

Supporting Information

Mechanistic study on coupling of CO₂ and epoxide mediated by guanidine/TBAI catalyst

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Structure	^a ZPE	^b H _c	^c G _c	E_{ZEP}	H	G	^d G	^e IF
CO ₂	0.01215	0.01635	-0.01222	-188.35833	-188.35413	-188.38270	-188.60915	-
R1	0.14035	0.15065	0.10220	-384.25713	-384.24683	-384.29529	-384.72653	-
product	0.15824	0.17115	0.11520	-572.64392	-572.63101	-572.68697	-573.33762	-
B-1-TS	0.15342	0.16683	0.11042	-572.53149	-572.51809	-572.57449	-573.23354	226i
B-2-TS	0.15201	0.16576	0.10830	-572.51061	-572.49686	-572.55432	-573.21131	856i

^a Zero-point correction energy;

^b Thermal correction to enthalpy;

^c Thermal correction to Gibbs free energy;

^d Gibbs free energy obtained at the M062X-D3/def2-TZVP//M062X-D3/def2-SVP theoretical level;

^e Imaginary frequencies (cm⁻¹) for the transition states.

Table S2 The corrected electronic energies (E_{ZPE}), enthalpies (H), and Gibbs free energies (G) for all stationary points (in Hartree) in G1 catalyzed unfavored mechanism, obtained at the M062X-D3/def2-SVP theoretical level. Single-point calculations were run at the M062X-D3/def2-TZVP theoretical level.

Structure	^a ZPE	^b H _c	^c G _c	E_{ZEP}	H	G	^d G	^e IF
G1-TS2-a	0.48108	0.52132	0.40225	-1541.52839	-1541.48816	-1541.60722	-1543.01521	-179.3i
G1-IM3-a	0.48422	0.52431	0.40416	-1541.54177	-1541.50169	-1541.62183	-1543.02883	-
G1-TS3-a	0.48290	0.52268	0.40283	-1541.50442	-1541.46465	-1541.58449	-1542.98890	-430.2i
G1-IM4-a	0.48689	0.52596	0.40720	-1541.57132	-1541.53225	-1541.65101	-1543.05075	-
G1-TS4-a	0.48396	0.52209	0.40516	-1541.55051	-1541.51237	-1541.62930	-1543.02825	-294.8i
G1-IM5-a	0.48816	0.52765	0.40592	-1541.57889	-1541.53940	-1541.66113	-1543.06723	-□

^a Zero-point correction energy;

^b Thermal correction to enthalpy;

^c Thermal correction to Gibbs free energy;

^d Gibbs free energy obtained at the M062X-D3/def2-TZVP//M062X-D3/def2-SVP theoretical level;

^e Imaginary frequencies (cm⁻¹) for the transition states.

Table S3 The corrected electronic energies (E_{ZPE}), enthalpies (H), and Gibbs free energies (G) for all stationary points (in Hartree) in the G1~G4-catalyzed reaction, obtained at the M062X-D3/def2-SVP theoretical level. Single-point calculations were run at the M062X-D3/def2-TZVP theoretical level.

Structure	^a ZPE	^b H _c	^c G _c	E_{ZEP}	H	G	^d G	^e IF
G1-COM	0.46993	0.50414	0.40023	-1055.44848	-1055.41426	-1055.51817	-1056.69290	-
G1-IM1	0.46948	0.50687	0.39024	-1353.17608	-1353.13870	-1353.25533	-1354.44373	-
G1-TS1	0.46666	0.50340	0.38987	-1353.13834	-1353.10160	-1353.21513	-1354.40543	424i
G1-IM2	0.46780	0.50410	0.39477	-1353.16259	-1353.12629	-1353.23562	-1354.42462	-
G1-TS2	0.47742	0.51780	0.39735	-1541.53094	-1541.49056	-1541.61101	-1543.02151	292i
G1-IM3	0.48501	0.52450	0.40718	-1541.55287	-1541.51338	-1541.63070	-1543.03844	-
G1-TS3	0.48497	0.52412	0.40840	-1541.53744	-1541.49829	-1541.61400	-1543.02064	425i
G1-IM4	0.48719	0.52699	0.40686	-1541.58335	-1541.54355	-1541.66368	-1543.06997	-
G2-COM	0.46846	0.50510	0.39425	-1147.59906	-1147.56242	-1147.67327	-1148.95349	-
G2-IM1	0.46787	0.50655	0.38811	-1445.33438	-1445.29570	-1445.41415	-1446.70753	-
G2-TS1	0.46576	0.50448	0.38743	-1445.29827	-1445.25954	-1445.37659	-1446.67211	439i
G2-IM2	0.46787	0.50620	0.39248	-1445.32615	-1445.28782	-1445.40153	-1446.69605	-
G2-TS2	0.47747	0.51998	0.39377	-1633.69011	-1633.64760	-1633.77381	-1635.28943	143i
G2-IM3	0.48418	0.52587	0.40384	-1633.71056	-1633.66887	-1633.79090	-1635.30399	-
G2-TS3	0.48329	0.52482	0.40242	-1633.69367	-1633.65215	-1633.77454	-1635.28659	434i
G2-IM4	0.48595	0.52803	0.40222	-1633.73808	-1633.69601	-1633.82182	-1635.33330	-
G3-COM	0.55187	0.59184	0.47562	-1173.17053	-1173.13057	-1173.24678	-1174.55269	-
G3-IM1	0.55142	0.59538	0.46292	-1470.90174	-1470.85777	-1470.99024	-1472.30865	-
G3-TS1	0.55013	0.59290	0.46737	-1470.86200	-1470.81923	-1470.94476	-1472.26492	392i
G3-IM2	0.55042	0.59269	0.47140	-1470.87871	-1470.83644	-1470.95773	-1472.27621	-
G3-TS2	0.55946	0.60626	0.47211	-1659.25251	-1659.20571	-1659.33986	-1660.88056	663i
G3-IM3	0.56865	0.61411	0.48545	-1659.27620	-1659.23073	-1659.35940	-1660.89853	-
G3-TS3	0.56776	0.61319	0.48396	-1659.26110	-1659.21567	-1659.34490	-1660.88106	422i
G3-IM4	0.57020	0.61606	0.48461	-1659.30772	-1659.26186	-1659.39331	-1660.92916	-
G4-COM	0.69523	0.74658	0.59950	-1494.74774	-1494.69639	-1494.84347	-1496.51213	-
G4-IM1	0.69586	0.74945	0.59752	-1792.48824	-1792.43465	-1792.58658	-1794.26617	-
G4-TS1	0.69394	0.74671	0.59653	-1792.43756	-1792.38479	-1792.53497	-1794.21961	416i
G4-IM2	0.69470	0.74726	0.59919	-1792.46026	-1792.40769	-1792.55577	-1794.23854	-
G4-TS2	0.70423	0.76086	0.60350	-1980.82918	-1980.77256	-1980.92991	-1982.83455	148i
G4-IM3	0.71230	0.76689	0.61778	-1980.85881	-1980.80422	-1980.95333	-1982.85121	-
G4-TS3	0.71172	0.76706	0.61551	-1980.84209	-1980.78674	-1980.93829	-1982.83486	427i
G4-IM4	0.71374	0.76851	0.61665	-1980.88724	-1980.83247	-1980.98433	-1982.88081	-□

^a Zero-point correction energy;

^b Thermal correction to enthalpy;

^c Thermal correction to Gibbs free energy;

^d Gibbs free energy obtained at the M062X-D3/def2-TZVP//M062X-D3/def2-SVP theoretical level;

^e Imaginary frequencies (cm⁻¹) for the transition states.

Table S4 The corrected electronic energies (E_{ZPE}), enthalpies (H), and Gibbs free energies (G) for all stationary points (in Hartree) in the catalytic reaction involving carbamate salt species, obtained at the M062X-D3/def2-SVP theoretical level. Single-point calculations were run at the M062X-D3/def2-TZVP theoretical level.

Structure	^a ZPE	^b H_c	^c G_c	E_{ZEP}	H	G	^d G	^e ΓF
G1-TS'	0.48336	0.52368	0.40402	-1541.53278	-1541.49245	-1541.61212	-1543.01905	147 <i>i</i>
G1-IM1'	0.48558	0.52568	0.40766	-1541.53276	-1541.49267	-1541.61068	-1543.01640	-
G1-TS1'	0.48273	0.52271	0.40388	-1541.50158	-1541.46160	-1541.58043	-1542.98789	456 <i>i</i>
G1-IM2'	0.48463	0.52435	0.40792	-1541.53817	-1541.49845	-1541.61488	-1543.02133	-
G1-TS2'	0.49603	0.53854	0.41629	-1729.91172	-1729.86920	-1729.99145	-1731.61515	402 <i>i</i>
G1-IM3'	0.49974	0.54263	0.41568	-1729.91548	-1729.87259	-1729.99954	-1731.62699	-
G1-TS3'	0.49951	0.54224	0.41655	-1729.89886	-1729.85613	-1729.98182	-1731.60753	435 <i>i</i>
G1-IM4'	0.50241	0.54570	0.41701	-1729.93835	-1729.89506	-1730.02375	-1731.64857	-□

^a Zero-point correction energy;

^b Thermal correction to enthalpy;

^c Thermal correction to Gibbs free energy;

^d Gibbs free energy obtained at the M062X-D3/def2-TZVP//M062X-D3/def2-SVP theoretical level;

^e Imaginary frequencies (cm^{-1}) for the transition states.

Table S5 The corrected electronic energies (E_{ZPE}), enthalpies (H), and Gibbs free energies (G) for all stationary points (in Hartree) in the guanidine-amide compound (G10)-catalyzed reaction, obtained at the M062X-D3/def2-SVP theoretical level. Single-point calculations were run at the M062X-D3/def2-TZVP theoretical level.

Structure	^a ZPE	^b H_c	^c G_c	E_{ZEP}	H	G	^d G	^e ΓF
G10-COM	0.62482	0.66774	0.54626	-1305.92554	-1305.88261	-1306.00409	-1307.46642	-
G10-IM1	0.62433	0.67038	0.53770	-1603.65224	-1603.60619	-1603.73887	-1605.21463	-
G10-TS1	0.62276	0.66784	0.53880	-1603.63705	-1603.59197	-1603.72101	-1605.19609	467 <i>i</i>
G10-IM2	0.62327	0.66820	0.54084	-1603.65424	-1603.60932	-1603.73668	-1605.21050	-
G10-TS2	0.63736	0.68600	0.55013	-1792.02726	-1791.97862	-1792.11449	-1793.81047	50 <i>i</i>
G10-IM3	0.63930	0.68759	0.55221	-1792.05406	-1792.00577	-1792.14115	-1793.83638	-
G10-TS3	0.63880	0.68688	0.55186	-1792.02989	-1791.98181	-1792.11683	-1793.81053	439 <i>i</i>
G10-IM4	0.64160	0.68906	0.55395	-1792.06856	-1792.02110	-1792.15621	-1793.85003	-□

^a Zero-point correction energy;

^b Thermal correction to enthalpy;

^c Thermal correction to Gibbs free energy;

^d Gibbs free energy obtained at the M062X-D3/def2-TZVP//M062X-D3/def2-SVP theoretical level;

^e Imaginary frequencies (cm^{-1}) for the transition states.

Table S6 The corrected electronic energies (E_{ZPE}), enthalpies (H), and Gibbs free energies (G) for all stationary points (in Hartree) in the guanidine/copper(I)(G10-Cu)-catalyzed reaction, obtained at the M06-D3/def2-SVP theoretical level.

Structure	^a ZPE	^b H_c	^c G_c	E_{ZEP}	H	G	^d Γ
I (M06)	0.00000	0.00272	-0.01976	-297.83256	-297.82985	-297.85233	-
CO₂ (M06)	0.01211	0.01631	-0.01227	-188.34893	-188.34473	-188.37331	-
R1 (M06)	0.13841	0.14878	0.10035	-384.15090	-384.14054	-384.18896	-
G10-Cu	0.47865	0.51513	0.40562	-2859.56245	-2859.52597	-2859.63548	-
G10-Cu-IM1	0.61669	0.66750	0.52436	-3541.62925	-3541.57843	-3541.72158	-
G10-Cu-TS1	0.61655	0.66657	0.52708	-3541.58912	-3541.53910	-3541.67859	323 <i>i</i>
G10-Cu-IM2	0.61769	0.66761	0.52690	-3541.60481	-3541.55489	-3541.69560	-
G10-Cu-TS2	0.63234	0.68537	0.53892	-3729.97168	-3729.91866	-3730.06511	136 <i>i</i>
G10-Cu-IM3	0.63578	0.68811	0.54320	-3729.98189	-3729.92956	-3730.07447	-
G10-Cu-TS3	0.63416	0.68676	0.53983	-3729.96012	-3729.90752	-3730.05445	334 <i>i</i>
G10-Cu-IM4	0.63839	0.69012	0.54777	-3730.00825	-3729.95652	-3730.09887	-□

^a Zero-point correction energy;

^b Thermal correction to enthalpy;

^c Thermal correction to Gibbs free energy;

^d Imaginary frequencies (cm^{-1}) for the transition states.

Table S7 The corrected electronic energies (E_{ZPE}), enthalpies (H), and Gibbs free energies (G) for all stationary points (in Hartree) in the catalytic reaction using different guanidine catalysts, obtained at the M062X-D3/def2-SVP theoretical level. Single-point calculations were run at the M062X-D3/def2-TZVP theoretical level.

Structure	^a ZPE	^b H _c	^c G _c	E_{ZEP}	H	G	^d G	^e IF
G1	0.32695	0.35035	0.27047	-671.17037	-671.14696	-671.22685	-671.97522	-
G1-TS1	0.46666	0.50340	0.38987	-1353.13834	-1353.10160	-1353.21513	-1354.40543	424 <i>i</i>
G2	0.32576	0.35145	0.26604	-763.32005	-763.29436	-763.37977	-764.23359	-
G2-TS1	0.46576	0.50448	0.38743	-1445.29827	-1445.25954	-1445.37659	-1446.67211	439 <i>i</i>
G3	0.40953	0.43947	0.34405	-788.89228	-788.86233	-788.95776	-789.83670	-
G3-TS1	0.55013	0.59290	0.46737	-1470.86200	-1470.81923	-1470.94476	-1472.26492	392 <i>i</i>
G4	0.55351	0.59321	0.47508	-1110.47157	-1110.43188	-1110.55001	-1111.79252	-
G4-TS1	0.69394	0.74671	0.59653	-1792.43756	-1792.38479	-1792.53497	-1794.21961	416 <i>i</i>
G5	0.14863	0.15804	0.11252	-359.61212	-359.60271	-359.64823	-360.05520	-
G5-TS1	0.28742	0.31030	0.22701	-1041.57802	-1041.55515	-1041.63843	-1042.48664	386 <i>i</i>
G6	0.17795	0.18875	0.13992	-398.85947	-398.84867	-398.89749	-399.34676	-
G6-TS1	0.31717	0.34126	0.25811	-1080.82282	-1080.79873	-1080.88188	-1081.77445	361 <i>i</i>
G7	0.20730	0.21951	0.16750	-438.09272	-438.08051	-438.13252	-438.62474	-
G7-TS1	0.34629	0.37211	0.28398	-1120.05144	-1120.02562	-1120.11376	-1121.04938	357 <i>i</i>
G8	0.20700	0.21943	0.16655	-438.09750	-438.08507	-438.13795	-438.62834	-
G8-TS1	0.34634	0.37190	0.28552	-1120.05700	-1120.03144	-1120.11782	-1121.05188	352 <i>i</i>
G9	0.23599	0.24975	0.19420	-477.32653	-477.31277	-477.36831	-477.90192	-
G9-TS1	0.37502	0.40224	0.31183	-1159.28631	-1159.25909	-1159.34950	-1160.32566	356 <i>i</i>

^a Zero-point correction energy;

^b Thermal correction to enthalpy;

^c Thermal correction to Gibbs free energy;

^d Gibbs free energy obtained at the M062X-D3/def2-TZVP//M062X-D3/def2-SVP theoretical level;

^e Imaginary frequencies (cm⁻¹) for the transition states.

Table S8 Comparison of energy barrier (kcal mol⁻¹) for the uncatalyzed reaction using different computational levels.

Epoxide	Computational level	C ₁ -O cleavage	C ₂ -O cleavage
Styrene oxide	B3LYP/6-31G**	56.3(44.6 ^[1])	68.9(59.7 ^[1])
	ωB97XD/6-31G**	61.1	71.8(70.7 ^[2])
	M062X-D3/def2-SVP	64.9	76.8

[1] V. Butera, N. Russo, U. Cosentino, C. Greco, G. Moro, D. Pitea and E. Sicilia, *ChemCatChem*, **2016**, *8*, 1167-1175.

[2] S. Marmitt and P. F. B. Gonçalves, *J. Comput. Chem.*, **2015**, *36*, 1322-1333.

Table S9 Comparison of three tetramethylammonium halides (X=Cl, Br, I).

Co-catalyst	N...X(Å) distance	Charge on X ⁻	Global nucleophilic index <i>N</i> (eV) ^a
TMAI	3.978	-0.889	4.9
TMAB	3.699	-0.880	4.4
TMAC	3.478	-0.873	4.0

^a Global nucleophilic index *N* (eV) was obtained based on the reference of *Journal of Molecular Structure: THEOCHEM*, 2008, 865, 68-72.

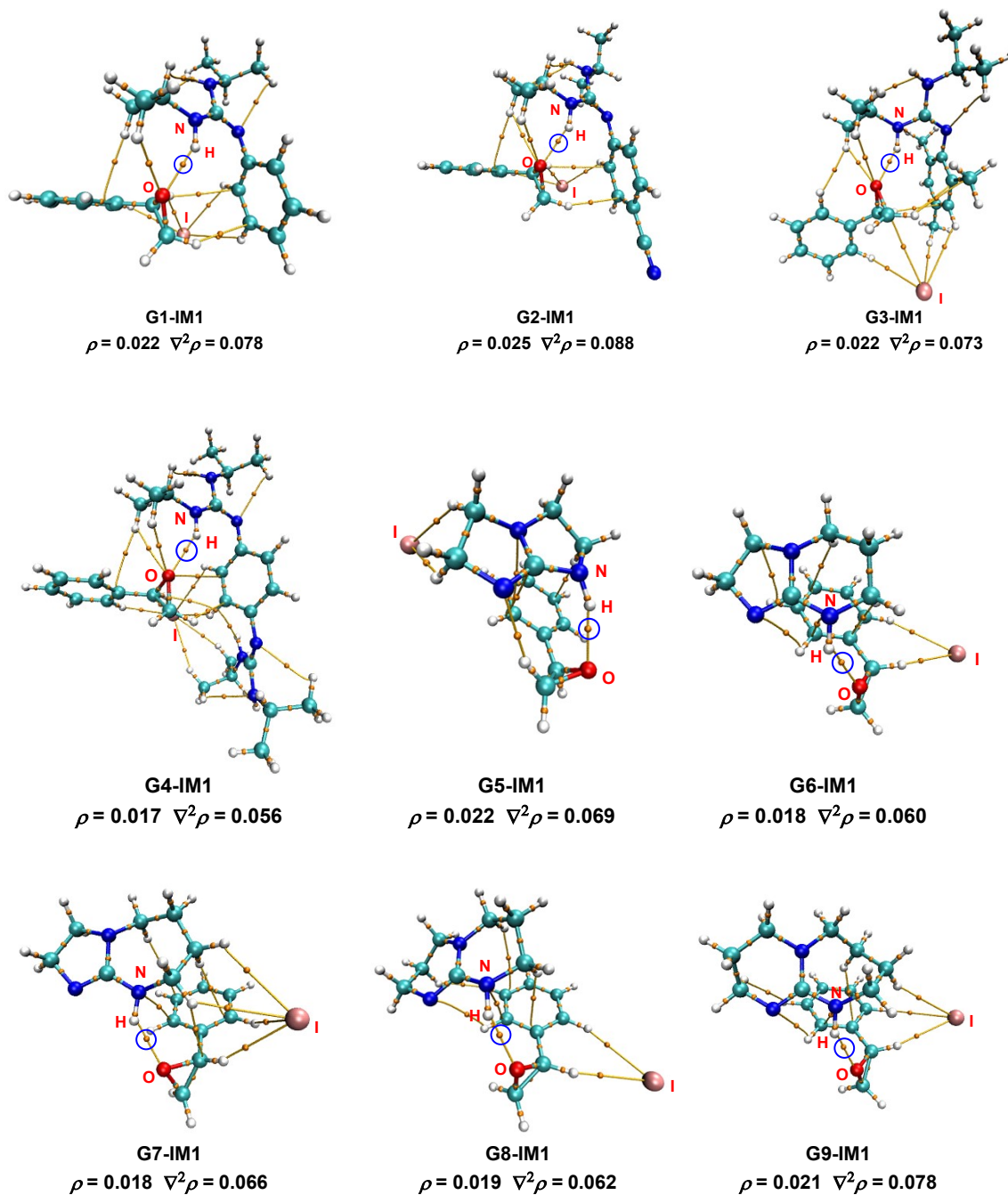


Figure S1 Laplacian ($\nabla^2\rho$) and charge density (ρ) on (3, -1) bond critical points (BCP) for **G1-IM1**~**G9-IM1**, obtained by AIM analysis.

Study on solvent effect

The solvent effect was studied at the M062X-D3/def2-TZVP//M062X-D3/def2-SVP (PCM-styrene oxide) level, in which the dielectric constant (ϵ) of styrene oxide was evaluated using the equation (1) in the *J. Phys. Chem. C*, 2019, **123**, 6395-6406:

$$\epsilon = \frac{2N\alpha + 3\epsilon_0}{3\epsilon_0 - N\alpha} \quad (1)$$

where N is number density of molecule ($1/\text{m}^3$), obtained by molecular dynamics simulation. α is molecular polarizability ($\text{C}\cdot\text{m}^2/\text{V}$), and ϵ_0 is dielectric constant of vacuum ($8.854187817 \times 10^{-12}$ F/m). The calculated dielectric constant (ϵ) of styrene oxide was 2.19.

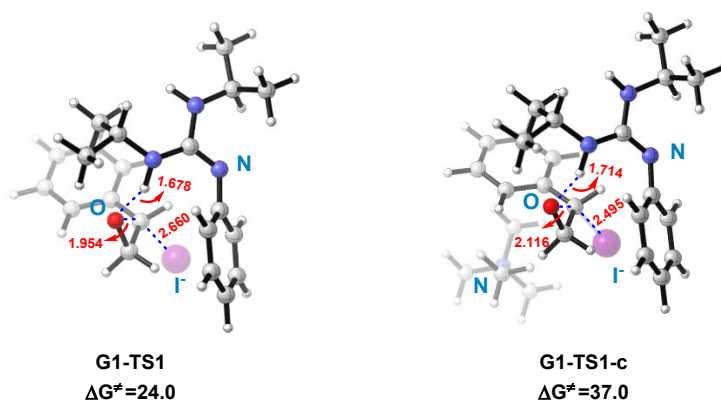


Figure S2 Optimized geometries of **G1-TS1** and **G1-TS1-c**, and the activation barriers (kcal mol^{-1}) in the ring-opening step.

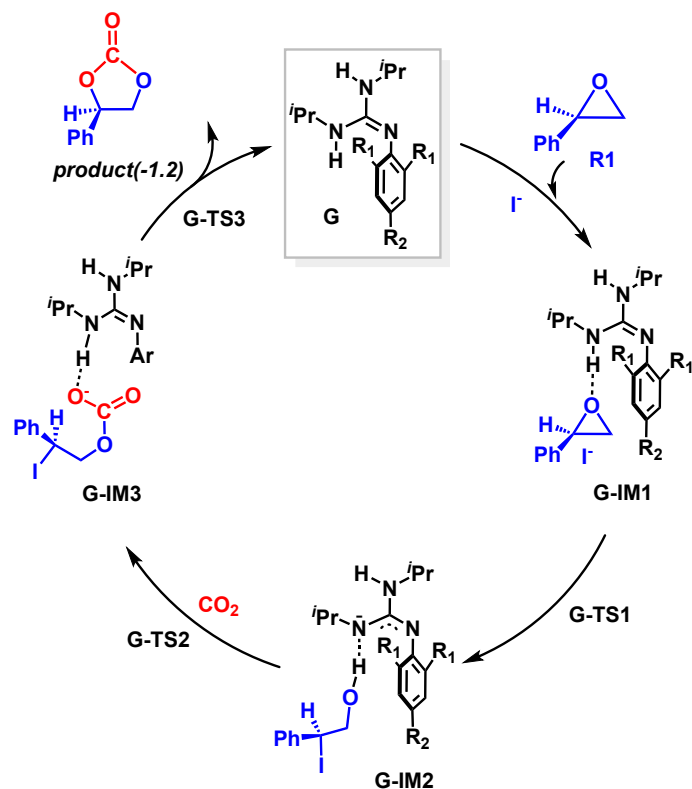


Figure S3 Catalytic cycle for TOF calculation.

Cartesian Coordinates of all Optimized Geometries

CO_2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15613600
O	0.00000000	0.00000000	-1.15613600

R1

C	2.56453400	-0.04149900	0.74726700
H	3.48797400	-0.59026800	0.96091800
C	1.60680500	-0.57047700	-0.24250300
H	1.85937000	-1.51417800	-0.74124900
O	2.46232600	0.50424700	-0.54418100
C	0.14958500	-0.26791900	-0.13783600
C	-0.29185800	1.05765200	-0.09751200
C	-0.78224600	-1.30643500	-0.06427900
C	-1.65051300	1.33858100	0.02964000
H	0.44427900	1.85885200	-0.18498800
C	-2.14081200	-1.02385000	0.06455600
H	-0.44082700	-2.34334800	-0.10980300
C	-2.57762400	0.29961100	0.11397400
H	-1.98963800	2.37547800	0.05617200
H	-2.86200900	-1.84061300	0.12293200

H	-3.64153200	0.52057600	0.21172300
H	2.17655000	0.58554000	1.55790900

Product

C	1.26822200	-1.22405400	0.74972700
H	1.25387400	-2.31948800	0.72178000
C	0.61043700	-0.56900000	-0.47517600
H	0.69794200	-1.22473000	-1.35763100
O	2.60419500	-0.76215400	0.66605100
C	-0.82675500	-0.18024600	-0.26537500
C	-1.17208000	1.10228700	0.16514300
C	-1.82502700	-1.14029600	-0.45255200
C	-2.50802000	1.41714100	0.40948000
H	-0.39186600	1.85425300	0.28969700
C	-3.15824300	-0.82579300	-0.19884000
H	-1.55862000	-2.14012500	-0.80522800
C	-3.50166000	0.45491300	0.23290500
H	-2.77452400	2.42334500	0.73631100
H	-3.93183900	-1.58062700	-0.34663400
H	-4.54603500	0.70472800	0.42526300
H	0.80996200	-0.86769600	1.68536100
C	2.65198800	0.35647900	-0.08753600
O	1.44926600	0.56002800	-0.67372700
O	3.59753100	1.05234600	-0.21927000

B-1-TS

C	-1.50171400	0.96332400	1.17888800
H	-1.73894500	1.86108600	1.77491200
C	-0.35885000	1.24216700	0.28509500
H	-0.53701800	2.10286300	-0.37039200
O	-2.50102900	0.75909000	0.23804800
C	0.85080800	0.54829200	0.11168700
C	1.14212300	-0.65249300	0.81257200
C	1.82569100	1.11388300	-0.75146600
C	2.39218200	-1.23012800	0.68235800
H	0.34816000	-1.13604100	1.37949300
C	3.07358800	0.52911600	-0.87026300
H	1.58084400	2.02126500	-1.30717100
C	3.35104900	-0.63985700	-0.15105100
H	2.62223900	-2.15835200	1.20506300
H	3.82874500	0.96287900	-1.52546900
H	4.33051500	-1.11086900	-0.25677100
H	-1.33482800	0.10799700	1.84824300
C	-2.46100100	-0.62877900	-0.43063600

O	-1.42997000	-1.22776000	-0.13434000
O	-3.44187200	-0.79682700	-1.09758500

B-2-TS

C	-0.69833000	-1.03895200	0.86303100
C	-1.48601000	-1.79205400	-0.10208900
O	-1.81955700	-0.17477000	0.89737300
H	-0.62019600	-1.52229800	1.85010200
H	-2.35872400	-2.31861500	0.28661800
H	-1.19760900	-1.95501500	-1.13809200
C	0.61129000	-0.44179300	0.42674200
C	1.59313000	-1.26205200	-0.13196100
C	0.86004800	0.91820000	0.62160900
C	2.82435100	-0.72467100	-0.49989000
H	1.39903200	-2.32792500	-0.28144000
C	2.09289300	1.45166500	0.24878700
H	0.07968500	1.55806700	1.03792200
C	3.07467800	0.63418700	-0.30906100
H	3.58823900	-1.36749200	-0.93934900
H	2.28287800	2.51633900	0.39071700
H	4.03670600	1.05715900	-0.60179800
C	-2.04152900	0.74190800	-0.41376200
O	-1.96922300	-0.02135800	-1.36991400
O	-2.23536100	1.87627300	-0.13059900

G1

C	-0.64913500	-0.10127800	0.02292800
N	0.20001700	-1.06904400	-0.04489500
C	1.56827000	-0.80771900	-0.05739500
C	2.16997700	-0.03220100	-1.06822100
C	2.40000100	-1.36684200	0.92737000
C	3.54569600	0.18368400	-1.08053100
H	1.53799000	0.38145900	-1.85736000
C	3.77496600	-1.14810400	0.90953700
H	1.93752000	-1.97993200	1.70212200
C	4.35811600	-0.36961700	-0.09082300
H	3.98891400	0.78288800	-1.87852000
H	4.39966700	-1.59316900	1.68641900
H	5.43583900	-0.20282300	-0.10371000
N	-0.32734800	1.20214800	0.31520900
H	0.65821900	1.36496000	0.48726900
N	-1.98509300	-0.34014900	-0.19871500
H	-2.63139400	0.28401700	0.27089700
C	-2.47548800	-1.69518200	-0.41846300

H	-1.74440900	-2.16940600	-1.08782600
C	-2.53170700	-2.50140800	0.87713300
H	-2.86502000	-3.53116400	0.68182900
H	-1.53445100	-2.53732200	1.33433500
H	-3.23937100	-2.04327000	1.58708400
C	-3.83112500	-1.61978500	-1.10889500
H	-3.76139100	-1.05909600	-2.05100600
H	-4.21120300	-2.62752700	-1.32575200
H	-4.57043900	-1.11914200	-0.46183600
C	-1.15077400	2.36873700	0.03404900
H	-1.85147200	2.08833200	-0.76914300
C	-1.95213000	2.80959400	1.26033200
H	-2.60046700	3.66552200	1.02278900
H	-2.58394000	1.99463500	1.64368100
H	-1.26822800	3.10357700	2.07036900
C	-0.26142300	3.49585800	-0.48004000
H	0.28821700	3.18188200	-1.37813700
H	-0.85936600	4.38360400	-0.72697600
H	0.47027800	3.78686300	0.29038100

G2

C	-1.22585600	-0.07597700	-0.03744600
N	-0.33518600	-1.01461200	0.01519000
C	1.01779400	-0.74157800	-0.00756200
C	1.61669100	0.07447300	-0.99409300
C	1.86241300	-1.34857100	0.94377000
C	2.98726100	0.28644100	-1.01483800
H	0.98405000	0.52781900	-1.75917900
C	3.23226400	-1.13692700	0.92776900
H	1.40612400	-1.99456400	1.69413700
C	3.80999500	-0.31272800	-0.05015400
H	3.43476400	0.91420100	-1.78667100
H	3.87088000	-1.61013700	1.67471100
N	-2.53327400	-0.39877500	-0.27899700
H	-3.23931300	0.25316400	0.03943500
N	-0.95641200	1.25560400	0.13209500
H	-0.00766100	1.47710500	0.41171200
C	-1.89992000	2.35581500	0.02868500
H	-2.61628400	2.09477000	-0.76775600
C	-2.66128200	2.59157900	1.33577600
H	-3.40764000	3.39057300	1.21942500
H	-3.17935500	1.68193000	1.67437000
H	-1.95909200	2.88552400	2.13010700
C	-1.14902700	3.60840200	-0.40859000

H	-0.63863600	3.44375800	-1.36714300
H	-1.83940600	4.45535200	-0.51824900
H	-0.39469800	3.88511500	0.34500600
C	-2.96120100	-1.78628300	-0.41604800
H	-2.16765900	-2.28672700	-0.98748700
C	-3.08469200	-2.47684100	0.93989700
H	-3.36084600	-3.53385700	0.81536200
H	-2.12442600	-2.42660100	1.46955400
H	-3.86114200	-1.99063700	1.55220900
C	-4.26326600	-1.82189600	-1.20566100
H	-4.14030300	-1.34350600	-2.18693900
H	-4.59241700	-2.85854700	-1.35910900
H	-5.06527600	-1.29689400	-0.66084500
C	5.23071000	-0.08831500	-0.06711200
N	6.37159100	0.09586700	-0.07957500

G3

C	1.13059900	0.01138000	-0.28392200
N	0.29491800	-0.96809300	-0.25215500
C	-1.07476000	-0.69654300	-0.15182400
C	-1.71948400	-0.83407300	1.09331000
C	-1.82450300	-0.33604600	-1.29132800
C	-3.09528200	-0.61154500	1.17964100
C	-3.19804100	-0.12409600	-1.16205100
C	-3.85619700	-0.25308800	0.06434600
H	-3.58748200	-0.72705300	2.14980900
H	-3.77409400	0.14549200	-2.05235900
N	2.47017400	-0.23515600	-0.45761100
H	3.11747500	0.50428100	-0.22052800
N	0.76106500	1.33835000	-0.20646500
H	-0.21667600	1.46960200	0.03755200
C	1.65101300	2.44096400	0.11569700
H	2.51514900	2.38378800	-0.56843400
C	0.92640900	3.74907200	-0.17741400
H	0.60175100	3.78713700	-1.22573500
H	0.03690900	3.84181000	0.46571300
H	1.57910700	4.60875200	0.02502500
C	2.14608200	2.38782000	1.56375600
H	2.86507500	3.19438800	1.76865600
H	1.29494000	2.49923000	2.25265000
H	2.63095100	1.42514000	1.78446800
C	2.99318800	-1.59172700	-0.37554200
H	2.28419600	-2.21988500	-0.93222000
C	4.35752300	-1.63691600	-1.04980100

H	4.76095200	-2.65856000	-1.03549000
H	4.29092300	-1.29883900	-2.09286500
H	5.07586700	-0.98952100	-0.51978500
C	3.04544000	-2.08999200	1.06762900
H	2.04567400	-2.02491600	1.51790900
H	3.38004200	-3.13672900	1.11198100
H	3.74717400	-1.48107000	1.66094500
C	-5.33532800	0.01254100	0.18154100
H	-5.53715800	1.08676700	0.31876000
H	-5.87110300	-0.30812000	-0.72278100
H	-5.76855900	-0.51679300	1.04113100
C	-0.90544800	-1.22941700	2.29493400
H	-1.53169600	-1.30558300	3.19345200
H	-0.40983800	-2.19670000	2.12109000
H	-0.10369900	-0.49911300	2.48991400
C	-1.12607200	-0.20245400	-2.61698900
H	-0.40653000	0.63153900	-2.59891200
H	-0.54903100	-1.11192800	-2.84030600
H	-1.84424900	-0.02410500	-3.42791800

G4

C	-3.57995200	0.01172600	0.07457300
N	-2.71790200	0.69399100	-0.59218500
C	-1.36562300	0.34385500	-0.60961800
C	-0.57225100	0.31044600	0.55071800
C	-0.73496900	0.06346100	-1.83355200
C	0.78418100	-0.00350000	0.48768700
H	-1.03497900	0.53717600	1.51433300
C	0.61699200	-0.25109000	-1.89617600
H	-1.34024500	0.09838700	-2.74075800
C	1.41025700	-0.28672300	-0.73757600
H	1.37881300	-0.04675000	1.40367600
H	1.09249500	-0.47773900	-2.85169900
N	-4.91410100	0.34716200	0.00678200
H	-5.47460600	0.07127400	0.80491200
N	-3.29510000	-1.08413100	0.87091000
H	-2.32235400	-1.37005700	0.79452700
C	-4.21902500	-2.20104100	1.05229700
H	-5.15340800	-1.81049900	1.48873800
C	-4.55107300	-2.90363900	-0.26329900
H	-5.26934900	-3.72103000	-0.10356800
H	-4.98470300	-2.19070800	-0.97774500
H	-3.63532600	-3.32698600	-0.70417100
C	-3.60866000	-3.15809500	2.06847700

H	-3.38708700	-2.63636400	3.00929700
H	-4.29217000	-3.99224700	2.27626900
H	-2.66963200	-3.58126100	1.67719500
C	-5.34122000	1.56593200	-0.66699900
H	-4.76582800	1.60307900	-1.60244200
C	-6.82755400	1.45750400	-0.98169500
H	-7.17197300	2.34508100	-1.53016900
H	-7.03713800	0.56589800	-1.58844600
H	-7.41919000	1.39143000	-0.05356300
C	-5.01450100	2.81859800	0.14387200
H	-3.93554700	2.86208200	0.34135800
H	-5.30621300	3.72620500	-0.40474300
H	-5.55780900	2.80937400	1.10262700
C	3.67538900	0.18060800	-0.44973400
N	2.76008700	-0.64388200	-0.81550000
N	4.98170600	-0.24077200	-0.34762000
H	5.67322900	0.47270200	-0.54416000
N	3.48024700	1.52305900	-0.16808200
H	2.49871200	1.78229600	-0.21836100
C	4.20815900	2.21031100	0.89718900
H	5.28534200	2.15106200	0.67199700
C	3.80980400	3.67995200	0.87584800
H	4.36596400	4.24482900	1.63609800
H	4.00391300	4.12259500	-0.11043000
H	2.73543200	3.78585500	1.09638000
C	3.96669500	1.57506800	2.26572000
H	4.24006800	0.50996100	2.24575500
H	4.56337000	2.07314900	3.04386000
H	2.90376100	1.66151100	2.54016500
C	5.34610600	-1.60683000	-0.71139200
H	4.77534700	-1.88776800	-1.61232900
C	6.83715800	-1.64788200	-1.01640300
H	7.14339500	-2.66598200	-1.29166200
H	7.09400700	-0.97889100	-1.85152200
H	7.42017800	-1.34532800	-0.13215600
C	4.97325100	-2.57520600	0.40652800
H	3.89754000	-2.51038000	0.61361800
H	5.20914600	-3.60936500	0.11561900
H	5.53330100	-2.33129800	1.32257800

