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Supporting Information

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A Frontier Molecular Orbital Theory Approach to Understanding the Mayr Equation and to Quantifying Nucleophilicity and Electrophilicity by Using HOMO and LUMO Energies**

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Table of Contents

1. **Computational methods and abbreviations ----------S2**
2. **Reactions of a-v with A-D ----------S3**
3. **Relationship of *E*/*L* for carbocations----------S6**
4. **Relationship of *E*/*L* for Michael acceptors----------S8**
5. **Relationship of *N*/*H* for arenes----------S14**
6. **Relationship of *N*/*H* for carboanions ----------S15**
7. **Relationship of *N*/*H* for heteroatom-centered nucleophiles----------S17**
8. **Calculated results of N, O, P, SD and SE ----------S19**
9. **References and notes----------S21**
10. **Computed energies of all stationary points----------S22**
11. **Coordinates of all stationary points----------S24**

1. Computational methods and abbreviations

All calculations were performed with the Gaussian 03 program.[1] All gas phase stationary points were optimized using B3LYP[2] functional with the basis set of 6-31G(d) for all atoms. Orbital energies were calculated by B3LYP/6-31G(d), B3LYP/6-31+G(d), HF/6-31G(d), HF/6-31+G(d) and BP86/6-31G(d) methods, respectively. All computed orbital energies were based on the gas phase geometries optimized at the B3LYP/6-31G(d) level. Full Hessian matrixes in Gaussian 03 were calculated to verify the nature of all stationary points as either minima or first-order saddle points. The first-order saddle points were further characterized by intrinsic reaction coordinate (IRC) [3] calculations to confirm that the stationary points are correctly connected to the corresponding reactants and products. Unless specified explicitly, all discussed orbital energies are referred to those computed by the B3LYP/6-31G(d) method. The reported enthalpies and free energies were computed at 298 K in the gas phase.

Even though in the text and the Supporting Information, we use the B3LYP/6-31G(d) orbital energies to discuss all relationships, we found that using orbital energies calculated by other methods usually give the same conclusions too.

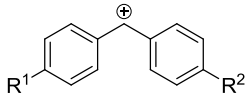
All the *E*, *N*, and *s* values in the Supporting Information are those reported by Mayr and coworkers and these data can be found in their original publications cited in the main text and the Supporting Information. The units for both k_{exp} and k_{cal} are [s^{-1}].

Abbreviations:
i = Mayr's electrophiles, **a**, **b**, **c**….
j = Mayr's nucleophiles, **A**, **B**, **C**…, or **SA, SB, SC**…
N =Mayr's nucleophilicity
s = Mayr's nucleophile-specific parameter
E = Mayr's electrophilicity
LUMO = lowest unoccupied molecular orbital
HOMO = highest occupied molecular orbital
L = LUMO energy
H = HOMO energy
k_{exp} = experimentally measured reaction rate, used in the Mayr equation
k_{cal} = calculated reaction rate (at 298 K) based on DFT results based on $k_{cal} = \frac{k_B T}{h} \exp(-\frac{\Delta G^{\neq}}{RT})$

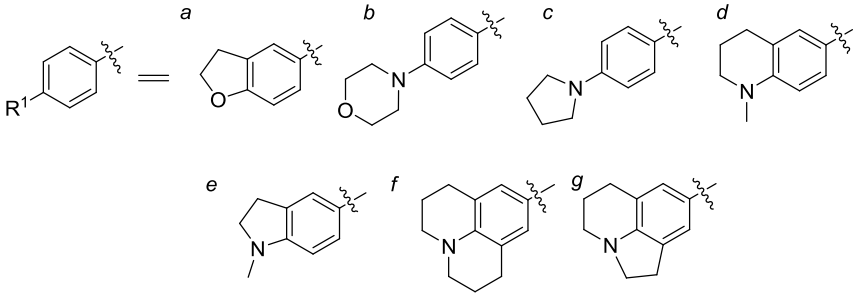
2. Reactions of a-v with A-D

2.1. Structures of a-v.

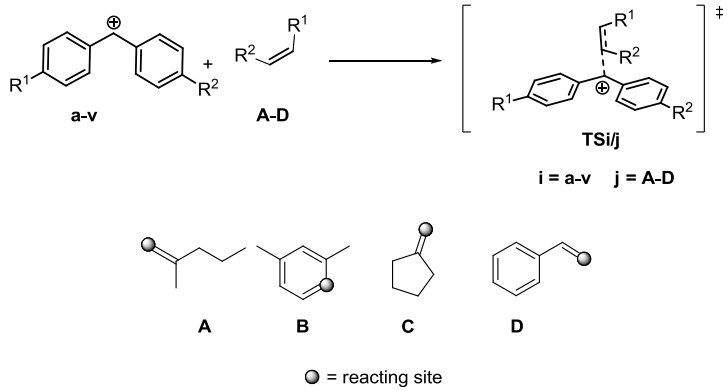
Table S2.1. Structures of **a-v**



i	R^1	R^2	E_i	i	R^1	R^2	E_i
a	OMe	OMe	0.0	**l**	$N(CH_2CF_3)Ph$	$N(CH_2CF_3)Ph$	-3.14
b	H	H	5.90	**m**	$N(CH_2CF_3)Me$	$N(CH_2CF_3)Me$	-3.85
c	F	H	5.60	**n**	NPh_2	NPh_2	-4.72
d	Me	H	4.59	**o**	mor[b]	mor	-5.53
e	Me	Me	3.63	**p**	NPhMe	NPhMe	-5.89
f	OPh	H	2.90	**q**	NMe_2	NMe_2	-7.02
g	OMe	H	2.11	**r**	pyr[c]	pyr	-7.69
h	OMe	Me	1.48	**s**	thq[d]	thq	-8.22
i	OPh	OMe	0.61	**t**	ind[e]	ind	-8.76
j	Cl	Cl	6.02	**u**	jul[f]	jul	-9.45
k	fur[a]	fur	-1.36	**v**	lil[g]	lil	-10.04



2.2. Calculation results of reactions of a-v with A-D



We list all the reactions mentioned in Table 1, where all the reaction energies and orbital energies were calculated at the B3LYP/6-31G(d) level.

2.2.1. Reactions of A toward a-v

Table S2.2. Calculated results of **A** with selected electrophiles.

A (N = 0.95, s = 1.00, H_A = -6.48 eV)

	$\Delta H^{\neq}$ (kcal mol^{-1})	$\Delta G^{\neq}$ (kcal mol^{-1})	$\Delta S^{\neq}$ (cal mol^{-1} K^{-1})	lnk_{cal}	L_i (eV)	E	lnk_{exp}
TSa/A	11.3	23.9	-42.3	-11.58	-6.65	0.00	1.59
TSw/A	4.7	17.0	-41.3	0.29	-7.24	3.63	9.95
TSf/A	6.3	18.5	-40.9	-2.37	-7.01	2.90	8.27
TSg/A	6.1	18.5	-41.4	-2.26	-7.10	2.11	6.45
TSh/A	8.3	20.8	-41.9	-6.23	-6.92	1.48	5.00

$\ln k_{cal} = 1.40 \ln k_{exp} - 13.20$, $R^2 = 0.9718$, N = 5.

$\Delta H_{i/A}^{\neq} = 8.99 L_i + 70.3$, $R^2 = 0.9718$, N = 5.

2.2.2. Reactions of B toward a-v

Table S2.3. Calculated results of **B** with selected electrophiles

B (N = -3.54, s = 1.62, H_B = -6.24 eV)

	$\Delta H^{\neq}$ (kcal mol^{-1})	$\Delta G^{\neq}$ (kcal mol^{-1})	$\Delta S^{\neq}$ (cal mol^{-1} K^{-1})	lnk_{cal}	L (eV)	E	lnk_{exp}
TSb/B	7.2	21.3	-47.2	-6.45	-7.66	5.90	8.80
TSc/B	9.5	23.5	-46.9	-10.21	-7.64	5.39	6.90
TSd/B	9.6	24.3	-49.2	-11.51	-7.44	4.59	3.92
TSe/B	12.3	26.3	-47.2	-14.96	-7.24	3.63	0.34
TSj/B	8.3	22.1	-46.3	-7.90	-7.69	6.02	9.25

$\ln k_{cal} = 0.86 \ln k_{exp} - 15.22$, $R^2 = 0.9673$, N = 5.

$\Delta H_{i/B}^{\neq} = 8.93 L_i + 76.2$, $R^2 = 0.8953$, N = 5.

2.2.3. Reactions of C towards a-v

Table S2.4. Calculated results of **C** with selected electrophiles

C (N = 2.82, s = 0.90, H_C = -5.70 eV)

	$\Delta H^{\neq}$ (kcal mol^{-1})	$\Delta G^{\neq}$ (kcal mol^{-1})	$\Delta S^{\neq}$ (cal mol^{-1} K^{-1})	lnk_{cal}	L (eV)	E	lnk_{exp}
TSb/C	-1.3	11.2	-42.1	10.5	-7.66	5.90	18.07
TSd/C	0.5	13.5	-43.7	6.6	-7.44	4.59	15.36
TSe/C	2.5	14.7	-40.9	4.7	-7.24	3.63	13.37
TSf/C	4.2	17.2	-43.6	0.4	-7.01	2.90	11.86
TSg/C	3.9	16.7	-43.0	1.3	-7.10	2.11	10.22
TSh/C	5.6	18.3	-42.6	-1.5	-6.92	1.48	8.91
TSi/C	8.9	21.7	-43.0	-7.1	-6.65	0.00	5.85
TSj/C	-0.2	12.4	-42.4	8.5	-7.69	6.02	18.32

$\ln k_{cal} = 1.29 \ln k_{exp} - 19.24$, $R^2 = 0.9776$, N = 8.

$\Delta H_{i/C}^{\neq} = 9.09 L_i + 68.2$, $R^2 = 0.9829$, N = 8.

2.2.4. Reactions of D towards a-v

Table S2.5. Calculated results of **D** with selected electrophiles

D (N = 0.25, s = 0.95, H_D = -6.03 eV)

	$\Delta H^{\neq}$ (kcal mol^{-1})	$\Delta G^{\neq}$ (kcal mol^{-1})	$\Delta S^{\neq}$ (cal mol^{-1} K^{-1})	lnk_{cal}	L (eV)	E	lnk_{exp}
TSa/D	9.7	22.4	-42.5	-8.34	-6.65	0.00	0.55
TSe/D	3.3	15.4	-40.5	3.53	-7.24	3.63	8.49
TSf/D	4.5	17.0	-42.1	0.72	-7.01	2.90	6.89
TSg/D	4.3	16.8	-42.0	1.05	-7.10	2.11	5.16
TSh/D	6.2	18.4	-40.9	-1.61	-6.92	1.48	3.78
TSj/D	9.7	22.2	-41.9	-7.98	-6.59	0.61	1.88

$\ln k_{cal} = 1.58 \ln k_{exp} - 9.13$, $R^2 = 0.9524$, N = 6.

$\Delta H_{i/D}^{\neq} = 10.8\, L_i + 81.3$, $R^2 = 0.9852$, N = 6.

2.2.5. Correlation between N and H for **A-D**.

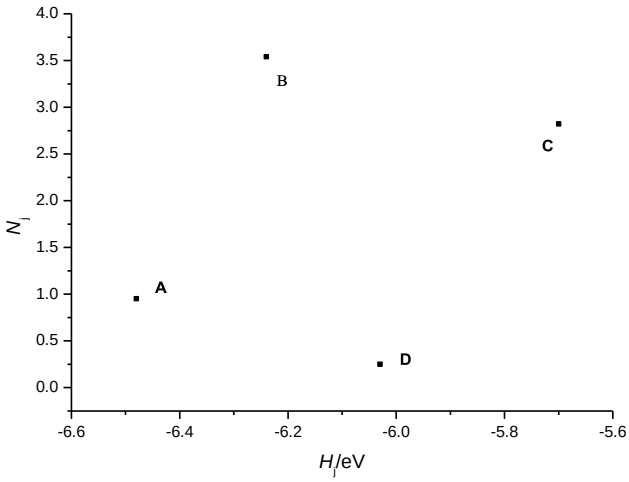


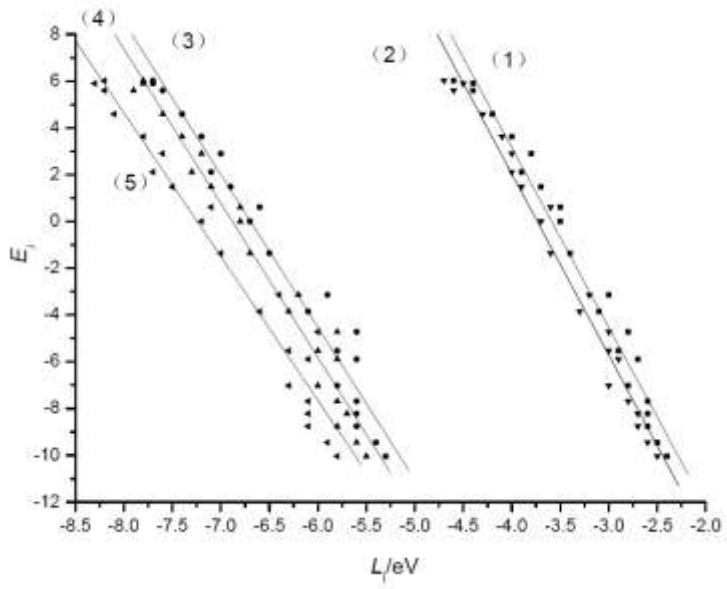
Figure S2.1 Correlation between N and H (B3LYP/6-31G(d))

3. Relationship of *E*/*L* for carbocations

Table S3.1. LUMO energies of **a-v**.

	HF/6-31G(d) (eV)	HF/6-31+G(d) (eV)	B3LYP/6-31G(d) (eV)	B3LYP/6-31+G(d) (eV)	BP86/6-31G(d) (eV)
a	-3.52	-3.67	-6.65	-6.85	-7.48
b	-4.36	-4.53	-7.66	-7.83	-8.05
c	-4.40	-4.58	-7.65	-7.85	-7.83
d	-4.17	-4.33	-7.44	-7.60	-7.68
e	-4.00	-4.14	-7.24	-7.39	-7.18
f	-3.82	-3.98	-7.01	-7.20	-6.31
g	-3.87	-4.03	-7.10	-7.28	-8.22
h	-3.74	-3.88	-6.92	-7.10	-8.24
i	-3.48	-3.64	-6.59	-6.79	-7.58
j	-4.62	-4.75	-7.69	-7.84	-8.30
k	-3.44	-3.58	-6.52	-6.71	-7.11
l	-2.99	-3.18	-5.93	-6.18	-7.03
m	-3.14	-3.31	-6.11	-6.35	-6.38
n	-2.78	-2.96	-5.61	-5.83	-6.57
o	-2.87	-3.03	-5.83	-6.04	-6.03
p	-2.68	-2.85	-5.65	-5.85	-6.28
q	-2.79	-2.95	-5.82	-6.00	-6.12
r	-2.60	-2.75	-5.61	-5.79	-6.10
s	-2.58	-2.73	-5.57	-5.75	-6.05
t	-2.57	-2.72	-5.57	-5.75	-6.05
u	-2.47	-2.60	-5.40	-5.57	-5.86
v	-2.38	-2.51	-5.35	-5.51	-5.81

Below we show that the linear relationship holds for all calculations methods that were used to compute orbital energies. All of them perform linear relationships well (Figure S3.1).



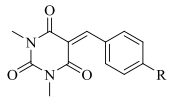
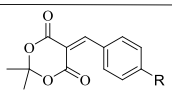
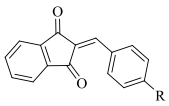
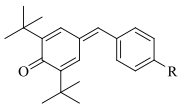
1) HF/6-31G(d), $E_i = -7.68\ L_i - 27.57$, $R^2 = 0.9860$, N = 22.
2) HF/6-31+G(d), $E_i = -7.75\ L_i - 28.97$, $R^2 = 0.9892$, N = 22.
3) B3LYP/6-31G(d), $E_i = -6.52\ L_i - 43.67$, $R^2 = 0.9817$, N = 22.
4) B3LYP/6-31+G(d), $E_i = -6.59\ L_i - 45.36$, $R^2 = 0.9817$, N = 22.
5) BP86/6-31G(d), $E_i = -6.14\ L_i - 44.51$, $R^2 = 0.9779$, N = 22.

Figure S3.1. Correlation between *E* and *L* for **a-v**.

4. Relationship of *E*/*L* for Michael acceptors

4.1. Relationship of *E*/*L* for Michael acceptors

Table S4.1. Structures of Michael acceptors.

	i	R	E_i
	**x1**	OMe	-10.37
	x2	NMe_2	-12.76
	**x3**	H	-9.15
	x4	MeO	-10.28
	x5	NMe2	-12.76
	x6	jul	-13.97
	**x7**	H	-10.11
	x8	OMe	-11.32
	x9	NMe_2	-13.56
	x10	jul	-14.66
	**y1**	H	-15.83
	y2	OMe	-16.11
	y3	NMe_2	-17.29
	y4	jul	-17.90

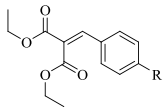
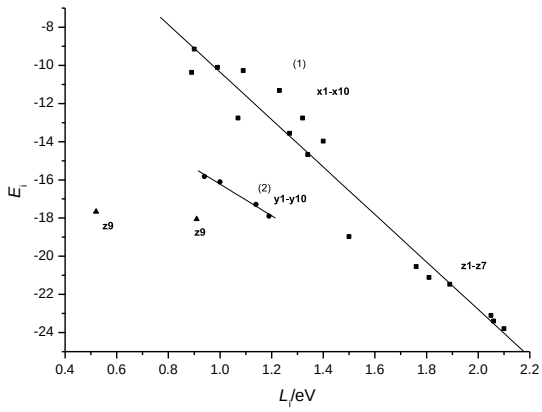
	i	R	E_i
	**z1**	*m*-Cl	-18.98
	z2	H	-20.55
	z3	Me	-21.11
	z4	MeO	-21.47
	z5	NMe_2	-23.1
	z6	thq	-23.4
	z7	jul	-23.8
	z8	NO_2	-17.67
	z9	CN	-18.06

Table S4.1. LUMO energies of Michael acceptors.

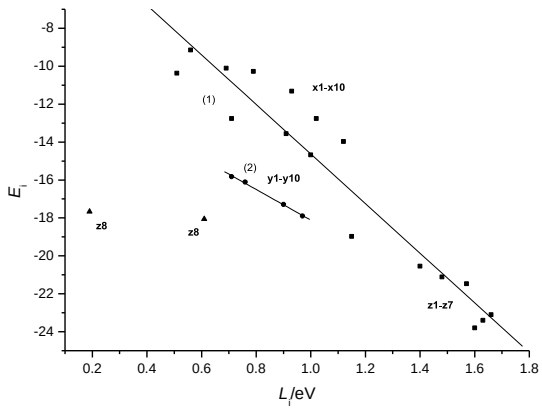
	HF/6-31G(d) (eV)	HF/6-31+G(d) (eV)	B3LYP/6-31G(d) (eV)	B3LYP/6-31+G(d) (eV)	BP86/6-31G(d) (eV)
x1	0.89	0.51	-2.55	-2.91	-3.26
x2	1.07	0.71	-2.34	-2.70	-3.01
x3	0.90	0.56	-2.54	-2.54	-3.23
x4	1.09	0.79	-2.32	-2.32	-2.96
x5	1.32	1.02	-2.03	-2.03	-2.65
x6	1.40	1.12	-1.90	-1.90	-2.50
x7	0.99	0.69	-2.39	-2.75	-3.02
x8	1.23	0.93	-2.11	-2.46	-2.72
x9	1.27	0.91	-2.09	-2.45	-2.74
x10	1.34	1.00	-1.98	-2.32	-2.60
y1	0.94	0.71	-2.43	-2.71	-3.08
y2	1.00	0.76	-2.35	-2.63	-2.97
y3	1.14	0.90	-2.14	-2.42	-2.74
y4	1.19	0.97	-2.04	-2.31	-2.61
z1	1.50	1.15	-2.04	-2.37	-2.76
z2	1.76	1.40	-1.82	-2.16	-2.55
z3	1.81	1.48	-1.76	-2.09	-2.48
z4	1.89	1.57	-1.66	-2.00	-2.35
z5	2.05	1.66	-1.45	-1.78	-2.12
z6	2.06	1.63	-1.42	-1.74	-2.07
z7	2.10	1.60	-1.34	-1.66	-1.98
z8	0.52	0.19	-2.87	-3.28	-3.53
z9	0.91	0.61	-2.48	-2.82	-3.17



1) E_i = -12.55 L_i – 2.27, R^2 = 0.9843, N = 17.

2) E_i= -7.39L_i – 9.02, R^2 = 0.9761, N = 4.

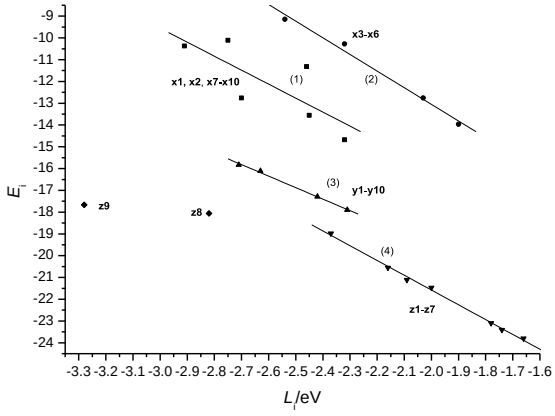
Figure S4.1.1. Correlation between *E* and *L* (HF/6-31G(d))



1) E_i = -13.08 L_i – 1.56, R^2 = 0.9604, N = 17.

2) E_i = -7.39L_i – 10.50, R^2 = 0.9761, N = 4.

Figure S4.1.2. Correlation between *E* and *L* (HF/6-31+G(d))



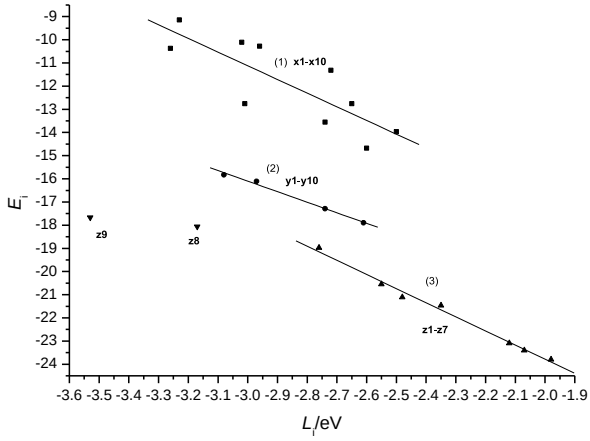
1) E_i = -6.41L_i – 28.83, R^2 = 0.72899, N = 6.

2) E_i = -7.64L_i – 28.32, R^2 = 0.9937, N = 4.

3) E_i = -5.32L_i – 30.08, R^2 = 0.9938, N = 4.

4) E_i = -6.51L_i – 34.70, R^2 = 0.9949, N = 7.

