	0.35878100
H	-5.55819800	0.74673400	-1.06871200
C	-7.11186500	-1.17218500	1.27690100
H	-6.26243500	-2.92654800	2.20751500
H	-7.70280300	0.59026700	0.17856100
H	-8.05230200	-1.24759600	1.81561500
O	-2.38435100	0.16926600	1.60801200
H	0.77278100	-2.48356100	-0.56222100
H	-3.15044800	1.46111600	0.21356800

23S

Cu	1.48288100	0.10246300	0.66016700
O	-0.16296100	1.06284800	0.22678300
O	0.15306100	-1.22238200	0.45314600
Cu	-1.52340100	-0.42440500	0.12492800
I	-2.73292300	-2.74267400	0.11072900
S	-4.31403200	0.34339100	-0.88668300
O	-3.01699900	0.81521700	-0.15578600
C	-5.52373300	0.03215300	0.43463400
C	-4.97692300	1.92984600	-1.47916200
H	-5.20003100	-0.88309400	0.93449700
H	-5.52034400	0.87744100	1.12778000
H	-6.50971000	-0.11038500	-0.01785300
H	-5.96598600	1.76330000	-1.91560900
H	-5.02249600	2.63466100	-0.64555000
H	-4.28559900	2.29493100	-2.24108800
I	-0.36447400	3.03845900	-0.09148100
H	0.27038000	-2.14379200	0.75352700
O	2.92974100	-1.00724600	1.14721400
C	4.12520700	-0.32995800	1.22071000
C	5.15160200	-0.72124600	0.13368700
C	3.93225100	1.15358600	1.03767900
C	6.50375900	-0.37006800	0.24971100
C	4.71149200	-1.42205900	-0.99391600
C	7.40873900	-0.71505900	-0.75689700
H	6.85713700	0.15678500	1.13510500

C	5.61914400	-1.76917900	-1.99789100
H	3.66665700	-1.71038200	-1.04883800
C	6.96652600	-1.41335600	-1.88495700
H	8.45698100	-0.44593200	-0.65716900
H	5.27436400	-2.32346200	-2.86689000
H	7.67066800	-1.68618800	-2.66633700
O	2.81715100	1.61586700	0.75380100
H	4.61840000	-0.46756800	2.20622300
H	4.78289700	1.84670400	1.11833900

23T

Cu	-1.42530600	0.18308600	-0.09776900
O	0.15657200	1.14077100	0.54062000
O	-0.34853400	-1.30901800	0.51047200
Cu	1.36779100	-0.47831500	0.37702400
I	2.58750700	-2.62774000	-0.56139100
S	4.39712000	0.02348600	0.91290800
O	2.96289600	0.61408400	0.71989400
C	5.22918000	0.25722700	-0.68704500
C	5.19825300	1.38063300	1.82148800
H	4.78562100	-0.46988500	-1.37025000
H	5.05193300	1.27828400	-1.03450300
H	6.29728200	0.05681800	-0.56025900
H	6.26603900	1.16434200	1.91875400
H	5.02798400	2.31961300	1.28957500
H	4.73181300	1.41834100	2.80786600
I	0.64330900	2.89422600	-0.29953300
H	-0.45251600	-2.09773500	-0.05396300
O	-2.79135100	-0.83527300	-0.90076100
C	-3.95446000	-0.14473800	-1.14720000
C	-5.15146600	-0.56551500	-0.26610200
C	-3.78002900	1.32598700	-0.86156000
C	-6.46125900	-0.18588000	-0.59092700
C	-4.91399000	-1.32056200	0.88728600
C	-7.52605500	-0.55703200	0.23345100
H	-6.65529700	0.38421500	-1.49852100
C	-5.98111300	-1.69337100	1.70859700
H	-3.89640600	-1.62917000	1.10497300
C	-7.28669600	-1.30966600	1.38752000
H	-8.53985100	-0.26567100	-0.02830600
H	-5.79288900	-2.28941700	2.59772700

H	-8.11478800	-1.60254200	2.02728000
O	-2.72874400	1.74822500	-0.36122900
H	-4.27271700	-0.23603600	-2.20643400
H	-4.59635700	2.03814800	-1.05493600

24T

Cu	0.75097400	0.02407000	-0.07095600
O	-0.98770000	0.67603200	0.72224700
O	-0.40527900	-1.61981600	-0.16321000
Cu	-2.06993800	-0.64756700	-0.20510900
I	-4.33046200	-1.17954700	-1.03027400
S	1.72103700	-1.20990300	2.84442500
O	1.79877400	-0.01409100	1.87435000
C	-0.04429900	-1.47614100	3.21789500
C	1.96844000	-2.71991600	1.85035000
H	-0.40623400	-0.57326600	3.71323600
H	-0.58347400	-1.64064600	2.28228700
H	-0.13259800	-2.33757400	3.88709500
H	1.86915600	-3.59002800	2.50681700
H	1.22728000	-2.73110100	1.04585200
H	2.97710200	-2.66967700	1.43549900
I	-1.60428300	2.57608200	0.60417200
C	2.92353200	0.09136000	-1.80138000
C	4.39164400	-0.06584000	-1.37067900
C	2.56122200	1.52391200	-1.49815200
C	5.41411200	-0.16017800	-2.32187200
C	4.71152900	-0.09685600	-0.00458600
H	2.89701700	-0.00503700	-2.90741800
C	6.74560800	-0.29537200	-1.91720900
H	5.16825800	-0.14464300	-3.38196400
C	6.04225600	-0.22886100	0.39702500
H	3.91399700	-0.01995100	0.73087300
C	7.06161800	-0.32922100	-0.55659700
H	7.53153600	-0.38102300	-2.66293400
H	6.28608700	-0.24900900	1.45624600
H	8.09588600	-0.43507700	-0.24036100
H	-0.16346700	-2.03837700	-1.01159400
O	1.64154000	1.80034600	-0.71955200
O	2.04988900	-0.78752700	-1.18785900
H	3.14251400	2.34207300	-1.95175900

25T

Cu	0.56542700	1.10809600	0.29521000
O	-1.14227300	1.26003200	-0.36664400
O	1.91900400	-2.60105900	3.10865100
Cu	-2.10083100	-0.28581500	-0.27706800
I	-4.37971400	-1.28417900	-0.37263400
S	-0.96579000	3.62903300	0.74817900
O	0.50043200	3.06625200	0.75348100
C	-0.65254900	5.30170500	1.40161200
C	-1.32726700	4.10127100	-0.96963600
H	-0.33818600	5.18569800	2.44077800
H	0.14118100	5.77825600	0.82088100
H	-1.57860200	5.88252000	1.35478500
H	-2.27654800	4.64524800	-0.98896400
H	-0.51079900	4.71674600	-1.35759800
H	-1.41194800	3.15477400	-1.50658300
I	0.26268000	-1.58678800	-0.07265300
C	3.54281200	0.59535200	0.75610900
C	4.00069200	0.23067300	-0.58115200
C	3.24519700	-2.44174100	3.09003900
C	5.27779200	-0.35076600	-0.69375900
C	3.22111100	0.43797200	-1.73496100
H	4.28517800	0.50495500	1.55905500
C	5.76623100	-0.72932900	-1.94209200
H	5.86364900	-0.52342100	0.20515400
C	3.71546700	0.06632300	-2.98089200
H	2.23685500	0.89125600	-1.65344200
C	4.98518700	-0.51853600	-3.08370200
H	6.74649300	-1.18800100	-2.02834400
H	3.11555700	0.22487300	-3.87169800
H	5.36469300	-0.81136300	-4.05868500
H	1.53142500	-2.20967200	2.28822200
O	3.89443700	-1.88434600	2.22684900
O	2.41411000	1.00166100	1.07027100
H	3.67948700	-2.89916200	3.98944600

TS26T

Cu	-0.24705000	-0.98269200	0.33391900
O	1.65203600	-0.76868900	-0.09571200
O	-0.53696600	-0.03038400	-1.41353100
Cu	1.10764700	1.09952200	-0.81975800

I	1.88375400	3.29647300	-0.03232900
S	1.06217500	-1.34283700	3.22930900
O	-0.00546700	-1.72497400	2.16235800
C	2.68838200	-1.86162100	2.60360900
C	1.30007500	0.45469900	3.11567100
H	2.67478400	-2.95185600	2.54263100
H	2.83092600	-1.41448100	1.61604800
H	3.44564800	-1.53540000	3.32303000
H	2.07268700	0.74700200	3.83312100
H	1.59396700	0.73433100	2.09844000
H	0.35053300	0.92219400	3.38494000
I	2.30626100	-2.26540200	-1.31889500
C	-2.75812800	0.08783600	-0.02307700
C	-4.25088100	0.15490200	0.08446600
C	-2.47400400	-0.02652300	-1.75820000
C	-4.90289700	1.39165500	-0.04409700
C	-5.00330500	-1.01286400	0.28517200
H	-2.27621900	1.07113500	0.12239500
C	-6.29442000	1.46351500	0.04164800
H	-4.31938400	2.29793700	-0.19537000
C	-6.39173700	-0.93677300	0.37234500
H	-4.48547100	-1.96174100	0.38058100
C	-7.04014000	0.29926000	0.24897900
H	-6.79385200	2.42391000	-0.04932900
H	-6.97308000	-1.84006200	0.53515000
H	-8.12333600	0.35306800	0.31439000
H	-0.25463300	-0.64313500	-2.12322400
O	-2.76358300	-1.02088600	-2.37236000
O	-2.16248300	-0.93439400	0.57587200
H	-2.47143200	0.99776500	-2.15965500