G5

N	-1.26430500	-0.34868000	-0.08828500
N	0.48049800	-1.41490200	0.84530300
C	0.10319000	-0.43943100	-0.08187400

C	-0.67481300	-2.24609800	1.10543400
H	-0.77860900	-3.05076300	0.34966800
H	-0.65728500	-2.70002200	2.10530700
C	1.79577300	-1.83892600	0.39940800
H	2.45374600	-2.12466500	1.23090900
H	1.71646900	-2.69207200	-0.30435500
C	-1.80629700	-1.21129700	0.95137500
H	-2.75429000	-1.67451600	0.64650000
H	-1.96511500	-0.67489400	1.90379300
N	1.01450200	0.10751000	-0.78166500
C	2.24883900	-0.54635300	-0.33414800
H	2.91545900	-0.76187200	-1.18074000
H	2.80116300	0.11243800	0.35939500
H	-1.71368300	0.50901800	-0.37746200

G6

N	0.94383700	-0.24291200	0.06193600
C	-0.07178300	0.24546300	0.84279600
C	2.27690200	-0.39566400	0.61557700
H	2.81724900	0.57003400	0.66842400
H	2.85733500	-1.05926200	-0.04048400
N	-1.10808900	0.85376500	0.40357900
N	-0.01712300	0.00963400	2.21905200
C	-1.96266100	1.06846100	1.56584000
H	-2.42569200	2.06498000	1.54743900
H	-2.78216900	0.32753800	1.57501400
C	-1.04378500	0.86845800	2.78857900
H	-1.54177700	0.39691600	3.64768500
H	-0.60020500	1.82811400	3.12452200
C	1.26098700	-0.13429200	2.87880600
H	1.10775000	-0.60201200	3.86322200
H	1.73005300	0.85716200	3.05919700
C	2.17600400	-0.99172400	2.01389000
H	3.17397800	-1.05977300	2.46853200
H	1.75828900	-2.00718200	1.94479500
H	0.86409700	0.05089800	-0.90400700

G7

N	5.54924700	8.63447900	0.22394400
C	5.82571100	8.56554100	-1.12479000
N	5.62456000	7.36103600	-1.80488200
C	5.93352500	7.55113300	1.12223500
H	5.98117900	7.98263100	2.13129200
H	6.94578700	7.17125800	0.88731700

C	4.93985100	6.39607100	1.12790100
H	3.93863000	6.80696300	1.33643100
H	5.19429400	5.71869700	1.95795600
C	6.40185000	9.08332100	-3.17588000
H	7.47442100	8.95506500	-3.40509900
H	6.00227600	9.80160900	-3.90647900
C	4.57168200	6.43829800	-1.40616700
H	4.42319100	5.75491200	-2.25427600
H	3.61288700	6.97371200	-1.25177800
C	5.66526900	7.73107100	-3.22001400
H	6.17116400	6.96576600	-3.82567500
H	4.63372200	7.85243500	-3.60456100
C	4.91221700	5.60610900	-0.17530200
H	5.89263800	5.13174500	-0.34577300
H	4.17122500	4.79613400	-0.09072900
N	6.25106400	9.55987800	-1.80824900
H	5.79358600	9.55915700	0.56135800

G8

N	3.01165700	12.47224800	1.80511800
N	3.81169900	10.37875100	2.59677200
C	3.95566200	13.24687300	2.59383300
H	3.45496200	13.65522700	3.49203100
H	4.27974500	14.11062900	1.98891800
C	5.15416800	12.40231500	2.99541100
H	5.78228000	12.21441900	2.11027000
H	5.76393200	12.94390000	3.73271400
C	4.65792500	11.06652800	3.53963400
H	5.51131700	10.41901000	3.79267300
H	4.11733200	11.24317600	4.49069100
C	3.06232800	11.08872800	1.83692400
N	2.18788500	10.43433800	0.98727300
H	2.38808000	9.44302000	0.94586600
C	2.17429400	13.24428800	0.90580100
H	2.79085800	13.66173000	0.08454000
H	1.76787600	14.10661400	1.46143300
C	1.03981300	12.41919500	0.32122000
H	0.27771500	12.22748200	1.09108600
H	0.56786500	12.97337100	-0.50203200
C	1.59350800	11.08566000	-0.15232600
H	0.78794900	10.44864400	-0.54310700
H	2.31215000	11.25335300	-0.98054300

G9

N	-1.54579300	-0.06545400	-0.01962600
N	-1.57738000	0.04732600	2.26570800
C	-1.76322800	0.64432700	1.02571900
N	-2.18632700	1.96569600	1.02858600
C	-1.67383400	0.59538000	-1.29549500
H	-1.76576500	-0.16490500	-2.08486300
H	-0.76637000	1.18575400	-1.53417000
C	-2.88526700	1.52206700	-1.29399100
H	-3.78463000	0.92074700	-1.08885000
H	-3.03025700	2.02708100	-2.25982700
C	-2.68940900	2.55947400	-0.20226800
H	-3.63839000	3.08014500	0.01921900
H	-1.97859400	3.33528400	-0.54660900
C	-2.08030600	2.93520900	2.11345900
H	-3.09344800	3.19498200	2.48178300
H	-1.67731800	3.86057400	1.66502400
C	-1.19238400	2.55856500	3.29406400
H	-0.97824000	3.47839100	3.85802500
H	-0.23236800	2.18646600	2.90896200
C	-1.81591600	1.51364800	4.21796600
H	-1.04101000	1.11225300	4.88838600
H	-2.59179700	1.96985800	4.85360400
C	-2.43097200	0.38643700	3.38860200
H	-2.57938000	-0.51190300	4.00326300
H	-3.43014500	0.69166200	3.02967900
H	-1.35609700	-0.93180600	2.13163400

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H	-4.31993300	1.19332600	2.18761600
H	-2.59077100	-2.38190100	-0.53179700
H	-1.93171700	-2.75058200	-2.89020300
H	0.43161900	-2.35992500	-0.00137700
H	2.82591000	-0.70576000	-1.11916300
O	1.16017600	0.31899000	1.35217200
N	-2.22831500	0.49263400	0.69342600
N	-1.49481900	-0.73214300	-1.22003900
N	-0.52624000	1.32240400	-0.63869000
N	2.54950800	-0.63644800	-0.14752200
C	-1.47375500	0.32944100	-0.31875100
C	-0.60910800	2.52641500	0.19499200
C	1.67901000	2.01916500	-1.52314200
C	0.81454900	0.87073700	-0.98337100
C	1.51083400	0.17305000	0.19996100
C	3.32460300	-1.35033100	0.85930100

C	-3.38395600	-0.33378900	0.97856800
C	-3.99109400	0.14865600	2.29317600
C	-4.42279500	-0.28801600	-0.14473800
C	-1.55801800	-2.13831600	-0.83649900
C	-0.61746400	-2.46347600	0.32229500
C	-1.23756000	-2.97597400	-2.06772500
C	1.67499800	3.21414300	-0.57857000
C	4.02119800	-2.53643600	0.20795700
H	4.58194900	-3.11067000	0.95744800
H	4.73891000	-2.19507900	-0.55590800
H	2.59432500	-1.71446200	1.59947000
H	-0.77415600	-1.77487700	1.16539200
H	-1.04463700	-0.54580800	-2.10606200
H	0.74834400	0.11691200	-1.78171200
H	-4.75783300	0.75042600	-0.29037900
H	-4.00592400	-0.64648300	-1.09608000
H	-3.08224900	-1.38830400	1.13261400
H	-3.23805300	0.11240100	3.09185400
C	4.29833000	-0.41682000	1.57301100
H	-5.30016800	-0.90048700	0.11143200
H	-4.85450100	-0.46735800	2.58571300
H	-1.31218400	-4.04684600	-1.83632400
H	-0.20907700	-2.77457300	-2.41067700
H	-0.77511700	-3.49454700	0.67136000
C	0.23334500	3.66041600	-0.36914400
H	3.29476800	-3.20947300	-0.26991300
H	3.74501200	0.41356000	2.03186100
H	4.84106000	-0.95255100	2.36526200
H	5.03305500	-0.00872700	0.86152000
H	0.18121300	4.51515800	0.32085400
H	-0.18713300	3.99206000	-1.33364200
H	-0.30273100	2.28720400	1.22602700
H	-1.66668600	2.80979900	0.24170000
H	2.11881500	2.92668000	0.39011200
H	2.29041400	4.02704300	-0.99130700
H	2.70036500	1.64884600	-1.69934100
H	1.26606200	2.32475600	-2.49787800

G1-TS2-a

C	2.40971100	-0.03481200	0.40117300
N	1.98354100	-1.13105700	-0.26843300
C	0.91525200	-1.87083600	0.18145500
C	0.56055200	-2.00303100	1.55044100
C	0.12179600	-2.59523100	-0.74353200

C	-0.53115300	-2.76706100	1.94581600
H	1.14196100	-1.46628500	2.29860300
C	-0.97271000	-3.35090600	-0.33370000
H	0.37717600	-2.54317000	-1.80080200
C	-1.32514600	-3.44015500	1.01340700
H	-0.77440900	-2.82462000	3.01030200
H	-1.57130500	-3.86723300	-1.08804300
H	-2.19678100	-4.01613400	1.32759200
N	3.74943800	0.31366700	0.14615800
H	3.87948000	1.28455600	-0.11064700
N	1.67121500	0.69708800	1.18753800
H	-0.01328400	0.65073500	1.75774000
C	2.21846100	1.84044400	1.89241200
H	3.31146800	1.91624700	1.75074100
C	1.56853000	3.12134000	1.36135700
H	1.92166000	4.01012600	1.90942900
H	1.78945700	3.25294300	0.29113800
H	0.47505600	3.04220900	1.46767900
C	1.98021100	1.68731100	3.39823500
H	2.47945400	0.77799400	3.76612700
H	2.38423500	2.55244400	3.94859700
H	0.90402600	1.60065500	3.60304500
C	4.70900100	-0.60996000	-0.42539800
H	4.32487600	-1.09104100	-1.34121700
C	5.96237400	0.17379700	-0.79551900
H	6.72870600	-0.49344200	-1.21494200
H	5.73102900	0.94412300	-1.54753900
H	6.38004100	0.66869000	0.09560900
C	5.01918100	-1.72791800	0.56647200
H	4.09318300	-2.26348200	0.81566900
H	5.73323200	-2.44671300	0.13540700
H	5.44660300	-1.30470800	1.48893600
C	-1.99140000	0.19147500	0.30119800
H	-1.35304200	-0.66109100	0.04394500
C	-2.01123600	0.39522400	1.81657500
H	-2.83903700	1.07550900	2.08658200
H	-2.22630600	-0.58636300	2.28170800
O	-0.82434400	0.95548900	2.26241400
C	-1.57706000	1.40504000	-0.47453900
C	-0.42268800	1.34182800	-1.25839300
C	-2.26353400	2.62072700	-0.36814200
C	0.03493900	2.47066400	-1.93863000
H	0.14412600	0.40936600	-1.30485800
C	-1.80527200	3.74920600	-1.03976600

H	-3.16906800	2.67255500	0.24202700
C	-0.65567800	3.67532100	-1.83124500
H	0.94552300	2.39123500	-2.53433900
H	-2.34656000	4.69310600	-0.94840100
H	-0.29768400	4.56253200	-2.35778700
I	-3.97067000	-0.52730500	-0.32731500
C	2.34112100	-0.81918100	-2.46096000
O	2.34816000	-1.91641400	-2.86907400
O	2.41378500	0.35202400	-2.48506300

G1-IM3-a

C	-2.40995600	-0.77665000	0.15185500
N	-1.51888000	-0.07818900	-0.69166900
C	-1.26952500	1.26550100	-0.41889400
C	-1.56124400	1.79198600	0.85712000
C	-0.75511300	2.14602100	-1.39416400
C	-1.36191100	3.14012800	1.13881600
H	-1.93619400	1.12631400	1.63568000
C	-0.56177000	3.48976300	-1.09146800
H	-0.49549400	1.74505900	-2.37087500
C	-0.86275400	4.00646200	0.16864500
H	-1.59327400	3.51112300	2.13984500
H	-0.15675100	4.14639800	-1.86479800
H	-0.69849800	5.06133500	0.39350800
N	-3.73672400	-0.48594900	-0.00695700
H	-4.37934800	-1.01766700	0.56870700
N	-1.92620100	-1.56626400	1.03742900
C	-2.78878400	-2.31122300	1.92921400
H	-3.69475600	-2.66833200	1.39431100
C	-2.02409000	-3.53541900	2.42291300
H	-2.61245400	-4.10931400	3.15488300
H	-1.77025000	-4.18732200	1.57552800
H	-1.07750400	-3.21002900	2.87911200
C	-3.22823400	-1.42206600	3.09751200
H	-3.75319700	-0.52375800	2.73773700
H	-3.89128400	-1.96387600	3.78915500
H	-2.33706000	-1.09139200	3.65259600
C	-4.32809700	0.10993900	-1.19845800
H	-3.49905300	0.54223500	-1.77245900
C	-4.99830800	-0.95765000	-2.05899400
H	-5.44052800	-0.50853100	-2.96114000
H	-4.23816300	-1.69336300	-2.35429400
H	-5.80754400	-1.45630600	-1.49791900
C	-5.28013300	1.22990500	-0.78859700

H	-4.74403800	1.98951900	-0.20231300
H	-5.72142200	1.71094500	-1.67358800
H	-6.10531100	0.83176500	-0.17444700
C	-1.14048300	-0.82216100	-1.94029800
O	-1.90906900	-1.75150100	-2.18568300
O	-0.13052900	-0.39927500	-2.50975900
H	-0.21259600	-1.91758700	1.10045700
C	1.83435600	-0.20724600	0.21659700
C	1.22597000	-0.71802300	1.52803800
H	2.00448400	-0.71373000	2.31186000
H	0.43669900	-0.00809400	1.84202300
O	0.73745000	-2.00704200	1.36928200
C	2.90488100	-1.09082400	-0.35271200
C	2.73400900	-1.61657100	-1.63810900
C	4.03777100	-1.44851500	0.38882900
C	3.68647500	-2.49054000	-2.16591900
H	1.84015900	-1.33894200	-2.20654000
C	4.98604900	-2.31697600	-0.14147500
H	4.17953200	-1.02523600	1.38649900
C	4.81171600	-2.84293700	-1.42390300
H	3.54105800	-2.90126900	-3.16707300
H	5.86596600	-2.58666900	0.44652400
H	5.55367300	-3.52767400	-1.84054100
I	2.61259900	1.81610200	0.60638400
H	1.06026100	-0.03105300	-0.54243300

G1-TS3-a

C	-2.65532600	-0.41819300	0.17380100
N	-1.61985600	-0.11725000	-0.72004400
C	-1.11656500	1.18945400	-0.79629900
C	-1.20298600	2.06064700	0.29981500
C	-0.50344500	1.64690600	-1.97608300
C	-0.68239600	3.35004400	0.22095800
H	-1.65494100	1.70758400	1.22861900
C	0.02584800	2.93158900	-2.03639200
H	-0.40969900	0.96449300	-2.81993100
C	-0.06177800	3.79490600	-0.94324300
H	-0.73146500	3.99861900	1.09707500
H	0.51900300	3.26064300	-2.95334900
H	0.36986400	4.79516700	-0.99208800
N	-3.80775100	0.31850700	0.01467600
H	-4.55820000	0.08227300	0.65356800
N	-2.45570900	-1.31172700	1.06902500
C	-3.52479800	-1.77682300	1.92318600

H	-4.49089700	-1.78109100	1.37403300
C	-3.21549100	-3.21245600	2.33424700
H	-3.99607000	-3.61969500	2.99452700
H	-3.13092500	-3.84551700	1.44043800
H	-2.24832500	-3.24109800	2.85813700
C	-3.66414100	-0.86261100	3.14393800
H	-3.88540500	0.17350200	2.84406300
H	-4.46284900	-1.21100200	3.81635900
H	-2.71500400	-0.85128300	3.70027800
C	-4.24826600	0.79696400	-1.29441100
H	-3.41081800	1.35792900	-1.73429500
C	-4.60637000	-0.36164800	-2.22295300
H	-4.86021800	0.00732100	-3.22849300
H	-3.75931600	-1.06176100	-2.29658600
H	-5.47883700	-0.90801900	-1.82680400
C	-5.40622000	1.76377300	-1.08627900
H	-5.10315300	2.60025900	-0.44101600
H	-5.74883900	2.16709900	-2.04926600
H	-6.26201700	1.25026100	-0.61629300
C	-0.98711400	-1.26581900	-1.43315700
O	-1.74973300	-2.16421300	-1.74405300
O	0.24173700	-1.13002200	-1.63610600
H	-0.81255400	-2.07975100	0.93531900
C	1.50845700	-0.44771700	-0.05555400
C	0.76911100	-1.00785200	1.16487600
H	1.52826800	-1.10625500	1.95494200
H	0.05239800	-0.24170700	1.50642300
O	0.15707400	-2.24456100	0.96681700
C	2.63512600	-1.16802100	-0.65864200
C	3.39549700	-0.54542900	-1.65841800
C	2.92635900	-2.48844700	-0.29513800
C	4.44164700	-1.22139700	-2.27118800
H	3.16214400	0.48716800	-1.92674700
C	3.97777800	-3.16453000	-0.91243800
H	2.29543500	-2.98784900	0.44084400
C	4.73866100	-2.53476500	-1.89549100
H	5.03280500	-0.72547300	-3.04322600
H	4.19750800	-4.19578300	-0.62948900
H	5.56172000	-3.06741600	-2.37677400
I	2.91470800	1.45825500	1.49000800
H	1.24991900	0.51607100	-0.47033300

G1-IM4-a

C	0.60245400	-0.16230000	0.06500000
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N	-0.59070100	0.57881900	0.38886500
C	-0.79049100	1.83513600	-0.21895100
C	-0.15206400	2.12183500	-1.43438100
C	-1.58277800	2.82050800	0.38767600
C	-0.30900100	3.37112200	-2.02808300
H	0.47080300	1.36003700	-1.90590600
C	-1.74743900	4.05848900	-0.22822800
H	-2.07361000	2.60806100	1.33747600
C	-1.11104400	4.34522800	-1.43526700
H	0.20177500	3.57861800	-2.96971000
H	-2.37078900	4.81300000	0.25491700
H	-1.23424600	5.32153600	-1.90587400
N	1.76033800	0.41451000	0.43538500
H	2.64519000	-0.03642700	0.15366600
N	0.41559400	-1.23550600	-0.60934400
C	1.55183200	-2.07012300	-0.97686600
H	2.33289600	-2.03462600	-0.19442800
C	1.06788400	-3.50757000	-1.12132200
H	1.90191800	-4.17114200	-1.39095800
H	0.62663900	-3.86133200	-0.17864300
H	0.29492800	-3.57107700	-1.90359600
C	2.17658800	-1.55240700	-2.27243700
H	2.54499900	-0.52320800	-2.14618600
H	3.04866000	-2.16225800	-2.54743200
H	1.43203500	-1.58001200	-3.08478400
C	1.91489600	1.36715200	1.53503400
H	0.92776800	1.81412800	1.72188900
C	2.37111200	0.63430400	2.79546400
H	2.48888200	1.34072100	3.63141800
H	1.62917400	-0.12765400	3.07529400
H	3.33736800	0.14271700	2.60229100
C	2.88448600	2.46820400	1.11841700
H	2.50608100	2.99422700	0.22949700
H	3.00730300	3.19621100	1.93397700
H	3.86593900	2.02971100	0.87904100
C	-1.49735500	-0.04882800	1.24615700
O	-1.15423700	-0.77634700	2.13118300
O	-2.79109800	0.27580100	1.05787800
H	-1.21808300	-1.73552700	-0.71856600
C	-3.45187000	0.20747600	-0.21236400
C	-2.67760300	-0.60406900	-1.27569500
H	-3.39777200	-0.77037700	-2.09859600
H	-1.85503200	0.00210400	-1.69056300
O	-2.21641900	-1.80204900	-0.75815300

C	-4.79519700	-0.43162000	0.05278400
C	-5.95555300	0.06392600	-0.54289800
C	-4.86652800	-1.57781600	0.85186400
C	-7.17982700	-0.57779300	-0.34911100
H	-5.90248800	0.96357500	-1.16176100
C	-6.08832900	-2.21650400	1.04539500
H	-3.94953000	-1.95326300	1.30895500
C	-7.24781000	-1.71958800	0.44618500
H	-8.08296500	-0.17898700	-0.81489300
H	-6.13577500	-3.11124900	1.66877300
H	-8.20453600	-2.22163200	0.60225500
H	-3.59658700	1.23475000	-0.59003400
I	5.17468500	-0.68289100	0.00491800

G1-TS4-a

C	0.63348800	-0.19269300	0.22129800
N	-0.54036400	0.53663200	0.43932500
C	-0.64407700	1.84151400	-0.09226100
C	0.00393100	2.15719800	-1.29532300
C	-1.36191100	2.84249100	0.57753300
C	-0.05802000	3.44809000	-1.81240300
H	0.56467900	1.38132900	-1.82050300
C	-1.43486800	4.12527100	0.04066200
H	-1.86574000	2.59909600	1.51192400
C	-0.78186800	4.43946000	-1.15126900
H	0.46122700	3.67456200	-2.74509900
H	-2.00009800	4.89300000	0.57228700
H	-0.83498300	5.44963700	-1.55971200
N	1.79948200	0.34296700	0.56358300
H	2.67558900	-0.09366700	0.21839900
N	0.48586500	-1.36341600	-0.34298200
C	1.47505400	-2.43515500	-0.35048200
H	2.32589900	-2.13476000	0.28262400
C	0.81367400	-3.67695100	0.24137900
H	1.53422000	-4.50503400	0.29870400
H	0.42767900	-3.46096600	1.24730900
H	-0.03702700	-3.98944800	-0.38417500
C	2.00549900	-2.66589400	-1.76078400
H	2.52276500	-1.76700800	-2.12375200
H	2.73960600	-3.48402300	-1.75710400
H	1.17981900	-2.92491800	-2.44258000
C	2.00075500	1.39296900	1.56359200
H	1.00505100	1.74424300	1.86687300
C	2.70422100	0.78590000	2.77648200

H	2.86903500	1.55495000	3.54572600
H	2.09232700	-0.01933300	3.20742800
H	3.67695300	0.37028300	2.47021300
C	2.79601600	2.54734800	0.96193500
H	2.25032100	3.00356400	0.12390800
H	2.97338900	3.31941300	1.72505400
H	3.76583300	2.17545100	0.59596700
C	-1.65790200	-0.20840100	1.04270900
O	-1.44701700	-0.90545300	1.99727200
O	-2.84214900	0.45698700	0.86031700
H	-0.58963300	-1.55322800	-0.56992500
C	-3.50237500	0.36527600	-0.39147700
C	-2.61411800	-0.51201600	-1.32021200
H	-3.27049500	-0.97547400	-2.08369200
H	-1.90067900	0.14737500	-1.86559700
O	-2.00342100	-1.41318200	-0.50089200
C	-4.84629100	-0.28511900	-0.17134400
C	-5.97848000	0.13634200	-0.87018700
C	-4.93917900	-1.38258000	0.69279000
C	-7.19527400	-0.52975700	-0.71595600
H	-5.90791000	0.99729900	-1.54042300
C	-6.15410900	-2.04584900	0.84576000
H	-4.04286000	-1.69717200	1.23257100
C	-7.28498900	-1.62311200	0.14331000
H	-8.07617500	-0.18972400	-1.26434600
H	-6.21998000	-2.90158000	1.52046600
H	-8.23618600	-2.14414900	0.26882400
H	-3.62991000	1.38126700	-0.80378800
I	5.05279300	-0.63617100	-0.34443700

G1-IM5-a

C	0.85534500	-0.11367300	0.53389400
N	-0.32023200	0.28380600	0.96440500
C	-0.83163900	1.53877600	0.71272700
C	-0.66230600	2.21593800	-0.51756000
C	-1.69818300	2.12368100	1.66169400
C	-1.34209100	3.40196400	-0.78230200
H	0.01335600	1.79018500	-1.26282500
C	-2.37077700	3.30982600	1.38819900
H	-1.84735000	1.59113900	2.60190500
C	-2.20620300	3.96035400	0.16236200
H	-1.19400600	3.89656200	-1.74540800
H	-3.04254500	3.72953500	2.14053300
H	-2.73830500	4.88844200	-0.05124700

N	1.91792100	0.68803500	0.26829700
H	2.72541900	0.26702300	-0.20981000
N	1.02019100	-1.44846300	0.30489300
C	2.23866900	-2.21208200	0.56894000
H	3.07472300	-1.50193000	0.64400500
C	2.09881200	-2.95816700	1.89473500
H	3.01379200	-3.52491200	2.12045700
H	1.90981700	-2.25328800	2.71732300
H	1.25307800	-3.66430800	1.85589500
C	2.54588900	-3.14516000	-0.59440500
H	2.71083800	-2.55775400	-1.50752200
H	3.46670900	-3.71134900	-0.39449700
H	1.71763200	-3.85616700	-0.75364800
C	2.24880400	1.90236800	1.00902600
H	1.32209200	2.28353900	1.45923700
C	3.24365000	1.57072700	2.12239600
H	3.49976800	2.47245800	2.69989200
H	2.81364700	0.82734700	2.81102100
H	4.16362900	1.15455200	1.68175700
C	2.80716300	2.95058400	0.05163500
H	2.06056600	3.21100500	-0.71204500
H	3.07927100	3.86372400	0.60148400
H	3.70496900	2.55343400	-0.44768600
C	-2.40547200	-1.70695700	1.33238400
O	-2.14105000	-2.28723100	2.33071700
O	-3.23283800	-0.65057900	1.24137900
H	0.15189300	-1.96431400	0.42006800
C	-3.36284100	-0.20508800	-0.09925800
C	-2.34783700	-1.09693200	-0.85896100
H	-2.79737300	-1.59951500	-1.72499300
H	-1.45338400	-0.53334100	-1.15593300
O	-1.98877700	-2.07369100	0.10118400
C	-4.78215700	-0.35738300	-0.58758300
C	-5.28449000	0.54532700	-1.52782700
C	-5.58611400	-1.41500500	-0.15434800
C	-6.56940900	0.38415800	-2.04420800
H	-4.66309000	1.38641800	-1.84598000
C	-6.87249000	-1.57299100	-0.66660300
H	-5.20553600	-2.10608700	0.60050000
C	-7.36562400	-0.67697500	-1.61570600
H	-6.95368800	1.09628900	-2.77654500
H	-7.49566500	-2.39938400	-0.32048700
H	-8.37353100	-0.80156700	-2.01527900
H	-3.06495900	0.85097000	-0.14405500

I	5.18151300	-0.23811500	-1.08247000
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G1-COM

C	-1.72912200	-0.72982700	0.22390000
N	-1.99484300	0.18329600	-0.65776300
C	-1.79226800	1.54140000	-0.47833900
C	-2.01583100	2.23726300	0.72960300
C	-1.41995600	2.30557900	-1.60525700
C	-1.86365900	3.62149800	0.79874500
H	-2.34086600	1.68506900	1.61236800
C	-1.26661200	3.68476900	-1.52815000
H	-1.27116700	1.77566400	-2.54746900
C	-1.48369900	4.35789200	-0.32271200
H	-2.05309600	4.13052000	1.74596700
H	-0.97999100	4.24411800	-2.42101500
H	-1.36863200	5.44070600	-0.26286900
N	-2.09943800	-2.01936300	-0.04906800
H	-2.05062200	-2.68978200	0.70599600
N	-1.07476700	-0.52913900	1.41399900
H	-0.57993400	0.36059300	1.46612200
C	-0.43464900	-1.58268300	2.19622900
H	-1.19210500	-2.35760300	2.40924600
C	0.75180000	-2.22050100	1.47218300
H	1.15248100	-3.06659200	2.04960700
H	0.45847600	-2.58453900	0.47712500
H	1.55492900	-1.47874500	1.34852700
C	-0.01172100	-0.98270400	3.53214400
H	-0.87717200	-0.56083900	4.06124500
H	0.45543900	-1.74703800	4.16786600
H	0.72145000	-0.18024300	3.35927200
C	-2.97581100	-2.35108800	-1.16307200
H	-2.61621500	-1.75883500	-2.01602500
C	-2.83127100	-3.83548300	-1.47132600
H	-3.45359600	-4.11290000	-2.33290000
H	-1.78643000	-4.09047700	-1.69727200
H	-3.16026000	-4.44660600	-0.61447400
C	-4.42443000	-1.95548100	-0.88556800
H	-4.48259300	-0.87798900	-0.68209100
H	-5.06336400	-2.18197900	-1.75172700
H	-4.81528900	-2.50700800	-0.01571700
C	1.57695400	2.23000800	0.35332400
H	0.71947200	2.88558300	0.17024100
C	1.55496600	0.84712700	-0.15808000
H	0.66048400	0.52887700	-0.70964100

O	1.32982300	1.13379900	1.21194000
C	2.81025600	0.11433400	-0.48786600
C	3.87874800	0.08586400	0.41397900
C	2.92353500	-0.55298800	-1.70977000
C	5.05085500	-0.59254900	0.08867600
H	3.77057500	0.58540400	1.37926000
C	4.09847000	-1.22854000	-2.03560100
H	2.08216100	-0.54451200	-2.40631300
C	5.16463600	-1.24899900	-1.13769000
H	5.87967900	-0.61509800	0.79802600
H	4.17934000	-1.74667000	-2.99250700
H	6.08226100	-1.78247200	-1.38993500
H	2.55219500	2.71010000	0.49126200

G1-IM1

C	2.90406000	0.10147800	-0.15829600
N	2.71241900	-1.16902900	-0.20714100
C	1.90383400	-1.79829100	0.74418700
C	2.33651700	-1.96603700	2.07252100
C	0.65616200	-2.32777500	0.37762200
C	1.55174900	-2.65561100	2.99358000
H	3.30381600	-1.55104200	2.36418300
C	-0.12490300	-3.02013200	1.30177000
H	0.28438700	-2.19665800	-0.64135400
C	0.32072900	-3.19357100	2.61345700
H	1.90960600	-2.77690500	4.01894200
H	-1.10006000	-3.38754200	0.97015000
H	-0.29109600	-3.73577000	3.33687300
N	3.80272300	0.68273000	-1.04159700
H	3.57352000	1.62901200	-1.31742900
N	2.31314200	0.95300000	0.73852400
H	1.49439500	0.58756900	1.22892500
C	2.43329200	2.39918200	0.71964200
H	3.48289200	2.63361100	0.47404500
C	1.51067100	3.04873000	-0.31658200
H	1.65815100	4.13875200	-0.35572200
H	1.68107100	2.63888800	-1.32405400
H	0.45999500	2.85223200	-0.05606300
C	2.14714800	2.93479000	2.11923900
H	2.85184400	2.50633100	2.84524300
H	2.23261600	4.03081900	2.14088600
H	1.12649900	2.65203100	2.41641600
C	4.40454500	-0.13206600	-2.09023600
H	3.64335900	-0.83567900	-2.46776500

C	4.85729700	0.78607800	-3.21812000
H	5.32735600	0.20423800	-4.02275800
H	4.00780900	1.33739100	-3.64942600
H	5.59584500	1.51522500	-2.84721700
C	5.56527300	-0.95171500	-1.53578100
H	5.20374900	-1.59524700	-0.72420400
H	5.99918000	-1.58849800	-2.32159500
H	6.34883700	-0.28327700	-1.14577500
C	-1.34427500	0.70314000	0.74004100
H	-1.03269500	0.00930000	-0.04945100
C	-1.55341100	0.11951800	2.06995900
H	-2.28129500	0.59590400	2.73600700
H	-1.37310500	-0.95021800	2.20333600
O	-0.40418000	0.90401500	1.79299900
C	-2.10436300	1.90975400	0.30301300
C	-2.86702200	1.86038100	-0.86925600
C	-2.06907500	3.08733200	1.05781600
C	-3.58692500	2.98384000	-1.27294000
H	-2.90477500	0.92382800	-1.43523500
C	-2.78780600	4.20856000	0.64630500
H	-1.45896300	3.11433900	1.96366200
C	-3.54924100	4.15931400	-0.52113000
H	-4.18617800	2.93802400	-2.18429800
H	-2.75232500	5.12504300	1.23908600
H	-4.11441000	5.03619500	-0.84381700
I	-3.03547400	-2.06808100	-1.13179200

G1-TS1

C	2.61172500	-0.10959200	-0.04417800
N	2.16949900	-1.21877500	-0.55062700
C	1.41362800	-2.13144000	0.17807600
C	1.73678100	-2.54131800	1.48863300
C	0.31099100	-2.74578300	-0.44360900
C	0.99018400	-3.52227700	2.13379900
H	2.58026000	-2.07050900	1.99528600
C	-0.44166500	-3.71509200	0.21246900
H	0.03730400	-2.42331000	-1.44979800
C	-0.10388200	-4.11947800	1.50425800
H	1.26355600	-3.81830400	3.14955100
H	-1.31709400	-4.13214300	-0.28877600
H	-0.69594000	-4.87619200	2.02171300
N	3.53761800	0.61097300	-0.77929800
H	3.54569000	1.60845300	-0.61485100
N	2.26100300	0.40391800	1.16625100

H	1.31905400	0.10848800	1.52309100
C	2.58252600	1.74981500	1.61150000
H	3.64805000	1.94157900	1.39044300
C	1.70448500	2.80490200	0.92926000
H	1.97161000	3.82240000	1.25467100
H	1.78652800	2.75877000	-0.16849200
H	0.65414000	2.60335600	1.18878800
C	2.38854500	1.79752700	3.12535100
H	3.05567000	1.07787200	3.62069100
H	2.59453100	2.80533600	3.51539100
H	1.34599400	1.52433700	3.34944700
C	3.90741100	0.18399800	-2.12017000
H	3.00402600	-0.20356300	-2.62035700
C	4.44076200	1.38765800	-2.88618300
H	4.73529600	1.09740500	-3.90428500
H	3.67987400	2.17925600	-2.96376400
H	5.32760200	1.80478700	-2.38158400
C	4.92995700	-0.94722000	-2.06504400
H	4.50667600	-1.78886400	-1.50237200
H	5.18471800	-1.29220400	-3.07893300
H	5.84898000	-0.60377500	-1.56453600
C	-1.28388000	0.19530200	0.40994300
H	-0.51806600	-0.21075200	-0.25388800
C	-1.33111700	-0.41554300	1.74584400
H	-2.26387600	-0.20347800	2.30797400
H	-1.15391700	-1.50665000	1.73054300
O	-0.24942800	0.37189000	2.05836500
C	-1.64758800	1.61554000	0.19297300
C	-1.36882100	2.22295000	-1.03736000
C	-2.21495200	2.39023700	1.21244000
C	-1.64910300	3.57036400	-1.24703800
H	-0.93910400	1.61533700	-1.83703200
C	-2.49574000	3.73717600	1.00302300
H	-2.38561300	1.93659300	2.18871800
C	-2.21425400	4.33524800	-0.22637600
H	-1.42585300	4.02689600	-2.21341300
H	-2.92862300	4.33013700	1.81136200
H	-2.43161600	5.39311300	-0.38676200
I	-3.15862700	-1.00962600	-1.04161700

G1-IM2

C	-1.85310200	1.08041500	-0.15894800
N	-0.90901000	1.68182800	-0.88480900
C	0.07765100	2.45370200	-0.32031100

C	0.01460700	3.14281900	0.91979100
C	1.28371200	2.59779500	-1.05300100
C	1.08911600	3.89860700	1.37888300
H	-0.88518300	3.05060200	1.52317100
C	2.35747200	3.33891100	-0.57599200
H	1.34720400	2.07749800	-2.01158600
C	2.27718800	4.00072000	0.65163900
H	0.99930300	4.40757200	2.34266500
H	3.27451200	3.39178100	-1.16878900
H	3.12147700	4.57696600	1.03447300
N	-2.91646900	0.55257400	-0.91360500
H	-3.30505300	-0.29468800	-0.51655400
N	-1.84314500	0.91761700	1.14896500
H	-0.44928800	0.52133300	1.95416600
C	-2.95488800	0.30767400	1.84221400
H	-3.90854000	0.50751400	1.31149300
C	-2.77992000	-1.21094900	1.98492800
H	-3.61759400	-1.66859100	2.53700800
H	-2.69559800	-1.70808600	1.00536600
H	-1.83993300	-1.40770000	2.52261100
C	-3.05349000	0.94385300	3.23023600
H	-3.21816000	2.02730000	3.14011100
H	-3.87209100	0.50525700	3.82346200
H	-2.10330100	0.78743300	3.76458700
C	-2.90225000	0.58511600	-2.36522200
H	-1.87740100	0.38588600	-2.72632800
C	-3.84380200	-0.49525300	-2.88475900
H	-3.86167700	-0.50367000	-3.98393800
H	-3.52957800	-1.49195600	-2.53694700
H	-4.86950100	-0.31374900	-2.52450400
C	-3.30220300	1.96492600	-2.88068300
H	-2.60165100	2.70872900	-2.48114500
H	-3.26997600	1.99789000	-3.98141200
H	-4.32209800	2.21126100	-2.54498800
C	1.13129600	-0.60297100	0.30270400
H	0.69300700	0.15254200	-0.35727000
C	1.43518800	-0.02057700	1.69033900
H	2.16496300	-0.66980600	2.20639800
H	1.92987600	0.95812000	1.52375000
O	0.29629600	0.06622200	2.47278000
C	0.29384500	-1.84127400	0.25640300
C	-0.57260200	-2.03952000	-0.82612500
C	0.34267500	-2.80309800	1.27032900
C	-1.35584800	-3.19018300	-0.90536600

H	-0.62991400	-1.26592500	-1.59808600
C	-0.45152300	-3.94445000	1.19991600
H	0.99053000	-2.63713500	2.13250100
C	-1.29818000	-4.14605800	0.10924900
H	-2.02145400	-3.33810900	-1.75839900
H	-0.41409600	-4.68051400	2.00535100
H	-1.91885100	-5.04268500	0.05570300
I	3.06397000	-0.98038100	-0.70049600