Figure S4.1.3. Correlation between *E* and *L* (B3LYP/6-31+G(d))



1) E_i = -5.90L_i – 28.83, R^2 = 0.8237, N = 10.

2) E_i = -4.09L_i – 28.43, R^2 = 0.9945, N = 4.

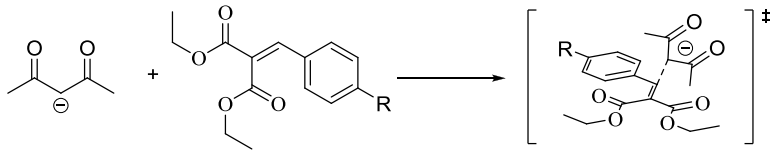
3) E_i = -6.09L_i – 35.96, R^2 = 0.9960, N = 7.

Figure S4.1.4. Correlation between *E* and *L* (BP86/6-31G(d))

4.2. Analyzing the deviation of z8 and z9.

We found **z8** and **z9**, which have strong electron-withdrawing groups, the nitro and cyano groups, deviate positively from the correlation line. Take the para-substituted malonate **z9** as an example, the *E* value predicted from the expression (E_i = -6.87L_i – 33.06) is 28.87) in Figure 6 using the LUMO energy in Table S4.1 which differs from Mayr's measurement by at least 10 orders of magnitude. To understand these derivations, we examined the reactions of **SA** (*N* = 17.64, *s* = 0.72) toward **z1-z9**, which are summarized in Table S4.2. High R^2 value (0.9855) of $\ln k_{cal}/\ln k_{exp}$ correlation and close entropies of activation (-46.6--49.0 cal mol^{-1} K^{-1}) were obtained.

Table S4.2. LUMO energy of Michael acceptors.



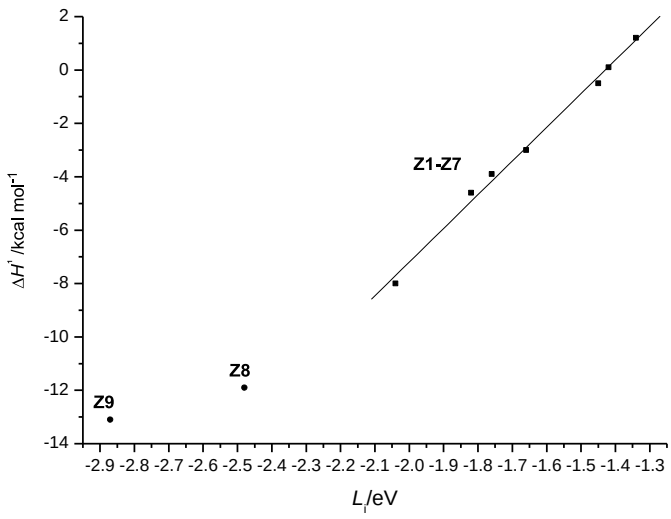
SA z1-9 TSzi/SA

$\ln k_{cal} = 2.20 \ln k_{exp} + 25.50$, $R^2 = 0.99$, N = 9

SA (N = 17.64, s = 0.72, H_{SA} = -0.11 eV)

	$\Delta H^{\neq}$ (kcal mol^{-1})	$\Delta G^{\neq}$ (kcal mol^{-1})	$\Delta S^{\neq}$ (cal mol^{-1} K^{-1})	$\ln k_{cal}$	L (eV)	E	$\ln k_{exp}$
TSSz1/SA	-8.0	6.1	-47.4	19.16	-2.04	-18.98	-2.22
TSSz2/SA	-4.6	10.0	-48.8	12.62	-1.82	-20.55	-4.83
TSSz3/SA	-3.9	10.7	-49.0	11.36	-1.76	-21.11	-5.75
TSSz4/SA	-3.0	10.9	-46.6	11.01	-1.66	-21.47	-6.35
TSSz5/SA	-0.5	13.8	-47.8	6.21	-1.45	-23.10	-9.05
TSSz6/SA	0.1	14.3	-47.6	5.40	-1.42	-23.40	-9.55
TSSz7/SA	1.2	15.1	-46.8	3.95	-1.34	-23.80	-10.21
TSSz8/SA	-13.1	1.3	-48.3	27.24	-2.87	-17.67	-0.05
TSSz9/SA	-11.9	2.5	-48.5	25.20	-2.48	-18.06	-0.70

However, a similar deviation was found in the correlation of $\Delta H_{i/A}^{\neq}/L_i$. In Figure S4.2.1, a high regression coefficient (0.9972) is showed in the liner relationship between $\Delta H_{i/A}^{\neq}$ and L_i if **z8** and **z9** are not included in the correlation there. The values of LUMO energies predicted from $\Delta H_{i/A}^{\neq} = 12.6\ L_i + 18.0$, $R^2 = 0.9970$ (correlation of **z1**-**z7**) are -2.47 eV and -2.37 eV while the calculated L are -2.87 eV and -2.48 eV, respectively. This suggests that the LUMO energies for these two species are much underestimated.



$\Delta H_{i/A}^{\neq} = 12.6\ L_i + 18.0$, $R^2 = 0.9970$, N=7

Figure S4.2.1. Correlation between $\Delta H^{\neq}$ and L (**z8** and **z9** are not included in the correlation)

After examining the LUMO and LUMO+1 orbitals **z1** ~ **z9** in Table S4.1, we found that both LUMO and LUMO+1 orbitals of **z8** and **z9** are reacting π orbitals, while for other Michael acceptors, their LUMO orbitals are reacting orbitals and their corresponding LUMO+1 orbitals are not (see Figure S4.2.2). This suggests that both LUMO and LUMO+1 orbitals of **z8** and **z9** should be taken into consideration in computing L_i value. Therefore, we define L' for **z8** and **z9** as:

$$L' = \frac{(c1_{\mathrm{L}})^2 L + (c1_{\mathrm{L+1}})^2 (E_{L+1})}{(c1_{\mathrm{L}})^2 + (c1_{\mathrm{L+1}})^2} \quad \text{.....(S1)}$$

Where L' is the modified LUMO energy and $E_{\mathrm{L+1}}$ is the energy of LUMO+1 orbital; $c1_L$ and $c1_{L+1}$ are the molecular orbital coefficients referred to the 2Pz part of the reacting carbon atoms in the LUMO and LUMO+1 orbitals, respectively. If the $c1_{L+1}$ coefficient of LUMO+1 is very low, then $L' \approx L$, that is, the correction affects the orbital energy slightly. Although all the calculation methods give better liner relationships, only B3LYP/6-31G(d) level give a very acceptable result in the present system (R^2 = 0.9709, E_{i} = -6.45L_{i}' - 32.32, see Figure S4.2.3). The predicted E value of **z8** and **z9** are -18.84 and -16.90, which are better than those predicted from Figure 6 and differ by about 1 order from the experimental results from Mayr.

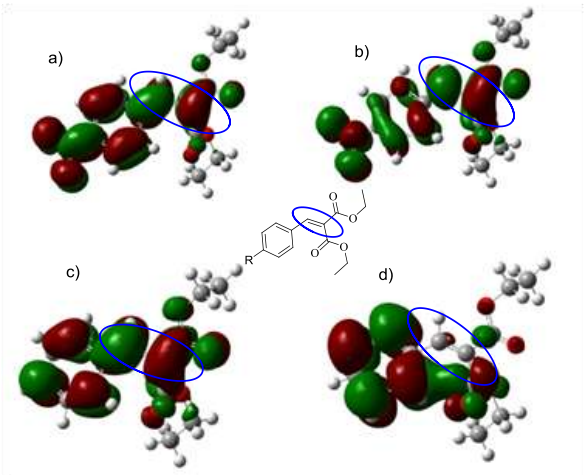
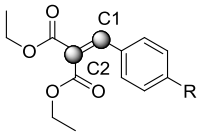


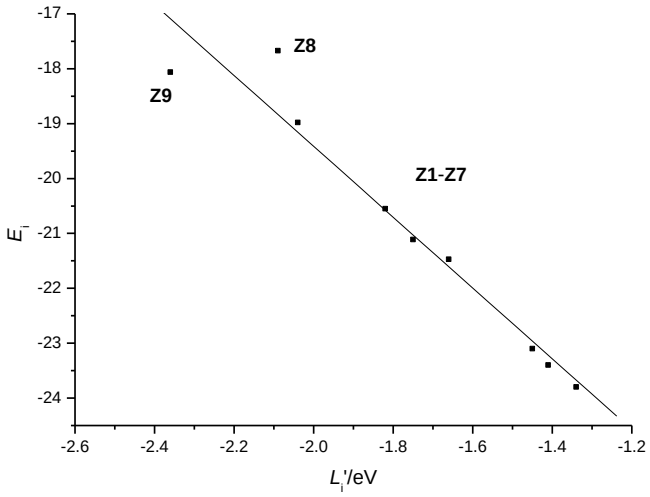
Figure S4.2.2. Orbitals of **z8** and **z2**. a) **z8** LUMO; b) **z8** LUMO+1; c) **z2** LUMO; d) **z2** LUMO+1.

Table S4.4 Calculated energies of LUMO and LUMO+1 and their molecular orbital coefficients at the C1 and C2 atoms in **z1-z9**.



		LUMO			LUMO+1			
i	R	L/eV [a]	$c1_{\mathrm{L}}$ [b]	$c2_{\mathrm{L}}$ [b]	$E_{\mathrm{L+1}}$/eV [a]	$c1_{\mathrm{L+1}}$ [b]	$c2_{\mathrm{L+1}}$ [b]	L'/eV [a, c]
z1	*m*-Cl	-2.04	0.30	-0.26	-0.59	0.01	0.00	-2.04
z2	H	-1.82	0.32	-0.26	-0.22	0.01	0.01	-1.82
z3	Me	-1.76	0.32	-0.26	-0.19	0.02	0.01	-1.75
z4	MeO	-1.66	0.33	-0.25	-0.19	-0.02	0.01	-1.66
z5	NMe_2	-1.45	0.33	-0.24	0.03	-0.01	0.02	-1.45
z6	thq	-1.42	0.33	-0.24	0.04	0.00	0.02	-1.41
z7	jul	-1.34	0.33	-0.23	0.11	-0.01	0.02	-1.34
z8	NO_2	-2.87	**0.17**	**-0.21**	-1.63	**0.30**	**-0.19**	-2.09
z9	CN	-2.48	**-0.26**	0.26	-0.83	**0.10**	-0.02	-2.36

[a] Calculated by the B3LYP/6-31G(d) method.; [b] Molecular orbital coefficients are referred to the 2Pz part of each carbon atom; [c] energies were predicted by Eq (S1).

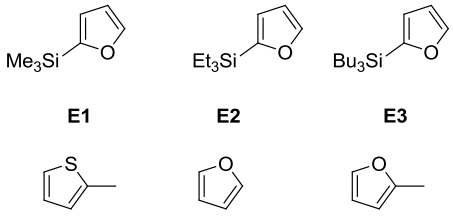


$E_i = -6.45L_i' - 32.32$, $R^2 = 0.9709$, N = 9.

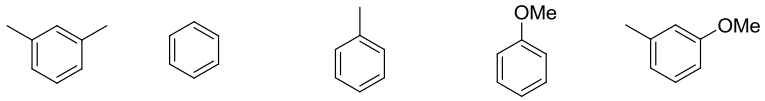
Figure S4.2.3. Correlation between *E* and *L′*

5. Relationship of *N*/*H* for arenes

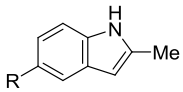
Table S5.1. Calculated HOMO energies of arenes.



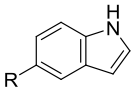
	E1	E2	E3	E4	E5	E6	E7
N_j	2.4	2.4	2.6	1.26	1.36	3.61	5.85
s_j	1.1	1.1	1.1	0.96	1.01	1.11	1.03
H_j/eV	-5.94	-5.96	-5.96	-6.03	-6.11	-5.78	-5.42



	B	F1	F2	F3	F4
N_j	-3.54	-6.29	-4.47	-1.18	0.13
s_j	1.62	1.00	1.11	0.96	1.27
H_j/eV	-5.70	-6.70	-6.40	-5.85	-5.62



	G1	G2	G3	G4
R	Cl	H	Me	OMe
N_j	6.08	6.91	7.22	7.26
s_j	1.10	1.10	1.10	1.10
H_j/eV	-5.61	-5.21	-5.22	-5.03

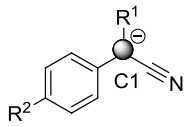


	H1	H2	H3	H4	H5	H6	H7	H8
R	7-azaindol	CN	COOH	Cl	Br	4-methoxyindol	H	Me
N_j	3.87	2.83	3.97	4.42	4.38	5.41	5.55	6.00
s_j	1.10	1.10	1.10	1.10	1.10	1.10	1.09	1.10
H_j/eV	-5.82	-6.09	-5.77	-5.73	-5.72	-5.01	-5.40	-5.35

	H9	H10	H11
R	OMe	OH	NH_2
N_j	6.22	6.44	7.22
s_j	1.12	1.10	1.10
H_j/eV	-5.10	-5.18	-4.83

6. Relationship of *N*/*H* for carboanions

Table S6.1. Calculated HOMO and LUMO energies and their molecular orbital coefficients at the C1 of **J.**

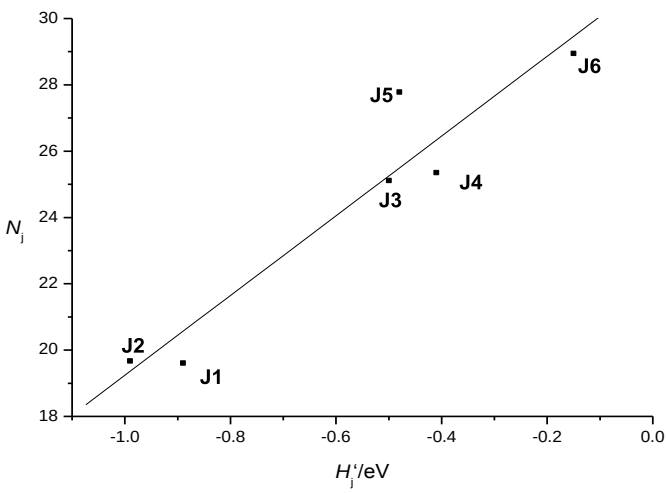
				HOMO		LUMO			
		N	*s*	*H*/eV [a]	c_H [b]	*L*/eV [a]	c_L [b]	*L* -*H* /eV	*H'*/eV [c]
	**J1**	19.61	0.60	-0.87	0.37	1.88	-0.19	2.75	-0.30
	J2	19.67	0.68	-0.95	0.36	1.89	-0.19	2.84	-0.35
	J3	25.11	0.54	-0.56	0.37	3.13	-0.18	3.69	0.16
	J4	25.35	0.56	-0.50	0.38	3.09	0.18	3.58	0.17
	J5	27.28	0.50	-0.26	0.38	3.76	-0.16	4.03	0.35
	J6	28.95	0.58	0.46	0.40	4.40	0.01	3.94	0.46

[a] B3LYP/6-31G(d); [b] Molecular orbital coefficients are referred to the 2Pz part of carbon atom; [c] predicted from Eq (9) in the text.

Table S6.2. Calculated *H* and *H'* values of **J.**

		H/eV[a]	*L*/eV[a]	*H'*/eV[b]
J1	energy	-0.91	2.90	-0.48
	coefficient	0.38	-0.14	
J2	energy	-1.11	2.47	-0.50
	coefficient	0.37	-0.17	
J3	energy	-1.55	1.15	-0.99
	coefficient	0.36	-0.18	
J4	energy	-0.15	2.99	-0.15
	coefficient	0.40	0.00	
J5	energy	-1.02	2.48	-0.41
	coefficient	0.38	-0.17	
J6	energy	-1.45	1.17	-0.89
	coefficient	0.36	-0.19	

[a] B3LYP/6-31+G(d); [b] Molecular orbital coefficients are referred to the 2Pz part of carbon atom; [c] predicted from Eq (9) in the text.

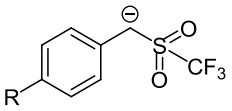


$N_j = 12.02\ H_j + 31.26$, $R^2 = 0.95135$, N = 6.

Figure S6.1. Correlation between *N* and *H'* of **J** (B3LYP/6-31+G(d)).

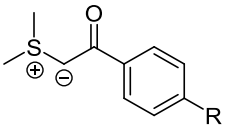
Comparison of Figures 4 and S6.1 shows that both 6-31+G(d) and 6-31G(d) basis sets give good correlation between N and H', demonstrating that for anionic species, 6-31G(d) basis set can be used to compute orbital energies. Therefore, for other anionic species, we used B3LYP/6-31G(d) to compute their orbital energies and coefficients.

Table S6.3. Calculated *H* and *H'* values of **K** and **L.**



		N	s		*H*/eV	*L*/eV	*H'*/eV
K1	R = NO_2	19.35	0.67	energy	-0.78	3.71	-0.73
				coefficient	0.30	0.03	
K2	R = CN	18.67	0.68	energy	-0.81	3.81	-0.80
				coefficient	0.30	0.01	
K3	R = CF_3	17.33	0.74	energy	-1.32	3.07	-0.96
				coefficient	0.31	-0.09	
K4	R = H	16.28	0.75	energy	-1.53	2.46	-1.07
				coefficient	0.30	-0.11	
K5	R = CH_3	14.49	0.86	energy	-1.79	1.28	-1.37
				coefficient	0.33	-0.13	

Using *H* values, $R^2 = 0.9794$ and the expression is $N_j = 4.26H_j + 22.54$



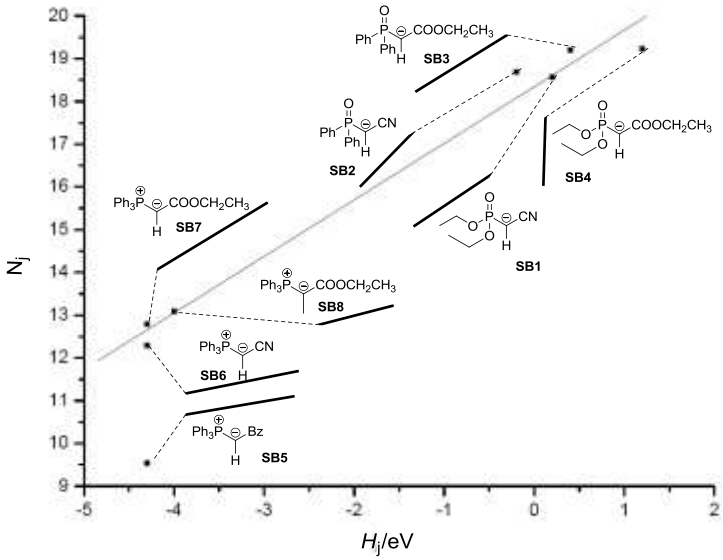
	R	*N*	s		*H*/eV	*L*/eV	*H'*/eV
L1	R = Br	16.23	0.6	energy	-5.22	0.34	-4.39
				coefficient	0.43	-0.18	
L2	R = H	13.78	0.72	energy	-5.21	-0.80	-5.00
				coefficient	0.39	-0.09	
L3	R = MeO	13.95	0.69	energy	-5.01	-0.49	-4.83
				coefficient	0.37	-0.08	
L4	R = $N(CH_3)_2$	14.48	0.71	energy	-4.90	-0.28	-4.76
				coefficient	0.38	-0.07	
L5		15.68	0.65	energy	-4.65	-0.10	-4.50
				coefficient	0.33	-0.06	

Using *H* values, no linear relationship was obtained for H_j and N_j.

High *H*/*N* correlations for the Wittig regents (**SB5**-**SB8**) and HWE (Honer-Wadsworth-Emmons) regents (**SB1**-**SB4**) [4] are showed in Figure S6.2. The appearance of anomalous points (**SB5**) may be explained by the high *s* value, that is, *s* = 0.97 for **SB5** while *s* = 0.65-0.77 for others.

Table S6.4. Calculated *H* values of **SB**.

	SB1	SB2	SB3	SB4	SB5	SB6	SB7	SB8
N	18.57	18.69	19.20	19.23	9.54	12.29	12.79	13.09
s	0.66	0.72	0.69	0.65	0.97	0.75	0.77	0.73
H/eV	0.21	-0.17	0.41	1.15	-4.26	-4.32	-4.29	-3.96



$N_j = 1.32\ H_j + 18.34$, $R^2 = 0.9913$, N = 7.

Figure S6.2. Correlation between *N* and *H* of **SB**.

7. Relationship of *N*/*H* for heteroatom-centered nucleophiles

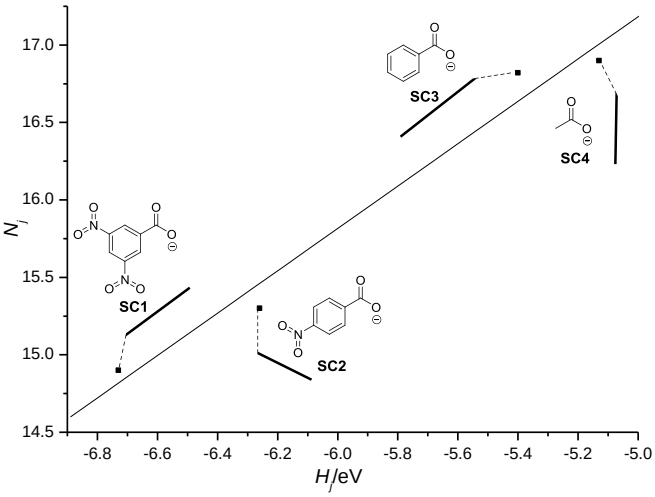
Heteroatom-centered nucleophiles, for examples, carboxylate ions [5], amide ions and pyridines, have been examined in our calculations too. All of them perform linear relationships in some extent. However, some issues should be pointed out here: 1) the experimental results of heteroatom-centered nucleophiles are not available at present, leading to the difficulty in judging calculation methods and results. 2) The reaction centers for these nucleophiles are different very much, making the liner relationships be only semi-quantitative. 3) The calculated HOMOs are not always those of the reacting orbitals, therefore, HOMO-1 orbitals were considered in our calculations (for additional discussions, see below).

7.1. Carboxylate ions

Table S7.1. Calculated *H* values of **SC**.

	SC1	SC2	SC3	SC4
N	14.90	15.30	16.82	16.90
s	0.71	0.76	0.70	0.75
H/eV[a]	-1.90	-1.42	-0.66	0.27

[a] HF/6-31G(d)



$N_j = 1.36\ H_j + 24.02$, $R^2 = 0.9878$, N = 4.

Figure S7.1. Correlation between *N* and *H* of **SC** (B3LYP results are not satisfactory in this case, the reasons are not known).

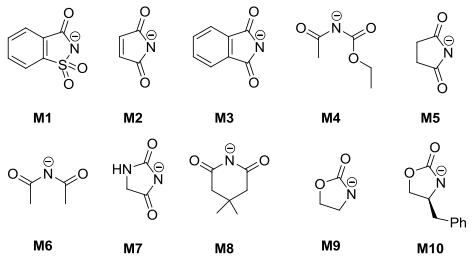
7.2. Pyridine derivates

Table S7.2. Calculated *H* values of **I**.

