

Supporting Information for

Unravelling the Mechanism of Phosphine-Catalyzed Azetine Formation and BF_3 -Mediated

Ring-Opening to Axially Chiral Alkenes: A DFT Study.

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Part 1: Supplementary computational details.

This study employed the M06-2X functional combined with the IEF-PCM solvent model as the baseline method for structure optimization and frequency analysis, denoted as L1. To verify the suitability of L1 for this phosphine-catalyzed reaction model, we designed three DFT-based comparative schemes, specifically the B3LYP-D3 functional¹ with IEF-PCM (L2), ω B97X-D functional² with IEF-PCM (L3), and the M06-2X functional with SMD solvent model³ (L4), where L4 was designed to verify the effect of changing the solvent model while keeping the functional unchanged. Using these four calculation combinations, we calculated the relative Gibbs free energies of the first-step transition states (*Re*-TS1 and *Si*-TS1) and compared these values across the methods. Here, *Re*-TS1 refers to the transition state generated when the phosphine catalyst attacks reactant R1 from the *Re* face, while *Si*-TS1 refers to that generated by attack from the *Si* face. Detailed results are presented in Table S1. As observed from Table S1, the calculated relative Gibbs free energies from the four combinations exhibit only minor discrepancies. This confirms that the initially selected computational method (L1) is reasonable for modeling this phosphine-catalyzed reaction.

Table S1 $\Delta\Delta G^\ddagger$ values of *Re*-TS1 and *Si*-TS1 for the nucleophilic attack of phosphine catalyst PR₃ on reactant R1, calculated using different functionals and solvent models.

	L1	L2	L3	L4
<i>Re</i> -TS1	3.13	2.65	4.31	3.75
<i>Si</i> -TS1	0.00	0.00	0.00	0.00

L1 : M06-2X/6-311++G(2df,2pd)/IEF-PCM_{DCM}// M06-2X/6-31G(d,p)/IEF-PCM_{DCM}

L2 : B3LYP-D3/6-311++G(2df,2pd)/IEF-PCM_{DCM}// B3LYP-D3/6-31G(d,p)/IEF-PCM_{DCM}

L3 : ω B97X-D/6-311++G(2df,2pd)/IEF-PCM_{DCM}// ω B97X-D/6-31G(d,p)/IEF-PCM_{DCM}

L4 : M06-2X/6-311++G(2df,2pd)/SMD_{DCM}// M06-2X/6-31G(d,p)/SMD_{DCM}

Part 2: Different pathways for the catalyst to attack the reactant R1.

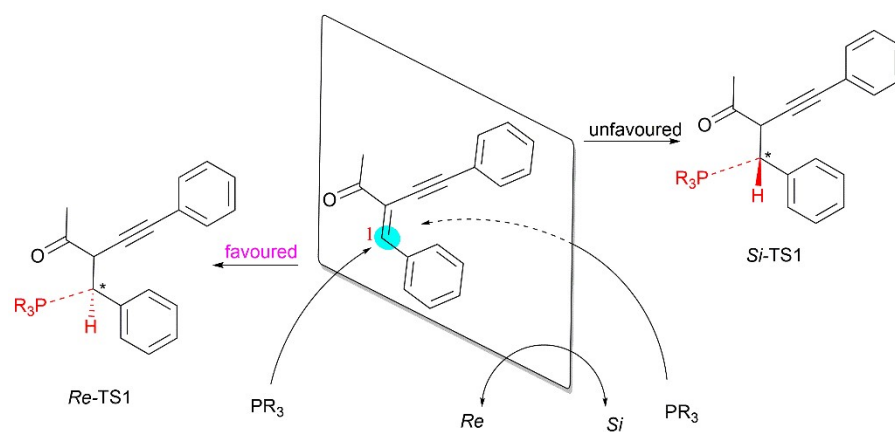


Fig. S1 Different models of nucleophilic attack of phosphine catalyst on reactant R1.

Part 3: The origin of the chemoselectivity of reactant R1.

For R1, owing to the presence of carbon-carbon double and triple bonds in its structure, and considering the conjugation effect of the carbonyl oxygen, we hypothesized the existence of two additional reactive sites, the C3 and C4 sites, besides the C1 site. Regrettably, we failed to locate either the transition state corresponding to P-C3 bond formation or the associated intermediate. Accordingly, we investigated the reaction pathway involving P-C4 bond formation between R1 and the catalyst, which proceeds via the transition state TS1'. As illustrated in Fig. S2, the energy barrier for the transition state TS1' is 28.34 kcal/mol. This indicates that the C3 and C4 sites are not susceptible to nucleophilic attack by the phosphine catalyst. Therefore, we conducted an active site analysis of reactant R1 using Parr functions, which include the condensed local electrophilicity index (P_k^+) and the condensed local nucleophilicity index (P_k^-). The results are presented in the table S2: the C1 site exhibits higher electrophilicity (0.25) and relatively lower nucleophilicity (0.23), whereas the C4 site has a significantly lower electrophilicity index (0.15) than that of C1. The C3 site exhibits the lowest electrophilicity index, with a value of merely 0.04. Furthermore, the carbonyl carbon has a significantly lower electrophilicity index (0.12) than that of C1. According to the hard-soft acid-base (HSAB) theory⁴, phosphine preferentially adds to electron-deficient carbon-carbon multiple bonds, forming zwitterionic species.⁵ These differences in parameters demonstrate that the C1 site is more likely to act as an electrophilic site for attack by the phosphine catalyst, thus resulting in a lower energy barrier compared to the C3 and C4 sites.

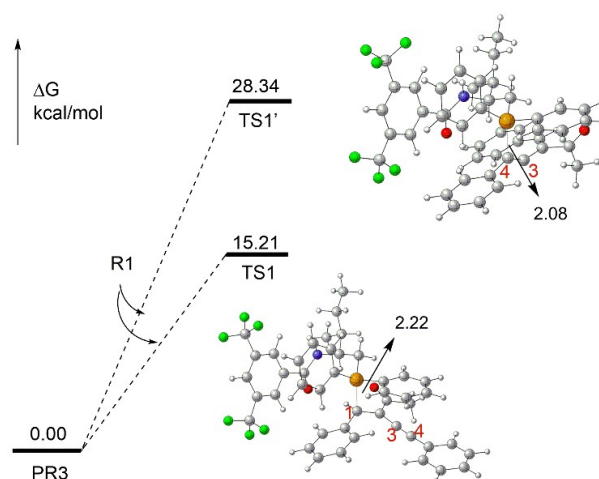


Fig. S2 Relative free energies (with PR₃ as the reaction zero point) and 3D structures corresponding to the attack of different transition states (TS1 and TS1') on R1.

Table S2 Local electrophilicity (P_k^+) and nucleophilicity (P_k^-) indices of reactant R1

Reactive site	C1		C3		C4	
	P_k^+	P_k^-	P_k^+	P_k^-	P_k^+	P_k^-
Condensed Indices	0.25	0.23	0.04	0.23	0.15	0.31

Part 4: Different configurations and corresponding conformations of TS2.

Notably, TS2 exists in four distinct configurations (TS2SR, TS2SS, TS2RR, and TS2RS), and each configuration may have multiple conformations. To ensure that the obtained diastereomers and enantiomers correspond to the lowest-energy conformations of their respective configurations, we investigated different conformations for each of the four configurations. This was done by adjusting the dihedral angle Φ (C3-C4-C5-N6), rotating it by approximately 90° each time for a total of four rotations, which resulted in 16 (4×4) theoretical possibilities. Detailed relative Gibbs free energies of each conformation are listed in Table S3. It can be observed that the relative energy value of each of TS2RR, TS2RS, TS2SR, and TS2SS is lower than those of the other three corresponding conformations for each species. For example, the relative Gibbs free energies of TS2SR, TS2SR', TS2SR'', and TS2SR''' are 16.48, 17.45, 16.85, and 21.75 kcal/mol, respectively. This indicates that transition state TS2SR is the most favorable conformation from the conformational search. Using the Boltzmann distribution equation, the ee of the SR-type product was calculated to exceed 99%. The experimentally measured ee is 90%, which is consistent with the theoretically predicted trend of high enantioselectivity.

$$\frac{[SR]}{[RS]} = \exp\left(\frac{-\Delta\Delta G_{[SR]-[RS]}^{\ddagger}}{RT}\right) \quad (1)$$

$$ee = \frac{[SR] - [RS]}{[SR] + [RS]} \quad (2)$$

Table S3 Relative Gibbs free energies (kcal/mol) of configurations TS2RR, TS2RS, TS2SR, TS2SS, and their respective conformers, with the combined energy of separated R1, R2, and PR₃ set as the zero reference point.

Config.-Conf.	Φ (C3-C4-C5-N6)	$\Delta G^{\ddagger}$
TS2SR	-144.44	16.48
TS2SR'	55.44	17.45
TS2SR''	108.68	16.85
TS2SR'''	-40.41	21.75
TS2SS	8.62	19.04
TS2SS'	-67.15	20.43
TS2SS''	149.92	20.11
TS2SS'''	-122.13	20.50
TS2RR	111.70	19.70
TS2RR'	30.14	20.97
TS2RR''	174.60	27.21
TS2RR'''	-42.09	27.81
TS2RS	-58.01	20.84

TS2RS'	75.73	29.47
TS2RS''	-107.44	24.53
TS2RS'''	151.84	29.15

Part 5: The promoting effect of BF_3 -mediated activation on H^- transfer.

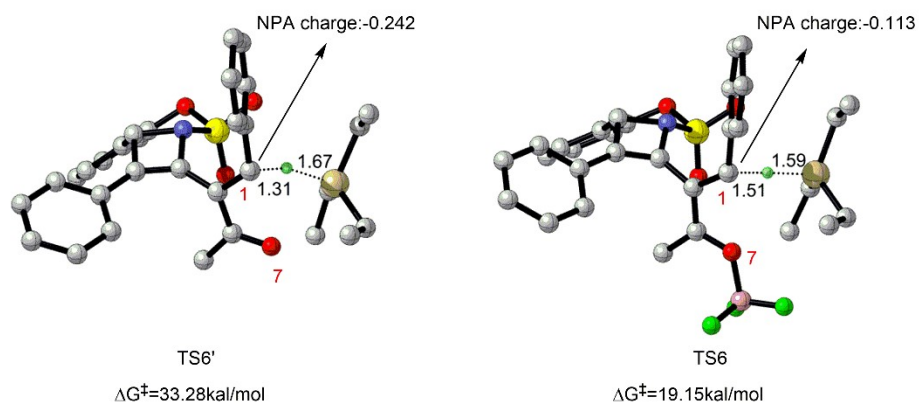


Fig. S3 3D structural diagrams of TS6 and TS6' (only the H^- species involved in the reaction are retained and highlighted; other H atoms are omitted).

Part 6: Intrinsic Reaction Coordinate (IRC) analysis of the ring-opening.

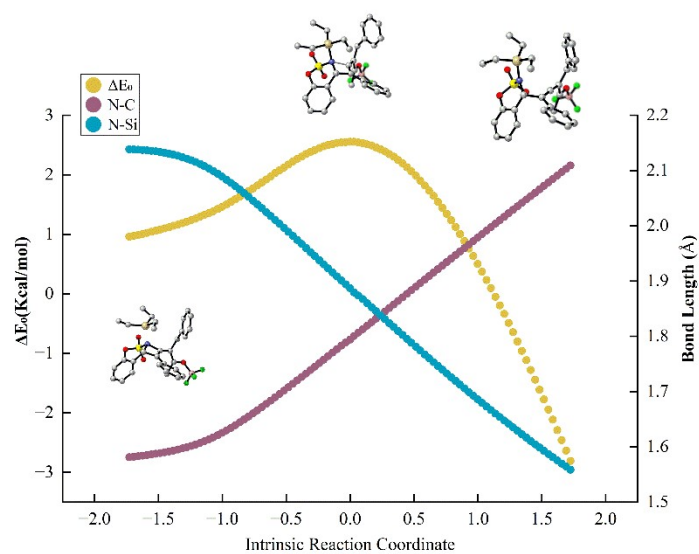


Fig. S4 IRC for the ring-opening: Featuring variations in N-C (purple) and N-Si bond lengths (blue), along with energy changes relative to intermediate M5 (yellow). Hydrogen atoms are omitted in the 3D plot.

Part 7: The energy change associated with the proton transfer from H_3O^+ to the N6 atom in M6.

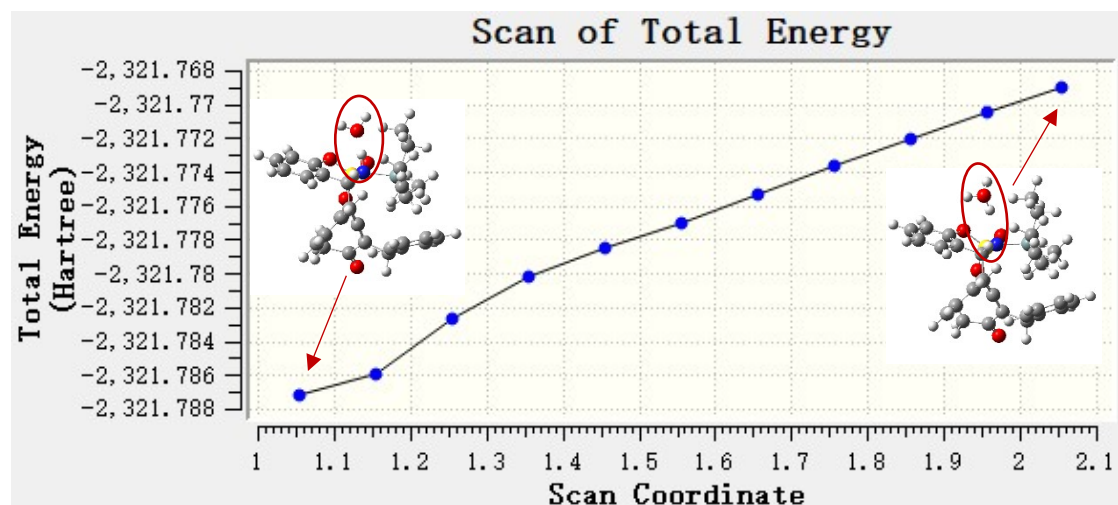


Fig. S5 Flexible scan curve and 3D contour plot for the proton transfer from H_3O^+ to the N6 atom in M6.

Part 8: The distortion/interaction analysis of key transition states (TS2 and TS2').

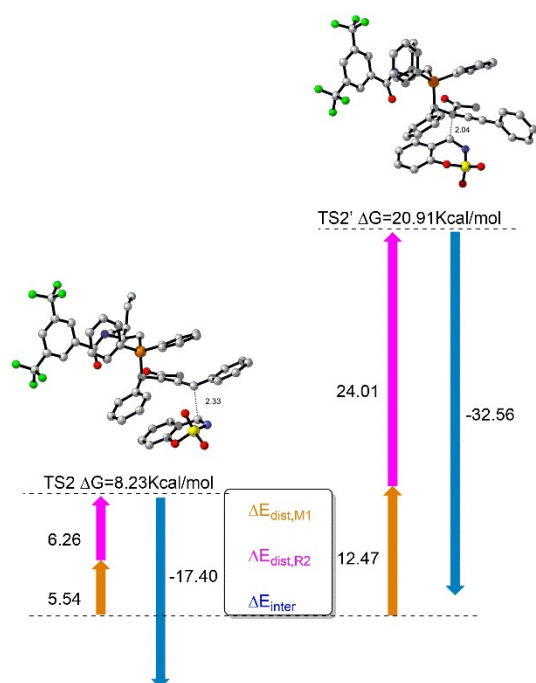


Fig. S6 The distortion/interaction analysis of key transition states (TS2 and TS2').

Part 9: The distortion/interaction analysis of TS2SR, TS2RR, TS2SS, and TS2RS.

Table S4 The distortion/interaction analysis of TS2SR, TS2RR, TS2SS, and TS2RS (unit: kcal/mol, computational level: M06-2X/6-311++G(2df,2pd)/IEF-PCM_{DCM}).

	$\Delta E_{\text{dist, R2}}$	$\Delta E_{\text{dist, M1}}$	$\Delta E_{\text{dist, total}}$	ΔE_{int}	$\Delta G^\ddagger$
TS2SR	6.26	5.54	11.80	-17.40	8.23
TS2SS	7.61	5.04	12.65	-16.33	10.79
TS2RR	8.89	8.75	17.64	-20.74	11.45
TS2RS	7.45	8.45	15.90	-17.53	12.59

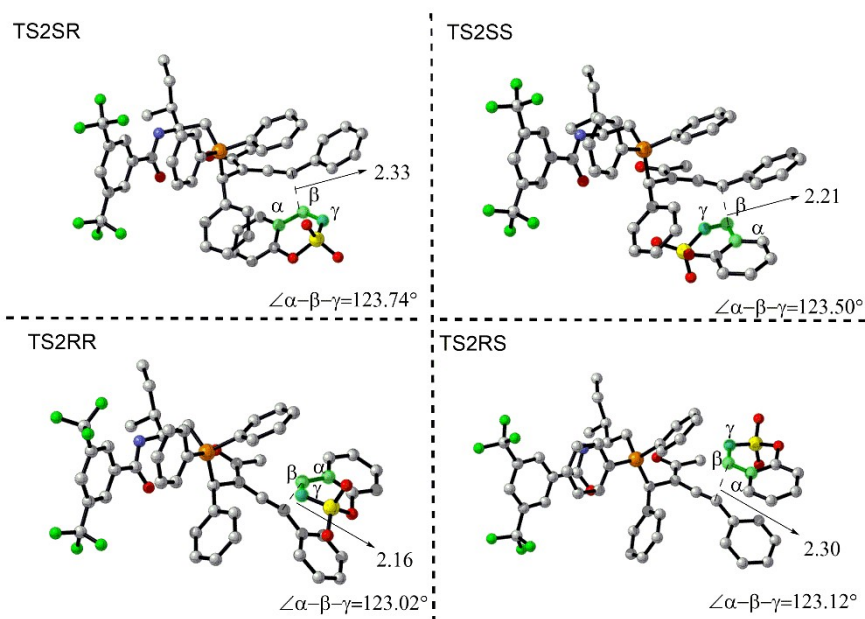


Fig. S7 3D structural diagrams of transition states TS2SR, TS2SS, TS2RR, and TS2RS. (H atoms are omitted)

Part 10: EDA in the second step.

An energy decomposition analysis (EDA) was undertaken for the interaction energies using sobEDA⁶ in Multiwfn. The resultant values (Table S5) further differentiated the transition states.

The complete form of sobEDA represents the interaction energy among the four components, which are the electrostatic term, the exchange-repulsion term, the orbital interaction term, and the Coulomb correlation term, as follows: $\Delta E_{\text{int}} = \Delta E_{\text{els}}$ (electrostatic energy) + ΔE_{xrep} (exchange-repulsion) + ΔE_{orb} (orbital interaction) + ΔE_{c} (Coulomb correlation). All calculations were performed at the M06-2X/6-31G(d,p) computational level.

Table S5 EDA study on the interaction energies of TS2SR, TS2SS, TS2RR and TS2RS. (Unit: kcal/mol)

	ΔE_{int}	ΔE_{els}	ΔE_{xrep}	ΔE_{orb}	ΔE_{c}
TS2SR	-18.55	-59.83	91.37	-27.66	-22.43
TS2SS	-15.20	-55.11	103.06	-36.48	-26.67
TS2RR	-21.02	-62.88	118.20	-43.16	-33.18
TS2RS	-18.89	-57.73	96.24	-32.78	-24.61

Part 11: The Atoms in Molecules (AIM) analysis of TS2SR, TS2RR, TS2SS, and TS2RS.

Table S6 Summary of interaction types, bond lengths (in Å) between interacting atoms, and Laplacian values (∇^2_{ρ} , in a.u.) at bond critical points (BCP).

BCP index (TS2SR)	Type of interaction	Distance	$\nabla^2_{\rho} \times 10^{-1}$
1	$\pi \dots \pi$	3.40	0.1861
2	C-H...O	2.50	0.3933
3	C-H...O	2.54	0.3680
4	C-H...O	2.29	0.4345
5	lp... π	3.18	0.2606
6	lp... π	3.15	0.2940
BCP index (TS2SS)	Type of interaction	Distance	$\nabla^2_{\rho} \times 10^{-1}$
1	$\pi \dots \pi$	3.41	0.1625
2	lp... π	3.14	0.2889
3	lp... π	3.12	0.2543
4	lp... π	3.39	0.1764
5	C-H...N	2.56	0.2980
6	$\pi \dots \pi$	3.19	0.2442
BCP index (TS2RR)	Type of interaction	Distance	$\nabla^2_{\rho} \times 10^{-1}$
1	C-H...N	2.44	0.3701
2	C-H... π	2.67	0.2917
3	C-H... π	3.30	0.1748
4	lp... π	3.33	0.1898
5	lp... π	3.23	0.2515
6	$\pi \dots \pi$	3.14	0.2796
BCP index (TS2RS)	Type of interaction	Distance	$\nabla^2_{\rho} \times 10^{-1}$
1	C-H... π	2.67	0.3287
2	lp... π	3.08	0.3009
3	C-H...O	2.28	0.4376
4	C-H...O	2.52	0.3171

Part 12: Cartesian Coordinates of All the Optimized Structures.

R1

C	-2.68617200	-1.60476800	-0.22337900
C	-3.93281000	-2.21836600	-0.24214700
C	-5.09025700	-1.46035100	-0.06964500
C	-4.99945200	-0.08232100	0.12215800
C	-3.75724800	0.54019200	0.14320500
C	-2.58940300	-0.21825700	-0.02902200
C	-1.30707200	0.41683900	-0.00587900
C	-0.20736300	0.93014000	0.01621400
C	1.04692000	1.60828700	0.02311700
C	2.26557600	1.01655200	0.02330600
C	2.63891200	-0.39438500	0.04876500
C	3.97742100	-0.70870600	-0.24241300
C	4.41793300	-2.02592400	-0.25241800
C	3.52898000	-3.05662700	0.04685200
C	2.20247900	-2.75924100	0.35837000
C	1.75634100	-1.44331600	0.35940500
C	1.01820000	3.11975700	-0.00768400
C	-0.33294200	3.78771300	-0.03534400
O	2.05002700	3.76257600	-0.00953700
H	-1.78068200	-2.18690000	-0.36160900
H	-4.00192400	-3.29048000	-0.39291100
H	-6.06189300	-1.94278600	-0.08555100
H	-5.89921700	0.50884200	0.25591300
H	-3.67735100	1.61197500	0.29266200
H	3.09780800	1.71694600	-0.02085900
H	4.67065600	0.09639000	-0.46917100
H	5.45341000	-2.24840600	-0.48737500
H	3.86946400	-4.08692700	0.04509800
H	1.51168300	-3.55860000	0.60618000
H	0.72790000	-1.22526800	0.61794300
H	-0.91299000	3.49676500	0.84528300
H	-0.19970300	4.86807900	-0.05851500
H	-0.89764700	3.45645600	-0.91156000

R2

C	2.24978000	1.24804400	0.07626400
C	3.28636300	0.33278000	0.16629000
C	3.01772000	-1.03482600	0.05200200
C	1.72143200	-1.50094300	-0.14551000
C	0.69542200	-0.57342900	-0.21747500
C	0.93502600	0.80125300	-0.11057500
O	-0.58128700	-1.02824900	-0.48722300
S	-1.83347500	-0.14810000	0.10035000

N	-1.42644300	1.42651200	-0.23541700
C	-0.17324800	1.72841300	-0.24477300
O	-2.95113500	-0.53417100	-0.71812400
O	-1.86803800	-0.32405800	1.53292100
H	2.43939600	2.31430300	0.15224100
H	4.30299700	0.67508200	0.31835800
H	3.83049300	-1.74985200	0.11810700
H	1.49664800	-2.55634700	-0.24247700
H	0.05987900	2.78490300	-0.38184500
PR₃			
C	2.99819700	0.94524400	-0.47320300
H	4.00886900	1.24520500	-0.76977100
H	2.98070600	0.93344900	0.62279000
P	2.73132700	-0.77882300	-1.15582400
C	4.12327800	-1.64490300	-0.30334000
C	5.43055300	-1.19947600	-0.54593100
C	3.94326300	-2.78125000	0.49266200
C	6.52306100	-1.85030800	0.01827100
H	5.60348400	-0.33943000	-1.18830000
C	5.03884600	-3.43881700	1.05022900
H	2.94327300	-3.15751200	0.68388500
C	6.33019800	-2.97292200	0.82164300
H	7.52618200	-1.48364700	-0.17493500
H	4.87841200	-4.31724100	1.66741400
H	7.18142900	-3.48339900	1.26006800
C	1.27475200	-1.35659300	-0.18064200
C	0.22322400	-1.95894600	-0.87466700
C	1.15983300	-1.19349400	1.20926600
C	-0.92354900	-2.39036000	-0.20250600
H	0.29570400	-2.08182100	-1.95214000
C	0.01265900	-1.60617000	1.87817100
H	1.97821400	-0.75128700	1.77320000
C	-1.03120800	-2.20905900	1.17094200
H	-1.74043600	-2.83808400	-0.75996100
H	-0.07361500	-1.45954400	2.95006000
H	-1.92918200	-2.51960600	1.69536400
C	-3.91209200	-0.25795800	0.42821600
C	-3.02485000	0.45413500	1.22587500
C	-1.88953000	1.04787200	0.68255700
C	-1.63279600	0.92719000	-0.68163100
C	-2.53268800	0.24025000	-1.49464500
C	-3.65681500	-0.35421400	-0.93607600
H	-4.79270000	-0.72104100	0.85959700
H	-1.22971900	1.61552200	1.33140800

H	-2.32857000	0.16959600	-2.55808900
C	-4.55879400	-1.17805200	-1.80999900
C	-3.24547500	0.50853400	2.71046800
F	-5.78425000	-1.30713500	-1.28593400
F	-4.68915200	-0.64568600	-3.03154000
F	-4.07022100	-2.42078600	-1.97762300
F	-2.64261500	-0.52260000	3.33150300
F	-4.54511300	0.44462300	3.02559800
F	-2.74695100	1.62958400	3.24818400
C	-0.39734800	1.47798700	-1.34441600
O	-0.37833600	1.70135000	-2.54852400
N	0.66555000	1.66463900	-0.52516600
H	0.61130500	1.26199600	0.40083900
C	2.39572500	3.43219400	-0.76526400
C	2.55593600	3.73026800	0.73042700
H	1.61732700	3.47990100	1.24421700
H	3.32906800	3.07708200	1.15021200
C	1.38267900	4.36594000	-1.43059900
H	1.18413400	4.05638600	-2.46038700
H	0.43143700	4.34606900	-0.88720200
H	1.74245100	5.39714800	-1.44590800
H	3.37266200	3.57808100	-1.24892400
C	2.92661700	5.18222800	1.02909600
H	2.11617700	5.86773600	0.76904900
H	3.14713600	5.31704000	2.09091100
H	3.81386300	5.48156100	0.46113900
C	2.00259000	1.96494400	-1.03539600
H	1.93744700	1.83732600	-2.12156900
Si-TS1			
C	6.15158800	-2.38785400	0.42382900
C	7.24127300	-2.95735300	1.07193900
C	8.42945400	-2.24194800	1.21730600
C	8.51936800	-0.94707500	0.70699500
C	7.43331400	-0.36799300	0.06173800
C	6.23117200	-1.08098900	-0.08748500
C	5.10013000	-0.47769000	-0.71451100
C	4.10354000	0.05569400	-1.16959400
C	2.95251400	0.72429700	-1.65253700
C	1.63503800	0.18366400	-1.54772800
C	1.34606300	-1.28081400	-1.48070500
C	0.28036300	-1.77573700	-2.24327900
C	-0.10916800	-3.10936800	-2.14228400
C	0.56419100	-3.96989300	-1.27702800
C	1.64262900	-3.49237000	-0.53363000