G1-TS2

C	2.84929400	0.14478900	-0.48288600
N	2.81216000	-1.13624400	-0.22639000
C	1.70345400	-1.93245800	-0.43928100
C	0.78830700	-1.78847100	-1.50758800
C	1.51911500	-3.03597900	0.41914300
C	-0.25830500	-2.69072900	-1.67904400
H	0.90462800	-0.94444500	-2.18732500
C	0.46768200	-3.92858500	0.24475000
H	2.22530100	-3.15024200	1.24234800
C	-0.43787900	-3.76435400	-0.80433400
H	-0.96076900	-2.54476300	-2.50423200
H	0.34697600	-4.75788800	0.94585700
H	-1.27769100	-4.44890100	-0.93156300
N	4.10479400	0.74289500	-0.44224000
H	4.06657100	1.71162500	-0.14751600
N	1.77352900	0.92766400	-0.72080600
C	1.90361600	2.35636100	-0.93407500
H	2.55118900	2.82201300	-0.15701700
C	2.49625200	2.67270100	-2.31029600
H	2.60594000	3.75968100	-2.45289900
H	3.47802000	2.19697500	-2.43922900
H	1.82167100	2.28410900	-3.08862600
C	0.52916300	2.99914500	-0.77778000
H	0.11664700	2.77069700	0.21335400
H	0.58920200	4.08887800	-0.91994700
H	-0.16549600	2.58568200	-1.52671200
C	5.24222800	0.00740500	0.09207900
H	4.88964600	-0.63218500	0.91903000
C	5.84757600	-0.90208900	-0.97242500
H	6.68640200	-1.48317600	-0.55813800
H	5.07758400	-1.59678000	-1.33066400
H	6.21505100	-0.30153900	-1.81966900
C	6.26087500	1.00747300	0.62509600
H	5.82146400	1.62123100	1.42638400

H	7.13826500	0.48642100	1.03386100
H	6.60428500	1.67620200	-0.18091400
H	0.88489700	0.64110600	0.00849500
C	-1.95609400	0.04450000	-0.04647900
H	-1.51190100	-0.11320600	-1.03871100
C	-0.96117300	-0.38308200	1.03939000
H	-1.50780600	-0.40846000	2.01045200
H	-0.67207900	-1.43378700	0.83237800
O	0.07571500	0.50495800	1.05380100
C	-2.50080400	1.43939100	0.07636700
C	-3.11545200	2.06097000	-1.01739800
C	-2.37317900	2.15853600	1.27032700
C	-3.59691700	3.36436200	-0.92529100
H	-3.21704900	1.50477400	-1.95307600
C	-2.85475900	3.46301300	1.36434100
H	-1.83533200	1.70862000	2.10415300
C	-3.46896100	4.07153600	0.27050200
H	-4.06941800	3.83212100	-1.79132900
H	-2.73384000	4.01433300	2.29894800
H	-3.83948600	5.09577100	0.34639300
I	-3.65613400	-1.38303600	-0.08670000
C	1.92757500	0.02278900	2.51173100
O	1.49735000	-0.97135100	2.92597600
O	2.50682800	0.99795700	2.25346800

G1-IM3

C	0.63323100	2.54628300	1.35335100
O	0.19848500	3.67745400	1.19617600
O	0.05023600	1.48998700	1.70087400
I	3.64112600	-1.00788700	-0.61541400
C	2.53719800	1.12747100	1.35986400
C	1.97086600	0.01281300	0.45237100
O	2.00206300	2.38740000	1.07470700
H	2.33843100	0.85343400	2.40833600
H	3.62002100	1.22767600	1.21805400
C	1.14487300	-1.05960000	1.10099700
C	1.48538200	-1.60631400	2.34337600
C	0.00120100	-1.53715800	0.45253500
C	0.68708900	-2.58232100	2.93508100
H	2.38914600	-1.26809500	2.85469600
C	-0.79875900	-2.51272100	1.04255600
H	-0.27497900	-1.12821000	-0.52097400
C	-0.46236200	-3.03827400	2.28928800
H	0.96588500	-2.98956700	3.90907700

H	-1.69690100	-2.85151400	0.52063900
H	-1.09141400	-3.79844900	2.75671800
H	1.43555800	0.46592200	-0.39001700
C	1.19310000	0.81985500	-3.14632100
C	-0.02183200	0.22124500	-2.82994600
C	-0.94217100	0.83406000	-1.95250500
C	-0.59365800	2.09730200	-1.43225500
C	0.62597600	2.69323400	-1.75172500
C	1.53064800	2.06158100	-2.60458900
H	1.89258800	0.30025200	-3.80483900
H	-0.29263800	-0.75293600	-3.24216000
H	-1.25007400	2.61884100	-0.73565900
H	0.87337300	3.63882800	-1.26648100
H	2.49668200	2.51919100	-2.82313100
N	-2.12336200	0.14228300	-1.69965100
C	-2.77744600	0.20610600	-0.57814300
N	-4.03848200	-0.38355100	-0.53487900
H	-4.28052100	-0.77236200	0.37058200
N	-2.36020000	0.77418700	0.57326900
C	-4.52433200	-1.15632100	-1.66463100
C	-6.04132300	-1.27348800	-1.56767600
C	-3.85093100	-2.52512700	-1.76225600
H	-4.25195500	-0.57979200	-2.55866300
H	-6.50436900	-0.27821100	-1.52186200
H	-6.44864500	-1.81697200	-2.43260800
H	-6.33151700	-1.82841500	-0.65948200
H	-2.76306300	-2.38779300	-1.82795700
H	-4.08844900	-3.13411100	-0.87333300
H	-4.19156000	-3.07619200	-2.65231100
C	-3.12657700	1.02669000	1.78428100
C	-3.03292600	2.51345700	2.13327300
C	-2.61556500	0.13866800	2.91975400
H	-4.18267100	0.79497400	1.57527300
H	-3.51701700	3.11541100	1.35004100
H	-3.53188600	2.71949500	3.09303100
H	-1.97748800	2.82098500	2.19128300
H	-2.73411000	-0.92653700	2.66818700
H	-1.54199200	0.33708100	3.06008600
H	-3.15396500	0.34520500	3.85778700
H	-1.36818900	1.03603900	0.68732500

G1-TS3

C	0.73803000	2.66726900	1.27457700
O	0.19954800	3.75129600	1.31876700

O	0.21050200	1.50428100	1.36013500
I	3.51887100	-1.21454900	-0.66102900
C	2.61725600	1.29600500	1.19840500
C	1.66460000	0.28737700	0.57095800
O	2.09970600	2.60457600	1.10033600
H	2.79777800	1.03466000	2.25408600
H	3.57244400	1.30391400	0.66999800
C	1.03307500	-0.87228000	1.24610600
C	1.37640800	-1.27710600	2.53948300
C	-0.00196200	-1.54320100	0.57929000
C	0.70351800	-2.33221600	3.15171100
H	2.18457000	-0.77527800	3.07255300
C	-0.66891500	-2.59979600	1.18974200
H	-0.27710400	-1.23028500	-0.43121200
C	-0.32013500	-3.00061500	2.48075300
H	0.98684400	-2.63789800	4.16076700
H	-1.47024300	-3.11090900	0.65166000
H	-0.84264600	-3.82976100	2.96177700
H	1.30158200	0.52858600	-0.42815800
C	1.27516400	0.89563500	-3.02635300
C	0.07264000	0.25312400	-2.74660800
C	-0.94127700	0.88116900	-1.99561100
C	-0.70851300	2.20700300	-1.57427100
C	0.49647100	2.84688700	-1.85675900
C	1.50035100	2.19716900	-2.57623200
H	2.05853600	0.35766100	-3.56251500
H	-0.10209500	-0.77182700	-3.07929500
H	-1.45767800	2.73457000	-0.98352500
H	0.65720700	3.85280300	-1.46419600
H	2.45516100	2.69048200	-2.76307500
N	-2.10308500	0.15122900	-1.75052800
C	-2.76132800	0.22331400	-0.63472500
N	-3.99026700	-0.42121900	-0.55646900
H	-4.21486500	-0.77372500	0.36812700
N	-2.36816700	0.87750800	0.48409900
C	-4.43259200	-1.27822100	-1.64398500
C	-5.94197300	-1.46573200	-1.54411100
C	-3.69074800	-2.61422500	-1.66325000
H	-4.18523900	-0.73798000	-2.56747300
H	-6.45564400	-0.49471500	-1.55959700
H	-6.31506400	-2.07942800	-2.37679500
H	-6.20910100	-1.98052800	-0.60584300
H	-2.61021500	-2.42953500	-1.73412600
H	-3.90271200	-3.18400700	-0.74267600

H	-3.99911800	-3.22922000	-2.52246400
C	-3.09432300	1.03824300	1.73201800
C	-2.94539900	2.48499600	2.20231800
C	-2.58905800	0.04571400	2.78105300
H	-4.16168900	0.85622700	1.52844600
H	-3.40977800	3.16903100	1.47758800
H	-3.42609100	2.62816800	3.18201600
H	-1.88144400	2.75725000	2.27488000
H	-2.74323400	-0.99273000	2.45075400
H	-1.50570500	0.19242300	2.91811400
H	-3.09852500	0.18985900	3.74629300
H	-1.38124200	1.15635800	0.55775600

G1-IM4

C	-1.06770800	1.44032700	2.60719200
O	-0.55010700	1.89964300	3.57524000
O	-0.40673300	1.10223600	1.48192200
I	-3.03309100	-1.96702600	-1.37833000
C	-2.63745400	0.58171000	1.19766300
C	-1.31802500	0.76528700	0.42595000
O	-2.37618700	1.22936400	2.44865200
H	-3.48940700	1.06650500	0.70829800
H	-2.86010200	-0.48021800	1.35896100
C	-1.32039400	1.86655900	-0.60621700
C	-1.22113800	3.20832400	-0.22198100
C	-1.41598800	1.54203900	-1.96255600
C	-1.19904500	4.21678100	-1.18414700
H	-1.13989000	3.47054200	0.83623200
C	-1.39362200	2.55398100	-2.92207500
H	-1.52422300	0.49091200	-2.24756900
C	-1.27903800	3.89002300	-2.53805100
H	-1.11177800	5.26003400	-0.87500900
H	-1.46269000	2.29277200	-3.97949600
H	-1.25328400	4.67836600	-3.29289900
H	-1.01037100	-0.18500300	-0.02648400
C	-0.90265700	-2.27946900	1.94550000
C	0.17811300	-2.24387700	1.06636900
C	1.40536400	-1.68718600	1.45999600
C	1.52201000	-1.18859300	2.77088300
C	0.43987600	-1.22311700	3.64590400
C	-0.78175000	-1.76325300	3.23755800
H	-1.84801800	-2.68983000	1.58020800
H	0.05513300	-2.61853900	0.04781800
H	2.47515300	-0.75715000	3.08466800

H	0.54421500	-0.80153000	4.64745700
H	-1.63392700	-1.77580700	3.91972300
N	2.47745700	-1.65193700	0.56276600
C	2.88595000	-0.51988600	0.10528700
N	4.01815700	-0.47736500	-0.69656700
H	4.02654800	0.27963100	-1.37154600
N	2.29785200	0.68933800	0.35404900
C	4.58836800	-1.72144900	-1.19324800
C	6.02035900	-1.46043800	-1.64432900
C	3.74028800	-2.34184100	-2.30200300
H	4.58893200	-2.40907000	-0.33666000
H	6.61586500	-1.03570100	-0.82438700
H	6.49680900	-2.39052000	-1.98584700
H	6.03925900	-0.74909700	-2.48716800
H	2.72029200	-2.51418100	-1.93429600
H	3.69876300	-1.67104500	-3.17620400
H	4.16099800	-3.30396100	-2.63115800
C	2.81717300	1.99111000	-0.02378900
C	2.40850600	3.00574600	1.03938200
C	2.34225900	2.42569500	-1.41445900
H	3.91840400	1.91988600	-0.02659200
H	2.79268900	2.71218900	2.02604900
H	2.78644800	4.00710400	0.78836500
H	1.31191500	3.05321400	1.10812900
H	2.59009200	1.67246000	-2.17836800
H	1.24872900	2.54922500	-1.41974000
H	2.80339800	3.38138300	-1.70731800
H	1.45514400	0.67879400	0.92511400

G1-TS2-a

C	2.40971100	-0.03481200	0.40117300
N	1.98354100	-1.13105700	-0.26843300
C	0.91525200	-1.87083600	0.18145500
C	0.56055200	-2.00303100	1.55044100
C	0.12179600	-2.59523100	-0.74353200
C	-0.53115300	-2.76706100	1.94581600
H	1.14196100	-1.46628500	2.29860300
C	-0.97271000	-3.35090600	-0.33370000
H	0.37717600	-2.54317000	-1.80080200
C	-1.32514600	-3.44015500	1.01340700
H	-0.77440900	-2.82462000	3.01030200
H	-1.57130500	-3.86723300	-1.08804300
H	-2.19678100	-4.01613400	1.32759200
N	3.74943800	0.31366700	0.14615800

H	3.87948000	1.28455600	-0.11064700
N	1.67121500	0.69708800	1.18753800
H	-0.01328400	0.65073500	1.75774000
C	2.21846100	1.84044400	1.89241200
H	3.31146800	1.91624700	1.75074100
C	1.56853000	3.12134000	1.36135700
H	1.92166000	4.01012600	1.90942900
H	1.78945700	3.25294300	0.29113800
H	0.47505600	3.04220900	1.46767900
C	1.98021100	1.68731100	3.39823500
H	2.47945400	0.77799400	3.76612700
H	2.38423500	2.55244400	3.94859700
H	0.90402600	1.60065500	3.60304500
C	4.70900100	-0.60996000	-0.42539800
H	4.32487600	-1.09104100	-1.34121700
C	5.96237400	0.17379700	-0.79551900
H	6.72870600	-0.49344200	-1.21494200
H	5.73102900	0.94412300	-1.54753900
H	6.38004100	0.66869000	0.09560900
C	5.01918100	-1.72791800	0.56647200
H	4.09318300	-2.26348200	0.81566900
H	5.73323200	-2.44671300	0.13540700
H	5.44660300	-1.30470800	1.48893600
C	-1.99140000	0.19147500	0.30119800
H	-1.35304200	-0.66109100	0.04394500
C	-2.01123600	0.39522400	1.81657500
H	-2.83903700	1.07550900	2.08658200
H	-2.22630600	-0.58636300	2.28170800
O	-0.82434400	0.95548900	2.26241400
C	-1.57706000	1.40504000	-0.47453900
C	-0.42268800	1.34182800	-1.25839300
C	-2.26353400	2.62072700	-0.36814200
C	0.03493900	2.47066400	-1.93863000
H	0.14412600	0.40936600	-1.30485800
C	-1.80527200	3.74920600	-1.03976600
H	-3.16906800	2.67255500	0.24202700
C	-0.65567800	3.67532100	-1.83124500
H	0.94552300	2.39123500	-2.53433900
H	-2.34656000	4.69310600	-0.94840100
H	-0.29768400	4.56253200	-2.35778700
I	-3.97067000	-0.52730500	-0.32731500
C	2.34112100	-0.81918100	-2.46096000
O	2.34816000	-1.91641400	-2.86907400
O	2.41378500	0.35202400	-2.48506300

G1-IM3-a

C	-2.40995600	-0.77665000	0.15185500
N	-1.51888000	-0.07818900	-0.69166900
C	-1.26952500	1.26550100	-0.41889400
C	-1.56124400	1.79198600	0.85712000
C	-0.75511300	2.14602100	-1.39416400
C	-1.36191100	3.14012800	1.13881600
H	-1.93619400	1.12631400	1.63568000
C	-0.56177000	3.48976300	-1.09146800
H	-0.49549400	1.74505900	-2.37087500
C	-0.86275400	4.00646200	0.16864500
H	-1.59327400	3.51112300	2.13984500
H	-0.15675100	4.14639800	-1.86479800
H	-0.69849800	5.06133500	0.39350800
N	-3.73672400	-0.48594900	-0.00695700
H	-4.37934800	-1.01766700	0.56870700
N	-1.92620100	-1.56626400	1.03742900
C	-2.78878400	-2.31122300	1.92921400
H	-3.69475600	-2.66833200	1.39431100
C	-2.02409000	-3.53541900	2.42291300
H	-2.61245400	-4.10931400	3.15488300
H	-1.77025000	-4.18732200	1.57552800
H	-1.07750400	-3.21002900	2.87911200
C	-3.22823400	-1.42206600	3.09751200
H	-3.75319700	-0.52375800	2.73773700
H	-3.89128400	-1.96387600	3.78915500
H	-2.33706000	-1.09139200	3.65259600
C	-4.32809700	0.10993900	-1.19845800
H	-3.49905300	0.54223500	-1.77245900
C	-4.99830800	-0.95765000	-2.05899400
H	-5.44052800	-0.50853100	-2.96114000
H	-4.23816300	-1.69336300	-2.35429400
H	-5.80754400	-1.45630600	-1.49791900
C	-5.28013300	1.22990500	-0.78859700
H	-4.74403800	1.98951900	-0.20231300
H	-5.72142200	1.71094500	-1.67358800
H	-6.10531100	0.83176500	-0.17444700
C	-1.14048300	-0.82216100	-1.94029800
O	-1.90906900	-1.75150100	-2.18568300
O	-0.13052900	-0.39927500	-2.50975900
H	-0.21259600	-1.91758700	1.10045700
C	1.83435600	-0.20724600	0.21659700
C	1.22597000	-0.71802300	1.52803800

H	2.00448400	-0.71373000	2.31186000
H	0.43669900	-0.00809400	1.84202300
O	0.73745000	-2.00704200	1.36928200
C	2.90488100	-1.09082400	-0.35271200
C	2.73400900	-1.61657100	-1.63810900
C	4.03777100	-1.44851500	0.38882900
C	3.68647500	-2.49054000	-2.16591900
H	1.84015900	-1.33894200	-2.20654000
C	4.98604900	-2.31697600	-0.14147500
H	4.17953200	-1.02523600	1.38649900
C	4.81171600	-2.84293700	-1.42390300
H	3.54105800	-2.90126900	-3.16707300
H	5.86596600	-2.58666900	0.44652400
H	5.55367300	-3.52767400	-1.84054100
I	2.61259900	1.81610200	0.60638400
H	1.06026100	-0.03105300	-0.54243300

G1-TS3-a

C	-2.65532600	-0.41819300	0.17380100
N	-1.61985600	-0.11725000	-0.72004400
C	-1.11656500	1.18945400	-0.79629900
C	-1.20298600	2.06064700	0.29981500
C	-0.50344500	1.64690600	-1.97608300
C	-0.68239600	3.35004400	0.22095800
H	-1.65494100	1.70758400	1.22861900
C	0.02584800	2.93158900	-2.03639200
H	-0.40969900	0.96449300	-2.81993100
C	-0.06177800	3.79490600	-0.94324300
H	-0.73146500	3.99861900	1.09707500
H	0.51900300	3.26064300	-2.95334900
H	0.36986400	4.79516700	-0.99208800
N	-3.80775100	0.31850700	0.01467600
H	-4.55820000	0.08227300	0.65356800
N	-2.45570900	-1.31172700	1.06902500
C	-3.52479800	-1.77682300	1.92318600
H	-4.49089700	-1.78109100	1.37403300
C	-3.21549100	-3.21245600	2.33424700
H	-3.99607000	-3.61969500	2.99452700
H	-3.13092500	-3.84551700	1.44043800
H	-2.24832500	-3.24109800	2.85813700
C	-3.66414100	-0.86261100	3.14393800
H	-3.88540500	0.17350200	2.84406300
H	-4.46284900	-1.21100200	3.81635900
H	-2.71500400	-0.85128300	3.70027800

C	-4.24826600	0.79696400	-1.29441100
H	-3.41081800	1.35792900	-1.73429500
C	-4.60637000	-0.36164800	-2.22295300
H	-4.86021800	0.00732100	-3.22849300
H	-3.75931600	-1.06176100	-2.29658600
H	-5.47883700	-0.90801900	-1.82680400
C	-5.40622000	1.76377300	-1.08627900
H	-5.10315300	2.60025900	-0.44101600
H	-5.74883900	2.16709900	-2.04926600
H	-6.26201700	1.25026100	-0.61629300
C	-0.98711400	-1.26581900	-1.43315700
O	-1.74973300	-2.16421300	-1.74405300
O	0.24173700	-1.13002200	-1.63610600
H	-0.81255400	-2.07975100	0.93531900
C	1.50845700	-0.44771700	-0.05555400
C	0.76911100	-1.00785200	1.16487600
H	1.52826800	-1.10625500	1.95494200
H	0.05239800	-0.24170700	1.50642300
O	0.15707400	-2.24456100	0.96681700
C	2.63512600	-1.16802100	-0.65864200
C	3.39549700	-0.54542900	-1.65841800
C	2.92635900	-2.48844700	-0.29513800
C	4.44164700	-1.22139700	-2.27118800
H	3.16214400	0.48716800	-1.92674700
C	3.97777800	-3.16453000	-0.91243800
H	2.29543500	-2.98784900	0.44084400
C	4.73866100	-2.53476500	-1.89549100
H	5.03280500	-0.72547300	-3.04322600
H	4.19750800	-4.19578300	-0.62948900
H	5.56172000	-3.06741600	-2.37677400
I	2.91470800	1.45825500	1.49000800
H	1.24991900	0.51607100	-0.47033300

G1-IM4-a

C	0.60245400	-0.16230000	0.06500000
N	-0.59070100	0.57881900	0.38886500
C	-0.79049100	1.83513600	-0.21895100
C	-0.15206400	2.12183500	-1.43438100
C	-1.58277800	2.82050800	0.38767600
C	-0.30900100	3.37112200	-2.02808300
H	0.47080300	1.36003700	-1.90590600
C	-1.74743900	4.05848900	-0.22822800
H	-2.07361000	2.60806100	1.33747600
C	-1.11104400	4.34522800	-1.43526700

H	0.20177500	3.57861800	-2.96971000
H	-2.37078900	4.81300000	0.25491700
H	-1.23424600	5.32153600	-1.90587400
N	1.76033800	0.41451000	0.43538500
H	2.64519000	-0.03642700	0.15366600
N	0.41559400	-1.23550600	-0.60934400
C	1.55183200	-2.07012300	-0.97686600
H	2.33289600	-2.03462600	-0.19442800
C	1.06788400	-3.50757000	-1.12132200
H	1.90191800	-4.17114200	-1.39095800
H	0.62663900	-3.86133200	-0.17864300
H	0.29492800	-3.57107700	-1.90359600
C	2.17658800	-1.55240700	-2.27243700
H	2.54499900	-0.52320800	-2.14618600
H	3.04866000	-2.16225800	-2.54743200
H	1.43203500	-1.58001200	-3.08478400
C	1.91489600	1.36715200	1.53503400
H	0.92776800	1.81412800	1.72188900
C	2.37111200	0.63430400	2.79546400
H	2.48888200	1.34072100	3.63141800
H	1.62917400	-0.12765400	3.07529400
H	3.33736800	0.14271700	2.60229100
C	2.88448600	2.46820400	1.11841700
H	2.50608100	2.99422700	0.22949700
H	3.00730300	3.19621100	1.93397700
H	3.86593900	2.02971100	0.87904100
C	-1.49735500	-0.04882800	1.24615700
O	-1.15423700	-0.77634700	2.13118300
O	-2.79109800	0.27580100	1.05787800
H	-1.21808300	-1.73552700	-0.71856600
C	-3.45187000	0.20747600	-0.21236400
C	-2.67760300	-0.60406900	-1.27569500
H	-3.39777200	-0.77037700	-2.09859600
H	-1.85503200	0.00210400	-1.69056300
O	-2.21641900	-1.80204900	-0.75815300
C	-4.79519700	-0.43162000	0.05278400
C	-5.95555300	0.06392600	-0.54289800
C	-4.86652800	-1.57781600	0.85186400
C	-7.17982700	-0.57779300	-0.34911100
H	-5.90248800	0.96357500	-1.16176100
C	-6.08832900	-2.21650400	1.04539500
H	-3.94953000	-1.95326300	1.30895500
C	-7.24781000	-1.71958800	0.44618500
H	-8.08296500	-0.17898700	-0.81489300

H	-6.13577500	-3.11124900	1.66877300
H	-8.20453600	-2.22163200	0.60225500
H	-3.59658700	1.23475000	-0.59003400
I	5.17468500	-0.68289100	0.00491800

G1-TS4-a

C	0.63348800	-0.19269300	0.22129800
N	-0.54036400	0.53663200	0.43932500
C	-0.64407700	1.84151400	-0.09226100
C	0.00393100	2.15719800	-1.29532300
C	-1.36191100	2.84249100	0.57753300
C	-0.05802000	3.44809000	-1.81240300
H	0.56467900	1.38132900	-1.82050300
C	-1.43486800	4.12527100	0.04066200
H	-1.86574000	2.59909600	1.51192400
C	-0.78186800	4.43946000	-1.15126900
H	0.46122700	3.67456200	-2.74509900
H	-2.00009800	4.89300000	0.57228700
H	-0.83498300	5.44963700	-1.55971200
N	1.79948200	0.34296700	0.56358300
H	2.67558900	-0.09366700	0.21839900
N	0.48586500	-1.36341600	-0.34298200
C	1.47505400	-2.43515500	-0.35048200
H	2.32589900	-2.13476000	0.28262400
C	0.81367400	-3.67695100	0.24137900
H	1.53422000	-4.50503400	0.29870400
H	0.42767900	-3.46096600	1.24730900
H	-0.03702700	-3.98944800	-0.38417500
C	2.00549900	-2.66589400	-1.76078400
H	2.52276500	-1.76700800	-2.12375200
H	2.73960600	-3.48402300	-1.75710400
H	1.17981900	-2.92491800	-2.44258000
C	2.00075500	1.39296900	1.56359200
H	1.00505100	1.74424300	1.86687300
C	2.70422100	0.78590000	2.77648200
H	2.86903500	1.55495000	3.54572600
H	2.09232700	-0.01933300	3.20742800
H	3.67695300	0.37028300	2.47021300
C	2.79601600	2.54734800	0.96193500
H	2.25032100	3.00356400	0.12390800
H	2.97338900	3.31941300	1.72505400
H	3.76583300	2.17545100	0.59596700
C	-1.65790200	-0.20840100	1.04270900
O	-1.44701700	-0.90545300	1.99727200

O	-2.84214900	0.45698700	0.86031700
H	-0.58963300	-1.55322800	-0.56992500
C	-3.50237500	0.36527600	-0.39147700
C	-2.61411800	-0.51201600	-1.32021200
H	-3.27049500	-0.97547400	-2.08369200
H	-1.90067900	0.14737500	-1.86559700
O	-2.00342100	-1.41318200	-0.50089200
C	-4.84629100	-0.28511900	-0.17134400
C	-5.97848000	0.13634200	-0.87018700
C	-4.93917900	-1.38258000	0.69279000
C	-7.19527400	-0.52975700	-0.71595600
H	-5.90791000	0.99729900	-1.54042300
C	-6.15410900	-2.04584900	0.84576000
H	-4.04286000	-1.69717200	1.23257100
C	-7.28498900	-1.62311200	0.14331000
H	-8.07617500	-0.18972400	-1.26434600
H	-6.21998000	-2.90158000	1.52046600
H	-8.23618600	-2.14414900	0.26882400
H	-3.62991000	1.38126700	-0.80378800
I	5.05279300	-0.63617100	-0.34443700

G1-IM5-a

C	0.85534500	-0.11367300	0.53389400
N	-0.32023200	0.28380600	0.96440500
C	-0.83163900	1.53877600	0.71272700
C	-0.66230600	2.21593800	-0.51756000
C	-1.69818300	2.12368100	1.66169400
C	-1.34209100	3.40196400	-0.78230200
H	0.01335600	1.79018500	-1.26282500
C	-2.37077700	3.30982600	1.38819900
H	-1.84735000	1.59113900	2.60190500
C	-2.20620300	3.96035400	0.16236200
H	-1.19400600	3.89656200	-1.74540800
H	-3.04254500	3.72953500	2.14053300
H	-2.73830500	4.88844200	-0.05124700
N	1.91792100	0.68803500	0.26829700
H	2.72541900	0.26702300	-0.20981000
N	1.02019100	-1.44846300	0.30489300
C	2.23866900	-2.21208200	0.56894000
H	3.07472300	-1.50193000	0.64400500
C	2.09881200	-2.95816700	1.89473500
H	3.01379200	-3.52491200	2.12045700
H	1.90981700	-2.25328800	2.71732300
H	1.25307800	-3.66430800	1.85589500

C	2.54588900	-3.14516000	-0.59440500
H	2.71083800	-2.55775400	-1.50752200
H	3.46670900	-3.71134900	-0.39449700
H	1.71763200	-3.85616700	-0.75364800
C	2.24880400	1.90236800	1.00902600
H	1.32209200	2.28353900	1.45923700
C	3.24365000	1.57072700	2.12239600
H	3.49976800	2.47245800	2.69989200
H	2.81364700	0.82734700	2.81102100
H	4.16362900	1.15455200	1.68175700
C	2.80716300	2.95058400	0.05163500
H	2.06056600	3.21100500	-0.71204500
H	3.07927100	3.86372400	0.60148400
H	3.70496900	2.55343400	-0.44768600
C	-2.40547200	-1.70695700	1.33238400
O	-2.14105000	-2.28723100	2.33071700
O	-3.23283800	-0.65057900	1.24137900
H	0.15189300	-1.96431400	0.42006800
C	-3.36284100	-0.20508800	-0.09925800
C	-2.34783700	-1.09693200	-0.85896100
H	-2.79737300	-1.59951500	-1.72499300
H	-1.45338400	-0.53334100	-1.15593300
O	-1.98877700	-2.07369100	0.10118400
C	-4.78215700	-0.35738300	-0.58758300
C	-5.28449000	0.54532700	-1.52782700
C	-5.58611400	-1.41500500	-0.15434800
C	-6.56940900	0.38415800	-2.04420800
H	-4.66309000	1.38641800	-1.84598000
C	-6.87249000	-1.57299100	-0.66660300
H	-5.20553600	-2.10608700	0.60050000
C	-7.36562400	-0.67697500	-1.61570600
H	-6.95368800	1.09628900	-2.77654500
H	-7.49566500	-2.39938400	-0.32048700
H	-8.37353100	-0.80156700	-2.01527900
H	-3.06495900	0.85097000	-0.14405500
I	5.18151300	-0.23811500	-1.08247000

G2-COM

C	0.01588700	2.03011700	0.33767000
N	0.93764100	1.77872200	-0.55025400
C	1.97019100	0.88836600	-0.38340600
C	2.62807100	0.61982100	0.84148900
C	2.47118700	0.24417500	-1.54003200
C	3.70681100	-0.25121600	0.90195300

H	2.29682300	1.12287500	1.74996100
C	3.54611800	-0.62586600	-1.48245100
H	1.98601400	0.46758900	-2.49093700
C	4.17521100	-0.89220000	-0.25424900
H	4.20160900	-0.43895100	1.85594300
H	3.91162300	-1.11014900	-2.38898200
N	-0.77763000	3.12140200	0.14725700
H	-1.62568900	3.19629300	0.69229300
N	-0.22789000	1.28167400	1.45428100
H	0.21346000	0.36195600	1.45263000
C	-1.44874800	1.34257500	2.25026600
H	-1.62714800	2.40009600	2.51065900
C	-2.65865300	0.78205000	1.49862600
H	-3.58099500	0.91556600	2.08233400
H	-2.79379900	1.27018300	0.52129700
H	-2.51934900	-0.29492400	1.31929600
C	-1.20521300	0.57870600	3.54643500
H	-0.36630200	1.01571400	4.10463700
H	-2.10165900	0.59799100	4.18076200
H	-0.96603400	-0.47060100	3.31492500
C	-0.68409100	3.95848900	-1.04226700
H	0.38776100	4.05375900	-1.26228500
C	-1.36590400	3.30234900	-2.24103500
H	-1.25232000	3.92128000	-3.14282800
H	-0.91132500	2.32072800	-2.43085400
H	-2.44265300	3.17040200	-2.04834400
C	-1.26635800	5.32916700	-0.72476000
H	-0.74426900	5.79243900	0.12367700
H	-1.17927300	5.99445300	-1.59430400
H	-2.33721300	5.25012100	-0.47464100
C	5.28481300	-1.80366100	-0.18386500
N	6.17176900	-2.54265700	-0.12564200
C	0.71363000	-2.37768800	0.20248900
H	1.72600300	-2.02669000	-0.02128600
C	-0.44528500	-1.58035500	-0.24039100
H	-0.23646400	-0.64888100	-0.78416600
O	-0.01513300	-1.57715500	1.11154600
C	-1.77164700	-2.20433000	-0.50939600
C	-2.32132300	-3.11647300	0.39788200
C	-2.47803400	-1.87759100	-1.66942200
C	-3.55572900	-3.70521000	0.13722900
H	-1.77778400	-3.34513900	1.31705000
C	-3.71295300	-2.46990500	-1.93022300
H	-2.05821200	-1.15251100	-2.37071900

C	-4.25311800	-3.38613900	-1.02887200
H	-3.97906600	-4.41491700	0.84983300
H	-4.25802600	-2.21125500	-2.83928900
H	-5.22060900	-3.84812100	-1.23084900
H	0.57955100	-3.45712800	0.33030000

G2-IM1

C	-2.84819100	-0.12623700	0.12898100
N	-2.32603300	-1.23488400	0.53146100
C	-1.46903900	-1.98724100	-0.25144700
C	-1.82088300	-2.45368400	-1.53747300
C	-0.21782800	-2.36211500	0.27350300
C	-0.96211800	-3.27189400	-2.25595700
H	-2.78638200	-2.16718100	-1.95779700
C	0.65042000	-3.16894000	-0.44692300
H	0.09224500	-1.98861200	1.25187700
C	0.28121700	-3.64251700	-1.71738700
H	-1.24761000	-3.63365400	-3.24510600
H	1.62814700	-3.39778400	-0.01697100
N	-3.80691700	0.48045400	0.91377400
H	-3.90574800	1.48041600	0.78897900
N	-2.54466400	0.49739300	-1.05431000
H	-1.66714100	0.18675200	-1.47679500
C	-2.89248300	1.87326100	-1.37419200
H	-3.96382700	2.00623100	-1.14412200
C	-2.06401900	2.88637600	-0.57864300
H	-2.38409700	3.91723300	-0.79302700
H	-2.14454300	2.71554300	0.50554900
H	-1.00172500	2.79283500	-0.84911100
C	-2.71066300	2.07651700	-2.87477100
H	-3.34424500	1.37859200	-3.43917700
H	-2.96843200	3.10605600	-3.16108200
H	-1.65979600	1.88908900	-3.14147800
C	-4.02175600	0.02256800	2.28138400
H	-4.02143600	-1.07426000	2.23246900
C	-2.89275300	0.46330900	3.21119700
H	-3.04582900	0.07363100	4.22842600
H	-1.92788300	0.08965300	2.84175000
H	-2.85121300	1.56373000	3.27095300
C	-5.38426100	0.51553400	2.75306900
H	-6.18035000	0.16768300	2.08017400
H	-5.59551100	0.15574500	3.76983000
H	-5.41126900	1.61793200	2.77894100
C	1.16044100	-4.48753300	-2.48059900

N	1.85146800	-5.16708100	-3.11223000
C	1.39906500	-0.06054000	-2.13394900
H	1.34905600	-1.14355400	-1.99072300
C	1.10795100	0.82220000	-0.99379700
H	0.87829800	0.33421000	-0.03693800
O	0.16081200	0.61994200	-2.04158700
C	1.69870400	2.19012600	-0.91236100
C	1.55930600	3.09244100	-1.97313600
C	2.40217100	2.57137900	0.23538600
C	2.12127200	4.36521800	-1.89138400
H	0.99174000	2.78868400	-2.85594500
C	2.96562600	3.84470300	0.30825300
H	2.51207500	1.85316900	1.05545900
C	2.82766300	4.74397200	-0.74947100
H	2.00470900	5.06592300	-2.72065700
H	3.51812100	4.13388000	1.20418000
H	3.26817200	5.74091700	-0.68347800
H	2.06723300	0.30846700	-2.91983200
I	2.62178700	-0.83761200	2.22044900

G2-TS1

C	1.74020900	-1.95212200	-0.19403300
N	0.67262100	-2.11930600	-0.92418100
C	-0.59217000	-2.26817500	-0.39666500
C	-0.88819900	-3.03100800	0.75878400
C	-1.67661800	-1.68506000	-1.08723000
C	-2.19464900	-3.20626400	1.18282500
H	-0.07076000	-3.48298100	1.32020200
C	-2.98331900	-1.84331500	-0.65591000
H	-1.46122600	-1.06513100	-1.95871100
C	-3.26060300	-2.61744500	0.48199200
H	-2.40569600	-3.80235900	2.07221900
H	-3.79239200	-1.34244300	-1.18898900
N	2.96809400	-2.11314300	-0.80161100
H	3.73729000	-1.61059100	-0.37527000
N	1.73768600	-1.64106600	1.12426700
H	0.87512800	-1.13707600	1.46159000
C	2.91162800	-1.23951600	1.88295000
H	3.73516500	-1.93510800	1.64057000
C	3.32793700	0.20175200	1.57002700
H	4.22930300	0.48816300	2.13346900
H	3.52669300	0.35067600	0.49678200
H	2.49942400	0.87227700	1.84415400
C	2.57450500	-1.38472200	3.36469200

H	2.32693200	-2.42876800	3.60340500
H	3.41929100	-1.06484700	3.99200400
H	1.69803800	-0.75606600	3.58501200
C	3.07255900	-2.29565900	-2.24057300
H	2.27361600	-2.99828900	-2.51275800
C	2.83710200	-0.99036600	-2.99925500
H	2.88938000	-1.14911800	-4.08686300
H	1.84218200	-0.59808800	-2.75022900
H	3.59861800	-0.24185600	-2.72390700
C	4.42921100	-2.91083900	-2.56234400
H	4.56549000	-3.85938300	-2.02464300
H	4.52507900	-3.09778800	-3.64131600
H	5.24486300	-2.22848200	-2.26981000
C	-4.61152900	-2.81498400	0.93048100
N	-5.69523500	-2.99340900	1.29500000
C	-1.19315300	0.59228800	1.62118800
H	-1.95339700	-0.16210000	1.34582800
C	-0.42777300	1.09132600	0.47375100
H	-0.18450600	0.34414500	-0.28249200
O	0.00943400	0.10891100	2.08387100
C	0.51629900	2.22576900	0.58939700
C	0.59482100	3.00124500	1.75257800
C	1.39599600	2.49998600	-0.46453100
C	1.53142500	4.02575700	1.85513500
H	-0.05555100	2.76505400	2.59493400
C	2.33293700	3.52442700	-0.36222500
H	1.32512300	1.90339000	-1.37706200
C	2.40541200	4.29273900	0.80012000
H	1.58563400	4.61677500	2.77163100
H	3.01050000	3.72471300	-1.19452400
H	3.14066900	5.09518200	0.88532700
H	-1.66672000	1.38120500	2.23723100
I	-2.21449000	2.13813600	-1.22509400

G2-IM2

C	1.22779200	-1.97311400	-0.15093100
N	0.14555400	-1.88342200	-0.94741700
C	-1.11899600	-1.91169300	-0.46644800
C	-1.54492600	-2.47083300	0.77728500
C	-2.14722400	-1.36158300	-1.28822400
C	-2.87567700	-2.46999200	1.14933400
H	-0.79716400	-2.88662100	1.44826700
C	-3.47288900	-1.34560900	-0.90482300
H	-1.84012000	-0.92657000	-2.24115600