	I1	I2	I3	I4	I5	I6
R	Cl	H	Me	OMe	NH_2	NMe_2
N	11.7	12.9	13.7	13.7	15.2	15.86
H/eV	-7.52	-7.78	-7.39	-7.05	-6.82	-6.72
orbital	HOMO	HOMO	HOMO - 1	HOMO - 1	HOMO - 1	HOMO - 1

7.3. Amide anions

Table S7.3. Calculated *H* values of **M**.



	M1	M2	M3	M4	M5
N	10.78	14.87	15.52	15.99	16.03
s	0.89	0.76	0.67	0.70	0.66
H/eV	-1.99	-1.08	-1.54	-1.08	-1.19

	M6	M7	M8	M9	M10
N	16.05	17.52	17.52	22.40	22.67
s	0.70	0.55	0.63	0.59	0.54
H/eV	-0.89	-1.11	-1.20	0.10	-0.34

8. Calculated results of N, O, P, SD and SE

Scheme S8.1 Structures of N, P, SD and SE

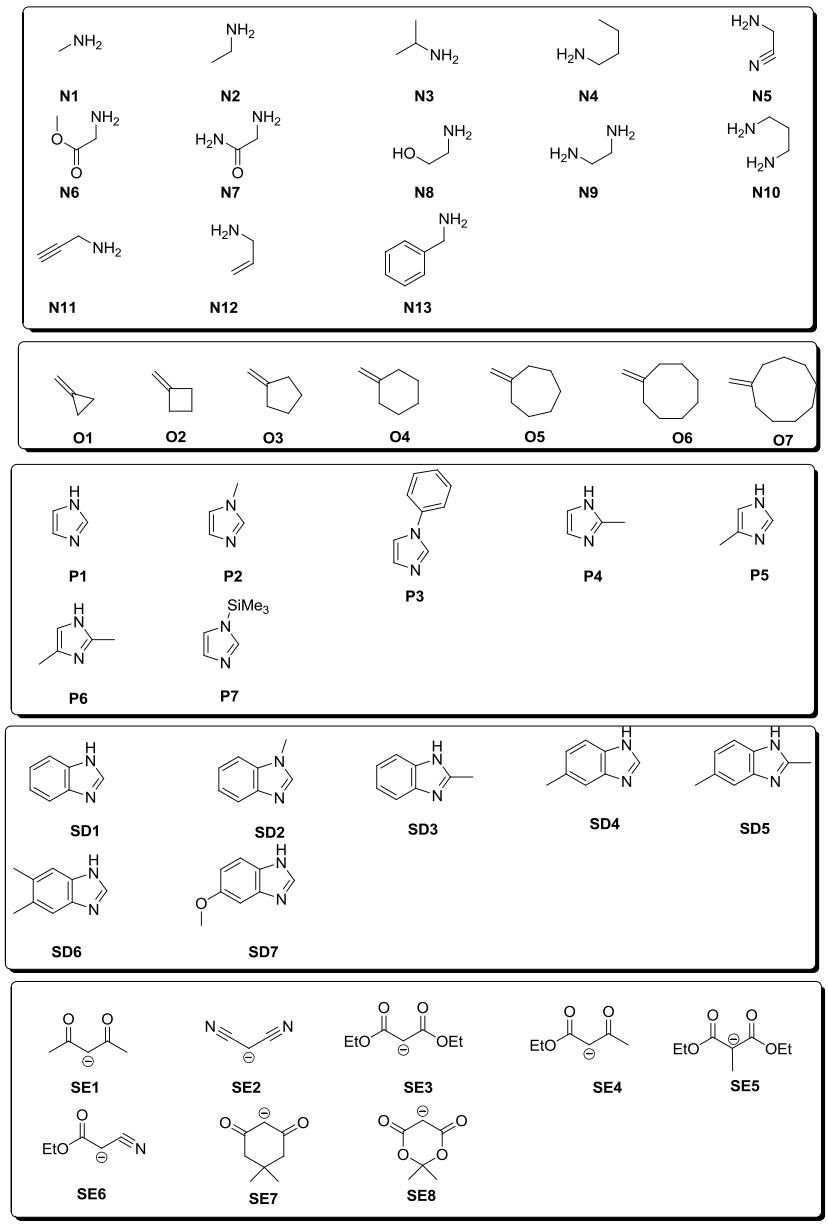


Table S8.1. Calculated *H* values of **N, O, P**, **SD** and **SE.**

Molecular	H_j/eV	N_j	Molecular	H_j/eV	N_j	Molecular	H_j/eV	N_j
N1	−6.22	9.48	01	−6.90	−0.47	P1	−7.14	11.47
N2	−6.22	13.85	02	−6.49	1.65	P2	−7.03	11.9
N3	−6.24	12	03	−6.34	2.82	P3	−7.19	11.31
N4	−6.20	10.48	04	−6.44	1.66	P4	−6.99	11.74
N5	−7.24	10.8	**O5** [a]	−6.37	2.24	P5	−7.03	11.79
N6	−6.50	12.08	**O6** [a]	−6.41	3.61	P6	−6.90	11.51
N7	−6.25	12.29	**O7** [a]	−6.34	2.82	P7	−6.93	11.43
N8	−6.14	12.61						
N9	−6.04	13.28				SE1	−0.11	17.64
N10	−5.78	14.02	SD1	−7.33	10.5	SE2	0.08	19.63
N11	−6.53	12.29	SD2	−7.24	10.37	SE3	−0.41	20.22
N12	−6.32	13.21	SD3	−7.19	10.02	SE4	−0.28	18.82
N13	−6.24	13.44	SD4	−7.27	10.69	SE5	−0.25	21.13
			SD5	−7.13	10.21	SE6	−0.21	19.62
			SD6	−7.21	11.08	SE7	−0.35	16.27
			SD7	−7.33	10.5	SE8	−0.69	13.91

[a] For **O5**, **O6** and **O7**, they have many conformations and we searched their conformations using MMFF94x force field (thanks to the help of Prof. Junmin Quan from Shengzhen graduate school of Peking University). We then used B3LYP/6-31G(d) to optimize the lowest 10 conformers for each nucleophile (**O5**, **O6** and **O7**). We found the orbital energies of the lowest conformers for **O5**, **O6** and **O7** are very close to those of other conformers that are close (in terms of total energy) to the lowest conformers of **O5**, **O6** and **O7**. The orbital energies and structures given are the lowest conformers of **O5**, **O6** and **O7**.

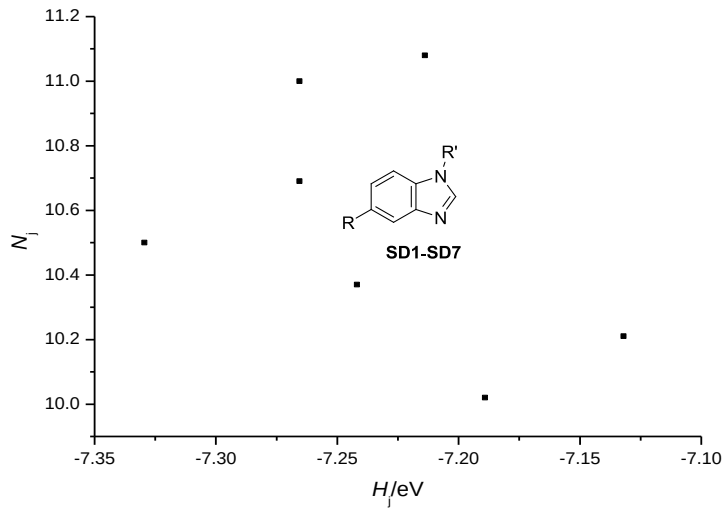


Figure S8.1. Correlation between *N* and *H* of **SD**.

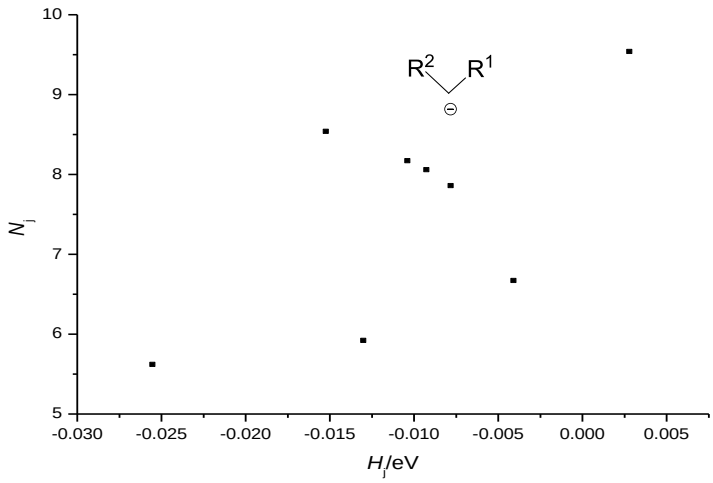


Figure S8.2. Correlation between *N* and *H* of **SE**

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10. Computed energies of all stationary points

thermal enthalpy (*H*, in Hartree)
thermal free energy (*G*, in Hartree)

	H	*G*
a	-1420.746085	-1420.800070
b	-501.543079	-501.590318
c	-600.783354	-600.832690
d	-540.838373	-540.891091
e	-580.133006	-580.190134
f	-807.733024	-807.795910
g	-616.046807	-616.100067
h	-655.340642	-655.398620
i	-922.232986	-922.301549
j	-730.547075	-730.606309
k	-806.761325	-806.821304
l	-1826.791531	-1826.893239
m	-1443.423087	-1443.506851
n	-1536.116706	-1536.215471
o	-1074.541922	-1074.617862
p	-1152.747562	-1152.832080
q	-769.378237	-769.446460
r	-924.162296	-924.233288
s	-924.181818	-924.252467
t	-845.598450	-845.667457
u	-1078.962928	-1079.037307
v	-1000.384989	-1000.455884
z1	-1303.338423	-1303.409760
z2	-843.735128	-843.803097
z3	-883.024449	-883.097402
z4	-958.224418	-958.298163
z5	-977.628245	-977.706463
z6	-1055.022838	-1055.103008
z7	-1132.416487	-1132.498709
z8	-1048.230281	-1048.305099
z9	-935.977165	-936.049728
A	-235.678472	-235.719273
B	-310.719684	-310.762658
C	-234.486613	-234.521575
D	-309.506814	-309.546006
SA	-345.097149	-345.136043
TSa/A	-966.207532	-966.287469
TSw/A	-815.804031	-815.882322
TSf/A	-1043.401380	-1043.485623
TSg/A	-851.715484	-851.789880
TSh/A	-891.005851	-891.084743
TSb/B	-1010.727940	-1010.800004
TSc/B	-812.251282	-812.319062

TSd/B	-851.542739	-851.615049
TSe/B	-890.833166	-890.910830
TSj/B	-1731.452477	-1731.527441
TSb/C	-1655.235132	-1655.305260
TSd/C	-736.033882	-736.097413
TSe/C	-775.326270	-775.394509
TSf/C	-814.617720	-814.691707
TSg/C	-850.529324	-850.598445
TSh/C	-965.021652	-965.096735
TSi/C	-1042.214958	-1042.293419
TSj/C	-889.820337	-889.894364
TSa/D	-1040.038374	-1040.116591
TSe/D	-889.634575	-889.711634
TSf/D	-925.546728	-925.619225
TSg/D	-1117.232680	-1117.314757
TSh/D	-964.837533	-964.915259
TSj/D	-1231.724312	-1231.812166
TSSz1/SA	-1648.447800	-1648.538997
TSSz2/SA	-1188.838970	-1188.926150
TSSz3/SA	-1228.127208	-1228.219263
TSSz4/SA	-1303.325689	-1303.419693
TSSz5/SA	-1322.725549	-1322.823461
TSSz6/SA	-1400.119305	-1400.219236
TSSz7/SA	-1477.511170	-1477.613563
TSSz8/SA	-1393.347698	-1393.441984
TSSz9/SA	-1281.092743	-1281.184683

11 Coordinates of all stationary points

a

C	0.00002200	1.31113500	-0.00004300
C	1.29116300	0.73138200	-0.03260900
C	2.39664800	1.58310800	0.26668300
C	3.68891200	1.09909800	0.29648200
C	3.91760500	-0.25100700	-0.02002800
C	2.85705100	-1.10751700	-0.37616100
C	1.56517500	-0.62473500	-0.38044800
H	4.52260400	1.74508100	0.54792400
C	-1.29125200	0.73151800	0.03274500
C	-2.39670700	1.58324500	-0.26656800
C	-3.68893000	1.09909500	-0.29655200
C	-3.91756600	-0.25101400	0.02000300
C	-2.85708200	-1.10738100	0.37660000
C	-1.56521000	-0.62451900	0.38087600
H	2.21222500	2.62666700	0.50545800
H	3.06848800	-2.13175500	-0.66247500
H	0.76557800	-1.27349500	-0.71657100
H	0.00014800	2.40111000	-0.00028900
H	-2.21237100	2.62681000	-0.50533400
H	-4.52264100	1.74496400	-0.54822300
H	-3.06847000	-2.13154600	0.66320500
H	-0.76559000	-1.27313500	0.71722500
Cl	-5.52598000	-0.86384900	0.00683200
Cl	5.52604100	-0.86374800	-0.00723200

b

C	-2.39379800	-1.26857000	-0.27407200
C	-1.29148400	-0.41812400	0.03873400
C	-1.55572800	0.93593000	0.40040100
C	-2.85255500	1.41613600	0.39437800
C	-3.91437200	0.57170900	0.02938600
C	-3.68491800	-0.77075100	-0.30168900
C	0.00006000	-0.99979200	0.00064200
C	1.29149900	-0.41807500	-0.03813000
C	2.39399200	-1.26846700	0.27418200
C	3.68518000	-0.77071200	0.30069000
C	3.91437500	0.57179200	-0.03036800
C	2.85227000	1.41633200	-0.39434100
C	1.55546900	0.93608200	-0.39965900
H	-0.74980900	1.57221100	0.74549200
H	-3.05391200	2.44042300	0.69067500
H	-4.92924700	0.95876300	0.02796900
H	-4.51532700	-1.41786100	-0.56401300
H	-2.20503200	-2.30925300	-0.52228900
H	0.00010500	-2.09009300	0.00095000
H	2.20547300	-2.30919700	0.52239600
H	4.51582100	-1.41787900	0.56212900
H	4.92925400	0.95884500	-0.02950700
H	3.05338200	2.44071000	-0.69047800
H	0.74935300	1.57238900	-0.74425200

c

C	-2.87921600	1.20772900	-0.27466400
C	-1.73958600	0.41208500	0.04433000
C	-1.94064500	-0.95285000	0.40211700
C	-3.21279500	-1.49571200	0.38695700
C	-4.31219000	-0.70397200	0.01611700
C	-4.14509400	0.64814000	-0.31121000
C	-0.47648500	1.05873700	0.01624000
C	0.83970100	0.54674000	-0.02581200
C	1.17621500	-0.79717800	-0.37692900
C	2.48886900	-1.21646500	-0.37882100
C	3.49073400	-0.29765000	-0.02733900
C	3.21726500	1.03838100	0.29216300
C	1.90329200	1.45610800	0.26854400
H	-2.74006300	2.25692900	-0.51998700
H	-5.00368200	1.25555900	-0.57777400
H	-3.36556500	-2.52899500	0.68114000
H	-1.10888100	-1.55075800	0.75472200
H	-0.53291700	2.14737800	0.02732200
H	1.66528700	2.48843500	0.50784700
H	4.03375800	1.70903600	0.53572900
H	2.77072500	-2.22376700	-0.66508400
H	0.40402700	-1.48118000	-0.70663100
H	-5.30697700	-1.13986200	0.00743200
F	4.74709900	-0.70637100	-0.02609700

d

C	2.92524900	1.19169100	0.27714000
C	1.77972900	0.40683300	-0.04319100
C	1.96902300	-0.95904300	-0.40007200
C	3.23672200	-1.51348500	-0.38360400

C	4.34266800	-0.73204300	-0.01245400
C	4.18659500	0.62118700	0.31462100
C	0.52026200	1.06464800	-0.01835000
C	-0.79853600	0.56441200	0.02397900
C	-1.15345700	-0.77559200	0.36781300
C	-2.47357900	-1.17104500	0.36183900
C	-3.50898900	-0.26995800	0.01777500
C	-3.17015100	1.06285900	-0.29538300
C	-1.85514400	1.47977000	-0.26903700
H	2.79506400	2.24214100	0.52213600
H	5.05001100	1.22146200	0.58192900
H	3.37999100	-2.54849300	-0.67664500
H	1.13132400	-1.54944200	-0.75093200
H	0.58633100	2.15284700	-0.03248500
H	-1.60914900	2.51071400	-0.50816000
H	-3.95621600	1.76777000	-0.54851200
C	-4.94053500	-0.71472100	0.03963400
H	-2.73083200	-2.18787500	0.64379400
H	-0.39050800	-1.47150900	0.69523200
H	-5.57238200	-0.08117200	-0.58833000
H	-5.04299600	-1.75505400	-0.28445300
H	-5.33340400	-0.65790600	1.06498700
H	5.33361700	-1.17654900	-0.00280900

e

C	1.57094500	-0.76494900	0.36547200
C	1.29161800	0.59398100	0.03270800
C	2.39617400	1.44823300	-0.25693900
C	3.68708600	0.95784800	-0.28861600
C	3.95129200	-0.39247700	0.01378300
C	2.86704400	-1.23477800	0.35417100
C	0.00022800	1.17201700	0.00033200
C	-1.29161500	0.59511700	-0.03495600
C	-1.57229200	-0.76075800	-0.37845400
C	-2.86924000	-1.22877800	-0.37359300
C	-3.95254000	-0.38853400	-0.02543300
C	-3.68723800	0.96003600	0.28419400
C	-2.39561300	1.44868200	0.25922900
C	-5.35202000	-0.92806200	0.00208800
C	5.35417300	-0.92400000	0.02341900
H	0.77143000	-1.41957600	0.69049600
H	3.06599400	-2.26673700	0.62887200
H	4.51070800	1.61991700	-0.53785500
H	2.20912600	2.49343800	-0.48763500
H	0.00070400	2.26227100	0.00413400
H	-2.20796700	2.49285800	0.49397400
H	-4.51102300	1.62258900	0.53156600
H	-3.06937900	-2.25666700	-0.66199500
H	-0.77380300	-1.41272500	-0.71128900
H	6.04836900	-0.25264300	-0.48775100
H	5.70521300	-1.04473300	1.05766400
H	5.40660000	-1.91226500	-0.44617800
H	-5.54157000	-1.58797300	-0.85120000
H	-5.50443300	-1.52967400	0.90915700
H	-6.09799400	-0.12954600	0.00359700

f

C	-4.10197000	0.88592700	0.38327200
C	-3.79957300	-0.47785600	0.12075100
C	-4.87621300	-1.37991000	-0.10017700
C	-6.18618700	-0.92764200	-0.13316700
C	-6.45734100	0.42587200	0.09920900
C	-5.41592700	1.32486900	0.37246400
C	-2.48015800	-1.02558000	0.09920400
C	-1.22400800	-0.42596700	-0.06222400
C	-0.06818400	-1.22990600	0.20905800
C	1.20669000	-0.72638600	0.12455800
C	1.38593100	0.61775300	-0.28478500
C	0.26442300	1.42522200	-0.61894700
C	-1.00299400	0.91917500	-0.51083500
O	2.56933700	1.20700100	-0.41321700
H	-1.84194300	1.52742900	-0.82527300
H	0.44883700	2.43148100	-0.97928600
H	2.06840800	-1.34060300	0.35569400
H	-0.21246200	-2.26078200	0.52074000
H	-2.44865700	-2.10795700	0.22521500
H	-4.66004600	-2.43068700	-0.27246300
H	-6.99767900	-1.62214300	-0.32474100
H	-7.48430500	0.77907200	0.09188800
H	-5.64119200	2.36315700	0.59411800
H	-3.31293800	1.57480100	0.66028500
C	3.77075600	0.50823000	-0.13541600
C	4.30536600	0.59049100	1.14540800
C	4.40988100	-0.15599500	-1.17640700
C	5.52993200	-0.03448900	1.39119600
H	3.78402200	1.14170200	1.92151700
C	5.63362800	-0.77514200	-0.91212100
H	3.96803200	-0.17306100	-2.16763800

C	6.19113200	-0.71627700	0.36713500
H	5.96745100	0.01962500	2.38330400
H	6.15163900	-1.29690200	-1.71090900
H	7.14503400	-1.19547100	0.56422000

g

C	-1.44677000	1.44563600	0.22044000
C	-0.36621400	0.54040000	-0.03251700
C	-0.70412300	-0.81231100	-0.37301500
C	-2.00792600	-1.22635000	-0.39860300
C	-3.05715600	-0.31729900	-0.08375100
C	-2.75869900	1.03498200	0.21926300
C	0.93656800	1.05379300	0.03950900
C	2.21107400	0.41022500	0.05818700
C	3.34271900	1.20972000	-0.26235800
C	4.61362700	0.65793200	-0.30157900
C	4.79227900	-0.69201900	0.02318500
C	3.69798200	-1.48755700	0.39382300
C	2.42121700	-0.95068400	0.41144100
O	-4.27601800	-0.82730000	-0.12674000
C	-5.43147200	-0.00815500	0.14816200
H	0.07397500	-1.50381500	-0.67142600
H	-2.27934600	-2.23859800	-0.67790300
H	-3.54931100	1.74168600	0.43898300
H	-1.21625900	2.48212000	0.45059400
H	0.98999200	2.14171300	0.08352900
H	3.19819800	2.25878800	-0.50551200
H	5.46667200	1.27287500	-0.56923300
H	5.78953400	-1.12188300	0.01142800
H	3.85433600	-2.52125400	0.68514700
H	1.59406100	-1.55613800	0.76209900
H	-6.28323500	-0.67872700	0.04869500
H	-5.38346600	0.38877200	1.16623200
H	-5.50565200	0.80298100	-0.58182000

h

C	1.12873600	-0.77959600	-0.36408000
C	0.85199500	0.58898300	-0.03951700
C	1.97078200	1.44509200	0.20662200
C	3.26420100	0.97535400	0.21122100
C	3.50199200	-0.39041300	-0.07777500
C	2.41337800	-1.25307200	-0.38356700
C	-0.42903000	1.16545800	0.02133800
C	-1.72939400	0.59062000	0.05046800
C	-2.82666300	1.44811700	-0.24310400
C	-4.12231800	0.96593100	-0.27175700
C	-4.39656500	-0.38048000	0.03269600
C	-3.31849200	-1.22467400	0.38020300
C	-2.01777500	-0.76214200	0.38824700
O	4.69878300	-0.95598100	-0.11512000
H	-2.63469900	2.49243600	-0.47406100
H	-4.94123300	1.63487200	-0.51869000
H	-3.52226200	-2.25293300	0.66517600
H	-1.22507500	-1.42108100	0.72164900
H	-0.42748500	2.25532600	0.04557800
H	1.78779200	2.49346900	0.42566100
H	4.08523400	1.64855000	0.42491100
H	2.63805600	-2.27980000	-0.65144600
H	0.32153600	-1.43915800	-0.65713400
C	5.88598700	-0.18346000	0.15038200
H	6.71031700	-0.88814300	0.05431500
H	5.99216900	0.61922600	-0.58531000
H	5.85817600	0.22369300	1.16544400
C	-5.80008400	-0.91328500	-0.00060000
H	-5.95834300	-1.50310100	-0.91405700
H	-5.99382100	-1.58011900	0.84619900
H	-6.54112600	-0.10998900	0.00805900

i

C	-0.11964300	-0.91204600	-0.50842000
C	-0.33306000	0.44604100	-0.11398300
C	0.82407500	1.24492300	0.13782200
C	2.09863600	0.72718900	0.08137600
C	2.27105300	-0.62818400	-0.27690900
C	1.14679000	-1.43402900	-0.58876100
C	-1.59227300	1.07256700	0.01208800
C	-2.90808800	0.55996700	0.07456000
C	-3.97921100	1.48786800	-0.08811700
C	-5.29967800	1.09217100	-0.08656600
C	-5.60991000	-0.27097000	0.12293900
C	-4.56646900	-1.20768200	0.34599600
C	-3.25570500	-0.80538900	0.32158800
O	-6.83976400	-0.77185500	0.15641100
C	-7.97995100	0.08490700	-0.03134100
O	3.45612700	-1.23486400	-0.37593800
H	-1.53926300	2.15967700	0.07238100
H	-2.48391800	-1.52835400	0.55444900
H	-4.84117100	-2.23575300	0.55600200