C	2.03529100	-2.15983400	-0.63415000
C	3.07265500	2.08203800	-2.13862600
C	4.46829400	2.65807300	-2.28803600
O	2.08627700	2.78307200	-2.41400100
H	5.22699300	-2.94527100	0.30719000
H	7.16374900	-3.96655800	1.46421400
H	9.27854500	-2.69011900	1.72256200
H	9.44088500	-0.38359200	0.81518800
H	7.49769700	0.64349200	-0.32704000
H	0.91070300	0.72183600	-2.15999000
H	-0.26069500	-1.09376300	-2.89304300
H	-0.94850300	-3.47433800	-2.72696100
H	0.25085800	-5.00468600	-1.18424800
H	2.17481800	-4.15753100	0.13933300
H	2.85922400	-1.79139000	-0.03437300
H	5.09268600	2.01460700	-2.91361900
H	4.40071500	3.65398800	-2.72524900
H	4.95502300	2.71549700	-1.30848600
C	0.43380900	2.70746600	0.19910200
H	1.34462400	3.19404300	-0.15756200
H	0.18627200	3.13023900	1.17818200
P	0.84593800	0.92311300	0.39463400
C	2.31297300	0.85661800	1.45266500
C	3.31389200	1.83028400	1.35077000
C	2.55195400	-0.29883900	2.21008800
C	4.54501100	1.63447700	1.97055400
H	3.15166400	2.73612100	0.77573100
C	3.78454200	-0.49050800	2.82319600
H	1.77776900	-1.05642000	2.30182800
C	4.78782300	0.46914000	2.69085000
H	5.31997400	2.38820100	1.87406600
H	3.96695500	-1.39387900	3.39587900
H	5.75826100	0.30519800	3.14861000
C	-0.51260400	0.15992600	1.36616400
C	-0.88281400	-1.16364400	1.10660200
C	-1.21776900	0.89015500	2.33600100
C	-1.94201600	-1.74719300	1.80389900
H	-0.36392600	-1.74523100	0.35149000
C	-2.28631200	0.31111300	3.01131200
H	-0.94048300	1.91530700	2.56634400
C	-2.64894700	-1.01132400	2.74652500
H	-2.22665700	-2.76962100	1.57728000
H	-2.83746400	0.88919700	3.74582400
H	-3.49089800	-1.45515800	3.26702400

C	-5.05588400	-1.69528400	0.09065400
C	-5.10602700	-0.37005700	0.50579900
C	-4.19225700	0.56837000	0.03175200
C	-3.21913800	0.17899900	-0.88576600
C	-3.18424800	-1.14032800	-1.33417100
C	-4.08600700	-2.06868900	-0.83494200
H	-5.76315300	-2.42137700	0.47527700
H	-4.27154800	1.59852200	0.36789700
H	-2.42605000	-1.42885200	-2.05402100
C	-3.93019700	-3.50613300	-1.24075700
C	-6.11033400	0.05857700	1.53813200
F	-5.03657600	-4.22092200	-1.00833500
F	-3.63034800	-3.62431900	-2.54280600
F	-2.92647500	-4.09310900	-0.56204500
F	-5.56288600	0.10370200	2.76608300
F	-7.15240300	-0.77817100	1.60262100
F	-6.58400100	1.28630500	1.28386100
C	-2.13985400	1.09022900	-1.40429000
O	-1.55233200	0.83030800	-2.44970200
N	-1.83872300	2.15655700	-0.62449800
H	-2.25301200	2.19497200	0.29735400
C	-1.00528300	4.46342700	-0.98307100
C	-1.79839600	4.98136500	0.22493500
H	-2.80190800	4.53564300	0.20587800
H	-1.32485800	4.64713800	1.15670500
C	-1.75711600	4.69695600	-2.29402900
H	-1.16531900	4.35362700	-3.14720000
H	-2.70273800	4.14379500	-2.29097500
H	-1.98301800	5.75472500	-2.44598000
H	-0.04831200	5.00228900	-1.02714500
C	-1.92158900	6.50386200	0.26484500
H	-2.48077900	6.88669600	-0.59248200
H	-2.44114600	6.82928600	1.16942100
H	-0.93271700	6.97268500	0.25721800
C	-0.64903600	2.96940600	-0.86018000
H	-0.24092300	2.64035500	-1.81802800
R-M1			
C	1.56109900	-4.24723700	-1.78916900
C	0.90481600	-3.41425200	-2.69340500
C	2.28591000	-3.68889800	-0.73875400
C	0.96707100	-2.03134500	-2.54104100
C	2.35293500	-2.30588600	-0.58910800
C	1.68839600	-1.46323900	-1.48631000
C	1.69758400	0.04163100	-1.34412600

C	7.65055100	-0.43462400	-0.28298000
C	8.77818800	-1.00483500	0.29536300
C	5.20461200	-0.34923300	-0.57292400
C	4.20160600	0.16911300	-1.04122100
C	6.36658700	-0.93308800	0.00741700
C	3.02031300	0.74414500	-1.54464900
C	8.65745000	-2.08373400	1.17054200
C	6.25660500	-2.02136600	0.89415100
C	7.39022600	-2.58715600	1.46419600
C	3.00527700	1.97296300	-2.24991000
C	4.31817500	2.69717500	-2.50099300
H	1.50819500	-5.32507000	-1.90316800
H	0.33804900	-3.84063300	-3.51487700
H	2.80272900	-4.33080200	-0.03219400
H	0.43388300	-1.38094900	-3.22841900
H	2.92565800	-1.87662900	0.22629000
H	0.98758300	0.46837100	-2.06081600
H	7.74812600	0.40255100	-0.96690800
H	9.75952700	-0.60491000	0.05905100
H	5.27071600	-2.41038700	1.13076100
H	7.28406100	-3.42627600	2.14499700
H	5.19573100	2.10021800	-2.25358400
H	4.33431300	3.61555800	-1.90465900
H	4.35623200	2.99466200	-3.55188000
O	1.95359400	2.52052700	-2.66437600
H	9.54038800	-2.52728400	1.61856100
C	-5.62071000	-1.11545700	0.27347000
C	-5.20542500	0.05411600	0.89710200
C	-4.11748900	0.77825600	0.41747900
C	-3.42534400	0.32613100	-0.70374200
C	-3.84081000	-0.84426600	-1.33875900
C	-4.93000100	-1.55325100	-0.85208700
H	-6.46524300	-1.67651500	0.65834300
H	-3.81703300	1.66706600	0.96240300
H	-3.27752000	-1.19811900	-2.19553800
C	-5.29342200	-2.86383500	-1.48978800
C	-5.86353000	0.48451600	2.17670600
F	-6.57027500	-3.19585000	-1.26053500
F	-5.10668700	-2.84117100	-2.81509800
F	-4.53366900	-3.86255500	-1.00512500
F	-5.24245900	-0.04963600	3.24513800
F	-7.14314400	0.09789400	2.23606700
F	-5.82771300	1.81457800	2.33343300
C	-2.15169200	0.94524100	-1.21649300

O	-1.47039400	0.34401700	-2.04459300
N	-1.77008600	2.12316200	-0.67793300
H	-2.36069300	2.58748600	-0.00462200
C	-0.47349800	2.70564900	-0.99253300
H	-0.13847700	2.24434100	-1.92016300
C	0.57461500	2.38968500	0.08863500
H	1.50627200	2.88817600	-0.19665600
H	0.27576800	2.75414700	1.07691000
C	-0.56936900	4.21693200	-1.27142000
C	-0.96228100	5.04551400	-0.04124900
H	-1.94588100	4.72314300	0.33006100
H	-0.24736700	4.86148800	0.76845000
P	1.00574500	0.62188400	0.28867800
C	2.27755100	0.54909300	1.57976700
C	3.27582400	1.52669800	1.65054200
C	2.29515400	-0.53075900	2.47138100
C	4.28712400	1.41664300	2.59933500
H	3.28853100	2.35438900	0.94949100
C	3.31424700	-0.63865200	3.41184900
H	1.51951600	-1.28962000	2.42674700
C	4.31026800	0.33386600	3.47490500
H	5.06272800	2.17317000	2.64626200
H	3.32788500	-1.48068300	4.09538400
H	5.10614400	0.24699200	4.20724300
C	-0.42182900	-0.26015600	1.00475800
C	-0.92850700	-1.45005000	0.47633000
C	-0.99312800	0.28335600	2.16648900
C	-1.99857200	-2.08804200	1.10691400
H	-0.51454600	-1.87180800	-0.43172500
C	-2.06173400	-0.35417000	2.78374300
H	-0.59913700	1.19974100	2.59832500
C	-2.56508400	-1.54388400	2.25357200
H	-2.40282900	-2.99894300	0.67724000
H	-2.50917400	0.07869500	3.67198600
H	-3.40881100	-2.03204500	2.73054400
C	-1.50689300	4.45759700	-2.45587100
H	-1.25620900	3.78880500	-3.28458300
H	-2.54972200	4.27443000	-2.17536000
H	-1.42911900	5.48450300	-2.81905500
H	0.44575300	4.50598600	-1.57440600
C	-1.01024500	6.54842900	-0.31557500
H	-1.82126600	6.80756600	-1.00042500
H	-1.16530900	7.10815600	0.60986400
H	-0.07082500	6.88894100	-0.76292400

Re-TS1

P	0.68532300	0.96199700	0.47950800
F	-6.88678200	0.43068800	0.83028700
F	-6.96606000	-1.67141300	1.33828500
F	-5.68741000	-0.33000700	2.44791300
F	-2.67936200	-3.83815500	-2.59138600
F	-2.39769100	-4.28374300	-0.49886000
F	-4.32389400	-4.60674300	-1.41395800
O	-1.56996100	0.95858300	-2.46135000
N	-2.01969200	2.05809800	-0.51824900
C	-0.92914700	3.01557000	-0.66014300
C	-1.43944900	4.46722200	-0.56968000
C	0.22625000	2.74298100	0.32463700
C	-2.26645600	4.71902000	0.69936400
C	-2.22991600	4.80566300	-1.83418400
C	-2.52180600	6.20032600	0.97316500
C	-0.63138100	0.14190800	1.44977400
C	2.12048300	0.92372300	1.59192800
C	-2.19003300	1.04402700	-1.40642400
C	-3.15133000	-0.03084900	-0.99109100
C	-1.27004700	0.80624000	2.50781400
C	2.47857300	-0.31677200	2.13582900
C	-1.00818200	-1.16402600	1.12854300
C	2.93509200	2.03824000	1.82274800
C	-2.87542800	-1.32045600	-1.45033000
C	-4.22750200	0.19225300	-0.13835800
C	-3.66387400	-2.37863400	-1.02462500
C	-5.02049600	-0.88210600	0.26152800
C	-2.29547000	0.17922400	3.20754100
C	3.64275500	-0.44265300	2.88512600
C	-2.01066600	-1.80141500	1.86163100
C	4.09367000	1.90945200	2.58458300
C	-4.74471600	-2.17236000	-0.16935700
C	-2.66355100	-1.12918100	2.88774100
C	4.45175900	0.66954300	3.10952700
C	-6.14807700	-0.61950100	1.21839000
C	-3.26735600	-3.77926600	-1.39370100
H	-0.54243600	2.85248100	-1.66784700
H	-0.54578700	5.10629500	-0.53040400
H	1.11528500	3.25133800	-0.06626700
H	0.03112200	3.15527400	1.32085100
H	-1.75887000	4.28863900	1.57227200
H	-3.22652800	4.19464000	0.60536900
H	-2.58716200	5.83766600	-1.82209400

H	-1.61193400	4.67495500	-2.72738700
H	-3.09913900	4.14513000	-1.92286500
H	-2.43464200	1.95069700	0.39851300
H	-3.10757800	6.66355800	0.17533100
H	-1.57757600	6.74698200	1.05775900
H	-3.07285900	6.33398800	1.90712600
H	-0.97352100	1.81321900	2.78951400
H	1.85297000	-1.18813000	1.95949900
H	-0.55573800	-1.67565800	0.28251400
H	2.68051900	3.00778900	1.40751200
H	-2.00656600	-1.48988400	-2.07889200
H	-4.47340700	1.19393000	0.20425400
H	-2.80062000	0.70697600	4.00981100
H	3.92177500	-1.41042500	3.28803400
H	-2.29597700	-2.81479200	1.59856700
H	4.71797200	2.77875900	2.76292000
H	-5.35773500	-3.00491400	0.15735000
H	-3.46560200	-1.61399100	3.43405100
H	5.36353300	0.56843000	3.68945100
C	6.64043700	-0.65495100	0.60870300
C	7.93888100	-0.83227300	1.07063700
C	8.54825100	-2.08493200	1.00118000
C	7.84649200	-3.16227200	0.46231600
C	6.54884900	-2.99314700	-0.00664400
C	5.92578100	-1.73525300	0.06099500
C	4.58942100	-1.55611200	-0.40863600
C	3.43988600	-1.37835900	-0.77182000
C	2.08905400	-1.23235400	-1.17666600
C	1.45775600	0.02179800	-1.42552200
C	2.17651200	1.23676900	-1.91468800
C	1.54855700	2.01218300	-2.90054500
C	2.14132300	3.17891700	-3.37292700
C	3.37113300	3.59310600	-2.86329800
C	4.00548900	2.82727400	-1.88774500
C	3.41784400	1.65551300	-1.41603200
C	1.28056900	-2.41766700	-1.36435400
O	0.07425600	-2.36941400	-1.65719900
H	6.15907000	0.31607700	0.67625100
H	8.47788400	0.01133700	1.49050000
H	9.56145100	-2.22017900	1.36486500
H	8.31327700	-4.14050200	0.40464800
H	6.00290700	-3.83043300	-0.42956400
H	0.48271900	-0.10546800	-1.89593600
H	0.58191900	1.69316400	-3.28161400

H	1.64174000	3.76497300	-4.13786300
H	3.83315900	4.50538500	-3.22652600
H	4.96480000	3.14117500	-1.48832200
H	3.91820200	1.06729800	-0.65632000
C	1.94471900	-3.76888100	-1.18322600
H	2.82576700	-3.86152700	-1.82400800
H	2.28961200	-3.88322300	-0.15074100
H	1.22448100	-4.55187900	-1.41953000
S-M1			
C	6.54430600	-0.91649500	0.85390900
C	7.80632400	-1.15429300	1.38389600
C	8.48592000	-2.33730200	1.09295200
C	7.88628500	-3.28277600	0.26135100
C	6.62513100	-3.05355800	-0.27548900
C	5.92916900	-1.86430100	0.01316700
C	4.63390200	-1.62218700	-0.52272900
C	3.50431800	-1.41185800	-0.94257800
C	2.20416800	-1.17873000	-1.42046000
C	1.55012100	0.17430800	-1.27824700
C	2.31006800	1.36133300	-1.84460700
C	1.75544300	2.08244700	-2.90760500
C	2.42000400	3.18307300	-3.44306700
C	3.64937900	3.57791500	-2.91979000
C	4.21323500	2.86082400	-1.86658900
C	3.55123500	1.75759800	-1.33214700
C	1.53661100	-2.13837100	-2.22512200
O	0.39684100	-1.95881300	-2.71609300
H	6.01058400	-0.00078100	1.09048500
H	8.26268300	-0.41122300	2.03112000
H	9.47093000	-2.52014500	1.50937300
H	8.40594000	-4.20693600	0.02738700
H	6.16208100	-3.79039700	-0.92419400
H	0.58540200	0.09537600	-1.80255300
H	0.79342400	1.77458900	-3.31240200
H	1.97618500	3.73055300	-4.26834400
H	4.16758200	4.43680500	-3.33348400
H	5.17493300	3.15750000	-1.46031300
H	4.00567000	1.18928100	-0.52598800
C	0.58019500	2.30797400	0.61712900
H	1.48604200	2.89156900	0.42105300
H	0.28597100	2.49045000	1.65662700
P	1.05828900	0.54506400	0.46763800
C	2.37716100	0.26263600	1.67378000
C	3.14666600	1.31400700	2.18299800

C	2.61540700	-1.05053500	2.09716600
C	4.14753100	1.04976300	3.11454700
H	2.97729700	2.33745600	1.86564700
C	3.62413500	-1.30727800	3.01738000
H	2.02135100	-1.86683000	1.69655800
C	4.38644500	-0.25814600	3.52877400
H	4.73895100	1.86695400	3.51284300
H	3.81568900	-2.32630600	3.33473400
H	5.17283500	-0.46238100	4.24804100
C	-0.31902500	-0.50777800	0.99114500
C	-0.84715200	-1.49354400	0.15483300
C	-0.84331800	-0.31120800	2.27857200
C	-1.90022400	-2.28608000	0.62017400
H	-0.46994300	-1.64242400	-0.85593100
C	-1.90856200	-1.08698000	2.71661600
H	-0.41928900	0.43932400	2.94134400
C	-2.43315800	-2.08157500	1.88727700
H	-2.32018200	-3.04554300	-0.03150900
H	-2.32861700	-0.92157700	3.70274800
H	-3.26724300	-2.68425200	2.23225100
C	-5.49995100	-1.38215200	0.15134800
C	-5.14758000	-0.31518200	0.96835800
C	-4.14498400	0.57478100	0.59490500
C	-3.46746600	0.38600900	-0.60759800
C	-3.82867200	-0.67039200	-1.44351100
C	-4.83740400	-1.54395900	-1.06140300
H	-6.28207300	-2.07132400	0.45089900
H	-3.92349500	1.40678800	1.25522100
H	-3.28953800	-0.80382100	-2.37549700
C	-5.14974600	-2.73273100	-1.92583100
C	-5.78848900	-0.17707400	2.31978200
F	-6.40636800	-3.16116200	-1.74738000
F	-4.98965800	-2.45878400	-3.22530800
F	-4.33846800	-3.76656600	-1.63902800
F	-5.11356400	-0.87969100	3.24843500
F	-7.04694100	-0.63205600	2.32592500
F	-5.80936400	1.09635500	2.73509800
C	-2.29176900	1.21335700	-1.05227700
O	-1.83440800	1.08799700	-2.18277900
N	-1.75198300	2.04784500	-0.12759100
H	-2.08258500	2.00159800	0.82536800
C	-0.67454200	4.27415600	-0.44403000
C	-1.11957600	4.87452900	0.89442800
H	-2.07590400	4.42083500	1.18880500

H	-0.39249100	4.61599800	1.67295900
C	-1.63387200	4.62187300	-1.58339000
H	-1.34833000	4.10211200	-2.50313500
H	-2.65639700	4.32247400	-1.32977700
H	-1.63398800	5.69445100	-1.78762400
H	0.31784300	4.67878100	-0.69211800
C	-1.27339500	6.39442000	0.85802800
H	-2.09773400	6.70050100	0.20946800
H	-1.47389200	6.78807700	1.85727900
H	-0.35904800	6.86830400	0.48641600
C	-0.49987600	2.74377200	-0.38324200
H	-0.19662300	2.42421200	-1.38132200
C	2.24777900	-3.45885100	-2.48941700
H	3.18239600	-3.29583300	-3.03413500
H	2.50822500	-3.95852200	-1.55198100
H	1.59164500	-4.10155900	-3.07678700
TS1'			
C	-1.84617500	-1.13560400	1.29394700
C	-3.03873500	-0.69018300	1.43707400
C	-0.79979200	-1.69689600	2.17386000
C	0.09745000	-0.84802800	2.83139600
C	-0.63710300	-3.08313900	2.27628800
C	1.16036800	-1.38354500	3.55690700
H	-0.02630800	0.22769000	2.73496200
C	0.42694400	-3.61419500	3.00149100
H	-1.34091000	-3.73984300	1.77173500
C	1.33527000	-2.76489600	3.63179300
H	1.86459500	-0.72414000	4.05610000
H	0.55059800	-4.69021400	3.06919900
H	2.17513100	-3.17625700	4.18205500
C	-4.19710800	-0.19768600	0.80484800
C	-4.63140700	1.09961700	0.71726800
H	-5.55749400	1.24017500	0.16656800
C	-4.07598900	2.29091500	1.34212300
C	-3.00147800	2.27856200	2.25320400
C	-4.68364800	3.53423200	1.06951200
C	-2.57731300	3.45067000	2.87206200
H	-2.50150500	1.34388800	2.48213900
C	-4.24711600	4.70333900	1.67638000
H	-5.51689200	3.56635600	0.37172000
C	-3.19127500	4.66881500	2.58930100
H	-1.74725900	3.40966100	3.57075800
H	-4.73410000	5.64522200	1.44241600
H	-2.84868700	5.58112900	3.06670200

C	-5.12777700	-1.24309800	0.22394900
O	-5.91564800	-0.96016100	-0.66012900
C	-5.06013000	-2.63718400	0.80035900
H	-4.04368300	-3.03286800	0.71942100
H	-5.31255800	-2.60382800	1.86435500
H	-5.75659300	-3.28256900	0.26562700
C	-1.83563300	0.25646500	-1.52102100
H	-2.92598900	0.22492600	-1.43587900
H	-1.58391100	0.19202700	-2.58527700
P	-1.17506000	-1.23397300	-0.67355700
C	-2.05712200	-2.64323100	-1.40784900
C	-3.29076700	-2.49918800	-2.04975300
C	-1.53028200	-3.92860500	-1.20901400
C	-3.99642700	-3.62569000	-2.47056800
H	-3.72155200	-1.51949900	-2.22331900
C	-2.23669200	-5.04736200	-1.63290100
H	-0.56465300	-4.05032200	-0.72380400
C	-3.47498000	-4.89782800	-2.25967000
H	-4.95703800	-3.50057700	-2.95924700
H	-1.82170900	-6.03719200	-1.47495300
H	-4.02737400	-5.77305500	-2.58491700
C	0.56244700	-1.46703400	-1.23060700
C	1.54474300	-1.83399500	-0.30399000
C	0.91864000	-1.28424800	-2.57526500
C	2.86375500	-2.01784500	-0.71871800
H	1.29467100	-1.97010600	0.74353100
C	2.24067500	-1.44555000	-2.97803100
H	0.16624000	-1.02315300	-3.31500700
C	3.21422200	-1.81684000	-2.04959300
H	3.61661100	-2.29130800	0.01395400
H	2.51084400	-1.28714800	-4.01675700
H	4.24696200	-1.93093000	-2.36453400
C	4.93092900	0.54268800	0.11675800
C	4.33623100	1.06256600	-1.02746400
C	3.01262900	1.49252800	-1.01788800
C	2.27430000	1.41799600	0.16145300
C	2.87197200	0.92927200	1.32122100
C	4.18421000	0.47840700	1.28833600
H	5.95188900	0.17751100	0.09122500
H	2.57641800	1.88346700	-1.93212700
H	2.28685000	0.88480300	2.23291600
C	4.74639800	-0.20258500	2.50256800
C	5.13171700	1.14078400	-2.30060900
F	6.08302100	-0.15561600	2.53530700

F	4.28743200	0.34201000	3.63843000
F	4.39450700	-1.50188400	2.52696900
F	5.81041500	2.29232800	-2.40026600
F	4.34241300	1.05297700	-3.38119500
F	6.03041900	0.14692000	-2.37706300
C	0.81051300	1.75437700	0.26014500
O	0.30956600	2.06429000	1.33430800
N	0.10098600	1.61486300	-0.88686300
H	0.58006800	1.23591600	-1.69274300
C	-1.99574700	2.81342300	-1.52837500
C	-1.67326400	2.93966900	-3.02240400
H	-0.58181800	2.95690500	-3.15073800
H	-2.04049700	2.05618800	-3.55687100
C	-1.57523500	4.05543100	-0.74190900
H	-1.70114800	3.89258400	0.33184400
H	-0.52147200	4.28941900	-0.93423700
H	-2.17449100	4.92419300	-1.02461900
H	-3.08270600	2.68510500	-1.41370100
C	-2.27839000	4.18330000	-3.67233700
H	-1.82810100	5.10016000	-3.28423900
H	-2.12664500	4.17044300	-4.75450300
H	-3.35599000	4.23338800	-3.48411100
C	-1.35985600	1.56700800	-0.88405800
H	-1.64983000	1.56012700	0.17136800
TS2SR			
C	-0.97379100	-4.03795400	-0.31673000
C	-0.21012000	-3.68847900	0.79634100
C	-1.73416000	-3.06850300	-0.96477400
C	-0.18799300	-2.36896600	1.23696800
C	-1.71337100	-1.74448700	-0.52579700
C	-0.92316800	-1.38208600	0.56811100
C	-4.27215200	-2.94432100	1.29886300
C	-3.41305100	-3.75408900	2.02783400
C	-0.76088900	0.05189400	1.02105600
C	-5.54856100	-0.84858100	0.96221900
C	-4.57046800	-1.63850800	1.70391000
C	-5.57540600	2.86508700	-0.42384300
C	-6.37825600	3.59461600	-1.29286100
C	-2.82656100	-3.24707600	3.18173000
C	-4.23287200	0.87467300	0.11171000
C	-3.13501500	0.87859500	0.70382200
C	-5.09769700	1.59523400	-0.79053400
C	-1.98894500	0.82364800	1.45281800
C	-6.71817900	3.07181000	-2.54090100

C	-3.97637900	-1.15711200	2.87811400
C	-5.46421100	1.06453200	-2.03528000
C	-3.10782300	-1.94965900	3.61320600
C	-6.25872300	1.80710700	-2.90385600
C	-1.88051000	1.58408400	2.67985300
C	-3.06125400	2.41693900	3.14461300
H	-0.98671500	-5.06496300	-0.66812100
H	0.37191800	-4.44137300	1.31886000
H	-2.36073000	-3.33142900	-1.80975400
H	0.43424600	-2.08385600	2.08052300
H	-3.21084900	-4.75865100	1.67517000
H	-2.32703800	-1.00537400	-1.03186300
H	-0.06733100	0.06292600	1.86875800
H	-5.29404100	3.27625600	0.54147100
H	-6.73441500	4.57711400	-0.99840700
H	-6.02333200	-0.02649100	1.49388500
H	-2.14118900	-3.87100600	3.74590800
H	-5.09508200	0.08560000	-2.31931700
H	-6.52113200	1.39302100	-3.87273200
H	-4.22220100	-0.15245800	3.20853100
H	-2.64863400	-1.55985900	4.51483100
H	-4.01165900	2.09984400	2.71523300
H	-2.88767400	3.45805700	2.85121300
H	-3.10460800	2.38278900	4.23469000
N	-6.23529500	-1.31028500	-0.07252400
O	-4.51202600	-2.06419700	-1.78664500
O	-4.88538000	-3.51484600	0.19962400
O	-6.62657900	-3.34035800	-1.49495200
O	-0.83732700	1.61768300	3.34914500
S	-5.58501700	-2.52010100	-0.91609900
H	-7.34067500	3.64400900	-3.22118500
C	6.50399800	-1.30244100	-0.64979900
C	6.27652400	0.06375800	-0.75109700
C	5.23131200	0.67232200	-0.06156300
C	4.39081000	-0.09632900	0.74034000
C	4.61719400	-1.46853700	0.85127200
C	5.66669100	-2.06031700	0.16293900
H	7.31742700	-1.76845700	-1.19485800
H	5.08420600	1.73848700	-0.19917100
H	3.94171200	-2.05951200	1.46052400
C	5.82855200	-3.55289000	0.21834700
C	7.09327900	0.88400100	-1.70819800
F	7.08253000	-3.93110700	-0.05983000
F	5.50907800	-4.04310000	1.42238300

F	5.02675800	-4.15845400	-0.67560800
F	6.49986700	0.95283800	-2.91477000
F	8.31117300	0.36518000	-1.90056900
F	7.24524900	2.14434800	-1.27969400
C	3.15040600	0.42980600	1.41181700
O	2.34668900	-0.35321300	1.91374000
N	2.93386400	1.76299700	1.37143000
H	3.61115700	2.37386700	0.94029200
C	1.67956200	2.33058700	1.84255700
H	1.22948400	1.58321300	2.49484100
C	0.70474300	2.59825500	0.68062700
H	-0.19282100	3.07251700	1.09128700
H	1.12995800	3.27924100	-0.06330600
C	1.89908700	3.58580100	2.70900600
C	2.49866400	4.76912500	1.93785800
H	3.48800900	4.49527500	1.54454000
H	1.86963400	5.00141300	1.07116400
P	0.11592800	1.12023200	-0.22903000
C	-1.02065100	1.71715900	-1.50921400
C	-1.80691200	2.85810200	-1.30755400
C	-1.12081700	1.00443300	-2.71047500
C	-2.67768700	3.28436400	-2.30462400
H	-1.76123100	3.40693400	-0.37249100
C	-2.00433300	1.43010400	-3.69729500
H	-0.51070800	0.12123200	-2.87594400
C	-2.77729900	2.57122400	-3.49692900
H	-3.29702800	4.15935100	-2.13986100
H	-2.08443400	0.87030700	-4.62266100
H	-3.47003000	2.89943400	-4.26469700
C	1.50534500	0.40772900	-1.16885200
C	1.82728800	-0.95112400	-1.17448700
C	2.23863000	1.30019500	-1.96783200
C	2.88356600	-1.40810100	-1.96564100
H	1.27885700	-1.65414400	-0.56051600
C	3.29055300	0.83749400	-2.74712400
H	1.98364300	2.35621200	-1.99341300
C	3.61558400	-0.52053900	-2.74503000
H	3.14441500	-2.46128100	-1.94574900
H	3.86297800	1.53438400	-3.34951800
H	4.44742100	-0.87652300	-3.34421400
C	2.72960800	3.21385500	3.93839600
H	2.31950300	2.32249400	4.42232700
H	3.76773000	3.00310500	3.66081100
H	2.73178700	4.02220600	4.67241000

H	0.89515400	3.87253400	3.05135900
C	2.64161200	6.03204400	2.78695300
H	3.38517700	5.90456000	3.57724600
H	2.95260500	6.87992700	2.17220500
H	1.68846800	6.28945300	3.25994200

TS2SR'