C	-3.86760400	-1.90163800	0.32727600
H	-3.16817500	-2.90702600	2.10636200
H	-4.22415200	-0.89238900	-1.55438800
N	2.38263100	-2.40996700	-0.80195400
H	3.25568500	-2.11276000	-0.38430700
N	1.25635100	-1.65476300	1.12029200
H	0.20726700	-0.56881500	1.87269800
C	2.46711200	-1.79140400	1.89955800
H	3.03825300	-2.68945400	1.58147700
C	3.37765800	-0.56381900	1.76380800
H	4.28401500	-0.65975000	2.38338500
H	3.68667700	-0.39550100	0.72058400
H	2.82234900	0.33366000	2.07873100
C	2.07543500	-1.98884700	3.36420300
H	1.45065800	-2.88737500	3.47146600
H	2.96261900	-2.09314100	4.00846900
H	1.48548200	-1.12339900	3.70298200
C	2.43398700	-2.63901700	-2.23281400
H	1.51144200	-3.17696900	-2.49037200
C	2.45324400	-1.33690800	-3.03455500
H	2.48838600	-1.53162900	-4.11787100
H	1.53935600	-0.77272800	-2.80452900
H	3.33542900	-0.73201600	-2.76330800
C	3.64130600	-3.51659400	-2.54798300
H	3.59598100	-4.45570000	-1.97899200
H	3.68782500	-3.75143400	-3.62132800
H	4.57774200	-2.99828800	-2.27980700
C	-5.24282700	-1.89982100	0.72803700
N	-6.35679000	-1.90511500	1.04803000
C	-1.05507000	0.89661500	1.49862000
H	-1.97147300	0.34836300	1.20203300
C	-0.29789300	1.25362600	0.21528000
H	-0.20398200	0.37844600	-0.43955000
O	-0.24677000	0.18278500	2.37017900
C	1.04408600	1.89262800	0.39404500
C	1.35853600	2.65117500	1.52724500
C	2.02429900	1.70556100	-0.58713200
C	2.62493400	3.21388300	1.66874800
H	0.61685100	2.76723700	2.31823500
C	3.28783400	2.27495800	-0.45125900
H	1.78355000	1.09265200	-1.45935400
C	3.59274200	3.03210800	0.67970500
H	2.86299500	3.79166000	2.56398800
H	4.04158300	2.11544600	-1.22510700

H	4.58498700	3.47252900	0.79586200
H	-1.38411700	1.82313500	2.00141400
I	-1.58802200	2.57454600	-0.99554400

G2-TS2

C	2.97168400	0.01528300	-0.44560900
N	2.75014400	-1.22676000	-0.08849100
C	1.56233700	-1.88299300	-0.26703900
C	0.66410700	-1.67311600	-1.34535300
C	1.25007800	-2.92928000	0.63451500
C	-0.47015300	-2.45401400	-1.49641300
H	0.87351500	-0.87431800	-2.05589500
C	0.11515600	-3.70510400	0.48715900
H	1.93410200	-3.08931100	1.46781700
C	-0.76669900	-3.47957400	-0.58315900
H	-1.15311100	-2.27163800	-2.32884100
H	-0.10652900	-4.49512900	1.20639900
N	4.29047300	0.42173700	-0.48082700
H	4.41800800	1.41142400	-0.30865200
N	2.01018600	0.92235500	-0.72164900
C	2.31265100	2.31907400	-0.98438800
H	3.04504100	2.70626500	-0.24307400
C	2.88381600	2.51361300	-2.39070800
H	3.12731600	3.57189900	-2.57265000
H	3.78927900	1.90992600	-2.54251200
H	2.13421600	2.19524000	-3.13095500
C	1.03908500	3.13408600	-0.78944000
H	0.64109200	2.96872400	0.21992700
H	1.23509200	4.20459300	-0.95030700
H	0.26609800	2.80806100	-1.50427400
C	5.34188700	-0.43261100	0.05579000
H	4.93634800	-0.96740000	0.93024700
C	5.77493100	-1.47240900	-0.97222400
H	6.54222400	-2.14056800	-0.55168900
H	4.90673600	-2.07588400	-1.26595100
H	6.18721400	-0.97673900	-1.86512800
C	6.50434500	0.44793700	0.49653500
H	6.18234800	1.15728700	1.27389500
H	7.31865000	-0.16530300	0.90721000
H	6.90412400	1.01887900	-0.35730700
H	1.12224000	0.77652100	-0.03671800
C	-1.81957900	0.47485000	0.03954200
H	-1.38360800	0.18556200	-0.92584400
C	-0.88197700	0.04047500	1.17129100

H	-1.42055700	0.18756900	2.13652000
H	-0.73370000	-1.05708800	1.08392100
O	0.26543000	0.77435800	1.09350300
C	-2.19866400	1.92886500	0.02298000
C	-2.76650400	2.49731000	-1.12431700
C	-1.95455400	2.75313300	1.12736900
C	-3.08486300	3.85141500	-1.17271100
H	-2.96482900	1.85702600	-1.98813900
C	-2.27423600	4.10927900	1.08098800
H	-1.45239300	2.33407800	1.99890500
C	-2.83974600	4.66487200	-0.06555100
H	-3.52324100	4.27497700	-2.07846500
H	-2.06243100	4.74078500	1.94616700
H	-3.08192300	5.72889400	-0.09992800
I	-3.64574100	-0.77272100	0.08872500
C	1.90154600	0.20997800	2.51364800
O	1.39575800	-0.71461100	3.00880700
O	2.63413000	1.07507100	2.23306700
C	-1.94034100	-4.28980300	-0.74685100
N	-2.87443500	-4.95965500	-0.88424000

G2-IM3

C	-0.53461200	-0.76733400	2.70267000
O	-0.23277500	-1.78359500	3.31010000
O	0.19212100	0.15733600	2.25705100
I	-3.36693100	1.03780100	-1.05589100
C	-2.27328200	0.58992200	1.82248400
C	-1.70498900	0.75406300	0.39613300
O	-1.89915400	-0.61931300	2.41995300
H	-1.93101000	1.44139700	2.43179700
H	-3.36919900	0.58229900	1.80464100
C	-0.71564100	1.85834300	0.16086200
C	-0.85756500	3.12102500	0.74646700
C	0.38334700	1.63002800	-0.67404500
C	0.08828200	4.11964200	0.52371400
H	-1.72139200	3.33093300	1.38057800
C	1.32906800	2.62686800	-0.89969300
H	0.50559900	0.65350700	-1.14549200
C	1.18868600	3.87731800	-0.29829600
H	-0.03690900	5.09613100	0.99599200
H	2.18524500	2.41351300	-1.54384200
H	1.93193500	4.65889800	-0.46742800
H	-1.29643900	-0.20492700	0.05916700
C	-1.45377600	-2.29772400	-1.78796400

C	-0.16124400	-1.83103700	-1.95242400
C	0.78467500	-1.86014300	-0.89870900
C	0.36465800	-2.42085600	0.32892100
C	-0.93224200	-2.88913400	0.50039500
C	-1.85711600	-2.83135600	-0.55223700
H	-2.17127200	-2.23464800	-2.60706600
H	0.16165900	-1.40779800	-2.90490100
H	1.03228000	-2.45884200	1.18889300
H	-1.23084500	-3.25016100	1.48557900
N	2.03634800	-1.35293100	-1.18089000
C	2.82596300	-0.79678000	-0.30078700
N	4.12564800	-0.52813800	-0.69989400
H	4.55366800	0.27059100	-0.24540400
N	2.50343200	-0.44161400	0.95648100
C	4.54411500	-0.73972500	-2.07512900
C	6.06506200	-0.83307500	-2.11771200
C	4.01115200	0.34315200	-3.01294900
H	4.10492500	-1.69924000	-2.37873400
H	6.42362800	-1.63242800	-1.45482500
H	6.41585000	-1.03420300	-3.14010100
H	6.52196800	0.11590600	-1.78986700
H	2.91482700	0.36743800	-2.95127100
H	4.41238100	1.33042600	-2.72834200
H	4.30172900	0.14486400	-4.05592800
C	3.37894800	0.09754800	1.98810300
C	3.16820400	-0.69697800	3.27747700
C	3.10012800	1.58874200	2.18189500
H	4.42227200	-0.05158300	1.66778100
H	3.48199900	-1.74117400	3.13447100
H	3.75585900	-0.26185400	4.10030000
H	2.10094500	-0.70034700	3.54492500
H	3.29442200	2.14937300	1.25448500
H	2.03623500	1.71348300	2.43622000
H	3.72273500	2.00710900	2.98752800
H	1.50811700	-0.38538200	1.24362600
C	-3.20190100	-3.31065600	-0.38028400
N	-4.28041800	-3.71207000	-0.26294200

G2-TS3

C	-0.72966300	-1.26449300	2.54849600
O	-0.33284900	-2.24126900	3.14356200
O	-0.04193700	-0.33476300	1.99304000
I	-3.09529500	1.48288000	-1.11424200
C	-2.40804300	0.15105300	1.77015900

C	-1.37444600	0.52034300	0.71548100
O	-2.07658300	-1.07571600	2.38680100
H	-2.48520400	0.95007600	2.52517400
H	-3.38740200	0.00635000	1.30932400
C	-0.52517700	1.73517100	0.67389400
C	-0.63468700	2.76486800	1.61259100
C	0.47751200	1.81210100	-0.30321200
C	0.23155800	3.85538200	1.56837100
H	-1.40472300	2.72104200	2.38315400
C	1.33609200	2.90494600	-0.35025400
H	0.56735800	1.00743500	-1.03846600
C	1.21761100	3.93430600	0.58602700
H	0.12963700	4.65278500	2.30696400
H	2.10533000	2.95161700	-1.12394100
H	1.89064300	4.79293400	0.55038000
H	-1.15148100	-0.25057900	-0.01971100
C	-1.64257000	-1.98663000	-1.96110900
C	-0.34475000	-1.52422700	-2.11084700
C	0.66352100	-1.81174200	-1.16282400
C	0.30884400	-2.64012600	-0.07179100
C	-0.98839800	-3.10712500	0.08265900
C	-1.98093300	-2.78074200	-0.85389700
H	-2.41279100	-1.70348800	-2.67864900
H	-0.07938400	-0.88928500	-2.95717300
H	1.04250300	-2.88738400	0.69463300
H	-1.24241000	-3.69420000	0.96654700
N	1.91654400	-1.27808000	-1.39457700
C	2.73652800	-0.90661900	-0.45238100
N	4.02300600	-0.56043100	-0.82076000
H	4.48146900	0.10597400	-0.21007600
N	2.45125300	-0.82992400	0.86795700
C	4.38925600	-0.45569800	-2.22402600
C	5.90496400	-0.55127700	-2.34985100
C	3.83922900	0.81889100	-2.86272200
H	3.92122500	-1.31599900	-2.72018400
H	6.27429400	-1.48783600	-1.90987800
H	6.21018200	-0.51058400	-3.40520700
H	6.39386300	0.28960400	-1.82979400
H	2.74782800	0.84651300	-2.74075800
H	4.27982700	1.70981000	-2.38472300
H	4.07308500	0.85754200	-3.93727200
C	3.32534200	-0.34928500	1.92633800
C	2.99672300	-1.11391000	3.20677500
C	3.17538000	1.16164400	2.11641900

H	4.36364200	-0.59200400	1.64480200
H	3.18235200	-2.18815000	3.06915200
H	3.61187800	-0.74973600	4.04277900
H	1.93262200	-0.99526000	3.45737400
H	3.44988600	1.71173200	1.20297200
H	2.11994000	1.39426500	2.33335000
H	3.80257700	1.52270000	2.94579000
H	1.45766000	-0.81263000	1.14076000
C	-3.32739600	-3.25614600	-0.68092900
N	-4.40392200	-3.65813500	-0.55118300

G2-IM4

C	1.25130100	0.05960000	-2.70011900
O	0.86210100	-0.22016300	-3.78877300
O	0.43861800	0.31485400	-1.65163500
I	2.61418400	-0.16996300	2.71608100
C	2.62286200	0.44439800	-0.92557300
C	1.18187200	0.81739100	-0.53196700
O	2.52439000	0.20669600	-2.33400500
H	3.34093400	1.25135000	-0.74435200
H	2.95691500	-0.46543100	-0.41002300
C	0.91235700	2.29377400	-0.37225400
C	0.73685700	3.11275200	-1.49298600
C	0.82769000	2.84776000	0.90877900
C	0.45753800	4.46949100	-1.33725800
H	0.79799000	2.68789200	-2.49837300
C	0.55059900	4.20656100	1.05990200
H	0.99250300	2.20059700	1.77640200
C	0.35835100	5.01780300	-0.05831600
H	0.31218100	5.09831300	-2.21754600
H	0.47928500	4.63129800	2.06275100
H	0.13411800	6.07895500	0.06571200
H	0.88851300	0.27213100	0.37361600
C	1.33003300	-2.59809600	-0.03074400
C	0.10316100	-2.26619400	0.52790900
C	-1.06881200	-2.25632000	-0.24995500
C	-0.97151500	-2.61198000	-1.61161500
C	0.25047600	-2.94143500	-2.17778400
C	1.41484400	-2.93286700	-1.39172000
H	2.22127500	-2.55883900	0.60073000
H	0.06023900	-1.97101300	1.57820300
H	-1.87605700	-2.60678000	-2.22233800
H	0.31934300	-3.18509000	-3.23841600
N	-2.28281200	-1.92094800	0.33509600

C	-2.89914100	-0.84201500	-0.01414400
N	-4.16027300	-0.58863400	0.49274700
H	-4.40987400	0.39158000	0.55683200
N	-2.40711300	0.08945400	-0.88209800
C	-4.69141800	-1.41762200	1.56581000
C	-6.20374300	-1.23903700	1.62017900
C	-4.02750100	-1.11547800	2.90800600
H	-4.45095100	-2.45304100	1.28879500
H	-6.66058200	-1.48022400	0.65048400
H	-6.64392900	-1.88680100	2.39135800
H	-6.46291100	-0.19724300	1.87361900
H	-2.94188500	-1.25634200	2.82604500
H	-4.23212700	-0.07607200	3.21354000
H	-4.40824800	-1.78371000	3.69471900
C	-3.07438000	1.30440600	-1.31435600
C	-2.55918600	1.66990400	-2.70228700
C	-2.87632000	2.45984200	-0.32737400
H	-4.15149800	1.07790600	-1.39608300
H	-2.74693400	0.85587400	-3.41551600
H	-3.04123900	2.58785600	-3.06714100
H	-1.47329000	1.83907300	-2.66215400
H	-3.19302300	2.18008800	0.68928400
H	-1.81152200	2.73403100	-0.27629600
H	-3.44943000	3.34654900	-0.63818400
H	-1.45111100	-0.04665500	-1.20586900
C	2.68167100	-3.27648900	-1.98381600
N	3.69350200	-3.56647100	-2.46241500

G3-COM

C	-2.32495200	-0.40147900	-0.26734600
N	-2.32913400	0.88503200	-0.16669200
C	-1.13844800	1.61067300	-0.16784700
C	-0.69741600	2.23336400	1.01997200
C	-0.42093100	1.81946600	-1.36671800
C	0.42972900	3.05697100	0.98730400
C	0.70743700	2.64448200	-1.35329300
C	1.15521600	3.27346600	-0.18814700
H	0.75514400	3.54265000	1.91291000
H	1.24754000	2.80810100	-2.29087500
N	-3.50366300	-1.06957800	-0.49467300
H	-3.54351800	-2.03829800	-0.20352800
N	-1.18535600	-1.16686000	-0.21419300
H	-0.41408100	-0.71956700	0.27696900

C	-1.14763400	-2.62067700	-0.18225200
H	-1.88799500	-2.98004800	-0.91570800
C	0.22997600	-3.08570400	-0.64258400
H	0.45399200	-2.69998000	-1.64652500
H	1.00077100	-2.71837900	0.05140300
H	0.28176800	-4.18315100	-0.66387600
C	-1.48109800	-3.17133700	1.20708600
H	-1.48475100	-4.27103700	1.21118300
H	-0.72391500	-2.81949600	1.92371400
H	-2.46388100	-2.81985700	1.55735100
C	-4.77515000	-0.35972000	-0.49174000
H	-4.59016800	0.58282000	-1.02530200
C	-5.80543500	-1.18680900	-1.24939800
H	-6.76721100	-0.65774200	-1.29629800
H	-5.46540800	-1.39212800	-2.27361800
H	-5.98095600	-2.15045000	-0.74294200
C	-5.23309400	-0.02419200	0.92639600
H	-4.45850400	0.56552800	1.43447300
H	-6.16497700	0.55981900	0.91211600
H	-5.41698200	-0.94696000	1.50062400
C	2.39818100	4.12626600	-0.18458800
H	3.25523500	3.57664000	0.23772800
H	2.67138500	4.43601000	-1.20244700
H	2.26030600	5.03221400	0.42257300
C	-1.46405400	1.99036100	2.29055400
H	-1.03653500	2.55452600	3.13076200
H	-2.51821300	2.27948200	2.16471800
H	-1.46329100	0.91889500	2.54966700
C	-0.90037700	1.16831000	-2.63373700
H	-0.81386900	0.07264100	-2.56438900
H	-1.96475400	1.39261400	-2.79958900
H	-0.32122200	1.51047500	-3.50129500
C	1.89356400	0.15490000	2.30761400
H	1.29500500	0.98274200	2.69999000
C	2.00890800	-0.01696600	0.84924700
H	1.47193200	0.69836700	0.21626800
O	1.16640900	-0.85070900	1.63537900
C	3.19782100	-0.65963900	0.22458100
C	3.74009600	-1.83721300	0.74945000
C	3.78189000	-0.07260000	-0.90031300
C	4.86437100	-2.41124600	0.16181400
H	3.26068200	-2.30758300	1.61118400
C	4.90987400	-0.64667100	-1.48514200
H	3.34116000	0.83650600	-1.31757500

C	5.45388100	-1.81533600	-0.95424600
H	5.28139900	-3.33205800	0.57284500
H	5.36204000	-0.18273900	-2.36305100
H	6.33367600	-2.26746200	-1.41446900
H	2.70987300	-0.20959600	2.94087900

G3-IM1

C	-3.51286200	0.10576600	0.05463800
N	-3.21135700	-1.09864700	0.39305400
C	-1.94311800	-1.35630300	0.94019800
C	-0.95803500	-1.97611100	0.14578100
C	-1.65997400	-1.04478300	2.28431300
C	0.28423300	-2.28478200	0.70208400
C	-0.40490500	-1.36861800	2.80750800
C	0.58126700	-1.99043900	2.03828000
H	1.06615800	-2.72362400	0.07372600
H	-0.19109700	-1.12020400	3.85218300
N	-4.80548000	0.39801000	-0.35886900
H	-4.87908600	1.16279400	-1.02028600
N	-2.64890100	1.16704200	0.12206200
H	-1.65599200	0.92316400	0.15077700
C	-2.92729600	2.51733800	-0.32818800
H	-3.98572500	2.72676000	-0.10159800
C	-2.07477200	3.49139700	0.47976700
H	-2.29790800	3.39995600	1.55150400
H	-1.01063500	3.26059700	0.32637600
H	-2.25959200	4.52840800	0.16372700
C	-2.67892200	2.68228100	-1.83107300
H	-2.93343400	3.69765100	-2.17113200
H	-1.61503000	2.49397900	-2.03886200
H	-3.27049300	1.96039700	-2.41580100
C	-5.73935100	-0.69011400	-0.60622200
H	-5.61008500	-1.38916200	0.23125700
C	-7.15755300	-0.13309400	-0.59973900
H	-7.89383000	-0.93648800	-0.74417500
H	-7.36978000	0.37706100	0.34988000
H	-7.29401200	0.59380800	-1.41811300
C	-5.41972000	-1.43663500	-1.90070500
H	-4.39024500	-1.81636000	-1.85857700
H	-6.10297000	-2.28656300	-2.04753400
H	-5.52074700	-0.76317200	-2.76828000
C	1.93531000	-2.33377800	2.60294200
H	1.97621000	-3.39111000	2.91154900
H	2.71669200	-2.18639900	1.83972700

H	2.16748300	-1.71959300	3.48543200
C	-1.26491600	-2.28663300	-1.29497100
H	-0.39246300	-2.73212800	-1.79235300
H	-2.11711500	-2.98075500	-1.36937300
H	-1.55351800	-1.37519200	-1.84401000
C	-2.71286100	-0.37383300	3.12466300
H	-2.91413900	0.64619000	2.75926400
H	-3.66412200	-0.92430400	3.06613900
H	-2.39914800	-0.31051800	4.17561400
C	1.06355600	0.51492200	-1.37438000
H	0.76092200	-0.52493100	-1.51760500
C	1.42201400	0.95327600	-0.02748900
H	1.34156600	0.20106900	0.76502300
O	0.17690400	1.33157600	-0.60743700
C	2.42299400	2.03718800	0.18572200
C	2.12737600	3.36734500	-0.12070200
C	3.69057300	1.70433500	0.67835900
C	3.08373400	4.36402700	0.07898500
H	1.14074800	3.61013300	-0.51955600
C	4.64307000	2.70193700	0.87020400
H	3.92723600	0.65259600	0.86326100
C	4.34249000	4.03406700	0.57739300
H	2.84342900	5.40270300	-0.15812700
H	5.63374200	2.43363400	1.24177300
H	5.09297100	4.81225600	0.73074200
H	1.53890700	1.01568700	-2.22313000
I	3.80200100	-1.84581700	-1.05071500

G3-TS1

C	3.21609000	0.20095200	0.00359100
N	3.02812600	-0.94378200	-0.55857000
C	1.91019900	-1.72792100	-0.25102900
C	1.93266800	-2.60852100	0.84526000
C	0.77538500	-1.69049600	-1.08666900
C	0.83799100	-3.44820400	1.07289900
C	-0.29231200	-2.55048800	-0.83617700
C	-0.28263200	-3.44194600	0.24217300
H	0.86017100	-4.11952000	1.93716700
H	-1.18338100	-2.49753700	-1.47063900
N	4.29372900	0.97124400	-0.41457200
H	4.65241000	1.61325800	0.28159600
N	2.44821000	0.73595100	1.00250900
H	1.52476900	0.28098600	1.13845100
C	2.34974000	2.17478700	1.24751400

H	3.36334700	2.61069100	1.23285600
C	1.50273400	2.85326700	0.17080800
H	1.95368000	2.69128100	-0.82034900
H	0.49712100	2.40609100	0.19068900
H	1.41752800	3.93694200	0.34630200
C	1.77525800	2.39897100	2.64300800
H	1.68426900	3.47557500	2.85108600
H	0.78284700	1.92792700	2.68797500
H	2.42532400	1.94149600	3.40330000
C	5.30056200	0.40535200	-1.29388600
H	4.74708200	-0.14392300	-2.06816700
C	6.08755200	1.54229700	-1.93523800
H	6.83304000	1.15272600	-2.64350900
H	5.41350400	2.22654800	-2.46853300
H	6.62810700	2.12177900	-1.16778700
C	6.21272900	-0.58678200	-0.57286700
H	5.60214300	-1.38852000	-0.13727000
H	6.94099500	-1.03392600	-1.26688500
H	6.77137900	-0.08094100	0.23225600
C	-1.48014400	-4.31797500	0.50539600
H	-2.39972400	-3.71141600	0.53087300
H	-1.60905800	-5.07056500	-0.28868700
H	-1.38269400	-4.84907200	1.46284600
C	3.13336500	-2.61461500	1.75185900
H	3.01427500	-3.34780100	2.56155100
H	4.04755300	-2.85663300	1.18703800
H	3.28510800	-1.61923400	2.19885000
C	0.72764000	-0.67948100	-2.19885800
H	0.72855900	0.34175200	-1.78010600
H	1.61662800	-0.75782600	-2.84276700
H	-0.17951600	-0.80206600	-2.80773000
C	-1.41239600	-0.25599400	1.53310100
H	-1.32146100	-1.35824900	1.52198400
C	-1.80903800	0.29145700	0.22458800
H	-1.30573400	-0.17303200	-0.61991500
O	-0.25049500	0.45382200	1.42330300
C	-2.13898200	1.72742500	0.06541500
C	-2.32810900	2.56276300	1.17356400
C	-2.21051300	2.28470700	-1.21656500
C	-2.58240800	3.91965000	1.00021900
H	-2.23316500	2.14459600	2.17585000
C	-2.46737000	3.64233200	-1.39110700
H	-2.07168500	1.63108100	-2.08091800
C	-2.65383100	4.46696300	-0.28209100

H	-2.71625500	4.55987500	1.87454400
H	-2.51957800	4.05904900	-2.39884100
H	-2.84976400	5.53269500	-0.41542700
H	-2.09154500	0.03508500	2.36400700
I	-4.03656300	-0.88952200	-0.47138000

G3-IM2

C	-2.95088800	-0.01320300	0.05381800
N	-2.64182800	-1.25574100	0.24033600
C	-1.33712400	-1.70041700	0.43101400
C	-0.62520100	-2.32929600	-0.61309500
C	-0.75691300	-1.63781100	1.71783100
C	0.59637400	-2.94753900	-0.33319300
C	0.47305200	-2.25538000	1.95327100
C	1.16031100	-2.93951000	0.94529900
H	1.13911200	-3.43124700	-1.15151400
H	0.90821800	-2.20029300	2.95693600
N	-4.30013300	0.32741500	0.12125000
H	-4.56905500	1.13421700	-0.42808800
N	-2.06596300	0.99915600	-0.14251900
H	-1.15204300	0.73900000	-0.66171400
C	-2.49447300	2.32398100	-0.57453600
H	-3.36909000	2.62508300	0.02971100
C	-1.37040300	3.31926400	-0.30826400
H	-1.10023000	3.32823100	0.75731600
H	-0.49142400	3.00071500	-0.88687000
H	-1.66856900	4.33430900	-0.61369200
C	-2.84794300	2.32179300	-2.06850900
H	-3.14825400	3.32333600	-2.41553400
H	-1.94915200	1.98684900	-2.60965000
H	-3.66423300	1.61609600	-2.29441400
C	-5.31565000	-0.70351400	0.21427900
H	-4.92961500	-1.43987800	0.93244200
C	-6.60200100	-0.08596400	0.75219000
H	-7.38308100	-0.85011800	0.87793700
H	-6.42142600	0.40169600	1.72019600
H	-6.98955200	0.67428000	0.05297800
C	-5.53958500	-1.41869100	-1.11837400
H	-4.58808700	-1.84613500	-1.46118600
H	-6.27838300	-2.22905800	-1.01834200
H	-5.90895400	-0.70903300	-1.87765300
C	2.46277200	-3.64129000	1.23478300
H	3.11452600	-3.02123300	1.86761600
H	2.29524500	-4.59771600	1.75799300

H	3.00940100	-3.85252800	0.30544200
C	-1.17406000	-2.25966200	-2.00949300
H	-0.59140200	-2.88856900	-2.69744500
H	-2.22861300	-2.57440700	-2.03169700
H	-1.11996900	-1.20745500	-2.34534600
C	-1.49292600	-0.89653800	2.79966400
H	-1.62589000	0.16026500	2.51433600
H	-2.50338500	-1.31380000	2.93361900
H	-0.95180100	-0.94184600	3.75581400
C	1.14869800	0.37445200	-1.88896800
H	1.27335100	-0.65029600	-2.33080100
C	1.73825500	0.28284900	-0.46918500
H	1.24212100	-0.51791200	0.08874000
O	-0.12029900	0.80666400	-1.81458100
C	1.72553500	1.54972700	0.32878400
C	2.19412200	2.75935600	-0.19862900
C	1.20641500	1.53939200	1.62697400
C	2.14165200	3.92814000	0.55437500
H	2.59821300	2.77354600	-1.21321200
C	1.15866600	2.70855400	2.38675700
H	0.82965000	0.59680700	2.03100200
C	1.62585200	3.90743200	1.85269000
H	2.50466600	4.86536000	0.12712300
H	0.74468700	2.68064300	3.39683700
H	1.58580300	4.82590700	2.44197300
H	1.82735000	1.02737700	-2.49940400
I	3.82699100	-0.48845400	-0.57821100

G3-TS2

C	2.80215500	0.23427500	-0.36038900
N	2.68834800	-1.06728100	-0.29992500
C	1.51237200	-1.77868500	-0.39766200
C	0.58815500	-1.65016000	-1.46504000
C	1.30455800	-2.82453100	0.54402100
C	-0.51899800	-2.50641700	-1.52443300
C	0.19251500	-3.65243300	0.44217000
C	-0.75061500	-3.50676600	-0.58252100
H	-1.22784900	-2.38500600	-2.35105000
H	0.05198400	-4.43804100	1.19206000
N	4.10828200	0.71600100	-0.49520900
H	4.24903100	1.63031400	-0.08415700
N	1.80136800	1.12802000	-0.27931000
C	2.06912200	2.55324400	-0.34775400
H	2.90983700	2.83253900	0.32593900

C	2.42151500	2.99922100	-1.77221000
H	2.67027100	4.07251100	-1.80224200
H	3.27061500	2.42594300	-2.16817500
H	1.55348700	2.82717600	-2.42775200
C	0.86145700	3.33505300	0.15986300
H	0.59462900	3.01641300	1.17501300
H	1.07668000	4.41499600	0.14840200
H	-0.01122100	3.14710100	-0.48446400
C	5.24613700	-0.18118000	-0.38212800
H	5.03158800	-0.93575800	0.39403500
C	5.48648300	-0.92137900	-1.69523600
H	6.32566100	-1.62843400	-1.59957900
H	4.58183400	-1.48125000	-1.96360700
H	5.71694300	-0.20196100	-2.49706700
C	6.46965500	0.63223800	0.02517400
H	6.31245800	1.12467900	0.99713500
H	7.35552800	-0.01361100	0.10712800
H	6.68079600	1.40907900	-0.72767400
H	0.82612400	0.81259000	0.43615500
C	-1.93284000	0.27099400	-0.01120500
H	-1.43259900	-0.05426300	-0.93109600
C	-1.10035600	-0.13787900	1.21266600
H	-1.75011400	-0.08305800	2.11334200
H	-0.84584000	-1.21003200	1.08569300
O	-0.02015200	0.69346200	1.33393100
C	-2.30466400	1.71824300	-0.10501100
C	-2.50197200	2.30617400	-1.35951300
C	-2.40737700	2.51962500	1.03732500
C	-2.79142500	3.66373800	-1.47687000
H	-2.41427900	1.68383600	-2.25400400
C	-2.69574600	3.87684900	0.92259900
H	-2.21161900	2.07942700	2.01541900
C	-2.88735900	4.45528200	-0.33289600
H	-2.93053200	4.10741900	-2.46468000
H	-2.75205600	4.49432400	1.82124200
H	-3.10103700	5.52237000	-0.41911500
I	-3.77564000	-0.95991700	-0.06126300
C	1.51875600	0.49724100	3.09771100
O	0.99752600	-0.38525900	3.64424400
O	2.18689800	1.37215600	2.72708500
C	-1.95663100	-4.40692500	-0.66094100
H	-1.66526200	-5.46627500	-0.75022100
H	-2.58524900	-4.31081500	0.23847300
H	-2.58325800	-4.14972300	-1.52665500

C	2.31659800	-3.01494700	1.63816300
H	3.32404200	-3.12521500	1.20965800
H	2.35002400	-2.13472300	2.29617000
H	2.07634700	-3.89658600	2.24956300
C	0.81047100	-0.64191000	-2.55886500
H	0.53774100	0.37427400	-2.23169400
H	1.87955900	-0.59193600	-2.82177300
H	0.23265800	-0.90654800	-3.45658300

G3-IM3

C	2.83958900	-0.35738100	-0.16435000
N	2.34598500	-1.03537500	-1.15087900
C	1.07801600	-1.62102600	-1.10217100
C	0.18384900	-1.31852200	-2.15824700
C	0.68104000	-2.55815000	-0.12002600
C	-1.11076300	-1.83773900	-2.14215500
C	-0.62655800	-3.05269700	-0.14171900
C	-1.55109900	-2.67848200	-1.11660900
H	-1.80219700	-1.55786500	-2.94234300
H	-0.93704500	-3.71392600	0.67082100
N	4.15867300	0.07919600	-0.27374100
H	4.35079500	0.94500900	0.21623300
N	2.18720600	0.00348700	0.97196100
C	2.76705000	0.55799800	2.18916000
H	3.73734300	1.01680000	1.94516900
C	1.84986800	1.65035400	2.73823900
H	2.27157000	2.07804700	3.66092500
H	1.71277700	2.45344500	1.99930300
H	0.86827700	1.20658900	2.95925400
C	3.01083000	-0.53970000	3.22569700
H	3.66540500	-1.31892000	2.80826800
H	3.48333900	-0.12583900	4.13036400
H	2.04224400	-0.98802800	3.49194100
C	4.85336900	-0.03561000	-1.54448100
H	4.62196500	-1.04015700	-1.92308600
C	4.35620400	0.98359500	-2.56983900
H	4.85126500	0.84611300	-3.54348000
H	3.27336200	0.86144700	-2.70639100
H	4.56417000	2.01018400	-2.22330900
C	6.35230700	0.08999700	-1.29808600
H	6.69114600	-0.66647100	-0.57711500
H	6.91461600	-0.03250500	-2.23513400
H	6.59727200	1.08554800	-0.89067500
H	1.24593100	-0.37931500	1.13247500

C	-2.98042100	-3.14326200	-1.02049800
H	-3.04134000	-4.23754400	-0.91681100
H	-3.45059500	-2.69937900	-0.12865000
H	-3.56273200	-2.84043700	-1.90235700
C	1.62361100	-3.04120300	0.95016500
H	2.67202600	-2.87385900	0.66438500
H	1.41253400	-2.52501200	1.89885300
H	1.46820300	-4.11480100	1.12641700
C	0.64855100	-0.44585700	-3.29406400
H	0.81137700	0.59882000	-2.98113000
H	1.61420700	-0.80677600	-3.67917900
H	-0.08981000	-0.43899000	-4.10769900
C	-1.05461200	-1.56314300	2.51376100
O	-1.05764700	-2.72632100	2.87342500
O	-0.11145100	-0.74689300	2.37159400
I	-3.51149100	0.73883000	-0.94197400
C	-2.36053800	0.32333800	1.90190600
C	-1.82335600	0.63007200	0.49476200
O	-2.33614600	-1.03819500	2.19312400
H	-1.73016400	0.88128700	2.61278300
H	-3.40122600	0.66138000	2.00998200
C	-1.02142400	1.88711000	0.35706800
C	-1.37261100	3.06055300	1.03657700
C	0.11734600	1.89682600	-0.45485000
C	-0.60532500	4.21482400	0.90317200
H	-2.26336600	3.07043900	1.66911900
C	0.88224800	3.05267300	-0.59693200
H	0.40905000	0.97783100	-0.96508100
C	0.52372900	4.21687500	0.08132700
H	-0.89067200	5.12018800	1.44242000
H	1.77118700	3.03241400	-1.23159100
H	1.12345300	5.12315800	-0.02287100
H	-1.26183700	-0.23542400	0.11943000

G3-TS3

C	2.90010600	-0.27104600	-0.30207800
N	2.35921900	-0.93380300	-1.27425100
C	1.13979600	-1.60279400	-1.13354400
C	0.14088300	-1.33798200	-2.10387900
C	0.87717500	-2.57078700	-0.13609900
C	-1.11344000	-1.93721500	-1.99503400
C	-0.40384300	-3.12650800	-0.04767600
C	-1.42353200	-2.80679100	-0.94417800
H	-1.88885200	-1.67337500	-2.71853800

H	-0.60918800	-3.81207300	0.78027800
N	4.17178900	0.26422600	-0.49488000
H	4.32533100	1.13512500	0.00289300
N	2.33889900	-0.02896400	0.90903700
C	2.97008500	0.50246000	2.10848400
H	4.03072300	0.68738200	1.88060300
C	2.30214900	1.81487800	2.51937000
H	2.73701500	2.20236600	3.45338000
H	2.41116400	2.57562200	1.73311300
H	1.22527800	1.63907200	2.67001500
C	2.91588200	-0.52951900	3.23671300
H	3.48635300	-1.42772300	2.96108900
H	3.34436700	-0.11161100	4.16064300
H	1.87497700	-0.83343700	3.42877600
C	4.77152000	0.23681500	-1.81893100
H	4.57874200	-0.76979400	-2.21324900
C	4.12708300	1.24829700	-2.76662700
H	4.55684300	1.17752700	-3.77747400
H	3.04860900	1.05176800	-2.82920100
H	4.28750900	2.27598900	-2.39925300
C	6.27355900	0.45876000	-1.68292600
H	6.71742600	-0.29356900	-1.01672400
H	6.76805300	0.40332200	-2.66343400
H	6.48233100	1.45621400	-1.26078300
H	1.37243400	-0.33518700	1.06275300
C	-2.81339400	-3.36180200	-0.76757900
H	-2.89508600	-4.39092900	-1.15437400
H	-3.07835500	-3.38164100	0.29988200
H	-3.54981300	-2.73548500	-1.29056500
C	1.92932400	-3.02763400	0.83997800
H	2.93804000	-2.75142900	0.50490700
H	1.74301300	-2.60035200	1.83652400
H	1.88195900	-4.12134500	0.94732600
C	0.44450600	-0.39685900	-3.23850500
H	0.61413400	0.63269900	-2.88450000
H	1.36783400	-0.70266200	-3.75344800
H	-0.38688200	-0.37050400	-3.95525000
C	-0.75295100	-1.40258600	2.56317700
O	-0.21206400	-2.29101000	3.18568500
O	-0.23584900	-0.36525200	2.02417700
I	-3.60643300	0.79858400	-1.10685500
C	-2.64475900	-0.27805800	1.82253100
C	-1.72374500	0.25812400	0.73777100
O	-2.11675300	-1.46247300	2.37483300

H	-2.77275900	0.48437300	2.60894300
H	-3.62460000	-0.53528700	1.41542200
C	-1.13481900	1.61535100	0.68335100
C	-1.53870700	2.66190200	1.51818700
C	-0.08540200	1.83582700	-0.21830200
C	-0.91407400	3.90510200	1.44126300
H	-2.36158500	2.51637700	2.21890800
C	0.53013100	3.07905600	-0.30252100
H	0.24182600	1.01125100	-0.85425200
C	0.11729200	4.12251600	0.52776700
H	-1.24406000	4.71446800	2.09518400
H	1.34409500	3.22829100	-1.01545800
H	0.59882200	5.10023300	0.46588200
H	-1.34173900	-0.46804200	0.02210000