H	-6.08373000	1.82431700	-0.23542600
H	-3.74335000	2.53658200	-0.24703500
H	-0.95770500	-1.52825200	-0.80918200
H	1.32165800	-2.45530300	-0.90954700
H	2.96166200	1.34522300	0.29715400
H	0.68918600	2.28830500	0.40997500
H	-8.84527000	-0.57267800	0.03647000
H	-8.02522400	0.84297600	0.75667500
H	-7.94759000	0.55810200	-1.01761900
C	4.65460100	-0.53526700	-0.10911100
C	5.16875500	-0.55972300	1.18311200
C	5.31884800	0.07769300	-1.16639600
C	6.39359900	0.06712000	1.42205200
H	4.62945900	-1.07021500	1.97474100
C	6.54255400	0.69992700	-0.91010300
H	4.89333100	0.05310800	-2.16460900
C	7.07795600	0.69654300	0.37986100
H	6.81347900	0.05571800	2.42325600
H	7.07820500	1.18073700	-1.72296500
H	8.03203900	1.17780700	0.57137600

j

C	2.40028300	1.43993200	-0.18942700
C	1.29048900	0.57691600	0.05443300
C	1.57865900	-0.78839200	0.37047500
C	2.86851300	-1.25312300	0.38557400
C	3.94925100	-0.38330900	0.08229000
C	3.69935300	0.97963600	-0.19879800
C	0.00003000	1.14931400	-0.00049000
C	-1.29053300	0.57693100	-0.05519900
C	-2.40015500	1.43992700	0.18928100
C	-3.69924700	0.97960700	0.19907100
C	-3.94926100	-0.38325000	-0.08219900
C	-2.86868700	-1.25298500	-0.38619600
C	-1.57880100	-0.78826500	-0.37146000
O	-5.15364400	-0.94171900	-0.11342100
C	-6.32848000	-0.15520300	0.15391000
O	5.15358400	-0.94175300	0.11400600
C	6.32861200	-0.15519100	-0.15247400
H	0.00002100	2.23936700	-0.00063900
H	0.77959800	-1.45788600	0.66344600
H	3.09931900	-2.28001700	0.64766200
H	4.51359000	1.66164900	-0.41063300
H	2.21058100	2.48836200	-0.40277500
H	-0.77985300	-1.45767500	-0.66494300
H	-3.09958000	-2.27979700	-0.64852700
H	-4.51338900	1.66159000	0.41136100
H	-2.21041100	2.48833200	0.40269000
H	-7.16261000	-0.84962200	0.06598300
H	-6.29224300	0.25790300	1.16663500
H	-6.43075400	0.64601100	-0.58441700
H	7.16264900	-0.84969300	-0.06435700
H	6.29285800	0.25822900	-1.16508200
H	6.43054800	0.64576700	0.58617100

k

C	2.37769100	2.00468200	0.33169000
C	1.29401000	1.12103700	0.02113600
C	1.59915200	-0.24720700	-0.28134600
C	2.89644500	-0.68351300	-0.21594100
C	3.92663100	0.21809700	0.14701000
C	3.68423100	1.57358100	0.41865300
C	-0.00000500	1.68855700	-0.00003500
C	-1.29403100	1.12104000	-0.02117600
C	-1.59915700	-0.24719000	0.28132000
C	-2.89646900	-0.68348800	0.21597500
C	-3.92666000	0.21809300	-0.14695700
C	-3.68426300	1.57359200	-0.41857300
C	-2.37771700	2.00468800	-0.33168300
H	2.15152800	3.04809900	0.53219700
O	5.13294200	-0.33278600	0.16641900
H	0.81727100	-0.91620700	-0.62087900
H	-0.00001300	2.77818800	-0.00007600
H	-2.15157200	3.04809600	-0.53225800
O	-5.13296100	-0.33281100	-0.16644400
H	-0.81727900	-0.91623800	0.62074700
C	5.01853900	-1.76547300	-0.13487100
H	5.32580700	-2.29807500	0.76790400
H	5.72947300	-1.97223700	-0.93568300
C	-5.01843300	-1.76562100	0.13464000
H	-5.72956000	-1.97261200	0.93521100
H	-5.32532800	-2.29805400	-0.76835500
C	3.53964100	-2.01802300	-0.52147000
H	3.43947300	-2.27772100	-1.58120700
H	3.10515700	-2.83684900	0.06032600
C	-3.53961100	-2.01792400	0.52167100
H	-3.43979800	-2.27722500	1.58155400
H	-3.10492500	-2.83699800	-0.05961900

H	4.49945800	2.24151600	0.67220800
H	-4.49949500	2.24152200	-0.67211900

l

C	1.55043800	0.15283400	-0.01012700
C	1.27377200	-1.24693300	0.00416600
C	2.40775500	-2.11593900	-0.01567800
C	3.69127000	-1.64700500	-0.12827600
C	3.94932000	-0.24583600	-0.20002500
C	2.83112600	0.63849000	-0.10065700
C	-0.00768400	-1.83204000	0.08408600
C	-1.30490000	-1.31007200	-0.10667600
C	-2.41539200	-2.10245400	0.31715900
C	-3.71178800	-1.66970600	0.20685600
C	-4.00890100	-0.40673900	-0.38643900
C	-2.91164700	0.37503600	-0.86074900
C	-1.61784600	-0.06277500	-0.72407700
N	-5.30631400	0.00229300	-0.52561400
N	5.22737200	0.21459100	-0.35255400
C	-5.68305600	1.19266900	-1.28342700
C	5.53366600	1.61928200	-0.60964300
H	-0.82623500	0.54534500	-1.14447700
H	-3.08355300	1.33929900	-1.31822900
H	-4.52115000	-2.29804900	0.55547800
H	-2.22271600	-3.07464000	0.76332000
H	0.00697200	-2.89148200	0.34122300
H	2.24314800	-3.18940400	0.02548700
H	4.51812600	-2.34407800	-0.16979900
H	2.98590200	1.70573700	-0.02641300
H	0.74384200	0.86290200	0.12795200
H	-5.00755200	1.35244900	-2.12671500
H	-6.68631800	1.03913600	-1.68565200
H	4.72914600	2.09800400	-1.17214800
H	6.44037500	1.66775300	-1.21626700
C	-5.72275400	2.47431000	-0.45105900
F	-6.09496600	3.49968700	-1.23605000
F	-4.51323300	2.76616100	0.07573200
F	-6.59527100	2.37833700	0.56667300
C	5.79131300	2.44365900	0.65202700
F	6.83243800	1.96563500	1.35452200
F	6.06037900	3.71317000	0.30277700
F	4.71666500	2.45173300	1.47110300
C	6.35708500	-0.69286800	-0.32516900
C	6.92277100	-1.11968300	-1.52987900
C	6.88123900	-1.11480600	0.89915700
C	8.02560700	-1.97434800	-1.50608900
H	6.49871500	-0.78960700	-2.47431200
C	7.98029500	-1.97435800	0.91335100
H	6.44020700	-0.76070900	1.82526900
C	8.55312800	-2.40274700	-0.28606700
H	8.46789500	-2.30734600	-2.44017000
H	8.39313500	-2.30124600	1.86293100
H	9.41145900	-3.06764100	-0.27013800
C	-6.39720300	-0.76382400	0.04286500
C	-7.14620200	-1.60715400	-0.78259500
C	-6.70648100	-0.63282700	1.39904600
C	-8.21655700	-2.32235800	-0.24391000
H	-6.88883900	-1.70455500	-1.83379800
C	-7.77431500	-1.35693200	1.93045900
H	-6.12563600	0.03958200	2.02206400
C	-8.52970200	-2.19881600	1.11140200
H	-8.80094600	-2.97766100	-0.88270700
H	-8.02049100	-1.25460800	2.98304200
H	-9.36314500	-2.75620400	1.52824000

m

C	1.54988600	-0.40883500	-0.03808400
C	1.26490400	-1.80640400	0.03006900
C	2.39011800	-2.68346200	-0.02083900
C	3.67058200	-2.22723100	-0.20929600
C	3.93581700	-0.83070200	-0.33636100
C	2.82619700	0.06345600	-0.20730500
C	-0.01373700	-2.38027400	0.19359600
C	-1.31645700	-1.85283700	0.06427400
C	-2.40363600	-2.62650200	0.57083800
C	-3.70240500	-2.18529000	0.52926300
C	-4.02936100	-0.93360400	-0.07383700
C	-2.95441300	-0.17239100	-0.63031300
C	-1.65840900	-0.61593900	-0.56056200
N	-5.32319900	-0.51268500	-0.13203800
C	-6.38669400	-1.24879300	0.56446600
N	5.20377200	-0.38501100	-0.55168000
C	6.34479200	-1.30926500	-0.50620900
C	-5.73695200	0.64726400	-0.90912000
C	5.49955100	1.00069400	-0.88739400
H	-0.88953000	-0.02076200	-1.03744100
H	-3.14554100	0.78640300	-1.09214500
H	-4.48250100	-2.81396000	0.93795700

H	-2.19159200	-3.59066000	1.02542400
H	0.00867600	-3.43322800	0.47525800
H	2.22171900	-3.75408900	0.05906800
H	4.47824600	-2.94435700	-0.27461300
H	2.99143700	1.13125100	-0.16510500
H	0.75696200	0.31145800	0.12342900
H	-5.07891000	0.80281700	-1.76516500
H	-6.74100800	0.47151100	-1.30342200
H	-7.28776700	-0.63781700	0.57205000
H	-6.60573600	-2.20117500	0.06705700
H	-6.10487400	-1.43918700	1.60343400
H	4.64981100	1.47265600	-1.38255400
H	6.33721200	1.02624200	-1.58939500
H	7.26593800	-0.72944600	-0.52287500
H	6.33299800	-1.88972600	0.42024200
H	6.33803700	-1.99284000	-1.36343700
C	-5.78288000	1.93779500	-0.09204700
F	-6.20331600	2.94849700	-0.86917000
F	-4.56611200	2.25610800	0.39603200
F	-6.62532800	1.82293400	0.95264700
C	5.88726400	1.84954700	0.32289700
F	6.96892200	1.34440800	0.94663400
F	6.17091100	3.09951600	-0.07598400
F	4.88574500	1.90914100	1.22473400

n

C	-1.58117700	-0.11409200	0.34236600
C	-1.28807400	-1.47635300	0.02639000
C	-2.41049600	-2.32022000	-0.23905900
C	-3.69819500	-1.84740100	-0.26143300
C	-3.96905700	-0.47461600	0.00917300
C	-2.86442900	0.37044300	0.33210900
C	0.00001100	-2.05188200	-0.00007100
C	1.28811700	-1.47637300	-0.02651900
C	2.41051200	-2.32024900	0.23898200
C	3.69822000	-1.84744000	0.26138300
C	3.96909600	-0.47467300	-0.00927200
C	2.86449600	0.37039800	-0.33223200
C	1.58123400	-0.11412300	-0.34250800
N	5.24871300	0.01641300	0.01002500
N	-5.24867400	0.01642700	-0.01006600
H	0.78546400	0.54375200	-0.67141000
H	3.05280400	1.39846400	-0.61685800
H	4.51523000	-2.51575200	0.50306900
H	2.23118800	-3.36677100	0.47113900
H	0.00000500	-3.14204600	-0.00007000
H	-2.23119200	-3.36675600	-0.47117500
H	-4.51522500	-2.51571700	-0.50304500
H	-3.05271600	1.39850600	0.61675400
H	-0.78539700	0.54377200	0.67126600
C	-6.39384100	-0.85461700	0.06307100
C	-6.53997600	-1.73423000	1.14272800
C	-7.37699800	-0.78564000	-0.93011800
C	-7.66464700	-2.55580300	1.21513900
H	-5.78229300	-1.76491300	1.92008900
C	-8.50066400	-1.60609100	-0.84509200
H	-7.25846400	-0.09372400	-1.75804400
C	-8.64607400	-2.49383100	0.22357800
H	-7.77860900	-3.23481700	2.05498300
H	-9.26146000	-1.55362200	-1.61815500
H	-9.52322900	-3.13075200	0.28620800
C	-5.51326200	1.42777800	-0.11309800
C	-6.34000800	2.04625700	0.83165400
C	-4.98092100	2.16698300	-1.17690100
C	-6.62319200	3.40598900	0.71454800
H	-6.75593500	1.46278000	1.64695500
C	-5.26494300	3.52829900	-1.28153600
H	-4.36010000	1.67356700	-1.91875900
C	-6.08565900	4.15033300	-0.33828500
H	-7.26301300	3.88446500	1.45000900
H	-4.85573200	4.09858000	-2.11028500
H	-6.31069000	5.20890600	-0.42664700
C	5.51319400	1.42776900	0.11309600
C	6.34005700	2.04630700	-0.83151700
C	4.98059600	2.16695300	1.17678800
C	6.62312000	3.40606100	-0.71437400
H	6.75617200	1.46285400	-1.64674000
C	5.26449400	3.52829100	1.28145900
H	4.35967000	1.67349700	1.91853200
C	6.08533800	4.15037600	0.33835200
H	7.26303600	3.88457700	-1.44972600
H	4.85508400	4.09855000	2.11012400
H	6.31027200	5.20896800	0.42674200
C	6.39393000	-0.85456800	-0.06304700
C	6.54020900	-1.73414000	-1.14272200
C	7.37701600	-0.78555200	0.93021000
C	7.66493600	-2.55564000	-1.21507100
H	5.78259100	-1.76483700	-1.92014500

C	8.50074200	-1.60593000	0.84524500
H	7.25837800	-0.09366200	1.75814300
C	8.64628300	-2.49363700	-0.22343300
H	7.77900900	-3.23462000	-2.05492800
H	9.26147800	-1.55343300	1.61836400
H	9.52348200	-3.13050300	-0.28601300

o

C	-1.59018600	-0.16918800	0.13084500
C	-1.28709100	1.22073900	0.00999300
C	-2.40890100	2.09390500	-0.12039000
C	-3.69882100	1.63525600	-0.19911700
C	-3.99281200	0.23724800	-0.12330700
C	-2.87528000	-0.64120300	0.06498000
C	0.00160600	1.79279600	0.04108400
C	1.29172600	1.23343800	-0.06726600
C	2.41295200	2.05708100	0.25559000
C	3.70486600	1.60152700	0.20825600
C	4.00154400	0.25973800	-0.18992700
C	2.88601700	-0.54963000	-0.58599700
C	1.59793600	-0.08322800	-0.52452200
N	5.27193400	-0.22382500	-0.21102700
C	5.59304500	-1.62828700	-0.51589000
N	-5.26627900	-0.23304600	-0.19118900
C	-5.60805100	-1.63477400	-0.49281200
C	6.47352700	0.63033500	-0.19706200
C	-6.45093700	0.64089000	-0.22675800
H	0.80749600	-0.71793300	-0.90727600
H	3.05134200	-1.53376500	-1.00389800
H	4.49555700	2.27828600	0.50261700
H	2.23164200	3.07796000	0.58159100
H	0.00026300	2.87510800	0.17209000
H	-2.22995300	3.16276400	-0.20273500
H	-4.49035800	2.35570500	-0.35552000
H	-3.03511000	-1.70056400	0.21624200
H	-0.79801800	-0.87553900	0.34844100
H	6.85183600	0.70354300	-1.22628000
H	6.23199300	1.63452200	0.14416000
H	4.72226400	-2.25910600	-0.34174600
H	5.88804300	-1.71523500	-1.57081400
H	-6.20294500	1.62944600	0.15723000
H	-6.79795000	0.74201900	-1.26429000
H	-5.92249900	-1.68768700	-1.54460700
H	-4.74230400	-2.28207900	-0.37042900
C	-7.56978800	0.04988200	0.64106600
H	-8.47933800	0.64334300	0.51697200
H	-7.26886300	0.08213300	1.70067000
C	-6.75639100	-2.11684700	0.39620500
H	-6.42824600	-2.15433000	1.44757200
H	-7.06691700	-3.11877600	0.08851000
C	7.56112300	0.02832200	0.69523800
H	8.47857600	0.61547700	0.60418600
H	7.23504800	0.04145100	1.74776600
C	6.73250000	-2.12115400	0.38539700
H	6.38009100	-2.17081400	1.42839500
H	7.03798000	-3.12249800	0.07074000
O	7.87299900	-1.29128000	0.28826100
O	-7.88558900	-1.27452000	0.25702600

p

C	-1.61156700	-0.65879600	0.27326200
C	-1.29257300	-2.02651700	0.00421300
C	-2.39833400	-2.89616100	-0.24143200
C	-3.69429400	-2.44741600	-0.29036500
C	-3.99267000	-1.06974200	-0.06658800
C	-2.90081800	-0.19643700	0.23951000
C	-0.00000100	-2.59176900	0.00004900
C	1.29257200	-2.02651800	-0.00415300
C	2.39833400	-2.89614700	0.24153800
C	3.69429600	-2.44740000	0.29042600
C	3.99267100	-1.06974400	0.06655300
C	2.90081600	-0.19645300	-0.23957500
C	1.61156400	-0.65881200	-0.27328500
N	5.27065600	-0.61171300	0.09915100
C	6.40071000	-1.53136700	0.28834500
N	-5.27065000	-0.61170700	-0.09926300
C	-6.40069900	-1.53136100	-0.28849100
H	0.82956200	0.02708000	-0.57548800
H	3.10684300	0.83888300	-0.48134700
H	4.48854800	-3.15020200	0.50710800
H	2.20120100	-3.94918700	0.42479900
H	-0.00000100	-3.68200000	0.00008200
H	-2.20120100	-3.94921500	-0.42461500
H	-4.48854600	-3.15023300	-0.50699300
H	-3.10684600	0.83891500	0.48121500
H	-0.82956700	0.02711400	0.57543000
H	7.32405000	-0.96352100	0.18290500
H	6.38174400	-1.98180700	1.28821000

H	6.38790600	-2.32735900	-0.46317800
H	-7.32403900	-0.96346500	-0.18332400
H	-6.38156100	-1.98198100	-1.28827100
H	-6.38806100	-2.32722300	0.46317600
C	-5.57642800	0.79592400	-0.02444000
C	-5.29755200	1.62808900	-1.11356100
C	-6.19252500	1.30965000	1.12081500
C	-5.63264400	2.98107900	-1.05016800
H	-4.83118300	1.21299400	-2.00233100
C	-6.52992300	2.66250700	1.17349000
H	-6.39927800	0.65447700	1.96223000
C	-6.24992500	3.49863300	0.09050900
H	-5.42048000	3.62705300	-1.89697000
H	-7.00797500	3.06234900	2.06273900
H	-6.51488600	4.55077700	0.13443300
C	5.57643000	0.79592200	0.02439800
C	6.19258300	1.30969400	-1.12080800
C	5.29749400	1.62804600	1.11353300
C	6.52997500	2.66255300	-1.17341800
H	6.39937900	0.65455200	-1.96223700
C	5.63258100	2.98104100	1.05020500
H	4.83108500	1.21292000	2.00226700
C	6.24991800	3.49863900	-0.09042100
H	7.00806900	3.06243000	-2.06262800
H	5.42037200	3.62698200	1.89702100
H	6.51487700	4.55078600	-0.13429600

q

C	-2.40747800	-1.70744400	-0.20544900
C	-1.29051100	-0.84970700	0.03587600
C	-1.59368600	0.51275600	0.33805200
C	-2.88125600	0.98482600	0.34060400
C	-3.98692700	0.12912900	0.02988000
C	-3.69897600	-1.24747300	-0.22659400
C	0.00000800	-1.41872900	0.00010500
C	1.29049400	-0.84968200	-0.03563900
C	2.40750900	-1.70743400	0.20549200
C	3.69900300	-1.24747300	0.22653400
C	3.98693200	0.12915300	-0.02988800
C	2.88119900	0.98491000	-0.34026400
C	1.59363700	0.51284000	-0.33762400
H	-0.80022700	1.18755500	0.63579100
H	-3.05738300	2.01819800	0.61031400
N	-5.25483900	0.60129000	0.00501600
H	-4.50160900	-1.94261600	-0.43588300
H	-2.22196900	-2.75935400	-0.40625300
H	0.00001700	-2.50905000	0.00012100
H	2.22200700	-2.75935900	0.40623300
H	4.50166100	-1.94262400	0.43570500
N	5.25486200	0.60125900	-0.00537600
H	3.05729200	2.01834800	-0.60974300
H	0.80013300	1.18769700	-0.63510900
C	-6.37928300	-0.29823100	-0.26630600
C	-5.53258900	2.01405500	0.27592500
H	-7.30485500	0.27553800	-0.25097700
H	-6.28119200	-0.76469600	-1.25292000
H	-6.45035800	-1.08528500	0.49315600
H	-6.59825100	2.19758600	0.14591000
H	-5.26039900	2.28482800	1.30301900
H	-4.98718100	2.66177200	-0.41882800
C	6.37933600	-0.29826900	0.26587000
C	5.53256600	2.01409000	-0.27605900
H	7.30495100	0.27541100	0.24994300
H	6.28158000	-0.76435600	1.25269700
H	6.45002100	-1.08560000	-0.49333000
H	6.59840500	2.19737000	-0.14716100
H	5.25932100	2.28523500	-1.30276300
H	4.98800700	2.66167000	0.41949900

r

C	-1.59386600	-0.26696100	-0.33652100
C	-1.29066100	1.09756500	-0.03877900
C	-2.40797500	1.95809700	0.19679300
C	-3.69973300	1.50043600	0.21413000
C	-3.98578200	0.12288100	-0.03964400
C	-2.88112000	-0.73816400	-0.34002900
C	-0.00000500	1.66542800	-0.00004700
C	1.29065200	1.09756000	0.03859900
C	2.40796300	1.95814000	-0.19679600
C	3.69973000	1.50050200	-0.21411800
C	3.98578800	0.12291500	0.03949800
C	2.88111400	-0.73821300	0.33958700
C	1.59385500	-0.26702500	0.33607800
N	5.24756300	-0.34492900	0.02279300
C	5.60845000	-1.76706200	0.18954100
N	-5.24757100	-0.34492600	-0.02294500
C	-5.60852600	-1.76709500	-0.18952100
C	6.44208200	0.50159000	-0.17216400