TS26T-2

Cu	0.75607000	0.74923700	0.00192900
O	-1.08804500	1.01822400	0.57473500
O	-0.37841700	-0.92485100	-1.39748600
Cu	-1.69175300	-0.79913900	0.04044100
I	-3.50416700	-2.44295900	0.42385500
I	-2.07793400	2.43101400	-0.46827700
H	-0.67507300	-1.21009200	-2.28270700
O	2.27342200	0.25656600	-0.95865400
C	2.26906800	-1.13784800	-1.12672500

C	3.52260200	-1.80773000	-0.56779400
C	1.07501700	-1.73633500	-0.37260700
C	3.98719400	-3.01412500	-1.10927800
C	4.19512900	-1.23505000	0.52020700
C	5.11191500	-3.64449800	-0.57093100
H	3.47517400	-3.45708900	-1.96218400
C	5.32124000	-1.86437900	1.05452200
H	3.84002600	-0.29300900	0.92656100
C	5.78073000	-3.06987900	0.51372000
H	5.46827000	-4.57670600	-1.00137600
H	5.84131500	-1.41215700	1.89484800
H	6.65816800	-3.55618900	0.93168500
O	0.72169900	-1.19328700	0.72494800
H	2.17026100	-1.39372900	-2.19367200
S	2.08372000	2.74407200	0.62097000
O	3.08451300	2.48078100	1.71265100
C	1.22960300	4.31108100	0.98663600
H	0.65961900	4.15643500	1.90484200
H	1.98499100	5.08722000	1.13660900
H	0.55563200	4.56081900	0.16351100
C	2.94543500	3.21531700	-0.90505800
H	2.21155800	3.57673100	-1.63101800
H	3.68525000	3.98385500	-0.66501500
H	3.41443100	2.29961900	-1.26954000
H	0.82404000	-2.78941700	-0.54815000

TS26T-3

Cu	0.52312400	0.92389900	-0.72867900
O	-1.32777800	1.12140700	-1.24973600
O	0.30832000	-0.83654400	-1.74279800
Cu	-1.66909900	-0.73633700	-0.58044300
I	-0.82133300	-0.70385800	1.94432200
S	2.24398400	3.00179200	0.67502000
O	0.83747800	2.72369600	0.05071100
C	2.00355200	4.69166900	1.30112300
C	2.26559000	2.13373200	2.27086900
H	1.88622300	5.34020700	0.43072700
H	1.09943900	4.71783500	1.91397200
H	2.88465100	4.98988700	1.87668700
H	3.15020100	2.45385800	2.83004300
H	1.34175400	2.34874000	2.81321500

H	2.32479900	1.07175600	2.03017300
I	-2.48612200	2.66876700	-0.69855700
C	2.45123400	-0.94509100	-0.43406000
C	3.86471900	-1.42826700	-0.25483800
C	1.88371500	-1.54363900	-1.89283400
C	4.13035100	-2.57851000	0.50162100
C	4.92785500	-0.74101900	-0.86060500
H	1.75627500	-1.44674200	0.26378800
C	5.44240700	-3.03327400	0.65998700
H	3.30832800	-3.10982400	0.97719200
C	6.23656900	-1.19458700	-0.70089700
H	4.70930500	0.14048800	-1.45493500
C	6.49769200	-2.34160200	0.05938000
H	5.63950800	-3.92201100	1.25388600
H	7.05605100	-0.65948300	-1.17395600
H	7.51873600	-2.69424300	0.18011600
H	0.12810200	-0.58610600	-2.67186700
O	2.42698900	-1.19024000	-2.94686100
O	2.33000100	0.40914600	-0.41785500
H	1.59086100	-2.59554800	-1.72345800
S	-2.99876400	-3.39346400	0.12686700
O	-2.85835000	-2.30968400	-0.97839400
C	-4.22101900	-2.74972600	1.31237500
H	-3.73256400	-1.92217700	1.83319200
H	-5.10245800	-2.40182500	0.76661900
H	-4.47680100	-3.54355500	2.02072700
C	-4.05920200	-4.63745700	-0.67423900
H	-4.32420000	-5.40844300	0.05517800
H	-4.95028100	-4.14567200	-1.07273300
H	-3.47714300	-5.07549900	-1.48758000

TS26S

Cu	-0.57609600	1.11740100	0.50285800
O	1.29650600	0.80083500	0.51682000
O	-0.56436900	-2.18484700	0.86992600
Cu	0.78905800	-1.00770700	0.51325100
I	2.85864300	-2.29775500	-0.18102600
S	-2.40748700	3.42681000	0.03266700
O	-0.89417800	3.02646700	0.01048400
C	-2.27983900	5.23228700	-0.15036700
C	-3.04610200	3.03346600	-1.62187900

H	-1.82432800	5.61388300	0.76552100
H	-1.64577700	5.46298600	-1.00986100
H	-3.28295800	5.65112400	-0.27352500
H	-4.05306300	3.45053900	-1.71947100
H	-2.37122200	3.44401200	-2.37776000
H	-3.07404100	1.94290800	-1.65683400
I	2.74678800	1.81077600	-0.42541400
O	-2.35377000	0.62900700	0.07659600
C	-2.87269600	-0.41666400	0.83643000
C	-3.31760400	-1.61135600	0.00624200
C	-1.90555000	-0.80262400	1.96469300
C	-2.82695100	-1.78936700	-1.29470000
C	-4.21142500	-2.55380500	0.53294800
H	-3.75952600	-0.06028000	1.40637900
C	-3.20744600	-2.90444100	-2.04725600
H	-2.15707300	-1.03897100	-1.70299400
C	-4.58733100	-3.67158200	-0.21636100
H	-4.61886200	-2.41415000	1.53292700
C	-4.08448600	-3.85137000	-1.50866100
H	-2.82089100	-3.03229000	-3.05512300
H	-5.27617400	-4.39815100	0.20638400
H	-4.37997900	-4.71797700	-2.09362000
O	-1.03838600	0.01139900	2.33093300
H	-0.85823000	-2.68878000	0.08804500
H	-2.15164200	-1.66516800	2.59680900

TS26S-2

Cu	-0.58254700	1.04752500	-0.15830100
O	1.23345700	1.18305600	-0.28714300
O	-0.35848000	-0.83865800	-0.74662300
Cu	1.62619000	-0.62855000	-0.17751800
I	2.23773200	-3.08423800	-0.10774300
S	3.66354600	0.42296500	0.52200000
O	4.88913100	-0.34555800	0.90307900
C	3.19155700	1.54638000	1.86745900
C	4.04872200	1.60092500	-0.80317300
H	2.91529500	0.92088300	2.71882100
H	4.06315500	2.15810500	2.11578200
H	2.34044900	2.13005200	1.51218700
H	3.12657600	2.14137100	-1.02548500
H	4.85675100	2.25120300	-0.45717000

H	4.37874100	1.00969800	-1.65982900
H	-0.20953300	-0.81104400	-1.71704600
O	-2.37674400	0.72415600	0.36500400
C	-2.69364200	-0.53403600	0.52548700
C	-4.13434100	-0.90593500	0.51647900
C	-2.23359000	-1.59678800	-0.98818900
C	-4.53309600	-2.12575700	1.09365300
C	-5.09200900	-0.06215700	-0.07379800
C	-5.88047500	-2.48710100	1.10185300
H	-3.79133900	-2.77468200	1.55529700
C	-6.43401900	-0.42897100	-0.06163700
H	-4.76619900	0.87283200	-0.51759000
C	-6.83128900	-1.64115000	0.52233900
H	-6.18756000	-3.42259400	1.56013400
H	-7.17707300	0.22704400	-0.50582800
H	-7.88031500	-1.92315900	0.52461500
O	-2.56479200	-1.28436600	-2.08946000
H	-2.07550300	-1.11968400	1.22475900
H	-2.07263600	-2.61050000	-0.59102100
I	-0.34019800	3.58105400	-0.09438100

HCOOH

C	0.00000000	0.42365800	0.00000000
H	-0.38658100	1.45126200	0.00000000
O	1.16700800	0.10929200	0.00000000
O	-1.03775100	-0.44091800	0.00000000
H	-0.64747500	-1.34020100	0.00000000

31S

Cu	1.18640600	0.24570500	-0.23810700
O	0.52285900	-1.42985600	-0.72748000
O	-0.59791000	0.72311300	-0.38077900
Cu	-1.28925400	-0.94878300	-0.34901800
I	-3.46543700	0.25951400	0.13912000
I	3.54641500	-0.72214300	0.11223600
S	0.96644600	3.31563300	0.22598700
O	1.82515700	2.00525000	0.10587600
C	-0.03664700	3.46440800	-1.28317800
C	-0.32055900	3.03062700	1.47689800
H	0.66616500	3.62928300	-2.10289000
H	-0.60789100	2.54283200	-1.42054600