C	1.49259800	-4.02717400	-0.19200200
C	0.98624900	-3.54723000	-1.39857300
C	1.63382800	-3.16043200	0.88958100
C	0.62890800	-2.20711500	-1.52313400
C	1.28609900	-1.81709800	0.76207400
C	0.77994300	-1.32800100	-0.44605700
C	6.83711300	-1.53409500	-1.10202900
C	7.97941700	-2.07013900	-0.51612000
C	0.46930600	0.13602800	-0.67147600
C	4.38141700	-1.15296200	-1.18007600
C	5.57292600	-1.70743800	-0.52844000
C	6.08962800	0.77417400	1.43334200
C	6.91575100	0.73939500	2.55164500
C	7.85750400	-2.78982200	0.66554400
C	3.87503200	0.36314700	0.39154500
C	2.82728200	0.75003200	-0.17079600
C	4.73836200	0.41116300	1.54537500
C	1.71521800	0.97098900	-0.92695300
C	6.41674200	0.33576000	3.78984800
C	5.47622400	-2.44372900	0.65934700
C	4.24186800	0.00857000	2.79518400
C	6.60445300	-2.98140300	1.25656500
C	5.07517600	-0.02596300	3.90750100
C	1.69986400	1.90307600	-2.03542800
C	2.97765500	2.62075800	-2.41353000
H	1.77091300	-5.07113000	-0.09399800
H	0.86867200	-4.21562600	-2.24499700
H	2.02022900	-3.52654000	1.83582000
H	0.23432600	-1.83300300	-2.46366300
H	8.93858900	-1.91472400	-0.99677800
H	1.42136200	-1.14771100	1.60532500
H	-0.18066300	0.23313800	-1.55005400
H	6.47213000	1.07687200	0.46376200
H	7.95900200	1.02371500	2.45452400
H	3.43944000	-1.65783700	-0.97241200
H	8.74589800	-3.20478400	1.12970700
H	3.19370200	-0.26487000	2.88326500
H	4.67421300	-0.33355900	4.86876000

H	4.49305200	-2.57001300	1.10592300
H	6.51720300	-3.54442400	2.17900800
H	3.79386800	2.44783500	-1.71410700
H	2.76733500	3.68956000	-2.50286300
H	3.28691300	2.26249300	-3.40041100
N	4.43287400	-0.53766900	-2.36757100
O	6.05672200	1.36040400	-1.81189700
O	6.99180500	-0.87801200	-2.30647200
O	5.96097800	0.41183400	-4.11375000
O	0.67264500	2.11469900	-2.69342000
S	5.80669900	0.22234200	-2.68756300
H	7.06804500	0.30542300	4.65737700
C	-6.91793600	-1.52636800	-0.12531100
C	-6.67500800	-0.24721700	0.35889300
C	-5.57323300	0.48697000	-0.07038500
C	-4.69457000	-0.06464800	-1.00015300
C	-4.93430700	-1.34656600	-1.49461900
C	-6.03854700	-2.06566100	-1.05882000
H	-7.77504600	-2.09393700	0.22009500
H	-5.40590600	1.46385300	0.37105700
H	-4.22828400	-1.77386400	-2.19876900
C	-6.21917400	-3.48129200	-1.52853300
C	-7.54530400	0.30700500	1.45033700
F	-7.49025000	-3.88745400	-1.41814200
F	-5.84914400	-3.63179700	-2.80603900
F	-5.46918000	-4.32840200	-0.80171200
F	-7.06700400	-0.02200400	2.66546100
F	-8.79474700	-0.16634300	1.38274300
F	-7.60807300	1.64430400	1.40806700
C	-3.39959300	0.58069200	-1.41325100
O	-2.53902400	-0.08472900	-1.98512300
N	-3.20649700	1.87025500	-1.05869800
H	-3.95502700	2.39705000	-0.63409900
C	-1.92640000	2.52239100	-1.28405100
H	-1.39730500	1.91903300	-2.02012200
C	-1.07651600	2.56232800	-0.00056900
H	-0.15757800	3.12083500	-0.21041200
H	-1.59452600	3.06778100	0.82147400
C	-2.08861800	3.92164000	-1.90837400
C	-2.78026900	4.93206900	-0.98365200
H	-3.79416600	4.58347000	-0.73983300
H	-2.23475200	4.99707400	-0.03542800
P	-0.52722000	0.94507200	0.66031800
C	0.46195300	1.32995300	2.13604200

C	1.38231300	2.38696500	2.11083000
C	0.29529200	0.58279100	3.30968600
C	2.11925700	2.69232800	3.25028300
H	1.53871600	2.96479300	1.20662500
C	1.03642600	0.89658000	4.44547600
H	-0.41350000	-0.23875400	3.34171600
C	1.94391300	1.95277700	4.41754700
H	2.83355000	3.50761400	3.22195000
H	0.89997000	0.31531000	5.35085300
H	2.52173100	2.19515200	5.30326700
C	-1.95780800	-0.00132500	1.25481400
C	-2.23074000	-1.30278300	0.82618700
C	-2.79265600	0.61408500	2.20153200
C	-3.33122500	-1.98489700	1.34787700
H	-1.61080400	-1.77923400	0.07580800
C	-3.88610900	-0.07184300	2.71347300
H	-2.58279600	1.62192800	2.55090200
C	-4.15459200	-1.37432100	2.28712200
H	-3.55399100	-2.98673600	0.99541300
H	-4.53637600	0.41029500	3.43499300
H	-5.01883600	-1.90072800	2.67922000
C	-2.79388600	3.79365400	-3.25962300
H	-2.32710900	3.00902700	-3.86232000
H	-3.85087300	3.53894900	-3.12814200
H	-2.73779000	4.72708800	-3.82330000
H	-1.06317900	4.27018000	-2.09249800
C	-2.87612000	6.33347200	-1.58638000
H	-3.54543500	6.35603200	-2.44966100
H	-3.25724800	7.04680200	-0.85188500
H	-1.89126200	6.68059400	-1.91494300
TS2SR"			
C	0.86160600	-4.04060000	-0.51868900
C	0.31415500	-3.50848900	-1.68495900
C	1.28700800	-3.18568400	0.49560200
C	0.16958700	-2.12965100	-1.82282600
C	1.16198800	-1.80637900	0.35032600
C	0.58276300	-1.26655800	-0.80315100
C	6.34371300	-1.94607600	-0.22237900
C	6.61509400	-3.13176300	0.44587400
C	0.36616700	0.21945100	-0.98638900
C	4.91605500	-0.47408200	-1.60820400
C	5.16653300	-1.76580400	-0.95389300
C	5.58512400	1.62212800	1.32200300
C	6.44820400	1.67689900	2.41162500

C	5.68169500	-4.16094900	0.38460700
C	3.82644600	0.45361000	0.04330600
C	2.75295000	0.77908400	-0.50304300
C	4.70851700	0.53768500	1.17531200
C	1.62093800	1.03402600	-1.22113900
C	6.45046400	0.65580700	3.36064600
C	4.23791600	-2.80989200	-0.99792800
C	4.73095400	-0.50032800	2.12007000
C	4.49504700	-4.00342300	-0.33667400
C	5.59145600	-0.43309500	3.20934800
C	1.57755600	2.12536400	-2.17096100
C	2.85061500	2.92022400	-2.39693300
H	0.95832500	-5.11544700	-0.40308800
H	-0.01458700	-4.16623900	-2.48285000
H	1.73027500	-3.59115400	1.39970800
H	-0.28837900	-1.71577300	-2.71667100
H	7.54078200	-3.22554700	1.00207300
H	1.51779300	-1.15091600	1.13817800
H	-0.31028600	0.37832000	-1.83341500
H	5.58079200	2.41060100	0.57593400
H	7.12434000	2.51936200	2.51770000
H	4.02071800	-0.40842900	-2.22329700
H	5.88214200	-5.09334400	0.90159100
H	4.07072300	-1.35344200	1.98371900
H	5.59793800	-1.23635900	3.93966900
H	3.30678600	-2.66788100	-1.54265500
H	3.76940000	-4.80848700	-0.37640800
H	3.71372200	2.26944300	-2.55787400
H	3.06944200	3.52729400	-1.51187000
H	2.70790900	3.57791000	-3.25403900
N	5.87953800	0.39607900	-1.90232500
O	8.04208900	1.25789600	-0.91731800
O	7.24863100	-0.90815300	-0.10652400
O	8.08910100	-0.70851200	-2.43667400
O	0.54327500	2.42827700	-2.77914400
S	7.38711800	0.07387600	-1.43078800
H	7.12487700	0.70306200	4.20949700
C	-6.92299900	-1.48357600	0.10447300
C	-6.66434800	-0.20067300	0.56953500
C	-5.60237900	0.54565300	0.06633900
C	-4.78140500	0.00262000	-0.91917300
C	-5.03705100	-1.28368000	-1.39439200
C	-6.10078200	-2.01475800	-0.88474800
H	-7.74862700	-2.06052200	0.50652200

H	-5.41728300	1.52594100	0.49296900
H	-4.37410500	-1.70448300	-2.14279700
C	-6.29574500	-3.43478700	-1.33517600
C	-7.46881600	0.34966400	1.71263100
F	-7.55855800	-3.84519800	-1.16328200
F	-5.98376100	-3.59425200	-2.62702400
F	-5.51002100	-4.27322200	-0.63643900
F	-6.90161400	0.04775100	2.89586900
F	-8.70975000	-0.14949600	1.73664100
F	-7.56250000	1.68480600	1.65799900
C	-3.52617200	0.66521400	-1.41733100
O	-2.69131500	0.01045100	-2.03871500
N	-3.33303000	1.96002500	-1.08413000
H	-4.05825200	2.47440200	-0.60668400
C	-2.07406200	2.62727200	-1.37785900
H	-1.58923300	2.04410900	-2.15951800
C	-1.14485600	2.64342100	-0.15028400
H	-0.24704300	3.21482100	-0.40694700
H	-1.61372900	3.12518100	0.71416700
C	-2.28654900	4.03853500	-1.95747400
C	-2.90955600	5.02482300	-0.96090200
H	-3.89742000	4.66226400	-0.64201600
H	-2.28921100	5.07776600	-0.05924000
P	-0.55129300	1.01122400	0.43243100
C	0.57678000	1.34141700	1.81549100
C	1.48557300	2.40562700	1.75213100
C	0.59255400	0.48063400	2.92079100
C	2.41373400	2.58892300	2.77183100
H	1.49439800	3.07838200	0.90131600
C	1.52646900	0.66879800	3.93464200
H	-0.11297800	-0.34237900	2.98428700
C	2.44026400	1.71736400	3.85769000
H	3.12622500	3.40390900	2.70788200
H	1.54034900	-0.00757500	4.78229600
H	3.17811600	1.85276500	4.64156900
C	-1.93643300	0.07395400	1.14762100
C	-2.26019200	-1.23018600	0.76357600
C	-2.67435800	0.70693500	2.16077000
C	-3.31442000	-1.89407000	1.39280900
H	-1.71794700	-1.72324700	-0.03411600
C	-3.72506900	0.04000200	2.77745600
H	-2.42308800	1.71486500	2.48068800
C	-4.04434100	-1.26412700	2.39424700
H	-3.57662400	-2.89781300	1.07428700

H	-4.30107700	0.53793700	3.54967600
H	-4.87456100	-1.77658800	2.86929000
C	-3.09188800	3.93883100	-3.25431800
H	-2.67815000	3.16306200	-3.90540600
H	-4.13799400	3.68765100	-3.04926900
H	-3.07175900	4.88241300	-3.80329400
H	-1.27823600	4.39440600	-2.20880700
C	-3.06562800	6.43571000	-1.52772400
H	-3.80348900	6.46716200	-2.33292500
H	-3.39098600	7.13216400	-0.75145100
H	-2.11371200	6.79786400	-1.92914300
TS2SR'''			
C	1.13758900	3.21569300	-2.67922500
C	0.74008400	3.58191100	-1.39523400
C	1.43113100	1.88352700	-2.95541600
C	0.61684900	2.61642800	-0.40023300
C	1.32503800	0.91946900	-1.95644300
C	0.90468300	1.27620900	-0.67192300
C	6.20489800	2.28894100	1.22337700
C	7.21016200	2.21210200	2.18206700
C	0.74911800	0.26745300	0.44536800
C	5.01255600	1.46387900	-0.79512300
C	6.05011700	1.30443800	0.24075100
C	5.37013300	-2.63339000	-1.15626600
C	5.90408000	-3.51847700	-2.08547900
C	8.08630900	1.13542100	2.15766200
C	4.02660500	-0.60629200	-0.63551900
C	3.09887600	-0.49670900	0.19539600
C	4.62172800	-1.52108400	-1.57961500
C	2.04813600	-0.25574400	1.02493900
C	5.70378900	-3.31505400	-3.45141300
C	6.96126600	0.24051800	0.22463100
C	4.45303200	-1.30692000	-2.95738700
C	7.96680600	0.14904200	1.17410700
C	4.97801100	-2.20545300	-3.88103500
C	2.17457700	-0.36836100	2.45933400
C	3.55364200	-0.65273500	3.02135000
H	1.22448800	3.96674400	-3.45770000
H	0.52485100	4.62019900	-1.16533500
H	1.74818500	1.59049000	-3.95173800
H	0.29723500	2.89904600	0.59865900
H	7.28807200	2.99963000	2.92289700
H	1.57865600	-0.11165800	-2.17933600
H	0.17087800	0.72171700	1.25865300

H	5.51010500	-2.79872400	-0.09166800
H	6.47323400	-4.37695900	-1.74202200
H	5.23666100	1.05966400	-1.78086100
H	8.86937000	1.06723300	2.90519400
H	3.88556500	-0.44178600	-3.29104200
H	4.82208100	-2.03558300	-4.94192400
H	6.86403500	-0.51648200	-0.54726100
H	8.66041000	-0.68393900	1.15078500
H	4.16782500	0.24698500	2.91136300
H	4.05140700	-1.45775600	2.47532200
H	3.46653300	-0.90836500	4.07743300
N	4.13631400	2.45481800	-0.78853600
O	3.14765600	2.47862400	1.58970800
O	5.41286900	3.41811500	1.23355700
O	3.48407200	4.60211000	0.32498300
O	1.21437200	-0.20930100	3.22403500
S	3.88894400	3.24111200	0.60110700
H	6.11739900	-4.01106700	-4.17374100
C	-6.74334400	1.08050600	-0.54368800
C	-6.45524000	-0.21198600	-0.12334500
C	-5.29865100	-0.49196900	0.59791500
C	-4.40955500	0.53554000	0.90621500
C	-4.69386300	1.83613800	0.49144800
C	-5.85297700	2.10068400	-0.22538200
H	-7.64384900	1.28902400	-1.11084300
H	-5.10074300	-1.52434200	0.86613100
H	-3.98028800	2.62199100	0.71570400
C	-6.08731700	3.49085500	-0.74478900
C	-7.34555900	-1.34265700	-0.55312200
F	-7.37787800	3.70881100	-1.02777100
F	-5.69683000	4.42175200	0.13441500
F	-5.39281100	3.70578800	-1.87590700
F	-6.96508500	-1.83430700	-1.74748100
F	-8.61963900	-0.95403600	-0.68110600
F	-7.31132800	-2.36269400	0.31455900
C	-3.06715700	0.31505900	1.54996700
O	-2.22027400	1.20483100	1.52320600
N	-2.82360300	-0.90668400	2.07347400
H	-3.55622700	-1.59969000	2.10457700
C	-1.50154200	-1.25882900	2.56713200
H	-0.97216100	-0.32127000	2.73110500
C	-0.71059100	-2.07658200	1.53052000
H	0.24413000	-2.36802700	1.98076300
H	-1.23847200	-2.99001300	1.23677100

C	-1.56164300	-1.96761600	3.93366400
C	-2.22042900	-3.35241900	3.88005700
H	-3.25624500	-3.26114500	3.52253000
H	-1.69329900	-3.98238800	3.15480600
P	-0.27910400	-1.20779900	-0.02305000
C	0.67631600	-2.39518900	-1.01063200
C	1.62857900	-3.22049400	-0.39957200
C	0.49308600	-2.45737300	-2.39850600
C	2.39222800	-4.08977700	-1.17231000
H	1.79687000	-3.17413000	0.67083500
C	1.26934700	-3.32111100	-3.16419100
H	-0.24504700	-1.82476900	-2.88212900
C	2.21973100	-4.13594000	-2.55306600
H	3.13517600	-4.71897000	-0.69483200
H	1.13049800	-3.35472700	-4.23938600
H	2.83313500	-4.80008600	-3.15280100
C	-1.78819300	-0.88266500	-0.98420200
C	-2.12288200	0.38594500	-1.46473800
C	-2.61664400	-1.97954900	-1.27063200
C	-3.27971200	0.55218900	-2.22800000
H	-1.50420200	1.24513300	-1.23423000
C	-3.76722100	-1.80384800	-2.02852300
H	-2.35822700	-2.97411000	-0.91598200
C	-4.09863700	-0.53544200	-2.50941300
H	-3.54783000	1.54323400	-2.57952600
H	-4.41100900	-2.65131500	-2.23722800
H	-5.00539200	-0.39968900	-3.08996700
C	-2.23193000	-1.04618500	4.95435200
H	-1.80497200	-0.04027700	4.90225600
H	-3.30810300	-0.96850100	4.76620900
H	-2.09206900	-1.41718800	5.97175300
H	-0.51179000	-2.09753800	4.22953800
C	-2.22934200	-4.06841000	5.23040100
H	-2.87851400	-3.56380100	5.94993500
H	-2.58693000	-5.09522200	5.12341100
H	-1.22077200	-4.10428500	5.65471300

TS2SS

C	-1.27204900	-3.80672900	-0.77005200
C	-0.62448800	-3.61312100	0.44870800
C	-1.79085300	-2.71246000	-1.45750600
C	-0.48871900	-2.33072900	0.97054800
C	-1.65787700	-1.42824100	-0.93496300
C	-0.99797800	-1.22675100	0.28088900
C	-4.73453000	-2.60864500	0.38435600

C	-4.91590600	-3.67201700	-0.48651100
C	-0.77058900	0.14990600	0.86214100
C	-5.32875400	-0.40606700	1.32637900
C	-5.59180100	-1.50460200	0.38753000
C	-5.87948700	2.39425000	-1.09182900
C	-6.67663200	2.78013400	-2.16502300
C	-5.98367700	-3.63011300	-1.38051300
C	-4.21063400	0.85395400	-0.10197700
C	-3.11253800	0.95455000	0.48476200
C	-5.04042000	1.27428700	-1.19978400
C	-1.99669600	0.94411700	1.25859900
C	-6.65628600	2.05445400	-3.35559600
C	-6.66003500	-1.48313000	-0.51394800
C	-5.04624900	0.53232000	-2.39229200
C	-6.85734900	-2.54197900	-1.39322100
C	-5.84020600	0.92820700	-3.46226500
C	-1.92892400	1.76076600	2.45920800
C	-3.16841500	2.53176800	2.86523100
H	-1.37347600	-4.80646500	-1.18104200
H	-0.22275200	-4.46143700	0.99346600
H	-2.30512000	-2.85644800	-2.40293100
H	0.02565200	-2.17407600	1.91348700
H	-4.22152300	-4.50389200	-0.45470300
H	-2.07148300	-0.58336800	-1.47534500
H	-0.12594300	0.06102600	1.74261200
H	-5.88583500	2.96442900	-0.16736200
H	-7.31441900	3.65365000	-2.07210800
H	-6.13714200	-4.45694000	-2.06585200
H	-4.42128800	-0.35395000	-2.46366200
H	-5.82653400	0.35213500	-4.38239000
H	-7.32590400	-0.62468900	-0.52204600
H	-7.68725700	-2.51827900	-2.09072000
H	-3.52886900	3.15164400	2.03922900
H	-2.93002300	3.15727300	3.72524200
H	-3.96478800	1.82652500	3.11959900
N	-4.64732600	-0.55521500	2.45769500
O	-4.75330100	-2.88186800	3.44189000
O	-3.64370600	-2.62014500	1.23115200
O	-2.55339100	-1.74559600	3.24050700
O	-0.90340600	1.82709800	3.14560600
S	-3.88966300	-1.95421900	2.72448000
H	-7.27768300	2.35964300	-4.19106900
C	0.86416200	2.64477000	0.70654700
H	-0.01455400	3.16925200	1.09435100

H	1.37406300	3.31460800	0.00641600
P	0.21961700	1.24654000	-0.28594500
C	-0.86600800	1.96611100	-1.55065000
C	-1.70177400	3.04820200	-1.24636600
C	-0.92599200	1.37949500	-2.82127500
C	-2.59983000	3.52202500	-2.19706800
H	-1.67703000	3.51100600	-0.26547200
C	-1.83224900	1.85441000	-3.76412000
H	-0.27661000	0.54514000	-3.06932300
C	-2.67247900	2.92036200	-3.45093900
H	-3.25438300	4.35083000	-1.95064200
H	-1.88286500	1.38732100	-4.74165800
H	-3.39055500	3.27808200	-4.18154000
C	1.59023800	0.49593800	-1.22193500
C	1.85916500	-0.87500400	-1.23601900
C	2.37493500	1.36806600	-1.99392900
C	2.90989500	-1.36530800	-2.01335900
H	1.27622200	-1.55914900	-0.63222800
C	3.42172200	0.87134800	-2.75986600
H	2.16464900	2.43424100	-2.01014100
C	3.69019700	-0.49871400	-2.76978900
H	3.12978600	-2.42796500	-1.99958900
H	4.03448400	1.55116900	-3.34171400
H	4.51871500	-0.88092800	-3.35726500
H	-6.04031300	0.41910700	1.32152900
C	6.49006400	-1.48723200	-0.59140700
C	6.30310200	-0.11364500	-0.67493200
C	5.25759900	0.51172200	-0.00116300
C	4.38031500	-0.24647900	0.77039800
C	4.56351800	-1.62630200	0.86199400
C	5.61199100	-2.23528100	0.18695700
H	7.30333200	-1.96711800	-1.12450700
H	5.13106100	1.58135100	-0.13198700
H	3.85640400	-2.20810300	1.44369100
C	5.72970300	-3.73272900	0.21816100
C	7.16852300	0.69929400	-1.59478500
F	6.97464100	-4.14287900	-0.05598400
F	5.38521600	-4.23398500	1.41037100
F	4.91842300	-4.29827600	-0.69330200
F	6.61486100	0.80305600	-2.81770600
F	8.37782600	0.15131700	-1.75906400
F	7.34049200	1.94832800	-1.14146900
C	3.13832000	0.30873800	1.41299900
O	2.25990200	-0.45414800	1.80944900

N	3.00568400	1.65267400	1.45492100
H	3.76426000	2.24702800	1.15578400
C	2.00528400	3.46344700	2.83564500
C	2.66769800	4.66234200	2.14389000
H	3.64681500	4.36929600	1.73833500
H	2.05703000	4.97662600	1.29011100
C	2.78583700	2.99808100	4.06615700
H	2.34173800	2.08867000	4.48145400
H	3.82891300	2.78101600	3.81246700
H	2.77938100	3.76081700	4.84741900
H	1.00223800	3.76793100	3.16381100
C	2.86082500	5.86172900	3.07150400
H	3.59262900	5.65137500	3.85508600
H	3.21299600	6.73201000	2.51277500
H	1.91683200	6.13074200	3.55632100
C	1.76272300	2.26571200	1.89846200
H	1.24072100	1.51390000	2.48896600

TS2SS'

C	0.61717100	-4.15436900	-0.66106400
C	-0.12116200	-3.60490700	-1.70771300
C	1.32977900	-3.31870200	0.19459800
C	-0.16044000	-2.22448500	-1.88070000
C	1.30427200	-1.93669500	0.01525000
C	0.54356900	-1.37953400	-1.01551200
C	6.93739600	-1.81703500	-0.33984200
C	8.22955700	-1.65086200	0.14721300
C	0.41445700	0.11268200	-1.21772500
C	4.93331700	-1.01907800	-1.56562500
C	6.28502100	-0.80071100	-1.04536800
C	5.20603400	2.51870800	0.64739100
C	6.04462900	3.08432500	1.60097900
C	8.88233100	-0.44528900	-0.07345200
C	3.93123100	0.61651100	-0.25252300
C	2.82813500	0.76684800	-0.82443000
C	4.79108300	1.18112100	0.76233300
C	1.67126600	0.89240700	-1.54276600
C	6.48601200	2.32551500	2.68467300
C	6.96852600	0.40304500	-1.26011400
C	5.25593700	0.41794300	1.84320500
C	8.25538700	0.58483900	-0.78189400
C	6.08758800	0.99393400	2.79836700
C	1.57777000	1.89222900	-2.58722600
C	2.81541200	2.70311600	-2.92611600
H	0.64512300	-5.22979800	-0.51879100

H	-0.67135800	-4.24926100	-2.38589200
H	1.92871400	-3.73763800	0.99600100
H	-0.76362200	-1.78924200	-2.67212800
H	8.69744400	-2.46743800	0.68506400
H	1.89860900	-1.30134800	0.66506500
H	-0.29178700	0.28631200	-2.03640800
H	4.85447200	3.10687500	-0.19590900
H	6.35269200	4.12063600	1.49964500
H	9.88781400	-0.30682800	0.30929400
H	4.94802900	-0.61887600	1.92495200
H	6.43228700	0.39584500	3.63662100
H	6.45857800	1.19848600	-1.79748600
H	8.77077400	1.52372600	-0.94935200
H	2.94548900	3.49181800	-2.17709000
H	2.67347200	3.16769900	-3.90182900
H	3.72249600	2.09587300	-2.92263700
N	4.28482500	-2.16974100	-1.44342400
O	4.40627700	-4.49094500	-0.49447900
O	6.35152500	-3.05407300	-0.16304500
O	4.26155400	-2.56596600	1.07979600
O	0.51738100	2.13408700	-3.17961500
S	4.69490500	-3.10508800	-0.20112200
H	7.13987300	2.76652700	3.43016900
C	-0.99863100	2.59214800	-0.43433400
H	-0.10543300	3.11393200	-0.79312200
H	-1.39204600	3.14933500	0.42215500
P	-0.40853900	0.98059800	0.21002100
C	0.77604800	1.35561800	1.53062300
C	1.55972600	2.51479000	1.49381900
C	0.91413000	0.45434600	2.59396000
C	2.46353100	2.77298100	2.51950100
H	1.48336700	3.21264500	0.66628300
C	1.83612400	0.70951700	3.60368400
H	0.30360000	-0.44305400	2.63407800
C	2.60623300	1.86999100	3.56968100
H	3.07406500	3.66834100	2.48442600
H	1.94712100	0.00291600	4.41885400
H	3.32698400	2.06708400	4.35628200
C	-1.77417700	0.13121400	1.06785700
C	-2.13847000	-1.19516100	0.82443800
C	-2.44129100	0.86535400	2.06235900
C	-3.16782600	-1.77704500	1.56693900
H	-1.64650100	-1.77212800	0.05156300
C	-3.46884400	0.28021700	2.79050500

H	-2.15369500	1.89075500	2.27993700
C	-3.83354500	-1.04462900	2.54252300
H	-3.46155000	-2.80021500	1.35588100
H	-3.99155100	0.85714500	3.54571400
H	-4.64638100	-1.49356400	3.10415000
H	4.62757900	-0.41269000	-2.41404700
C	-6.82768500	-1.37138300	0.45131400
C	-6.53708500	-0.05557600	0.78856500
C	-5.49699500	0.63180000	0.17015200
C	-4.72855000	-0.00464200	-0.80194000
C	-5.01643000	-1.32458300	-1.14879000
C	-6.05962300	-1.99596900	-0.52611000
H	-7.63558400	-1.90220700	0.94299600
H	-5.28960700	1.64514500	0.49724400
H	-4.39262300	-1.81717000	-1.88719800
C	-6.28773300	-3.44711700	-0.84122500
C	-7.27796000	0.59838900	1.91962400
F	-7.53990000	-3.82896800	-0.55974200
F	-6.05559400	-3.71852700	-2.13133000
F	-5.46516400	-4.23119600	-0.12233700
F	-6.67227900	0.35960600	3.09808200
F	-8.53139900	0.14292200	2.02624400
F	-7.33405900	1.92918000	1.77570400
C	-3.49629600	0.59826700	-1.41963600
O	-2.71493400	-0.11044200	-2.05061900
N	-3.25853700	1.90676000	-1.18265700
H	-3.93489800	2.46400200	-0.68298800
C	-2.23716500	3.90885800	-2.23705700
C	-2.77848600	4.95923900	-1.25806700
H	-3.74479800	4.62971600	-0.84963300
H	-2.09538400	5.05432800	-0.40670000
C	-3.12763800	3.75449900	-3.47150100
H	-2.77145500	2.93497600	-4.10267300
H	-4.16219600	3.53716500	-3.18528800
H	-3.12720900	4.66540600	-4.07351600
H	-1.24230100	4.23208400	-2.57260700
C	-2.95987700	6.33783500	-1.89273900
H	-3.75229300	6.33398900	-2.64494300
H	-3.22271600	7.08160000	-1.13691500
H	-2.03506700	6.66335000	-2.37988900
C	-2.00942800	2.52727600	-1.59464400
H	-1.58985100	1.89189600	-2.37363500