G3-IM4

C	3.09202000	-0.40289800	-0.26113400
N	2.60526600	-1.57174100	-0.49233400
C	1.35457900	-1.95195300	0.01478800
C	0.28700800	-2.12676200	-0.89333700
C	1.15101600	-2.22507100	1.38422300
C	-0.95587800	-2.55647000	-0.42846300
C	-0.11619600	-2.63549800	1.81396500
C	-1.18551900	-2.79898500	0.92999800
H	-1.78824800	-2.63338400	-1.13182800
H	-0.27152300	-2.81096300	2.88330000
N	4.36214700	-0.09335800	-0.73330600
H	4.51519100	0.88815500	-0.93448300
N	2.47092500	0.59058800	0.44366700
C	3.02939900	1.89543500	0.75281300
H	4.12163700	1.77154200	0.84541300
C	2.72413000	2.91364300	-0.35034300
H	3.18277700	3.88978100	-0.13012100
H	3.09322300	2.56783700	-1.32859300
H	1.63452600	3.04976200	-0.43791900
C	2.50688700	2.38074900	2.10150500
H	2.67539100	1.62856500	2.88500100
H	3.00981200	3.31623000	2.38591300
H	1.42648800	2.56900600	2.04357600
C	5.02122100	-0.99714000	-1.66361200
H	4.85297000	-2.00716200	-1.26617800
C	4.41232800	-0.92906600	-3.06296700
H	4.88727200	-1.65669600	-3.73833500
H	3.33907400	-1.15284500	-3.00629200

H	4.54809500	0.07679900	-3.49467400
C	6.51377700	-0.68927900	-1.67284700
H	6.93369800	-0.76832600	-0.66063800
H	7.05099700	-1.38226400	-2.33600600
H	6.69731000	0.33368500	-2.04273300
H	1.56192500	0.36877100	0.84351500
C	-2.55439900	-3.20650900	1.41241900
H	-2.65578800	-4.30330400	1.45547200
H	-2.74405800	-2.81206200	2.42190500
H	-3.32669500	-2.81940900	0.72961500
C	2.27673600	-2.05069000	2.36788900
H	3.21749800	-2.43937000	1.95026900
H	2.43430700	-0.98605500	2.60329700
H	2.05391400	-2.56321200	3.31275200
C	0.48948300	-1.79867100	-2.34746900
H	0.87511000	-0.77332500	-2.46494100
H	1.23560700	-2.47030000	-2.80186400
H	-0.45837200	-1.87575000	-2.89617800
C	-0.57416700	0.05881500	3.04841400
O	0.11561600	-0.18245100	3.98831700
O	-0.12810700	0.62185700	1.90895800
I	-3.89361600	-0.42797800	-1.56949300
C	-2.42017400	0.34199300	1.73802100
C	-1.16491700	0.67698400	0.91112200
O	-1.88787200	-0.15351300	2.97133700
H	-3.03489800	1.22955100	1.94662700
H	-3.03018200	-0.42405500	1.24608900
C	-1.12447700	2.02855300	0.24812300
C	-1.01566900	3.18921900	1.02080100
C	-1.16417700	2.12800300	-1.14393300
C	-0.93351200	4.43878700	0.41037400
H	-0.98133000	3.11018100	2.11072400
C	-1.08646100	3.38025400	-1.75425200
H	-1.29488900	1.21914400	-1.73613900
C	-0.96520100	4.53458500	-0.98168400
H	-0.84403000	5.33899800	1.02122200
H	-1.12657700	3.44965900	-2.84234500
H	-0.90016400	5.51215800	-1.46341600
H	-0.98092000	-0.11225200	0.16957600

G4-COM

C	-3.74844800	-1.10999500	0.12239900
N	-2.88188400	-1.89488800	-0.43196500
C	-1.51575500	-1.64482300	-0.37920400

C	-0.74898800	-1.82360000	-1.54696700
C	-0.82343900	-1.26349400	0.78640900
C	0.61600300	-1.55911900	-1.57287800
H	-1.26895100	-2.15531300	-2.44742200
C	0.54471100	-1.01002600	0.76309600
H	-1.37354700	-1.15219600	1.72212000
C	1.29356500	-1.12935700	-0.41988300
H	1.18506000	-1.66657300	-2.49810600
H	1.05115200	-0.68696000	1.67679200
N	-5.07076500	-1.49452500	0.13896900
H	-5.75966800	-0.75810800	0.22314200
N	-3.46759100	0.08514100	0.73218000
H	-2.52753000	0.45312400	0.59566200
C	-4.44184100	1.05208800	1.20684800
H	-5.26661000	0.49123000	1.67660300
C	-3.79575400	1.91226200	2.28825400
H	-4.51242500	2.64950800	2.67627500
H	-3.44798800	1.28584700	3.12091100
H	-2.93009100	2.44753500	1.87108200
C	-4.99070900	1.91409200	0.06632100
H	-5.42966600	1.29331100	-0.72952000
H	-5.75848700	2.61496100	0.42573000
H	-4.16731700	2.49521100	-0.37700100
C	-5.51627700	-2.68065000	-0.57873800
H	-4.74771500	-3.44437200	-0.39953800
C	-6.84562600	-3.13868400	0.00737000
H	-7.19169300	-4.05665200	-0.48737800
H	-6.75175700	-3.33188700	1.08464200
H	-7.62262600	-2.36994400	-0.13957500
C	-5.60404400	-2.43497200	-2.08385600
H	-4.62478300	-2.11250200	-2.46145900
H	-5.90114700	-3.35063200	-2.61601900
H	-6.35120200	-1.65477400	-2.30399100
C	0.12236100	2.26530000	-0.14513500
H	0.84560200	1.51727500	0.19837700
C	-0.83320000	1.83742500	-1.18331200
H	-1.23293500	2.59835800	-1.86282600
H	-0.79531300	0.80658600	-1.55096300
O	-1.22682500	1.97901000	0.16917300
C	0.54362000	3.69004300	-0.02418900
C	1.90171300	4.01777100	-0.06393600
C	-0.40592400	4.70716000	0.11023300
C	2.30516800	5.34912000	0.01584700
H	2.64235900	3.22035600	-0.15987400

C	-0.00070100	6.03733300	0.19376700
H	-1.46357300	4.44111900	0.16097100
C	1.35496700	6.36217900	0.14386100
H	3.36733300	5.59699100	-0.01812100
H	-0.74733900	6.82557100	0.30354500
H	1.67153000	7.40419300	0.21025800
C	3.53090600	-1.38252300	0.20569600
N	2.64222700	-0.75660900	-0.48359000
N	4.85326200	-1.01827200	0.10648600
H	5.42735300	-1.23587500	0.91072600
N	3.27941000	-2.43502300	1.06849800
H	2.30895000	-2.73650500	1.02782200
C	4.22155300	-3.53352000	1.27281400
H	5.15854200	-3.11676400	1.67846700
C	3.64091800	-4.46192200	2.33179200
H	4.33842200	-5.28004800	2.55585100
H	3.42822400	-3.91102000	3.25790700
H	2.70091800	-4.90947800	1.97139600
C	4.53804700	-4.27614400	-0.02466200
H	4.95155700	-3.58296300	-0.77033000
H	5.26744600	-5.08079900	0.14855900
H	3.61898600	-4.72251300	-0.43476900
C	5.25239300	0.14196500	-0.68223100
H	4.49514900	0.93096100	-0.53881500
C	6.60192200	0.63453800	-0.17660400
H	6.92865100	1.51126100	-0.75162500
H	6.55175600	0.92203300	0.88441100
H	7.36654400	-0.14999900	-0.29210000
C	5.29819000	-0.20534800	-2.16686000
H	4.31734200	-0.57396500	-2.49229900
H	5.55422500	0.68227000	-2.76385400
H	6.05527800	-0.98329100	-2.35061000

G4-IM1

C	-3.52450600	-1.93020800	-0.01872600
N	-2.61149100	-2.68131000	0.48781600
N	-4.84409000	-2.09209200	0.39708000
H	-5.37051600	-1.22708100	0.42049400
N	-3.32614900	-1.00158000	-1.00683700
H	-2.35565400	-0.76755900	-1.21835900
C	-4.32870700	-0.09378600	-1.53219700
H	-5.29927900	-0.61064500	-1.46647700
C	-4.38880100	1.21105200	-0.73326100
H	-5.17383000	1.88162100	-1.11486300

H	-4.58214000	1.01604500	0.33279400
H	-3.42381600	1.73525000	-0.80564300
C	-4.05405600	0.17001600	-3.01058000
H	-4.06660800	-0.77240200	-3.57519400
H	-4.81189500	0.84873800	-3.42887900
H	-3.06330600	0.63147900	-3.12384400
C	-5.12635200	-2.98826800	1.51279300
H	-4.32151400	-2.88882000	2.26114800
C	-6.45641600	-2.58296200	2.13462900
H	-6.70606200	-3.24393100	2.97606300
H	-6.42148900	-1.55009500	2.51413000
H	-7.26608000	-2.65487600	1.39066500
C	-5.15035600	-4.43801300	1.03956900
H	-4.18071400	-4.68965600	0.59270900
H	-5.33837900	-5.11787600	1.88446300
H	-5.94285800	-4.57671100	0.28762100
C	-1.27808300	-2.48219700	0.10124100
C	-0.60625300	-3.41340200	-0.70521800
C	-0.55782800	-1.35786700	0.53240200
C	0.71878800	-3.21592700	-1.08015100
H	-1.15269800	-4.29716400	-1.04129500
C	0.76530400	-1.15885400	0.15353400
H	-1.03019900	-0.61889400	1.18682800
C	1.44099000	-2.08525700	-0.66105600
H	1.22829000	-3.93520600	-1.72437800
H	1.25348200	-0.24255400	0.49929100
C	-0.45896200	1.73594600	-1.10352500
H	-0.25072000	1.41502400	-0.07458400
C	0.28971000	1.08749100	-2.19540900
H	0.45650200	1.66197300	-3.11449700
H	1.01849600	0.30321300	-1.96532700
O	-1.06047800	0.76054500	-1.94344400
C	-0.97710200	3.12747500	-1.24580500
C	-0.78200700	4.04360600	-0.20719500
C	-1.66329900	3.52305200	-2.39979200
C	-1.26102400	5.34746700	-0.33512100
H	-0.26022600	3.71827200	0.69953800
C	-2.14250400	4.82539400	-2.52041500
H	-1.83140300	2.79136200	-3.19367200
C	-1.94018300	5.74227400	-1.48774000
H	-1.10773600	6.05767700	0.47943700
H	-2.68260700	5.12462700	-3.42103400
H	-2.31878900	6.76222400	-1.57997000
C	3.70765900	-1.43520100	-0.43244500

N	2.74165000	-1.91209600	-1.14547000
N	4.92268700	-1.20100500	-1.05296100
H	5.73027900	-1.15035500	-0.44470200
N	3.68279400	-1.16425300	0.91046300
H	2.76399200	-1.20025800	1.34028500
C	4.67226600	-0.37647100	1.63880500
H	5.66481100	-0.84169900	1.47951200
C	4.71929100	1.08324600	1.18405600
H	5.51154100	1.62536800	1.72324200
H	4.91870400	1.14994400	0.10535800
H	3.75256100	1.56437800	1.40314600
C	4.35382000	-0.48087500	3.12581600
H	4.33684700	-1.53258100	3.44670200
H	5.10839100	0.05919000	3.71457900
H	3.37138300	-0.02150600	3.32439500
C	5.17466300	-1.67004000	-2.40277000
H	4.27000800	-1.42839200	-2.97753700
C	6.36449700	-0.90845900	-2.97385400
H	6.55849000	-1.21058000	-4.01296400
H	6.18285200	0.17484300	-2.94810400
H	7.27734300	-1.11870600	-2.39109300
C	5.38008700	-3.18350500	-2.46140100
H	4.49758400	-3.68433600	-2.04241700
H	5.52032700	-3.52412300	-3.49868900
H	6.27064700	-3.47463400	-1.88010100
I	0.95185200	1.76541600	2.65851000

G4-TS1

C	-1.82084500	2.19041100	0.10098400
N	-1.00275300	1.80870800	-0.82914300
C	0.21016500	1.18625500	-0.53980900
C	1.11872600	1.66674500	0.42354300
C	0.60212000	0.06139300	-1.28797500
C	2.35428800	1.05641500	0.61363200
H	0.83557500	2.52485100	1.03496400
C	1.83042000	-0.56029300	-1.08419600
H	-0.09426800	-0.34246900	-2.02635000
C	2.73894700	-0.06261900	-0.14213000
H	3.04174300	1.43458700	1.37499700
H	2.09576300	-1.45044000	-1.65649300
N	-2.87560700	3.01839300	-0.24622400
H	-3.70890900	2.86673900	0.31019800
N	-1.73570100	1.85573900	1.41878700
H	-1.33438900	0.92473900	1.62486500

C	-2.66388100	2.29783200	2.44841100
H	-2.89923800	3.35591600	2.24157000
C	-3.95232600	1.46870600	2.48988700
H	-4.65826800	1.87798500	3.22992900
H	-4.45911500	1.41996700	1.51151100
H	-3.67775800	0.43873600	2.75785500
C	-1.94229600	2.20163400	3.79066200
H	-1.04239200	2.83321700	3.79500400
H	-2.60255700	2.51207600	4.61411300
H	-1.64327500	1.15306700	3.94487200
C	-3.13743900	3.32826100	-1.64425900
H	-3.01262600	2.40782300	-2.24357700
C	-4.57453400	3.82147300	-1.76179300
H	-4.82269100	4.04192800	-2.80950100
H	-5.28421000	3.06586700	-1.39095100
H	-4.71100600	4.74335500	-1.17410300
C	-2.15073600	4.36692500	-2.16891100
H	-1.12827200	3.98364000	-2.06790600
H	-2.34704100	4.58274300	-3.23029500
H	-2.24678800	5.30059600	-1.59292500
C	-1.94031900	-1.52675800	0.59466800
H	-1.18505700	-0.96161500	0.05150400
C	-1.50588500	-1.99688100	1.91668100
H	-2.15395800	-2.77771000	2.36649600
H	-0.46240600	-2.36726600	1.91094800
O	-1.70470200	-0.71515300	2.35452500
C	-3.34557500	-1.16816700	0.29886400
C	-3.61984700	-0.33772900	-0.79581200
C	-4.41145200	-1.61436200	1.08931200
C	-4.92724700	0.04293100	-1.09016200
H	-2.78817500	0.00827100	-1.41431900
C	-5.71702200	-1.22903900	0.79967700
H	-4.20483000	-2.25106100	1.95082300
C	-5.98299800	-0.39717900	-0.29015700
H	-5.12190800	0.67974300	-1.95655100
H	-6.53641600	-1.57816900	1.43131700
H	-7.00886600	-0.10039700	-0.51799300
I	-1.59494200	-3.53594700	-1.10440100
C	5.04955800	-0.06582600	-0.32278000
N	3.99194100	-0.67785100	0.05279100
N	6.30429000	-0.56210700	-0.00186400
H	6.98412000	-0.42324000	-0.74174800
N	5.08771400	1.09704700	-1.08787200
H	4.14547000	1.44049300	-1.26471100

C	6.02643800	2.17015500	-0.76790500
H	7.04710200	1.76225600	-0.84461400
C	5.87445200	3.26631300	-1.81494700
H	6.59862100	4.07497800	-1.64359600
H	6.02298400	2.85968000	-2.82459800
H	4.86316900	3.70061400	-1.76456100
C	5.83240100	2.70879400	0.64891200
H	5.93330200	1.89465200	1.38178400
H	6.57700500	3.48430900	0.88413400
H	4.82784500	3.14772700	0.75149600
C	6.41067400	-1.83442400	0.70496000
H	5.66242500	-2.53345400	0.29362900
C	7.81002200	-2.39334000	0.48428100
H	7.92889700	-3.35129100	1.00854900
H	8.00765700	-2.56572500	-0.58497600
H	8.56757600	-1.69328900	0.87145300
C	6.11181200	-1.64477300	2.18831400
H	5.10227400	-1.23377900	2.31440100
H	6.16387500	-2.60744900	2.71814300
H	6.84362300	-0.95342000	2.63521600

G4-IM2

C	-1.93875800	1.99680000	-0.18161800
N	-1.14256800	1.47272200	-1.11369500
C	0.11170700	0.97713400	-0.84638000
C	0.89731900	1.19067600	0.31659700
C	0.70911200	0.16946200	-1.84881900
C	2.18368400	0.66620500	0.42726000
H	0.47419200	1.76343000	1.13804700
C	1.98581300	-0.36101800	-1.72498800
H	0.11397400	-0.02782700	-2.74314700
C	2.76490000	-0.10706900	-0.58793800
H	2.75336700	0.83583700	1.34592300
H	2.40677400	-0.98539600	-2.51591100
N	-3.02692200	2.72530100	-0.69580100
H	-3.85711700	2.66736000	-0.11887300
N	-1.81210500	1.87228400	1.12609700
H	-1.42216500	0.46051800	1.90022100
C	-2.70740800	2.56308100	2.02931200
H	-3.03481600	3.52860600	1.59274300
C	-3.95220700	1.72696400	2.36203800
H	-4.62563700	2.25842000	3.05475000
H	-4.52345900	1.46141000	1.45754200
H	-3.62702900	0.78265600	2.82401300

C	-1.93847900	2.87165100	3.31580500
H	-1.06779600	3.50524900	3.09198500
H	-2.57262800	3.38446300	4.05684400
H	-1.57241700	1.92889500	3.75175100
C	-3.29320400	2.81339300	-2.11927600
H	-3.15342400	1.82233300	-2.58920300
C	-4.73803600	3.26283200	-2.30904800
H	-4.98813000	3.33583300	-3.37721600
H	-5.43816100	2.55532700	-1.83819800
H	-4.89134900	4.25280300	-1.84964200
C	-2.32703200	3.77980300	-2.79923800
H	-1.30106400	3.42409700	-2.64527200
H	-2.53039300	3.83939400	-3.88035800
H	-2.43311300	4.78452500	-2.35995200
C	-1.84186900	-1.46022100	0.34896200
H	-1.40091800	-0.73114700	-0.33794200
C	-1.08896600	-1.47651800	1.68330800
H	-1.34016500	-2.39804900	2.23840200
H	-0.00926200	-1.53096600	1.43928500
O	-1.41723100	-0.38315500	2.46671400
C	-3.32231800	-1.24668700	0.40315400
C	-3.93909500	-0.54564700	-0.64096500
C	-4.10629600	-1.71961700	1.46001600
C	-5.31736300	-0.34090900	-0.63877300
H	-3.30828500	-0.15098000	-1.44305100
C	-5.48223200	-1.50279900	1.46959700
H	-3.62645600	-2.23941200	2.29126100
C	-6.09360900	-0.81870600	0.41780700
H	-5.78767200	0.19529700	-1.46592200
H	-6.08261500	-1.86433100	2.30674400
H	-7.17267200	-0.65264800	0.42574100
I	-1.40706500	-3.35653100	-0.69072400
C	5.06598600	0.15167400	-0.39727200
N	4.06832700	-0.64290600	-0.47092900
N	6.34002200	-0.33572800	-0.12394200
H	7.06076500	0.15595200	-0.64198500
N	5.03374500	1.52810900	-0.61180700
H	4.07516900	1.83872000	-0.76308900
C	5.78958000	2.43894500	0.24414600
H	6.85421600	2.16216300	0.17825900
C	5.63296400	3.85187500	-0.30428500
H	6.21832100	4.56958400	0.28763200
H	5.96041200	3.89862300	-1.35195500
H	4.57591800	4.15940100	-0.26137600

C	5.36541300	2.35108200	1.70941400
H	5.46263800	1.31671100	2.07082100
H	5.98749600	3.00205000	2.34239000
H	4.31459100	2.66042100	1.81883400
C	6.54328400	-1.77573700	-0.01899800
H	5.95494300	-2.27955800	-0.80577400
C	8.02447400	-2.06882500	-0.22033800
H	8.21876500	-3.14727300	-0.14067600
H	8.36835800	-1.73424600	-1.21164400
H	8.62314400	-1.55385300	0.54781500
C	6.05284300	-2.28657600	1.33185700
H	4.98664900	-2.05618800	1.44892600
H	6.18527700	-3.37660400	1.40334000
H	6.61932400	-1.80618100	2.14508400

G4-TS2

C	-3.07087800	-1.91721800	0.25269900
N	-2.14383600	-2.47772900	-0.47403500
C	-0.83271900	-2.03053300	-0.52300100
C	-0.12073100	-1.46553600	0.55757600
C	-0.11077400	-2.23698100	-1.71492500
C	1.22789700	-1.13787200	0.44085300
H	-0.64945000	-1.26596300	1.48925400
C	1.23401300	-1.90316600	-1.83148200
H	-0.65249800	-2.66262000	-2.56066000
C	1.93798100	-1.35926800	-0.75025500
H	1.75318400	-0.67518500	1.28156100
H	1.76619900	-2.06332700	-2.77105700
N	-4.27089700	-2.61119100	0.37763800
H	-5.06519100	-1.98634700	0.45963000
N	-2.97600400	-0.70002000	0.84091200
C	-4.06747500	-0.12583200	1.60398500
H	-5.02853100	-0.18490800	1.04463000
C	-4.24801000	-0.82988200	2.95167000
H	-5.08441400	-0.38974500	3.51758400
H	-4.43540200	-1.90342700	2.81540300
H	-3.32627100	-0.71437200	3.54239600
C	-3.78257100	1.35957100	1.80250400
H	-3.64860700	1.84932000	0.82927900
H	-4.59802900	1.84550900	2.35929000
H	-2.84612000	1.48720300	2.36983300
C	-4.52730200	-3.77071400	-0.46525900
H	-4.06886600	-3.59638900	-1.45353600
C	-3.89073400	-5.02247000	0.12998600

H	-4.06035500	-5.89428600	-0.52111600
H	-2.81045100	-4.86128800	0.23266900
H	-4.32138700	-5.22977200	1.12244200
C	-6.03410800	-3.92685100	-0.62703500
H	-6.46795300	-3.03581700	-1.10611700
H	-6.27018900	-4.80112100	-1.25032100
H	-6.51460700	-4.06616100	0.35515600
H	-2.48637500	0.05572400	0.09923100
C	-0.41761100	2.10684100	-0.01025500
H	-0.28877100	1.43425400	0.84894000
C	-0.96781700	1.31792600	-1.20475400
H	-0.92275900	1.98546800	-2.09664000
H	-0.25835800	0.49171400	-1.41741000
O	-2.24046500	0.91877500	-0.91739000
C	-1.19941700	3.32885200	0.38460500
C	-0.94803900	3.97528800	1.60171400
C	-2.22127300	3.82212600	-0.43558800
C	-1.68939500	5.08766300	1.99073900
H	-0.14941900	3.59739100	2.24554100
C	-2.96355900	4.93656100	-0.04731400
H	-2.47549100	3.27929200	-1.34521100
C	-2.70173500	5.57555200	1.16337400
H	-1.47887100	5.57492200	2.94492900
H	-3.76594400	5.29839400	-0.69333100
H	-3.28936600	6.44470400	1.46595100
I	1.68135800	2.68012600	-0.44051300
C	-3.33238300	-0.48493000	-2.49978700
O	-2.44588200	-0.55333100	-3.24508700
O	-4.34088100	-0.52080400	-1.91958800
N	3.30499700	-1.03660400	-0.87064200
N	3.91579200	-2.85567300	0.53701200
H	2.92255500	-3.08041500	0.51403900
N	5.49519300	-1.29665000	-0.16307300
H	6.13941400	-2.08015600	-0.16427000
C	4.49621600	-3.03280800	1.86651200
H	5.59246700	-2.99082400	1.76515600
C	4.11975500	-4.41922600	2.37322800
H	4.56901900	-4.61142800	3.35780200
H	3.02598800	-4.50048000	2.47852800
H	4.45446400	-5.19271200	1.66846000
C	4.06477400	-1.93653200	2.83926900
H	4.32430800	-0.94667800	2.43506400
H	2.97504000	-1.97357800	2.99174000
H	4.55726200	-2.05542700	3.81634800

C	5.91268100	-0.14978400	-0.96226100
H	5.40527900	-0.19478200	-1.94150100
C	5.49851800	1.14839400	-0.27885200
H	5.76870000	2.01594600	-0.89978900
H	4.41085000	1.15728300	-0.12790400
H	6.00149800	1.24062800	0.69687300
C	7.42057400	-0.22296700	-1.16331900
H	7.93787800	-0.20495200	-0.19076700
H	7.71091500	-1.14202900	-1.69623200
H	7.77052500	0.63567000	-1.75279300
C	4.16533100	-1.69420300	-0.19296500

G4-IM3

C	-0.70361400	-1.77589400	-0.55276200
C	0.68516100	-1.84994800	-0.61710500
C	1.41242000	-1.14522400	-1.59246500
C	0.66284200	-0.40365000	-2.52764300
C	-0.72190800	-0.32702000	-2.46022200
C	-1.44789700	-1.00112300	-1.46149700
H	-1.18071500	-2.25201800	0.30271300
H	1.19600800	-2.43163900	0.15219500
H	1.21149900	0.14153800	-3.29855800
H	-1.28024700	0.30000100	-3.15743600
N	2.80163800	-1.14348700	-1.71944400
N	-2.81925300	-0.74370900	-1.37666200
N	3.30174400	-0.95815100	0.59871400
H	2.33762800	-0.70237900	0.84436000
N	4.96132600	-1.39408600	-0.96286200
H	5.58106400	-0.91617500	-0.31681000
N	-3.51704500	-2.86280600	-0.50721500
H	-2.58612300	-3.18803700	-0.74382700
N	-4.94283400	-1.04136400	-0.54766000
H	-5.68572300	-1.73067300	-0.58008300
C	-3.99926300	-3.39963600	0.77220200
H	-5.10342900	-3.38189900	0.74702100
C	-3.52496300	-2.59933600	1.98418000
H	-3.99081000	-2.99755100	2.89966200
H	-2.42956100	-2.63598100	2.10925100
H	-3.80756300	-1.54216400	1.88526400
C	-3.55953100	-4.85566900	0.85810400
H	-3.90561200	-5.42534700	-0.01654000
H	-2.46006100	-4.91194900	0.90409600
H	-3.95435000	-5.32418700	1.77012100
C	-5.31000600	0.32682200	-0.86598300

H	-4.43691300	0.93905100	-0.59651400
C	-5.57899700	0.52395900	-2.35718100
H	-5.80944700	1.57718900	-2.57889500
H	-4.68636400	0.23217700	-2.92566800
H	-6.43528600	-0.09153500	-2.68090100
C	-6.50372200	0.73046200	-0.00851200
H	-7.38475000	0.11094500	-0.24889300
H	-6.27434700	0.60481700	1.05864600
H	-6.77508300	1.78005400	-0.19054400
C	4.04921800	-1.41868200	1.76381000
H	5.05931700	-1.70253900	1.43140900
C	4.15665300	-0.28401100	2.78085600
H	4.66524400	0.58525800	2.33721400
H	3.14290300	0.02202900	3.07659800
H	4.71525800	-0.61035200	3.67162700
C	3.38014800	-2.66093100	2.35631900
H	2.32949400	-2.44250100	2.60628700
H	3.39770600	-3.48259200	1.62391000
H	3.90803500	-2.99421100	3.26369300
C	5.44898700	-1.43811600	-2.33032700
H	4.71422000	-2.03255100	-2.88984600
C	6.80259600	-2.13912100	-2.34797100
H	7.54351200	-1.56766500	-1.76378200
H	6.72306600	-3.14317400	-1.90905200
H	7.18623900	-2.22778800	-3.37472200
C	5.51459300	-0.04952700	-2.96603700
H	4.51803700	0.41003400	-2.92901600
H	6.22946300	0.58985500	-2.42100600
H	5.84005100	-0.10594700	-4.01615300
C	-3.68010500	-1.52329800	-0.83112400
C	3.61011800	-1.17102600	-0.70728100
C	-0.00331600	-0.99006400	2.26800200
O	-0.17472800	-2.19223600	2.45493800
O	1.04931200	-0.32387400	2.18132100
I	-1.62270000	2.89119800	-0.50629900
C	-1.03685300	1.13505800	1.99515600
C	-0.30389100	1.57570100	0.70941400
O	-1.18825700	-0.25313000	2.09254600
H	-0.47085900	1.51667600	2.85976400
H	-2.05334900	1.54563500	2.02427700
C	1.00547700	2.28805700	0.87810200
C	1.19481400	3.26101500	1.86685600
C	2.07426400	1.97632700	0.03179700
C	2.42910700	3.88604000	2.02311400

H	0.36296900	3.53751400	2.51856700
C	3.31093800	2.59821700	0.18840700
H	1.93798700	1.22389400	-0.74807100
C	3.49568300	3.55331100	1.18685700
H	2.56004100	4.63809400	2.80378000
H	4.13590900	2.32118700	-0.47162400
H	4.46571400	4.03816900	1.31401900
H	-0.19104800	0.71620700	0.04036800

G4-TS3

C	-0.44614500	-2.01033700	-0.42798100
C	0.94212500	-2.05627400	-0.50416400
C	1.64147900	-1.37319300	-1.51142800
C	0.87624100	-0.68697400	-2.47283600
C	-0.51023400	-0.63494600	-2.39444200
C	-1.20981900	-1.27737000	-1.35559300
H	-0.92159300	-2.46680900	0.43978800
H	1.49321800	-2.58418300	0.27796400
H	1.40540300	-0.15914400	-3.26880800
H	-1.08845000	-0.03109600	-3.09538900
N	3.03529700	-1.38525900	-1.61047900
N	-2.57209200	-1.00720300	-1.23227100
N	3.37010500	-0.43189600	0.54099700
H	2.35971900	-0.30423300	0.64127200
N	5.14322300	-1.30487000	-0.68567400
H	5.71344000	-0.63169400	-0.18532300
N	-3.27862800	-3.11798100	-0.36673200
H	-2.35612000	-3.45172800	-0.62451400
N	-4.66903000	-1.25914300	-0.33412500
H	-5.42853300	-1.93131600	-0.33864600
C	-3.77569100	-3.70200700	0.88217000
H	-4.87829100	-3.64386000	0.86594600
C	-3.27398900	-2.97995500	2.13095900
H	-3.72996700	-3.42052000	3.03144500
H	-2.17803800	-3.03611900	2.23582900
H	-3.53259400	-1.91353900	2.09279500
C	-3.39222300	-5.17658700	0.88894000
H	-3.76962700	-5.68516900	-0.00961000
H	-2.29532900	-5.27872000	0.91439400
H	-3.79467000	-5.67747700	1.78013500
C	-5.02344900	0.10780200	-0.69140900
H	-4.13188900	0.71998200	-0.49057800
C	-5.34393400	0.25534300	-2.17671200
H	-5.55656300	1.30632600	-2.42189300

H	-4.47646700	-0.06699500	-2.76730500
H	-6.22305800	-0.35302800	-2.45026600
C	-6.17179500	0.56901000	0.19650700
H	-7.07726200	-0.03548800	0.01471700
H	-5.90295900	0.47765300	1.25819500
H	-6.42110900	1.61833200	-0.01439300
C	4.01698800	-0.58441100	1.84343100
H	5.10403800	-0.65311300	1.68203200
C	3.74090100	0.65487700	2.69042600
H	4.11800200	1.55937400	2.19168200
H	2.65669600	0.77022100	2.83289700
H	4.22360500	0.55980200	3.67487700
C	3.55424400	-1.86873300	2.53161100
H	2.46259400	-1.85016400	2.68416100
H	3.80768600	-2.74017300	1.90763800
H	4.04650300	-1.99033800	3.50931000
C	5.72813000	-1.78741800	-1.92472900
H	5.03681400	-2.55464300	-2.29928000
C	7.08164800	-2.41808300	-1.61833900
H	7.78063500	-1.66417900	-1.21864900
H	6.97576100	-3.21576500	-0.87029500
H	7.53270500	-2.83961900	-2.52827700
C	5.83295800	-0.68999400	-2.98328000
H	4.83473600	-0.27474200	-3.17355000
H	6.50073300	0.11646300	-2.63721500
H	6.23714600	-1.08629100	-3.92742000
C	-3.43171300	-1.77096600	-0.66305600
C	3.77854900	-1.05862300	-0.60703700
C	-0.12696000	-0.81312000	2.21790700
O	0.03617600	-1.90760100	2.72414700
O	0.74002600	0.00674000	1.77722400
I	-1.77278100	2.89365800	-1.00618900
C	-1.53161300	0.93630300	1.51864700
C	-0.34923300	1.31338900	0.63288700
O	-1.41568000	-0.36828400	2.04677200
H	-1.64163900	1.66965400	2.33367300
H	-2.44665700	0.93647800	0.92243500
C	0.67234300	2.35367900	0.90006600
C	0.64150800	3.18892900	2.02075500
C	1.75621300	2.44300500	0.01730900
C	1.66958400	4.10086000	2.24736700
H	-0.19063400	3.13143400	2.72322100
C	2.78151100	3.35405500	0.24369600
H	1.78088100	1.78535500	-0.85571300

C	2.74178800	4.19112500	1.35982500
H	1.63186500	4.74830200	3.12557300
H	3.61891200	3.40712400	-0.45438000
H	3.54423900	4.90925600	1.53887300
H	-0.16927400	0.68183800	-0.23544500

G4-IM4

C	0.46901100	-2.29477500	-0.24584100
C	1.81167200	-2.00415200	-0.47637200
C	2.20397200	-1.10145700	-1.47316000
C	1.19342700	-0.50784300	-2.24734900
C	-0.14569600	-0.79441900	-2.02106800
C	-0.54853100	-1.70331900	-1.02031100
H	0.22636200	-2.93335700	0.60272600
H	2.57839900	-2.46515100	0.14996200
H	1.48207600	0.20697800	-3.01991500
H	-0.93640800	-0.28551000	-2.57881800
N	3.55368100	-0.81431500	-1.71560700
N	-1.92372800	-1.82444700	-0.83490800
N	3.81790500	0.26598400	0.38537800
H	2.80182500	0.25057500	0.47685600
N	5.65436000	-0.25412800	-0.93797700
H	6.08927000	0.54886600	-0.49506300
N	-2.07503900	-3.97613200	0.21443600
H	-1.12779800	-4.12633500	-0.11406000
N	-3.88076800	-2.52750100	0.13068300
H	-4.43302900	-3.37673100	0.19512200
C	-2.27932100	-4.42176900	1.59651600
H	-3.35991600	-4.59070200	1.73783500
C	-1.82346100	-3.39179200	2.63010000
H	-2.07196300	-3.73064000	3.64744900
H	-0.73629600	-3.22069400	2.58351700
H	-2.31405500	-2.42387900	2.45678000
C	-1.56962500	-5.75756000	1.77220900
H	-1.92373500	-6.48831500	1.03156300
H	-0.48262600	-5.62952500	1.64111800
H	-1.73882500	-6.15975800	2.78069500
C	-4.59522300	-1.34394400	-0.34610200
H	-3.90546500	-0.49371600	-0.25319700
C	-4.96756500	-1.45073900	-1.82062900
H	-5.42082600	-0.50907600	-2.16197200
H	-4.05854500	-1.61085700	-2.41563700
H	-5.67493100	-2.28231700	-1.98764500
C	-5.80795500	-1.10256300	0.54077000

H	-6.53452300	-1.92938400	0.45437000
H	-5.51016800	-1.01280500	1.59528800
H	-6.31146200	-0.17438600	0.23738900
C	4.52362900	0.11147900	1.65500000
H	5.56656100	0.43815700	1.51086000
C	3.87977900	1.02547800	2.68982400
H	3.83409800	2.05955700	2.32003900
H	2.85885000	0.67344500	2.90201100
H	4.45131000	1.00473800	3.62879900
C	4.52721800	-1.34233400	2.12615100
H	3.49023500	-1.66230900	2.31114900
H	4.97741300	-1.98986700	1.35846600
H	5.10164700	-1.45490200	3.05838500
C	6.26370100	-0.66324400	-2.19318200
H	5.74048100	-1.58332000	-2.48904100
C	7.73856700	-0.96263200	-1.95256400
H	8.27133000	-0.05337800	-1.62704600
H	7.85905500	-1.72744600	-1.17298500
H	8.22046300	-1.31678900	-2.87510300
C	6.06174300	0.37138800	-3.29960100
H	4.98797800	0.54837800	-3.44257100
H	6.55277000	1.32174300	-3.03251500
H	6.49067400	0.02084500	-4.25060900
C	-2.56079700	-2.73337300	-0.19548300
C	4.27759900	-0.30057500	-0.78591700
C	0.32830200	-0.17713400	1.87813500
O	1.03535000	-0.90272400	2.51540100
O	0.79018800	0.74315000	1.01208400
I	-3.23001500	2.14191600	-1.85062300
C	-1.51874500	0.78104900	0.96413400
C	-0.27472800	1.60070600	0.57302300
O	-0.99622800	-0.14363400	1.93630300
H	-2.30402500	1.38505700	1.43133500
H	-1.92476900	0.22380500	0.11208700
C	-0.17698700	2.95108600	1.24960100
C	0.71415600	3.18305000	2.29911900
C	-1.02097000	3.98315400	0.81943400
C	0.76100000	4.43235400	2.92031500
H	1.38437400	2.38719300	2.62330500
C	-0.96971400	5.22704200	1.44357200
H	-1.72003400	3.79487700	-0.00379200
C	-0.08014800	5.45729700	2.49505400
H	1.46412600	4.60098600	3.73834000
H	-1.63171800	6.02418700	1.10049800

H	-0.04191200	6.43503000	2.97945300
H	-0.22063200	1.70189200	-0.51903000

G1-TS'

C	2.49909500	-0.48819700	0.47351200
N	1.96239500	-1.46078700	-0.22442800
C	0.64855300	-1.88883900	0.08458300
C	0.33326200	-2.34968800	1.37031200
C	-0.36498400	-1.83617000	-0.88062600
C	-0.98109000	-2.66766100	1.70180900
H	1.12963900	-2.41945200	2.11512200
C	-1.67979100	-2.14573400	-0.54064600
H	-0.12331500	-1.51825700	-1.89768100
C	-1.99831700	-2.54182400	0.75693100
H	-1.21526600	-2.99413700	2.71739300
H	-2.48728200	-2.02869600	-1.26658600
H	-3.04531500	-2.71088500	1.01312500
N	3.84265000	-0.25753700	0.41575400
H	4.13340000	0.69485800	0.59147300
N	1.78273900	0.31743900	1.28776900
H	0.76193400	0.27318200	1.20632500
C	2.30913400	1.31394600	2.20132200
H	3.26299700	0.92548000	2.59880600
C	2.55945100	2.65829500	1.51176300
H	2.96904100	3.39078900	2.22371400
H	3.25872000	2.56919500	0.66641800
H	1.61573700	3.04998300	1.10136900
C	1.32063700	1.46767900	3.35279200
H	1.16349400	0.50599800	3.86002800
H	1.68276400	2.20575400	4.08193400
H	0.34935700	1.80387700	2.95930300
C	4.85254800	-1.14268700	-0.15675500
H	4.72662800	-1.19538700	-1.24962500
C	6.21240500	-0.51244400	0.12322400
H	7.01149500	-1.12051200	-0.32134400
H	6.27843400	0.49835100	-0.30802300
H	6.38955200	-0.44486100	1.20803500
C	4.77073000	-2.55149200	0.42418800
H	3.81545400	-3.02963100	0.17577500
H	5.58500200	-3.16523600	0.01254400
H	4.87860700	-2.51267600	1.51952600
C	-1.52804700	1.30726500	-0.07654000
H	-2.12977200	0.68622900	-0.75480700
C	-2.13164900	1.58168600	1.23114300