H	-0.68425200	4.33838100	-1.16520800
H	-0.92945100	3.93794500	1.53366900
H	-0.90645200	2.15446700	1.18756600
H	0.20253000	2.87417100	2.42302300
C	-1.29666700	-3.56885000	0.32784300
H	-1.82399300	-4.53429700	0.39486600
O	-2.01986300	-2.66734300	-0.27313100
O	-0.15939900	-3.44073400	0.79616300
H	0.66744300	-2.16484500	-0.05608200

TS32S

Cu	1.24939400	0.28645200	-0.17263400
O	0.33321000	-1.22787800	-0.63114300
O	-0.42403400	1.06505000	-0.32409800
Cu	-1.34657900	-0.50709700	-0.34077200
I	-3.63585100	0.41044500	0.05395200
I	3.34155700	-1.16316700	0.05240500
S	1.61104700	3.33239400	0.31152400
O	2.20998000	1.88146300	0.22393900
C	0.69431200	3.63104200	-1.22867400
C	0.24963400	3.28703300	1.51380000
H	1.43587700	3.65257500	-2.03034300
H	-0.02635300	2.81914500	-1.36904400
H	0.20584000	4.60641500	-1.14484900
H	-0.21195900	4.27880500	1.53334100
H	-0.45346300	2.50593000	1.20883300
H	0.70193400	3.06744700	2.48350300
C	-1.49700900	-3.27580200	0.25510700
H	-1.86106500	-2.17282400	-0.11016200
O	-2.40462600	-4.02594500	0.49973600
O	-0.22329200	-3.35583200	0.29724300
H	0.23682300	-2.33135800	-0.07063100

TS32S-2

Cu	-1.07564100	-0.11550300	-0.16343000
O	0.04434500	1.28501000	-0.58658200
O	0.46342800	-1.10811800	-0.27282400
Cu	1.58506400	0.32243000	-0.29251200
I	3.70713000	-0.93531800	0.04159800
I	-3.17251900	1.31499600	-0.00905300
S	-2.13435400	-2.12734700	0.34827900

O	-2.50146600	-2.34983400	1.77696200
C	-1.02066000	-3.42903200	-0.23588300
C	-3.56401600	-2.36699500	-0.73943700
H	-0.06655900	-3.28170100	0.27329600
H	-1.47800900	-4.38663100	0.02784900
H	-0.88207900	-3.32146100	-1.31352000
H	-3.24558400	-2.20453400	-1.77250200
H	-3.94040600	-3.38215200	-0.58714300
H	-4.30691800	-1.62145100	-0.45145400
C	2.16586200	3.03860200	0.27981900
H	2.34944500	1.89144200	-0.06739600
O	3.17575100	3.64471100	0.51819200
O	0.91856800	3.32361400	0.31635500
H	0.31997900	2.40169100	-0.02797900

TS33S

Cu	1.09976500	-0.44715700	-0.05113500
O	0.44772500	1.24019600	-0.31056400
O	-0.69737000	-0.84415500	0.01073500
Cu	-1.35676300	0.82306200	-0.20075000
I	-3.75870400	-0.00787600	-0.08676500
I	3.49340600	0.44951700	-0.20523000
S	0.84627100	-3.52634000	0.33375000
O	1.72962100	-2.23656300	0.19353400
C	-0.32528600	-3.24097200	1.69400500
C	-0.29170200	-3.56543300	-1.08306500
H	0.27206100	-3.17511000	2.60614900
H	-0.86488400	-2.30992100	1.49688200
H	-0.99460300	-4.10483700	1.74728900
H	-0.95660900	-4.42489000	-0.95536500
H	-0.83968100	-2.61922800	-1.11514600
H	0.32816300	-3.70209300	-1.97202100
H	-2.01903900	2.31340200	-0.37416400
H	0.86273400	2.33715400	0.42481500
C	0.31996300	4.23652100	0.67274900
H	0.66539200	5.19980000	1.06506800
O	1.14989900	3.27517500	0.88616200
O	-0.78684200	4.20073900	0.09698700
H	-1.44223000	2.93510900	-0.20008500

TS33S-2

Cu	1.00985900	-0.23447700	-0.08815000
O	0.08546900	1.33289200	-0.34341900
O	-0.68564700	-0.94289900	-0.01815600
Cu	-1.60354200	0.60154700	-0.19043800
I	-3.82075900	-0.62770700	-0.01344400
I	3.32807900	0.76578700	-0.15150500
S	1.66388000	-2.46949100	0.19989300
O	3.06244500	-2.98306300	0.27863000
C	0.73418700	-3.29416800	-1.12023100
C	0.70530400	-2.94724100	1.66263300
H	1.26984100	-3.09576500	-2.05097500
H	0.71406500	-4.36718200	-0.91287100
H	-0.26367100	-2.84751500	-1.13652400
H	-0.29217700	-2.51495500	1.54632100
H	0.68911700	-4.03832500	1.72612900
H	1.22100300	-2.52311100	2.52678300
H	-2.57678600	1.94882700	-0.33368100
H	0.39744000	2.55925700	0.31830600
C	-0.44040500	4.32392600	0.50282800
H	-0.23840300	5.35203900	0.82678500
O	0.57318100	3.53904600	0.68942100
O	-1.55317000	4.05176700	0.02519200
H	-2.06641600	2.59824700	-0.21195000

int1b

O	2.91934700	1.41020300	-0.00011900
C	2.38759600	0.30222200	-0.00007200
C	0.90337600	0.15582100	-0.00004000
C	3.29237200	-0.92741100	-0.00027500
C	0.27718900	-1.10294100	-0.00003900
C	0.12217100	1.32489100	-0.00001300
C	-1.11278400	-1.19771100	-0.00002400
H	0.86691000	-2.01434700	-0.00006100
C	-1.26645900	1.24558500	0.00002300
H	0.62763400	2.28487200	-0.00001900
C	-1.85734600	-0.01892900	0.00001300
H	-1.62391800	-2.15271200	-0.00003200
H	-1.89385900	2.12874200	0.00005400
H	3.05820000	-1.54208100	0.88478000

N	-3.33045400	-0.11409400	0.00004300
O	-3.96634700	0.94190200	0.00007100
O	-3.82588600	-1.24323500	0.00002100
H	3.05866700	-1.54098900	-0.88628000
O	4.63860000	-0.54524400	0.00053100
H	4.61713400	0.43701700	-0.00021200

TS4Sb

Cu	0.24157200	1.04862000	-0.08906700
O	1.89543100	0.94823000	0.63967100
O	0.27684100	-0.72209100	0.49063900
Cu	2.10483300	-0.89834900	0.56754400
I	1.94565700	-3.35744100	-0.29298300
S	4.97286000	0.27225700	0.96249600
O	4.01199200	-0.95745400	0.82184900
C	4.31257300	1.31801800	2.29377000
C	4.66875500	1.35554800	-0.46413500
H	4.42771600	0.75331000	3.22168200
H	3.25886300	1.52685900	2.07805600
H	4.91038200	2.23345000	2.33587000
H	5.30086700	2.24180900	-0.35491400
H	3.60387500	1.60899300	-0.48482000
H	4.96606400	0.79160900	-1.35106900
I	0.71887700	3.50513200	-0.58499600
O	-1.57831900	0.96160900	-0.80261800
C	-2.15808000	-0.16696900	-0.85789200
C	-3.56481300	-0.25243000	-0.40653800
C	-1.39246800	-1.35868400	-1.21713800
C	-4.39680800	-1.33160800	-0.76099700
C	-4.08083200	0.80047200	0.37471000
H	-0.69067000	-1.36774600	-0.16000100
C	-5.71917900	-1.37191400	-0.32669100
H	-4.02638000	-2.12884500	-1.39649500
C	-5.39868700	0.76938600	0.81578000
H	-3.43147000	1.63169500	0.62666000
C	-6.19275700	-0.32131400	0.45766400
H	-6.38340900	-2.18697100	-0.58684200
H	-5.81933400	1.56070200	1.42429800
O	-0.42107500	-1.12550900	-2.17994300
H	0.28320600	-1.80008300	-2.05072600
H	-1.92420600	-2.30977000	-1.29678300

N	-7.59406200	-0.36192900	0.92151200
O	-7.98854700	0.57923900	1.61249300
O	-8.27321400	-1.33479200	0.58671500

TS6Sb

Cu	0.19880600	0.71219200	-0.02443700
O	1.95522600	1.03468900	-0.39917600
O	0.77008000	-1.10597900	-0.18316400
Cu	2.57598400	-0.69855100	-0.26403900
I	3.09885200	-3.20060100	-0.01191900
S	5.04378500	1.19846300	-0.38094700
O	4.43350900	-0.24773900	-0.35813000
C	4.31207700	2.07982600	-1.79368600
C	4.32449900	2.12698000	1.00654800
H	4.67605800	1.57566000	-2.69171200
H	3.22275000	2.02499800	-1.71558300
H	4.67720300	3.11095700	-1.76939600
H	4.71427100	3.14827100	0.95921700
H	3.23453400	2.09328600	0.92064100
H	4.67392500	1.63671200	1.91802900
I	-0.12638900	3.21778700	0.33431300
O	-1.79207300	0.38066800	-0.37385200
C	-2.46625400	-0.25439700	0.45181200
C	-3.91678900	-0.44197400	0.20188000
C	-1.79054300	-0.81583500	1.70959000
C	-4.71537300	-1.21360300	1.06656900
C	-4.49583900	0.17624000	-0.92258100
H	-2.33177500	-0.38099600	2.57167300
C	-6.07581100	-1.36849000	0.81409500
H	-4.28239100	-1.69793700	1.93545700
C	-5.85395500	0.02908900	-1.18411300
H	-3.86681100	0.77032400	-1.57640400
C	-6.61758900	-0.74286400	-0.30804400
H	-6.71589000	-1.95680100	1.46010600
H	-6.32784000	0.49371500	-2.04026600
O	-0.45344200	-0.54149100	1.76264500
H	0.33585200	-1.20395700	0.81862700
H	-2.01378000	-1.90112500	1.72018800
N	-8.06098600	-0.90494400	-0.57906500
O	-8.51520500	-0.34285700	-1.57707200
O	-8.71131200	-1.59106700	0.21181200