TS2SS''

C	-4.36630700	0.90643300	2.91335800
C	-4.42987100	0.78839800	4.29960300
C	-3.86211900	-0.31219000	4.93877200
C	-3.23350100	-1.30249600	4.18281100
C	-3.16093700	-1.18335400	2.80007700
C	-3.71301500	-0.06809000	2.14729200
C	-3.55412600	0.09281400	0.71734000
C	-2.69991400	-0.02777100	-0.18730500
C	-1.80116800	-0.13002800	-1.21139500
C	-0.80297500	0.96470900	-1.50312600
C	-1.29639100	2.27528100	-2.08443400
C	-0.54753800	2.90970100	-3.07882500
C	-0.95190400	4.14020100	-3.59362400
C	-2.11135100	4.74741800	-3.11890900
C	-2.86178800	4.12217500	-2.12405300
C	-2.45313300	2.89852600	-1.60281900
C	-1.61320400	-1.38039400	-1.92444700
C	-2.61572500	-2.49773500	-1.72380300
O	-0.66167500	-1.55028800	-2.69901000
H	-4.80914600	1.76284100	2.41326400
H	-4.93010200	1.55631000	4.88137300
H	-3.91687500	-0.40319400	6.01855800
H	-2.79863000	-2.16994300	4.67045100
H	-2.68595800	-1.95583700	2.20109200
H	-0.09395500	0.51565400	-2.20819900
H	0.35570400	2.43606000	-3.45515700
H	-0.36284500	4.61893400	-4.36892700
H	-2.42890800	5.70395400	-3.52069400
H	-3.76150800	4.59437300	-1.74296200
H	-3.01859100	2.43065800	-0.80086700
H	-3.23504600	-2.56497500	-2.62484000
H	-2.07232000	-3.44104900	-1.62264300
H	-3.27261700	-2.34400900	-0.86526800
P	0.20555600	1.34664700	0.02267300
F	5.63154000	1.63149400	2.61650100
F	7.71125800	1.03022200	2.56117500
F	6.91231400	2.30038500	1.01494600
F	7.63327900	-3.78896500	-1.39404700
F	8.29369900	-1.97402600	-2.35202300
F	9.13637400	-2.54822400	-0.45221700
O	2.83805700	-1.95494700	-1.53784000
N	2.25946700	-1.40083200	0.59422600
C	0.82100000	-1.36270400	0.37271100
C	0.09241800	-2.65372100	0.79703500

C	0.23690300	-0.12684500	1.08978100
C	0.21541200	-2.92146200	2.30176100
C	0.57054900	-3.82293400	-0.06155600
C	-0.57330300	-4.14454600	2.76800200
C	1.89765800	1.79635100	-0.44045300
C	-0.51588200	2.70975200	0.95461100
C	3.15187100	-1.61472900	-0.40533200
C	4.58581900	-1.33228200	-0.05733200
C	2.63507000	2.66497800	0.37627100
C	-0.34266200	4.02375200	0.49654800
C	2.49565000	1.21856000	-1.56735900
C	-1.32404000	2.45423500	2.06738900
C	5.58635200	-2.05966600	-0.69697200
C	4.92284000	-0.27830600	0.78992000
C	6.92063900	-1.75239600	-0.45384500
C	6.26030200	0.04038500	0.99357900
C	3.95687600	2.96128200	0.05674100
C	-0.96797800	5.07229100	1.15889200
C	3.81817400	1.52235700	-1.87924400
C	-1.95053500	3.51195000	2.72162600
C	7.26942700	-0.70000100	0.38704200
C	4.54519900	2.39586500	-1.07379100
C	-1.77207300	4.81644400	2.26970900
C	6.62739200	1.24950600	1.80628100
C	8.00060200	-2.52219300	-1.16275000
H	0.70051400	-1.27932300	-0.71431400
H	-0.97006600	-2.47233700	0.56895600
H	-0.79874700	-0.31747200	1.38782300
H	0.80322200	0.13216100	1.99115300
H	-0.13819800	-2.04364400	2.85889100
H	1.27489300	-3.05405700	2.55850400
H	-0.03836300	-4.71312900	0.11286300
H	0.50833000	-3.56298800	-1.12246200
H	1.61293700	-4.07078600	0.16781300
H	2.60930900	-1.26855700	1.53306400
H	-0.15542900	-5.07025500	2.36492100
H	-1.61893800	-4.08437000	2.44624700
H	-0.56134800	-4.22195000	3.85801800
H	2.17929500	3.11027200	1.25529800
H	0.26624300	4.22452200	-0.38118400
H	1.96138300	0.50402500	-2.18682700
H	-1.48398300	1.44364100	2.42989700
H	5.31250100	-2.85912100	-1.37745600
H	4.14922900	0.32998700	1.24992400

H	4.52933900	3.62509900	0.69517300
H	-0.83407800	6.08779600	0.80294700
H	4.28015200	1.06209100	-2.74585200
H	-2.58041900	3.30597700	3.58056600
H	8.31244500	-0.45930600	0.56427300
H	5.57910200	2.62108400	-1.31269200
H	-2.26238000	5.63772700	2.78168300
C	-4.75307000	0.25114700	-2.53800200
C	-4.66306200	-0.30437500	-3.80655200
C	-5.33180100	-1.49688600	-4.09130400
C	-6.08535100	-2.13635900	-3.11189300
C	-6.15819600	-1.57288700	-1.84578600
C	-5.50171000	-0.37366300	-1.53195000
O	-6.96915100	-2.19957700	-0.91952000
S	-6.59486000	-1.90671100	0.66340100
N	-6.45313500	-0.29413700	0.73098300
C	-5.71059400	0.24593900	-0.22044300
O	-7.77380100	-2.33154200	1.38131500
O	-5.33279600	-2.58304600	0.90670100
H	-4.25144800	1.18655800	-2.31256200
H	-4.07618600	0.18981000	-4.57254300
H	-5.26653700	-1.93353100	-5.08216200
H	-6.61861700	-3.05924400	-3.30869100
H	-5.58409100	1.32460400	-0.15870400
TS2SS''			
C	4.66504000	-0.61603300	2.13014000
C	5.44581900	-0.62376200	3.28169800
C	5.90343800	0.57222000	3.82863100
C	5.57974600	1.78400600	3.21650700
C	4.79741800	1.80281800	2.06852000
C	4.32368200	0.59939100	1.52151900
C	3.59595300	0.59598000	0.27875300
C	2.51988400	0.77577300	-0.33957000
C	1.44427000	0.90343100	-1.16506900
C	0.52290800	-0.25586900	-1.48071700
C	1.09596300	-1.45018000	-2.22370900
C	0.37142800	-2.00248100	-3.28385900
C	0.86018500	-3.10730100	-3.97778100
C	2.08349000	-3.66927000	-3.62154300
C	2.81059000	-3.12647100	-2.56366000
C	2.31617500	-2.03179900	-1.86102100
C	1.07232300	2.18950000	-1.74308200
C	1.94728200	3.40246600	-1.50014600
O	0.04941700	2.31935900	-2.42356200

H	4.33656900	-1.54560500	1.67757100
H	5.71195000	-1.57114500	3.73986300
H	6.51803600	0.56275400	4.72291800
H	5.94360300	2.71796800	3.63321100
H	4.55661200	2.74095700	1.57627100
H	-0.26946100	0.18393600	-2.09777100
H	-0.57581900	-1.55840400	-3.57795600
H	0.28796200	-3.52045900	-4.80188500
H	2.46884900	-4.52507500	-4.16604500
H	3.76536100	-3.55284100	-2.27379400
H	2.88248500	-1.64391900	-1.02010800
H	2.35084900	3.73809500	-2.45992200
H	1.31483200	4.20822500	-1.11623100
H	2.76958400	3.21425100	-0.80995400
P	-0.35301500	-0.84294700	0.04996800
F	-5.65332800	-2.11415200	2.65112500
F	-7.80329400	-1.85824100	2.60979800
F	-6.81694600	-2.96096800	1.04398800
F	-8.39555500	2.23108600	-2.19777200
F	-9.69133700	0.82930900	-1.17731700
F	-9.16231000	2.69711700	-0.23782100
O	-3.50209500	1.97958200	-1.42269700
N	-2.83134100	1.46533400	0.69034900
C	-1.41469100	1.71373000	0.47002300
C	-0.95387100	3.10867500	0.93948600
C	-0.59525800	0.59184900	1.14352000
C	-1.20727600	3.32568700	2.43572300
C	-1.59329600	4.18730600	0.06686600
C	-0.62377000	4.63362600	2.96752500
C	-1.95205400	-1.57233600	-0.39104800
C	0.60124600	-2.09090600	0.93025200
C	-3.75197900	1.55502500	-0.30265800
C	-5.11767700	1.02792300	0.03411600
C	-2.50727000	-2.56949400	0.42330300
C	0.63193400	-3.40171300	0.43058200
C	-2.65985600	-1.10736400	-1.50617000
C	1.33478700	-1.75669500	2.07269300
C	-6.22331900	1.58293200	-0.60483000
C	-5.27612600	-0.07961800	0.86525800
C	-7.48771400	1.05020000	-0.37622500
C	-6.54077400	-0.62344800	1.05443600
C	-3.75525000	-3.10233700	0.11360700
C	1.38340300	-4.36975700	1.08319500
C	-3.90504900	-1.65015900	-1.81080200

C	2.07808300	-2.73781900	2.72493300
C	-7.65757800	-0.05785600	0.44780800
C	-4.44922500	-2.64946300	-1.00730900
C	2.10258900	-4.03883500	2.23188800
C	-6.70211600	-1.88867900	1.84871300
C	-8.68931800	1.70154400	-1.00322900
H	-1.28294800	1.69289900	-0.61803400
H	0.13433600	3.12859000	0.77122700
H	0.40559600	0.95899800	1.38993800
H	-1.06472200	0.23497500	2.06675900
H	-0.77732200	2.49169800	3.00492500
H	-2.28975500	3.30905600	2.61918400
H	-1.18093900	5.17286100	0.29632100
H	-1.41443700	3.97395400	-0.99098300
H	-2.67593300	4.22469000	0.23017900
H	-3.14460400	1.24648000	1.62605600
H	-1.12218300	5.50299800	2.53201900
H	0.44358500	4.70563000	2.73489500
H	-0.73654700	4.69659300	4.05242700
H	-1.96759600	-2.93256200	1.29235500
H	0.07449900	-3.66125500	-0.46551500
H	-2.27462400	-0.30255800	-2.12460600
H	1.34078600	-0.74330300	2.46086900
H	-6.08360100	2.41818400	-1.28305400
H	-4.41335400	-0.55731900	1.31969500
H	-4.18723100	-3.86592100	0.75099700
H	1.40932800	-5.38157900	0.69448300
H	-4.45182500	-1.27917000	-2.67077800
H	2.64728900	-2.47541700	3.61017100
H	-8.64390600	-0.48226300	0.60280800
H	-5.42443200	-3.06274500	-1.24116800
H	2.68662300	-4.79826200	2.74064800
C	6.90500100	1.30228800	-0.33232100
C	7.65328200	2.46312600	-0.18364300
C	4.98268700	0.02180600	-1.23511600
C	5.78975100	1.25216200	-1.17252500
C	7.27357000	3.60033500	-0.88769600
C	5.43178700	2.40397600	-1.87956100
C	6.16623300	3.57327900	-1.74098400
H	8.50992900	2.45740700	0.48069000
H	7.84947400	4.51280600	-0.77630300
H	4.56342800	2.36607100	-2.53194000
H	5.88173900	4.46222700	-2.29286400
N	5.46037700	-1.17729600	-0.88345100

O	7.93008600	-1.37400000	-1.39429700
O	7.26076400	0.19407500	0.41172200
O	7.06035000	-2.22176100	0.77235600
S	6.96194400	-1.26780300	-0.31224000
H	4.18668200	0.00642800	-1.97827000

TS2RR

C	4.70704900	-2.51642200	-1.54081700
C	5.74054400	-3.40589300	-1.81405000
C	3.86440800	-0.22001300	-1.33758000
C	2.82835700	0.43824900	-1.56881800
C	4.90079400	-1.13890100	-1.72245200
C	1.67458000	1.16693200	-1.63330800
C	6.97259600	-2.93787700	-2.26636100
C	6.14646600	-0.67038400	-2.16949400
C	7.17055200	-1.56864600	-2.44413600
C	1.67357600	2.54907100	-2.03647400
H	3.74754400	-2.86982500	-1.17578200
H	5.58414500	-4.46945600	-1.66424900
H	6.30232700	0.39922200	-2.28155600
H	8.13058600	-1.19787000	-2.78977500
O	0.61382600	3.19383500	-2.09845800
H	7.77720200	-3.63543100	-2.47529800
C	0.44446900	-3.78775400	-1.26109300
C	-0.22083800	-3.12828000	-2.29313200
C	1.09121400	-3.04896700	-0.27140000
C	-0.25151000	-1.73541100	-2.33041900
C	1.06242700	-1.65838000	-0.31022200
C	0.38008800	-0.99202700	-1.33157900
C	0.32346400	0.51821500	-1.37874000
H	0.46376700	-4.87232300	-1.23200600
H	-0.72040100	-3.69794800	-3.07000600
H	1.63246500	-3.54764000	0.52719900
H	-0.79323300	-1.21932500	-3.11667900
H	1.59125000	-1.10163800	0.45813800
H	-0.38234400	0.82661800	-2.15611800
C	6.55812300	-0.13240800	0.89890800
C	7.83919700	0.39647100	0.80063900
C	4.08894000	0.05140600	0.79673100
C	5.42249100	0.66628300	0.74485400
C	7.98603000	1.75122600	0.52790200
C	5.59281600	2.02693900	0.46758200
C	6.86460800	2.57067800	0.36128800
H	8.69216100	-0.26073000	0.92597700
H	3.24442700	0.73534000	0.78988500

H	8.98198100	2.17292400	0.44460400
H	4.70707600	2.64071000	0.32438900
H	6.98942300	3.62618000	0.14712100
N	3.85863600	-1.13983700	1.35218500
O	4.97433700	-3.38350200	1.66201600
O	6.42988400	-1.49299400	1.09842600
O	5.35387400	-1.58616100	3.33497100
S	5.09334800	-1.97051600	1.95447600
C	-6.52190000	-1.76424100	0.34760600
C	-6.25116000	-0.52538600	0.91712800
C	-5.34607800	0.35017600	0.32857000
C	-4.69227500	-0.01986900	-0.84532600
C	-4.94921000	-1.26336300	-1.41943300
C	-5.86657600	-2.12106600	-0.82648400
H	-7.21361600	-2.45191000	0.82318400
H	-5.10987800	1.27544700	0.84282900
H	-4.39812400	-1.55798200	-2.30626400
C	-6.91883400	-0.16414200	2.21457900
F	-7.27061300	-3.99112100	-1.11212200
F	-5.89100100	-3.52837000	-2.71464200
F	-5.15904400	-4.35757500	-0.86270900
F	-6.91041500	-1.20157100	3.06670000
F	-8.20097100	0.18307600	2.03719700
F	-6.30661300	0.86093900	2.82293300
C	-3.56130400	0.78313400	-1.42084600
O	-2.70067900	0.23541000	-2.10803300
N	-3.49612100	2.08596300	-1.07758000
H	-4.25107600	2.50263600	-0.55220200
C	-2.29397600	2.87269400	-1.31794400
H	-1.78912900	2.42699100	-2.17624400
C	-1.36067200	2.80536500	-0.09920400
H	-0.58835100	3.56556300	-0.20839700
H	-1.91732900	2.99614000	0.82474200
C	-2.62806700	4.32616500	-1.70125300
C	-3.25212700	5.13052000	-0.55215400
H	-4.19560700	4.66439200	-0.23370500
H	-2.58390900	5.10786300	0.31581300
P	-0.48897300	1.21004700	0.18467400
C	0.79759100	1.59813600	1.40677500
C	1.54556100	2.77732300	1.27428400
C	1.08910100	0.70228100	2.44172600
C	2.56151300	3.05876500	2.18204600
H	1.34665600	3.47457800	0.46629700
C	2.12073900	0.98308200	3.33455800

H	0.51981400	-0.21612000	2.54934800
C	2.85383300	2.15996900	3.20784900
H	3.13107700	3.97676800	2.08129900
H	2.35720700	0.27349000	4.11956000
H	3.65730100	2.37538600	3.90414600
C	-1.67632300	0.11985800	1.05170600
C	-2.20063800	0.62898500	2.25194200
C	-2.08302100	-1.14366100	0.60901000
C	-3.11397900	-0.11281400	2.99194700
H	-1.88428600	1.59889300	2.62689000
C	-2.99128200	-1.88565200	1.36328300
H	-1.72648200	-1.54525400	-0.32983000
C	-3.50686200	-1.37628100	2.54996800
H	-3.51631100	0.29557200	3.91245900
H	-3.31254600	-2.85587000	0.99717500
H	-4.22825700	-1.95059100	3.12257500
C	-3.49959300	4.34353600	-2.95852000
H	-3.09278800	3.67482100	-3.72267800
H	-4.52076700	4.01763000	-2.73410500
H	-3.55185300	5.34709600	-3.38545700
H	-1.65788300	4.77980300	-1.94488800
C	-3.52658300	6.58833800	-0.91997800
H	-4.30990200	6.67244900	-1.67709200
H	-3.84924100	7.15527200	-0.04368000
H	-2.62313300	7.06324200	-1.31586700
C	2.97883200	3.25233500	-2.34321700
H	3.83242300	2.57621500	-2.38041300
H	2.87784900	3.78164100	-3.29331600
H	3.15426000	4.00661100	-1.56861600
C	-6.05433100	-3.50262800	-1.38660600

TS2RR'

C	-5.56973700	1.85041200	0.85013000
C	-6.77893400	2.48360100	1.11148400
C	-3.91271500	0.94114800	-0.73740200
C	-2.74468600	1.08115000	-1.17893600
C	-5.13225200	1.67051600	-0.47153100
C	-1.49325300	1.09838500	-1.70903800
C	-7.58310100	2.92937300	0.06252800
C	-5.94119700	2.13251300	-1.52152400
C	-7.15881600	2.75101700	-1.25294700
C	-1.29872300	0.73683200	-3.11046100
H	-4.95345200	1.47686700	1.66315900
H	-7.10258100	2.61880800	2.13889900
H	-5.60735800	1.99907800	-2.54661600

H	-7.77516000	3.10054900	-2.07542000
O	-0.19604600	0.80858300	-3.65677500
H	-8.53194100	3.41344900	0.26904100
C	-0.57389400	5.82024000	0.06110600
C	0.42548100	5.37015800	-0.79763800
C	-1.48815400	4.91210800	0.59145300
C	0.51752700	4.01615900	-1.10972200
C	-1.39945600	3.55920300	0.27597500
C	-0.38398900	3.09522500	-0.56831700
C	-0.27911400	1.63197700	-0.96387900
H	-0.64743600	6.87442500	0.30727900
H	1.13111400	6.07131700	-1.23095000
H	-2.27965100	5.25710700	1.24880100
H	1.28511300	3.67081800	-1.79845300
H	-2.13560900	2.86536400	0.67200700
H	0.57132900	1.50576300	-1.65124600
C	-5.36803700	-1.98930600	1.03245600
C	-6.36450300	-2.08592700	1.99027400
C	-4.45816700	-1.22715200	-1.13711100
C	-5.57952600	-1.36953600	-0.20343300
C	-7.62138500	-1.56122900	1.69699600
C	-6.85867100	-0.87764900	-0.48613000
C	-7.87364100	-0.97212000	0.45747800
H	-6.15003100	-2.57540900	2.93364700
H	-4.67882300	-0.76577100	-2.09738500
H	-8.41184300	-1.62984300	2.43658900
H	-7.04327400	-0.40823500	-1.44668900
H	-8.85821800	-0.57865000	0.23154300
N	-3.37688000	-2.01099700	-1.10922600
O	-1.96789700	-3.32447500	0.51826200
O	-4.11304400	-2.49711300	1.32783600
O	-4.06411500	-4.34103600	-0.35855400
S	-3.31992400	-3.15525400	0.02568600
C	6.99109300	-0.42621100	0.34493000
C	6.05712300	-1.34281900	0.81524700
C	4.79908300	-1.45003000	0.23272200
C	4.46217200	-0.62580500	-0.84014600
C	5.39155000	0.29684200	-1.31578600
C	6.64604900	0.38921900	-0.72628800
H	7.96718900	-0.34354100	0.81076700
H	4.08749000	-2.14495000	0.66529900
H	5.10425900	0.95463800	-2.12944200
C	6.38360900	-2.13596600	2.04800400
F	8.84868300	1.22784800	-0.80586600

F	7.59303400	1.55492800	-2.53789000
F	7.23496300	2.66099800	-0.72360400
F	6.22796900	-1.38886600	3.15750600
F	7.65396000	-2.55930100	2.04411200
F	5.59320000	-3.20758400	2.18271800
C	3.07886000	-0.55228200	-1.42891500
O	2.74570100	0.43451100	-2.07848400
N	2.23006600	-1.56554800	-1.14385800
H	2.56405700	-2.37834700	-0.64624200
C	0.80567600	-1.47386800	-1.43646900
H	0.70492000	-0.64147800	-2.13761700
C	0.00258200	-1.17290600	-0.15937400
H	-1.05916500	-1.29755400	-0.38874300
H	0.24125800	-1.85587600	0.66207800
C	0.26767300	-2.73118600	-2.14595800
C	0.56171800	-4.02532200	-1.37499200
H	1.62277100	-4.28529100	-1.49622100
H	0.38194700	-3.86927900	-0.30527600
P	0.15875800	0.52888400	0.45198700
C	-0.96117800	0.70545700	1.86032400
C	-2.11537600	-0.07703100	1.94735400
C	-0.67684600	1.65410700	2.85142100
C	-2.98072100	0.08480100	3.02529000
H	-2.34936100	-0.80846300	1.18453100
C	-1.55385300	1.82053900	3.91695600
H	0.22235700	2.25999600	2.78929600
C	-2.70421200	1.03660700	4.00412300
H	-3.86860500	-0.53649400	3.09162600
H	-1.33653200	2.55789400	4.68177500
H	-3.38204300	1.16429100	4.84171700
C	1.81574000	0.83658200	1.11815700
C	2.22784600	0.04422200	2.20121600
C	2.66742100	1.81563700	0.60494000
C	3.48695400	0.23087400	2.75635400
H	1.56393700	-0.70963700	2.61665800
C	3.93044100	1.99835800	1.16986200
H	2.36484400	2.42000200	-0.24104800
C	4.33944100	1.20848200	2.23900000
H	3.81013400	-0.39231300	3.58282700
H	4.60014600	2.74474300	0.75537800
H	5.32829600	1.34083800	2.66657500
C	0.80456200	-2.76989600	-3.57699700
H	0.52031500	-1.86087000	-4.11630700
H	1.89819900	-2.83597800	-3.57216400

H	0.41614100	-3.63013800	-4.12725200
H	-0.82433000	-2.60225400	-2.18001800
C	-0.30387400	-5.19789400	-1.83202700
H	-0.15840300	-5.42096300	-2.89258000
H	-0.06630100	-6.10270800	-1.26698400
H	-1.36289800	-4.97199600	-1.67274900
C	-2.48379000	0.17723100	-3.87212100
H	-2.23531100	0.13471800	-4.93235100
H	-2.68979000	-0.83598800	-3.50731700
H	-3.38384600	0.77719300	-3.71847700
C	7.59056200	1.45596700	-1.20233900
TS2RR"			
C	0.43523500	3.93482800	-0.67694100
C	-0.06545100	3.65564100	0.59296800
C	0.98842900	2.90961500	-1.44438600
C	-0.03924600	2.35121500	1.08599700
C	1.01812900	1.61047400	-0.94884600
C	0.47980300	1.31670100	0.30686300
C	0.48249400	-0.09855700	0.84339800
C	3.75589400	3.48201200	1.21367400
C	4.32893300	4.68855400	1.59366400
C	3.89420000	1.06720100	0.81363200
C	2.94085900	0.28455900	1.02591900
C	4.50888900	2.29531900	1.25567200
C	1.89795100	-0.58798400	1.14248200
C	5.65855300	4.73526100	2.01690200
C	5.84565700	2.35143600	1.66757500
C	6.41066600	3.56436700	2.05149400
C	2.03298800	-1.84031700	1.83761200
C	3.36933900	-2.25560200	2.40983400
H	0.40748600	4.94838300	-1.06300700
H	-0.48206500	4.45195600	1.20111800
H	1.40016100	3.12316200	-2.42512700
H	-0.45942800	2.12475100	2.06036600
H	1.46363600	0.81323600	-1.53927800
H	-0.10498600	-0.11674100	1.76822200
H	2.72192800	3.43539500	0.88346800
H	3.73579500	5.59744800	1.56076200
H	6.43755900	1.44231800	1.68778400
H	7.44855200	3.59211300	2.36774300
H	3.33590500	-2.10852300	3.49419100
H	4.20362700	-1.68674500	1.99833300
H	3.52077800	-3.32033200	2.22060800
O	1.04290200	-2.57332700	2.00301800

H	6.10471700	5.67991800	2.31056300
C	-6.69592600	1.63245100	-0.37395300
C	-6.50198100	0.26313400	-0.49894300
C	-5.45292100	-0.37450500	0.15758800
C	-4.58963300	0.36576400	0.96188000
C	-4.77262100	1.74253300	1.08871800
C	-5.82071500	2.36397900	0.42465100
H	-7.51231700	2.12364900	-0.89173700
H	-5.30314800	-1.43620800	-0.01175400
H	-4.06970300	2.31340400	1.68651700
C	-5.94475900	3.86023300	0.48609500
C	-7.37762300	-0.53519200	-1.42383700
F	-7.19971900	4.26761900	0.25914800
F	-5.56421400	4.34305900	1.67501100
F	-5.16633500	4.44410500	-0.44191200
F	-6.83006300	-0.64734400	-2.64689900
F	-8.57963500	0.03034500	-1.58274200
F	-7.56607800	-1.78178700	-0.96956500
C	-3.35234400	-0.22201100	1.57806400
O	-2.40117600	0.50124700	1.86994000
N	-3.31079000	-1.56276900	1.71508500
H	-4.13122300	-2.11149000	1.50296500
C	-2.05709900	-2.26187300	1.96750200
H	-1.42015900	-1.57731400	2.53120100
C	-1.37791300	-2.61697600	0.63507400
H	-0.61971600	-3.37402800	0.81675300
H	-2.11541300	-3.01038200	-0.07190600
C	-2.26566000	-3.50644000	2.84988400
C	-3.07445000	-4.61230400	2.15766700
H	-4.08362700	-4.24779700	1.91815600
H	-2.60064500	-4.87152300	1.20430000
P	-0.54088800	-1.24132200	-0.25819300
C	0.48770800	-2.05585100	-1.51594100
C	1.09574400	-3.28906800	-1.25322700
C	0.63249700	-1.46191600	-2.77704000
C	1.80342100	-3.93712600	-2.26310500
H	1.03215900	-3.74205700	-0.26906100
C	1.38196900	-2.09482900	-3.76325100
H	0.14481100	-0.51666300	-2.99648600
C	1.95553800	-3.33965800	-3.51143300
H	2.24202100	-4.91043600	-2.07038300
H	1.49719900	-1.62525200	-4.73379100
H	2.51786300	-3.84505900	-4.28917800
C	-1.87279600	-0.42840500	-1.22814800

C	-2.58056900	-1.27884700	-2.09635700
C	-2.23678200	0.91951400	-1.15449500
C	-3.63194100	-0.79105800	-2.86207100
H	-2.30369000	-2.32544100	-2.19293600
C	-3.28277700	1.40550100	-1.93954500
H	-1.74210900	1.59387100	-0.47071500
C	-3.98238100	0.55745900	-2.78842300
H	-4.17647600	-1.46286400	-3.51652300
H	-3.56241400	2.45105100	-1.85539400
H	-4.80832400	0.93561500	-3.38145800
C	-2.87618900	-3.09725200	4.19148300
H	-2.34467500	-2.24057300	4.61591300
H	-3.92858200	-2.81733800	4.07583200
H	-2.82168400	-3.91518100	4.91264600
H	-1.25318300	-3.89206800	3.03080900
C	-3.20126200	-5.87984600	3.00215500
H	-3.80689100	-5.71001400	3.89554700
H	-3.67228800	-6.68185900	2.42919000
H	-2.21517700	-6.22906000	3.32468600
C	6.42527900	-1.18785600	-0.16368100
C	6.77422300	-2.46190300	0.25264700
C	4.86613400	0.47700900	-1.11871900
C	5.18462500	-0.90922100	-0.74707800
C	5.85768400	-3.49518700	0.07126400
C	4.28472700	-1.96169700	-0.93505200
C	4.62387700	-3.24887900	-0.52984000
H	7.74668200	-2.62630300	0.70250400
H	3.89722800	0.65450700	-1.57844200
H	6.11470800	-4.49916900	0.39156300
H	3.32321900	-1.75778500	-1.39805500
H	3.92163400	-4.06211100	-0.66897300
N	5.79416600	1.39454900	-1.37430800
O	8.10153000	2.07837000	-0.57842800
O	7.31848500	-0.15145400	0.05123700
O	7.88044500	0.32609400	-2.32925400
S	7.34102700	0.99119300	-1.15361300