H	-1.83524100	2.48532000	1.77909600
H	-3.13145500	1.17011400	1.41151300
O	-1.10674300	0.61032900	1.09088100
C	-0.49317100	2.20134400	-0.68790900
C	0.58299900	1.62843700	-1.37937600
C	-0.55713600	3.59343700	-0.57824600
C	1.58360300	2.42353300	-1.93161200
H	0.65167300	0.54405600	-1.48027500
C	0.44059500	4.39579300	-1.13640500
H	-1.40129200	4.05129900	-0.05842600
C	1.51427800	3.81297400	-1.80885300
H	2.41005800	1.93379300	-2.45009200
H	0.37629800	5.48196900	-1.04573400
H	2.29418800	4.44283500	-2.24166000
I	-5.07745400	-0.38316100	-0.20817500
C	2.49275600	-1.69973300	-2.08551400
O	2.34551700	-2.85130400	-2.29595800
O	2.79871200	-0.61141900	-2.45769800

G1-IM1'

C	2.48620600	-0.47038400	0.42316000
N	1.92002900	-1.40345300	-0.34389500
C	0.61518400	-1.88124100	-0.02298200
C	0.34264900	-2.36800700	1.25846300
C	-0.41294700	-1.81188900	-0.96826300
C	-0.96320600	-2.69590900	1.61599700
H	1.15769700	-2.45030900	1.98127300
C	-1.71632800	-2.13467700	-0.60179300
H	-0.18875300	-1.48191700	-1.98456400
C	-2.00122600	-2.55339200	0.69734300
H	-1.17170800	-3.04455600	2.62949400
H	-2.54116700	-2.00858400	-1.30595800
H	-3.04154200	-2.72895200	0.97563200
N	3.82402600	-0.28959000	0.41736100
H	4.13656900	0.63317000	0.68973300
N	1.75533900	0.29018700	1.24927500
H	0.73443600	0.27235200	1.13227300
C	2.27123100	1.24402200	2.21595600
H	3.20668300	0.82350200	2.62487700
C	2.55916500	2.60173000	1.57033500
H	2.95995600	3.30803100	2.31254300
H	3.27730400	2.52482700	0.73967900
H	1.63128100	3.01685600	1.14711700
C	1.25431700	1.37348100	3.34452700

H	1.06384100	0.39710600	3.81063600
H	1.61400200	2.07452900	4.11004000
H	0.30157200	1.74694200	2.94059300
C	4.85284400	-1.15807600	-0.16312800
H	4.81603600	-1.06628100	-1.25898000
C	6.19724800	-0.63356200	0.32963900
H	7.01453700	-1.20404000	-0.13087300
H	6.33578900	0.42500100	0.06030900
H	6.27656900	-0.73290700	1.42367400
C	4.65966200	-2.62071100	0.23196200
H	3.76750200	-3.06159000	-0.22878000
H	5.53327200	-3.19746300	-0.10436100
H	4.58530800	-2.70914000	1.32753400
C	-1.51600300	1.34290700	-0.12262100
H	-2.13034200	0.74608200	-0.81111300
C	-2.10854000	1.59824400	1.19414100
H	-1.79187200	2.48396200	1.75971200
H	-3.11390900	1.19923700	1.37231200
O	-1.10329200	0.60943800	1.02773700
C	-0.45914200	2.22736000	-0.71081500
C	0.60700300	1.64389700	-1.40806800
C	-0.48353000	3.61736200	-0.56193400
C	1.64318200	2.42021700	-1.91999400
H	0.64647300	0.56318800	-1.54944600
C	0.54440700	4.40370700	-1.08725300
H	-1.31889800	4.08637600	-0.03765100
C	1.61165300	3.80728800	-1.75929700
H	2.46087800	1.90751400	-2.43098200
H	0.51060400	5.48856800	-0.96836100
H	2.41633700	4.42603500	-2.16183700
I	-5.06691100	-0.36510200	-0.17462500
C	2.43626300	-1.59784900	-1.86215200
O	2.26415700	-2.73081600	-2.24530400
O	2.88682300	-0.55290500	-2.31091900

G1-TS1'

C	2.38369300	-0.02805300	0.25185300
N	1.96502800	-1.17540300	-0.29855900
C	0.93383000	-1.95743400	0.27983600
C	0.86164300	-2.17849800	1.66051200
C	-0.05851300	-2.50421700	-0.54687900
C	-0.21772000	-2.86838200	2.20507800
H	1.63143400	-1.76876700	2.31466400
C	-1.12895800	-3.20190000	0.00389500

H	-0.00489600	-2.35724900	-1.62579000
C	-1.22398800	-3.37448000	1.38431900
H	-0.27548800	-2.99708200	3.28721700
H	-1.91865600	-3.56940500	-0.65197700
H	-2.08409700	-3.88769900	1.81552000
N	3.56393200	0.51321800	-0.14018000
H	3.59790400	1.52310000	-0.08920300
N	1.69393600	0.60528900	1.19835100
H	0.69505100	0.37045100	1.37858000
C	2.15394000	1.74440200	1.98587900
H	3.24234200	1.82854700	1.84428500
C	1.45777600	3.01677500	1.50603800
H	1.81901900	3.89619700	2.06012500
H	1.61434300	3.17810400	0.42774300
H	0.37701400	2.89559000	1.66958200
C	1.88418200	1.47555600	3.46515600
H	2.44303400	0.59123200	3.80546400
H	2.19348000	2.34008200	4.07114500
H	0.80805500	1.29469700	3.60070500
C	4.68189800	-0.12432800	-0.83620400
H	4.41571300	-0.27926600	-1.89288000
C	5.85130200	0.85262500	-0.77268200
H	6.70987200	0.44955800	-1.32616000
H	5.58556400	1.82064900	-1.22475000
H	6.15806800	1.02329700	0.27136100
C	5.05298600	-1.46278400	-0.20294500
H	4.26232800	-2.21100000	-0.33606100
H	5.96288000	-1.84792600	-0.68551100
H	5.25701500	-1.32711100	0.87115700
C	-1.82713500	0.37699900	0.61405200
H	-1.50353100	-0.64294400	0.42077500
C	-2.16565600	0.65821600	2.00607300
H	-2.72063700	1.59683200	2.19069600
H	-2.67860000	-0.17981700	2.51127100
O	-0.79816100	0.72510400	2.16551000
C	-1.34236600	1.42241400	-0.31386100
C	-0.38983400	1.08222700	-1.28073500
C	-1.74528600	2.75991600	-0.20821700
C	0.18769700	2.05330100	-2.09643400
H	-0.07081300	0.04607900	-1.39450200
C	-1.18357100	3.73105500	-1.03150700
H	-2.50847600	3.03271400	0.52243700
C	-0.20893900	3.38440300	-1.97214000
H	0.95138000	1.73720000	-2.80924600

H	-1.50880200	4.76952500	-0.94032900
H	0.23287500	4.15260700	-2.61046200
I	-4.19831500	-0.31118500	-0.54654400
C	2.29594900	-1.46808400	-1.86194500
O	2.53693300	-2.64065300	-2.04460000
O	2.22991300	-0.45014200	-2.52855300

G1-IM2'

C	2.37339600	0.04718600	0.31267000
N	1.91277100	-1.10487400	-0.30800100
C	0.88925800	-1.88686800	0.23674900
C	0.65515100	-1.96175200	1.62459100
C	0.03069300	-2.61909200	-0.60939000
C	-0.42242900	-2.68237400	2.12988000
H	1.30161100	-1.41335500	2.30586300
C	-1.03876800	-3.34220100	-0.08904200
H	0.21016400	-2.61502700	-1.68262600
C	-1.29142400	-3.36953600	1.28195600
H	-0.58771800	-2.69266100	3.20960300
H	-1.69692700	-3.87702100	-0.77671100
H	-2.14658000	-3.91656300	1.68145100
N	3.66511700	0.42251300	-0.00995700
H	3.78304900	1.42393300	-0.08781400
N	1.64490700	0.70961000	1.14727400
H	-0.09379900	0.65211100	1.74853300
C	2.17840900	1.84725700	1.87333900
H	3.27396300	1.92913400	1.74721200
C	1.52429900	3.12469200	1.34179700
H	1.86893400	4.01218700	1.89610300
H	1.74671800	3.26208900	0.27263000
H	0.43145300	3.03592500	1.44284400
C	1.92269300	1.67330000	3.37267700
H	2.42219200	0.76345300	3.73874700
H	2.31918400	2.53403100	3.93397800
H	0.84518900	1.58347200	3.56670200
C	4.69770100	-0.35839100	-0.68329100
H	4.44365200	-0.50939200	-1.74562800
C	5.98028400	0.46673800	-0.62228400
H	6.79391700	-0.05181700	-1.14831700
H	5.84215200	1.44887700	-1.10136100
H	6.28335200	0.62899300	0.42413100
C	4.90107700	-1.72188100	-0.02712600
H	4.03254500	-2.37224800	-0.18570000
H	5.77658400	-2.21384800	-0.47696700

H	5.08152900	-1.59599300	1.05246000
C	-2.01487200	0.22860900	0.26640500
H	-1.41634700	-0.66300900	0.05192100
C	-2.08551700	0.45892300	1.77432100
H	-2.88359500	1.18608600	2.00623500
H	-2.36955900	-0.50131000	2.24709200
O	-0.88490500	0.95758100	2.26530500
C	-1.50007700	1.38963900	-0.52602300
C	-0.41541400	1.18669300	-1.38120700
C	-2.01495000	2.68352300	-0.37540100
C	0.16000200	2.25145000	-2.07333100
H	0.02328700	0.19569900	-1.50122100
C	-1.44951800	3.74813200	-1.07038300
H	-2.86259400	2.85385800	0.29319200
C	-0.36001000	3.53473000	-1.92144600
H	1.02550800	2.03472100	-2.70210900
H	-1.85610000	4.75383600	-0.94458100
H	0.08589200	4.37631100	-2.45616100
I	-4.00419300	-0.41409200	-0.41847300
C	2.23157100	-1.25791800	-1.82101100
O	2.47646500	-2.40977900	-2.15001500
O	2.19289800	-0.19048800	-2.43058200

G1-TS2'

C	2.07067700	0.33769500	-0.25462000
N	1.60253000	-0.86226900	-0.75947500
C	1.13600000	-1.89215800	0.07019900
C	1.53227700	-1.98401600	1.41650500
C	0.24212900	-2.85870500	-0.42801200
C	1.01990800	-2.97991700	2.24169800
H	2.20738900	-1.23887100	1.83755700
C	-0.24396900	-3.86280100	0.40494200
H	-0.06015800	-2.81956300	-1.47247600
C	0.12768800	-3.93038200	1.74664600
H	1.31587200	-2.99525000	3.29264500
H	-0.94624100	-4.59093900	-0.00628600
H	-0.27911500	-4.70178400	2.40156700
N	3.21231700	0.82195300	-0.81263300
H	3.39202100	1.80152300	-0.63922800
N	1.45542600	0.96255800	0.70866000
H	0.33905100	0.51091100	1.32891700
C	2.00112000	2.18311900	1.28919900
H	2.34959700	2.85500000	0.47755900
C	0.89911200	2.93858100	2.02797100

H	1.29268200	3.89646300	2.40051000
H	0.04790700	3.13940000	1.36142800
H	0.54626000	2.34212600	2.87990800
C	3.17051000	1.86487600	2.22595900
H	3.96383000	1.31363900	1.69940700
H	3.60171100	2.78884100	2.64097600
H	2.79122700	1.24427900	3.05040800
C	4.04338000	0.20829100	-1.84912600
H	3.46718500	0.14266100	-2.78593200
C	5.22135900	1.14976000	-2.07788300
H	5.85881500	0.77008600	-2.88736700
H	4.87733300	2.15599200	-2.36268900
H	5.83269500	1.23116700	-1.16478900
C	4.52890800	-1.18702000	-1.45930600
H	3.70802300	-1.91359400	-1.46261700
H	5.27884700	-1.52472600	-2.19016300
H	4.99731200	-1.15873000	-0.46265100
C	-1.64714900	0.14242400	-0.20353200
H	-0.78384100	-0.20379700	-0.78430300
C	-1.61400900	-0.39648000	1.22524100
H	-2.57469000	-0.21613100	1.73423000
H	-1.45118300	-1.48715900	1.20698400
O	-0.59557200	0.25650300	1.93219300
C	-1.75742300	1.63259700	-0.32511700
C	-0.94437400	2.29857300	-1.25078100
C	-2.61247000	2.37315700	0.49872500
C	-0.99120800	3.69008800	-1.34275000
H	-0.26531600	1.71158000	-1.88045500
C	-2.65420800	3.76131600	0.40444000
H	-3.24343400	1.85675600	1.22503300
C	-1.84252500	4.42454100	-0.51762500
H	-0.35159200	4.20196300	-2.06431300
H	-3.31833300	4.33077600	1.05741000
H	-1.87221700	5.51372100	-0.58844800
I	-3.31687400	-0.85218700	-1.23321900
C	1.39297000	-0.89873400	-2.28929800
O	1.06279600	0.20214600	-2.73334600
O	1.60790900	-1.98662000	-2.79915800
C	-0.22678300	-0.38443200	3.56402300
O	-1.14559300	-1.06709100	3.86922700
O	0.82911600	0.09151500	3.83819900

G1-IM3'

C	3.31708900	0.38935100	-0.59264600
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N	3.22686500	-0.93176900	-0.32712900
C	2.30835100	-1.41773900	0.63314300
C	2.09108600	-0.71969400	1.82581300
C	1.61386100	-2.61300700	0.40733800
C	1.17055000	-1.18523200	2.76086100
H	2.60466500	0.22708600	2.00277100
C	0.71846400	-3.08804200	1.35880000
H	1.79638900	-3.16871200	-0.51027500
C	0.48226000	-2.37483900	2.53556500
H	0.97148300	-0.58906000	3.65219400
H	0.18322500	-4.02042500	1.16760300
H	-0.24285200	-2.73868700	3.26589100
N	4.52493700	0.93847400	-0.84276300
H	4.50399300	1.82019600	-1.33688300
N	2.24589700	1.17599300	-0.59513900
H	1.27836600	0.75921500	-0.39556700
C	2.31117600	2.63525700	-0.59725800
H	3.00333000	2.95704600	-1.39886300
C	0.93891400	3.20043100	-0.95086200
H	1.01609700	4.28902900	-1.08816100
H	0.56086500	2.75173900	-1.88081600
H	0.23623700	2.99202200	-0.13251800
C	2.79910800	3.17127800	0.74963700
H	3.78902400	2.76106000	0.99978100
H	2.87304400	4.26913600	0.72384200
H	2.06877900	2.86817100	1.51375100
C	5.85704800	0.36527100	-0.64328800
H	6.05352200	-0.35801300	-1.44863100
C	6.84864500	1.51919300	-0.75365300
H	7.87682400	1.14026100	-0.68112700
H	6.75091500	2.03737900	-1.72045600
H	6.68963100	2.25072700	0.05466000
C	5.98879300	-0.33535500	0.70924400
H	5.42427300	-1.27466600	0.75062100
H	7.04882800	-0.57022400	0.88583000
H	5.64148000	0.33066700	1.51569100
C	-2.93087200	-0.22694100	-0.23000600
H	-2.15778100	-0.23708800	-1.00045500
C	-2.31120800	-0.68310500	1.10076400
H	-3.10843300	-0.98808500	1.79533100
H	-1.65289000	-1.54378500	0.89967000
O	-1.61974900	0.34802900	1.74674000
C	-3.58000700	1.12583900	-0.16574700
C	-2.87166500	2.21159700	-0.69235000

C	-4.79903300	1.36155500	0.47847300
C	-3.37842400	3.50621400	-0.58795400
H	-1.89940700	2.02880100	-1.15528000
C	-5.30709500	2.65381300	0.57923800
H	-5.35969100	0.51895200	0.89011200
C	-4.59924700	3.73121100	0.04438300
H	-2.80853300	4.34218800	-0.99778900
H	-6.26264900	2.82181600	1.07969200
H	-4.99834000	4.74396400	0.12592400
I	-4.31187900	-1.79384400	-0.89324700
C	4.05310600	-1.95277900	-1.21779300
O	4.34017100	-1.47887500	-2.30616000
O	4.25387900	-3.00498700	-0.63990500
C	-0.47148200	0.85230300	1.14279300
O	-0.20811300	0.39259000	-0.00177400
O	0.12991500	1.69508100	1.79532700

G1-TS3'

C	3.03444300	0.31176300	-0.49387700
N	2.88626000	-1.02001200	-0.54451500
C	1.95762900	-1.65922300	0.31612500
C	2.01645300	-1.43377100	1.69317700
C	0.97390000	-2.50696900	-0.20401600
C	1.08034600	-2.01868900	2.54177300
H	2.77861000	-0.76208800	2.09383600
C	0.04437800	-3.09441100	0.64747600
H	0.94872400	-2.69562300	-1.27720900
C	0.08784600	-2.84572000	2.02173200
H	1.11079600	-1.79580200	3.60889600
H	-0.73074000	-3.74229800	0.23296200
H	-0.65232100	-3.29653900	2.68555100
N	4.21943800	0.88078400	-0.79001600
H	4.17934900	1.86305300	-1.02549000
N	2.02330700	1.11223200	-0.13832800
H	1.10788000	0.67867900	0.09712500
C	2.16911700	2.51345600	0.25270400
H	2.75793900	3.03273200	-0.52652600
C	0.79297100	3.17214800	0.28204400
H	0.90824400	4.25826600	0.40762900
H	0.23689900	2.97896900	-0.64679000
H	0.21082800	2.78215200	1.12725800
C	2.87399200	2.63742600	1.60388500
H	3.86433000	2.15801400	1.57797500
H	3.00606100	3.69602100	1.87361700

H	2.24626400	2.14390600	2.36038000
C	5.54358600	0.26315400	-0.88934400
H	5.61993300	-0.25109100	-1.85780200
C	6.55883100	1.40047200	-0.83853500
H	7.57408900	1.00487900	-0.97509100
H	6.37645600	2.13512000	-1.63823800
H	6.51615400	1.91976300	0.13221900
C	5.80002600	-0.73884900	0.23524900
H	5.18658700	-1.64310200	0.14321800
H	6.85631500	-1.04369700	0.20520700
H	5.60239700	-0.27048900	1.21327900
C	-2.31938000	-0.14415900	0.14724300
H	-1.83025900	-0.82868200	-0.53628000
C	-2.59348800	-0.57842400	1.58228300
H	-3.62768700	-0.34390100	1.85585900
H	-2.45125300	-1.66738100	1.64451200
O	-1.76520000	0.08375200	2.51790300
C	-2.55447900	1.24463700	-0.30655700
C	-2.26729600	1.60026900	-1.63099700
C	-2.97911900	2.23424500	0.58774600
C	-2.40554700	2.91691900	-2.05407400
H	-1.94521300	0.82454600	-2.32869600
C	-3.11236500	3.55453600	0.16225700
H	-3.18026200	1.97507400	1.62878900
C	-2.82817300	3.90148700	-1.15744100
H	-2.18196500	3.17858500	-3.08995100
H	-3.43868700	4.31810800	0.87054300
H	-2.93447100	4.93596600	-1.48872400
I	-4.54998700	-1.23554900	-0.80055500
C	3.54677600	-1.88515300	-1.73048900
O	3.82720800	-1.19170000	-2.69225500
O	3.63268700	-3.05354600	-1.41710300
C	-0.55506400	0.49187000	2.02223200
O	-0.44143500	0.28733300	0.76595800
O	0.23911500	1.01264200	2.77897300

G1-IM4'

C	3.17618200	0.13976700	-0.53434100
N	2.73722000	-1.11033500	-0.51512000
C	1.62999000	-1.47685500	0.29195100
C	1.66580200	-1.25491500	1.67192700
C	0.50943400	-2.08402500	-0.28420300
C	0.58178200	-1.62439300	2.46619100
H	2.54362700	-0.77987600	2.11557100

C	-0.57107600	-2.45737800	0.51103300
H	0.49457500	-2.26154500	-1.36038100
C	-0.53678300	-2.22517100	1.88865400
H	0.61135900	-1.42969700	3.53976400
H	-1.46556900	-2.89334700	0.05909000
H	-1.39139100	-2.51718000	2.50232200
N	4.46005000	0.42260300	-0.83673700
H	4.63047100	1.35832700	-1.17948400
N	2.36718400	1.18250700	-0.24970800
H	1.38662300	0.96707100	-0.06090800
C	2.83035700	2.51755600	0.12163400
H	3.54280800	2.86508800	-0.64780300
C	1.64642600	3.47582100	0.09597600
H	1.99902700	4.50660000	0.23876700
H	1.10494000	3.41329700	-0.85855600
H	0.95829400	3.22748200	0.91439800
C	3.51749100	2.51210300	1.48659200
H	4.36915700	1.81623400	1.49370600
H	3.88789800	3.51767900	1.73544000
H	2.78757900	2.19956200	2.24672400
C	5.62304900	-0.46862800	-0.82792500
H	5.61686800	-1.06881300	-1.74900600
C	6.85827700	0.42640200	-0.82102000
H	7.76749700	-0.18660400	-0.87826800
H	6.86085000	1.10888600	-1.68504500
H	6.90095300	1.02588800	0.10226500
C	5.62287300	-1.40167400	0.38218500
H	4.82238600	-2.15001400	0.33740800
H	6.58258100	-1.93707500	0.41699700
H	5.51795100	-0.81925800	1.31203300
C	-1.84808900	0.71454700	0.25861200
H	-1.82932800	-0.20016100	-0.34671900
C	-2.56714900	0.44692000	1.59543900
H	-3.53534300	0.95327600	1.67015800
H	-2.70027400	-0.62597500	1.77172400
O	-1.66835600	1.00063100	2.56860500
C	-2.40550600	1.87442900	-0.53109200
C	-3.33084000	1.62942000	-1.55057200
C	-2.04661400	3.19112900	-0.22634300
C	-3.88338800	2.69663400	-2.25734800
H	-3.62737800	0.59727300	-1.76190200
C	-2.59955000	4.25497000	-0.93772000
H	-1.32016400	3.39144100	0.56413800
C	-3.51896700	4.00902300	-1.95675700

H	-4.60583100	2.49754800	-3.05069200
H	-2.30933800	5.27893500	-0.69468500
H	-3.95276100	4.84068600	-2.51527900
I	-4.38729600	-1.93531700	-0.31972800
C	3.27611800	-2.23212300	-1.63552400
O	3.68089000	-1.67018100	-2.62858400
O	3.14152500	-3.34297200	-1.18978300
C	-0.48118900	1.23508200	2.02820600
O	-0.51020600	1.01471400	0.70049600
O	0.48560500	1.62541100	2.61319500

G10-COM

H	2.77365900	-4.78334600	0.86472600
H	2.83378900	-1.12015100	-2.13797600
H	1.33031800	0.23174000	-3.53358600
H	2.96811400	1.36464100	-0.34607300
H	0.02652300	2.50222500	-0.36117000
O	1.44864200	1.35678700	2.21672900
N	1.87445600	-2.30087700	0.52582900
N	1.12268200	-0.63994400	-1.02215100
N	0.09706000	-0.94775200	1.08771000
N	0.67688600	2.50042700	0.41962200
C	1.10291200	-1.34001900	0.18749500
C	0.18884900	-1.57527200	2.40948600
C	-1.61977700	0.64792800	1.94396900
C	-0.41822100	0.41264800	1.01646400
C	0.66911600	1.45175900	1.28737600
C	1.57009500	3.63296600	0.61619900
C	2.77216200	-3.00360200	-0.36380100
C	3.50122200	-4.06736700	0.45357200
C	2.03091000	-3.64544000	-1.53995400
C	2.36722400	-0.23459300	-1.67939700
C	3.36258600	0.40477400	-0.71398200
C	2.00019100	0.71891900	-2.80968000
C	-1.38768000	0.12554100	3.35322100
C	1.80857900	4.33367900	-0.71348500
H	2.48312300	5.19004200	-0.57963900
H	0.86104000	4.71378100	-1.12879600
H	2.51753000	3.21067100	0.98759400
H	3.53712200	-0.24068800	0.15847000
H	0.40644900	0.06794500	-1.12894500
H	-0.81394300	0.59477100	0.01301100
H	1.28337000	-4.35603200	-1.15421900
H	1.50227300	-2.89288500	-2.14238600

H	3.55114700	-2.32775300	-0.76709300
H	4.02417900	-3.59774100	1.29790000
C	1.02604600	4.57670700	1.68650800
H	2.72688500	-4.19547400	-2.19100500
H	4.23180800	-4.61529200	-0.16010100
H	2.90176400	1.05215700	-3.34143100
H	1.48670300	1.60512100	-2.40308800
H	4.32374300	0.58827600	-1.21662400
C	-1.06013900	-1.35698500	3.24713900
H	2.26060000	3.65015200	-1.44661300
H	0.86897600	4.02413800	2.62284200
H	1.73324100	5.39583700	1.88125300
H	0.06752700	5.01199100	1.36382800
H	-0.89497300	-1.80363300	4.23867400
H	-1.91314300	-1.88505000	2.78593900
H	1.07506400	-1.18163300	2.93806100
H	0.37015300	-2.64217700	2.24507600
H	-0.54545900	0.66081000	3.82045700
H	-2.28139300	0.29605200	3.97183300
H	-1.84499100	1.72618700	1.93436700
H	-2.48754100	0.12825400	1.50237900
C	-2.47360200	1.17082200	-2.20463800
H	-3.08470100	2.07963000	-2.23138100
C	-1.52122900	0.96151500	-3.30898200
H	-1.22964200	-0.06520100	-3.55565200
H	-1.46069200	1.69012800	-4.12300600
O	-1.08111500	1.42478200	-2.05027500
C	-3.05147000	0.04725600	-1.41080100
C	-4.33329600	0.17924400	-0.87044400
C	-2.31968000	-1.12062700	-1.16650400
C	-4.88076100	-0.84283700	-0.09596300
H	-4.90310100	1.09365300	-1.05032300
C	-2.85955800	-2.13359000	-0.37942000
H	-1.30168500	-1.22778500	-1.55085500
C	-4.14302800	-1.99877800	0.15382300
H	-5.88135300	-0.72964900	0.32383300
H	-2.26526200	-3.02451400	-0.17097700
H	-4.56372700	-2.79261100	0.77279100

G10-IM1

H	-1.84945000	-3.24808700	-3.38608600
H	-2.43606100	-0.22108800	0.10867000
H	-1.68408300	0.27285500	2.34735400
H	-1.12793200	2.42525600	-0.70713400

H	1.57645800	2.29123200	0.84374400
O	1.88994000	2.17504200	-2.29687500
N	-0.59259400	-1.32287000	-2.01747600
N	-0.32013000	-0.16603900	0.06024900
N	1.51002900	-0.62191100	-1.38066600
N	1.60278500	2.65880400	-0.10371400
C	0.11239600	-0.71522000	-1.14522600
C	1.92785400	-0.99061100	-2.73297300
C	3.80186700	0.19623700	-0.86857600
C	2.28856100	0.40245100	-0.70263000
C	1.90112100	1.81957300	-1.13110100
C	1.22832000	4.04316100	-0.34788800
C	-1.97764300	-1.72555200	-1.84765200
C	-2.44910500	-2.35249700	-3.15669600
C	-2.15198500	-2.71079900	-0.69033600
C	-1.62238600	0.50895400	0.19362500
C	-1.83060300	1.58845800	-0.86310500
C	-1.73315600	1.07713700	1.59866000
C	4.21198700	-0.04926800	-2.31319100
C	0.45716100	4.57944600	0.84921300
H	0.17938000	5.62978700	0.68522200
H	1.07545300	4.53131400	1.76066100
H	0.57459600	4.03590800	-1.23544900
H	-1.65936400	1.18576400	-1.87282100
H	0.38945700	0.32516800	0.58715000
H	2.12241600	0.31916800	0.37532100
H	-1.59677100	-3.63952800	-0.90419100
H	-1.77320200	-2.28935600	0.25210800
H	-2.64201000	-0.86463000	-1.65817700
H	-2.32158900	-1.63920000	-3.98349600
C	2.45846600	4.88768900	-0.67549100
H	-3.21752600	-2.93797200	-0.54305600
H	-3.51006300	-2.63504000	-3.09161100
H	-2.71648200	1.55529500	1.70630100
H	-0.93075000	1.81079200	1.80053800
H	-2.86677400	1.95302800	-0.80289700
C	3.42395700	-1.24759400	-2.82481700
H	-0.46266900	4.00272500	1.02117800
H	2.97930500	4.45586100	-1.54055300
H	2.16952600	5.92079500	-0.91953600
H	3.14654300	4.90967500	0.18411000
H	3.67714100	-1.47458700	-3.87182000
H	3.68235200	-2.13628800	-2.22189200
H	1.63845400	-0.19424000	-3.44319300

H	1.35505100	-1.88139700	-3.00805600
H	3.97659500	0.83679900	-2.92364700
H	5.29716500	-0.22709900	-2.37396600
H	4.31151200	1.07373800	-0.43899500
H	4.08494600	-0.67860800	-0.25799700
C	2.34119700	-0.10554000	3.19751700
H	3.05223200	0.38517600	3.87190100
C	0.90519300	0.03893600	3.49477300
H	0.21473300	-0.73311000	3.14038400
H	0.58444900	0.60230600	4.37641900
O	1.51680800	0.80606900	2.48187200
C	2.89464200	-1.27016600	2.44468000
C	4.22717500	-1.64352600	2.64060500
C	2.11213300	-1.97854600	1.52512600
C	4.77285400	-2.71301700	1.93166300
H	4.84428600	-1.08525900	3.34861500
C	2.66166900	-3.03555100	0.80521600
H	1.07892300	-1.67988000	1.32672500
C	3.99091600	-3.40905300	1.01055000
H	5.81516200	-2.99438700	2.09057900
H	2.04391200	-3.55341900	0.06983900
H	4.42060700	-4.23666700	0.44363400
I	-5.28049200	-0.17034300	0.54912700

G10-TS1

H	4.90354700	-3.79683300	-1.61033900
H	2.49616300	-0.16331200	-3.30941000
H	0.19640800	0.68013300	-3.44839000
H	2.97970300	2.19366300	-1.41695200
H	0.44372400	2.26523600	0.27445300
O	3.23147300	1.64630100	1.64200100
N	3.51656900	-1.64841800	-0.89492700
N	1.64483300	-0.24378100	-1.38849600
N	2.14565800	-0.94697400	0.81128700
N	1.35424400	2.49419400	0.69079300
C	2.48285400	-0.96625500	-0.54746300
C	3.12787100	-1.55514900	1.70595600
C	0.86679500	-0.07412500	2.76616800
C	1.34695900	0.16002100	1.32796400
C	2.08885100	1.49374300	1.23326100
C	1.88805800	3.83844200	0.58074900
C	3.84265400	-2.02433600	-2.24834000
C	5.10287900	-2.88853600	-2.19937900
C	2.70772500	-2.78962500	-2.93755000

C	2.15571100	0.52650800	-2.52085900
C	3.32720200	1.42381000	-2.12316000
C	1.00913100	1.33941400	-3.10971500
C	1.97359400	-0.55452300	3.69274300
C	1.12279100	4.59428900	-0.49702200
H	1.48698700	5.62828900	-0.57801700
H	0.04845800	4.62399100	-0.25624400
H	2.94717600	3.74063200	0.28626800
H	4.11501500	0.84116600	-1.62379000
H	0.81104700	0.18609800	-0.98028700
H	0.42664600	0.24323200	0.74499200
H	2.49628700	-3.71040300	-2.37136000
H	1.78269100	-2.19724100	-2.96815000
H	4.09666700	-1.14151000	-2.86882900
H	5.91491600	-2.33889200	-1.70343300
C	1.85128300	4.55299700	1.93093000
H	2.98521200	-3.06975800	-3.96580700
H	5.43067200	-3.18285300	-3.20871000
H	1.36412400	1.92684500	-3.96871900
H	0.59091700	2.01693800	-2.35046200
H	3.75646200	1.91983000	-3.00722000
C	2.56073000	-1.82416200	3.09108500
H	1.23661900	4.10628600	-1.47585100
H	2.41095400	3.96355700	2.66976300
H	2.30738200	5.55221800	1.85956200
H	0.81155200	4.66428000	2.27537000
H	3.36337300	-2.23562300	3.72261600
H	1.76882400	-2.59029700	3.01888800
H	4.01302400	-0.89719300	1.78151600
H	3.46439100	-2.48331600	1.23290400
H	2.75791500	0.21536000	3.77275900
H	1.57248600	-0.73951400	4.70160500
H	0.40807600	0.86247100	3.12021000
H	0.06765400	-0.83198400	2.72818600
C	-2.49733800	0.51604300	-0.08155400
H	-2.87911200	1.33558000	0.52345500
C	-1.91611900	0.89102600	-1.36683600
H	-1.76679200	0.05138900	-2.07231500
H	-2.43943500	1.71714900	-1.87747000
O	-0.82325700	1.23755100	-0.59759800
C	-2.14558500	-0.73651900	0.62562800
C	-2.73136100	-1.01022200	1.86874800
C	-1.21626400	-1.64517900	0.10285600
C	-2.40665700	-2.16820100	2.56792600

H	-3.47668200	-0.31596000	2.26212100
C	-0.87603500	-2.79523700	0.81221200
H	-0.71766500	-1.43223600	-0.84452600
C	-1.47410400	-3.06537300	2.04297400
H	-2.88202400	-2.37049300	3.52939100
H	-0.12635600	-3.47404200	0.40181700
H	-1.20842900	-3.96832500	2.59596900
I	-5.11326800	0.00219600	-0.73179800

G10-IM2

H	4.89899500	-3.74389200	-1.36471500
H	2.52125500	-0.24349600	-3.25451100
H	0.19393800	0.46102800	-3.55646000
H	2.80172300	2.23739200	-1.48634700
H	0.31809200	2.25865100	0.18700700
O	3.05029100	1.79879600	1.75054100
N	3.49117700	-1.56940300	-0.80010600
N	1.58978900	-0.22973500	-1.36638500
N	2.09234600	-0.83870800	0.86409500
N	1.20015700	2.55248400	0.66534900
C	2.43448200	-0.89638000	-0.49165100
C	3.07891200	-1.38477100	1.79163000
C	0.71341300	-0.02091000	2.76461200
C	1.23684000	0.24031800	1.34772000
C	1.93644300	1.60033100	1.27589900
C	1.71442300	3.89654100	0.50508600
C	3.84315600	-2.01589000	-2.12262500
C	5.10620100	-2.86976100	-2.00135100
C	2.72699100	-2.82746000	-2.79000200
C	2.10946400	0.47973100	-2.53390200
C	3.21633300	1.46133800	-2.14900800
C	0.95377300	1.18870100	-3.23249900
C	1.80596100	-0.44069200	3.73652500
C	0.95960700	4.58362300	-0.62583200
H	1.31500600	5.61558000	-0.76146800
H	-0.11848000	4.61118000	-0.40340400
H	2.78349800	3.81109800	0.24027700
H	4.02058700	0.94652600	-1.60231000
H	0.74099300	0.23399900	-1.00115100
H	0.33889600	0.30077200	0.72553600
H	2.51605100	-3.71942600	-2.17850100
H	1.79735900	-2.24605100	-2.86297500
H	4.10739700	-1.17021100	-2.78986800
H	5.90511300	-2.28794800	-1.52093500

C	1.63200800	4.67749000	1.81675700
H	3.02178500	-3.15892100	-3.79827700
H	5.45634800	-3.21948600	-2.98563500
H	1.32443100	1.72770500	-4.11707300
H	0.45908500	1.88294600	-2.53868100
H	3.64445100	1.94419000	-3.04137300
C	2.48382700	-1.67743700	3.16114800
H	1.08973600	4.03828400	-1.57182100
H	2.18497000	4.13543300	2.59594100
H	2.06927800	5.68222300	1.70710500
H	0.58169200	4.78244000	2.13034200
H	3.28739900	-2.04038200	3.82138900
H	1.73868800	-2.48752500	3.06746800
H	3.92128700	-0.67594200	1.89263200
H	3.48120700	-2.29571300	1.33743400
H	2.54372500	0.37072800	3.84297100
H	1.37784100	-0.64725900	4.73067100
H	0.18856400	0.88831100	3.09823200
H	-0.03876900	-0.82428900	2.69513500
C	-2.78858300	0.34910900	0.02558200
H	-2.95150300	1.06285000	0.84301800
C	-1.99289700	1.02685200	-1.10602000
H	-2.03978900	0.34288100	-1.99370100
H	-2.58902000	1.92115500	-1.40889600
O	-0.74385700	1.29729900	-0.68208900
C	-2.23281200	-0.93540500	0.56997900
C	-2.69051900	-1.43368900	1.79804500
C	-1.23066500	-1.64101600	-0.10603500
C	-2.16653800	-2.60513000	2.33654100
H	-3.47844600	-0.89149000	2.32751900
C	-0.68452900	-2.80026700	0.44482600
H	-0.83453500	-1.25685100	-1.04624900
C	-1.15361100	-3.29040300	1.66253500
H	-2.53793300	-2.97722800	3.29350300
H	0.12811300	-3.30767700	-0.07874300
H	-0.72260100	-4.19665200	2.09228100
I	-4.87891100	-0.00047300	-0.67587600

G10-TS2

H	3.28851400	-5.01451200	-1.32760100
H	1.86982600	-1.05472100	-3.35887800
H	-0.07529100	0.39194600	-3.47841100
H	3.27776500	1.25742500	-1.92680200
H	1.01450700	2.28475000	0.00335700