TS22Sb

Cu	0.50995500	-1.14053500	-0.08892200
O	-0.62624100	0.45502300	-0.04553900
O	-1.26412500	-1.76543000	0.12515200
Cu	-2.47128200	-0.31963900	0.09622000
I	-4.54264700	-1.91890700	0.14143000
S	-4.77991200	1.63021100	-0.40150200
O	-3.32711000	1.43514900	0.14361600
C	-5.83992800	1.68912900	1.07408300
C	-4.76691600	3.40649500	-0.78907500
H	-5.87944400	0.66953200	1.46285800
H	-5.39574000	2.36897000	1.80576900
H	-6.83883900	2.02050300	0.77482300
H	-5.77635200	3.71600800	-1.07476500
H	-4.41075900	3.96259500	0.08128900
H	-4.08040300	3.54091600	-1.62712100
I	-0.02754600	2.36925900	-0.08888500
H	-1.55306800	-2.69441100	0.05070300
O	2.25029200	-0.30733700	-0.32682200
C	3.17476000	-1.22192600	-0.33971000
C	4.60522200	-0.80157600	-0.21688600
C	2.73717600	-2.60133300	-0.21589000
C	5.68438300	-1.64623100	-0.53235000
C	4.85180100	0.49401600	0.26221000
C	6.99354100	-1.21323200	-0.35061600
H	5.51000500	-2.63770300	-0.94149400
C	6.15909100	0.93987300	0.44572100
H	4.00666200	1.13605800	0.48376600
C	7.20903700	0.07610200	0.13937400
H	7.84231800	-1.84314700	-0.58764100
H	6.37615300	1.93445800	0.81639100
O	1.47913700	-2.85619500	-0.12869400
H	3.16545600	-2.05398300	-1.44117500
H	3.46073100	-3.41491900	-0.10932900
N	8.59244800	0.53944200	0.32838800
O	8.75671900	1.68329600	0.76085700
O	9.50063100	-0.24649000	0.04311600

TS26Tb

Cu	0.38150100	-1.01080400	0.32506000
O	2.28294900	-0.75351200	-0.08284700
O	0.09426000	-0.01440300	-1.40595200
Cu	1.76321000	1.10917900	-0.75023300
I	2.39543600	3.34479300	0.04211600
S	1.66833600	-1.45759500	3.21843500
O	0.61539400	-1.80913500	2.12620200
C	3.30370000	-1.94672700	2.59349200
C	1.89539500	0.34444900	3.16887800
H	3.29585600	-3.03420700	2.49433100
H	3.45770100	-1.46479400	1.62439800
H	4.05142800	-1.64338000	3.33257400
H	2.65854300	0.61705300	3.90393400
H	2.19783000	0.65915700	2.16470800
H	0.94010700	0.79655300	3.44396300
I	2.98958800	-2.16632100	-1.37124500
C	-2.12590600	0.05975100	-0.05622700
C	-3.62657000	0.06847000	0.00417500
C	-1.76574100	0.02915000	-1.77059800
C	-4.32479400	1.28314700	-0.09144400
C	-4.33228800	-1.13872400	0.13200200
H	-1.69028900	1.05036100	0.16479700
C	-5.71737200	1.30188600	-0.05172800
H	-3.77816400	2.21882800	-0.18324800
C	-5.72250600	-1.13431400	0.17501000
H	-3.77739000	-2.06750200	0.20676100
C	-6.39165800	0.08852800	0.08115500
H	-6.28231700	2.22393800	-0.11596600
H	-6.29582700	-2.04779400	0.27793200
H	0.38123000	-0.60278600	-2.13501000
O	-2.06921800	-0.93246600	-2.43949300
O	-1.53297500	-0.96936100	0.54034000
H	-1.77252200	1.07089100	-2.12557100
N	-7.86274100	0.09854100	0.12723100
O	-8.42852000	1.19189200	0.03856000
O	-8.43649000	-0.98679000	0.25149100

TS29Tb

Cu	1.38169300	-1.06109700	0.86516700
O	2.20851800	0.00146700	-0.58001200
O	-0.30216400	-1.03446300	-0.17114800

Cu	0.61124400	1.13477900	-0.60381100
I	-0.69159500	3.15116400	-0.12696700
S	3.79045900	0.53623600	1.68854900
O	2.98925300	-0.77799500	1.98346300
C	4.58121900	0.83107800	3.29690800
C	5.25886500	0.01374200	0.75767900
H	3.78370500	1.08597600	3.99748500
H	5.09092000	-0.07976800	3.62048900
H	5.27950900	1.66759500	3.20359300
H	5.95399400	0.85642600	0.69919300
H	5.71577200	-0.84496900	1.25636900
H	4.91352300	-0.25641200	-0.24149100
I	2.64418600	-1.04654600	-2.27761100
C	-0.86043600	-1.90604600	2.16068900
C	-1.49649800	-2.28572800	0.63051200
H	-1.20682300	-0.86751800	2.27652000
H	-0.16628200	-1.49879500	-1.02264500
O	-1.24330800	-3.40218600	0.19514200
O	0.45982900	-2.07681300	2.19690900
C	-2.83949600	-1.62972600	0.41088300
C	-3.03234100	-0.24282300	0.47210800
C	-3.92584800	-2.48926400	0.17729800
C	-4.30869700	0.28928100	0.29593000
H	-2.19164700	0.43058500	0.60967500
C	-5.20592400	-1.96759000	0.00963000
H	-3.75335100	-3.55906300	0.12500200
C	-5.37318400	-0.58434200	0.07548700
H	-4.48122300	1.35859500	0.32037200
H	-6.06420400	-2.60304900	-0.17259100
H	-1.40013100	-2.59115800	2.82930300
N	-6.72682700	-0.02749400	-0.10020100
O	-7.64676800	-0.82407700	-0.30643100
O	-6.85307800	1.19671700	-0.02743800

int3b

O	-2.58046100	1.68036000	0.19104100
C	-2.09982900	0.57454700	-0.03408900
C	-0.63297000	0.33701600	-0.01888400
C	-3.08500400	-0.58003400	-0.33333600
C	-0.08756700	-0.95590400	-0.10852500

C	0.21652900	1.45450400	0.07772200
C	1.29465600	-1.13272900	-0.10546300
H	-0.74348100	-1.81886300	-0.14154500
C	1.59711400	1.29104900	0.07546400
H	-0.22852200	2.44129000	0.15077300
C	2.10908300	-0.00461500	-0.01861700
H	1.74746400	-2.11492400	-0.16534600
H	2.27743800	2.13127400	0.14369000
H	-2.82586600	-1.10647600	-1.26253200
N	3.57392900	-0.18816600	-0.02284000
O	4.27247100	0.82455400	0.05836900
O	4.00149200	-1.34157600	-0.10794200
O	-4.36418100	-0.06905200	-0.48896900
H	-4.35331000	0.80115000	-0.03002800
O	-2.95852400	-1.45315100	0.78664300
H	-3.72967900	-2.04836500	0.74610500

TS17Sb

Cu	0.34378600	1.02160600	0.00420400
O	2.03797900	1.00545300	-0.69017000
O	0.63452100	-0.79906400	0.07944900
Cu	2.43756600	-0.74781800	-0.24651400
I	2.60749500	-3.18541800	0.52034000
S	5.08198600	0.58184700	-1.19343500
O	4.29452800	-0.66900600	-0.65814800
C	4.20492200	1.17398900	-2.66927500
C	4.76397600	1.95106800	-0.04385900
H	4.31975800	0.39895600	-3.43029800
H	3.15368800	1.32600800	-2.40158600
H	4.68639700	2.09887100	-3.00063100
H	5.24646400	2.84704700	-0.44568600
H	3.67897800	2.06652600	0.04986700
H	5.22565400	1.67186700	0.90585100
I	-0.19311100	3.46283900	-0.08361200
O	-3.24887300	1.19594900	2.74623600
C	-2.92836600	0.38157100	1.89077200
C	-3.88777600	-0.17870800	0.91005600
C	-1.40523600	0.00909300	1.85622400
C	-3.51933100	-1.08856500	-0.09917000
C	-5.22204900	0.26452700	1.00860000