TS2RR'''

C	0.93915100	3.86002600	-0.66657000
C	0.39475700	3.66500700	0.60152400
C	1.46741200	2.77625400	-1.36829500
C	0.35013300	2.38618400	1.15447900
C	1.43173000	1.50148600	-0.81099800
C	0.84671300	1.29478100	0.44048200
C	0.76357900	-0.09067900	1.04485000

C	4.18613400	3.51687100	1.35030000
C	4.75781800	4.73790100	1.68893900
C	4.15969200	1.06735700	1.41361500
C	3.18854800	0.28601200	1.47794400
C	4.73429800	2.31664400	1.83814200
C	2.12949800	-0.57847300	1.51974500
C	5.88316000	4.78934500	2.51201600
C	5.87492900	2.37584600	2.65615700
C	6.43578100	3.60376200	2.99344000
C	2.18764600	-1.78120700	2.30642900
C	3.50865700	-2.22920600	2.88928300
H	0.96179900	4.85372600	-1.10206700
H	-0.00395800	4.50662400	1.15859900
H	1.91307000	2.92111400	-2.34699400
H	-0.10559600	2.22351300	2.12644100
H	1.85883400	0.65969800	-1.35153100
H	0.08362900	-0.05039200	1.90394300
H	3.31247700	3.46796200	0.70609900
H	4.32084500	5.65612300	1.30817200
H	6.30699200	1.45331000	3.03386600
H	7.31088900	3.63323800	3.63510500
H	4.12475400	-1.38453000	3.20146100
H	4.06241700	-2.77527400	2.11859700
H	3.31397700	-2.89392700	3.73178100
O	1.17371400	-2.48146900	2.46901900
H	6.32620000	5.74442800	2.77391200
C	-6.39739700	1.59992800	-0.40756900
C	-6.20070600	0.23026600	-0.52370600
C	-5.16565300	-0.40567700	0.15647400
C	-4.31719300	0.33618600	0.97489100
C	-4.50574400	1.71283500	1.09514000
C	-5.53964000	2.33301100	0.40803400
H	-7.20235600	2.08952600	-0.94441200
H	-5.01714600	-1.46827700	-0.00657300
H	-3.81596000	2.28431000	1.70727000
C	-5.66425300	3.82914900	0.46523100
C	-7.05257600	-0.56930100	-1.46904600
F	-6.91209600	4.23804100	0.20350700
F	-5.31631000	4.31258700	1.66392500
F	-4.85990600	4.41257100	-0.44105700
F	-6.47612100	-0.67650200	-2.67990400
F	-8.25251800	-0.00750100	-1.65529900
F	-7.24742500	-1.81762600	-1.02271700
C	-3.09252200	-0.24310400	1.62734500

O	-2.17710100	0.49554300	1.98713000
N	-3.02512300	-1.58635900	1.72234600
H	-3.82149700	-2.14605000	1.45500800
C	-1.78210700	-2.27136100	2.05572800
H	-1.18486200	-1.57578400	2.64697100
C	-1.01542500	-2.63407000	0.77433600
H	-0.23768100	-3.35656500	1.01339400
H	-1.69243900	-3.07471000	0.03565500
C	-2.03323200	-3.50682300	2.93998700
C	-2.79256200	-4.62704600	2.21558400
H	-3.78488100	-4.27025100	1.90403900
H	-2.25629900	-4.90003900	1.29988200
P	-0.18440500	-1.24609100	-0.10358900
C	0.88322300	-2.06483700	-1.31992900
C	1.64876200	-3.16730500	-0.92741100
C	0.88978200	-1.64794200	-2.65788200
C	2.37317400	-3.87810300	-1.88059900
H	1.69169600	-3.47178300	0.11464400
C	1.62382700	-2.36026500	-3.59946800
H	0.30615900	-0.78615400	-2.96752300
C	2.35309800	-3.48382800	-3.21386400
H	2.96745500	-4.72875100	-1.56941700
H	1.61379600	-2.04470400	-4.63786300
H	2.91421500	-4.04513600	-3.95365700
C	-1.51379300	-0.44860400	-1.08923300
C	-2.23476800	-1.30829200	-1.93726800
C	-1.85862700	0.90560800	-1.04850600
C	-3.27394400	-0.82189400	-2.72061900
H	-1.97461100	-2.36086900	-2.00928300
C	-2.89607800	1.38917200	-1.84655500
H	-1.35327600	1.58891500	-0.38151200
C	-3.60429400	0.53305200	-2.67997500
H	-3.82644400	-1.50062300	-3.36116700
H	-3.16232200	2.43979900	-1.78553000
H	-4.42228500	0.90978000	-3.28484600
C	-2.72597700	-3.08543900	4.23710300
H	-2.22809300	-2.21759600	4.67948000
H	-3.77211900	-2.81752500	4.05482300
H	-2.70723600	-3.89242600	4.97239800
H	-1.03029600	-3.88033800	3.18541600
C	-2.97050000	-5.88158100	3.07023900
H	-3.63289300	-5.70015300	3.92011900
H	-3.40101300	-6.69467900	2.48110900
H	-2.00618300	-6.22164300	3.46115000

C	4.41931100	0.00547000	-2.01214300
C	3.88872400	0.47761900	-3.20256600
C	5.76111800	0.23035400	0.04265200
C	5.21027900	0.80881000	-1.18802000
C	4.14979100	1.79636800	-3.57084700
C	5.45865200	2.12995200	-1.57110100
C	4.92820400	2.62267500	-2.75779700
H	3.28519500	-0.18396800	-3.81327200
H	6.39244900	0.87605100	0.65018800
H	3.74430800	2.17868000	-4.50183800
H	6.06899900	2.75939000	-0.92980600
H	5.12406600	3.64705300	-3.05425700
N	5.93357800	-1.06386100	0.23706300
O	4.66333600	-3.19519300	-0.16427700
O	4.09705700	-1.27604600	-1.59488100
O	6.29017900	-2.41757700	-1.87678700
S	5.31878000	-2.09761000	-0.84365500

TS2RS

C	5.39762900	-1.59552900	1.83883400
C	6.48493500	-2.30238300	2.32385300
C	7.75835500	-1.72424600	2.28746300
C	7.94166400	-0.44632800	1.77551900
C	6.83959700	0.24956300	1.29053300
C	5.55622800	-0.30681000	1.31235700
O	7.05085900	1.54177800	0.85288000
S	5.94085600	2.15331800	-0.21594500
N	4.51568000	1.71403900	0.38170800
C	4.41382200	0.46344500	0.82292200
O	6.10875100	3.58556800	-0.10188200
O	6.24222700	1.52505900	-1.49363600
H	4.40211300	-2.03275800	1.84159700
H	6.35144800	-3.30152900	2.72274700
H	8.61491300	-2.27551500	2.66044100
H	8.91735100	0.02486700	1.74359900
H	3.43818900	0.20168400	1.22624500
C	4.39821500	-3.30710300	-0.99602600
C	5.29007400	-4.36726800	-1.11253800
C	3.91053400	-0.89867900	-0.96950800
C	2.86251800	-0.29761200	-1.28128900
C	4.83687200	-1.98354900	-1.17461600
C	1.74283600	0.45168000	-1.52136000
C	6.63205400	-4.13001200	-1.40775300
C	6.18985900	-1.75194000	-1.47185900
C	7.07262100	-2.81991700	-1.59099600

C	1.80660700	1.67894300	-2.28180100
C	3.15084400	2.24200200	-2.68934500
H	3.35213000	-3.48760100	-0.76614500
H	4.93465300	-5.38378000	-0.97358400
H	6.53208100	-0.73120500	-1.60611200
H	8.11528800	-2.62597600	-1.82369900
H	3.08115700	2.58901700	-3.72270300
H	3.96890000	1.53265200	-2.57512800
H	3.36550000	3.11190300	-2.05969400
O	0.77719200	2.29990500	-2.59197400
H	7.32722200	-4.95858100	-1.49629500
C	0.05566000	-4.36965900	-0.72667100
C	-0.51844400	-3.73485300	-1.82636200
C	0.76488000	-3.62101500	0.21080900
C	-0.40113900	-2.35501700	-1.97753100
C	0.89584600	-2.24377600	0.05091900
C	0.29744000	-1.59696400	-1.03466000
C	0.36078700	-0.09622400	-1.20461100
H	-0.04644400	-5.44259500	-0.60201300
H	-1.06725400	-4.31211100	-2.56321700
H	1.22259700	-4.10917800	1.06550400
H	-0.88061800	-1.85283100	-2.81216200
H	1.46830100	-1.66913000	0.77386800
H	-0.31629200	0.19319000	-2.01575600
C	-0.93842100	2.46666400	-0.25043600
H	-0.02755700	3.00124800	-0.52785700
H	-1.35960700	2.93398800	0.64568500
P	-0.40974900	0.78698600	0.25920100
C	0.78896000	1.04922900	1.59754800
C	1.64539300	2.15443500	1.57886000
C	0.83639800	0.14801900	2.67204800
C	2.52210600	2.37072500	2.64012100
H	1.65598000	2.84325200	0.74139900
C	1.73602900	0.35457400	3.71132800
H	0.16620100	-0.70620300	2.69956700
C	2.57087600	1.47281600	3.70122500
H	3.18601700	3.22701900	2.61365000
H	1.77377300	-0.34856000	4.53617100
H	3.26229500	1.63926900	4.52046600
C	-1.82520500	-0.02443400	1.08600700
C	-2.31071700	-1.29652200	0.77106500
C	-2.42104600	0.70245100	2.13061900
C	-3.37748500	-1.83180400	1.49483700
H	-1.88957100	-1.86637600	-0.04620600

C	-3.48922400	0.16627500	2.83840500
H	-2.04432000	1.68334500	2.40838800
C	-3.96761100	-1.10633600	2.52237700
H	-3.76076300	-2.81096600	1.22586300
H	-3.95201700	0.74158200	3.63283200
H	-4.80928400	-1.51811500	3.06943800
C	-6.95612000	-1.18978000	0.34084900
C	-6.58645500	0.08144100	0.76021700
C	-5.50068800	0.73850000	0.18849200
C	-4.76913500	0.11767200	-0.82111900
C	-5.13549800	-1.15808700	-1.24987900
C	-6.22138100	-1.80022100	-0.67129200
H	-7.79962400	-1.69776600	0.79521200
H	-5.22716700	1.71206500	0.58125000
H	-4.53911200	-1.64246800	-2.01591500
C	-6.53497800	-3.21398700	-1.07145800
C	-7.29539700	0.71683600	1.92242400
F	-7.81317400	-3.53082400	-0.82945900
F	-6.29724800	-3.42821100	-2.37117500
F	-5.77573800	-4.08716000	-0.38573800
F	-6.68687300	0.42004200	3.08582200
F	-8.56144100	0.29680800	2.02579200
F	-7.31119400	2.05287000	1.82438500
C	-3.49666700	0.68229000	-1.39100600
O	-2.73375800	-0.04051700	-2.03020100
N	-3.20581300	1.96771400	-1.10124500
H	-3.87129700	2.53554700	-0.59829200
C	-2.04182800	3.97765500	-1.97964700
C	-2.52578200	4.98623600	-0.92888800
H	-3.51787100	4.69413700	-0.55526800
H	-1.84996400	4.97124100	-0.06669900
C	-2.92461100	3.97762400	-3.22924600
H	-2.62538200	3.17893200	-3.91431200
H	-3.97698200	3.82255200	-2.96832800
H	-2.84599300	4.92535600	-3.76575500
H	-1.02236700	4.25618900	-2.27737400
C	-2.60474400	6.41712300	-1.46037300
H	-3.38426400	6.52319200	-2.21866300
H	-2.82819100	7.11901900	-0.65355600
H	-1.65277300	6.71377800	-1.91217700
C	-1.91123900	2.54106500	-1.43945100
H	-1.50402300	1.93875500	-2.25074200
TS2RS'			
C	6.66283900	-0.47011900	1.05554200

C	7.02672100	-1.70464900	1.56814700
C	6.78441000	-2.86292800	0.82181100
C	6.19313900	-2.78606500	-0.43369800
C	5.84027900	-1.53806400	-0.93794100
C	6.05732300	-0.36876300	-0.20361700
O	5.35532100	-1.49148500	-2.22775900
S	4.52450400	-0.13216000	-2.67882800
N	5.35477600	1.09998600	-2.04518600
C	5.76055600	0.93675200	-0.79933000
O	4.63727100	-0.13658300	-4.11988000
O	3.21680700	-0.22823000	-2.06616400
H	6.84027100	0.44253700	1.61920200
H	7.49540100	-1.77334100	2.54326400
H	7.06601500	-3.83260900	1.21810800
H	6.02217400	-3.66760400	-1.04131800
H	6.26824800	1.79637400	-0.36762500
C	4.80626400	3.90326400	0.51540300
C	5.42642500	5.03872800	1.02507600
C	4.09446400	1.54504500	0.73745700
C	3.12855300	0.77013100	0.91963000
C	4.71693600	2.73172700	1.28620800
C	2.09899100	-0.09888600	1.17047700
C	5.99096600	5.02394700	2.30034000
C	5.29006600	2.72610600	2.56890000
C	5.92261800	3.86151700	3.06609900
C	2.29648900	-1.20368600	2.06937300
C	3.70009900	-1.58103000	2.48524100
H	4.37830900	3.90741600	-0.48312400
H	5.47529200	5.93877900	0.42001900
H	5.22314700	1.82574200	3.17281200
H	6.35744500	3.83944700	4.06069300
H	4.31001200	-0.70539900	2.71378600
H	4.19088900	-2.10187200	1.65433900
H	3.65096600	-2.25027100	3.34472800
O	1.33922100	-1.89801800	2.45446600
H	6.48092900	5.90909400	2.69211500
C	0.28266900	4.14288800	-0.98878400
C	-0.16533900	3.92156600	0.31200200
C	0.87785600	3.10368800	-1.70250000
C	-0.03521400	2.66056800	0.89005500
C	1.01535900	1.84475900	-1.12456300
C	0.54171400	1.61364000	0.16891200
C	0.66185900	0.25223400	0.81459700
H	0.17387300	5.12280700	-1.44230700

H	-0.62186500	4.72859800	0.87602900
H	1.23977100	3.27370400	-2.71150400
H	-0.41135500	2.47444400	1.89116300
H	1.50161800	1.04087500	-1.67015600
H	0.06637300	0.25255400	1.73441800
C	-0.88201300	-2.44571300	0.85683000
H	-0.01176900	-3.04986100	1.11050400
H	-1.53359700	-3.02892200	0.19821400
P	-0.25814100	-1.06299200	-0.18831400
C	0.82874100	-1.88247700	-1.38021400
C	1.83340500	-2.73151300	-0.89621100
C	0.69053800	-1.67410700	-2.75501700
C	2.68507900	-3.36931100	-1.78961000
H	1.94636200	-2.90280500	0.17032200
C	1.54488000	-2.32246900	-3.64169500
H	-0.07639600	-1.00728400	-3.13566300
C	2.54111500	-3.16667400	-3.16098800
H	3.46097800	-4.02737700	-1.41276200
H	1.43591600	-2.15847100	-4.70832100
H	3.21085000	-3.66472300	-3.85462100
C	-1.71517800	-0.47908600	-1.13740200
C	-2.16832500	0.84260200	-1.19500400
C	-2.41864100	-1.47146900	-1.84336100
C	-3.29657100	1.16287700	-1.95107900
H	-1.67550600	1.62503700	-0.63575100
C	-3.54657200	-1.14608200	-2.58631400
H	-2.07686100	-2.50286600	-1.83688800
C	-3.98655300	0.17661200	-2.64452600
H	-3.64647400	2.19027900	-1.96711700
H	-4.08342600	-1.92494500	-3.11684300
H	-4.87447500	0.42723900	-3.21552600
C	-6.69418900	1.21534600	-0.29758500
C	-6.40556500	-0.14255200	-0.30357100
C	-5.28392600	-0.64040500	0.35470600
C	-4.43907600	0.23063300	1.03745800
C	-4.72132700	1.59687900	1.04801300
C	-5.84129100	2.07825900	0.38578900
H	-7.56603800	1.59694900	-0.81749500
H	-5.07301100	-1.70228300	0.28139600
H	-4.03591200	2.26859200	1.55390900
C	-6.07574400	3.56058500	0.31642000
C	-7.25484300	-1.08537600	-1.10844400
F	-5.64696200	4.18558800	1.41948500
F	-5.41790500	4.10355200	-0.72324500

F	-7.37252400	3.85399800	0.15527800
F	-6.73841100	-1.28659900	-2.33428800
F	-8.49680600	-0.61780500	-1.27843200
F	-7.34452700	-2.28887500	-0.52570900
C	-3.13352000	-0.19677400	1.64964000
O	-2.26875200	0.63997700	1.90330200
N	-2.94021000	-1.51915900	1.82963700
H	-3.69157800	-2.16581400	1.63976200
C	-1.71708800	-3.24415900	3.12703500
C	-2.39930700	-4.48103400	2.52595300
H	-3.43199700	-4.23851600	2.23640400
H	-1.87857600	-4.77637200	1.60834100
C	-2.38688900	-2.78948300	4.42508900
H	-1.95154100	-1.85003100	4.77811600
H	-3.46027300	-2.62923400	4.27806400
H	-2.26147700	-3.53368600	5.21425500
H	-0.67326500	-3.50528700	3.34673000
C	-2.42648500	-5.67556800	3.47891800
H	-3.06798400	-5.48764600	4.34327900
H	-2.80374500	-6.56733500	2.97296100
H	-1.42004500	-5.89714400	3.84834000
C	-1.62414300	-2.06150700	2.14501400
H	-1.06964500	-1.27154200	2.65296200
TS2RS"			
C	0.35490500	-4.32084300	-0.66607800
C	-0.27940300	-3.73629800	-1.76061100
C	0.99793900	-3.51575800	0.27162700
C	-0.27867000	-2.35173200	-1.91203100
C	1.00201500	-2.13233200	0.11752100
C	0.35703700	-1.53848700	-0.97050100
C	0.32471100	-0.03890200	-1.16160400
C	5.38370500	-2.52228600	-0.49686000
C	6.34374700	-3.45639600	-0.87549000
C	3.97174400	-0.55304000	-1.01846800
C	2.84679500	-0.07403100	-1.27810800
C	4.97250800	-1.52741000	-1.39613700
C	1.66537000	0.57356400	-1.52853100
C	6.91439400	-3.40620800	-2.14480400
C	5.55075500	-1.48580700	-2.67436300
C	6.51389300	-2.41602500	-3.04183900
C	1.66346500	1.71502700	-2.41890700
H	0.35016200	-5.39909600	-0.54577300
H	-0.78024800	-4.35772600	-2.49570200
H	1.49957200	-3.96305700	1.12369300

H	-0.79535900	-1.89122100	-2.74893800
H	1.50971500	-1.51163100	0.84925400
H	-0.37899400	0.19463300	-1.96930400
H	4.93623200	-2.56739400	0.49171000
H	6.64676300	-4.22682800	-0.17313100
H	5.23707600	-0.71227400	-3.36819900
H	6.95297300	-2.37102200	-4.03366000
O	0.61467100	2.27580100	-2.76521200
H	7.66517200	-4.13413200	-2.43502700
C	-7.02543100	-1.23218600	0.23842200
C	-6.68897700	0.05010400	0.65285600
C	-5.60010900	0.71999100	0.10283700
C	-4.82897000	0.10019100	-0.87779100
C	-5.16261900	-1.18604000	-1.30173000
C	-6.25353700	-1.84049600	-0.74645200
H	-7.87148900	-1.75006700	0.67662200
H	-5.35641900	1.70347400	0.49032200
H	-4.53769500	-1.66826000	-2.04599800
C	-6.53203100	-3.26275700	-1.14267700
C	-7.43520100	0.68044500	1.79400800
F	-7.80384600	-3.60827100	-0.90697700
F	-6.28182700	-3.47578400	-2.44034000
F	-5.75639000	-4.11559200	-0.44998500
F	-6.85797800	0.38352900	2.97375700
F	-8.70113400	0.25322600	1.86083500
F	-7.45529800	2.01646400	1.69860900
C	-3.55055700	0.67739600	-1.42161300
O	-2.77316700	-0.03721200	-2.05238000
N	-3.26969700	1.96262500	-1.11749400
H	-3.94684300	2.52735000	-0.62674700
C	-1.98134400	2.54699200	-1.45871400
H	-1.56792500	1.93888200	-2.26152800
C	-1.00195500	2.49792100	-0.27162100
H	-0.08442500	3.01339100	-0.56936900
H	-1.40718300	3.00175900	0.61179500
C	-2.12527000	3.97431300	-2.02020400
C	-2.62787700	4.99314200	-0.98844800
H	-3.61793600	4.69411400	-0.61499300
H	-1.95654600	5.00089400	-0.12260900
P	-0.48291200	0.82981400	0.28327300
C	0.67649700	1.12045300	1.64994000
C	1.62778300	2.14450500	1.55709300
C	0.58946200	0.35758700	2.82343900
C	2.47049000	2.41016600	2.63428800

H	1.71744700	2.73864500	0.65288600
C	1.43356800	0.63118100	3.89465600
H	-0.14231100	-0.43991300	2.90478800
C	2.36909800	1.66028100	3.80322000
H	3.20531100	3.20434200	2.55530700
H	1.35898100	0.03951600	4.80056300
H	3.02529300	1.87243000	4.64055300
C	-1.91130100	0.00627500	1.06554600
C	-2.58077500	0.73723600	2.06169400
C	-2.33594400	-1.28915100	0.75951900
C	-3.65818600	0.17744500	2.73588400
H	-2.25524300	1.73916500	2.32827300
C	-3.41758700	-1.84493900	1.44509900
H	-1.85268400	-1.86243200	-0.02056800
C	-4.07755400	-1.11813300	2.42851800
H	-4.17696600	0.75354600	3.49429200
H	-3.75534800	-2.84229800	1.18265900
H	-4.92856400	-1.54690900	2.94752000
C	-2.99870700	3.94310700	-3.27595400
H	-2.67923900	3.14106700	-3.94790800
H	-4.05017900	3.77262200	-3.02125600
H	-2.93252900	4.88506400	-3.82417500
H	-1.10807200	4.26126000	-2.31775600
C	-2.72264900	6.41428500	-1.54303400
H	-3.49976300	6.49804600	-2.30651800
H	-2.95911100	7.12602000	-0.74865100
H	-1.77249600	6.71615500	-1.99527800
C	6.42972000	-0.15478700	1.94107700
C	6.71477900	-1.02466800	2.99085000
C	4.84549300	0.96781600	0.39144200
C	5.12070600	0.05071600	1.50350000
C	5.66999000	-1.68751700	3.61993200
C	4.08327500	-0.61384100	2.16600200
C	4.34568100	-1.47573900	3.21685000
H	7.74603100	-1.15909300	3.29638300
H	3.86599500	1.43683400	0.37873500
H	5.88686300	-2.36977300	4.43488200
H	3.06738900	-0.43626200	1.82416100
H	3.53044800	-1.98237800	3.72197700
N	5.79261700	1.64414400	-0.24413400
O	8.19753800	2.30994900	-0.12627600
O	7.48230900	0.55884900	1.41132100
O	7.64783500	0.05298300	-1.01641400
S	7.32736700	1.15321400	-0.12948400

C	2.99300500	2.22295600	-2.94496000
H	3.73857700	2.31918800	-2.15185200
H	3.39425100	1.51407600	-3.67625600
H	2.83220100	3.18446500	-3.43230000
TS2RS'''			
C	-4.28915100	1.78688100	-1.38826100
C	-3.62597100	2.21980100	-2.52533900
C	-3.56636100	1.39302900	-3.65118100
C	-4.16750700	0.14037300	-3.64197200
C	-4.82834500	-0.28077600	-2.49356900
C	-4.90419600	0.52858100	-1.35379900
O	-5.47670200	-1.49568900	-2.55572000
S	-5.84729900	-2.22557800	-1.11376600
N	-6.40818800	-1.02512500	-0.19161300
C	-5.72557000	0.10921600	-0.21817900
O	-6.92348900	-3.12611600	-1.46286500
O	-4.60299900	-2.78194900	-0.61641200
H	-4.35487200	2.42122100	-0.50916800
H	-3.15645400	3.19629100	-2.54132300
H	-3.04937900	1.73117200	-4.54322300
H	-4.14690800	-0.51409600	-4.50632800
H	-6.12746500	0.89843500	0.41509500
C	-4.86478700	-2.21943200	2.48419400
C	-5.64530600	-2.94999000	3.37413000
C	-4.19776500	-0.05254100	1.49164300
C	-3.15256200	0.60236700	1.30505800
C	-4.97523100	-0.82193600	2.43312100
C	-2.02819100	1.35973800	1.08938000
C	-6.55399300	-2.30770900	4.21386100
C	-5.89996500	-0.18140800	3.27249400
C	-6.67802600	-0.92040400	4.15699000
C	-1.95924500	2.68772800	1.61336500
C	-3.21589400	3.43686600	1.99744200
H	-4.17093800	-2.71519000	1.81439100
H	-5.54568800	-4.03055500	3.40841000
H	-5.99635400	0.89986000	3.22949100
H	-7.38433100	-0.41007700	4.80457300
H	-4.10084200	2.80223300	2.03246200
H	-3.37310100	4.23186800	1.25999600
H	-3.06253800	3.91692800	2.96622500
O	-0.86208900	3.26878600	1.72382400
H	-7.16337500	-2.88310700	4.90299200
C	-1.55844300	-3.09978200	-1.25421700
C	-1.07644300	-3.08092100	0.05200000

C	-1.81757500	-1.90093600	-1.91487400
C	-0.82072100	-1.86566900	0.68420100
C	-1.57538200	-0.68602100	-1.28127800
C	-1.04215800	-0.66455000	0.00934100
C	-0.73287200	0.64454500	0.70639400
H	-1.75682700	-4.04535800	-1.74763900
H	-0.89386600	-4.01167000	0.57942300
H	-2.22735700	-1.90983800	-2.92017300
H	-0.40862300	-1.84328300	1.68870900
H	-1.81108300	0.24880400	-1.78745800
H	-0.14480000	0.41900000	1.60428800
C	1.59960200	2.77496300	0.68561600
H	1.04549400	3.70139700	0.81029100
H	2.46831600	2.96510100	0.04816200
P	0.52003100	1.64169700	-0.29128100
C	-0.21268900	2.70120300	-1.58334600
C	-0.67879900	3.98446200	-1.26648100
C	-0.20226900	2.27623400	-2.91786000
C	-1.09173700	4.84098100	-2.28379800
H	-0.71676600	4.31397300	-0.23348700
C	-0.61753400	3.13961600	-3.92734400
H	0.15055900	1.28216400	-3.17484900
C	-1.05056900	4.42594800	-3.61378000
H	-1.43981900	5.83745300	-2.03392100
H	-0.59119700	2.80728500	-4.95971300
H	-1.35997600	5.10225700	-4.40370200
C	1.73227000	0.59210400	-1.19762100
C	1.81173500	-0.80244700	-1.14942500
C	2.67581700	1.29566500	-1.96931800
C	2.80377000	-1.47625500	-1.86334700
H	1.13031900	-1.37847900	-0.54182300
C	3.66882100	0.62000200	-2.66682100
H	2.62879400	2.37844100	-2.04843900
C	3.73192300	-0.77315600	-2.61940400
H	2.85672400	-2.55848100	-1.79648100
H	4.39335000	1.18093100	-3.24714800
H	4.51283900	-1.29980200	-3.15756000
C	5.99499000	-2.43112000	-0.11312600
C	6.08605900	-1.04715600	-0.18531300
C	5.14172800	-0.23384600	0.43450300
C	4.09453100	-0.81079400	1.14942200
C	3.99279900	-2.19966500	1.22394200
C	4.93934000	-2.99726400	0.59623500
H	6.73121800	-3.05926400	-0.60269500

H	5.22201600	0.84072600	0.30626700
H	3.15214400	-2.63687100	1.75230400
C	4.76070700	-4.48916000	0.59534500
C	7.16478600	-0.41515700	-1.01961500
F	4.18571000	-4.92281700	1.72322600
F	3.97216000	-4.87712300	-0.42226200
F	5.92711300	-5.13183300	0.45460800
F	6.76032100	-0.22517600	-2.28824200
F	8.26376800	-1.17714500	-1.07012600
F	7.51843200	0.78599300	-0.54278200
C	2.95602700	-0.00991900	1.71761300
O	1.87582700	-0.55000600	1.94732500
N	3.16123900	1.31333700	1.88472000
H	4.08183000	1.69325900	1.71874600
C	2.43852000	3.40368800	3.00868900
C	3.53141300	4.31955300	2.44027900
H	4.45902300	3.74920200	2.28922800
H	3.22536800	4.68721200	1.45434200
C	2.81071400	2.84417000	4.38258300
H	2.06403800	2.12120600	4.72384200
H	3.78050300	2.33678400	4.34927600
H	2.87037000	3.64002800	5.12771900
H	1.51901300	3.99626400	3.10934000
C	3.83676300	5.51836100	3.33770700
H	4.29375600	5.20961500	4.28094900
H	4.52682400	6.20662800	2.84417200
H	2.91995000	6.06886500	3.57156100
C	2.05913700	2.25324600	2.05807500
H	1.24597400	1.70262700	2.53544600