C	-6.44202800	0.50155100	0.17264100
H	0.79956700	-0.94203500	0.63122800
H	3.06613100	-1.77038200	0.61170100
H	4.50704600	2.18947000	-0.43003400
H	2.22008300	3.00926300	-0.39983700
H	-0.00000400	2.75576800	0.00005700
H	-2.22010000	3.00919000	0.39999600
H	-4.50705500	2.18935900	0.43017700
H	-3.06613600	-1.77026900	-0.61238000
H	-0.79958300	-0.94190100	-0.63185100
H	6.48695400	0.84940500	-1.21318000
H	6.39910700	1.37980000	0.47957800
H	5.46885700	-2.06882200	1.23670200
H	4.97052400	-2.39870600	-0.43624800
H	-6.48659700	0.84898000	1.21379900
H	-6.39921300	1.38001100	-0.47878100
H	-5.46915600	-2.06892700	-1.23668500
H	-4.97047400	-2.39868000	0.43619300
C	7.08491000	-1.82031300	-0.22343200
H	7.61847800	-2.63738100	0.26830200
H	7.16473400	-1.96918800	-1.30605500
C	7.61248300	-0.43110600	0.16643300
H	7.82395900	-0.39099600	1.24078100
H	8.52513900	-0.15211200	-0.36574900
C	-7.08491400	-1.82027300	0.22372000
H	-7.61864900	-2.63730300	-0.26791500
H	-7.16455600	-1.96912100	1.30635000
C	-7.61242700	-0.43103700	-0.16606900
H	-7.82374900	-0.39085300	-1.24044900
H	-8.52519800	-0.15208600	0.36596400

s

C	-1.48262100	0.81225900	-0.45710400
C	-1.16579700	-0.54315000	-0.14930500
C	-2.27439000	-1.41915900	0.06870200
C	-3.58364900	-1.00678500	0.05570100
C	-3.87383800	0.37749900	-0.20639700
C	-2.78065100	1.25538400	-0.48686500
C	0.13341100	-1.09063500	-0.08812200
C	1.41350100	-0.50143100	-0.01698700
C	2.54513200	-1.34034700	-0.24782600
C	3.83527300	-0.86920500	-0.24586000
C	4.05967200	0.51040100	0.06091200
C	2.95281600	1.37560300	0.36527000
C	1.67877700	0.86227000	0.31208800
N	5.31990900	0.99577600	0.10160400
N	-5.14956600	0.83353200	-0.21495600
C	6.53003400	0.20706300	-0.14877700
C	-6.29869400	-0.03553300	0.09765600
H	0.85765800	1.50954500	0.59714900
H	2.37344600	-2.39176300	-0.46843800
H	0.15182500	-2.18085800	-0.09744200
H	-2.06643700	-2.46667700	0.27654300
H	-0.69540600	1.50382500	-0.73151800
H	7.33196800	0.61930400	0.47118700
H	6.83237300	0.32200500	-1.19923700
H	-7.03670800	0.57522600	0.62680700
H	-6.76299700	-0.36644100	-0.84286200
C	-4.72461600	-1.96876200	0.29723800
H	-5.05312300	-2.40476400	-0.65751700
H	-4.38800500	-2.80290700	0.92149900
C	5.02389400	-1.75687100	-0.55125800
H	5.21220800	-1.76070600	-1.63467700
H	4.79691500	-2.79155400	-0.27322000
C	6.28165900	-1.26484200	0.17687400
H	6.15929800	-1.38355000	1.26007700
H	7.15580400	-1.85165900	-0.12106600
C	-5.89905900	-1.23529900	0.94895800
H	-6.76484700	-1.89603400	1.05656000
H	-5.61848800	-0.89629600	1.95348600
H	-2.97319400	2.28873300	-0.74549800
H	5.44206300	1.98037700	0.29113600
C	-5.45825000	2.20861800	-0.60737100
H	-5.04900300	2.93055900	0.10916500
H	-5.06488800	2.43476900	-1.60445700
H	-6.54147900	2.32949300	-0.63493900
C	3.20494100	2.80904300	0.76181200
H	3.84202300	2.87991600	1.65385100
H	3.69458300	3.37772600	-0.04106100
H	2.26673800	3.31985600	0.99191000

t

C	1.61782000	0.28113100	0.25477300
C	1.29535000	-1.09444000	-0.00683700
C	2.38438500	-1.98637200	-0.26360900
C	3.69588900	-1.57341800	-0.32697000
C	3.97184600	-0.20596500	-0.09542800
C	2.91445800	0.70563300	0.21098200

C	0.00001700	-1.65509800	-0.00016500
C	-1.29534300	-1.09447500	0.00651200
C	-2.38433100	-1.98641500	0.26343200
C	-3.69583500	-1.57347200	0.32689700
C	-3.97182700	-0.20603200	0.09530700
C	-2.91450900	0.70553500	-0.21140000
C	-1.61786500	0.28105200	-0.25524800
N	-5.16242200	0.42444600	0.08769000
C	-6.46575600	-0.19009300	0.25462900
N	5.16244500	0.42453300	-0.08757600
C	6.46586200	-0.19010300	-0.25354700
C	-5.04227800	1.82465000	-0.35794500
C	5.04218800	1.82447300	0.35888500
H	-0.83809800	0.97556100	-0.54451300
H	-2.15829100	-3.03591300	0.43191000
H	0.00002300	-2.74488200	-0.00016200
H	2.15837400	-3.03588900	-0.43201300
H	0.83801000	0.97567200	0.54383900
H	-5.53997700	1.94240500	-1.32939600
H	-5.54615900	2.48403000	0.35662900
H	-7.13356700	0.51359400	0.76032400
H	-6.91041300	-0.46013800	-0.71282000
H	-6.38416300	-1.08696600	0.87164700
H	5.53855500	1.94128100	1.33115100
H	5.54728600	2.48422900	-0.35446000
H	7.13394000	0.51332000	-0.75925700
H	6.91000800	-0.45966000	0.71427800
H	6.38456900	-1.08728500	-0.87014500
C	3.51421300	2.07803100	0.44256800
H	3.19010400	2.78502000	-0.32937900
H	3.22766600	2.50185500	1.40988500
C	-3.51430900	2.07782700	-0.44350700
H	-3.22878600	2.50052400	-1.41163200
H	-3.18917400	2.78562500	0.32724700
H	4.48916100	-2.28494300	-0.52632000
H	-4.48908100	-2.28498400	0.52640200

u

C	-1.61748100	0.44861600	-0.34388500
C	-1.29346200	-0.92019900	-0.10733500
C	-2.39397000	-1.80271100	0.11201100
C	-3.69938000	-1.38154100	0.15466600
C	-3.98939600	0.01193900	-0.03885100
C	-2.90659200	0.92173500	-0.30680400
C	0.00269400	-1.47630500	-0.11053700
C	1.29384400	-0.90640500	-0.07408500
C	2.40375600	-1.75806100	-0.35034100
C	3.70534500	-1.32015700	-0.36936700
C	3.98581100	0.05021000	-0.04057800
C	2.88955900	0.92873200	0.27663300
C	1.60343300	0.44416800	0.25872400
N	5.26776000	0.50165200	0.00334400
N	-5.26892100	0.45949200	0.00395100
C	6.40268500	-0.35103800	-0.38268100
C	-6.40315600	-0.39962800	0.37960300
H	0.80847600	1.11439900	0.56571600
H	2.20658400	-2.80163500	-0.58662200
H	0.00919700	-2.56603900	-0.14698500
H	-2.18497500	-2.85858200	0.26989700
H	-0.83086300	1.14479400	-0.61173200
H	7.28110700	0.00825600	0.16145200
H	6.60953100	-0.21840200	-1.45538600
H	-7.08628600	0.21004900	0.98230800
H	-6.94604100	-0.68438200	-0.53374100
C	-4.83957800	-2.34452300	0.39474600
H	-5.22564400	-2.71646400	-0.56571500
H	-4.48250300	-3.21948200	0.94754700
C	4.83585400	-2.25975200	-0.73054100
H	4.97087400	-2.27123800	-1.82191600
H	4.57599800	-3.28347100	-0.44075900
C	6.14069500	-1.81964000	-0.06710600
H	6.07888800	-1.95397400	1.01948400
H	6.98370500	-2.41936600	-0.42435500
C	-5.96640000	-1.63850900	1.15245400
H	-6.82986400	-2.29814600	1.28302600
H	-5.62095100	-1.34917400	2.15232100
C	-5.64054200	1.84236800	-0.33180800
H	-5.79558900	2.40520100	0.60063100
H	-6.60675800	1.80254400	-0.84735400
C	3.16173800	2.37534600	0.63326900
H	2.39998700	2.73575900	1.33308100
H	3.07427900	2.99783200	-0.26941400
C	-3.21600700	2.38043300	-0.55937500
H	-3.20268500	2.93453000	0.39097000
H	-2.43824900	2.82415900	-1.18994400
C	4.56340300	2.54170700	1.21940100
H	4.80689400	3.59982900	1.35749200
H	4.62484000	2.05886100	2.20203000

C	-4.59544600	2.52574800	-1.20524800
H	-4.86561100	3.57926100	-1.32724900
H	-4.59242600	2.06996000	-2.20274100
C	5.58420400	1.91051300	0.27933400
H	5.63215000	2.46825800	-0.66828000
H	6.58440500	1.94039000	0.72137200

v

C	-1.59099900	0.65397200	-0.37819000
C	-1.29315800	-0.72798500	-0.11191600
C	-2.39159800	-1.62572000	0.10719900
C	-3.70547200	-1.21545800	0.13323400
C	-3.93026800	0.16269200	-0.09196100
C	-2.88737400	1.08612100	-0.36492500
C	0.00272100	-1.28793700	-0.08592000
C	1.29386800	-0.72024900	-0.02440200
C	2.40010500	-1.59387100	-0.29623500
C	3.70947300	-1.16887900	-0.30668600
C	3.92452200	0.18787500	0.02998100
C	2.87306500	1.08571500	0.35200600
C	1.57972900	0.64515800	0.32730600
N	5.12892700	0.77511400	0.12271900
C	5.01562300	2.21118800	0.42273500
N	-5.13796900	0.75046300	-0.11860000
C	-5.05271500	2.16173300	-0.52613700
C	6.36902000	0.06337600	-0.16636600
C	-6.37448200	-0.00075900	0.06455900
H	0.77529000	1.30405800	0.63195800
H	2.18126000	-2.63251100	-0.53502800
H	0.00722800	-2.37741800	-0.11837400
H	-2.16376600	-2.67583100	0.27755200
H	-0.79316700	1.33628300	-0.64638900
H	7.15669000	0.46070200	0.48317300
H	6.67387400	0.25700100	-1.20570600
H	5.65959600	2.46904200	1.27026500
H	5.34781300	2.80078400	-0.44161200
H	-7.10116100	0.64358100	0.57165600
H	-6.79809700	-0.26208100	-0.91700600
H	-5.56302300	2.79611400	0.20676800
H	-5.55304600	2.29994700	-1.49319900
C	-3.52079700	2.44506000	-0.60770500
H	-3.24398900	2.86611500	-1.57927800
H	-3.21502500	3.16877100	0.15589100
C	3.49991800	2.41735900	0.72714200
H	3.08757300	3.25215200	0.15246500
H	3.34067000	2.64542700	1.78720400
C	-4.92348200	-2.09050900	0.33966200
H	-5.21800100	-2.54318100	-0.61806300
H	-4.69368400	-2.92078400	1.01616400
C	4.92959800	-2.00050400	-0.63761000
H	5.09785900	-1.99184000	-1.72410700
H	4.77149800	-3.04752300	-0.35739600
C	6.17728100	-1.44324000	0.07857400
H	6.08643800	-1.61624000	1.15754900
H	7.07453900	-1.97075500	-0.25901700
C	-6.09930800	-1.26313100	0.89865100
H	-7.00907200	-1.87034500	0.92828300
H	-5.87663600	-0.96255100	1.92944500

z1

O	-1.79324800	-1.98274500	-0.60821400
O	-2.04512200	2.25572000	-0.59023300
C	-2.26696600	0.99534300	-0.15796400
C	-1.02564700	0.17823600	-0.07342200
C	-1.29588500	-1.23016600	0.39318400
C	0.19710000	0.70351000	-0.29222500
C	1.50339500	0.03743100	-0.26194100
C	2.63808700	0.83375200	-0.02165100
C	3.90012600	0.25168200	0.02636400
C	4.07518500	-1.11580300	-0.18182100
C	2.95222200	-1.90199300	-0.44792500
C	1.68017200	-1.33918400	-0.49012000
O	-1.10154900	-1.61661800	1.52312100
O	-3.36447800	0.55900400	0.13689000
C	-2.27141000	-3.30685900	-0.24891600
C	-3.20114300	3.12641300	-0.66240800
C	-3.69838200	-3.24245600	0.27282000
C	-3.48536100	3.78280400	0.67988600
Cl	5.30234900	1.26424700	0.34443400
H	0.22673900	1.76870500	-0.50783700
H	2.52950900	1.90160600	0.13940200
H	5.06844700	-1.55021600	-0.14725400
H	3.07755600	-2.96523000	-0.63119600
H	0.82747400	-1.96039900	-0.73811300
H	-2.20584200	-3.87532900	-1.17960200
H	-1.59200100	-3.73790600	0.49039300

H	-2.93201300	3.86404100	-1.42232900
H	-4.05685100	2.54246700	-1.00888100
H	-4.06602800	-4.25620200	0.46995500
H	-3.74411000	-2.66972800	1.20286000
H	-4.35747000	-2.76756800	-0.46006400
H	-4.31619800	4.49036700	0.57726800
H	-3.76403300	3.03233700	1.42481300
H	-2.60890900	4.33169400	1.03952900

z2

O	0.75353100	2.03154700	0.54457600
O	2.38294900	-1.67797600	-0.14191000
C	2.06744800	-0.39618200	-0.43945100
C	0.60543700	-0.11710700	-0.36499200
C	0.28379800	1.34616500	-0.51090000
C	-0.29224000	-1.11348300	-0.18803900
C	-1.75508700	-1.10983500	-0.09005900
C	-2.35036500	-2.20737400	0.56522000
C	-3.73032300	-2.29118300	0.72392100
C	-4.55150400	-1.28729100	0.20639400
C	-3.97976800	-0.20799700	-0.47149400
C	-2.59815100	-0.11344900	-0.62190800
O	-0.31018500	1.84612400	-1.44482600
O	2.88742900	0.44420000	-0.75866300
C	0.60892500	3.47391200	0.50587000
C	3.78310800	-2.03432000	-0.23567700
C	-0.73409600	3.90768700	1.07294200
C	4.52812100	-1.69756600	1.04711300
H	0.15119600	-2.09636200	-0.04656800
H	-1.71360600	-2.99380700	0.96348300
H	-4.16477900	-3.14137000	1.24260200
H	-5.63042000	-1.35235000	0.31890100
H	-4.61555400	0.56424600	-0.89618400
H	-2.17124800	0.71131100	-1.17846800
H	1.43992600	3.84116900	1.11251800
H	0.73566200	3.81036900	-0.52557400
H	3.77331200	-3.11093900	-0.42357900
H	4.22012400	-1.51919400	-1.09436500
H	-0.78825400	5.00210300	1.10313400
H	-1.55348900	3.54036400	0.44870300
H	-0.86825500	3.52839200	2.09124800
H	5.56439900	-2.04804700	0.97678100
H	4.54077600	-0.61663600	1.21092000
H	4.05859300	-2.18227200	1.90939800

z3

O	1.33681000	1.99999500	0.53603200
O	2.56150300	-1.86064100	-0.12405300
C	2.38525600	-0.55151800	-0.42242700
C	0.95951700	-0.12315600	-0.36937800
C	0.78905500	1.36452700	-0.51368300
C	-0.03799800	-1.02558100	-0.21484800
C	-1.49291500	-0.88358500	-0.13988900
C	-2.20685800	-1.94200100	0.45606900
C	-3.59051400	-1.89827800	0.58955300
C	-4.32408500	-0.80449200	0.11307100
C	-3.61848900	0.23615800	-0.51018400
C	-2.23433100	0.20776700	-0.63781400
C	-5.82417600	-0.74004500	0.26757000
O	0.23930100	1.92382200	-1.44151300
O	3.29431200	0.19763100	-0.72774900
C	1.34369400	3.44901300	0.49340700
C	3.91680500	-2.36158700	-0.20448300
C	0.05886500	4.02337300	1.07048900
C	4.67731400	-2.11437200	1.08967800
H	0.30478800	-2.04805800	-0.07459800
H	-1.66083500	-2.80574900	0.82827000
H	-4.11028500	-2.72815600	1.06258700
H	-4.16805800	1.08352800	-0.91445200
H	-1.72651300	1.01149300	-1.15595200
H	-6.24892500	-1.72576100	0.48246100
H	-6.10798000	-0.07260000	1.09226600
H	-6.30414500	-0.35288500	-0.63824200
H	2.21410900	3.72903100	1.09134700
H	1.49544800	3.76819800	-0.54015900
H	3.79664300	-3.43003000	-0.40122000
H	4.41647200	-1.88936000	-1.05361800
H	0.12050000	5.11750400	1.09748700
H	-0.79982800	3.74283200	0.45413000
H	-0.10547800	3.66267900	2.09111500
H	5.67142900	-2.57245400	1.02928800
H	4.80243400	-1.04199400	1.26228000
H	4.14797400	-2.55200000	1.94248500

z4

O	1.77707300	2.00183800	0.48162800
O	2.86359000	-1.87508300	-0.10021600

C	2.69674900	-0.57298800	-0.43940100
C	1.27952200	-0.12283000	-0.35992700
C	1.11890300	1.36359900	-0.50193000
C	0.27448200	-1.01901600	-0.19258900
C	-1.17662100	-0.88821100	-0.10458800
C	-1.88261000	-1.97795800	0.45696400
C	-3.25821500	-1.95999300	0.60256300
C	-3.99226700	-0.84560800	0.16515900
C	-3.31992300	0.23613300	-0.42117600
C	-1.93379800	0.21137000	-0.55209300
O	-5.33794900	-0.91884600	0.34157400
O	0.48422300	1.92803700	-1.37224700
O	3.60874600	0.14706000	-0.80102500
C	1.80742200	3.44866000	0.41893000
C	4.20550800	-2.40221400	-0.21709000
C	0.59917600	4.05695800	1.11477900
C	5.02188600	-2.12528900	1.03649100
C	-6.13962900	0.17273600	-0.08961600
H	0.61923600	-2.04110300	-0.05416200
H	-1.32673500	-2.84899100	0.79559500
H	-3.79264700	-2.79533200	1.04355600
H	-3.86674400	1.09651200	-0.78992500
H	-1.43686800	1.04095200	-1.03872200
H	2.73899900	3.71818800	0.92215800
H	1.85984300	3.75334400	-0.62881900
H	4.06063500	-3.47461300	-0.37190100
H	4.67886500	-1.96804200	-1.10097400
H	0.68718200	5.14960700	1.12516500
H	-0.32238700	3.79136000	0.58926400
H	0.52921000	3.70764300	2.15014600
H	6.00466200	-2.60392800	0.95324800
H	5.17225400	-1.05013400	1.16619300
H	4.51936900	-2.52317000	1.92430900
H	-7.16785400	-0.09904000	0.15457400
H	-5.87335000	1.09875000	0.43565100
H	-6.05265500	0.33185400	-1.17192900

C	-0.91367300	-0.69839300	-0.18286500
C	-1.72498200	-1.77394400	0.24069000
C	-3.09967100	-1.66888400	0.36404700
C	-3.76112200	-0.45588600	0.05172700
C	-2.95720100	0.61720300	-0.40989800
C	-1.58219500	0.49941200	-0.52052100
N	-5.12735800	-0.32628800	0.18273300
O	0.98179900	2.00005200	-1.33428700
O	3.96080600	-0.07128700	-0.75420100
C	2.46472500	3.36788100	0.44869600
C	4.30566900	-2.66743600	-0.20413700
C	1.32586000	4.07477600	1.16874500
C	5.11851000	-2.48297300	1.06895600
C	-5.78732800	0.89768400	-0.24248300
C	-5.93469700	-1.47898300	0.54661500
H	0.77466900	-1.98889200	-0.12861900
H	-1.25214100	-2.72106700	0.49114000
H	-3.66177400	-2.53251300	0.69844600
H	-3.41660200	1.55435600	-0.70089800
H	-1.01759800	1.33648800	-0.91046200
H	3.42360000	3.54832000	0.94072500
H	2.52906700	3.68048000	-0.59616000
H	4.07068600	-3.72080000	-0.37935700
H	4.83497600	-2.26429700	-1.07089700
H	1.51233300	5.15492000	1.19066700
H	0.37729400	3.90004700	0.65328600
H	1.23801000	3.71974800	2.20086000
H	6.05853300	-3.04251000	0.99553000
H	5.35680000	-1.42668000	1.21990400
H	4.56631200	-2.85019700	1.94042200
H	-5.39500900	1.76865300	0.29715500
H	-5.67019400	1.08375500	-1.32041900
H	-6.85386000	0.82310400	-0.02399600
H	-5.86680500	-2.28794100	-0.19600100
H	-5.63235500	-1.88545400	1.52016900
H	-6.97977300	-1.17462400	0.62311200

z5

O	2.30600500	1.93051200	0.49667300
O	3.01530200	-2.02506600	-0.10412200
C	2.97472000	-0.70497800	-0.42449900
C	1.60566400	-0.12947000	-0.36747300
C	1.57815900	1.36500300	-0.48497800
C	0.51823500	-0.93844000	-0.24533100

z6

O	2.38929300	1.90491400	-0.94103300
O	3.35912500	-2.00401600	-0.36181800
C	3.26846500	-0.68565500	-0.04498400
C	1.87161800	-0.18243700	-0.01970500
C	1.78465400	1.30999000	0.10473700
C	0.81967500	-1.04371900	-0.07579500