H	-1.10727500	0.73726400	0.86021800
C	-4.47606100	-1.54414500	-1.00469300
H	-2.49872200	-1.44434800	-0.16155900
C	-6.18250900	-0.19054200	0.11380600
H	-5.48230600	0.96852900	1.79163600
C	-5.78670200	-1.08795500	-0.87959000
H	-4.22524800	-2.24325800	-1.79307800
H	-7.21532900	0.13191700	0.16455500
O	-1.10297200	-1.23775000	1.58049000
H	-0.06561300	-1.21454100	0.96308200
O	-0.74438900	0.56103100	2.92437900
H	-1.33161600	1.27380000	3.26694300
N	-6.80106700	-1.57373600	-1.83807300
O	-6.42678300	-2.36082500	-2.70935700
O	-7.95349200	-1.15794000	-1.70096900

TS9Sb

Cu	0.22656600	0.75660900	-0.13759000
O	1.99583300	1.10585400	-0.33090700
O	0.82195100	-1.04916600	-0.38581500
Cu	2.62521000	-0.62797600	-0.30384200
I	3.15107700	-3.13985600	-0.22494600
S	5.07803200	1.27969400	-0.09119200
O	4.47960300	-0.16535700	-0.22695900
C	4.43784100	2.27390600	-1.47329700
C	4.26100500	2.08944100	1.31646400
H	4.85884600	1.84071700	-2.38335900
H	3.34590800	2.22153400	-1.47210700
H	4.80235000	3.29732600	-1.34329300
H	4.64586700	3.11175100	1.37912900
H	3.17946100	2.06208100	1.15709900
H	4.55248500	1.52647500	2.20601900
I	-0.11509300	3.25917600	0.26754300
O	-1.71298800	0.41372600	-0.37990900
C	-2.37875900	-0.29113700	0.39836900
C	-3.82947700	-0.43229700	0.15125900
C	-1.67510400	-0.93345800	1.63719700
C	-4.63180100	-1.27850200	0.94154400
C	-4.41134100	0.32647400	-0.88538100
H	-2.17559600	-0.51088500	2.53254000

C	-6.00045100	-1.36619700	0.69721800
H	-4.17480300	-1.88359700	1.71565700
C	-5.77598400	0.24499300	-1.13430100
H	-3.78017200	0.97773300	-1.47991000
C	-6.54434400	-0.60202800	-0.33355300
H	-6.64468400	-2.01087500	1.28247100
H	-6.25236300	0.81651000	-1.92148500
O	-0.35634500	-0.68743600	1.67230100
H	0.37889700	-1.22341500	0.59781700
O	-1.99961700	-2.33159900	1.52091300
H	-1.29655800	-2.77767400	2.02968800
N	-7.99720100	-0.69168700	-0.59020100
O	-8.65506300	-1.44045500	0.13465500
O	-8.45161300	-0.01087000	-1.51165200

H	-3.34319100	0.83501200	-1.68170500
C	-5.48664900	-0.36544200	1.34418000
H	-4.04012400	0.67648900	2.56360100
C	-5.82850500	-0.68960400	0.02946100
H	-5.38867600	-0.56261800	-2.06862800
H	-6.10413300	-0.72251600	2.15971300
O	-0.99530300	3.54656900	-0.66339400
H	-2.91967200	3.01344700	-1.23938600
O	-2.92644200	4.16739800	0.40040100
H	-2.25430200	4.54974900	1.00089900
N	-7.03064000	-1.51311200	-0.20548400
O	-7.67365600	-1.87322800	0.78302900
O	-7.31128000	-1.78750100	-1.37445900

TS27Sb

Cu	-0.36298500	1.77432100	-0.27482600
O	0.24536900	-0.06743400	-0.13370200
O	1.54576800	1.88088000	-0.41334500
Cu	2.25809400	0.16771300	-0.09788800
I	4.71503400	1.09473600	-0.07240900
S	3.93336100	-2.41104600	-0.09424800
O	2.57047500	-1.73387200	0.25952400
C	4.83486400	-2.52362900	1.48060900
C	3.43061500	-4.15347500	-0.23233700
H	5.14497500	-1.50626000	1.72778300
H	4.16611500	-2.92478800	2.24663300
H	5.71076500	-3.16387000	1.33889200
H	4.32294900	-4.77295700	-0.36052800
H	2.87207200	-4.43908600	0.66217300
H	2.79080300	-4.22791700	-1.11367700
I	-0.80245500	-1.78897800	-0.20602600
H	2.08842900	2.67973000	-0.27695400
O	-1.85313300	1.80531400	1.81633500
C	-2.38568200	1.70038700	0.72280400
C	-3.58240800	0.85063000	0.46792700
C	-2.24761600	3.31728900	-0.43119100
C	-3.95355200	0.51251300	-0.84275300
C	-4.35060000	0.40730400	1.55928100
C	-5.08122100	-0.27182100	-1.07161700

int1c

O	2.76752500	1.31455100	0.00018800
C	2.13892200	0.25309900	-0.00002500
C	0.66365600	0.21552400	0.00002400
C	2.95498400	-1.04389500	-0.00048700
C	-0.06045200	-0.98704000	0.00017900
C	-0.04875800	1.43329900	-0.00012300
C	-1.45492900	-0.99009300	0.00017800
H	0.45921700	-1.94119700	0.00028700
C	-1.43242400	1.44660000	-0.00009400
H	0.51687500	2.35965000	-0.00025100
C	-2.14675600	0.23224500	0.00005100
H	-1.98829500	-1.93410800	0.00030800
H	-1.99267100	2.37612200	-0.00019200
H	2.68138600	-1.64108900	0.88485900
H	2.68191100	-1.63978300	-0.88692800
O	4.32540700	-0.75056100	0.00030300
H	4.35348300	0.23345900	0.00007800
O	-3.49975600	0.34996300	0.00004600
C	-4.27765600	-0.84598300	-0.00006400
H	-4.08037100	-1.44548100	0.89686900
H	-5.31663700	-0.51605800	-0.00040700
H	-4.07983400	-1.44567400	-0.89674900

TS4Sc

Cu	0.08949300	1.04944500	-0.08155600
O	1.76553200	0.94695500	0.60305600
O	0.18183500	-0.72920200	0.45542600
Cu	2.01628000	-0.89870100	0.52978200
I	1.84602800	-3.37311600	-0.31249500
S	4.87064700	0.32889200	0.87211500
O	3.93720300	-0.92256400	0.76250300
C	4.20590200	1.37374300	2.20228000
C	4.50563500	1.39206800	-0.55575700
H	4.35126200	0.82436300	3.13519800
H	3.14286300	1.54924700	1.99908900
H	4.77776500	2.30636600	2.22328100
H	5.11329800	2.29769100	-0.46858800
H	3.43272600	1.61304600	-0.55106800
H	4.79757300	0.82948500	-1.44536300
I	0.48729700	3.53398300	-0.52781100
O	-1.73052000	0.91608600	-0.78188100
C	-2.34707300	-0.19780900	-0.74439000
C	-3.72904200	-0.22561600	-0.27031000
C	-1.60582300	-1.43071100	-1.06286300
C	-4.57639900	-1.33279800	-0.46734200
C	-4.24852100	0.91542400	0.38726500
H	-0.81060500	-1.37953000	-0.06798500
C	-5.89111100	-1.32313500	-0.01162200
H	-4.22193100	-2.20672000	-1.00456900
C	-5.55089700	0.93559000	0.84660200
H	-3.59964500	1.77353400	0.52717700
C	-6.38368200	-0.18675600	0.65410200
H	-6.52282600	-2.18703100	-0.18405100
H	-5.95838800	1.79998600	1.36041400
O	-0.73225300	-1.29208800	-2.12640800
H	-0.02071500	-1.96197700	-2.01040100
H	-2.14231400	-2.38215500	-1.01064800
O	-7.64043000	-0.06921600	1.14114600
C	-8.53441800	-1.17351100	0.98537300
H	-8.14723800	-2.06573000	1.49090000
H	-9.46603600	-0.85815500	1.45458000
H	-8.70810100	-1.39092900	-0.07488600

TS6Sc

Cu	0.02618700	0.71016500	-0.06981200
O	1.79402300	1.02374700	-0.41151000
O	0.59573000	-1.11201800	-0.21199200
Cu	2.40719200	-0.70954800	-0.25098200
I	2.94824600	-3.20898800	0.03619500
S	4.87311900	1.19756800	-0.29440800
O	4.26954600	-0.25062900	-0.30216500
C	4.18091900	2.08944400	-1.72097400
C	4.10773000	2.11270500	1.07748200
H	4.57560200	1.59590000	-2.61193400
H	3.09007600	2.02691300	-1.67642600
H	4.53917200	3.12229700	-1.67523300
H	4.49545500	3.13555700	1.05094200
H	3.02114700	2.07569900	0.95583500
H	4.42967900	1.61554700	1.99535500
I	-0.27083000	3.21798700	0.30664700
O	-1.93955800	0.40188100	-0.47732300
C	-2.65166500	-0.22173700	0.33365000
C	-4.07474800	-0.42006700	0.04677300
C	-2.00987000	-0.76488700	1.62633200
C	-4.91216800	-1.14190400	0.91628100
C	-4.63144000	0.12926100	-1.13103500
H	-2.56358300	-0.30180100	2.46488500
C	-6.26333300	-1.31757400	0.63220900
H	-4.51379700	-1.57712000	1.82761600
C	-5.97184100	-0.03830000	-1.42422400
H	-3.98632800	0.68865200	-1.80023400
C	-6.79968900	-0.76460100	-0.54412600
H	-6.88553900	-1.87920200	1.31963900
H	-6.41284200	0.37871600	-2.32362600
O	-0.67007200	-0.50644500	1.70580500
H	0.15449800	-1.21134800	0.76990700
H	-2.24370000	-1.84663900	1.65472300
O	-8.09579600	-0.87394500	-0.92012200
C	-8.98828700	-1.59797300	-0.07111300
H	-9.95727700	-1.55488500	-0.56798900
H	-8.67099100	-2.64213900	0.03301700
H	-9.05718300	-1.12899400	0.91738500