SR-M2

C	-0.94906000	-4.14167300	-0.36748500
C	-0.24360300	-3.80932500	0.78905200
C	-1.66073900	-3.15997300	-1.05083200
C	-0.22374900	-2.49282000	1.23921000
C	-1.64658700	-1.84144700	-0.60057700
C	-0.90886000	-1.49817200	0.53254000
C	-4.33850500	-3.01337700	0.93342300
C	-3.67392100	-3.99663800	1.66906700
C	-0.77465500	-0.06521100	1.00002200
C	-5.37147200	-0.70622900	0.71910000
C	-4.65652100	-1.78038500	1.51381600
C	-5.02620400	2.85593000	0.06311500
C	-5.58959700	3.92176000	-0.63306900
C	-3.31811900	-3.75776800	2.98823700

C	-4.41139800	0.45380200	0.30164900
C	-3.21550400	0.53615300	0.82123700
C	-4.97298300	1.57825900	-0.50667200
C	-2.06080900	0.60908600	1.46457000
C	-6.10090700	3.72180200	-1.91359500
C	-4.31298300	-1.57702500	2.85269800
C	-5.47846200	1.38525300	-1.79609000
C	-3.64181100	-2.54226100	3.59232400
C	-6.03584700	2.45561100	-2.49141700
C	-1.98459200	1.33930800	2.76906400
C	-3.21218000	2.02437500	3.31925100
H	-0.95783400	-5.16753300	-0.72213900
H	0.29614200	-4.57415200	1.33844100
H	-2.25430000	-3.40657200	-1.92413200
H	0.35483200	-2.22151600	2.11782000
H	-3.43945100	-4.93448400	1.17767900
H	-2.23851800	-1.10174200	-1.12923000
H	-0.08028500	-0.04593700	1.84717900
H	-4.63616400	3.00806000	1.06473700
H	-5.63234400	4.90399400	-0.17326900
H	-6.07968000	-0.20213600	1.39194800
H	-2.79216000	-4.52494700	3.54753500
H	-5.40333800	0.40815100	-2.25413800
H	-6.41976900	2.29694100	-3.49435700
H	-4.58942700	-0.63488500	3.32088100
H	-3.38197900	-2.35417600	4.62838000
H	-4.14458200	1.60063700	2.94899900
H	-3.17255100	3.07905700	3.02625300
H	-3.17649800	1.97848600	4.40803000
N	-6.17666900	-1.26051600	-0.35060700
O	-4.29060600	-1.61293800	-2.07110300
O	-4.65498700	-3.35277600	-0.35820000
O	-6.33361800	-3.00328500	-2.12366200
O	-0.92174400	1.42008200	3.36470600
S	-5.41914100	-2.19516200	-1.32465400
H	-6.54472300	4.54871400	-2.45889100
C	6.53857800	-1.15752700	-0.56370100
C	6.22082300	0.18447800	-0.73107400
C	5.14480500	0.75720000	-0.05980500
C	4.36693000	-0.02364200	0.79210800
C	4.68081300	-1.37111500	0.96764500
C	5.76037600	-1.92699900	0.29544500
H	7.37543200	-1.59691800	-1.09560200
H	4.91696200	1.79963800	-0.25490600

H	4.05039200	-1.97392400	1.61257300
C	6.01921500	-3.40180700	0.42222900
C	6.97434400	1.00209200	-1.74119600
F	7.29022200	-3.71291500	0.13921400
F	5.75139500	-3.84788700	1.65563700
F	5.24311300	-4.10088300	-0.42407500
F	6.41121500	0.90499200	-2.96018300
F	8.24340700	0.59757600	-1.86451500
F	6.98520500	2.30295800	-1.42177800
C	3.09994700	0.45955500	1.44057300
O	2.31019100	-0.34750600	1.92718900
N	2.83898300	1.78500400	1.38997500
H	3.52250300	2.42569700	1.01472900
C	1.56381800	2.30706700	1.85228900
H	1.14535800	1.54262400	2.50566100
C	0.58840900	2.53405600	0.68100700
H	-0.32742900	2.98713700	1.07723500
H	1.00179200	3.22384200	-0.06198100
C	1.73168300	3.57397500	2.71370000
C	2.26950600	4.78020900	1.93280900
H	3.25607300	4.54247300	1.51037200
H	1.60910800	4.99447900	1.08514800
P	0.05828400	1.03772100	-0.23485500
C	-1.07554100	1.59315600	-1.53026500
C	-1.82604200	2.76551300	-1.38443700
C	-1.17458200	0.83945100	-2.70786700
C	-2.65254600	3.18902900	-2.41941500
H	-1.77622600	3.35596300	-0.47543600
C	-2.02753600	1.25441000	-3.72368000
H	-0.58720700	-0.06566600	-2.83109000
C	-2.75746800	2.43307100	-3.58314100
H	-3.23913500	4.09310400	-2.30050400
H	-2.11286700	0.66132000	-4.62725800
H	-3.41902300	2.75895600	-4.37900900
C	1.46641500	0.33230700	-1.14269100
C	1.85792300	-1.00694900	-1.08343200
C	2.14142000	1.22189200	-1.99498100
C	2.92465900	-1.44788900	-1.86856800
H	1.35803300	-1.70436100	-0.42411100
C	3.20668700	0.77456500	-2.76503800
H	1.82862300	2.25998800	-2.07140200
C	3.59891600	-0.56417300	-2.70259300
H	3.23816100	-2.48461600	-1.80207200
H	3.73511000	1.46840500	-3.40963200

H	4.43946500	-0.90709200	-3.29695100
C	2.58844500	3.24361200	3.93730400
H	2.23490900	2.32709000	4.41892400
H	3.63601600	3.09636300	3.65471500
H	2.54626100	4.04744000	4.67480300
H	0.71919500	3.81954000	3.06376400
C	2.39229300	6.04331600	2.78455700
H	3.16259500	5.93847200	3.55214500
H	2.65525200	6.90376400	2.16509800
H	1.44483600	6.26518900	3.28610800
TS2'			
C	2.90027100	3.31677200	1.05751000
C	2.22034600	4.52266300	0.97083700
C	3.38304600	1.11989600	2.11219600
C	2.53564800	2.33187100	1.97715100
C	1.12507200	4.73685400	1.80468900
C	1.44307000	2.56864200	2.81430900
C	0.73177700	3.76227200	2.72365400
H	2.54433300	5.26237700	0.24733500
H	3.19792200	0.62975900	3.06805600
H	0.58098100	5.67333000	1.74116200
H	1.16267000	1.81081500	3.54234000
H	-0.11860900	3.93715000	3.37334300
N	4.71208600	1.17734500	1.80891700
O	6.08592600	1.92752300	-0.19122800
O	3.94116400	3.05781900	0.19039700
O	5.84675600	3.43327700	1.75311900
S	5.27595800	2.36939800	0.93126800
C	0.81457400	2.75715600	-2.83915000
C	0.34654400	3.12670500	-1.58041900
C	1.42101600	1.51489600	-3.00847300
C	0.46911500	2.25312600	-0.50364800
C	1.55776700	0.64722800	-1.92829000
C	1.07587400	1.00456500	-0.66369500
C	1.10747700	0.04648400	0.51592100
C	6.73760000	-0.83480700	-1.50029200
C	7.72405200	-1.13845200	-2.43160500
C	4.37669500	-0.84778900	-0.81217600
C	3.48950800	-0.63074900	-0.01347600
C	5.39642400	-1.14009100	-1.77585700
C	2.51452500	-0.35077800	0.99827800
C	7.38821500	-1.73876000	-3.64453700
C	5.06336000	-1.74331700	-2.99809700
C	6.05592500	-2.03677800	-3.92631600

C	2.55133600	-1.25794200	2.16426600
H	0.71059900	3.43310300	-3.68161700
H	-0.12019200	4.09536600	-1.43081300
H	1.79367000	1.21766300	-3.98316200
H	0.06644800	2.52819500	0.46504700
H	2.03978100	-0.31217200	-2.07486100
H	0.56108500	0.50406000	1.34670800
H	6.97785100	-0.33983600	-0.56655800
H	8.75977000	-0.89948200	-2.21280800
H	4.02450500	-1.98106600	-3.20457700
H	5.78976800	-2.50135400	-4.87036200
O	1.59089200	-1.33746300	2.93015100
H	8.16195800	-1.97073600	-4.36921700
C	-6.16999800	1.01837100	-1.07321500
C	-5.97829900	-0.24920300	-0.53976700
C	-4.89441400	-0.52035100	0.29107100
C	-3.99298500	0.49373700	0.60490100
C	-4.17552700	1.76934600	0.07075500
C	-5.25776800	2.02269100	-0.75998200
H	-7.01266600	1.22160100	-1.72486200
H	-4.75209300	-1.53815300	0.63946300
H	-3.44509600	2.54045200	0.29244300
C	-6.89520800	-1.37331300	-0.93353100
F	-6.65143700	3.65220500	-1.73691300
F	-4.93222400	4.35101200	-0.62232500
F	-4.66594300	3.42083000	-2.54945800
F	-6.41289700	-2.05655300	-1.98714200
F	-8.10908000	-0.92851900	-1.27752800
F	-7.04722700	-2.25717500	0.06217500
C	-2.72327600	0.24871100	1.36962800
O	-1.77930500	1.03131700	1.27039600
N	-2.64299100	-0.89120000	2.08653300
H	-3.45558000	-1.48162700	2.18844700
C	-1.36907400	-1.36165500	2.61352800
H	-0.74778100	-0.47893300	2.77349900
C	-0.67857900	-2.28220900	1.59247300
H	0.13362300	-2.81350900	2.08630000
H	-1.38480800	-3.02062100	1.20053100
C	-1.53541400	-2.04792600	3.98161100
C	-2.32644500	-3.36138600	3.90965800
H	-3.34313400	-3.16828500	3.53839000
H	-1.85254100	-4.03625200	3.18808900
P	0.03163000	-1.46233000	0.10556600
C	1.05170200	-2.72782400	-0.70377300

C	1.85191600	-3.58680800	0.05716600
C	1.08218500	-2.80526300	-2.10162600
C	2.69551300	-4.49485700	-0.57544800
H	1.82938500	-3.55951100	1.14191700
C	1.92183900	-3.72093000	-2.72701600
H	0.45134500	-2.15484900	-2.70006000
C	2.73611000	-4.55775500	-1.96579900
H	3.31728200	-5.15349300	0.02111300
H	1.94121200	-3.77767700	-3.81019400
H	3.39684600	-5.26399800	-2.45716300
C	-1.37515900	-1.21072200	-1.04412400
C	-1.73747700	-0.00317000	-1.64691400
C	-2.12339600	-2.36771100	-1.32541000
C	-2.82992300	0.04407100	-2.51326800
H	-1.20254100	0.90997800	-1.43173500
C	-3.21775400	-2.30878600	-2.17907700
H	-1.84621800	-3.32725500	-0.89741400
C	-3.57220300	-1.09959900	-2.77834500
H	-3.10950600	0.99505000	-2.95575700
H	-3.79390500	-3.20630300	-2.37579800
H	-4.43313100	-1.05320400	-3.43666500
C	-2.14112200	-1.06366100	4.98390100
H	-1.62767500	-0.09850500	4.93976700
H	-3.20209900	-0.89180200	4.77386500
H	-2.05601600	-1.44126400	6.00477400
H	-0.51209100	-2.28455800	4.30186100
C	-2.42528300	-4.07717400	5.25636700
H	-3.02799600	-3.51107500	5.97053400
H	-2.88554100	-5.06098600	5.13958200
H	-1.43103700	-4.21881600	5.69199400
C	3.85176100	-1.96087100	2.46451500
H	4.67298900	-1.23552400	2.45438600
H	3.78026100	-2.45525500	3.43290500
H	4.07222900	-2.68972400	1.67916500
C	-5.38327600	3.36999900	-1.41327300
TS3			
C	0.80590000	3.67382900	-2.06932700
C	0.32234300	3.79653700	-0.76890600
C	1.25065000	2.43542900	-2.52813400
C	0.27858500	2.68426600	0.06794400
C	1.21349900	1.32507700	-1.69023200
C	0.72239700	1.44163300	-0.38649400
C	6.65387900	2.39480100	0.65922300
C	7.99002300	2.57938800	0.99213800

C	0.66941500	0.25865900	0.55564300
C	4.78870800	1.28340400	-0.64282100
C	6.24708600	1.42286200	-0.25800100
C	5.06201800	-2.42282300	-0.56274800
C	5.55957100	-3.52578400	-1.25225600
C	8.95658500	1.78480900	0.38606600
C	4.17182100	-0.08936700	-0.54224000
C	3.15041500	0.10319900	0.28514300
C	4.58375200	-1.31123700	-1.26325700
C	2.03353900	-0.25977500	0.99161800
C	5.57815200	-3.52931400	-2.64535800
C	7.23482800	0.63138700	-0.84900600
C	4.60360200	-1.32048400	-2.66301100
C	8.57867800	0.80783600	-0.53334800
C	5.09503000	-2.42679700	-3.34938500
C	2.13015500	-0.88492800	2.29308000
C	3.46193900	-1.42947600	2.76655100
H	0.83739900	4.53973400	-2.72248900
H	-0.02237300	4.75855500	-0.40413000
H	1.63012100	2.33365600	-3.53995800
H	-0.11149300	2.77273200	1.07759600
H	8.24705000	3.34285900	1.71788800
H	1.58052700	0.36733700	-2.04946500
H	0.09962700	0.53944500	1.44865600
H	5.06456700	-2.40406800	0.52259800
H	5.93845600	-4.38026400	-0.70044200
H	4.66288200	1.68431200	-1.65973900
H	10.00258700	1.92650900	0.63608100
H	4.23647600	-0.45617100	-3.21028900
H	5.10293200	-2.42820000	-4.43475000
H	6.94585400	-0.12387500	-1.57400300
H	9.32939000	0.18418200	-1.00635600
H	4.31059500	-0.89611300	2.34159600
H	3.51823100	-2.48818400	2.48779000
H	3.49311100	-1.36761900	3.85534400
N	3.78258300	1.94190800	0.23169100
O	4.67647600	1.43063600	2.59902800
O	5.72363100	3.23599800	1.25090500
O	3.45426900	3.54119000	2.14234600
O	1.12746200	-1.06256000	2.99893800
S	4.29888000	2.47107000	1.64344700
H	5.97074900	-4.38691100	-3.18223600
C	-6.75706600	1.32289500	-0.47473200
C	-6.52129600	-0.02470900	-0.23653000

C	-5.38989600	-0.44431200	0.45742600
C	-4.47420500	0.49688000	0.92148100
C	-4.70584800	1.85291000	0.68960300
C	-5.84010900	2.25634100	-0.00059200
H	-7.63813100	1.64089800	-1.02138700
H	-5.23234100	-1.51059800	0.58180200
H	-3.97106100	2.57338800	1.03279400
C	-6.02170200	3.71081200	-0.33031300
C	-7.43724500	-1.05503300	-0.83272900
F	-7.31096600	4.02430300	-0.51274100
F	-5.53814500	4.50428600	0.63271400
F	-5.37449200	4.03151000	-1.46482400
F	-7.01558600	-1.43168500	-2.05477300
F	-8.68439300	-0.59247300	-0.97595000
F	-7.49274400	-2.16488800	-0.08432700
C	-3.15346500	0.13851100	1.54653100
O	-2.27281500	0.99013600	1.65274300
N	-2.96274500	-1.15053000	1.90011000
H	-3.71737600	-1.81565400	1.82026900
C	-1.65943300	-1.61790800	2.34845200
H	-1.11508700	-0.73858400	2.68930100
C	-0.86521200	-2.25660100	1.19575400
H	0.05852700	-2.67260600	1.60627200
H	-1.42579700	-3.06745400	0.71954700
C	-1.76977800	-2.56424700	3.55855600
C	-2.42810900	-3.90997100	3.22611400
H	-3.44590300	-3.74608600	2.84350100
H	-1.86864200	-4.40420400	2.42414800
P	-0.35876100	-1.12779300	-0.15646300
C	0.61211200	-2.14814300	-1.29871300
C	1.53516500	-3.07489800	-0.79990500
C	0.42314300	-2.02848300	-2.68201600
C	2.23607600	-3.89489500	-1.67812200
H	1.71366200	-3.16375500	0.26699200
C	1.14634700	-2.83509400	-3.55349000
H	-0.28941100	-1.31086600	-3.07683500
C	2.04479100	-3.77434000	-3.05145500
H	2.94428500	-4.61631300	-1.28752300
H	0.99923500	-2.73558600	-4.62340700
H	2.60363700	-4.40916200	-3.73124700
C	-1.85079100	-0.66203100	-1.10044900
C	-2.19538900	0.65097200	-1.43239400
C	-2.66547700	-1.72136000	-1.53425700
C	-3.34092400	0.89722000	-2.19123200

H	-1.59806500	1.48498100	-1.08822800
C	-3.80593200	-1.46658900	-2.28507400
H	-2.40616000	-2.75087900	-1.30260100
C	-4.14432300	-0.15358900	-2.61690500
H	-3.61269900	1.92207400	-2.42288000
H	-4.43581000	-2.28975200	-2.60448200
H	-5.04313100	0.04327400	-3.19202300
C	-2.47548400	-1.84391800	4.70921800
H	-2.05839200	-0.84265600	4.85157100
H	-3.54731700	-1.73861100	4.50987900
H	-2.35863600	-2.39173800	5.64653500
H	-0.73039100	-2.75436000	3.85743800
C	-2.50114000	-4.85691700	4.42360600
H	-3.18133900	-4.48270900	5.19245100
H	-2.85611500	-5.84378200	4.11745700
H	-1.51328600	-4.97950500	4.87927900
M3			
C	-0.62558400	-2.93662600	-2.85022700
C	-0.24440900	-3.29521400	-1.55858900
C	-1.08586900	-1.64524600	-3.10301600
C	-0.30187100	-2.36201700	-0.52613500
C	-1.15266900	-0.71583500	-2.06939200
C	-0.74073700	-1.06183700	-0.77941800
C	-5.99615100	-2.89935600	1.04060400
C	-7.07655000	-3.35159200	1.77864000
C	-0.81938100	-0.05389300	0.34620500
C	-4.87276500	-1.47698500	-0.69237500
C	-6.08751100	-1.85721800	0.11974300
C	-4.43885300	2.37363400	-1.43806100
C	-4.92920200	3.41514700	-2.21737700
C	-8.31339100	-2.74328000	1.58145400
C	-4.45575500	-0.02279000	-0.77750100
C	-3.33612800	-0.24916000	-0.04346500
C	-4.96477100	1.07829900	-1.57415700
C	-2.23296600	0.44146900	0.57413500
C	-5.94399600	3.19046100	-3.14736300
C	-7.32708400	-1.23699800	-0.03249300
C	-5.97054400	0.85803200	-2.52936300
C	-8.43404200	-1.68219300	0.68698400
C	-6.45606400	1.90425200	-3.30611900
C	-2.41923800	1.36768900	1.60689800
C	-3.79638700	1.86159500	2.00119400
H	-0.57405100	-3.66306900	-3.65485600
H	0.09987800	-4.30386400	-1.35362200

H	-1.39817600	-1.36371600	-4.10357100
H	0.00587400	-2.63134700	0.47805500
H	-6.93562900	-4.15654100	2.49076200
H	-1.54259300	0.28234700	-2.25710300
H	-0.37227500	-0.48451900	1.24935000
H	-3.63868900	2.54666500	-0.72426200
H	-4.51784600	4.41185100	-2.09289900
H	-4.86749200	-2.02052400	-1.64510700
H	-9.17563800	-3.08644200	2.14243200
H	-6.36398800	-0.14513800	-2.67327800
H	-7.23498700	1.71354400	-4.03748500
H	-7.42607500	-0.39937100	-0.71466300
H	-9.39217100	-1.19243500	0.55260700
H	-4.60713700	1.24917600	1.60572100
H	-3.92252100	2.89000000	1.64141900
H	-3.85191100	1.88739600	3.09191700
N	-3.54838300	-1.70103300	0.01482200
O	-3.98922300	-1.51823000	2.57013100
O	-4.74869700	-3.50510900	1.23943000
O	-2.36385500	-3.20842400	1.71007200
O	-1.42716900	1.84061200	2.23456300
S	-3.55965900	-2.42233000	1.52081600
H	-6.32937700	4.00984700	-3.74512100
C	6.48099200	-1.48138700	-0.57958500
C	6.28830700	-0.18117200	-0.13050000
C	5.15652400	0.16170700	0.60328100
C	4.20708400	-0.81178100	0.90578300
C	4.38700300	-2.11761600	0.45141300
C	5.51893200	-2.44316900	-0.28310700
H	7.36323500	-1.74226500	-1.15406700
H	5.01391800	1.19968800	0.88574800
H	3.62019500	-2.85692200	0.65797500
C	5.65390900	-3.82595300	-0.85479400
C	7.27129100	0.88900000	-0.51481100
F	6.93543700	-4.16294700	-1.04946500
F	5.10202500	-4.75087600	-0.06047000
F	5.03855000	-3.91472200	-2.04728200
F	6.95600700	1.45191400	-1.69447800
F	8.51186600	0.40036300	-0.63624400
F	7.30588900	1.87743600	0.38897000
C	2.89455600	-0.48148600	1.55902600
O	1.91138800	-1.19335000	1.36423200
N	2.83910700	0.65287700	2.28684000
H	3.68555700	1.18144700	2.44337400

C	1.56454800	1.28757900	2.60932500
H	0.82653200	0.49096300	2.71777200
C	1.14728500	2.21896400	1.45889800
H	0.41130600	2.93276700	1.82018800
H	2.02061900	2.75585200	1.07538000
C	1.62590900	2.03009700	3.95531500
C	2.58340500	3.22964800	3.93827600
H	3.61307200	2.88525600	3.76496200
H	2.32821400	3.88993200	3.10164600
P	0.38053700	1.39832800	-0.00475200
C	-0.47470200	2.72790800	-0.90818700
C	-1.19553500	3.70949400	-0.21655400
C	-0.40209400	2.77471400	-2.30585800
C	-1.81324100	4.73875800	-0.92185000
H	-1.29209700	3.65548900	0.86325300
C	-1.03726000	3.79715000	-3.00377300
H	0.15911700	2.02133100	-2.85052300
C	-1.73247900	4.78585100	-2.31202100
H	-2.36384700	5.50178000	-0.38100300
H	-0.97700200	3.82614900	-4.08622600
H	-2.21466500	5.59111300	-2.85711600
C	1.82640100	1.00111500	-1.07776300
C	2.17804400	-0.27157900	-1.53618000
C	2.64755700	2.09179300	-1.41695900
C	3.32016900	-0.44774800	-2.31817800
H	1.59375200	-1.13854300	-1.26599300
C	3.79144100	1.90840800	-2.18407500
H	2.38834100	3.09730100	-1.09568600
C	4.12871700	0.63412800	-2.64144600
H	3.58549400	-1.44822800	-2.64609200
H	4.41981100	2.75941500	-2.42410500
H	5.02682000	0.48970400	-3.23260200
C	1.95236100	1.04817500	5.08155900
H	1.31654100	0.16033800	5.01954500
H	2.99587000	0.72057300	5.02541200
H	1.79334000	1.50508100	6.06053200
H	0.60667900	2.41012100	4.10628100
C	2.55267200	4.04234200	5.23232000
H	2.94542300	3.47075700	6.07673900
H	3.15503700	4.94880400	5.13647400
H	1.52816100	4.34151900	5.47554600
TS4			
C	0.24963900	-3.03470700	-2.25504400
C	0.57539200	-3.19566600	-0.90981700

C	-0.48312800	-1.91970100	-2.66572200
C	0.19650800	-2.23100300	0.02284900
C	-0.86649000	-0.95984000	-1.73645500
C	-0.51338300	-1.10070900	-0.38827800
C	-5.91951600	-2.81537700	1.19954700
C	-6.99299400	-3.21471900	1.97628000
C	-0.84608300	-0.03108800	0.59060200
C	-4.79355500	-1.49918400	-0.60873800
C	-6.00713000	-1.81221600	0.23563800
C	-4.34908700	2.26745400	-1.69778400
C	-4.87901700	3.22891000	-2.55110100
C	-8.22121500	-2.58997400	1.77648500
C	-4.37043600	-0.05373800	-0.78464800
C	-3.26912000	-0.23841100	-0.01236100
C	-4.88697700	0.97097300	-1.67445100
C	-2.18745800	0.46091100	0.65354000
C	-5.93106100	2.91552600	-3.41075300
C	-7.23612100	-1.17111800	0.08345000
C	-5.92653900	0.65778900	-2.56553500
C	-8.33702900	-1.56343800	0.84231000
C	-6.44379800	1.62033300	-3.42467000
C	-2.44408000	1.49545100	1.61351500
C	-3.86362700	1.94318600	1.89328900
H	0.56675400	-3.77610300	-2.98124700
H	1.13771600	-4.06779000	-0.59014000
H	-0.74052600	-1.79306700	-3.71219100
H	0.46428100	-2.33437700	1.07022600
H	-6.85323000	-3.99099500	2.71971300
H	-1.41603800	-0.07479100	-2.05200600
H	-0.30930000	-0.10184700	1.53604100
H	-3.50775500	2.51041500	-1.05385000
H	-4.46562500	4.23138900	-2.54404400
H	-4.79347000	-2.10557600	-1.52216700
H	-9.07920300	-2.89155900	2.36699900
H	-6.32406100	-0.35332800	-2.59294900
H	-7.24795900	1.35780500	-4.10433800
H	-7.33384900	-0.35850300	-0.62782500
H	-9.28690600	-1.05825600	0.70682400
H	-3.86535000	2.54799400	2.80055600
H	-4.53024300	1.08508600	2.00920900
H	-4.24533400	2.55162600	1.06555900
N	-3.47462700	-1.67834200	0.11779800
O	-3.88713400	-1.41131900	2.66952500
O	-4.67744100	-3.43105500	1.40469600

O	-2.28661300	-3.14593200	1.84633400
O	-1.49584000	2.04145800	2.21087800
S	-3.47634300	-2.35531700	1.64814800
H	-6.34144800	3.67322000	-4.06991300
C	5.77678900	-2.05624600	-0.75840000
C	6.02754500	-0.79953900	-0.21707700
C	5.13577300	-0.21081400	0.67194500
C	3.96869300	-0.88621400	1.02795000
C	3.72668500	-2.15970000	0.51859300
C	4.62161400	-2.72972400	-0.37815300
H	6.46323800	-2.49680200	-1.47394800
H	5.36761300	0.77124900	1.07087400
H	2.81920900	-2.67633100	0.81026700
C	4.26547600	-4.02982200	-1.04019600
C	7.27602000	-0.06928800	-0.62618000
F	5.34911600	-4.70125900	-1.44659000
F	3.56638300	-4.83174500	-0.22483800
F	3.50089500	-3.81912300	-2.12811700
F	7.52142200	-0.22880500	-1.93646900
F	8.35627500	-0.51667300	0.02919000
F	7.18259500	1.24607500	-0.39070200
C	2.87337000	-0.27684200	1.86276000
O	2.00689700	-0.97728400	2.37577500
N	2.88522200	1.07495300	1.94503100
H	3.53140200	1.57601800	1.35037200
C	1.75746300	1.83847900	2.47494400
H	0.99685200	1.10713100	2.75941300
C	1.19091300	2.72232600	1.36141300
H	0.36596100	3.31049600	1.76165900
H	1.95381600	3.40261100	0.96832800
C	2.13660400	2.61765600	3.74892900
C	3.17512500	3.71503700	3.48632300
H	4.07631600	3.25941800	3.05273900
H	2.78482700	4.41658600	2.74045800
P	0.51619800	1.71601600	-0.04091000
C	-0.44347400	2.90556500	-1.02697300
C	-1.25374300	3.86485400	-0.40485400
C	-0.38670900	2.85514000	-2.42645100
C	-1.94038200	4.80065300	-1.17521100
H	-1.34966600	3.88232700	0.67619900
C	-1.09048000	3.78073300	-3.18991500
H	0.23033600	2.10876200	-2.91876600
C	-1.84957400	4.76789200	-2.56504300
H	-2.54877100	5.55463600	-0.68590900