C	-0.62232100	-0.86911300	-0.05232000
C	-1.40910100	-1.98055900	-0.41658200
C	-2.79191800	-1.92088600	-0.45877100
C	-3.47772500	-0.73216100	-0.11903200
C	-2.70200300	0.38865600	0.29834800
C	-1.31830700	0.30496200	0.31226400
N	-4.85804500	-0.65415100	-0.19799000
O	1.24241000	1.91741000	1.00853500
O	4.23972200	0.00347200	0.21279100
C	2.51947800	3.34544400	-0.89003300
C	4.68369100	-2.57994300	-0.32965300
C	3.73574000	3.75509000	-0.07280100
C	5.07035800	-3.01530300	1.07632500
C	-5.56296100	0.49241700	0.37309900
C	-4.78540500	1.78550800	0.14015200
C	-3.38715800	1.66382100	0.74876500
C	-5.63959000	-1.85194400	-0.44889700
H	1.11743600	-2.08187600	-0.20397100
H	-0.91691600	-2.91236300	-0.68596900
H	-3.34293200	-2.80639700	-0.75133300
H	-0.75886000	1.16782400	0.65343600
H	2.62063900	3.64059800	-1.93742300
H	1.59948500	3.77067200	-0.48089300
H	4.62243400	-3.43353500	-1.00994100
H	5.39425600	-1.85071800	-0.72595300
H	3.87150000	4.84174600	-0.12713300
H	3.60690100	3.47389000	0.97582100
H	4.63771500	3.26762600	-0.45429100
H	6.04662200	-3.51385900	1.05693100
H	5.14022400	-2.14896700	1.73984900
H	4.33425200	-3.71603100	1.48428200
H	-6.54711200	0.55085300	-0.10448000
H	-5.73636300	0.35073800	1.45446200
H	-5.33325200	2.62495000	0.58296200
H	-4.71383900	1.96985700	-0.93893400
H	-3.47084600	1.67199100	1.84584400
H	-2.77167500	2.53119600	0.48474900
H	-5.35005500	-2.31956200	-1.39695200
H	-6.69377000	-1.57532300	-0.52348500
H	-5.53705600	-2.60347900	0.34984000

z7

O	-3.04728800	1.91466700	0.52610400
O	-3.46955200	-2.11677600	0.38671600
C	-3.53840200	-0.84079600	-0.08158900
C	-2.21545700	-0.17038500	-0.14952300
C	-2.30102000	1.30199900	-0.41225800
C	-1.06736400	-0.89301700	-0.01749600
C	0.34501500	-0.56475000	-0.04881900
C	1.24287300	-1.58128100	0.34481000
C	2.61474900	-1.40014900	0.40327500
C	3.16493500	-0.15062900	0.01053600
C	2.28513600	0.87926300	-0.42605500
C	0.91625300	0.66762100	-0.43557900
N	4.52991700	0.05684200	0.04071100
O	-1.77131700	1.89593800	-1.33272900
O	-4.58313700	-0.31865400	-0.42755800
C	-3.30266800	3.32080300	0.31787600
C	-4.70772400	-2.85930400	0.40236400
C	-4.23103500	3.78017700	1.42647800
C	-4.98715600	-3.50928700	-0.94514400
C	5.13473200	1.36249800	-0.21243400
C	4.13616300	2.50727200	-0.06363100
C	2.87307400	2.19921100	-0.87285300
C	3.54127700	-2.50551700	0.85774700
C	4.87856400	-2.40078300	0.11861300
C	5.47921000	-1.01369400	0.33293300
H	-1.24695100	-1.94448900	0.19389900
H	0.83969300	-2.54939300	0.63800700
H	0.27621500	1.46563200	-0.79111700
H	-2.34932500	3.86022600	0.32824000
H	-3.74812400	3.45318800	-0.67309000
H	-4.56307200	-3.60888400	1.18511200
H	-5.51871600	-2.18618600	0.69021600
H	-4.45596100	4.84587100	1.30681800
H	-5.17136500	3.22105200	1.39894300
H	-3.77080100	3.63278500	2.40896900
H	-5.89159700	-4.12581700	-0.88191600
H	-5.14441200	-2.74655100	-1.71282000
H	-4.15365900	-4.15135700	-1.24914700
H	5.57600600	1.37791500	-1.22335200
H	5.96555800	1.49403700	0.49479900
H	4.60760900	3.43829600	-0.39761900
H	3.87445400	2.63279900	0.99447900
H	3.13196000	2.16040800	-1.94210700
H	2.13110200	2.99748800	-0.76322400
H	3.07564400	-3.48275300	0.68596300
H	3.72347100	-2.43402800	1.94116700

H	4.72086400	-2.57131900	-0.95363900
H	5.58945900	-3.15682100	0.47034900
H	6.35274300	-0.87902500	-0.31975800
H	5.84321700	-0.91788300	1.37006800

z8

O	1.90566000	1.96507000	0.60881500
O	3.09200600	-1.89733800	-0.16372300
C	2.95242900	-0.58012400	-0.42302800
C	1.53086100	-0.12059800	-0.37635700
C	1.39544600	1.37662300	-0.48118500
C	0.51372300	-1.00147000	-0.26045100
C	-0.93943400	-0.79803700	-0.20024400
C	-1.69465900	-1.78609700	0.46597800
C	-3.07391700	-1.68287300	0.58816700
C	-3.71029000	-0.58478500	0.01252200
C	-3.00297200	0.39554800	-0.68074700
C	-1.62051500	0.28801200	-0.78709100
N	-5.17246000	-0.46662600	0.12883700
O	0.90026200	1.96633100	-1.42023700
O	3.87512300	0.16409100	-0.69208100
C	1.93781700	3.41782900	0.61757900
C	4.43856600	-2.43145300	-0.23615700
C	0.63625700	3.99292800	1.15340100
C	5.17897700	-2.24442300	1.07891700
O	-5.77021900	-1.35586200	0.73495800
O	-5.70917100	0.51431100	-0.38485900
H	0.81931100	-2.03807700	-0.14133500
H	-1.18443200	-2.63934800	0.90434500
H	-3.65886700	-2.43052100	1.10913600
H	-3.53949600	1.22081900	-1.13250100
H	-1.06722000	1.02993300	-1.34888000
H	2.78354600	3.65880400	1.26519700
H	2.14478100	3.76706100	-0.39630600
H	4.29291400	-3.48885400	-0.46969400
H	4.96324400	-1.94476100	-1.06144900
H	0.71473500	5.08398300	1.22117300
H	-0.19724400	3.75049000	0.48818800
H	0.41833600	3.60142500	2.15226400
H	6.16234600	-2.72491800	1.02031700
H	5.32809900	-1.18195500	1.28968400
H	4.62414600	-2.69703200	1.90719900

z9

O	1.53052000	1.98363500	0.55338400
O	2.75584700	-1.87156400	-0.11796300
C	2.58877600	-0.56605900	-0.42044000
C	1.16046100	-0.13023800	-0.37099500
C	0.99716600	1.36108100	-0.50692900
C	0.16042500	-1.02762500	-0.22777700
C	-1.29600600	-0.85853100	-0.16280900
C	-2.02506800	-1.86189800	0.50844800
C	-3.40500200	-1.79115200	0.63634500
C	-4.10055600	-0.71219000	0.06524200
C	-3.39155500	0.27913800	-0.63420500
C	-2.00848400	0.20782700	-0.74748700
C	-5.52669900	-0.63158000	0.18418800
O	0.46327800	1.92278100	-1.44228000
O	3.49551700	0.18320400	-0.72766100
C	1.54056400	3.43588700	0.52685900
C	4.11037600	-2.38358000	-0.19246700
C	0.24742400	4.00496800	1.08907400
C	4.86759500	-2.13564800	1.10291600
N	-6.68409900	-0.56617100	0.28334500
H	0.48940400	-2.05445700	-0.08763600
H	-1.49239900	-2.70172800	0.94652800
H	-3.95087700	-2.56428000	1.16704700
H	-3.93307400	1.09944700	-1.09420200
H	-1.47726800	0.96229100	-1.31393000
H	2.40187600	3.70517400	1.14206600
H	1.71082600	3.76404100	-0.50082700
H	3.98099900	-3.45134000	-0.38516700
H	4.61370000	-1.91820000	-1.04302100
H	0.31121700	5.09838500	1.12880600
H	-0.60210100	3.73430800	0.45577400
H	0.06599400	3.63429100	2.10308700
H	5.85822200	-2.60131100	1.04648000
H	5.00110600	-1.06371500	1.27205700
H	4.33328100	-2.56655300	1.95591200

x1

C	-3.17976700	-1.67800000	0.00003800
C	-4.50899700	-1.24858300	0.00041100
C	-4.82685000	0.11989600	0.00060400
C	-3.82254100	1.09088900	0.00044100
C	-2.49990600	0.65700500	0.00008300
C	-2.18272700	-0.70632200	-0.00011600

C	-1.24002100	1.45316200	-0.00017200
C	-0.10457000	0.47054500	-0.00032000
C	-0.69899500	-0.89665100	-0.00047900
C	1.16758100	0.95367500	-0.00048200
O	-1.15303700	2.67095000	-0.00028300
O	-0.14872200	-1.99086500	-0.00083200
C	2.48802900	0.34843700	-0.00029600
C	3.59104300	1.23218300	-0.00003300
C	4.89590400	0.75311000	0.00046100
C	5.12775900	-0.62482300	0.00066300
C	4.04845600	-1.51372600	0.00036300
C	2.73985400	-1.04133800	-0.00011000
H	-2.91924700	-2.73212400	-0.00015100
H	-5.31192000	-1.98072400	0.00055500
H	-5.87020800	0.42341900	0.00088600
H	-4.05308900	2.15198000	0.00057700
H	1.18628700	2.04618300	-0.00074400
H	3.40883300	2.30396100	-0.00021500
H	5.73001600	1.44910800	0.00067200
H	6.14610800	-1.00453400	0.00106800
H	4.22914900	-2.58516200	0.00044300
H	1.90263900	-1.72953000	-0.00051100

x2

C	3.93346400	-1.74912700	0.00019700
C	5.27919400	-1.37277500	0.00051100
C	5.65071400	-0.01835800	0.00056400
C	4.68490600	0.99154400	0.00032100
C	3.34655100	0.61033300	0.00001000
C	2.97582000	-0.73910600	-0.00003800
C	2.11706800	1.45500100	-0.00025900
C	0.94784900	0.51883700	-0.00044000
C	1.48422000	-0.86806300	-0.00038000
C	-0.30874700	1.05044000	-0.00045500
O	2.08013900	2.67637400	-0.00014400
O	0.89066800	-1.94088200	-0.00064600
C	-1.64334200	0.49745800	-0.00027800
C	-2.71836200	1.41220100	0.00005800
C	-4.04338000	0.99482500	0.00032000
C	-4.32705000	-0.37956500	0.00027000
C	-3.27117300	-1.31026400	-0.00016000
C	-1.95627900	-0.88554700	-0.00045800
O	-5.57553600	-0.90786300	0.00057300
C	-6.69154900	-0.02578000	0.00028900
H	3.63142800	-2.79220800	0.00014800
H	6.05247300	-2.13629100	0.00071700
H	6.70527700	0.24398400	0.00079200
H	4.95720000	2.04280300	0.00033100
H	-0.28487100	2.14296600	-0.00033400
H	-2.50338600	2.47791000	-0.00002500
H	-4.83798000	1.73166600	0.00037300
H	-3.51845800	-2.36722500	-0.00029700
H	-1.14746400	-1.60742200	-0.00091500
H	-7.57516100	-0.66570000	-0.00035700
H	-6.70077700	0.60786600	0.89596200
H	-6.69987500	0.60829800	-0.89510500

x3

O	-2.19702900	-1.28727700	-0.28136400
O	-2.78738400	0.99630900	-0.26081500
C	-1.49968500	1.42103500	-0.40354600
C	-0.43884200	0.36471600	-0.33210900
C	-0.86488000	-1.04879100	-0.46198100
C	0.83255000	0.85071900	-0.20094000
C	2.17508700	0.30767900	-0.05530900
C	3.18003100	1.26176900	0.23570800
C	4.50492100	0.88560000	0.41848800
C	4.86278800	-0.46011100	0.30614900
C	3.88792300	-1.41635200	0.00886900
C	2.55878500	-1.04683800	-0.17275300
O	-0.16318800	-1.98774800	-0.76857700
O	-1.28936600	2.59451700	-0.60765700
C	-3.03783000	-0.29072000	0.31642200
C	-4.46058600	-0.65668800	-0.06912800
C	-2.81193600	-0.24739800	1.82728500
H	0.82672500	1.93948600	-0.16401200
H	2.90288500	2.30937400	0.32222000
H	5.25627200	1.63686600	0.64410300
H	5.89790400	-0.76140400	0.44354900
H	4.16688000	-2.46186000	-0.08852800
H	1.81193400	-1.78743700	-0.42138700
H	-4.55210200	-0.67036600	-1.15796800
H	-4.70967200	-1.64622400	0.32302500
H	-5.15786300	0.07978200	0.33901400
H	-3.02607000	-1.22796300	2.26157100
H	-3.47390700	0.49637400	2.27961900
H	-1.77721500	0.01922800	2.06318200

x4

O	-2.83058000	-1.38787600	-0.32671100
O	-3.64651500	0.82116300	-0.20081100
C	-2.40539100	1.37797300	-0.31658500
C	-1.24738900	0.43253500	-0.30304700
C	-1.52611100	-1.00799300	-0.47856200
C	-0.02298100	1.04121200	-0.18643800
C	1.36379700	0.63886600	-0.10298100
C	2.29328800	1.68505900	0.14274900
C	3.64756700	1.44714900	0.26241700
C	4.13885100	0.13547600	0.13480100
C	3.24501500	-0.91784900	-0.11681500
C	1.88353500	-0.66801200	-0.23509700
O	5.47898100	-0.00428700	0.26458900
O	-0.72984300	-1.86609300	-0.79714700
O	-2.31761900	2.57725700	-0.45545700
C	6.04864900	-1.30404400	0.14542200
C	-3.76776900	-0.51008800	0.31064800
C	-5.14645800	-0.99727900	-0.10100300
C	-3.55116900	-0.51767700	1.82405900
H	-0.14003700	2.12182200	-0.11136500
H	1.92535500	2.70286400	0.24391200
H	4.35135800	2.25095300	0.45206400
H	3.60345000	-1.93449200	-0.22962800
H	1.20598100	-1.48306600	-0.44791900
H	7.12192200	-1.16985600	0.28696900
H	5.66046500	-1.98198300	0.91524900
H	5.86166400	-1.73216300	-0.84684600
H	-5.23435100	-0.96712600	-1.18984100
H	-5.29645300	-2.02464300	0.24137200
H	-5.91461000	-0.35459600	0.33734700
H	-3.66727600	-1.53440200	2.20989100
H	-4.28480300	0.13421000	2.30669500
H	-2.54866100	-0.16080600	2.07897400

x5

O	-3.24242600	-1.35390400	-0.30223200
O	-3.99388800	0.87788500	-0.19186200
C	-2.73489400	1.39664200	-0.31778200
C	-1.60788300	0.42037500	-0.30501300
C	-1.92500700	-1.01102500	-0.45697100
C	-0.36027100	0.99710700	-0.21851300
C	1.00874000	0.56028700	-0.14994500
C	1.97745000	1.58000700	0.03873600
C	3.32786700	1.31581200	0.14354500
C	3.80965800	-0.01723700	0.06284400
C	2.84899000	-1.04437000	-0.13804600
C	1.50036000	-0.76612400	-0.24156200
N	5.14748500	-0.30096400	0.17057100
O	-1.15463600	-1.89938000	-0.75893300
O	-2.61703200	2.59369800	-0.46349700
C	5.61844200	-1.67417100	0.05548300
C	-4.14966000	-0.44458100	0.33081000
C	-5.54447000	-0.89587900	-0.06890200
C	-3.92719900	-0.44527200	1.84394100
C	6.11329800	0.77439900	0.34377900
H	-0.44756900	2.08174300	-0.16213500
H	1.64294600	2.61245200	0.10780600
H	4.01456200	2.14104800	0.28703800
H	3.16781700	-2.07630100	-0.22245500
H	0.80029200	-1.57215200	-0.41241300
H	5.17402900	-2.31759400	0.82561400
H	5.38442200	-2.10472500	-0.92749200
H	6.70132200	-1.69248600	0.18473100
H	-5.63702800	-0.87317100	-1.15757100
H	-5.72197800	-1.91549900	0.28353000
H	-6.29191200	-0.22757400	0.36713100
H	-4.63980300	0.23152900	2.32399400
H	-2.91374700	-0.11488500	2.09072900
H	-4.07039800	-1.45498900	2.23924000
H	6.10649300	1.47041500	-0.50621200
H	7.11385900	0.34761700	0.42420800
H	5.91562400	1.34911400	1.25803200

x6

O	3.98614600	1.32001700	-0.14863500
O	4.71201000	-0.91842800	-0.28289700
C	3.44472400	-1.40605600	-0.45466700
C	2.33043200	-0.42510700	-0.33393300
C	2.66208000	1.00916900	-0.32512400
C	1.07385200	-0.99570700	-0.32484700
C	-0.28960700	-0.55989400	-0.21884700
C	-1.26939500	-1.58637700	-0.19205600
C	-2.62371600	-1.33774100	-0.09440900
C	-3.07380400	0.00989200	0.01717800
C	-2.11074300	1.06192700	0.00551200
C	-0.76650500	0.77122900	-0.12752100
O	1.90021300	1.93621100	-0.51395300

O	3.31463800	-2.58082900	-0.72397600
C	4.88699700	0.33880000	0.37508500
C	6.28421200	0.81481300	0.01385400
C	4.67621000	0.18067700	1.88186000
N	-4.41455500	0.29049300	0.13131000
C	-4.94154200	1.65546400	0.09775700
C	-3.96307000	2.64239900	-0.53206900
C	-2.58763800	2.49263400	0.12296400
C	-3.63884100	-2.45854500	-0.09226600
C	-4.84009900	-2.07200200	0.77461800
C	-5.42826300	-0.75369100	0.27915800
H	1.15284600	-2.07998700	-0.39733300
H	-0.94004100	-2.62169100	-0.25875200
H	-0.05136900	1.58221700	-0.16857100
H	6.36840800	0.90731800	-1.07182200
H	6.47678400	1.78912100	0.47126700
H	7.02698700	0.09559100	0.36953400
H	5.38467500	-0.55073000	2.28127700
H	3.66086100	-0.16386400	2.09984100
H	4.83285800	1.14089900	2.38171400
H	-5.19739600	1.97622700	1.12097000
H	-5.88061600	1.63749400	-0.47144800
H	-4.35408700	3.65876100	-0.41227700
H	-3.88350300	2.44592500	-1.60847300
H	-2.66120400	2.78411500	1.18195500
H	-1.85749300	3.16785000	-0.33512000
H	-3.17749600	-3.38443600	0.26898100
H	-3.98613300	-2.66263600	-1.11659700
H	-4.52280300	-1.96369100	1.81921900
H	-5.61744400	-2.84342300	0.74584900
H	-6.18467800	-0.38833500	0.98649500
H	-5.94303300	-0.90725200	-0.68368800

x7

N	-2.69530900	1.41025100	-0.00006000
C	-3.79047600	0.54206100	0.00005400
N	-3.49198700	-0.82055100	-0.00001000
C	-2.20667900	-1.36396300	-0.00003800
C	-1.06345000	-0.40856000	-0.00002200
C	-1.34548700	1.03402000	-0.00004700
C	0.16677300	-1.02162700	0.00000300
C	1.56327100	-0.64880900	-0.00000100
C	2.48233200	-1.73401200	0.00001100
C	3.84805600	-1.53758200	0.00000600
C	4.36397600	-0.22897400	-0.00000100
C	3.48182900	0.86332000	-0.00001100
C	2.10827200	0.65507700	-0.00001300
O	-4.93983400	0.95226600	0.00017800
O	5.71403900	-0.13068000	-0.00001200
C	6.30841900	1.16330300	0.00008000
O	-0.50111700	1.92577200	-0.00006600
O	-2.07698300	-2.58276000	-0.00006200
C	-2.96740600	2.85329700	-0.00005100
C	-4.60809700	-1.77438000	0.00002100
H	0.03786200	-2.10364200	0.00000500
H	2.09620600	-2.74998700	0.00002600
H	4.54240400	-2.37144600	0.00001000
H	3.85829300	1.87975200	-0.00002900
H	1.43449700	1.49998800	-0.00002900
H	7.38590700	0.99302700	0.00015000
H	6.02815500	1.73121200	0.89557300
H	6.02828500	1.73128400	-0.89540900
H	-4.04581300	2.98767000	0.00010200
H	-2.52217000	3.31240300	-0.88573300
H	-2.52190700	3.31243700	0.88547800
H	-5.53360400	-1.20444400	-0.00001500
H	-4.54691700	-2.41102000	-0.88555500
H	-4.54696600	-2.41093200	0.88566700

x8

N	-3.10433400	1.37038500	0.00020800
C	-4.17163500	0.47011400	0.00004900
N	-3.83022800	-0.88169900	-0.00003600
C	-2.52634300	-1.38443000	-0.00000700
C	-1.41704500	-0.39604000	-0.00003100
C	-1.74140500	1.03399300	-0.00001200
C	-0.16330100	-0.97077800	-0.00001200
C	1.21302700	-0.55514800	-0.00006700
C	2.17171600	-1.60307000	0.00011500
C	3.53162300	-1.37146200	0.00008300
C	4.03663300	-0.04438600	-0.00018900
C	3.08674900	1.01186800	-0.00034200
C	1.72778800	0.76622700	-0.00029500
O	-5.33434900	0.84430200	0.00000900
N	5.38517400	0.20631600	-0.00032000
C	5.87714900	1.57701900	0.00008500
C	6.33646300	-0.89560600	0.00039000