TS22Sc

Cu	0.70058400	-1.08761300	-0.06395600
O	-0.46717700	0.47897700	-0.00930300
O	-1.05399000	-1.75665700	0.15550300
Cu	-2.30015200	-0.33863700	0.11081500
I	-4.34757600	-1.98126500	0.08830100
S	-4.63185800	1.57114300	-0.43519000
O	-3.19862400	1.40154000	0.16224700
C	-5.75105500	1.58234900	0.99771500
C	-4.64945000	3.35396500	-0.79444300
H	-5.78089900	0.55578900	1.36875300
H	-5.35190200	2.26034200	1.75664300
H	-6.74507200	1.89547800	0.66430400
H	-5.65421400	3.64406900	-1.11503900
H	-4.34136300	3.90414500	0.09782300
H	-3.93369700	3.51910000	-1.60201000
I	0.10393200	2.40390400	-0.02553600
H	-1.31642300	-2.68705900	0.02471900
O	2.40347700	-0.21262800	-0.29072600
C	3.36078800	-1.10507800	-0.32464500
C	4.77345100	-0.64258500	-0.17681500
C	2.94958500	-2.49106200	-0.21341800
C	5.88258100	-1.43731400	-0.49288600
C	4.99012900	0.65166500	0.32495300
C	7.18336300	-0.97237200	-0.29308400
H	5.74768500	-2.42802700	-0.92149200
C	6.27995500	1.12615000	0.52706800
H	4.12977000	1.27161900	0.55284500
C	7.38622500	0.31665500	0.22372000
H	8.02111400	-1.61047400	-0.55200400
H	6.45717300	2.12275400	0.91876300
O	1.69631300	-2.77812500	-0.13798700
H	3.36856700	-1.88377300	-1.43895100
H	3.68867600	-3.29390600	-0.14014900
O	8.61013700	0.87214900	0.45666000
C	9.76090500	0.08544900	0.16716200
H	10.61535500	0.70935800	0.43151300
H	9.77617800	-0.83325000	0.76731300
H	9.80946400	-0.17206800	-0.89857400

TS26Tc

Cu	1.22120900	-0.57479600	0.94140500
O	2.11480400	-0.51012100	-0.77882600
O	-0.47701400	-1.04781000	-0.00284300
Cu	0.52462700	0.60250000	-1.25008800
I	-0.13758900	2.96341100	-0.96636000
S	3.04005800	0.78293000	1.87043000
O	4.10886100	0.20570100	2.75608100
C	2.18967100	2.14620000	2.71597500
C	3.78744600	1.69946500	0.49600800
H	1.64660400	1.70644900	3.55419700
H	2.93708800	2.86175600	3.06914300
H	1.49476600	2.60810100	2.00661700
H	2.98837800	2.19862200	-0.06087000
H	4.50281900	2.41430300	0.91177500
H	4.28419300	0.96818800	-0.14208300
I	2.57000300	-2.34541800	-1.54913500
C	-1.02663900	-0.37360400	2.43952100
C	-1.75438100	-1.57666100	1.38947000
H	-1.29834500	0.53579800	1.88705500
H	-0.36613900	-1.91048500	-0.45212300
O	-1.52401900	-2.72905900	1.70635800
O	0.27109300	-0.59406000	2.59621300
C	-3.04394800	-1.08661200	0.82736300
C	-3.18448300	0.14800500	0.16669900
C	-4.17260200	-1.89832200	1.01898200
C	-4.42581400	0.54851300	-0.30260200
H	-2.31991300	0.77872100	-0.01969100
C	-5.42533500	-1.49917100	0.55644100
H	-4.05927400	-2.84933300	1.52986000
C	-5.55613000	-0.26804600	-0.10744300
H	-4.54543200	1.48847700	-0.83115600
H	-6.28110500	-2.14698400	0.71093000
H	-1.60872100	-0.50649400	3.36088300
O	-6.72328100	0.22048900	-0.59934300
C	-7.90290000	-0.56477400	-0.43294800
H	-8.12537300	-0.72311000	0.62924900
H	-8.70340500	0.01381100	-0.89404000
H	-7.80712400	-1.53279600	-0.93948600

TS29Tc

Cu	1.17335400	-0.97608600	0.94993900
O	2.07507800	-0.16202800	-0.60898500
O	-0.48578600	-1.02465900	-0.09949600
Cu	0.55091000	1.06110000	-0.74075400
I	-0.56324000	3.20945500	-0.34084200
S	3.61494900	0.64676000	1.56202700
O	2.77077600	-0.57848700	2.05331400
C	4.39166500	1.17862800	3.11601900
C	5.08095500	-0.06366700	0.76050300
H	3.59239200	1.56994300	3.74840200
H	4.86638900	0.31928800	3.59605400
H	5.11828500	1.96725600	2.90087300
H	5.80171100	0.73804300	0.57450700
H	5.50522000	-0.83862600	1.40422800
H	4.74034200	-0.48801700	-0.18528500
I	2.47876000	-1.47052700	-2.13430200
C	-1.09824800	-1.51498300	2.35429200
C	-1.79632400	-2.12527300	0.86772500
H	-1.38162300	-0.45705000	2.26461900
H	-0.36344000	-1.59934800	-0.88190400
O	-1.57116500	-3.29925000	0.63827800
O	0.19682300	-1.77381800	2.40221000
C	-3.07469200	-1.42647500	0.54904700
C	-3.19262000	-0.02883200	0.44150800
C	-4.21570400	-2.22826100	0.39628200
C	-4.42524700	0.54681300	0.17326200
H	-2.31622200	0.60853900	0.51230000
C	-5.46060300	-1.65627100	0.13703900
H	-4.11902400	-3.30645900	0.47756800
C	-5.56858900	-0.26041300	0.02624700
H	-4.52336200	1.62146800	0.06063100
H	-6.32708000	-2.29756900	0.01829100
H	-1.68523200	-2.04843700	3.11431600
O	-6.72792000	0.40386300	-0.22573400
C	-7.91590300	-0.36545500	-0.39453300
H	-8.14932100	-0.93831500	0.51152000
H	-8.70727900	0.36011100	-0.58406900
H	-7.82770900	-1.04741300	-1.24926000

int3c

O	-2.22265900	1.74422800	0.17431700
C	-1.81216000	0.60167100	-0.03848300
C	-0.38478700	0.25298800	-0.03363300
C	-2.88840000	-0.47761100	-0.31539800
C	0.07251300	-1.07507000	-0.16834100
C	0.56076400	1.28476500	0.09771600
C	1.43013200	-1.35478700	-0.17488000
H	-0.64305500	-1.88826600	-0.23038700
C	1.92545300	1.01810000	0.08743100
H	0.19999300	2.30316600	0.20434600
C	2.36574100	-0.31077300	-0.05148800
H	1.79879600	-2.37111900	-0.26840300
H	2.63350800	1.83359200	0.18581000
H	-2.68349700	-1.03315300	-1.24157000
O	-4.12418900	0.13791500	-0.45705200
H	-4.00172500	1.02635900	-0.04621500
O	-2.82949500	-1.35470700	0.80880600
H	-3.66248200	-1.86043200	0.78539700
O	3.66999400	-0.68880000	-0.07540300
C	4.66589800	0.32492800	0.05489000
H	5.62048700	-0.19983600	0.01195800
H	4.60390300	1.04761300	-0.76761500
H	4.57395000	0.84772100	1.01444000

TS9Sc

Cu	0.06538200	0.75304400	-0.18980600
O	1.84265800	1.09264600	-0.34279500
O	0.66084800	-1.05824300	-0.42757700
Cu	2.46433800	-0.64258300	-0.28832200
I	3.01041800	-3.15377100	-0.17165900
S	4.90531000	1.27304700	0.01226500
O	4.31887200	-0.17276800	-0.15332500
C	4.31249700	2.27454800	-1.38628100
C	4.03426000	2.07323400	1.39308000
H	4.76923500	1.84922100	-2.28274900
H	3.22156400	2.21638400	-1.42548800
H	4.66713100	3.29867100	-1.23580600
H	4.41369800	3.09619100	1.47563200
H	2.95961900	2.04315000	1.19220500
H	4.29384300	1.50572300	2.28962500
I	-0.25050600	3.25950400	0.22672300