H	-1.03129000	3.74111000	-4.27236200
H	-2.37741300	5.50503100	-3.16199100
C	2.00378300	1.39595700	-1.08889000
C	2.30826800	0.11752800	-1.56799900
C	2.86822200	2.45750600	-1.40306500
C	3.44998600	-0.09620000	-2.34058500
H	1.67443100	-0.72781100	-1.33560700
C	4.02123900	2.23525500	-2.14918200
H	2.63852800	3.46793400	-1.07572500
C	4.31518000	0.95493500	-2.62073400
H	3.66348100	-1.09943800	-2.69672300
H	4.68538600	3.06420100	-2.37069800
H	5.21932100	0.78087700	-3.19557600
C	2.60039400	1.63367500	4.82459700
H	1.90425700	0.79434800	4.91116900
H	3.58653800	1.22839800	4.57295200
H	2.67072300	2.11650200	5.80159500
H	1.20840300	3.09747000	4.09092000
C	3.56112300	4.50037100	4.73907600
H	4.09909500	3.87612000	5.45672100
H	4.20609500	5.34512100	4.48519600
H	2.67048500	4.89515300	5.23890200
P1			
C	5.05407900	0.27064100	-2.11126400
C	5.49707900	0.10580200	-0.80051600
C	3.74941200	0.69835800	-2.35766000
C	4.63519300	0.36540300	0.25815700
C	2.88097700	0.94110300	-1.30146600
C	3.31086600	0.76460600	0.02290600
C	-1.61075600	-2.80132300	-0.44235000
C	-2.49924300	-3.79052400	-0.05903900
C	2.45658700	1.01546600	1.18426700
C	-0.95330200	-0.49103200	-1.14262100
C	-1.99663000	-1.48685900	-0.69539900
C	-1.42524400	3.18092100	0.24703800
C	-2.16894000	4.34415400	0.09667400
C	-3.84450500	-3.45491200	0.06687800
C	-0.91062500	0.84073400	-0.41290100
C	0.22474000	0.48088800	0.22614500
C	-1.68998300	2.05940900	-0.55569800
C	1.10968400	0.96625500	1.28397500
C	-3.17981000	4.41382600	-0.86212700
C	-3.34272300	-1.16449300	-0.52645800
C	-2.69453800	2.14694000	-1.53003500

C	-4.26109600	-2.14460500	-0.15678700
C	-3.43477800	3.31500200	-1.67926700
C	0.50920200	1.26669000	2.63658700
C	-0.89921900	0.79821500	2.90901200
H	5.72679900	0.07715400	-2.94042900
H	6.51422000	-0.21582200	-0.60407100
H	3.41028100	0.84680100	-3.37739300
H	4.97972600	0.25004500	1.28182800
H	-2.13141700	-4.79110200	0.13636700
H	1.87414400	1.29240800	-1.50074000
H	2.97565500	1.26515400	2.10858500
H	-0.62370100	3.14637200	0.97976700
H	-1.95556000	5.20176000	0.72579300
H	-0.86659900	-0.45226300	-2.23356500
H	-4.56155100	-4.21417800	0.35827100
H	-2.88633600	1.30088300	-2.18452700
H	-4.20856700	3.36707600	-2.43779100
H	-3.67546200	-0.14345200	-0.67748300
H	-5.30529800	-1.87942300	-0.03504700
H	-0.99235400	-0.26409400	2.66474700
H	-1.61403500	1.34108200	2.28251300
H	-1.12960300	0.97387600	3.95892300
N	0.41098200	-0.73856300	-0.52312800
O	0.31590300	-2.11668400	1.65416900
O	-0.25498000	-3.13507500	-0.57894100
O	2.07079700	-2.62500200	-0.05486900
O	1.16629800	1.84158300	3.48312100
S	0.74180500	-2.17617600	0.26980400
H	-3.75879300	5.32390200	-0.97686100

BF₃·Et₂O

F	1.51220400	-1.12841900	-1.01520200
F	1.67336700	1.09525300	-0.45133500
F	1.67676900	-0.50959900	1.18516000
O	-0.31654800	-0.05549600	-0.00336700
C	-0.99666300	-1.30035400	0.32583000
H	-0.35566700	-2.07835300	-0.08554900
H	-1.02266500	-1.38979600	1.41504000
C	-0.81340400	1.13594700	0.68211700
H	-1.64675600	0.81839700	1.31059400
H	-0.00537600	1.48872400	1.32445400
C	-1.22730900	2.16221300	-0.34557700
H	-1.58340700	3.06183100	0.16154200
H	-0.37306600	2.42393400	-0.97101900
H	-2.02999900	1.77447700	-0.97692600

C	-2.37108800	-1.32219500	-0.30292500
H	-2.84495400	-2.28244400	-0.08807000
H	-3.01562100	-0.53432000	0.09487400
H	-2.29413400	-1.20467700	-1.38556300
B	1.27875200	-0.16051800	-0.07934100
TS5			
C	-4.14913800	4.72043000	1.34120200
C	-3.40646600	5.20274000	0.26501400
C	-3.76194100	3.54629100	1.98711400
C	-2.28290700	4.50831400	-0.16516300
C	-2.65067300	2.83961300	1.54653500
C	-1.90558200	3.30670600	0.45303400
C	-3.74744500	-2.20972000	-1.21355600
C	-4.02104800	-3.21126600	-2.12833000
C	-0.72182000	2.61638600	-0.05687500
C	-2.68948100	-1.23723200	0.83505800
C	-2.89565000	-2.38394000	-0.12522600
C	1.01436100	-0.99242800	2.21449200
C	1.91036600	-1.57602600	3.10078500
C	-3.42478400	-4.45517000	-1.94095600
C	-1.25376200	-0.88226700	1.18608400
C	-1.32735900	0.23983300	0.43594600
C	-0.30281100	-1.47030300	2.11632300
C	-0.43133900	1.29537300	-0.02742400
C	1.50621400	-2.63196100	3.91724500
C	-2.28174700	-3.62722600	0.02318000
C	-0.70321700	-2.52120300	2.95463200
C	-2.55205200	-4.65777100	-0.87418000
C	0.19471100	-3.09653000	3.84732100
C	0.86430100	0.86202600	-0.63601800
C	0.95231200	-0.50774600	-1.25338100
H	-5.02237200	5.26496800	1.68524100
H	-3.69784300	6.12211700	-0.23128400
H	-4.32707800	3.18348700	2.83899100
H	-1.69419700	4.88527500	-0.99649700
H	-4.68253600	-3.00597000	-2.96193100
H	-2.34341500	1.93684500	2.06351500
H	0.01668300	3.24565000	-0.55114200
H	1.35018500	-0.16050700	1.60399200
H	2.92763200	-1.20217700	3.15008800
H	-3.40113000	-1.26802200	1.66661600
H	-3.62956100	-5.25857200	-2.63960900
H	-1.72806400	-2.88067300	2.91584300
H	-0.13185800	-3.90779100	4.48915400

H	-1.58623700	-3.79099800	0.83900200
H	-2.07106300	-5.62046600	-0.74250600
H	0.01948900	-0.75219400	-1.76644400
H	1.11277200	-1.25522400	-0.46885400
H	1.79692300	-0.53390600	-1.94010200
N	-2.73909200	0.12468100	0.16299100
O	-2.25325700	0.03316600	-2.36536500
O	-4.35528800	-0.95759000	-1.38994300
O	-4.12289800	1.46468800	-1.51895200
O	1.81888600	1.63186800	-0.62316700
S	-3.30967500	0.28231200	-1.40427000
H	2.20860300	-3.08564400	4.60823900
B	3.84254300	0.87135800	-0.62533300
F	4.33653100	2.03427400	-0.22251000
F	3.87696100	0.55962900	-1.91899200
F	3.52565200	-0.06454800	0.26891400
O	6.22707200	-0.06473200	-0.57356000
C	7.08243800	1.04884400	-0.78330900
H	8.03769100	0.69947000	-1.20078500
H	6.62779800	1.73002400	-1.51738500
C	7.31538800	1.74570700	0.54184600
H	6.36892700	2.08366600	0.96555500
H	7.79403800	1.06230800	1.24735900
H	7.96526700	2.61305200	0.40208300
C	6.28911600	-1.00070100	-1.63858300
H	7.32901100	-1.33840600	-1.75917700
H	5.98334500	-0.51948100	-2.57793600
C	5.38595300	-2.17276400	-1.31421100
H	5.67620800	-2.61868700	-0.35972500
H	4.34545900	-1.85177600	-1.24522000
H	5.46699800	-2.93435400	-2.09343700
M4			
C	-2.63584300	-4.48195300	2.34483700
C	-3.48103100	-4.25603700	1.25961200
C	-1.70927600	-3.51137000	2.72975100
C	-3.39630300	-3.06059000	0.55965400
C	-1.60468300	-2.32510400	2.01866900
C	-2.44244800	-2.09087500	0.91396600
C	3.25519600	-1.36399400	-1.14254000
C	4.25157500	-1.25645700	-2.09637800
C	-2.40934000	-0.86963900	0.12776900
C	1.93567100	-0.62592100	0.85352300
C	3.02462600	-0.39576500	-0.16769000
C	-0.04639800	2.64011600	1.89292900

C	0.04092400	3.79651400	2.65699000
C	5.06962200	-0.13045200	-2.07000200
C	0.94441900	0.50569100	1.07683600
C	-0.01794800	-0.18870500	0.43203800
C	1.02044600	1.72774400	1.86085900
C	-1.38521600	0.01256300	-0.04780300
C	1.18643000	4.05756000	3.40882400
C	3.83234100	0.74119100	-0.18335300
C	2.15905700	1.99053200	2.63584000
C	4.85308800	0.86764900	-1.12278000
C	2.24136700	3.14827700	3.40187900
C	-1.62747200	1.16963300	-0.91593000
C	-0.49572300	1.88609800	-1.57469900
H	-2.70619900	-5.41108800	2.90083300
H	-4.20909800	-5.00488700	0.96837100
H	-1.06994700	-3.68211500	3.58885900
H	-4.06020100	-2.87041100	-0.27843000
H	4.36821100	-2.03980600	-2.83617200
H	-0.89755000	-1.56687400	2.33535600
H	-3.31963500	-0.64714300	-0.42570500
H	-0.95656600	2.44185600	1.33419400
H	-0.78957200	4.49401900	2.66893700
H	2.31635300	-1.11994400	1.75341400
H	5.86254700	-0.02649400	-2.80204800
H	2.97743200	1.27585400	2.65058000
H	3.12866800	3.33694500	3.99653100
H	3.66142100	1.53427600	0.53607900
H	5.47567200	1.75519100	-1.11815100
H	0.34445300	1.21026700	-1.72921000
H	-0.17736900	2.70964100	-0.92450500
H	-0.83732800	2.31248700	-2.51615000
N	0.74969800	-1.40108800	0.30197200
O	0.55358000	-1.23044600	-2.25769700
O	2.43416700	-2.50249800	-1.16090500
O	0.18171600	-3.43680500	-1.13530500
O	-2.81896700	1.53110000	-1.06916600
S	0.85071600	-2.16362000	-1.18873400
H	1.25130500	4.96225200	4.00362400
B	-3.26965000	2.81777600	-1.89143600
F	-4.60900800	2.89495700	-1.64874600
F	-2.54739100	3.85527000	-1.35387200
F	-2.96095100	2.56772800	-3.20577200
Et₂O			
O	-0.00002200	0.26843300	0.00000000

C	0.00000400	-0.51781500	1.17264900
H	-0.88598000	-1.17225500	1.18682100
H	0.88600800	-1.17222600	1.18680000
C	0.00000400	0.40854600	2.37160300
H	0.88647500	1.04697500	2.35752900
H	-0.88648800	1.04694600	2.35755300
H	0.00002500	-0.16755900	3.29947200
C	0.00000400	-0.51781500	-1.17264900
H	-0.88598000	-1.17225500	-1.18682100
H	0.88600800	-1.17222600	-1.18680000
C	0.00000400	0.40854600	-2.37160300
H	-0.88648800	1.04694600	-2.35755300
H	0.88647500	1.04697500	-2.35752900
H	0.00002500	-0.16755900	-3.29947200

TS6

C	1.96418100	3.74539700	-3.25880700
C	2.34769300	4.14434700	-1.98000000
C	1.39053700	2.48985100	-3.45617400
C	2.16623100	3.28320200	-0.90299000
C	1.18489700	1.63455900	-2.37898400
C	1.56681800	2.03099600	-1.09218700
C	-3.28081600	-2.16996400	-1.62743300
C	-4.07548600	-3.29458500	-1.49172600
C	1.43692400	1.15952600	0.09559800
C	-2.69807300	0.24755000	-1.30137800
C	-3.60827700	-0.93413600	-1.07436900
C	-2.40410100	2.44172300	1.96873500
C	-3.06027300	3.39290800	2.74017600
C	-5.26684800	-3.17709300	-0.78132000
C	-2.26589900	1.03830100	-0.07709700
C	-1.01224100	0.54970700	-0.16892900
C	-2.95203200	2.02090100	0.74769400
C	0.24278600	0.56967800	0.58008400
C	-4.27012500	3.93629800	2.30857700
C	-4.79205500	-0.84693900	-0.34185500
C	-4.16457300	2.57810200	0.31787500
C	-5.61875800	-1.95913400	-0.20356500
C	-4.81874200	3.52820000	1.09481500
C	0.36782000	-0.15257500	1.78694400
C	-0.77833400	-0.79433400	2.49796900
H	2.12292800	4.40753900	-4.10356400
H	2.80201800	5.11662500	-1.82319100
H	1.10987000	2.17130500	-4.45442600
H	2.48500200	3.58050500	0.09222400

H	-3.75569600	-4.23046500	-1.93486900
H	0.76509100	0.64774200	-2.54085300
H	2.14329900	1.39760600	0.88675500
H	-1.46168400	2.02275200	2.30818000
H	-2.62809300	3.70885600	3.68378900
H	-3.00365900	0.83399900	-2.17378400
H	-5.91047400	-4.04211400	-0.66769600
H	-4.58957400	2.27555500	-0.63566400
H	-5.75578500	3.95212900	0.74967200
H	-5.06719000	0.09348200	0.12375300
H	-6.53808400	-1.87427100	0.36485600
H	-1.73252700	-0.54180200	2.04070800
H	-0.75523900	-0.48039300	3.54486900
H	-0.63265600	-1.87729300	2.47930600
N	-1.23351400	-0.13407700	-1.42730500
O	-0.65212700	-2.37777500	-0.29539000
O	-2.09016900	-2.28209400	-2.36563700
O	0.29923100	-1.83112900	-2.54280900
O	1.56127300	-0.28818600	2.24586000
S	-0.78039800	-1.73500200	-1.58821100
H	-4.78174800	4.67522600	2.91602800
B	1.93869700	-0.92999900	3.59365100
F	3.31818100	-0.92970500	3.58032600
F	1.41474400	-0.12517700	4.58863300
F	1.41615100	-2.20780400	3.64421700
H	2.29269500	-0.02259400	-0.27834700
Si	3.51729100	-0.98236000	-0.60417600
C	4.76677500	0.88502300	1.20963100
H	4.62364500	1.62864100	0.41665000
H	3.94076100	0.96544200	1.92091800
H	5.68335500	1.14888100	1.74417900
C	4.83442000	-0.54966600	0.66647900
H	5.80355200	-0.73652800	0.18498600
H	4.75286100	-1.24795700	1.50530900
C	2.37641400	-3.16582500	0.88813500
H	3.06945400	-2.90181100	1.69185700
H	1.42728200	-2.67485700	1.10763500
H	2.20754500	-4.24580300	0.93190200
C	2.90051600	-2.74851300	-0.48923600
H	3.76604200	-3.36512900	-0.77319700
H	2.14121500	-2.90865700	-1.26183000
C	4.70491300	0.85151700	-2.49811600
H	5.61613200	0.87592000	-1.89194300
H	4.99384900	1.03849600	-3.53622600

H	4.07000800	1.68361900	-2.17826800
C	3.98233900	-0.49451900	-2.35969300
H	3.07407500	-0.51430000	-2.97401900
H	4.61999600	-1.30414700	-2.74087000
TS6'			
C	-2.27494000	2.77027500	3.72636800
C	-2.42046600	3.57033300	2.59503700
C	-1.95153600	1.42247800	3.58435500
C	-2.24760700	3.02079900	1.32812400
C	-1.76278000	0.87446100	2.31843200
C	-1.90387500	1.67285000	1.18028400
C	2.96221300	-2.42089600	1.12888000
C	3.77333500	-3.51652300	0.89111400
C	-1.74660400	1.13233300	-0.20385800
C	2.38137300	0.01728900	1.11240100
C	3.30468100	-1.12267300	0.75762700
C	2.13660500	2.87403900	-1.60535800
C	2.80357800	3.97015900	-2.13853600
C	4.99734200	-3.30515300	0.26220900
C	2.00007600	1.00925800	0.03008000
C	0.72854600	0.55137300	-0.00373000
C	2.70414000	2.14141300	-0.55022000
C	-0.48542000	0.74411000	-0.77123500
C	4.04475600	4.35594400	-1.63225200
C	4.51848700	-0.94024800	0.09589800
C	3.94444900	2.54780300	-0.03699700
C	5.36212700	-2.02293600	-0.14241600
C	4.60956500	3.64420000	-0.57630300
C	-0.61240200	0.19571900	-2.08183200
C	0.59850700	-0.27590700	-2.85759800
H	-2.42150100	3.19381400	4.71466100
H	-2.67920300	4.61914600	2.69716200
H	-1.84923100	0.79233100	4.46185400
H	-2.37643700	3.63967600	0.44438500
H	3.43981900	-4.50301000	1.19166000
H	-1.52005700	-0.17775600	2.21212800
H	-2.35711100	1.67308300	-0.92833500
H	1.16313800	2.58324800	-1.98883400
H	2.35336800	4.52631000	-2.95441800
H	2.65246200	0.45251000	2.08060000
H	5.65484500	-4.14615100	0.07227000
H	4.38232900	2.01117400	0.80080200
H	5.56860400	3.94481400	-0.16731500
H	4.80320700	0.05156800	-0.23835300

H	6.30511700	-1.86369200	-0.65336200
H	1.37543100	0.49298100	-2.89535400
H	0.28838500	-0.53427800	-3.87074700
H	1.02989500	-1.15670000	-2.37276200
N	0.90752600	-0.36114000	1.12588200
O	0.50905100	-2.40535000	-0.42586700
O	1.72637100	-2.62790000	1.76316400
O	-0.68898500	-2.25709900	1.75525200
O	-1.76128400	0.03455600	-2.56076800
S	0.48115700	-1.96837200	0.95674300
H	4.56527800	5.20854500	-2.05539000
H	-2.49034300	0.05977100	-0.25493200
Si	-3.54567600	-1.07967900	-0.87453700
C	-4.70644800	1.14861100	-2.30583600
H	-4.93331800	1.60792200	-1.33796900
H	-3.74535300	1.53423100	-2.65126000
H	-5.47644100	1.47275800	-3.01136200
C	-4.64984700	-0.38362100	-2.22113300
H	-5.65291500	-0.79136800	-2.03562600
H	-4.30650100	-0.78970000	-3.17758700
C	-2.03404500	-3.00086800	-2.51816500
H	-2.67697800	-2.72912600	-3.36025900
H	-1.11134300	-2.42754900	-2.60783500
H	-1.78670000	-4.06230300	-2.61312800
C	-2.71394500	-2.73177100	-1.17583300
H	-3.54253100	-3.44075200	-1.02273800
H	-2.02083900	-2.91485300	-0.34728400
C	-5.24553500	0.08483400	1.14777700
H	-6.01976900	0.30387500	0.40563400
H	-5.73959100	-0.02275100	2.11764900
H	-4.58710900	0.95808700	1.21050400
C	-4.46411900	-1.18007000	0.77430800
H	-3.73596600	-1.42867500	1.55645900
H	-5.14684500	-2.03907300	0.70973800

Et₃SiH

Si	-0.00003200	0.00021400	-1.02458700
C	-0.20034000	-1.79116300	-0.44411100
C	1.65161100	0.72186200	-0.44383500
C	0.29302100	-2.06352900	0.98370800
C	1.64078100	1.28553200	0.98388100
H	0.00006800	0.00039800	-2.51770700
H	-1.25691200	-2.07216500	-0.53895200
H	0.34471800	-2.43439500	-1.14510300
H	2.42275800	-0.05319500	-0.53836700

H	1.93681700	1.51515600	-1.14494300
H	0.15351600	-3.11192800	1.26426000
H	1.35982200	-1.83742000	1.08006200
H	-0.23804000	-1.45280700	1.72043700
H	2.61877700	1.68790100	1.26482800
H	0.91242500	2.09717700	1.07970700
H	1.37616000	0.52066800	1.72060000
C	-1.93390700	0.77766700	0.98378500
H	-2.77220200	1.42249100	1.26442300
H	-2.27136300	-0.25934400	1.07952900
H	-1.13957500	0.93191200	1.72069000
C	-1.45115300	1.06935200	-0.44377900
H	-2.28062300	0.91939700	-1.14500000
H	-1.16597400	2.12483800	-0.53814200
M5			
C	1.90785100	4.34482300	2.19784200
C	2.26141400	2.99816800	2.25910000
C	1.46426200	4.88323400	0.99091900
C	2.15514500	2.19300000	1.12693000
C	1.35851900	4.07361100	-0.13782500
C	1.68833200	2.71542900	-0.08276000
C	-2.97189000	-2.29898300	-0.42484300
C	-3.64316800	-3.47286900	-0.70937200
C	1.56596300	1.85515600	-1.32364600
C	-1.37151600	-0.84719000	0.90192700
C	-2.02057000	-2.17629900	0.58204000
C	2.44035200	-1.43362200	1.69189300
C	3.29443500	-1.88256700	2.69377900
C	-3.36049400	-4.59158400	0.06832500
C	0.13438800	-0.78349800	0.95153200
C	0.24496500	-0.03527900	-0.16251100
C	1.06501200	-1.30587900	1.94701500
C	1.28294700	0.39012000	-1.06765500
C	2.79914300	-2.21542000	3.95263900
C	-1.72878500	-3.32156400	1.32548000
C	0.57734000	-1.63649300	3.22226400
C	-2.39964300	-4.51523100	1.07357800
C	1.43654900	-2.08866400	4.21607200
C	2.09387200	-0.57338800	-1.61833300
C	1.86389700	-2.05907600	-1.52625100
H	1.98207300	4.97086600	3.08104000
H	2.61756600	2.56926400	3.19073600
H	1.19528500	5.93302200	0.92870800
H	2.43366800	1.14492300	1.18398500

H	-4.35807000	-3.49572900	-1.52333000
H	1.00888500	4.49741500	-1.07630400
H	2.50589400	1.89400500	-1.88111400
H	2.85447900	-1.18453900	0.72134600
H	4.35376300	-1.97798000	2.48076800
H	-1.89735300	-0.36719800	1.73358100
H	-3.87681100	-5.52446400	-0.12638900
H	-0.48158300	-1.52518900	3.44427500
H	1.04216100	-2.33802200	5.19511400
H	-0.97599200	-3.28481000	2.10362500
H	-2.16202100	-5.39212400	1.66464500
H	0.95833000	-2.31853100	-0.98408400
H	2.72803000	-2.53609200	-1.05911400
H	1.79899400	-2.44547700	-2.54608900
N	-1.28394200	0.15873700	-0.29303400
O	-1.02767100	-1.43799700	-2.33449500
O	-3.25343400	-1.16762900	-1.21759000
O	-2.40967900	0.66338200	-2.57478200
O	3.12760000	-0.18816200	-2.34402300
S	-1.94480700	-0.46424300	-1.81666000
H	3.47141600	-2.57200300	4.72565800
B	4.40404800	-0.97026500	-2.31746200
F	5.37669800	-0.14348200	-2.85042700
F	4.69036200	-1.28810700	-0.97882800
F	4.27905500	-2.13717600	-3.06675100
H	0.81450400	2.29623800	-1.98940800
Si	-2.16024500	1.86053800	0.22529700
C	-5.00496600	1.36632200	-0.49926100
H	-5.26540100	2.40306000	-0.71586600
H	-4.69678100	0.89615800	-1.43467200
H	-5.91117500	0.86222400	-0.15450000
C	-3.91869700	1.28217900	0.58434100
H	-4.22299300	1.89132800	1.44647700
H	-3.87296600	0.25713800	0.97404000
C	-1.24706200	1.65306600	3.08043800
H	-2.20196800	1.18626400	3.34542800
H	-0.48204800	0.87506100	3.01118800
H	-0.96124900	2.30286500	3.91131800
C	-1.32408900	2.46277500	1.78510600
H	-1.92909900	3.36823900	1.96177800
H	-0.33236900	2.83660100	1.51806200
C	-3.08288800	3.68937700	-1.84997900
H	-3.80493400	4.13293100	-1.15885300
H	-2.77663100	4.47058800	-2.55012500

H	-3.58779700	2.90644200	-2.41853000
C	-1.85546800	3.14020800	-1.11213500
H	-1.14885300	2.73496200	-1.84096300
H	-1.33172500	3.95605900	-0.60022000
TS7			
C	1.44408600	4.74186500	1.93595300
C	1.79191200	3.44570200	2.31259800
C	1.29147600	5.04578900	0.58455700
C	1.96981700	2.45843200	1.34603500
C	1.46569300	4.05373200	-0.37808300
C	1.79294900	2.74462600	-0.01115500
C	-2.77507900	-2.42466700	-0.35732100
C	-3.37654700	-3.66316600	-0.48625500
C	1.98562400	1.69049200	-1.07936800
C	-1.45814400	-0.64206100	0.88104000
C	-2.02542000	-2.04426600	0.75214900
C	2.06201300	-1.04903700	2.54477800
C	2.69712600	-1.29225500	3.75754600
C	-3.23770400	-4.57376600	0.55599400
C	-0.00246800	-0.51061000	1.24504500
C	0.47735000	-0.00115200	0.10655600
C	0.67922400	-0.82166800	2.50523200
C	1.59958400	0.27834900	-0.67856400
C	1.96371700	-1.32021100	4.94208200
C	-1.87593400	-2.98688300	1.77164600
C	-0.05064500	-0.85100100	3.70276800
C	-2.48136900	-4.23681100	1.67560100
C	0.58816200	-1.09960100	4.91224600
C	2.37792100	-0.79576500	-1.12711800
C	2.13057700	-2.23503500	-0.78160400
H	1.29823200	5.50962900	2.68876900
H	1.92311100	3.19888700	3.36166800
H	1.02972600	6.05374000	0.27851700
H	2.24450800	1.45280900	1.65121900
H	-3.93090700	-3.89308500	-1.38850900
H	1.34010300	4.29409100	-1.43103300
H	3.04187000	1.65772500	-1.36305300
H	2.63692500	-1.03205400	1.62502000
H	3.76731500	-1.46722900	3.77469500
H	-2.13597900	-0.04745200	1.50352000
H	-3.70570500	-5.54877300	0.48319000
H	-1.12319200	-0.67309400	3.69163600
H	0.01117700	-1.11825800	5.83033800
H	-1.28640400	-2.74756500	2.64818000

H	-2.35506400	-4.95112100	2.48106400
H	1.25146600	-2.37585500	-0.15875100
H	3.02199200	-2.62141700	-0.28127900
H	2.01672800	-2.79463300	-1.71152500
N	-1.22668000	0.10918000	-0.44401800
O	-0.51275100	-1.81184000	-1.99759300
O	-2.92503500	-1.51285800	-1.41695800
O	-1.87978200	0.09192600	-2.91963800
O	3.40070400	-0.51397100	-1.86971200
S	-1.54088900	-0.81638600	-1.85739500
H	2.46200000	-1.51593700	5.88544500
B	4.43702200	-1.51631400	-2.35640000
F	5.33835800	-0.76760400	-3.08344600
F	5.03687400	-2.10320600	-1.24874600
F	3.80566400	-2.46547800	-3.14774200
H	1.45214900	1.99881000	-1.98696800
Si	-2.11601400	1.81909000	-0.44474900
C	-4.77416800	1.15114000	-1.60932600
H	-4.91041100	2.09369800	-2.14173300
H	-4.31331500	0.44226000	-2.29936400
H	-5.76573500	0.77074000	-1.35070100
C	-3.93975300	1.35041300	-0.33517800
H	-4.39160800	2.14656400	0.27194900
H	-4.00978800	0.44967400	0.29057900
C	-1.85999600	2.22856600	2.51973700
H	-2.86061900	1.79939300	2.64251100
H	-1.11911600	1.47495200	2.79971500
H	-1.76433200	3.04463300	3.24058500
C	-1.60301100	2.74163900	1.10166800
H	-2.17116200	3.67395500	0.94707800
H	-0.55481500	3.03227300	0.99636600
C	-2.50020100	3.18699900	-2.99092300
H	-3.33294100	3.76073800	-2.57366100
H	-2.02599300	3.80645700	-3.75649600
H	-2.90727900	2.29948600	-3.47865900
C	-1.48151400	2.80777800	-1.90943400
H	-0.65132700	2.25844700	-2.36479300
H	-1.04636700	3.71485600	-1.47337900
M6			
C	0.39532700	-5.07508100	-0.19186500
C	-0.15399000	-4.39339500	0.89407300
C	0.06107000	-4.68802300	-1.48636900
C	-1.03409400	-3.33591300	0.68352900
C	-0.80682200	-3.61628500	-1.69383500