O	-0.92659400	1.95400400	-0.00012100
O	-2.36217700	-2.60026300	-0.00000100
C	-3.41938900	2.80389100	0.00029000
C	-4.91484100	-1.86992500	-0.00012700
H	-0.25874500	-2.05632400	0.00005700
H	1.82056400	-2.63217400	0.00031700
H	4.20775700	-2.21754600	0.00027400
H	3.42196100	2.04211700	-0.00049900
H	1.03143800	1.59286500	-0.00042100
H	5.54280200	2.12736900	0.88940700
H	6.96778900	1.56524500	-0.00015000
H	5.54247100	2.12791000	-0.88876200
H	6.22215400	-1.53040700	-0.88844300
H	7.35032600	-0.49340600	-0.00017500
H	6.22254600	-1.52908800	0.89023500
H	-4.50144700	2.90576500	0.00020100
H	-2.98790600	3.27694000	-0.88497500
H	-2.98810300	3.27679600	0.88573700
H	-5.85787100	-1.32933600	-0.00027300
H	-4.83396700	-2.50488100	-0.88546600
H	-4.83422100	-2.50478700	0.88530700

x9

C	-4.17954100	-1.84387800	0.00031800
C	-5.54418300	-1.54042300	0.00057400
C	-5.98770500	-0.20845000	0.00055300
C	-5.07655300	0.85179200	0.00027900
C	-3.72021100	0.54276600	0.00003100
C	-3.27764800	-0.78444600	0.00004800
C	-2.53488800	1.45131300	-0.00027700
C	-1.32135200	0.58000600	-0.00044800
C	-1.77949800	-0.83025800	-0.00029600
C	-0.08957500	1.17763000	-0.00036700
O	-2.56639400	2.67393200	-0.00040100
O	-1.13032700	-1.87219000	-0.00047800
C	1.26508600	0.69752300	-0.00029100
C	2.30304500	1.66057200	0.00013000
C	3.63864700	1.30865000	0.00031700
C	4.02410000	-0.05771700	0.00005900
C	2.98742100	-1.02930000	-0.00043700
C	1.65523500	-0.66411800	-0.00060700
N	5.34739800	-0.42592100	0.00032100
C	5.71719800	-1.83381300	-0.00006200
C	6.39010600	0.58863400	0.00073300
H	-3.82195400	-2.86930500	0.00033600
H	-6.27524200	-2.34459800	0.00078900
H	-7.05483600	-0.00278900	0.00074900
H	-5.40459000	1.88709400	0.00027300
H	-0.17167600	2.26742400	-0.00029700
H	2.03952000	2.71572600	0.00032200
H	4.38804500	2.09082700	0.00070700
H	3.23272100	-2.08456500	-0.00071600
H	0.88576800	-1.42820700	-0.00092900
H	5.33572500	-2.35390600	0.88874100
H	5.33587100	-2.35338300	-0.88923200
H	6.80473900	-1.91778000	-0.00000600
H	6.33217500	1.23054100	0.89021400
H	7.36542400	0.10029400	0.00054400
H	6.33218200	1.23123700	-0.88825100

x10

C	4.95568900	1.75964500	0.12089700
C	6.31769800	1.44340600	0.10911400
C	6.74830000	0.10977100	0.03113100
C	5.82655200	-0.93946900	-0.03698800
C	4.47355600	-0.61753700	-0.02482400
C	4.04375400	0.71136600	0.05300800
C	3.27822500	-1.51209200	-0.08423800
C	2.07493700	-0.63097000	-0.03554000
C	2.54524500	0.77060600	0.04995700
C	0.83567200	-1.21726900	-0.07499900
O	3.29946300	-2.73330900	-0.15812600
O	1.90704600	1.81857300	0.10939800
C	-0.51277000	-0.72950500	-0.04867100
C	-1.55649100	-1.68413800	-0.11253700
C	-2.89342200	-1.33562200	-0.11048700
C	-3.25111500	0.04008700	-0.00854000
C	-2.21799300	1.02012000	0.07280700
C	-0.89182600	0.63188700	0.03697600
N	-4.57516600	0.41585000	0.01199500
C	-4.99863800	1.81545400	-0.02610500
C	-3.90852800	2.74025400	-0.55965600
C	-2.59901700	2.47936300	0.18906300
C	-3.98528900	-2.37777700	-0.20014400
C	-5.21137500	-1.91539100	0.59190100
C	-5.66862400	-0.55277400	0.07948400
H	4.60794900	2.78673600	0.18116700
H	7.05637800	2.23896800	0.16104600

H	7.81339600	-0.10633900	0.02387800
H	6.14441800	-1.97621300	-0.09758600
H	0.91014900	-2.30560200	-0.14130000
H	-1.29583000	-2.73914200	-0.17618700
H	-0.11249500	1.38560700	0.08629400
H	-5.30512300	2.13558200	0.98359200
H	-5.89253300	1.87836700	-0.66143400
H	-4.23442800	3.77995700	-0.44453400
H	-3.76405600	2.55830800	-1.63193700
H	-2.72833000	2.75646200	1.24657200
H	-1.79100100	3.10810400	-0.19922800
H	-3.61857400	-3.34075300	0.17244000
H	-4.27619800	-2.53964400	-1.24943800
H	-4.95644800	-1.84165900	1.65637800
H	-6.03859600	-2.62790500	0.50041400
H	-6.44160000	-0.14112100	0.74238700
H	-6.13025000	-0.65927300	-0.91632100

y1

C	1.09788200	1.25678300	-0.06932500
C	2.35944800	0.46218600	0.05627000
C	2.27505000	-1.02830300	0.02716600
C	1.04782500	-1.60132200	-0.04166900
C	-0.19097900	-0.84678200	-0.06628800
C	-0.08819200	0.59785400	-0.11630500
C	-1.37352300	-1.54287900	-0.07902100
C	-2.75287400	-1.07458900	0.00023300
C	-3.75866100	-1.84457900	-0.62139400
C	-5.09221100	-1.45698800	-0.58499100
C	-5.49060800	-0.29630000	0.09505000
C	-4.50095100	0.44840200	0.75135700
C	-3.16176100	0.07279500	0.71015500
O	3.45448100	1.03088700	0.16012600
C	-6.93624200	0.13663100	0.11439400
C	1.19036400	2.79040900	-0.15428700
C	3.57227900	-1.85334000	0.08500000
C	3.29010000	-3.36772900	0.02555700
C	4.32350000	-1.56577200	1.40910100
C	4.47894300	-1.49695000	-1.11963000
C	-0.19732200	3.44051100	-0.32185700
C	2.05235800	3.20454400	-1.37330500
C	1.81970600	3.35201700	1.14600000
H	0.94666800	-2.68207500	-0.05057100
H	-1.00865600	1.15133100	-0.24277400
H	-1.28022500	-2.62453600	-0.18177900
H	-3.47743300	-2.75192700	-1.15076100
H	-5.84054300	-2.06778900	-1.08487400
H	-4.78694000	1.33116900	1.31856100
H	-2.43323900	0.64531400	1.27375700
H	-7.61361600	-0.72394900	0.13535600
H	-7.15586900	0.76410400	0.98425100
H	-7.18467300	0.72202100	-0.78125000
H	2.68511400	-3.70959000	0.87381100
H	2.78019800	-3.65682300	-0.90123100
H	4.24000400	-3.91244000	0.06086000
H	3.70462300	-1.83608700	2.27347300
H	5.24068100	-2.16620800	1.45273500
H	4.59297900	-0.51206400	1.48894300
H	3.97372300	-1.72296500	-2.06673100
H	4.75009300	-0.44052900	-1.11193000
H	5.39901900	-2.09321600	-1.08040700
H	-0.85851300	3.22957200	0.52721300
H	-0.08072800	4.52824000	-0.38200000
H	-0.69946200	3.11244000	-1.23963100
H	3.06778200	2.81529000	-1.29101600
H	2.10272700	4.29855000	-1.43594300
H	1.60911700	2.83607700	-2.30659800
H	2.82844200	2.96540000	1.29453400
H	1.86776600	4.44673100	1.09080100
H	1.21033000	3.08726500	2.01891100

y2

C	1.38161000	1.25856900	-0.09227700
C	2.66444100	0.51022600	0.08318800
C	2.63196100	-0.98110900	0.05550200
C	1.42691900	-1.59672800	-0.04408500
C	0.16448700	-0.88688800	-0.10576100
C	0.21994100	0.55883900	-0.16751900
C	-0.99328800	-1.62583100	-0.14013100
C	-2.38844500	-1.21590600	-0.08534500
C	-3.35866800	-2.04874400	-0.69225400
C	-4.70356500	-1.72609300	-0.68400100
C	-5.14301400	-0.55841600	-0.03710300
C	-4.20949400	0.26323700	0.60991200
C	-2.85684000	-0.06829700	0.58329300
O	3.73510600	1.11778900	0.22432700
O	-6.48135900	-0.32771400	-0.07952500
C	-6.99050500	0.83689500	0.55688500

C	3.95443900	-1.76192200	0.14915600
C	1.42472700	2.79347300	-0.19554000
C	3.72515100	-3.28473900	0.08019200
C	4.65934400	-1.45166400	1.49351100
C	4.88147800	-1.37301800	-1.02963500
C	0.02312700	3.39379500	-0.42407400
C	2.31648500	3.22111500	-1.38810900
C	1.98582700	3.39341900	1.11848800
H	1.36417000	-2.68038400	-0.05047600
H	-0.71346500	1.08010100	-0.33129700
H	-0.85587100	-2.70342300	-0.23771800
H	-3.03383900	-2.95696700	-1.19394800
H	-5.44063200	-2.36133900	-1.16478500
H	-4.52602100	1.14866200	1.14907500
H	-2.16030100	0.55456300	1.13339200
H	-8.06744400	0.82413300	0.38225400
H	-6.79738600	0.82111000	1.63713000
H	-6.56204900	1.74985200	0.12424300
H	3.11128300	-3.64881500	0.91266100
H	3.24765400	-3.58781700	-0.85928400
H	4.69142800	-3.79792100	0.13746300
H	4.02666300	-1.74450000	2.34042000
H	4.89011700	-0.38941200	1.58155900
H	5.59494100	-2.02067400	1.56135300
H	4.41152800	-1.61668100	-1.99045800
H	5.11402800	-0.30747000	-1.01493700
H	5.82100500	-1.93577100	-0.96412900
H	-0.66111700	3.17538400	0.40476700
H	-0.43471100	3.03391800	-1.35310600
H	0.10586900	4.48375200	-0.49971600
H	3.33994000	2.86546400	-1.26428500
H	1.91913000	2.82715600	-2.33161200
H	2.33449800	4.31537000	-1.46351500
H	3.00083500	3.04311500	1.30837400
H	1.35435100	3.11828200	1.97231000
H	1.99869900	4.48841300	1.05008900

y3

C	1.77525900	1.25323400	-0.10279300
C	3.02848000	0.45758900	0.06098300
C	2.93419600	-1.02932900	0.05209400
C	1.70346000	-1.59773500	-0.03080000
C	0.47092200	-0.84044500	-0.08814700
C	0.58464000	0.59939500	-0.16038100
C	-0.71768500	-1.53647700	-0.10660200
C	-2.09325300	-1.08870800	-0.03236300
C	-3.10524400	-1.92524100	-0.55466100
C	-4.44356000	-1.57404900	-0.53662100
C	-4.86565500	-0.34860300	0.03777800
C	-3.86408600	0.46885400	0.62001200
C	-2.52777500	0.10786300	0.58087600
O	4.12671400	1.02380200	0.17653300
N	-6.19261900	0.02422200	0.04489200
C	-6.60461800	1.23748100	0.73253000
C	-7.20862100	-0.89386000	-0.44396000
C	4.22494300	-1.86204900	0.14454000
C	1.87678300	2.78484200	-0.21638800
C	0.49667400	3.43977400	-0.42345600
C	2.76395400	3.17050600	-1.42650900
C	2.48487500	3.36940800	1.08364900
C	3.93599900	-3.37564100	0.10002800
C	4.95441100	-1.56098700	1.47769500
C	5.15617800	-1.52727900	-1.04727500
H	1.59861100	-2.67836500	-0.02499500
H	-0.32745500	1.15814100	-0.31951100
H	-0.61607600	-2.61825400	-0.20512300
H	-2.82087000	-2.87396400	-1.00428900
H	-5.16737700	-2.25682900	-0.96480600
H	-4.13630400	1.38623000	1.12773900
H	-1.80921000	0.74434500	1.08484800
H	-6.08277800	2.11575300	0.33289500
H	-7.67451400	1.38864500	0.58082000
H	-6.41512600	1.19092800	1.81541200
H	-7.25045300	-1.82316100	0.14349600
H	-7.03034100	-1.16195400	-1.49293000
H	-8.18507600	-0.41057500	-0.38561900
H	-0.18149200	3.25028300	0.41744300
H	0.00940100	3.09512300	-1.34323600
H	0.62095900	4.52550000	-0.50427500
H	3.77303500	2.77112900	-1.31857700
H	2.33337600	2.78989700	-2.36093500
H	2.82722200	4.26288800	-1.50738900
H	3.48775800	2.97819500	1.25739000
H	1.85798100	3.12478000	1.95010900
H	2.54119500	4.46276300	1.00850300
H	3.31432400	-3.70333800	0.94184400
H	3.44008500	-3.67386900	-0.83149500
H	4.88220500	-3.92511200	0.15857800

H	4.31922500	-1.81802900	2.33434500
H	5.86903600	-2.16345000	1.54544400
H	5.22462600	-0.50673500	1.54784300
H	4.66838800	-1.76635100	-2.00037100
H	5.42839400	-0.47113100	-1.04953300
H	6.07421000	-2.12470700	-0.98150500

y4

C	-2.54892700	1.20492000	0.20914500
C	-3.77692800	0.38925900	-0.02318400
C	-3.63899100	-1.09033600	-0.11501600
C	-2.39204700	-1.62831000	-0.06288400
C	-1.18265800	-0.84314300	0.05456800
C	-1.33944200	0.58269900	0.22932900
C	0.02685200	-1.50606900	0.02807200
C	1.38893500	-1.02373600	-0.01987400
C	2.42237100	-1.88070900	0.42056700
C	3.75588500	-1.50796900	0.43863900
C	4.12975400	-0.23093200	-0.06343700
C	3.11651200	0.62924300	-0.57087600
C	1.78976500	0.23240200	-0.52749000
O	-4.89057800	0.93205500	-0.11209900
N	5.45423200	0.15780100	-0.08029500
C	5.87605400	1.50501900	-0.45766500
C	4.73275500	2.51476400	-0.39853000
C	3.51784300	1.96588000	-1.15279600
C	4.82833300	-2.43621800	0.96229200
C	6.13284700	-2.21606900	0.19101300
C	6.54256700	-0.74808700	0.27921000
C	-2.69516800	2.72057400	0.43319000
C	-4.90441400	-1.95179700	-0.27324500
C	-1.33636300	3.39771000	0.70163000
C	-3.60246600	2.99177400	1.65919300
C	-3.30907800	3.38198300	-0.82649300
C	-4.57255800	-3.45638200	-0.32215400
C	-5.63164500	-1.58643500	-1.59142300
C	-5.85573100	-1.72011300	0.92717400
H	-2.25664900	-2.70267600	-0.14265500
H	-0.44542100	1.15470100	0.43689400
H	-0.04770300	-2.59433000	0.05478300
H	2.15799800	-2.86895300	0.79321200
H	1.04749500	0.89685500	-0.95741200
H	6.30962100	1.48666200	-1.47171200
H	6.68267000	1.81119100	0.22286500
H	5.07238900	3.46448900	-0.82626800
H	4.46124900	2.70424500	0.64736100
H	3.77382900	1.85957300	-2.21814000
H	2.67753800	2.66713800	-1.10310500
H	4.49750800	-3.47791400	0.88169900
H	5.00737200	-2.24838000	2.03201900
H	5.99123900	-2.49586100	-0.86031200
H	6.94161500	-2.83805100	0.59023100
H	7.38349000	-0.55202000	-0.40000500
H	6.89912600	-0.51710500	1.29721300
H	-0.64599800	3.28858100	-0.14385700
H	-0.84692000	3.00141700	1.59926200
H	-1.49285600	4.47085500	0.85900400
H	-4.59834800	2.57210900	1.51223600
H	-3.16826700	2.55573200	2.56739500
H	-3.69875000	4.07315800	1.81927200
H	-2.66603100	3.22328000	-1.70114000
H	-3.40257600	4.46423000	-0.67037100
H	-4.29647100	2.97204100	-1.04085000
H	-3.93551400	-3.71212700	-1.17735200
H	-4.07418800	-3.79858600	0.59284000
H	-5.50176300	-4.02826600	-0.42376200
H	-4.98313100	-1.77115200	-2.45671000
H	-6.52922400	-2.20734000	-1.70592900
H	-5.92946500	-0.53721500	-1.59644000
H	-5.36929500	-2.00274500	1.86895200
H	-6.15945200	-0.67453700	0.99110400
H	-6.75445200	-2.33958800	0.81481100

A

C	-1.94524800	-1.17592100	-0.21097900
C	-1.16487100	-0.13516400	0.09915200
C	-1.67493700	1.28471700	0.03083700
C	0.27106300	-0.32708100	0.54130800
C	1.31922200	0.19627100	-0.46153600
C	2.75637000	-0.04227900	0.01167500
H	-2.97589600	-1.04471700	-0.53230600
H	-1.58266300	-2.19970900	-0.15382900
H	0.42742400	0.18325500	1.50487400
H	0.45604300	-1.39396000	0.72080900
H	1.15965700	-0.29570900	-1.43019500
H	1.16769600	1.26997800	-0.63245700
H	-1.57350900	1.78551400	1.00386100

H	-1.10601000	1.88682100	-0.68964500
H	-2.72877400	1.32012400	-0.26175100
H	2.95403700	-1.11145000	0.15715800
H	3.48372600	0.33478600	-0.71626200
H	2.94866500	0.46181300	0.96699900

B

C	-1.21120100	1.12755500	0.00486000
C	-0.00578500	1.82402500	0.00126600
C	1.20818400	1.13224200	-0.00515300
C	1.22800100	-0.26538800	-0.00641500
C	0.00278100	-0.94877200	-0.00516000
C	-1.22183500	-0.27561400	0.00109100
C	2.53185900	-1.03043400	0.00537100
C	-2.52935200	-1.03453500	0.00020900
H	0.00593200	-2.03787600	-0.01013400
H	-2.15305000	1.67230000	0.00811000
H	-0.00797900	2.91124500	0.00115300
H	2.14592400	1.68332100	-0.00996300
H	3.38387700	-0.37151500	-0.19051400
H	2.53932300	-1.82373700	-0.75153500
H	2.70410100	-1.51235800	0.97678600
H	-3.13857600	-0.78398500	0.87774000
H	-3.13109200	-0.79525200	-0.88569200
H	-2.36437200	-2.11661700	0.00762800

C

C	-1.18243247	-1.98198195	0.00000000
C	0.33942553	-1.98198195	0.00000000
C	0.80819853	-0.53411695	0.00000000
C	-1.65163847	-0.53766195	-0.10359000
H	-1.57439447	-2.58442695	-0.85750800
H	-1.57254747	-2.45239295	0.93750400
H	0.72805253	-2.51657995	-0.90328000
H	0.73279253	-2.52271395	0.89683700
H	1.35513353	-0.30242395	0.94858800
H	1.52015953	-0.35094095	-0.84321600
H	-2.30401647	-0.27585995	0.76707400
H	-2.26338447	-0.39003995	-1.02879300
C	-0.41954147	0.35545105	-0.13318600
C	-0.42026769	1.70504506	-0.25632221
H	-1.16587783	2.19138159	-0.84999072
H	0.32733502	2.28627724	0.24183373

D

C	-1.36216800	1.32962100	-0.00000300
C	0.00889800	1.09241600	-0.00001800
C	0.51518100	-0.22052400	-0.00002200
C	-0.40649200	-1.28139200	-0.00000200
C	-1.78090800	-1.04611700	0.00001100
C	-2.26531900	0.26187300	0.00001200
H	-1.73030900	2.35235700	-0.00000200
H	0.69411700	1.93520200	-0.00003300
H	-0.03506200	-2.30387100	0.00000300
H	-2.47209900	-1.88490000	0.00002300
H	-3.33544200	0.45055500	0.00002600
C	1.95472200	-0.52931400	-0.00001400
H	2.18625900	-1.59469400	-0.00004400
C	2.97735100	0.33499600	0.00002600
H	2.84056800	1.41305100	0.00006400
H	4.00438500	-0.01705200	0.00002300

E1

C	0.37008800	-1.34652200	0.00000600
C	-0.98113100	-0.99378300	-0.00001000
C	-1.35124300	0.35277800	0.00001100
C	-0.37008700	1.34652300	-0.00001000
C	0.98112900	0.99378300	0.00000600
C	1.35124300	-0.35277900	-0.00000400
H	0.65808700	-2.39436100	0.00000700
H	-1.74459700	-1.76710100	0.00000600
H	-2.40268600	0.62731600	-0.00001300
H	-0.65808500	2.39436100	0.00000600
H	1.74459800	1.76710000	0.00000600
H	2.40268500	-0.62731500	-0.00001300

E2

C	1.20112000	-1.20543900	0.00217300
C	-0.19431700	-1.20234400	-0.00892900
C	-0.91386600	0.00007100	-0.01124500
C	-0.19422600	1.20239000	-0.00892900
C	1.20124500	1.20537400	0.00217200
C	1.90504000	-0.00005100	0.00845700
H	1.73845700	-2.15049000	0.00144400
H	-0.73456000	-2.14680200	-0.01774900
H	-0.73440200	2.14688000	-0.01774400

H	1.73865600	2.15038200	0.00144500
H	2.99179600	-0.00010300	0.01382400
C	-2.42540400	0.00003700	0.00929300
H	-2.80998400	-0.00511800	1.03818000
H	-2.83370300	0.88853400	-0.48429200
H	-2.83381600	-0.88351400	-0.49306300

E3

C	-2.28352900	0.33072800	0.00019000
C	-1.85192700	-1.00039100	0.00015200
C	-0.49515200	-1.30364000	0.00005300
C	0.45467100	-0.27121200	-0.00045500
C	0.03266400	1.06356100	-0.00032100
C	-1.33616800	1.35168500	-0.00009800
O	1.76149300	-0.67213400	-0.00046200
C	2.76880500	0.32508000	0.00053700
H	-2.57834700	-1.80898000	0.00036500
H	-0.14285800	-2.33054400	0.00000000
H	0.75052600	1.87595900	-0.00070600
H	-1.65589200	2.39070700	0.00018700
H	-3.34406600	0.56493800	0.00082600
H	2.71020900	0.95959000	0.89521200
H	3.72055900	-0.20967600	0.00121900
H	2.71173900	0.96021100	-0.89375700

E4

C	1.68261200	-0.22955900	-0.00005400
C	1.38750500	1.10327000	0.00020600
C	-0.02011200	1.35793200	-0.00023600
C	-0.78660600	0.22331500	0.00002000
S	0.23787100	-1.19652300	-0.00001800
H	2.65408900	-0.70528500	-0.00013000
H	2.14188200	1.88296300	0.00043200
H	-0.45166000	2.35416500	-0.00037400
C	-2.28230700	0.10570000	0.00007700
H	-2.65284400	-0.42765400	-0.88393400
H	-2.65278100	-0.42784700	0.88400800
H	-2.73116300	1.10408700	0.00021400

E5

C	1.09499500	0.34741800	-0.00008200
C	0.71790600	-0.95977300	0.00017000
C	-0.71794800	-0.95974500	-0.00020100
C	-1.09498100	0.34746400	0.00017000
H	2.05012100	0.85011800	-0.00011200
H	1.37346500	-1.81947900	0.00029900
H	-1.37354300	-1.81942200	-0.00032900
H	-2.05008500	0.85020700	0.00028400
O	0.00002600	1.16079900	-0.00006100

E6

C	1.39801300	-0.73417000	0.00002000
C	1.55003000	0.61650900	-0.00000800
C	0.22277500	1.16400300	-0.00001400
C	-0.63915600	0.10678800	0.00000000
H	2.08695900	-1.56508000	0.00004200
H	2.48460000	1.16031700	-0.00012100
H	-0.05312700	2.20972500	0.00019800
C	-2.12342700	-0.01351100	-0.00000300
H	-2.48436900	-0.55417800	-0.88386400
H	-2.48457000	-0.55328000	0.88432700
H	-2.57662000	0.98171600	-0.00055500
O	0.07221500	-1.06461700	0.00000000

E7

C	0.00000000	0.00000000	0.00000000
C	1.37860975	0.00000000	0.00000000
C	1.79972388	1.36000271	0.00000000
C	0.66233499	2.13904374	0.00000000
N	-0.43415239	1.30649356	0.00695860
H	-0.71111900	-0.81450587	-0.00157430
H	2.01160450	-0.87721334	0.01426713
H	2.81767420	1.72601395	0.01421402
H	0.53591744	3.21288185	-0.00157243
C	-1.81592351	1.73436665	-0.09497724
H	-1.93825636	2.70081770	0.40188088
H	-2.13724691	1.83270068	-1.13960248
H	-2.46285489	1.00735740	0.40383600