O	-1.85034000	0.43320000	-0.49473900
C	-2.55508800	-0.25171300	0.27966000
C	-3.97995000	-0.38722100	0.00742100
C	-1.88345200	-0.88245700	1.54723800
C	-4.82034500	-1.18251500	0.81219200
C	-4.54641000	0.31735000	-1.08351700
H	-2.39765700	-0.43932600	2.42455400
C	-6.18191100	-1.27741200	0.54392600
H	-4.39404800	-1.75246500	1.62980600
C	-5.89690400	0.22935200	-1.35602700
H	-3.90039500	0.93360700	-1.69969200
C	-6.72713000	-0.57064300	-0.54237400
H	-6.80659700	-1.90072700	1.17362800
H	-6.34625300	0.76506100	-2.18570600
O	-0.56208200	-0.65450500	1.60722700
H	0.20435100	-1.23259300	0.53504400
O	-2.21651100	-2.28191300	1.45914600
H	-1.50508900	-2.71671600	1.96598600
O	-8.03445900	-0.59048600	-0.89062800
C	-8.93153900	-1.38484200	-0.11135300
H	-8.95802800	-1.04023600	0.92884800
H	-9.91032100	-1.24808500	-0.57068700
H	-8.64928600	-2.44333400	-0.14638500

TS17Sc

Cu	-0.17095600	0.99183600	0.03933100
O	-1.90133900	1.03618900	0.64536200
O	-0.51564000	-0.82064000	-0.01413300
Cu	-2.32821400	-0.71562800	0.22991200
I	-2.54617700	-3.17445100	-0.46791300
S	-4.97803100	0.73586000	0.96976500
O	-4.20305300	-0.56454500	0.54976700
C	-4.17350900	1.37881600	2.46610600
C	-4.54096800	2.03361500	-0.22320500
H	-4.36428100	0.65096900	3.25787200
H	-3.10286900	1.47922100	2.25690000
H	-4.63986500	2.33635900	2.71656100
H	-5.01675800	2.96394400	0.10115700
H	-3.44848500	2.10861600	-0.24991900
H	-4.95025200	1.72004200	-1.18614600
I	0.41998600	3.42344000	0.13163800

O	3.42295700	1.10205700	-2.63615100
C	3.13202200	0.28643400	-1.76395800
C	4.08473200	-0.26728300	-0.80438100
C	1.60059500	-0.08557200	-1.71801400
C	3.73506300	-1.17951700	0.20963000
C	5.42922400	0.16511700	-0.90153100
H	1.31217000	0.66451700	-0.72497100
C	4.69196400	-1.64340700	1.10796800
H	2.71491500	-1.53573900	0.28368400
C	6.38528600	-0.29458700	-0.01750800
H	5.69220600	0.87030700	-1.68316200
C	6.02241000	-1.20424900	0.99788100
H	4.39775100	-2.34512400	1.88012400
H	7.41904200	0.02958200	-0.07783600
O	1.27987200	-1.32239400	-1.42123400
H	0.22264100	-1.27512000	-0.85981900
O	0.94221100	0.46074900	-2.78917300
H	1.55506200	1.15054000	-3.14138900
O	7.02909300	-1.59443400	1.81491400
C	6.72786700	-2.51353600	2.86705100
H	7.67233700	-2.67735400	3.38567600
H	5.99224500	-2.08914300	3.56006000
H	6.35571700	-3.46268200	2.46444900

TS27Sc

Cu	-0.58603500	1.74071900	-0.31880500
O	0.04208900	-0.09005500	-0.15439300
O	1.31394000	1.86954000	-0.54773000
Cu	2.05754300	0.18157000	-0.14056000
I	4.51506700	1.14420200	-0.14219600
S	3.78029000	-2.36595200	0.00288100
O	2.40439900	-1.70213100	0.31739800
C	4.68376700	-2.37572900	1.58143600
C	3.31899400	-4.12582200	-0.03808500
H	4.97242800	-1.34002700	1.77225400
H	4.02222600	-2.74788500	2.36818600
H	5.57255700	-3.00502300	1.47476800
H	4.22477000	-4.73178400	-0.13308300
H	2.76665100	-4.37445200	0.87128900
H	2.68024900	-4.26299500	-0.91269300
I	-0.97349500	-1.83477900	-0.25901700

H	1.83511900	2.67728400	-0.38336700
O	-1.93731200	1.85976200	1.89414500
C	-2.52094500	1.69471900	0.83324500
C	-3.65004500	0.78431600	0.61146300
C	-2.46810800	3.29447600	-0.33840300
C	-4.09745100	0.48151600	-0.68310400
C	-4.29023300	0.18396400	1.71860500
C	-5.15629300	-0.39876400	-0.88890800
H	-3.59186400	0.90892100	-1.54528400
C	-5.35004500	-0.68272800	1.52903400
H	-3.93151900	0.41521600	2.71658100
C	-5.79088700	-0.98027100	0.22216700
H	-5.47503400	-0.62874400	-1.89909600
H	-5.85894200	-1.15221900	2.36479600
O	-1.24280200	3.49257200	-0.71741100
H	-3.23091300	3.00597000	-1.06736300
O	-3.02766200	4.18094800	0.54399100
H	-2.28791100	4.52420000	1.08485300
O	-6.83560200	-1.84038500	0.14438400
C	-7.32802800	-2.18827700	-1.15029600
H	-6.55232100	-2.68365000	-1.74604900
H	-8.15177500	-2.87884700	-0.97003800
H	-7.69617400	-1.30294700	-1.68197700

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Cu	0.00000900	-0.03187100	-0.00012000
I	-0.00004900	2.41369700	-0.00006000
O	1.40093000	-1.39038400	-0.00037600
S	2.92471700	-1.00464700	0.00019100
C	3.60321700	-1.96003600	1.38520300
C	3.60406600	-1.95969900	-1.38464300
H	3.20887100	-1.51925200	2.30294300
H	3.28591200	-3.00138800	1.29175300
H	4.69315200	-1.87166600	1.36850100
H	4.69399700	-1.87146700	-1.36719800
H	3.28655200	-3.00103100	-1.29168300
H	3.21036300	-1.51861500	-2.30251600
O	-1.40087800	-1.39042000	0.00003900
S	-2.92467400	-1.00472100	-0.00034200
C	-3.60343000	-1.96103300	-1.38459600
C	-3.60371800	-1.95888700	1.38524900

H	-3.20935100	-1.52076800	-2.30270100
H	-3.28593400	-3.00227500	-1.29056800
H	-4.69337000	-1.87280600	-1.36768500
H	-4.69364900	-1.87056600	1.36801300
H	-3.28634400	-3.00031200	1.29286700
H	-3.20976900	-1.51726500	2.30275700

31D-2

Cu	-0.12008100	-0.14799100	0.00000000
I	-2.55692900	-0.32120600	-0.00037900
S	1.70334500	-1.69750700	0.00041600
O	1.21112400	-3.11406100	0.00046100
C	2.81257300	-1.38158000	1.40227900
C	2.81300100	-1.38181600	-1.40116300
H	2.23604200	-1.55129800	2.31406000
H	3.64220200	-2.09173100	1.34643200
H	3.16187300	-0.34788100	1.33182100
H	3.16228500	-0.34810800	-1.33076800
H	3.64260800	-2.09196300	-1.34494700
H	2.23674500	-1.55168000	-2.31309000
S	1.13520500	1.89774300	0.00001500
O	2.62726500	1.67861600	0.00023800
C	0.64234300	2.94525900	1.39885500
C	0.64272800	2.94503600	-1.39912600
H	0.89693300	2.40835200	2.31472200
H	1.20323600	3.88210700	1.34085800
H	-0.43582700	3.11828600	1.34412900
H	-0.43545600	3.11807900	-1.34472000
H	1.20361200	3.88188900	-1.34112900
H	0.89756100	2.40798000	-2.31483800

31D-3

Cu	-0.16904700	0.02072300	0.00002000
I	-2.29894700	1.19864500	0.00001900
S	-0.09897600	-2.41149000	0.00001200
O	-1.34817400	-3.23530700	0.00009600
C	0.97411600	-2.85612000	1.39656100
C	0.97383400	-2.85588000	-1.39683500
H	0.41130500	-2.65640800	2.31086000
H	1.21608900	-3.92011700	1.32978200
H	1.86975900	-2.23194600	1.34670500

H	1.86945500	-2.23166500	-1.34705300
H	1.21588400	-3.91987400	-1.33028500
H	0.41082700	-2.65604200	-2.31098500
O	1.78282000	0.12608300	0.00003400
S	2.46768100	1.55171100	0.00006700
C	3.63397800	1.46843100	1.38568200
C	3.63369300	1.46860400	-1.38581600
H	3.04315900	1.43953900	2.30355200
H	4.24988300	0.57082400	1.29091900
H	4.24901100	2.37284500	1.37178900
H	4.24879300	2.37296900	-1.37194100
H	4.24954800	0.57093900	-1.29126500
H	3.04268200	1.43984400	-2.30356600