C	-1.36450100	-2.92903400	-0.61467100
C	1.82731900	3.05996600	0.58211600
C	2.14990500	4.27383700	1.17636700
C	-2.34939600	-1.80907600	-0.85368100
C	1.41514900	0.52392100	0.66545700
C	1.72750800	1.87306100	1.31287600
C	-0.75308800	-0.34296500	3.58293200
C	-0.71618800	-0.89697300	4.85977700
C	2.39219600	4.32010900	2.54176500
C	0.16261800	-0.13942400	1.25268800
C	-0.93674400	-0.29695300	0.56923200
C	0.20780600	-0.70259300	2.63500000
C	-2.06807100	-0.53897600	-0.06901300
C	0.27790000	-1.81265500	5.19591500
C	1.98737900	1.94846100	2.68675400
C	1.20071300	-1.62996200	2.97227200
C	2.31233800	3.15235800	3.29849600
C	1.23412000	-2.17994400	4.24984500
C	-3.10974900	0.48773600	-0.03913500
C	-3.00538400	1.72461200	0.78362500
H	1.07791000	-5.90267200	-0.02792900
H	0.09805100	-4.68664000	1.90858900
H	0.48096400	-5.21290000	-2.33891700
H	-1.46663200	-2.82080200	1.53826100
H	2.20579600	5.15776300	0.55134400
H	-1.06268200	-3.31597400	-2.70644500
H	-3.36039600	-2.13612200	-0.58395000
H	-1.52103800	0.37763700	3.31848300
H	-1.46241300	-0.60862100	5.59240800
H	2.24958500	-0.13888400	0.91554000
H	2.64541500	5.26416100	3.01120500
H	1.93751000	-1.93459700	2.23332800
H	2.00435500	-2.90041200	4.50407700
H	1.94954500	1.04282800	3.28244500
H	2.50975000	3.17601400	4.36417600
H	-2.01987700	1.83302300	1.22725700
H	-3.78379800	1.67643700	1.55036200
H	-3.22976900	2.58125500	0.14538200
N	1.37890500	0.59914100	-0.80297400
O	-0.62073500	2.18134400	-0.88054700
O	1.65824600	3.10285900	-0.80356600
O	0.93146900	1.96692800	-2.84312100
O	-4.12510600	0.24922600	-0.73696600
S	0.70257200	1.93791200	-1.41909100

H	0.30752000	-2.24155000	6.19186500
B	-5.39755800	1.19750500	-0.83292200
F	-6.24694100	0.50709500	-1.64706700
F	-5.86047300	1.33510800	0.45378900
F	-4.95324500	2.37818200	-1.37555100
H	-2.39142100	-1.56058300	-1.91959800
Si	2.21135200	-0.64626900	-1.85484800
C	4.02280100	1.38381000	-2.93300400
H	3.45711800	1.45123700	-3.86465900
H	3.62730500	2.14787900	-2.25808100
H	5.06467300	1.63676200	-3.14907200
C	3.92156800	-0.01140600	-2.30373500
H	4.37170800	-0.76333500	-2.96717900
H	4.51912400	-0.03903800	-1.38306300
C	3.64902100	-2.29560600	0.09735800
H	4.52768200	-2.37680000	-0.54853700
H	3.82989800	-1.44583800	0.76576400
H	3.61219500	-3.19639200	0.71824400
C	2.36710900	-2.15510400	-0.73483200
H	2.29514000	-3.01911600	-1.40608500
H	1.46848600	-2.23247200	-0.10544700
C	1.53262800	-0.49949900	-4.68394500
H	2.56943700	-0.76502200	-4.91492900
H	0.90525900	-0.90138800	-5.48450400
H	1.45008600	0.58823200	-4.70379500
C	1.10441000	-1.05839700	-3.32134500
H	0.07795600	-0.74961400	-3.08581500
H	1.08070600	-2.15474600	-3.36677000
TS8			
C	-1.74750800	4.94500500	-0.36667100
C	-1.10813000	4.40274400	0.74822300
C	-1.29905400	4.61529200	-1.64239400
C	-0.02836900	3.53973600	0.58543600
C	-0.22760600	3.73686400	-1.80140900
C	0.42025000	3.18757300	-0.69350500
C	-1.45751000	-3.33687100	0.63649800
C	-1.53374300	-4.57587200	1.26132400
C	1.61251300	2.27986500	-0.88205100
C	-1.58629300	-0.76690100	0.65153900
C	-1.62165500	-2.13617300	1.33263600
C	-1.79086300	-4.63741600	2.62336500
C	-0.52699500	0.17171200	1.24067500
C	0.52700800	0.55177700	0.56650600
C	1.59120100	1.00769900	-0.05566600

C	-1.88842700	-2.23020300	2.70406400
C	-1.97013200	-3.45934600	3.34615200
H	-2.58745600	5.62046300	-0.23976100
H	-1.44759000	4.65306800	1.74876200
H	-1.78680000	5.03345400	-2.51766800
H	0.46730300	3.13019900	1.46233000
H	-1.39069400	-5.46752200	0.66156100
H	0.11673500	3.47980500	-2.79976200
H	2.53589700	2.81120000	-0.62203800
H	-2.55675300	-0.30214500	0.85382400
H	-1.85289300	-5.60127500	3.11627500
H	-2.05035100	-1.32167800	3.27385200
H	-2.18034100	-3.49587800	4.40911000
N	-1.48934200	-0.87540400	-0.81364800
O	0.79753800	-2.01754800	-0.79448400
O	-1.25058500	-3.37911700	-0.74385700
O	-0.70688700	-2.17001000	-2.79870700
S	-0.53113000	-2.05747300	-1.37022000
H	1.71892200	2.00964600	-1.93855500
Si	-2.50774100	0.15844400	-1.92387500
C	-3.84000800	-2.21067700	-3.01109300
H	-3.24016700	-2.18093900	-3.92309800
H	-3.32218600	-2.86597500	-2.30519300
H	-4.80198700	-2.67231500	-3.25169900
C	-4.04051100	-0.81173400	-2.41567600
H	-4.60582900	-0.17646600	-3.11229500
H	-4.66559400	-0.88610200	-1.51607600
C	-4.33612700	1.52468800	-0.08479100
H	-5.18180400	1.41423800	-0.76942800
H	-4.37411100	0.66968000	0.60021800
H	-4.50982100	2.42680000	0.51055400
C	-3.01290300	1.62789500	-0.85544300
H	-3.07998900	2.47660600	-1.54651900
H	-2.18063100	1.89306300	-0.18801900
C	-1.70888400	0.09359700	-4.72472600
H	-2.76779200	0.14698700	-4.99823700
H	-1.14083400	0.59257200	-5.51503000
H	-1.41657500	-0.95743300	-4.71035400
C	-1.45057400	0.75384800	-3.36475800
H	-0.39271400	0.65986200	-3.08763800
H	-1.64259400	1.83176700	-3.43911500
C	-0.73748600	0.74588800	2.60216900
C	0.26320400	0.65953100	3.57364200
C	-1.92930500	1.41720000	2.90153200

C	0.07295000	1.22848700	4.83011100
H	1.18631300	0.13779100	3.33895000
C	-2.11697000	1.98329100	4.15889500
H	-2.70555400	1.51291800	2.14641500
C	-1.11782000	1.88780500	5.12645200
H	0.85408800	1.15148800	5.57916500
H	-3.04219600	2.50503500	4.38041400
H	-1.26707200	2.32790300	6.10673600
B	5.87756100	-0.25182700	-0.54045700
F	6.32698700	0.66676100	-1.38639900
F	5.91582000	-0.02046000	0.77023100
F	5.48532200	-1.43702700	-0.98959900
O	8.16197900	-1.02139700	-0.33844200
H	8.60579500	-0.41231500	-0.94040000
H	8.36723600	-0.68367100	0.54140900
C	2.87033700	0.24280300	0.01226100
C	3.01065900	-0.92550400	0.94926100
H	2.04687500	-1.31239600	1.27375800
H	3.58881300	-0.58870200	1.81543900
H	3.58220700	-1.70827900	0.44958300
O	3.80589700	0.62279800	-0.68142400
M7			
C	4.57917300	-1.20950000	-1.52409400
C	4.27130200	0.07016100	-1.06211200
C	4.23311500	-2.31743400	-0.75590500
C	3.62435600	0.23726700	0.15887900
C	3.57021400	-2.14620800	0.45908500
C	3.25641800	-0.87071400	0.93227200
C	-3.36833100	0.86710900	-0.05051600
C	-4.54235200	1.61078700	-0.05859800
C	2.58472000	-0.70079900	2.27412200
C	-0.87619900	0.53806100	-0.60320000
C	-2.16638400	1.35940800	-0.56643600
C	-4.53739100	2.88619600	-0.60482300
C	0.29172200	1.21057100	0.12764400
C	0.81679800	0.72086000	1.22154800
C	1.41787500	0.26800300	2.29712200
C	-2.19496500	2.64538300	-1.12023700
C	-3.35878200	3.40355300	-1.13926600
C	0.93068800	0.67317100	3.65747700
C	-0.02723000	1.83180600	3.77394800
H	5.08623100	-1.33983700	-2.47478900
H	4.53689300	0.94271400	-1.65131200
H	4.46969300	-3.31841200	-1.10375200

H	3.39647100	1.23995700	0.51193400
H	-5.43771600	1.16900400	0.36381500
H	3.29890100	-3.01490500	1.05337600
H	3.30905700	-0.34313000	3.01605000
H	-0.58495900	0.47998700	-1.65721300
H	-5.45052400	3.47092700	-0.61524900
H	-1.28953500	3.05111400	-1.55830400
H	-3.34550300	4.39503300	-1.57773000
H	0.54756300	2.76108400	3.69603400
H	-0.51063600	1.80043400	4.75014000
H	-0.77075100	1.81642300	2.97664100
N	-1.09042900	-0.85265700	-0.16825200
O	-1.77024000	-0.23116200	2.21723500
O	-3.48775900	-0.42420300	0.46792100
O	-2.37713400	-2.46129500	1.24024600
O	1.35872500	0.08943900	4.63568500
S	-2.11084000	-1.05217400	1.07342300
H	2.24014800	-1.67076100	2.64965300
Si	-0.38259000	-2.26629100	-1.08394400
C	-3.05644400	-3.27648300	-1.72265200
H	-2.99573200	-4.05239800	-0.95655700
H	-3.52935700	-2.40410800	-1.26307900
H	-3.71721600	-3.63486600	-2.51727000
C	-1.67402800	-2.92028500	-2.28284100
H	-1.22728200	-3.79185500	-2.78200000
H	-1.78446600	-2.16000200	-3.06721800
C	0.76373200	-1.00931400	-3.47254800
H	0.42485400	-1.82219500	-4.12098300
H	-0.01266700	-0.23627500	-3.50689500
H	1.66657500	-0.58378000	-3.92235900
C	1.05120700	-1.51939300	-2.05395300
H	1.80083200	-2.31708400	-2.11845000
H	1.53597500	-0.74665200	-1.44046500
C	-0.53828200	-4.82420600	0.30180600
H	-0.71628500	-5.30512400	-0.66567100
H	-0.01078000	-5.54461000	0.93349300
H	-1.50709600	-4.61911900	0.75963300
C	0.27762500	-3.53563400	0.14126200
H	0.41767700	-3.04545400	1.11319700
H	1.28616000	-3.78333400	-0.21353800
C	0.91666100	2.42280200	-0.47892700
C	1.05459100	3.59964600	0.26133600
C	1.40311700	2.37663200	-1.79118000
C	1.66369000	4.71759800	-0.30276500

H	0.66991200	3.63327900	1.27612200
C	2.00989600	3.49594900	-2.35315200
H	1.32349800	1.45867900	-2.36848300
C	2.13917900	4.66926800	-1.61119000
H	1.76140300	5.62824200	0.27902500
H	2.38790000	3.44919300	-3.36921700
H	2.61059400	5.54147300	-2.05171700

H₂O

O	0.00000000	0.00000000	0.11882300
H	0.00000000	0.75786500	-0.47529200
H	0.00000000	-0.75786500	-0.47529200

BF₃·H₂O

B	0.20602600	0.00781000	-0.02762800
F	0.35001700	-1.01518400	-0.91741900
F	0.86850300	-0.16964000	1.14310300
F	0.31078400	1.25746700	-0.56265300
O	-1.38774400	-0.06138200	0.38390900
H	-1.81076500	-0.88490600	0.09418200
H	-1.88115500	0.68313700	0.00541000

M8

C	4.86681700	-0.54517600	-1.60628400
C	4.30110300	0.64447000	-1.14849400
C	4.77394300	-1.69387800	-0.82501000
C	3.63748000	0.67973100	0.07486600
C	4.09435700	-1.65808700	0.39222400
C	3.50502600	-0.47757100	0.85166600
C	-3.42447800	0.86138200	0.19226100
C	-4.56673700	1.62172800	0.38654500
C	2.79527600	-0.44778700	2.18586500
C	-1.01468300	0.51254300	-0.66309700
C	-2.28664500	1.33783100	-0.45899800
C	0.88923500	3.49862000	0.29860200
C	1.44109900	4.66026600	-0.23333400
C	-4.59261200	2.92172300	-0.09892300
C	0.17783700	1.10087000	0.08405600
C	0.77816000	0.63220900	1.15092100
C	0.72976400	2.36506200	-0.50186600
C	1.49336200	0.33024800	2.21140500
C	1.83641600	4.69883900	-1.56879100
C	-2.35408400	2.64513000	-0.95911600
C	1.13121100	2.40602700	-1.84199300
C	-3.48696200	3.42816400	-0.77947200
C	1.68160300	3.56998400	-2.37117000
C	1.00193400	0.73263300	3.57972800

C	-0.10987200	1.74358600	3.70505200
H	5.38515300	-0.57272200	-2.55915700
H	4.37678600	1.55083900	-1.74147300
H	5.22464400	-2.62168000	-1.16267700
H	3.21388000	1.61740200	0.42498900
H	-5.40988600	1.17939700	0.90410900
H	4.03147100	-2.55808100	0.99924700
H	3.43937500	0.01067300	2.94514500
H	0.57287700	3.46410600	1.33649900
H	1.55697500	5.53683600	0.39501600
H	-0.77236800	0.54527000	-1.73089500
H	-5.47745000	3.53074500	0.04527200
H	1.03193500	1.52774000	-2.47523000
H	1.99569000	3.59093800	-3.40927800
H	-1.50830700	3.04659400	-1.50551700
H	-3.50663100	4.43540700	-1.17892700
H	-0.80280100	1.71127400	2.86441100
H	0.34535800	2.73916300	3.74482500
H	-0.64019600	1.57488500	4.64227800
N	-1.31038700	-0.95160600	-0.42760400
O	-1.54757900	-0.53823600	2.12252100
O	-3.53547800	-0.48344100	0.62000600
O	-2.49919800	-2.63181200	1.08824600
O	1.54955800	0.25875100	4.55482200
S	-2.20103600	-1.23071300	1.04999800
H	2.26444100	5.60513400	-1.98338500
H	2.61087800	-1.46698700	2.54427900
Si	0.06365900	-2.30152800	-0.84423100
C	-2.15784800	-4.18627200	-1.46339500
H	-2.00890700	-4.74225600	-0.53659800
H	-2.95853500	-3.46573200	-1.27387800
H	-2.51192400	-4.88506700	-2.22501400
C	-0.86598300	-3.50722500	-1.93607900
H	-0.11047600	-4.27395800	-2.16362600
H	-1.03493600	-2.99587600	-2.89215100
C	0.93616200	-1.10507100	-3.33323800
H	0.84863700	-2.03231600	-3.90465500
H	-0.02237400	-0.58132700	-3.43094400
H	1.70143900	-0.49236700	-3.81773200
C	1.32518100	-1.38772700	-1.87440100
H	2.20997700	-2.03933700	-1.85547900
H	1.65625700	-0.48053700	-1.35814900
C	0.24786900	-4.36864900	1.16783500
H	0.44382900	-5.07599000	0.35678400

H	0.79438700	-4.71563600	2.04765400
H	-0.81797700	-4.40166200	1.39967900
C	0.69133100	-2.94550900	0.79759700
H	0.44781600	-2.24279600	1.60344900
H	1.78298000	-2.90857500	0.70055900
O	-2.83773200	-1.05136800	-2.56026300
H	-3.18958200	-1.85022600	-2.97484200
H	-2.02816600	-1.15230000	-1.20483500
H	-3.52435200	-0.37666000	-2.64968800
H₃O⁺			
O	0.00000000	0.00000000	0.00000000
H	0.00000000	0.97171400	0.00000000
H	0.84152900	-0.48585700	0.00000000
H	-0.84152900	-0.48585700	0.00000000
TS9			
C	1.03468700	-4.34806800	-1.49585300
C	2.10768500	-3.48232700	-1.28011000
C	0.11792500	-4.57309000	-0.47356000
C	2.25996600	-2.85114600	-0.04943900
C	0.26865300	-3.93006200	0.75597300
C	1.33783200	-3.06181900	0.98448000
C	-0.97921100	3.18877200	0.06139900
C	-1.05686000	4.57009100	0.06080400
C	1.51549300	-2.40150700	2.33132500
C	0.12699000	0.94023600	-0.49072000
C	0.07001800	2.46504900	-0.49178200
C	-0.03279800	5.28451200	-0.54812100
C	1.46119600	0.40167000	0.02512800
C	1.56230800	-0.18323200	1.19377700
C	1.67450300	-0.89093400	2.29364400
C	1.08137400	3.21099900	-1.10724600
C	1.02953000	4.60055200	-1.13485600
C	1.97205900	-0.22337900	3.61329700
C	2.33145200	1.23891200	3.61686500
H	0.91777000	-4.84440600	-2.45381200
H	2.83118900	-3.29978400	-2.06867800
H	-0.71674800	-5.25026500	-0.62781100
H	3.10693000	-2.18818100	0.11114700
H	-1.90894000	5.05326500	0.52440000
H	-0.44683400	-4.11728800	1.55264100
H	2.40703900	-2.79429200	2.83509300
H	0.00739500	0.61693900	-1.52724200
H	-0.06827500	6.36755500	-0.56621100
H	1.91221600	2.70270900	-1.58107000

H	1.82708500	5.15047500	-1.62100200
H	1.67739800	1.80918300	2.95471000
H	3.35959800	1.34813800	3.25647500
H	2.27125700	1.62027100	4.63547700
N	-1.01644600	0.27402600	0.24547000
O	-0.75857300	1.53825100	2.49016300
O	-2.09091800	2.50026600	0.60187800
O	-3.00116700	0.60304400	1.79824700
O	1.93659300	-0.89424800	4.62396200
S	-1.74090500	1.21892400	1.48959400
H	0.67649000	-2.64086300	2.99301600
Si	-2.48631100	-0.96657400	-0.96191600
C	-5.23524500	-0.00241200	-0.98925300
H	-5.26091500	-0.16320800	0.09084700
H	-5.00015300	1.05185000	-1.15865400
H	-6.24164700	-0.17297900	-1.37798700
C	-4.22309200	-0.92659000	-1.68436200
H	-4.56629900	-1.96720900	-1.61279800
H	-4.17818500	-0.69922400	-2.75529400
C	-0.99553800	-0.95837300	-3.49144700
H	-1.94091100	-0.94987200	-4.04276600
H	-0.64001900	0.07534400	-3.43150500
H	-0.27553800	-1.51568900	-4.09618300
C	-1.16043900	-1.61328900	-2.11512500
H	-1.45850700	-2.66207100	-2.25489300
H	-0.20011500	-1.68358000	-1.58210800
C	-3.96237500	-2.28612500	1.25125600
H	-4.77372300	-2.50495300	0.55247400
H	-3.91220100	-3.11783600	1.95897700
H	-4.22396300	-1.38723700	1.81008800
C	-2.61666800	-2.13530200	0.53242700
H	-1.82361500	-1.99910700	1.27528900
H	-2.37223600	-3.09467700	0.04879500
O	-2.37456100	1.08151300	-1.77489400
H	-2.70160900	1.12927200	-2.68655300
H	-2.83023200	1.78571700	-1.28572400
C	2.65379400	0.47256500	-0.86621800
C	3.86945800	0.96542500	-0.38421900
C	2.57503900	-0.00583500	-2.17932100
C	4.99180600	0.98483100	-1.20705800
H	3.92331200	1.34415400	0.63168500
C	3.69933500	0.01608800	-2.99886600
H	1.64422800	-0.42073600	-2.55800900
C	4.90828900	0.51354700	-2.51543700

H	5.93021000	1.37385800	-0.82664700
H	3.63156500	-0.36229100	-4.01328300
H	5.78276400	0.53205800	-3.15691400
H	-0.60182200	-0.52312300	0.74993900
P2			
C	-1.92935800	-3.50409600	-1.74625000
C	-0.67517200	-3.72770700	-1.17519400
C	-2.91601300	-2.85195200	-1.00885400
C	-0.41147100	-3.29442800	0.12201100
C	-2.64502800	-2.41509200	0.28838600
C	-1.39042700	-2.62532900	0.86514300
C	-0.76912800	2.80907800	-0.98273100
C	-0.76096700	4.17023700	-0.70850000
C	-1.06097800	-2.04214900	2.21543000
C	0.37304300	0.52508900	-1.19032900
C	0.37226000	2.01752100	-0.88556500
C	0.43258400	4.77374800	-0.33452500
C	1.11601500	-0.25174000	-0.09575600
C	0.49218100	-0.50281500	1.02799300
C	-0.22190700	-0.77882400	2.09083600
C	1.55845600	2.64591600	-0.49416200
C	1.59372700	4.00867500	-0.22602200
C	-0.29512200	0.21431900	3.21306400
C	0.27915400	1.58833500	2.97031300
H	-2.13471600	-3.83607700	-2.75848700
H	0.09810700	-4.23663700	-1.74174200
H	-3.89051300	-2.66353600	-1.44630300
H	0.57140800	-3.45708900	0.55753000
H	-1.68759500	4.72643100	-0.79211000
H	-3.40781600	-1.88245100	0.84966300
H	-0.52039300	-2.76497100	2.83720100
H	0.92093900	0.38524100	-2.12780400
H	0.45346000	5.83639000	-0.12018400
H	2.46361800	2.05267600	-0.39978000
H	2.52685900	4.47322500	0.07216600
H	-0.31664000	2.08093300	2.19358500
H	1.30579800	1.52728000	2.59951700
H	0.24278800	2.16647200	3.89271800
N	-0.98736700	0.01817800	-1.45078500
O	-2.29630900	0.88002800	0.63632200
O	-1.98879900	2.26024900	-1.39433400
O	-3.47375200	0.31138000	-1.49496200
O	-0.85568400	-0.08813900	4.24813100
S	-2.29513700	0.78125900	-0.81015800

H	-1.97148200	-1.77695300	2.75923900
C	2.52475600	-0.67144500	-0.32085400
C	3.45976600	-0.58397500	0.71773000
C	2.92888500	-1.18858400	-1.55749400
C	4.77068100	-1.00585900	0.52451400
H	3.14933500	-0.17717700	1.67594900
C	4.24177500	-1.61005600	-1.74785900
H	2.21367500	-1.28966400	-2.36856100
C	5.16614600	-1.51796300	-0.70995100
H	5.48574100	-0.92837900	1.33686400
H	4.54023900	-2.01594400	-2.70874400
H	6.18983400	-1.84315200	-0.86226400
H	-1.08569000	-0.99758600	-1.39990800
Et₃Si-OH₂⁺			
Si	0.17723900	-0.18615500	-0.18494500
C	-1.39705800	2.22208300	-0.09433300
H	-2.12388000	1.83238500	-0.81153000
H	-1.74859600	1.97173700	0.91096700
H	-1.39526800	3.31047000	-0.18272800
C	0.00439500	1.65591600	-0.36443400
H	0.31812600	1.89228600	-1.38942700
H	0.74999200	2.13768200	0.28056700
C	-2.52965800	-1.19345100	0.01791000
H	-2.39092600	-1.54554100	1.04306800
H	-2.92764300	-0.17778500	0.06802600
H	-3.28935600	-1.82552400	-0.44652900
C	-1.22148200	-1.25732400	-0.78634700
H	-0.85959700	-2.29005300	-0.84475600
H	-1.40307800	-0.94929300	-1.82442400
C	3.01992100	0.04733500	-0.01032400
H	2.95409100	0.20696700	1.07000700
H	3.99169000	-0.40638100	-0.21553700
H	3.00131800	1.02688700	-0.49480900
C	1.88152100	-0.84842400	-0.51815700
H	1.95851600	-0.98742100	-1.60397100
H	1.95132000	-1.85366600	-0.08539800
O	-0.01666400	-0.33188800	1.66034500
H	0.00688500	-1.19618600	2.10538800
H	0.31253900	0.35789100	2.26166900
TS9'			
C	2.33099900	4.17414500	-1.45935300
C	0.99942100	4.12923500	-1.04933100
C	3.31505000	3.61094300	-0.65100100
C	0.65528800	3.51793200	0.15336100

C	2.96347800	2.98675500	0.54469500
C	1.63041900	2.91940600	0.95889100
C	-2.22704200	-2.86584900	-0.13992100
C	-3.36858700	-3.66194600	-0.17233800
C	1.27741300	2.26621300	2.27555500
C	-0.94132900	-0.70733700	-0.68055100
C	-2.19503800	-1.58680900	-0.70275300
C	-4.51560700	-3.19120100	-0.79353000
C	-1.17954300	0.59593500	0.09566200
C	-0.55436700	0.93517300	1.19435000
C	0.02606900	1.40727500	2.27573200
C	-3.36256600	-1.14841800	-1.34215000
C	-4.50966900	-1.93022600	-1.38779300
C	-0.52178400	1.06166000	3.62867700
C	-1.89095600	0.43669500	3.72388400
H	2.59937600	4.65048400	-2.39688300
H	0.22151900	4.57139000	-1.66485300
H	4.35729900	3.64919200	-0.95227000
H	-0.38582700	3.50062700	0.46359600
H	-3.32639600	-4.64246600	0.28858200
H	3.73758600	2.54939100	1.17056200
H	1.12987300	3.03288300	3.04580600
H	-0.76338300	-0.40266600	-1.71788200
H	-5.40604000	-3.80982000	-0.82072600
H	-3.36422400	-0.17789100	-1.82613600
H	-5.39404600	-1.55767600	-1.89256900
H	-2.64026000	1.22241800	3.57917100
H	-2.01957500	0.00835300	4.71769200
H	-2.03295400	-0.32448800	2.95601600
N	0.25470800	-1.44983200	-0.27902000
O	-0.39970800	-1.88607600	2.18909500
O	-1.11266100	-3.46539800	0.43390200
O	1.25527100	-3.32314800	0.97574200
O	0.13161700	1.33327700	4.61955300
S	0.08669500	-2.45693700	0.94171200
H	2.11943000	1.65929100	2.62899400
Si	2.25748300	-1.03173300	-0.89108100
C	4.60594700	-2.79407700	-1.49189700
H	4.36158800	-3.25866500	-0.53145000
H	4.26760200	-3.47645900	-2.28314100
H	5.69643200	-2.77947700	-1.57624200
C	4.00041200	-1.38618600	-1.64312600
H	4.65869000	-0.65723600	-1.15181400
H	4.00372500	-1.10855000	-2.70517200

C	1.33009500	0.23559500	-3.32566900
H	2.13191900	-0.26668900	-3.87563500
H	0.44445500	-0.40288000	-3.41338000
H	1.11465400	1.17510800	-3.84447300
C	1.73114000	0.48762700	-1.86631600
H	2.61796400	1.13569700	-1.84913800
H	0.96212400	1.05328800	-1.32913800
C	3.82745700	-1.52439500	1.58048500
H	4.75790600	-1.54575600	1.00587100
H	4.06838400	-1.13019400	2.57277200
H	3.47819300	-2.55186600	1.70567100
C	2.76140500	-0.65757200	0.90334600
H	1.88620400	-0.55418000	1.55046700
H	3.16293500	0.36140600	0.78623500
O	1.70818500	-2.60664200	-1.91584100
H	2.38736500	-3.26938700	-2.11544500
H	0.88910300	-3.02528500	-1.60660600
C	-2.12753000	1.59223000	-0.49015000
C	-3.22803400	2.04991600	0.23722600
C	-1.89689700	2.09738800	-1.77599900
C	-4.09118700	2.99484500	-0.31256700
H	-3.40786800	1.64927700	1.23017200
C	-2.76092400	3.04085400	-2.32371900
H	-1.03060800	1.76318900	-2.34283000
C	-3.86131200	3.48979000	-1.59399600
H	-4.94638400	3.33989500	0.25924900
H	-2.57145600	3.43027900	-3.31880000
H	-4.53509000	4.22385500	-2.02322600

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