O	3.74641200	1.17274300	1.14405400
N	2.76260100	-2.45409700	-0.86149200
N	1.31688600	-0.61760300	-1.37318500
N	1.97397000	-1.13385100	0.84100500
N	2.02044500	2.30364300	0.19776600
C	2.04260300	-1.43978000	-0.52136200
C	2.91992900	-1.84261100	1.69880600
C	1.23453900	0.27119800	2.75683700
C	1.53501400	0.19277500	1.25566400
C	2.55726500	1.25878200	0.86344700
C	2.82190300	3.45603600	-0.16489400
C	2.72772800	-3.09542200	-2.15129800
C	3.65670100	-4.30841800	-2.08793200
C	1.31709800	-3.53489700	-2.55913000
C	1.85293800	-0.19669800	-2.66712000
C	3.27725400	0.34594900	-2.54488000
C	0.90878700	0.83753800	-3.27152400
C	2.34533300	-0.31918700	3.61379000
C	2.24222200	4.12664800	-1.40396400
H	2.85631800	4.99127500	-1.69594600
H	1.22066800	4.48084200	-1.20198900
H	3.82791800	3.06681100	-0.39279800
H	3.93573600	-0.38904900	-2.05860000
H	0.69372200	0.09815900	-0.96777300
H	0.58517400	0.43640900	0.76374500
H	0.92499100	-4.23708300	-1.80606700
H	0.62867600	-2.67978100	-2.61052500
H	3.13084900	-2.43742600	-2.94759600
H	4.66528400	-3.99057000	-1.78900700
C	2.94626900	4.42426900	1.01205600
H	1.32548400	-4.04344000	-3.53607200
H	3.71469000	-4.82710500	-3.05794700
H	1.32584900	1.22185300	-4.21427300
H	0.74121800	1.66373300	-2.56629600
H	3.68822300	0.58775300	-3.53757500
C	2.55207500	-1.76248800	3.17395600
H	2.20172000	3.42366000	-2.24802700
H	3.38540300	3.89938300	1.87219000
H	3.59272300	5.27808300	0.75590600
H	1.95074100	4.79924300	1.29156800
H	3.35072500	-2.24978500	3.75535600
H	1.62154000	-2.32778800	3.35338300
H	3.93394100	-1.42893500	1.54439400
H	2.94694300	-2.88361800	1.35920800

H	3.27532500	0.25173100	3.46418300
H	2.07729900	-0.26536100	4.68114500
H	1.03965200	1.32790900	2.99964000
H	0.29770800	-0.28268200	2.93725300
C	-1.39246600	3.57007700	0.11011500
O	-0.41325900	3.89153200	0.65182200
O	-2.45739500	3.48950100	-0.34522000
C	-2.64668100	0.37613600	0.12509500
H	-2.97130000	1.25435900	0.69514400
C	-1.76472300	0.81144700	-1.05794400
H	-1.57652100	-0.10007700	-1.67981100
H	-2.40371800	1.46249900	-1.69454700
O	-0.62905100	1.41344200	-0.62425500
C	-2.11594600	-0.68471800	1.04292200
C	-2.55346100	-0.73865400	2.37448300
C	-1.20642100	-1.65019900	0.59913400
C	-2.11420000	-1.74294200	3.23213100
H	-3.26425700	0.01200800	2.72981600
C	-0.75072600	-2.64702000	1.46113600
H	-0.82806100	-1.61444500	-0.42373100
C	-1.21251700	-2.70626300	2.77475600
H	-2.47152700	-1.77198700	4.26340600
H	-0.01453200	-3.36711600	1.09726300
H	-0.85753800	-3.48969300	3.44728400
I	-4.59434800	-0.34280000	-0.69282100

G10-IM3

H	-3.98876700	5.03654500	0.17003200
H	-2.03217600	1.95919800	-2.85040000
H	-0.01002800	0.52313800	-3.08293400
H	-3.41986800	-0.70574400	-2.26697700
H	-1.48530700	-2.64701200	-0.22217900
O	-4.19430700	-1.09785800	0.38519100
N	-3.17032900	2.52145100	-0.03228700
N	-1.59977500	1.01276900	-1.01871400
N	-2.29186200	0.80323700	1.22146200
N	-2.50137100	-2.43426700	-0.33331500
C	-2.38489300	1.50159200	0.00887400
C	-3.25453300	1.22249500	2.23833400
C	-1.74910400	-1.25137400	2.53036600
C	-1.94840900	-0.61378500	1.15064000
C	-3.00662100	-1.39802700	0.36062100
C	-3.35393500	-3.35161900	-1.05866300
C	-3.18760900	3.48531100	-1.10499300

C	-4.25130700	4.53072900	-0.77199700
C	-1.82791100	4.16041700	-1.31435400
C	-2.03479900	0.94613900	-2.40910600
C	-3.43956900	0.35984000	-2.54321100
C	-1.02404500	0.11166300	-3.18607200
C	-2.89260800	-0.93036600	3.48118400
C	-2.52663100	-4.02479000	-2.14705700
H	-3.12726800	-4.75970100	-2.70290200
H	-1.66427100	-4.54089100	-1.69672100
H	-4.16015900	-2.75179300	-1.51339000
H	-4.14950000	0.86027200	-1.86895800
H	-0.84571600	0.36235500	-0.79134700
H	-0.98673200	-0.73184000	0.63964200
H	-1.54808700	4.71071400	-0.40118400
H	-1.04707100	3.41348400	-1.51649800
H	-3.49191300	3.02347400	-2.06516600
H	-5.22397300	4.04015800	-0.62772000
C	-4.00284800	-4.36479800	-0.11459800
H	-1.86391300	4.87621500	-2.15088300
H	-4.34365500	5.28568200	-1.56875700
H	-1.30055700	0.08264700	-4.25032400
H	-0.99234700	-0.90990100	-2.78123600
H	-3.79803400	0.45325100	-3.58036600
C	-2.99045200	0.58544600	3.59580100
H	-2.13713800	-3.27818100	-2.85416600
H	-4.58394400	-3.83217500	0.65122800
H	-4.67817900	-5.04175800	-0.66067600
H	-3.22700100	-4.96726600	0.38289300
H	-3.79782300	0.88697700	4.28116000
H	-2.04662600	0.97658500	4.01647500
H	-4.27553500	0.97395200	1.89908900
H	-3.20546800	2.31555600	2.30530200
H	-3.83808700	-1.32943900	3.07732700
H	-2.72366000	-1.39592800	4.46500100
H	-1.60603200	-2.33058900	2.37565200
H	-0.80502700	-0.86777900	2.95277300
C	0.91022100	-2.07366700	-0.31042400
O	0.13778600	-2.91243000	0.17432600
O	0.66988400	-1.01992000	-0.91398100
I	5.68732400	0.17649600	-0.08991900
C	3.25233300	-1.58121300	-0.63395600
C	3.69233400	-0.57980000	0.44340600
O	2.25830400	-2.41148300	-0.11077500
H	2.89780700	-1.03720500	-1.52268800

H	4.10298500	-2.22397700	-0.90395400
C	2.70807800	0.52887700	0.66785900
C	2.49883500	1.52594600	-0.29125200
C	1.86903500	0.47522700	1.78344900
C	1.46216500	2.43896400	-0.14668500
H	3.15029800	1.57319900	-1.16706100
C	0.82130200	1.38654300	1.92303100
H	2.01231900	-0.31198800	2.52785200
C	0.61004600	2.36499700	0.95650300
H	1.29951000	3.20172900	-0.91055900
H	0.14320500	1.31801300	2.77451800
H	-0.23749000	3.04735800	1.04672700
H	3.88264200	-1.12891800	1.37275100

G10-TS3

H	-3.92260400	4.90154600	-0.46789800
H	-1.66550400	1.48838700	-2.94805200
H	0.33247200	-0.03133300	-2.81374700
H	-3.13022100	-1.02047000	-1.97776900
H	-1.51442600	-2.57088000	-0.10171700
O	-4.06564600	-1.04254800	1.03784300
N	-2.95311200	2.44108900	-0.25640300
N	-1.30581000	0.86507100	-0.97103000
N	-2.02925700	0.96970700	1.26013300
N	-2.50063600	-2.38628200	0.10831500
C	-2.12972600	1.47828200	-0.04436000
C	-2.93382700	1.59393500	2.22440700
C	-1.50785100	-0.85113800	2.87304400
C	-1.75559500	-0.45943100	1.41040000
C	-2.88958500	-1.31005400	0.83120200
C	-3.49443300	-3.29238000	-0.44687500
C	-2.99080500	3.22730900	-1.46762600
C	-4.12463400	4.24218300	-1.32586900
C	-1.66924500	3.94475900	-1.75196900
C	-1.70346700	0.56479200	-2.34142300
C	-3.11632200	-0.01576000	-2.42560400
C	-0.69319300	-0.41415000	-2.92869700
C	-2.57173700	-0.30939300	3.81706400
C	-2.89522700	-4.05633600	-1.61973200
H	-3.64529400	-4.73555700	-2.05053800
H	-2.02020000	-4.63962600	-1.29999500
H	-4.32864700	-2.66186300	-0.79822300
H	-3.84146600	0.60191600	-1.87733100
H	-0.54033600	0.29767000	-0.61441000

H	-0.83351500	-0.71707400	0.88104800
H	-1.44316200	4.63493400	-0.92370400
H	-0.83808800	3.23039700	-1.83001200
H	-3.23361400	2.60494600	-2.35068600
H	-5.07310700	3.72206800	-1.13259000
C	-4.04344400	-4.22370500	0.63345500
H	-1.73194300	4.52858900	-2.68397900
H	-4.22986100	4.85866100	-2.23228600
H	-0.89435900	-0.57052900	-3.99790700
H	-0.76438900	-1.38547800	-2.41553300
H	-3.43479800	-0.09223600	-3.47667500
C	-2.61008700	1.20479500	3.65930700
H	-2.55038300	-3.36673600	-2.40411800
H	-4.46381300	-3.62636800	1.45412000
H	-4.83708500	-4.86963300	0.22801600
H	-3.23931200	-4.86383100	1.02786400
H	-3.36385700	1.65737700	4.32182400
H	-1.62967000	1.62418800	3.94716900
H	-3.97663300	1.32455400	1.98391900
H	-2.85192500	2.67842500	2.08678400
H	-3.55359800	-0.73247300	3.55159100
H	-2.34584800	-0.59754800	4.85571100
H	-1.43353000	-1.94846800	2.91925400
H	-0.52531600	-0.44654200	3.16980200
C	0.94055800	-2.46910400	-0.87967100
O	0.09315300	-3.33342200	-1.01551900
O	0.82630800	-1.35866800	-0.26364500
I	5.28704600	-0.08154000	0.48195800
C	2.98458300	-1.48731300	-1.35380800
C	2.71318900	-0.71900000	-0.06701000
O	2.17737000	-2.64920700	-1.42248500
H	2.77369300	-0.83717900	-2.21818600
H	4.02098600	-1.82514500	-1.40395700
C	2.24004100	0.68358700	0.01368300
C	2.34869000	1.58346400	-1.05156400
C	1.56575100	1.08111800	1.17352200
C	1.80081800	2.85863700	-0.94841400
H	2.89782300	1.30074400	-1.95106400
C	1.00851400	2.35176300	1.27155200
H	1.46251500	0.36886000	1.99477800
C	1.12898600	3.24759500	0.21084200
H	1.89556400	3.55616100	-1.78266800
H	0.45836800	2.63369500	2.17045700
H	0.68971300	4.24325400	0.28247200

H	2.77242000	-1.27881500	0.86265800
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G10-IM4

H	-4.34331800	4.86806700	-0.05192000
H	-1.99794200	1.73210700	-2.92887400
H	0.05201300	0.31196700	-2.88211900
H	-3.39585600	-0.88421500	-2.16086600
H	-1.94358700	-2.66856900	-0.28566000
O	-4.45366900	-1.09232200	0.80870300
N	-3.34249300	2.41051000	-0.08492300
N	-1.67373800	0.96608600	-0.99151900
N	-2.34856500	0.79247500	1.23871800
N	-2.93481600	-2.48206900	-0.13742100
C	-2.50424300	1.44716500	0.00606800
C	-3.18554500	1.31195500	2.32021000
C	-1.75535700	-1.21063800	2.59297700
C	-2.10697800	-0.64819100	1.21026400
C	-3.29329500	-1.41228600	0.61115000
C	-3.92724500	-3.32326500	-0.78211700
C	-3.34351400	3.33573100	-1.19941400
C	-4.49649300	4.31459500	-0.99082100
C	-2.01460000	4.08631200	-1.32248200
C	-2.01924100	0.76579700	-2.38936200
C	-3.40786900	0.14808200	-2.54237800
C	-0.94810000	-0.13403300	-2.99522800
C	-2.73615800	-0.75483400	3.66475400
C	-3.27293400	-4.04990100	-1.94961700
H	-4.00227900	-4.69040300	-2.46473400
H	-2.44661200	-4.68528700	-1.59414000
H	-4.71360700	-2.64734400	-1.15888400
H	-4.16097900	0.70651100	-1.96801900
H	-0.79799500	0.56168700	-0.68498500
H	-1.24283500	-0.85739400	0.57007200
H	-1.82227500	4.64365700	-0.39168600
H	-1.17488200	3.39433900	-1.47946600
H	-3.53257300	2.81619200	-2.15873600
H	-5.44538100	3.76714900	-0.90504500
C	-4.57405800	-4.28056700	0.21678100
H	-2.04479300	4.80418800	-2.15657400
H	-4.57049500	5.03401700	-1.82056200
H	-1.13369600	-0.29304700	-4.06644700
H	-0.94706300	-1.11335100	-2.48956900
H	-3.70581400	0.13264700	-3.60152900
C	-2.75899700	0.76886700	3.67553700

H	-2.85927500	-3.33494200	-2.67585300
H	-5.02197600	-3.70469300	1.03792300
H	-5.36415900	-4.87465300	-0.26653100
H	-3.82073500	-4.96872100	0.63029500
H	-3.45114200	1.15178700	4.44066200
H	-1.75181700	1.14597400	3.92471500
H	-4.24260800	1.06718300	2.12107700
H	-3.10590600	2.40518100	2.29101800
H	-3.74477300	-1.13538300	3.43337200
H	-2.44197500	-1.15670600	4.64623100
H	-1.71146600	-2.30693000	2.50886600
H	-0.73954600	-0.87249200	2.85686500
C	0.98609900	-2.04222600	-0.50732700
O	-0.05194100	-2.63721800	-0.61853700
O	1.42580800	-1.51026400	0.63495700
I	6.20355800	-0.35124900	0.13880800
C	3.04296500	-1.23215100	-0.97969900
C	2.57808700	-0.67833200	0.37179900
O	1.83211900	-1.81637100	-1.50071400
H	3.40474400	-0.46849200	-1.67310400
H	3.81159600	-2.00593400	-0.86432200
C	2.16265800	0.77848200	0.36128300
C	3.00299500	1.74039900	-0.21362200
C	0.96545100	1.18462100	0.95647100
C	2.62311800	3.08088000	-0.21608400
H	3.97183500	1.43131500	-0.61816300
C	0.58202700	2.52648500	0.94025800
H	0.31371100	0.45178300	1.43214700
C	1.40989700	3.47768000	0.34987500
H	3.28750500	3.82202900	-0.66369200
H	-0.37492900	2.81139700	1.38415400
H	1.11084600	4.52755400	0.33084900
H	3.33821200	-0.86534700	1.14150700

I (M06)

I	0.31335200	0.19073600	0.00000000
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CO₂ (M06)

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15849400
O	0.00000000	0.00000000	-1.15849400

R1 (M06)

C	2.56817500	-0.03865100	0.73377800
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H	3.48544800	-0.59976900	0.96266600
C	1.60164900	-0.57037000	-0.23239000
H	1.84020200	-1.53374600	-0.71094000
O	2.47031000	0.48466600	-0.56287900
C	0.15216500	-0.26099200	-0.13236600
C	-0.29550800	1.06217400	-0.08655500
C	-0.77893000	-1.30043600	-0.06695600
C	-1.65444200	1.33787700	0.03473100
H	0.43890300	1.86982600	-0.16575400
C	-2.13766900	-1.02388800	0.05785100
H	-0.43224500	-2.33873100	-0.11745000
C	-2.57884500	0.29693900	0.11043000
H	-1.99660800	2.37667200	0.06429700
H	-2.85867000	-1.84499100	0.10917700
H	-3.64653500	0.51574000	0.20345800
H	2.19696500	0.60962900	1.54164200

G10-Cu

H	1.44718300	-4.35567300	1.23627100
H	4.64035100	0.99703200	-0.01371500
H	3.46202600	-0.05406300	1.93960300
H	5.77905200	-1.80902400	-0.48351300
H	-1.78330100	1.91956200	1.30558500
H	1.67605600	2.42909200	-1.62211600
H	0.05648900	2.82770300	2.14552200
O	-0.44260400	1.56448000	-1.51023600
N	1.24963900	-1.27343100	-0.19053500
N	3.41734400	-0.53600900	-0.76591400
N	1.80793800	0.99439300	-0.10653500
N	-1.68332900	2.09400100	0.30979300
C	2.11582700	-0.31394000	-0.36134200
C	2.41066700	2.09493500	-0.86747700
C	0.95432700	2.52728600	1.58244200
C	0.62244800	1.35981900	0.64764900
C	-0.55518500	1.66344800	-0.30098400
C	-2.90201000	2.38346600	-0.44770100
C	1.66438900	-2.67724800	-0.12206300
C	1.08971600	-3.31842900	1.13047200
C	1.23108900	-3.41363300	-1.37899900
C	4.55768800	-0.10407300	0.05500100
C	5.81422300	-0.70561200	-0.53887300
C	4.38704400	-0.48189000	1.51769500
C	1.54701500	3.70355500	0.82569200
C	-4.07711100	2.39347900	0.50562700

H	-5.01081300	2.60536100	-0.03699700
H	-3.95251400	3.17694400	1.27531800
H	-3.03473700	1.56074800	-1.17728100
H	1.68516100	2.16258200	2.32845600
H	3.27699100	1.71101600	-1.41955500
H	5.93615700	-0.41829300	-1.59481100
H	3.55298900	-1.45559800	-1.17429700
H	0.32848500	0.48897300	1.26475300
H	1.65684300	-2.95245400	-2.28573400
H	1.53992500	-4.47095100	-1.34613100
H	2.76891500	-2.74410900	-0.03760900
H	-0.01404300	-3.33880000	1.09004700
C	-2.75596800	3.69689000	-1.19522300
H	0.13090900	-3.38244400	-1.47535300
H	1.38571000	-2.75470600	2.03051800
H	5.23145200	-0.11197400	2.12105000
H	4.34101300	-1.57887300	1.63752900
H	6.70667800	-0.37704800	0.01449700
C	2.77136000	3.25026100	0.04627000
H	3.56310600	2.93527200	0.75503100
H	3.18827700	4.07563200	-0.55435100
H	1.79893700	4.52104900	1.52094300
H	0.79165100	4.11319200	0.12564800
H	-4.18912200	1.41487300	1.00094900
H	-1.89333300	3.66524200	-1.87703000
H	-3.65663200	3.90478700	-1.79494800
H	-2.61556000	4.53103800	-0.48527600
Cu	-0.68752800	-1.16579300	-0.14433400
I	-3.05866800	-1.49521700	0.19882600

G10-Cu-IM1

H	0.92030000	-3.46116500	3.01909100
H	2.44133700	1.75852100	2.72679300
H	2.68088400	-0.56197200	3.57453800
H	4.78727000	1.07137000	0.87070900
H	-2.95991600	0.31981700	-0.06436700
H	0.18847200	3.39793200	0.31921600
H	-2.61328200	2.32826500	3.07190400
O	-2.12591700	3.36581400	0.17642000
N	0.25757100	-0.82280700	0.98182200
N	2.20733900	0.47572600	1.09987300
N	0.10706300	1.50786500	1.21077700
N	-2.89169200	1.30732300	-0.32882300
C	0.84319600	0.34160100	1.11778100

C	0.70301500	2.83953500	1.11932200
C	-1.53140900	2.27463200	2.85602200
C	-1.31862300	1.52868700	1.53617500
C	-2.14310400	2.16125400	0.40120600
C	-3.72275500	1.75577200	-1.43524400
C	0.96030400	-2.05969500	1.35344200
C	0.40443800	-2.54522300	2.68492800
C	0.81362000	-3.12402000	0.27979300
C	3.05195000	1.04446900	2.14846100
C	4.22689000	1.77141500	1.51649100
C	3.53127300	-0.04451600	3.09916400
C	-0.90146100	3.66177200	2.87419400
C	-3.81986000	0.65813600	-2.47821300
H	-4.38591100	1.00745200	-3.35675400
H	-4.33222300	-0.22921300	-2.06687100
H	-3.20867200	2.63737600	-1.86244600
H	-1.07852000	1.64900200	3.64981300
H	1.74766400	2.73841400	0.80235500
H	3.89360400	2.61287500	0.88716800
H	2.70056500	-0.26878600	0.57982100
H	-1.64289800	0.48223900	1.66614700
H	1.26428600	-2.79649900	-0.67040700
H	1.34536200	-4.04106600	0.58268000
H	2.04375200	-1.87559900	1.47294900
H	-0.67477400	-2.76627400	2.59413700
C	-5.09010300	2.19497300	-0.93575900
H	-0.24995300	-3.38555900	0.11251800
H	0.52350300	-1.77465500	3.46644900
H	4.16539300	0.37722900	3.89730000
H	4.12530500	-0.79299500	2.54508800
H	4.91185700	2.16304700	2.28664200
C	0.55422100	3.59861900	2.43107300
H	1.15286800	3.10267300	3.21969800
H	0.97032900	4.61448700	2.31407400
H	-0.97605500	4.09366000	3.88799400
H	-1.46280500	4.32121300	2.19380800
H	-2.82026900	0.32877100	-2.80490000
H	-4.98920800	3.00730600	-0.19903000
H	-5.71967000	2.55662000	-1.76599800
H	-5.60836100	1.34678700	-0.45501600
Cu	-1.49412500	-1.35089000	0.29643500
I	-3.75007200	-2.34088200	0.25901300
O	-0.63241900	-0.72389400	-1.87809300
C	0.69848000	-0.33515100	-2.18128400

C	-0.15392000	-1.00274700	-3.17056100
H	1.49055900	-0.94037100	-1.70764800
H	0.01077400	-2.06483800	-3.39867900
H	-0.60483900	-0.40498300	-3.97782000
C	0.97818500	1.12213800	-2.22852300
C	2.30225100	1.56679700	-2.15177900
C	-0.05799500	2.05414300	-2.33581400
C	2.57984600	2.93073500	-2.21471200
H	3.10919100	0.83142400	-2.02276100
C	0.22299800	3.41658200	-2.38896600
H	-1.09383900	1.70043900	-2.34274400
C	1.54505800	3.85763000	-2.33745100
H	3.61880200	3.27074800	-2.15476800
H	-0.60017700	4.13572100	-2.44470900
H	1.76750600	4.92891900	-2.37534200
I	4.40549100	-1.67156800	-0.80916200

G10-Cu-TS1

H	-1.82354300	-4.68756700	-1.76276600
H	3.08382000	-2.92432900	1.49728800
H	0.92588300	-4.25054600	1.62819800
H	3.43768800	-4.33324700	-1.19259200
H	-2.36514100	0.60379500	0.84782800
H	1.71272500	0.22529200	2.44736400
H	-1.65251700	-1.50935400	3.89451300
O	-0.27530300	1.16379700	3.16589500
N	-0.34582300	-1.84687000	-0.64728700
N	1.86773400	-2.43489100	-0.15613600
N	0.60127800	-1.18602800	1.37977400
N	-1.79400200	1.16292600	1.49263500
C	0.66919800	-1.84366300	0.17111900
C	1.77450900	-0.84451000	2.18317600
C	-0.71805600	-1.73921800	3.35278000
C	-0.68153100	-0.94158800	2.04614500
C	-0.89742800	0.56059500	2.29557000
C	-2.12207000	2.57905900	1.59187300
C	-0.51370600	-2.95087700	-1.58938400
C	-1.65169300	-3.83041100	-1.08912000
C	-0.78583600	-2.44566500	-2.99573000
C	2.65047300	-3.40131100	0.59651500
C	3.80985500	-3.83349700	-0.27913100
C	1.79939200	-4.58105700	1.04006400
C	0.49715000	-1.50426800	4.24472800
C	-2.35807600	3.15364000	0.20826200

H	-2.54522500	4.23834000	0.27416200
H	-3.23478300	2.67860900	-0.26798800
H	-1.23922400	3.06086200	2.04690100
H	-0.77226500	-2.80955800	3.06979800
H	2.67743600	-0.94922400	1.56512800
H	4.40930900	-2.95835400	-0.58047900
H	2.11868300	-2.33034600	-1.13477800
H	-1.46931600	-1.30548600	1.36573500
H	0.04772200	-1.83036400	-3.37276600
H	-0.93180300	-3.28734800	-3.69327500
H	0.40581400	-3.57287300	-1.62293300
H	-2.58218900	-3.24028400	-1.01999500
C	-3.31654300	2.77072600	2.51245000
H	-1.70349100	-1.82801800	-3.01289100
H	-1.42472500	-4.21997400	-0.08137000
H	2.38215300	-5.27730100	1.66682600
H	1.41877200	-5.13629400	0.16417200
H	4.46057800	-4.54368900	0.25426500
C	1.79817300	-1.66468500	3.46562600
H	1.95012100	-2.73375200	3.22009800
H	2.66085900	-1.35960300	4.08298300
H	0.47340000	-2.20439200	5.09872800
H	0.44413800	-0.48382000	4.65493600
H	-1.49290300	2.98193900	-0.45207200
H	-3.10149300	2.36996100	3.51645300
H	-3.57259100	3.83872200	2.61291300
H	-4.19618700	2.24154600	2.10520200
Cu	-1.68322500	-0.33745200	-1.07288700
I	-4.20391200	-0.48031700	-0.84696200
C	1.12816800	1.35731400	-0.95792000
H	1.04531200	0.62867700	-0.14964000
C	0.74037600	0.90173200	-2.27943500
H	1.07454800	1.52357600	-3.13374500
H	0.98415200	-0.15947900	-2.48343200
O	-0.53201300	1.16758900	-1.80971400
C	1.24122700	2.75629000	-0.56549300
C	1.26828900	3.07634000	0.79876300
C	1.25349900	3.79613700	-1.50574200
C	1.29927900	4.40220400	1.21484700
H	1.23659600	2.27294400	1.54293200
C	1.27918200	5.12053100	-1.08847500
H	1.22492800	3.55658800	-2.57242900
C	1.30053000	5.42964700	0.27292700
H	1.30900200	4.63042700	2.28502800

H	1.27908900	5.92349200	-1.83208400
H	1.31631800	6.47490800	0.59743500
I	3.98145800	0.55604900	-1.00509000

G10-Cu-IM2

H	3.54865400	3.53846300	-2.14304600
H	-1.30672600	4.29030800	1.35957200
H	1.19951200	4.32573800	1.31188200
H	-1.11571300	5.50382500	-1.44323600
H	1.90725800	-1.42991200	0.94156900
H	-1.78330800	0.81873900	2.34162100
H	2.01717600	0.64711700	3.82593700
O	-0.54456100	-1.00873100	2.91062600
N	1.13659900	1.68152000	-0.65613400
N	-0.70991000	3.11804600	-0.27624800
N	-0.09555100	1.50283900	1.31039100
N	1.11816300	-1.70778000	1.53791500
C	0.16612100	2.09473200	0.09200600
C	-1.28820000	1.77647000	2.10632400
C	1.31360100	1.31644400	3.30003900
C	0.91563600	0.67354800	1.96865400
C	0.41420200	-0.76229200	2.18106000
C	0.77701000	-3.12313600	1.54807900
C	1.67466900	2.50838700	-1.72415500
C	3.09786800	2.90632700	-1.35829100
C	1.63466800	1.78880100	-3.06334800
C	-0.77605700	4.41321400	0.39544000
C	-1.61176200	5.33620000	-0.46903100
C	0.59361400	5.00643900	0.69067800
C	0.11907700	1.65815200	4.18131800
C	0.86523300	-3.67894500	0.13822900
H	0.52531000	-4.72831700	0.11962100
H	1.90952200	-3.65473500	-0.22342100
H	-0.26703800	-3.17827800	1.90264400
H	1.87726600	2.23945700	3.05974300
H	-1.99636600	2.35615100	1.49949300
H	-2.60437300	4.89870900	-0.66154700
H	-0.74451300	3.20813100	-1.28751000
H	1.78836200	0.64959900	1.29625400
H	0.61094100	1.47630500	-3.32445100
H	2.01905300	2.44322600	-3.86454900
H	1.08924000	3.45021300	-1.83610000
H	3.71799200	2.00288400	-1.22733200
C	1.67008500	-3.86608700	2.52829000

H	2.26159900	0.87925300	-3.03144000
H	3.11395700	3.46504900	-0.40726400
H	0.50097300	5.96220400	1.23364900
H	1.15454700	5.19201700	-0.24297300
H	-1.74583800	6.31856000	0.01023700
C	-0.90994400	2.47252000	3.40719500
H	-0.49036100	3.47386800	3.18035300
H	-1.81586500	2.63873100	4.01626500
H	0.45546700	2.21342700	5.07506100
H	-0.34886400	0.72337500	4.53204600
H	0.26135500	-3.07941800	-0.56701200
H	1.56054100	-3.45792900	3.54687300
H	1.41967300	-4.94000300	2.55562500
H	2.72867400	-3.76852200	2.22849600
Cu	1.62845100	-0.40867400	-1.09856800
I	4.07076900	-0.98968900	-0.62370600
C	-1.98621000	-0.68389600	-0.73751300
H	-1.48691300	-0.27048700	0.15597100
C	-1.12712900	-0.43553000	-1.97560000
H	-1.74434300	-0.69787100	-2.87929200
H	-1.00466100	0.68078100	-2.05581600
O	0.00823200	-1.14503000	-1.87142600
C	-2.40819200	-2.09252800	-0.48740900
C	-2.65012900	-2.52754900	0.82078800
C	-2.57480600	-3.00237300	-1.53824500
C	-3.05524000	-3.83575800	1.07333100
H	-2.48602100	-1.83083200	1.65130700
C	-2.97845100	-4.30943700	-1.28681800
H	-2.35737900	-2.68167500	-2.56086800
C	-3.22422700	-4.73191100	0.01975200
H	-3.22923600	-4.15801500	2.10516200
H	-3.09233000	-5.01146100	-2.11920200
H	-3.53621000	-5.76295300	0.21615900
I	-3.83490500	0.58898700	-0.86726900

G10-Cu-TS2

H	2.94131200	3.74271100	-2.59635900
H	-2.14448200	4.25829600	0.73442500
H	0.29609700	4.84325000	0.63823200
H	-2.18410400	5.06317300	-2.21694300
H	2.05630500	-0.68429000	1.39201800
H	-2.07597900	1.02242600	2.23459200
H	1.58886100	1.81195500	3.84239600
O	-0.58109900	-0.42107000	3.13799500

N	0.77850200	1.84233500	-0.80519000
N	-1.26665200	3.02745200	-0.71593000
N	-0.48378700	1.84426200	1.15319300
N	1.26620300	-1.00843600	1.96448600
C	-0.26736900	2.23700000	-0.15232100
C	-1.75259300	2.00797200	1.85777200
C	0.80567300	2.24188300	3.19333500
C	0.61511400	1.33271600	1.97536800
C	0.36588600	-0.11983600	2.41357900
C	1.21112500	-2.43953200	2.22817100
C	1.23519500	2.52508100	-2.00739500
C	2.57109400	3.19382300	-1.71335900
C	1.35019500	1.56973300	-3.18732900
C	-1.63731200	4.35842800	-0.24252500
C	-2.64461900	4.92933600	-1.22041100
C	-0.44252200	5.28054000	-0.05459700
C	-0.48319800	2.47750000	3.96930400
C	1.47704200	-3.19621200	0.93997200
H	1.35717100	-4.28136700	1.09480400
H	2.50407100	-3.00889300	0.57910200
H	0.18357500	-2.64563300	2.57566400
H	1.19976500	3.20744500	2.81940100
H	-2.52140800	2.33402100	1.14556900
H	-3.50583800	4.25133400	-1.33063200
H	-1.23830600	2.97679300	-1.73007600
H	1.52083700	1.36414300	1.34899900
H	0.38539500	1.09355100	-3.42667400
H	1.70008500	2.10952900	-4.08355800
H	0.52733500	3.33151300	-2.30739300
H	3.31894000	2.43582800	-1.42444900
C	2.19293900	-2.80085000	3.33077300
H	2.07655100	0.76289800	-2.97273700
H	2.47906300	3.90429700	-0.87471300
H	-0.75624500	6.25361200	0.35986500
H	0.06829300	5.46678700	-1.01616400
H	-3.00916400	5.91367200	-0.88758600
C	-1.59158400	2.95449000	3.03968400
H	-1.34873100	3.97150300	2.67004100
H	-2.55010900	3.03393200	3.58199800
H	-0.31171500	3.21410200	4.77411300
H	-0.79299200	1.53281800	4.44605000
H	0.79258600	-2.86410200	0.14143000
H	1.95857200	-2.25638100	4.26056500
H	2.16582900	-3.88237100	3.54473000

H	3.22083600	-2.53752900	3.02427600
Cu	1.70254500	-0.11440700	-0.80079500
I	4.15812000	-0.16364300	-0.08940300
C	-1.87110400	-1.00586700	-0.44763900
H	-1.46537100	-0.38106000	0.36721700
C	-1.07971000	-0.77283800	-1.72746300
H	-1.57434000	-1.30243400	-2.57345500
H	-1.16363100	0.31321700	-1.97225100
O	0.20602700	-1.20078700	-1.57279600
C	-2.02384400	-2.41557500	0.01445500
C	-2.21964200	-2.67124200	1.37711900
C	-1.97429100	-3.49499000	-0.87639100
C	-2.36676900	-3.97442600	1.84217700
H	-2.22145200	-1.83045600	2.08095200
C	-2.11791000	-4.79810700	-0.40804200
H	-1.78886300	-3.31842400	-1.94001500
C	-2.31812900	-5.04420600	0.94944300
H	-2.50791100	-4.15445500	2.91281200
H	-2.06106500	-5.63216000	-1.11446400
H	-2.42562000	-6.07126600	1.31327100
I	-3.89566700	-0.11820400	-0.74161100
C	0.87068300	-2.43300000	-2.88235200
O	-0.06690300	-2.70581600	-3.55699300
O	2.00898500	-2.50939000	-2.58221800

G10-Cu-IM3

Cu	2.27891300	-0.85791600	-0.90131500
I	3.71283500	-2.78316100	-0.04545600
H	5.50315700	1.14228900	-2.46533000
H	1.81810400	4.60151700	1.40070700
H	3.71245000	2.99401800	1.74916400
H	3.40735000	5.50617400	-1.05606500
H	1.28312500	-1.99510800	0.88197500
H	-0.83625600	2.06014000	1.45026700
H	1.47878500	-0.36142000	3.80045100
O	-1.08048700	-0.08961300	1.80115500
N	2.65374000	1.16001200	-0.61168300
N	1.91115300	3.38506100	-0.30679600
N	1.20232700	1.71658100	1.14366400
N	0.32330200	-1.72346700	1.12324900
C	1.94160000	2.02903200	0.03365600
C	0.12243400	2.57249900	1.62996500
C	1.46850100	0.62370700	3.30091800
C	1.29106600	0.41419200	1.79215800

C	0.05924300	-0.47352700	1.54495300
C	-0.73724800	-2.68852300	0.86040200
C	3.52966700	1.59773500	-1.68808900
C	4.79983600	0.76733600	-1.70192300
C	2.79412300	1.52111100	-3.02164300
C	2.51989400	4.38577900	0.56988800
C	2.69138900	5.66308900	-0.22794600
C	3.83735500	3.93074800	1.18189300
C	0.40251000	1.53329000	3.89770700
C	-0.34994500	-3.59743000	-0.28762000
H	-1.17277100	-4.30243700	-0.49318500
H	0.55840000	-4.17899800	-0.04682100
H	-1.61585000	-2.09412000	0.55969200
H	2.46978200	1.07059300	3.45521200
H	0.10532200	3.49272500	1.03459000
H	1.73317700	5.99125500	-0.66134700
H	2.15195500	3.52785500	-1.28124100
H	2.18644400	-0.09208300	1.39302900
H	1.85386200	2.09902100	-2.99868000
H	3.42541100	1.88487300	-3.85078800
H	3.84557600	2.65371700	-1.52988800
H	4.57577300	-0.29191900	-1.91653300
C	-1.07883700	-3.45454500	2.12785800
H	2.50246300	0.47737000	-3.23050100
H	5.29441900	0.79591100	-0.71680700
H	4.23210200	4.69348100	1.87397800
H	4.59651900	3.75007700	0.40022800
H	3.08469600	6.47577800	0.40253900
C	0.30739500	2.83842600	3.11610800
H	1.23742700	3.42439500	3.26951900
H	-0.52591700	3.45805300	3.49157200
H	0.62716100	1.73239400	4.96076300
H	-0.57282700	1.01958500	3.86039300
H	-0.14983900	-3.00574400	-1.19549200
H	-1.38074000	-2.76449500	2.93321100
H	-1.91349600	-4.15364700	1.94889500
H	-0.20513100	-4.03617700	2.47283700
C	-0.37623500	-0.12548200	-1.77271600
O	0.54083500	-0.95473900	-1.96336200
O	-0.35806800	1.00790300	-1.29882000
C	-2.70330200	0.24495200	-2.09258000
C	-3.26920800	0.25264100	-0.68579100
O	-1.62030700	-0.63535700	-2.18674700
H	-3.46848700	-0.08706500	-2.81878100

H	-2.39917000	1.27235000	-2.35407900
C	-3.81013200	-1.03745900	-0.16387600
C	-4.07943200	-2.12420500	-1.00112800
C	-4.00836800	-1.18760700	1.21630200
C	-4.54363400	-3.32824700	-0.47322200
H	-3.88449300	-2.04687300	-2.07367800
C	-4.48199100	-2.38273700	1.74112100
H	-3.74826500	-0.35379700	1.87572700
C	-4.75367100	-3.46054400	0.89650000
H	-4.73319000	-4.17341200	-1.14224100
H	-4.62034800	-2.48380100	2.82224800
H	-5.11529600	-4.40757900	1.30995400
H	-2.51319200	0.66100300	0.00540600
I	-4.86083900	1.79156600	-0.64128000