31D-4

Cu	0.77831300	-0.12387400	-0.06516500
I	2.18060200	-2.11768400	-0.26950300
S	2.62756600	2.34029700	0.13186600
O	1.16088300	1.77233000	0.17283600
C	2.54226200	3.64348400	-1.12725000
C	2.72154000	3.36784800	1.62376200
H	2.41265600	3.14950900	-2.09231800
H	1.69240000	4.29551500	-0.91183500
H	3.48433600	4.19891700	-1.11731000
H	3.66036900	3.92832600	1.60151200
H	1.85835000	4.03709700	1.65292500
H	2.71315600	2.69150500	2.48080600
C	-6.10298600	0.60885900	-0.58865700
C	-5.87320900	-0.22284300	0.51384400
C	-4.56956700	-0.54027800	0.88431000
C	-3.48076700	-0.02280900	0.15012300
C	-3.72428600	0.81615200	-0.95966700
C	-5.02861700	1.12758500	-1.32433700
H	-7.12141000	0.85276200	-0.87598800
H	-6.70902700	-0.62167200	1.07950500
H	-4.40208800	-1.18685900	1.73975000
H	-2.88104900	1.20751800	-1.51828200
H	-5.21494200	1.77045900	-2.17873500
C	-2.09956200	-0.34352500	0.51434600
O	-1.16375100	0.15099200	-0.16611400
C	-1.79721600	-1.24871600	1.68202000

H	-2.27185900	-2.22625400	1.54305700
H	-0.71844100	-1.39364300	1.78475400
H	-2.18910800	-0.81946200	2.61103100

31D-5

Cu	-0.75999400	-0.42308400	-0.05543900
I	-3.06129500	-1.25552700	-0.04578000
S	-1.03369300	1.99324900	0.24958500
O	0.19455200	2.77557200	-0.11763900
C	-1.48471600	2.26441100	1.98630200
C	-2.48775600	2.64992300	-0.61350700
H	-0.65124100	1.90921800	2.59562700
H	-1.63931300	3.33576900	2.14041700
H	-2.39038600	1.68959900	2.19850100
H	-3.36737800	2.09593700	-0.27573700
H	-2.56274500	3.71706300	-0.38765100
H	-2.32820800	2.49603100	-1.68232700
C	6.08908400	-0.64841000	0.69396900
C	5.85905900	-0.03755000	-0.54517300
C	4.55668600	0.13189600	-1.00372400
C	3.46759100	-0.30466400	-0.21659300
C	3.71248500	-0.91731200	1.03392800
C	5.01608700	-1.08837200	1.48199800
H	7.10731800	-0.78359000	1.04621300
H	6.69437100	0.30152300	-1.14903700
H	4.38842100	0.60708900	-1.96472100
H	2.87168400	-1.25526200	1.62979800
H	5.20359200	-1.56320800	2.43964400
C	2.09304300	-0.13400000	-0.67188300
O	1.15103200	-0.50281200	0.08594300
C	1.78259200	0.46877100	-2.01673300
H	2.34734800	-0.02846700	-2.81130300
H	0.71475400	0.37690600	-2.23507900
H	2.04975000	1.53155800	-2.02155100

31D-6

I	2.46083600	-0.01874800	-0.12658000
Cu	0.08986300	0.05394400	0.36096900
S	-2.92437700	-0.03671700	-0.53287200
C	-4.08565900	-1.31290700	0.01553200
H	-4.28565100	-1.18348000	1.08177700

H	-5.00007400	-1.21969700	-0.57740200
H	-3.61432400	-2.27889200	-0.17621600
C	-3.81305600	1.45463400	-0.00605300
H	-4.02650900	1.38850300	1.06343000
H	-3.17212900	2.31143600	-0.22384500
H	-4.73391800	1.52325200	-0.59254800
O	-1.75192600	-0.17184100	0.51682000

O₂⁻

O	0.00000000	0.00000000	0.68060100
O	0.00000000	0.00000000	-0.68060100

HOO[·]

O	0.05612500	-0.61456500	0.00000000
O	0.05612500	0.72255600	0.00000000
H	-0.89799500	-0.86392700	0.00000000

Int5

O	-2.25857800	-1.27152100	-0.00013100
C	-1.80352100	-0.07699800	0.00001300
C	-0.27584400	0.04182600	0.00000200
C	-2.53042400	1.10386300	0.00018900
C	0.47489800	1.23334900	-0.00006400
C	0.44206900	-1.16876900	0.00003400
H	-3.61804800	1.06477000	0.00027700
C	1.87271900	1.21508800	-0.00007800
H	-0.03814300	2.19198200	-0.00012700
C	1.83816300	-1.19575000	0.00002600
H	-0.16817000	-2.06917200	0.00005700
C	2.56824100	-0.00165500	-0.00002900
H	2.42514200	2.15541600	-0.00013600
H	2.36453600	-2.15122100	0.00005800
H	3.65774100	-0.01508000	-0.00004200
H	-2.07224300	2.08975300	0.00040300

32S

I	3.10174300	-0.66254300	-0.01203500
Cu	0.90899300	0.48392700	-0.01832500
C	-1.88791500	2.19781400	1.01816400
H	-2.80875000	2.71280700	0.77122700
H	-1.12540100	2.74862700	1.55789700

O	-0.55813400	0.33540000	1.18757900
O	0.21295200	1.75016100	-1.26521300
O	-0.85061600	2.57923300	-0.94494700
C	-1.72532600	0.80812400	0.90257900
C	-2.77520900	-0.10345500	0.39634400
C	-2.45837900	-1.46588400	0.23965500
C	-4.07510700	0.33604600	0.08064600
C	-3.41469700	-2.36322100	-0.22969500
H	-1.45859900	-1.80204700	0.49359800
C	-5.02938300	-0.56469400	-0.38878600
H	-4.35126100	1.37927000	0.20113000
C	-4.70202000	-1.91546000	-0.54665100
H	-3.15755800	-3.41166300	-0.34875400
H	-6.02823000	-0.21369400	-0.63126800
H	-5.44752900	-2.61555600	-0.91297700
H	-0.40124100	3.38916200	-0.61446800

32T

I	3.16727500	-0.84019000	0.13666900
Cu	0.92196800	0.20102900	-0.26415600
C	-1.79950200	2.12664500	0.24464700
H	-0.79028700	2.52400800	0.16627900
H	-2.61428600	2.79367400	0.49872800
O	-1.00211900	-0.00142100	-0.30538700
O	1.23304600	2.13302500	-0.57976400
O	2.15048000	2.56118300	0.35872000
C	-2.00095600	0.74080300	-0.01930200
C	-3.33901400	0.10674600	0.02488300
C	-3.42378800	-1.29042400	-0.13426000
C	-4.52193700	0.84773800	0.21510600
C	-4.65962600	-1.92933400	-0.09977800
H	-2.50886900	-1.85412400	-0.28070500
C	-5.75778700	0.20412500	0.24593200
H	-4.48870500	1.92634600	0.32926000
C	-5.82961200	-1.18385700	0.09053600
H	-4.71407200	-3.00721300	-0.21993700
H	-6.66407800	0.78470600	0.38976400
H	-6.79398400	-1.68313000	0.11713400
H	2.91369500	1.93899400	0.22137700

8q

Cu	-1.23303700	-1.41760300	-0.47802100
O	-2.43672500	0.07369200	-0.26118300
Cu	-0.96971800	1.30449400	-0.29317400
I	1.50226400	2.41010500	0.36207200
S	-3.78841400	-2.82448600	0.71085000
O	-2.42533400	-2.96031800	-0.02184400
C	-3.52233300	-1.60551800	2.03439700
C	-4.82918300	-1.78851900	-0.36398100
H	-2.82625700	-2.05744500	2.74488000
H	-3.08931700	-0.71629400	1.54765200
H	-4.47936700	-1.39856200	2.52395000
H	-5.76058400	-1.55310900	0.16100200
H	-4.23127200	-0.89500700	-0.59233200
H	-5.04156000	-2.37373300	-1.26177900
O	-0.02816200	-0.10265300	-1.16554900
Cu	1.67850400	-0.26840800	-0.45458000
I	1.08374700	-2.87055300	0.07924200
S	4.65074700	0.66613100	-0.18453600
O	3.64527600	-0.51898700	-0.27326000
C	4.97678600	0.88814200	1.59211000
C	6.21595600	-0.14629900	-0.62999000
H	4.06709400	1.31424600	2.02048000
H	5.19363800	-0.08569100	2.03907700
H	5.81373800	1.58190000	1.71610600
H	7.04181300	0.55545900	-0.48127000
H	6.33944400	-1.04359000	-0.01856400
H	6.14035300	-0.41950700	-1.68434200

S	-3.63123700	2.50066700	0.18708500
O	-2.11374000	2.86897400	0.16259000
C	-4.36785000	4.15704500	0.37871200
H	-4.09277400	4.51679400	1.37234700
H	-3.95828600	4.82355700	-0.38451300
H	-5.45639400	4.08197000	0.29509800
C	-4.10578000	2.21665500	-1.54593600
H	-5.19187400	2.09197600	-1.60416600
H	-3.77128400	3.06074900	-2.15557100
H	-3.58604600	1.29235700	-1.81250800

1D

Cu	-0.18724000	0.60335500	-0.00338100
I	-2.65003000	0.72514600	0.05309700
I	0.35461400	-1.92666300	-0.10329300
O	1.54482300	1.52243500	0.06369000
S	2.86973900	0.78448900	-0.31044600
C	4.00987500	2.18062800	-0.54027400
C	3.52774600	0.15686100	1.26336600
H	3.67821500	2.71689700	-1.43154700
H	3.95991000	2.83398800	0.33406300
H	5.02155400	1.79318400	-0.69065900
H	4.54471000	-0.21100000	1.09794300
H	3.50895800	0.95899400	2.00569600
H	2.87351200	-0.66520500	1.56202500

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