G10-Cu-TS3

Cu	2.25082200	-0.49038900	-1.03951300
I	4.27835800	-1.91436000	-0.56522400
H	4.10139900	2.28078800	-3.28008700
H	0.90012300	4.57192000	1.75143000
H	3.13820100	3.47642400	1.44351600
H	1.53122600	5.97507000	-0.89682800
H	1.92705700	-1.88261100	0.80681100
H	-0.91493900	1.43505300	2.26124600
H	2.54258200	-0.22537100	3.66955700
O	-0.46902700	-0.68956900	2.50202500
N	1.90871500	1.53659900	-0.78672600
N	0.82531300	3.50687000	-0.05679100
N	0.95188200	1.66566700	1.35502800
N	1.02275300	-1.86852100	1.28862900
C	1.25194700	2.18834100	0.12466400
C	-0.12191300	2.19828300	2.19516200
C	2.11687000	0.71195000	3.26960700
C	1.57201300	0.44328500	1.86272900
C	0.59543700	-0.74572900	1.89696500
C	0.15282500	-3.02698500	1.14061400
C	2.36266600	2.23082000	-1.98839000
C	3.71621000	1.70003000	-2.42462800
C	1.33592900	2.10182600	-3.10808400
C	1.39156400	4.58641900	0.75957800
C	1.04562000	5.90313600	0.09415300
C	2.89122800	4.44346700	0.97508100
C	1.06691100	1.28870500	4.21005700
C	0.54778900	-3.78732000	-0.10815500

H	-0.12758200	-4.64481300	-0.26154400
H	1.58338200	-4.16496100	-0.03096200
H	-0.86937900	-2.62669900	1.01954100
H	2.95820500	1.42497600	3.16704000
H	-0.55457600	3.07764700	1.70319000
H	-0.04194600	6.00139200	-0.04963300
H	0.80419000	3.75706600	-1.03958300
H	2.41790000	0.20279500	1.19521100
H	0.34560900	2.48715000	-2.80504200
H	1.65798600	2.65168700	-4.00856000
H	2.50564100	3.31346600	-1.77467500
H	3.64779200	0.63993000	-2.72758700
C	0.16743800	-3.89447000	2.38736400
H	1.19443200	1.04072100	-3.37298400
H	4.44542500	1.75358700	-1.60032600
H	3.27064500	5.24272300	1.63309700
H	3.43566800	4.50130800	0.01579300
H	1.39437000	6.75541600	0.69761600
C	0.40324400	2.51064300	3.58844800
H	1.14089700	3.33694300	3.52871800
H	-0.42547000	2.87041800	4.22273400
H	1.52899400	1.54947600	5.17852500
H	0.29919300	0.52290400	4.40902600
H	0.49780000	-3.13602600	-0.99596900
H	-0.13923900	-3.30554000	3.26654200
H	-0.53567000	-4.73808300	2.27829900
H	1.17674200	-4.30483100	2.56831400
C	-0.54630800	-0.47267600	-1.71800200
O	0.52172400	-0.91694600	-2.14678700
O	-0.84074700	-0.14496800	-0.53593300
C	-2.69540300	0.32021800	-2.05510800
C	-2.83105200	0.00440500	-0.58513100
O	-1.55624200	-0.31168700	-2.61751000
H	-3.56883600	-0.03341300	-2.62017700
H	-2.62930900	1.41464700	-2.18481400
C	-3.13431800	-1.33889900	-0.09579000
C	-3.18656800	-2.43943100	-0.96356200
C	-3.28330800	-1.55143500	1.28231900
C	-3.39096100	-3.72065500	-0.46126500
H	-3.04388100	-2.29471100	-2.03856000
C	-3.48704900	-2.83023900	1.77995700
H	-3.23095600	-0.69424000	1.95921400
C	-3.54317900	-3.92080600	0.90968000
H	-3.42391600	-4.57193600	-1.14787700

H	-3.58980400	-2.98101900	2.85863600
H	-3.69756200	-4.93029100	1.30392800
H	-2.76306300	0.80246300	0.14975900
I	-5.50015500	1.02518300	-0.53159800

G10-Cu-IM4

Cu	-1.96073700	-1.16504900	0.00277300
I	-4.37481300	-1.72842100	0.09415700
H	-0.14351500	-4.30014700	1.99163000
H	1.93685600	0.50329700	3.44966700
H	1.68780400	-1.96862300	3.66351500
H	4.56437600	-0.15407400	1.99581500
H	-3.43849100	0.83709400	0.18113700
H	0.71297900	2.96482100	0.91191200
H	-2.79645300	2.28134300	2.87323400
O	-1.27940000	3.14267100	-0.03158600
N	-0.12414100	-1.12861400	0.74939800
N	1.94537700	-0.31904800	1.53599400
N	0.08229600	1.07287500	1.54649500
N	-3.06125500	1.75369500	-0.08240900
C	0.60283700	-0.17549800	1.27803100
C	0.91834100	2.26271700	1.73546900
C	-1.71718200	2.04964700	2.88859100
C	-1.34878600	1.32960100	1.58421500
C	-1.85703100	2.14796800	0.38711500
C	-3.74435200	2.46667100	-1.15143700
C	0.32226800	-2.52870900	0.82019700
C	-0.47485400	-3.25247800	1.89576000
C	0.17082100	-3.20287500	-0.53128700
C	2.58100000	-0.15877700	2.84198100
C	3.95567900	0.46764000	2.67673100
C	2.68180600	-1.50633000	3.54378900
C	-0.88020600	3.29755500	3.12278300
C	-3.27616100	1.99732400	-2.51829500
H	-3.77630200	2.56485100	-3.32121200
H	-3.49739500	0.92560000	-2.65283100
H	-3.46557700	3.52934600	-1.02970000
H	-1.55339500	1.33239200	3.71518400
H	1.97234600	1.97768300	1.65034500
H	3.89834100	1.47799900	2.24007800
H	2.42971700	-1.02082200	0.95741000
H	-1.86322800	0.35214500	1.58632500
H	0.80063800	-2.71404600	-1.29294300
H	0.49788300	-4.25383800	-0.47323000

H	1.39401300	-2.59114900	1.08552100
H	-1.55286500	-3.24853100	1.65212800
C	-5.24211300	2.29883400	-0.97706100
H	-0.88293100	-3.18818600	-0.87247600
H	-0.35324300	-2.76000800	2.87617300
H	3.14116800	-1.40772500	4.54180600
H	3.30649400	-2.19201200	2.94373900
H	4.47813400	0.54048600	3.64494300
C	0.60074500	2.95186200	3.05133800
H	0.86728200	2.29204600	3.90125400
H	1.22267200	3.85897800	3.14345100
H	-1.13446900	3.75005800	4.09726900
H	-1.11579200	4.04741400	2.34644000
H	-2.18777700	2.13321600	-2.62331900
H	-5.57660700	2.67233900	0.00424400
H	-5.79101300	2.84307800	-1.76244500
H	-5.51802200	1.23137400	-1.04528000
C	-0.33594100	-0.31001700	-2.40162300
O	-1.46085100	-0.71391100	-2.32213800
O	0.17458600	0.66181300	-1.64109100
C	1.78721100	-0.02033200	-3.11139700
C	1.60529700	0.60704900	-1.73818100
O	0.58367100	-0.77510700	-3.25401800
H	1.84305100	0.73181000	-3.91937500
H	2.65597200	-0.69801300	-3.13978200
C	2.23157500	1.93812600	-1.49935200
C	1.51021200	3.12453800	-1.64193200
C	3.57157200	1.97511000	-1.09915900
C	2.13004100	4.34565100	-1.38352500
H	0.44435300	3.08560400	-1.88393600
C	4.18546400	3.19932200	-0.84915900
H	4.11460100	1.02820200	-0.96576000
C	3.46621000	4.38645800	-0.98968600
H	1.55291800	5.27117200	-1.47181200
H	5.23180500	3.22404600	-0.52912300
H	3.94745800	5.34758500	-0.78138800
H	1.98163800	-0.11458400	-0.98642600
I	4.18838300	-2.09664000	-0.67230300

G5-TS1

N	-2.45348100	-1.70814400	0.30508500
C	-3.29509100	-0.92480600	-0.40237300
N	-3.46940000	-0.72778400	-1.65871100
N	-4.06802100	-0.14656700	0.48585400

C	-4.49185200	0.31004200	-1.73746600
H	-4.25309100	1.05820600	-2.51139800
H	-5.47367300	-0.12413000	-2.00990200
C	-4.56411100	0.94827300	-0.32246000
H	-5.58116900	1.26024600	-0.03962900
H	-3.89263400	1.82690700	-0.24331400
C	-3.27008700	0.01835000	1.68934000
H	-3.88823100	0.14807800	2.59016400
H	-2.58681300	0.88663200	1.59733200
C	-2.47379300	-1.30422700	1.70218000
H	-1.52983600	-2.04465100	-0.04179900
C	1.24309300	-2.09193900	-0.40448200
H	2.07855700	-2.81422300	-0.29902200
C	1.41215100	-0.91203800	0.46127200
H	1.72747000	-1.14202900	1.47801200
O	0.09836600	-2.38936600	0.26942700
I	3.79174200	0.05757800	-0.07572000
H	1.14839500	-1.83376700	-1.48174100
C	0.55008800	0.28449100	0.30246700
C	-0.33560000	0.41734200	-0.77418600
C	0.62316000	1.32347700	1.24136700
C	-1.09446100	1.57535300	-0.92847100
H	-0.46353100	-0.40168900	-1.48290100
C	-0.13524300	2.48034900	1.08934300
H	1.32209200	1.22801600	2.07542100
C	-0.99108900	2.61663300	-0.00574600
H	-1.78532700	1.64227100	-1.77129200
H	-0.05020000	3.28385900	1.82373300
H	-1.58429200	3.52520600	-0.13067900
H	-1.44355000	-1.18172600	2.06512600
H	-2.97759500	-2.05870400	2.33240000

G6-TS1

N	-0.55297400	-1.47841900	-0.18079200
C	0.33310900	-0.53546000	0.20885000
C	-1.97348100	-1.18397500	-0.18637100
H	-2.40204000	-1.26879300	0.83166400
H	-2.47201000	-1.94341500	-0.80445000
N	1.51862500	-0.74447800	0.67462100
N	-0.01954100	0.82166600	0.05242500
C	2.12885900	0.56293100	0.83690800
H	2.71539600	0.62821600	1.76675300
H	2.82532400	0.77898800	0.00253000
C	0.95903500	1.56838900	0.81356200

H	1.20746700	2.53011500	0.33752800
H	0.58115700	1.77930200	1.83723400
C	-1.40898200	1.21450800	0.09274200
H	-1.50599700	2.23322900	-0.31807400
H	-1.78584400	1.24037200	1.13844600
C	-2.22629400	0.21889800	-0.71924700
H	-3.29605200	0.46667300	-0.65654600
H	-1.91659200	0.27818000	-1.77467700
H	-0.36203600	-2.47066500	0.08788700
C	-0.40032700	-4.79666600	1.56477000
H	-0.36888400	-5.89526000	1.41025400
C	-1.58975300	-4.37677100	2.33053100
H	-2.51765600	-4.83968000	1.99743600
O	-0.83357400	-4.05032400	0.51115600
I	-1.65417600	-5.74880500	4.54658800
H	0.55692100	-4.49553700	2.04307800
C	-1.71059200	-2.98753500	2.83435900
C	-0.61953800	-2.11067000	2.83849300
C	-2.95031000	-2.52085900	3.29375800
C	-0.77205800	-0.79981600	3.28396200
H	0.34550000	-2.42051200	2.43428800
C	-3.10244600	-1.21221500	3.74167600
H	-3.79595400	-3.21224900	3.30882000
C	-2.01003600	-0.34218400	3.73706000
H	0.09179400	-0.13206900	3.25437900
H	-4.07661300	-0.86921400	4.09596000
H	-2.12368600	0.68762300	4.08302300

G7-TS1

N	-0.03836700	-1.53426000	-0.51464900
C	-0.90281800	-0.52518400	-0.26427900
N	-0.39243100	0.71940300	0.18219000
C	1.18185800	-1.77718000	0.22728400
H	1.43347400	-2.82129000	-0.00165300
H	1.00485400	-1.70357800	1.31899300
C	2.34211900	-0.86922100	-0.15769700
H	2.48730700	-0.93715400	-1.24785000
H	3.26306800	-1.24547000	0.31768800
C	-2.71699200	0.69521100	-0.02771700
H	-3.18678000	0.62165900	0.97237400
H	-3.49962200	1.05152100	-0.71704500
C	0.87013400	1.20618800	-0.36369200
H	0.89379000	2.28827500	-0.16345100
H	0.89387400	1.07636300	-1.46612100

C	-1.50881200	1.64505200	0.01421600
H	-1.54973900	2.39230700	0.82186100
H	-1.40712100	2.18524800	-0.94946300
C	2.11940000	0.58190600	0.24595300
H	2.04001500	0.66199100	1.34389700
H	2.98605300	1.18891000	-0.06358600
N	-2.17992000	-0.59135900	-0.42037900
H	-0.41846700	-2.40674200	-0.91216400
C	-0.02794100	-4.76858300	-2.58550300
H	-0.17816000	-5.86567700	-2.50285300
C	1.37567100	-4.42274800	-2.88216500
H	2.10442600	-4.95884000	-2.27571000
O	0.05334700	-4.07397500	-1.42163200
I	2.06728100	-5.81191400	-4.98333800
H	-0.73659200	-4.39015000	-3.35658800
C	1.75339400	-3.04060700	-3.26874100
C	0.78621900	-2.05536200	-3.50430600
C	3.10570600	-2.69795200	-3.40664600
C	1.16405000	-0.76832600	-3.88022700
H	-0.26673800	-2.29280200	-3.35141500
C	3.48434800	-1.41276300	-3.78375600
H	3.86045800	-3.47062000	-3.24473200
C	2.51228600	-0.43976400	-4.02408300
H	0.39464000	-0.01185200	-4.04872200
H	4.54302900	-1.16915900	-3.89292200
H	2.80470400	0.57076400	-4.31734100

G8-TS1

N	-3.56400300	0.00889300	0.17525000
N	-1.45708300	0.03983400	1.26876700
C	-3.70156700	-1.43367400	0.21875200
H	-4.03699900	-1.78391100	-0.77710100
H	-4.50356200	-1.71066100	0.93152100
C	-2.40147700	-2.12305700	0.60397400
C	-1.72247700	-1.30449200	1.69787200
C	-2.38072600	0.63259100	0.58596500
N	-2.24175100	1.94954900	0.26680000
H	-1.26921300	2.34337100	0.29841500
C	-4.57743800	0.66644300	-0.62473700
H	-5.56712700	0.28847500	-0.30804100
H	-4.45253100	0.38671800	-1.69211000
C	-4.51123400	2.17675900	-0.49645900
C	-3.06953100	2.60026800	-0.71628000
H	-2.94204200	3.68539500	-0.59762700

H	-2.76744500	2.35431800	-1.75446000
H	-5.18585300	2.63838600	-1.23259700
H	-4.83209500	2.48337400	0.51161400
H	-2.60818100	-3.15802200	0.91730000
H	-1.72313100	-2.16462000	-0.26272600
H	-0.77615800	-1.78410000	1.99471600
H	-2.37110700	-1.32285700	2.60134600
C	1.17561500	2.60402900	-0.52448000
H	2.11383800	3.13384800	-0.25644000
C	0.89370800	2.68752500	-1.97236100
H	0.99316100	3.69290400	-2.37849700
O	0.01218500	3.26509200	-0.26515400
I	2.99961800	1.89202700	-3.26888100
C	-0.16619900	1.85808700	-2.59426100
C	-0.74675100	2.27036300	-3.80153800
C	-0.61306000	0.66677700	-2.00727000
C	-1.75406500	1.52430400	-4.40710200
H	-0.38530400	3.18800000	-4.27109100
C	-1.62555400	-0.07629800	-2.61015300
H	-0.20448000	0.33872700	-1.04924900
C	-2.20145900	0.34506700	-3.81026500
H	-2.19170100	1.86406500	-5.34797900
H	-1.97899900	-0.99152200	-2.12884400
H	-2.99330500	-0.24417700	-4.27778300
H	1.25640600	1.56345800	-0.14426700

G9-TS1

N	-1.52505300	-1.05544900	-0.92099200
N	0.32360500	-1.62004000	0.31915000
C	-0.47888400	-0.68983500	-0.25297700
N	-0.12902900	0.65427900	-0.04497600
C	-2.28780900	0.01749700	-1.50035700
H	-3.24974000	-0.37492900	-1.86563300
H	-1.77988100	0.47475500	-2.37941700
C	-2.50981900	1.11416500	-0.45899900
H	-2.97762300	0.65272100	0.42446200
H	-3.16979200	1.92193300	-0.81252300
C	-1.14431200	1.68684600	-0.10725300
H	-1.18168100	2.24364900	0.85040300
H	-0.85317300	2.42391300	-0.88186800
C	1.23292400	1.16662400	0.02487300
H	1.45496300	1.54833300	1.04373700
H	1.27051300	2.04863300	-0.64142000
C	2.32672300	0.19542800	-0.41331600

H	3.22755800	0.77962700	-0.65737700
H	2.00683000	-0.28681000	-1.34827000
C	2.64844400	-0.87249800	0.63122500
H	3.13608600	-1.73028000	0.14358300
H	3.33497600	-0.47976500	1.40151800
C	1.35614200	-1.35652100	1.28503000
H	1.53439000	-2.29811200	1.82144600
H	0.99602100	-0.60964000	2.01436300
H	0.35060500	-2.58431100	-0.04717000
C	1.46869700	-5.00136200	-1.02665400
H	1.80530400	-5.99686200	-0.66816000
C	2.54499100	-4.27262000	-1.72526500
H	3.50329800	-4.29243100	-1.20703000
O	1.40107800	-4.00971900	-0.10027000
I	3.47724000	-5.89280100	-3.55207000
H	0.57237500	-5.15881400	-1.66736800
C	2.25645500	-3.03820600	-2.49801900
C	0.94967100	-2.57156000	-2.69007800
C	3.31653700	-2.30791000	-3.05357000
C	0.71257900	-1.42217800	-3.44261800
H	0.10635300	-3.07605400	-2.21614200
C	3.08037200	-1.16476800	-3.81105300
H	4.33469000	-2.67798000	-2.91412700
C	1.77252100	-0.71990400	-4.01585500
H	-0.31488200	-1.07235700	-3.55679500
H	3.92093800	-0.62033200	-4.24605300
H	1.58278900	0.17753100	-4.60829600

G1-IM1-sol

C	2.89691800	-0.13704700	-0.15148400
N	2.40479100	-1.32519500	-0.26688100
C	1.56649900	-1.90752000	0.67859400
C	1.88879800	-1.98362200	2.04994300
C	0.38871500	-2.54529600	0.24673700
C	1.07567300	-2.68616600	2.93717000
H	2.79920500	-1.49818800	2.40771700
C	-0.42317100	-3.24173800	1.13790000
H	0.11228300	-2.47988000	-0.80705100
C	-0.08080700	-3.32708200	2.48922000
H	1.35425900	-2.73585500	3.99242300
H	-1.34496500	-3.69032100	0.76249000
H	-0.71616300	-3.87441300	3.18724300
N	3.76822600	0.30981600	-1.11662500
H	4.31966700	1.12887200	-0.89769600

N	2.61020500	0.75111700	0.85841200
H	1.77192500	0.50787200	1.39004800
C	2.83991800	2.18970500	0.77250800
H	3.90515700	2.35487400	0.53107700
C	1.97600800	2.86508700	-0.29301200
H	2.21452000	3.93660300	-0.36914700
H	2.13104700	2.39978600	-1.27621300
H	0.91270200	2.76931200	-0.02748500
C	2.59471300	2.79228000	2.15175100
H	3.25710900	2.33376400	2.89914600
H	2.77283800	3.87640600	2.13523000
H	1.55163900	2.61129800	2.45084600
C	4.31265900	-0.58739900	-2.12271700
H	3.46881000	-1.20360200	-2.46235200
C	4.84092400	0.24156500	-3.28600400
H	5.22426700	-0.41129000	-4.08234600
H	4.04885000	0.87779400	-3.70436500
H	5.67053200	0.89003000	-2.95798300
C	5.37978500	-1.51563600	-1.54519400
H	4.95335600	-2.09267000	-0.71406200
H	5.74467700	-2.21868500	-2.30858300
H	6.23824000	-0.93180300	-1.17517600
C	-0.98434100	0.80926800	0.71951300
H	-0.60874200	0.14684600	-0.07007100
C	-1.30961800	0.17351800	2.00250800
H	-2.08095300	0.63593700	2.62714500
H	-1.15513600	-0.90386700	2.10906400
O	-0.12787400	0.94484700	1.84751000
C	-1.67330000	2.05376600	0.26896300
C	-2.35155800	2.07045200	-0.95425900
C	-1.64885000	3.20652200	1.06141400
C	-3.00153100	3.23037400	-1.37309600
H	-2.39074100	1.15676200	-1.55306100
C	-2.29628000	4.36567600	0.63624600
H	-1.10443900	3.18614200	2.00794300
C	-2.97461500	4.38042200	-0.58253900
H	-3.53833100	3.23223800	-2.32333600
H	-2.27032000	5.26211300	1.25894600
H	-3.48376300	5.28693500	-0.91524000
I	-3.43993100	-1.67820200	-1.02423700

G1-TS1-sol

C	2.46702200	-0.36149500	-0.08768100
N	1.87059100	-1.37059000	-0.65595100

C	1.09438400	-2.28662400	0.04362100
C	1.40850100	-2.78734200	1.32623300
C	-0.04669000	-2.81486000	-0.59256700
C	0.61015400	-3.75251300	1.93307900
H	2.28440500	-2.40056500	1.84740100
C	-0.84783100	-3.77063200	0.02467700
H	-0.30306100	-2.43543100	-1.58371900
C	-0.52650500	-4.25210700	1.29439600
H	0.88021500	-4.11463500	2.92791000
H	-1.74384300	-4.12423600	-0.48974400
H	-1.15624700	-4.99724200	1.78299100
N	3.39981500	0.33158800	-0.82550900
H	3.60703700	1.27417200	-0.52560900
N	2.25236800	0.06057600	1.18666100
H	1.29918500	-0.15599000	1.56911100
C	2.78812300	1.28509700	1.76019500
H	3.85970800	1.34918000	1.49899300
C	2.05347500	2.53314700	1.26060900
H	2.47700800	3.44751200	1.70370900
H	2.09888500	2.62629500	0.16451700
H	0.99209800	2.44866300	1.54030500
C	2.66526000	1.17152000	3.27765700
H	3.24548500	0.31536500	3.64969600
H	3.02236500	2.08702700	3.77090700
H	1.60477100	1.01266900	3.52625500
C	3.64450300	0.02393700	-2.22736900
H	2.68016200	-0.25304000	-2.68301300
C	4.19254600	1.26920300	-2.91231300
H	4.38173900	1.07155400	-3.97620200
H	3.48153200	2.10586600	-2.83982300
H	5.14438000	1.57824300	-2.45046100
C	4.58840200	-1.16634600	-2.37058500
H	4.15503100	-2.03818100	-1.86390300
H	4.74250100	-1.41629500	-3.43107200
H	5.56441800	-0.93572400	-1.91590800
C	-1.23529500	0.25074500	0.46075000
H	-0.53223300	-0.27248900	-0.19063500
C	-1.40126200	-0.36598400	1.79015400
H	-2.30553000	-0.02491700	2.33747600
H	-1.41725500	-1.47272100	1.73216500
O	-0.21734300	0.20272800	2.17780700
C	-1.30926200	1.71449500	0.26464100
C	-0.75773200	2.27621300	-0.89285900
C	-1.88080400	2.56122500	1.22287500

C	-0.77466400	3.65426400	-1.09386800
H	-0.31494900	1.61197600	-1.63965100
C	-1.89151700	3.93873100	1.02646900
H	-2.28557500	2.13336100	2.14063100
C	-1.34012100	4.49170900	-0.13205100
H	-0.34061500	4.07692000	-2.00195700
H	-2.32894100	4.59037500	1.78521800
H	-1.35055300	5.57275500	-0.28227100
I	-3.27107400	-0.54920000	-1.01355800

G1-IM2-sol

C	2.46702200	-0.36149500	-0.08768100
N	1.87059100	-1.37059000	-0.65595100
C	1.09438400	-2.28662400	0.04362100
C	1.40850100	-2.78734200	1.32623300
C	-0.04669000	-2.81486000	-0.59256700
C	0.61015400	-3.75251300	1.93307900
H	2.28440500	-2.40056500	1.84740100
C	-0.84783100	-3.77063200	0.02467700
H	-0.30306100	-2.43543100	-1.58371900
C	-0.52650500	-4.25210700	1.29439600
H	0.88021500	-4.11463500	2.92791000
H	-1.74384300	-4.12423600	-0.48974400
H	-1.15624700	-4.99724200	1.78299100
N	3.39981500	0.33158800	-0.82550900
H	3.60703700	1.27417200	-0.52560900
N	2.25236800	0.06057600	1.18666100
H	1.29918500	-0.15599000	1.56911100
C	2.78812300	1.28509700	1.76019500
H	3.85970800	1.34918000	1.49899300
C	2.05347500	2.53314700	1.26060900
H	2.47700800	3.44751200	1.70370900
H	2.09888500	2.62629500	0.16451700
H	0.99209800	2.44866300	1.54030500
C	2.66526000	1.17152000	3.27765700
H	3.24548500	0.31536500	3.64969600
H	3.02236500	2.08702700	3.77090700
H	1.60477100	1.01266900	3.52625500
C	3.64450300	0.02393700	-2.22736900
H	2.68016200	-0.25304000	-2.68301300
C	4.19254600	1.26920300	-2.91231300
H	4.38173900	1.07155400	-3.97620200
H	3.48153200	2.10586600	-2.83982300
H	5.14438000	1.57824300	-2.45046100

C	4.58840200	-1.16634600	-2.37058500
H	4.15503100	-2.03818100	-1.86390300
H	4.74250100	-1.41629500	-3.43107200
H	5.56441800	-0.93572400	-1.91590800
C	-1.23529500	0.25074500	0.46075000
H	-0.53223300	-0.27248900	-0.19063500
C	-1.40126200	-0.36598400	1.79015400
H	-2.30553000	-0.02491700	2.33747600
H	-1.41725500	-1.47272100	1.73216500
O	-0.21734300	0.20272800	2.17780700
C	-1.30926200	1.71449500	0.26464100
C	-0.75773200	2.27621300	-0.89285900
C	-1.88080400	2.56122500	1.22287500
C	-0.77466400	3.65426400	-1.09386800
H	-0.31494900	1.61197600	-1.63965100
C	-1.89151700	3.93873100	1.02646900
H	-2.28557500	2.13336100	2.14063100
C	-1.34012100	4.49170900	-0.13205100
H	-0.34061500	4.07692000	-2.00195700
H	-2.32894100	4.59037500	1.78521800
H	-1.35055300	5.57275500	-0.28227100
I	-3.27107400	-0.54920000	-1.01355800

G1-TS2-sol

C	2.84291700	0.16745600	-0.45719300
N	2.81445100	-1.11728800	-0.19877500
C	1.71476900	-1.92136400	-0.42023800
C	0.79434300	-1.77647300	-1.48548800
C	1.54695900	-3.04286400	0.42004300
C	-0.24122200	-2.68991700	-1.66682200
H	0.89759200	-0.92351400	-2.15632900
C	0.50526700	-3.94529100	0.23768300
H	2.25952100	-3.16621700	1.23677800
C	-0.40674200	-3.77739500	-0.80598100
H	-0.94464600	-2.54312500	-2.49106900
H	0.40058300	-4.78808100	0.92509200
H	-1.23565600	-4.47337600	-0.94281200
N	4.09121700	0.77005500	-0.43928000
H	4.06561300	1.75166100	-0.19166600
N	1.75814400	0.94115400	-0.67903500
C	1.87651200	2.36934900	-0.91219700
H	2.53050100	2.84896300	-0.14938600
C	2.44982600	2.67601300	-2.29866900
H	2.54847600	3.76190400	-2.45317900

H	3.43458700	2.20949700	-2.43576200
H	1.77039900	2.27465600	-3.06633900
C	0.49943800	3.00467300	-0.75035100
H	0.08905200	2.77346800	0.24117000
H	0.55297400	4.09430500	-0.89315900
H	-0.19430600	2.58734800	-1.49773600
C	5.26031900	0.05268000	0.05086300
H	4.93795300	-0.61564000	0.86606200
C	5.86979200	-0.81033900	-1.04916400
H	6.72331500	-1.38930100	-0.66423300
H	5.11159200	-1.50868000	-1.42538800
H	6.21804700	-0.17749600	-1.88075000
C	6.26110600	1.06405300	0.59583100
H	5.81827100	1.64492400	1.41912100
H	7.15662000	0.55449400	0.97787200
H	6.57739900	1.76213800	-0.19598300
H	0.87186600	0.65127200	0.06510600
C	-1.94875700	0.05344700	-0.04496200
H	-1.49151800	-0.09091400	-1.03329000
C	-0.96706900	-0.38122200	1.05059400
H	-1.52815400	-0.42555400	2.01233600
H	-0.66585700	-1.42649200	0.83145300
O	0.06560200	0.51113900	1.09845400
C	-2.50989800	1.44042900	0.08363000
C	-3.08651800	2.07720900	-1.02235000
C	-2.43712400	2.13646500	1.29537900
C	-3.58158500	3.37551000	-0.92505100
H	-3.14493700	1.54011600	-1.97296000
C	-2.93040000	3.43642100	1.39468700
H	-1.93727900	1.67324200	2.14530800
C	-3.50480900	4.06105300	0.28803400
H	-4.02420800	3.85565000	-1.79977400
H	-2.85276000	3.97083000	2.34344300
H	-3.88587900	5.08081900	0.36833300
I	-3.63376400	-1.39174900	-0.12272800
C	1.91896200	-0.05523500	2.54888700
O	1.46671400	-1.05686500	2.91991300
O	2.50857500	0.92202500	2.32900400

G1-IM3-sol

C	-2.74645500	-0.19326600	0.54590400
N	-2.30179400	-1.39491800	0.73004600
C	-1.08354700	-1.68289700	1.31799900
C	-0.59186800	-1.08298000	2.49772100

C	-0.30739100	-2.71112900	0.74003200
C	0.62091400	-1.49065100	3.05437200
H	-1.17402900	-0.29098700	2.97005300
C	0.90451000	-3.10509600	1.29522600
H	-0.69275800	-3.17416700	-0.17036900
C	1.38417400	-2.49563300	2.45876400
H	0.97545100	-1.00984700	3.96973500
H	1.48934100	-3.88952700	0.81003600
H	2.33942500	-2.79839300	2.88996900
N	-4.00656300	-0.00984600	0.01589700
H	-3.95076100	0.73127500	-0.68141700
N	-2.04819900	0.95546800	0.84747700
C	-2.48688200	2.29266800	0.44958800
H	-2.83150700	2.26896300	-0.59764200
C	-3.59573600	2.79992500	1.36819500
H	-3.93792300	3.79362800	1.04191000
H	-4.45302600	2.11436900	1.36510700
H	-3.21825100	2.87997300	2.39937800
C	-1.27264000	3.20978200	0.48906000
H	-0.49165400	2.83360500	-0.18851800
H	-1.54959500	4.22643000	0.17549400
H	-0.85670300	3.25968200	1.50794100
C	-4.70497300	-1.17378700	-0.52728700
H	-3.95882100	-1.84633300	-0.98229900
C	-5.43027000	-1.93055200	0.57909500
H	-5.94169900	-2.81535800	0.17081900
H	-4.71139100	-2.26293500	1.33924400
H	-6.17895700	-1.27883500	1.05634100
C	-5.65768800	-0.68790200	-1.61125300
H	-5.08987800	-0.18002800	-2.40459200
H	-6.19767900	-1.53459500	-2.05776800
H	-6.39730500	0.01420800	-1.19355900
H	-1.05069500	0.81169700	0.69741700
C	1.75461500	-0.10056000	-0.32122700
H	1.35155900	-0.63067500	0.54894800
C	0.92250200	-0.40142100	-1.55895600
H	1.44294100	-0.07644200	-2.47776200
H	0.77200900	-1.48786800	-1.64644500
O	-0.28967300	0.27445400	-1.39371300
C	1.95458900	1.34704300	0.00269000
C	1.94238500	1.75463500	1.34071200
C	2.12690900	2.31043100	-0.99917300
C	2.09908600	3.09884300	1.67600400
H	1.80001100	1.00120800	2.11980300

C	2.27814000	3.65306500	-0.66549900
H	2.12623700	2.00625900	-2.04747300
C	2.26541400	4.05218000	0.67299000
H	2.08019900	3.40293800	2.72417700
H	2.40032200	4.39631300	-1.45526700
H	2.38028600	5.10653700	0.93031800
I	3.71406300	-1.07702200	-0.57715600
C	-1.31672600	-0.03818800	-2.35550000
O	-1.03227700	-0.92119100	-3.15929100
O	-2.32542400	0.66037400	-2.20637400

G1-TS3-sol

C	0.74253400	2.63597800	1.34247100
O	0.22038600	3.73023300	1.40322700
O	0.20643200	1.48221800	1.42785600
I	3.53324300	-1.18653900	-0.70742800
C	2.61413700	1.25623800	1.25565100
C	1.67585400	0.25955000	0.59028700
O	2.10354300	2.56722800	1.14687900
H	2.75377000	0.98810700	2.31511600
H	3.58875000	1.26661800	0.76352300
C	1.04426100	-0.91274900	1.23690700
C	1.40903000	-1.35934100	2.51098400
C	-0.00502700	-1.55609900	0.56511700
C	0.73991200	-2.42910400	3.10144200
H	2.22945900	-0.88017800	3.04649400
C	-0.66799300	-2.62789800	1.15387900
H	-0.29778300	-1.20835900	-0.42918300
C	-0.29934300	-3.06949000	2.42611800
H	1.03822700	-2.76820200	4.09504200
H	-1.48165400	-3.11863600	0.61560800
H	-0.81843200	-3.91011000	2.89014000
H	1.30200700	0.53822100	-0.39577000
C	1.27564500	0.97516700	-3.00905100
C	0.07792700	0.32130100	-2.73465100
C	-0.93125600	0.92475200	-1.95537000
C	-0.69277300	2.23759700	-1.49506300
C	0.50887500	2.88696000	-1.77091300
C	1.50581100	2.26292200	-2.52204300
H	2.04977200	0.45888100	-3.57929200
H	-0.09974200	-0.69219100	-3.10012100
H	-1.43779000	2.74892300	-0.88509900
H	0.67144100	3.88241500	-1.35351500
H	2.45517300	2.76608300	-2.71020100

N	-2.09241700	0.19065600	-1.73552000
C	-2.77130000	0.23695500	-0.62757100
N	-4.00092900	-0.39601900	-0.58854500
H	-4.27676000	-0.74049000	0.32462900
N	-2.38802600	0.86174200	0.51276400
C	-4.45094200	-1.21714400	-1.70260400
C	-5.96365700	-1.38039500	-1.61724700
C	-3.73234400	-2.56500300	-1.74700300
H	-4.19114900	-0.65886600	-2.61165000
H	-6.46215600	-0.40137900	-1.61487100
H	-6.33886800	-1.96661100	-2.46801700
H	-6.24625700	-1.91360500	-0.69434500
H	-2.64748800	-2.40231400	-1.80556400
H	-3.96292200	-3.15134600	-0.84183700
H	-4.04584900	-3.15338800	-2.62233100
C	-3.12743600	0.98039300	1.75894200
C	-2.95349600	2.39982400	2.29692900
C	-2.66408000	-0.07125000	2.76830300
H	-4.19565100	0.83428800	1.53385800
H	-3.38796800	3.12770300	1.59687800
H	-3.44725600	2.51065800	3.27363600
H	-1.88471900	2.63846000	2.40093600
H	-2.82775500	-1.08868700	2.38213100
H	-1.58249600	0.04736600	2.94134700
H	-3.19543000	0.03379300	3.72621400
H	-1.40169200	1.13230800	0.60227500

G1-IM4-sol

C	0.90222300	3.04265000	-1.34517300
O	0.40796200	3.89806200	-2.01029200
O	0.22556400	2.27126000	-0.47532500
I	3.57540900	-1.89341600	0.38159100
C	2.47006600	1.73176900	-0.34214400
C	1.06979100	1.22115300	0.03424400
O	2.19749400	2.72300000	-1.33649200
H	2.98324600	2.20872100	0.50564000
H	3.09632100	0.93553500	-0.76078600
C	0.79753500	1.02605000	1.49987800
C	0.75638200	2.12706900	2.36189700
C	0.58589800	-0.25767700	2.00534400
C	0.51161200	1.94638900	3.72147100
H	0.90944100	3.13327100	1.96285200
C	0.34730600	-0.43818100	3.36814700
H	0.64111300	-1.11307300	1.32906800

C	0.30986900	0.65997800	4.22633800
H	0.48044500	2.80952700	4.38843700
H	0.19722300	-1.44552600	3.75920900
H	0.12450700	0.51491200	5.29211000
H	0.84284300	0.30074600	-0.52050700
C	1.28418100	-1.02534100	-2.75591900
C	0.12286500	-1.46990200	-2.12959500
C	-1.05349900	-0.69587800	-2.14024700
C	-1.03184200	0.52308700	-2.84737900
C	0.12982000	0.96119200	-3.48067000
C	1.29877100	0.19901700	-3.42841800
H	2.19212800	-1.62601800	-2.67765400
H	0.11964100	-2.41296000	-1.58044800
H	-1.93600700	1.13464800	-2.88346800
H	0.12365800	1.92126200	-4.00066400
H	2.21261900	0.55777400	-3.90442600
N	-2.18813200	-1.18502000	-1.50007300
C	-2.84867600	-0.47943700	-0.64110600
N	-4.03616200	-0.97925200	-0.14603000
H	-4.33738600	-0.60929900	0.74698900
N	-2.48711300	0.75396100	-0.17260500
C	-4.40804300	-2.36827800	-0.38038100
C	-5.90204400	-2.52735500	-0.12808100
C	-3.57734700	-3.32875000	0.46934700
H	-4.19108000	-2.56565100	-1.43863400
H	-6.48255800	-1.84629900	-0.76558400
H	-6.21945400	-3.55932900	-0.33290300
H	-6.14470200	-2.30717700	0.92493500
H	-2.50934800	-3.17421100	0.26626000
H	-3.76695000	-3.15523700	1.54133900
H	-3.82858600	-4.37540500	0.24226000
C	-3.20173000	1.52563900	0.83227700
C	-2.81979700	2.99423200	0.68892500
C	-2.92588200	1.03033900	2.25502500
H	-4.28010400	1.43235400	0.61518800
H	-3.01298600	3.35253800	-0.33173700
H	-3.39226900	3.60844200	1.39751000
H	-1.74783600	3.12401200	0.89867400
H	-3.12465300	-0.04697200	2.36167600
H	-1.86732800	1.19357900	2.50490900
H	-3.54624000	1.57244500	2.98447900
H	-1.60544400	1.13545300	-0.50391400