F1

C	-0.11643600	-1.42483200	-0.06449100
C	-1.26164400	-0.72389200	-0.10395600
C	-1.25896300	0.72853200	0.10389000

C	-0.11115000	1.42523900	0.06425400
H	-0.12075400	-2.50613600	-0.18406500
H	-2.21343600	-1.22331200	-0.27096600
H	-2.20882700	1.23133500	0.27176600
H	-0.11140600	2.50652300	0.18401100
C	1.19405600	-0.73408700	0.23918300
H	1.36084800	-0.76623400	1.32965800
H	2.03436100	-1.27597500	-0.21053000
C	1.19683700	0.72970900	-0.23908000
H	2.03903300	1.26852800	0.21086500
H	1.36398300	0.76126000	-1.32953700

F2

C	1.20112000	-1.20543900	0.00217300
C	-0.19431700	-1.20234400	-0.00892900
C	-0.91386600	0.00007100	-0.01124500
C	-0.19422600	1.20239000	-0.00892900
C	1.20124500	1.20537400	0.00217200
C	1.90504000	-0.00005100	0.00845700
H	1.73845700	-2.15049000	0.00144400
H	-0.73456000	-2.14680200	-0.01774900
H	-0.73440200	2.14688000	-0.01774400
H	1.73865600	2.15038200	0.00144500
H	2.99179600	-0.00010300	0.01382400
C	-2.42540400	0.00003700	0.00929300
H	-2.80998400	-0.00511800	1.03818000
H	-2.83370300	0.88853400	-0.48429200
H	-2.83381600	-0.88351400	-0.49306300

F3

C	-2.28352900	0.33072800	0.00019000
C	-1.85192700	-1.00039100	0.00015200
C	-0.49515200	-1.30364000	0.00005300
C	0.45467100	-0.27121200	-0.00045500
C	0.03266400	1.06356100	-0.00032100
C	-1.33616800	1.35168500	-0.00009800
O	1.76149300	-0.67213400	-0.00046200
C	2.76880500	0.32508000	0.00053700
H	-2.57834700	-1.80898000	0.00036500
H	-0.14285800	-2.33054400	0.00000000
H	0.75052600	1.87595900	-0.00070600
H	-1.65589200	2.39070700	0.00018700
H	-3.34406600	0.56493800	0.00082600
H	2.71020900	0.95959000	0.89521200
H	3.72055900	-0.20967600	0.00121900
H	2.71173900	0.96021100	-0.89375700

F4

C	-1.64162900	-0.29908600	-0.00001400
C	-0.40677600	-0.94342200	-0.00001000
C	0.79184400	-0.21326700	0.00000800
C	0.75859800	1.18396600	0.00000800
C	-0.48312700	1.82991200	0.00000300
C	-1.67012200	1.10662700	-0.00000600
H	-0.34364600	-2.02801500	-0.00002200
H	1.67070000	1.76962900	-0.00000600
H	-0.51220900	2.91670600	0.00000000
H	-2.62481400	1.62709200	-0.00001400
O	1.93457700	-0.96438000	0.00000300
C	3.17937500	-0.28673800	-0.00000100
H	3.29982900	0.33938200	0.89434500
H	3.94509600	-1.06495400	0.00000400
H	3.29982800	0.33936700	-0.89435800
C	-2.92803600	-1.09293800	0.00000700
H	-3.53899100	-0.86188700	-0.88158200
H	-2.73462800	-2.17004000	-0.00044900
H	-3.53853500	-0.86256700	0.88209500

G1

N	2.11468200	0.94439500	-0.00071100
C	2.70784300	-0.31008500	-0.00021600
C	1.71863500	-1.26279400	-0.00009000
C	0.45519400	-0.58151200	0.00006900
C	-0.88467600	-1.00434900	0.00000700
C	-1.87565700	-0.03406900	0.00003900
C	-1.58865400	1.34341500	0.00002200
C	-0.26813800	1.77922300	-0.00013200
C	0.74030700	0.81290900	-0.00007200
C	4.19487500	-0.45857300	0.00026700
H	2.61649000	1.81916700	0.00351400
H	1.87948900	-2.33240700	-0.00056400
H	-1.14389300	-2.05793800	-0.00008800
H	-0.03856500	2.84143600	-0.00018000
H	4.65081600	0.00502000	0.88525700
H	4.46701300	-1.51714100	0.00092300
H	4.65149300	0.00420000	-0.88476100
H	-2.40327800	2.05912300	0.00012800
Cl	-3.56945300	-0.53748300	0.00008100

G2

N	-1.11855100	-1.03663600	-0.00001100
C	-1.93232400	0.08650200	-0.00001100
C	-1.13305200	1.20421400	-0.00003200
C	0.23386900	0.76576800	-0.00000200
C	1.48012200	1.41694700	0.00001000
C	2.64218200	0.65554300	0.00001500
C	2.59162000	-0.75355100	0.00000600
C	1.37554500	-1.42851100	-0.00000700
C	0.20924900	-0.65782400	-0.00000900
C	-3.42550600	-0.04760600	0.00002900
H	-1.45461400	-1.98742200	-0.00001000
H	-1.48511000	2.22747500	-0.00004900
H	1.53190600	2.50295500	0.00000900
H	3.60926200	1.15142900	0.00002300
H	3.51766300	-1.32203100	0.00001000
H	1.33568800	-2.51509200	-0.00000900
H	-3.73237300	-1.09944800	-0.00033300
H	-3.87136200	0.42453100	0.88328200
H	-3.87144600	0.42516200	-0.88283900

G3

N	1.69394300	0.98184100	0.00052900
C	2.35362800	-0.23930500	-0.00003000
C	1.41539400	-1.24237400	-0.00013600
C	0.11612100	-0.62984500	-0.00002600
C	-1.20305400	-1.11659300	0.00001800
C	-2.27617700	-0.22960900	-0.00003900
C	-2.02488900	1.16381900	-0.00009300
C	-0.73595200	1.68215200	-0.00000300
C	0.32728900	0.77496300	0.00004100
C	3.84669800	-0.30913500	-0.00003200
H	2.14749800	1.88238100	-0.00198500
H	1.63384400	-2.30211500	0.00004400
H	-1.38666900	-2.18900200	0.00004200
H	-0.56579400	2.75610100	0.00002600
H	4.27972100	0.17590400	0.88532300
H	4.17358000	-1.35227700	-0.00120100
H	4.27977900	0.17785000	-0.88429700
C	-3.70262300	-0.73337100	0.00002500
H	-3.73821100	-1.82766900	-0.00055800
H	-4.25500400	-0.38429500	0.88215600
H	-4.25543300	-0.38332400	-0.88144600
H	-2.86952000	1.84935100	-0.00016500

G4

N	2.10108800	0.99845700	0.00018900
C	2.77867200	-0.21104700	0.00002200
C	1.85954300	-1.23184300	-0.00001100
C	0.54849300	-0.64379400	-0.00006800
C	-0.75418200	-1.15952900	-0.00011600
C	-1.83470300	-0.27814200	-0.00018900
C	-1.63179200	1.11878000	-0.00020500
C	-0.34227200	1.64996500	-0.00009800
C	0.73518300	0.76769600	-0.00002400
C	4.27275300	-0.25728000	0.00015100
H	2.53993900	1.90593800	-0.00064700
H	2.09739600	-2.28719000	0.00004100
H	-0.94723500	-2.22794100	-0.00009600
H	-0.19478400	2.72703600	-0.00008200
H	4.69731400	0.23677000	-0.88425100
H	4.69711100	0.23543200	0.88539500
H	4.61650500	-1.29490400	-0.00060300
O	-3.07753900	-0.86698800	-0.00031500
H	-2.47680500	1.79701000	-0.00031600
C	-4.21798100	-0.03129200	0.00048400
H	-4.25928900	0.60714100	-0.89344100
H	-5.08138200	-0.70036500	0.00075000
H	-4.25836300	0.60669400	0.89476400

H1

C	-0.23644700	0.77710500	0.00017900
C	-0.20795500	-0.64857800	0.00025600
C	2.03047700	-0.77604300	0.00018200
C	2.14859100	0.62663600	-0.00012500
C	1.00704800	1.42271200	-0.00033400
C	-1.61760700	1.16571700	0.00005400
C	-2.35592500	0.00972900	-0.00004000
H	2.92609600	-1.39451000	0.00049800
H	3.13688900	1.07638200	0.00025600
H	1.08037700	2.50737600	-0.00013600
H	-2.01511400	2.17130800	0.00088800
H	-3.42853200	-0.12559900	0.00047800
N	-1.51307200	-1.08558800	-0.00045000

H	-1.78519000	-2.05678600	0.00061100
N	0.86684000	-1.43467500	-0.00006800

H2

N	-2.49873600	0.71500700	0.00000800
C	-2.99855900	-0.57632100	-0.00001500
C	-1.96206400	-1.46974600	0.00001700
C	-0.74733600	-0.70252100	-0.00000100
C	0.61401300	-1.03116100	-0.00000700
C	1.55875700	0.00022700	-0.00000600
C	-0.18271200	1.70938100	0.00000700
C	-1.12377600	0.67274700	0.00000600
H	-3.05690600	1.55473000	0.00001200
H	-4.06582200	-0.74815800	-0.00002800
H	-2.04989600	-2.54713500	0.00002900
H	0.94048100	-2.06627400	-0.00000600
H	-0.48783900	2.75206500	0.00001200
C	2.95664500	-0.31612900	-0.00000600
N	4.09317100	-0.56869000	-0.00000700
C	1.15807600	1.36289200	0.00000000
H	1.92067700	2.13433100	0.00000300

H3

C	-1.14875600	-0.67726900	0.00004900
C	-1.53951100	0.69403300	-0.00006600
C	-0.60600300	1.73857300	-0.00018400
C	0.73794100	1.40126600	-0.00014100
C	1.15211400	0.04583600	-0.00002700
C	0.21512000	-0.98912200	0.00001800
C	-2.35748100	-1.45682500	0.00018200
C	-3.40273100	-0.57490400	0.00015500
H	-0.92066500	2.77872300	-0.00039000
H	1.49062800	2.18099000	-0.00015400
H	0.56591800	-2.01615700	0.00004900
H	-2.43352700	-2.53520400	0.00038900
H	-4.46860400	-0.75555400	0.00019700
N	-2.91443500	0.72298200	-0.00005700
H	-3.48118800	1.55679200	-0.00037100
C	2.58503800	-0.32855800	-0.00003600
O	3.01700400	-1.46619200	-0.00049000
O	3.42214700	0.74646600	0.00056200
H	4.32088300	0.36916600	0.00041400

H4

C	0.86428600	-0.68888100	0.00000300
C	1.24025000	0.68424300	-0.00002200
C	0.29543600	1.71481900	0.00003600
C	-1.04902600	1.36511900	0.00004100
C	-1.42611100	0.00824500	0.00000000
C	-0.50117300	-1.02368700	-0.00001100
C	2.07873100	-1.45532200	0.00004500
C	3.11689800	-0.56143300	0.00007200
H	0.59330500	2.75985600	0.00003300
H	-1.81571000	2.13189300	0.00007700
H	-0.82814300	-2.05817000	-0.00006000
H	2.16714600	-2.53278300	0.00003400
H	4.18406200	-0.73494300	0.00008400
N	2.61936100	0.72827100	-0.00021600
H	3.17743600	1.56752600	0.00049900
Cl	-3.14878700	-0.38175900	-0.00000800

H5

C	1.47769400	-0.67842100	0.00000500
C	1.92001500	0.67486900	-0.00001800
C	1.02677900	1.75063600	0.00003600
C	-0.33323600	1.46654100	0.00003600
C	-0.77530600	0.13025300	0.00000400
C	0.09722300	-0.94557500	-0.00000200
C	2.65322000	-1.50338600	0.00003500
C	3.73360800	-0.66117700	0.00006200
H	1.37511900	2.77998700	0.00003000
H	-1.06043700	2.27040200	0.00006700
H	-0.27917300	-1.96278200	-0.00004500
H	2.68863600	-2.58387300	0.00003800
H	4.79105900	-0.88647000	0.00007200
N	3.29944800	0.65143600	-0.00019600
H	3.89784100	1.46245800	0.00043400
Br	-2.66597600	-0.20120600	-0.00000500

H6

N	-2.57931600	-0.11033500	0.00000800
C	-2.37443700	-1.47965800	0.00000000
C	-1.02957800	-1.73852300	0.00000200

C	-0.36273100	-0.46856800	-0.00000600
C	0.99445300	-0.07987900	-0.00001400
C	1.30913200	1.27632900	-0.00001100
C	0.28533600	2.25017100	-0.00000200
C	-1.05771500	1.90799100	0.00000600
C	-1.36103500	0.53804700	0.00000200
O	1.90211100	-1.10140500	-0.00002500
C	3.27885600	-0.76627800	0.00002500
H	-3.47884800	0.34417800	0.00001900
H	-3.21640500	-2.15797100	-0.00000400
H	-0.56353500	-2.71298300	0.00000200
H	2.34213300	1.60463400	-0.00001900
H	0.56906400	3.29925400	0.00000200
H	-1.83597700	2.66586500	0.00001400
H	3.81954200	-1.71493300	0.00005700
H	3.55436900	-0.19113600	-0.89431700
H	3.55429800	-0.19111600	0.89437700

H7

C	-0.25012600	0.75195700	0.00000500
C	-0.24776000	-0.67193600	-0.00001400
C	0.93524300	-1.41876100	0.00003700
C	2.13597400	-0.71859700	0.00003300
C	2.15921100	0.69171500	-0.00001400
C	0.98239900	1.42898600	-0.00001900
C	-1.62615000	1.16681600	0.00003100
C	-2.39025000	0.03022600	0.00007700
H	0.91817200	-2.50580400	0.00004800
H	3.07335800	-1.26821200	0.00006800
H	3.11620700	1.20653000	-0.00003500
H	1.01132700	2.51575200	-0.00006000
H	-1.99867600	2.18204300	0.00004200
H	-3.46517800	-0.08688800	0.00010400
N	-1.56651500	-1.08104700	-0.00019600
H	-1.88085100	-2.03853100	0.00039500

H8

N	2.20957100	0.81799300	0.00017100
C	0.83423800	0.68999900	0.00001500
C	0.53982200	-0.70030000	-0.00000200
C	1.79891000	-1.39274200	-0.00000600
C	2.78382100	-0.44000100	-0.00008400
C	-0.17462300	1.65933200	0.00003300
C	-1.49048600	1.21800400	-0.00000100
C	-1.82441400	-0.15929000	0.00002200
C	-0.80689700	-1.10785800	0.00004900
C	-3.27849300	-0.57618700	-0.00005900
H	0.05905200	2.72120300	0.00006600
H	-2.29349500	1.95178900	-0.00002200
H	-1.05356200	-2.16745300	0.00010700
H	1.95179900	-2.46334100	0.00005900
H	3.85954900	-0.54956500	-0.00011300
H	2.71567900	1.68937200	-0.00085700
H	-3.37994900	-1.66628400	-0.00069100
H	-3.80855600	-0.19423400	0.88207500
H	-3.80878300	-0.19317800	-0.88161700

H9

N	-2.59084300	0.88919000	0.00043000
C	-1.21941900	0.70074100	0.00005100
C	-0.98610800	-0.70443500	-0.00002300
C	-2.27614800	-1.33909200	-0.00016500
C	-3.21650900	-0.34235200	-0.00000800
C	-0.17028400	1.61844300	-0.00000500
C	1.13436000	1.12941100	-0.00002100
C	1.38365000	-0.26105500	-0.00007600
C	0.33351600	-1.17713700	0.00008300
O	2.64519100	-0.80760300	-0.00006400
C	3.75757100	0.06585700	0.00003900
H	-0.35251800	2.69009200	-0.00006400
H	1.95707400	1.83454400	-0.00005900
H	0.56153000	-2.23859800	0.00018100
H	-2.47692600	-2.40155300	-0.00001800
H	-4.29606200	-0.40617300	-0.00000800
H	-3.05899700	1.78120500	-0.00195000
H	4.64228300	-0.57464100	-0.00018900
H	3.77701000	0.70485500	-0.89406100
H	3.77720200	0.70447100	0.89442000

H10

C	-0.52301800	-0.70246800	-0.00002200
C	-0.78600500	0.69680200	-0.00009900
C	0.24286100	1.64014800	-0.00005400
C	1.55250800	1.17280600	0.00001400
C	1.83104000	-0.21158800	-0.00023100

C	0.80800900	-1.15188900	-0.00015700
C	-1.79860300	-1.36347100	0.00031900
C	-2.76072500	-0.38679200	0.00014500
H	0.03765000	2.70748700	0.00000700
H	2.37723000	1.88330000	0.00031300
H	1.05492300	-2.20896500	-0.00032400
H	-1.97697400	-2.42991300	0.00022700
H	-3.83862700	-0.47364500	0.00023100
N	-2.16102600	0.85678600	-0.00077000
H	-2.64758700	1.73896300	0.00352200
O	3.12437300	-0.68145100	0.00000000
H	3.72919200	0.07559800	0.00193000

H11

C	-0.52640300	-0.69908200	-0.00460500
C	-0.80984200	0.69374000	0.00028700
C	0.20942900	1.64920900	-0.00007500
C	1.52314200	1.20147800	-0.00730600
C	1.83807200	-0.18116200	-0.00949000
C	0.81301300	-1.12657200	-0.00557900
C	-1.79210000	-1.37891400	0.00018700
C	-2.76955700	-0.41653100	0.00630800
H	-0.00997500	2.71404200	0.00473100
H	2.33542700	1.92457500	-0.02042300
H	1.05132500	-2.18830800	-0.00870000
H	-1.95558100	-2.44797900	-0.00217200
H	-3.84607500	-0.51918600	0.00947200
N	-2.18746400	0.83488200	0.00841700
H	-2.68602200	1.71025100	0.00433200
N	3.19040600	-0.57731800	-0.08059300
H	3.82446600	0.06832200	0.37682800
H	3.35132300	-1.51766400	0.26279800

I1

C	-0.19535700	1.20100900	0.00039600
C	-1.59260600	1.14247800	0.00026700
N	-2.29071500	-0.00000200	-0.00091800
C	-1.59259500	-1.14248100	0.00026800
C	-0.19535700	-1.20101000	0.00039500
C	0.51794700	-0.00000600	-0.00004800
Cl	2.24181100	0.00000100	-0.00025800
H	0.31936600	2.17478800	0.00162400
H	-2.18334300	2.07309400	-0.00005800
H	-2.18334500	-2.07306400	-0.00005800
H	0.31934900	-2.17476000	0.00162400

I2

C	-1.19868900	0.67299000	0.00002700
C	-1.14214700	-0.72207200	-0.00009700
N	0.00000300	-1.42088400	0.00004500
C	1.14215200	-0.72206400	-0.00009600
C	1.19868500	0.67299600	0.00002700
C	-0.00000500	1.38567300	-0.00008500
H	-2.15767000	1.18290100	0.00028400
H	-2.05981500	-1.30864700	0.00022700
H	2.05982200	-1.30863700	0.00022700
H	2.15766200	1.18291500	0.00028300
H	-0.00000700	2.47251800	0.00001000

I3

C	0.18119100	-1.18838700	-0.00227700
C	-1.21587400	-1.14396600	0.00011100
N	-1.92439000	-0.00881100	0.00257900
C	-1.22972300	1.13490400	0.00011400
C	0.16683600	1.19843300	-0.00228400
C	0.90356200	0.00935100	-0.00164700
C	2.40972300	0.00236100	0.00219000
H	0.70682500	-2.15613200	-0.00422100
H	-1.79727600	-2.08052800	0.00053000
H	-1.82337400	2.06385700	0.00063000
H	0.67440500	2.17561100	-0.00410300
H	2.83496500	1.03092100	0.00560600
H	2.78651500	-0.52547900	0.90786600
H	2.79437800	-0.52274300	-0.90159400
C	-0.00114700	1.02985900	-0.01646800
C	1.37262700	1.29382600	-0.00217000
N	2.31655300	0.34831600	0.01229900
C	1.88386900	-0.91642800	0.00922000
C	0.53291400	-1.27208900	-0.00398400
C	-0.47049100	-0.29238200	-0.01698400
O	-1.78745500	-0.67566800	-0.01636700
C	-2.77182100	0.33108300	0.02200800
H	-0.69012500	1.88814300	-0.02543400
H	1.73319500	2.33563900	0.00154800
H	2.66203600	-1.69686200	0.02195500

H	0.25210800	-2.33789400	-0.00173900
H	-3.76745400	-0.16578500	0.05055700
H	-2.66212400	0.94331600	0.94478000
H	-2.71957300	0.95736300	-0.89655200

I4

C	-0.00114700	1.02985900	-0.01646800
C	1.37262700	1.29382600	-0.00217000
N	2.31655300	0.34831600	0.01229900
C	1.88386900	-0.91642800	0.00922000
C	0.53291400	-1.27208900	-0.00398400
C	-0.47049100	-0.29238200	-0.01698400
O	-1.78745500	-0.67566800	-0.01636700
C	-2.77182100	0.33108300	0.02200800
H	-0.69012500	1.88814300	-0.02543400
H	1.73319500	2.33563900	0.00154800
H	2.66203600	-1.69686200	0.02195500
H	0.25210800	-2.33789400	-0.00173900
H	-3.76745400	-0.16578500	0.05055700
H	-2.66212400	0.94331600	0.94478000
H	-2.71957300	0.95736300	-0.89655200

I5

C	-0.19961000	1.20734700	-0.00434600
C	1.19379600	1.14644000	0.00004200
N	1.89336900	0.00000000	0.00451900
C	1.19379500	-1.14644000	0.00004100
C	-0.19961100	-1.20734600	-0.00434600
C	-0.92093300	0.00000000	-0.00171900
N	-2.30438000	0.00000000	0.00334200
H	-0.72028300	2.17775600	-0.00735500
H	1.78575000	2.07631800	0.00261900
H	1.78574900	-2.07631900	0.00261800
H	-0.72028400	-2.17775500	-0.00735400
H	-2.82924000	0.90873800	0.00820500
H	-2.82923800	-0.90873900	0.00820500

I6

C	0.56993700	1.19817600	-0.00033200
C	1.95811800	1.13208200	-0.00009900
N	2.67585100	0.00005600	0.00016700
C	1.95826100	-1.13206300	0.00026900
C	0.57008800	-1.19831500	0.00009300
C	-0.18078200	-0.00010100	-0.00031300
N	-1.55689500	-0.00003400	-0.00076600
C	-2.28308700	1.25853000	0.00063000
C	-2.28344600	-1.25840700	-0.00006900
H	0.08679600	2.16798600	-0.00053200
H	2.53165300	2.05871800	-0.00016400
H	2.53191600	-2.05862500	0.00055700
H	0.08710200	-2.16818300	0.00033000
H	-2.05321600	1.86349900	-0.88765400
H	-3.35498600	1.05407800	0.00024000
H	-2.05342900	1.86162700	0.89027200
H	-2.05508600	-1.86153600	0.88990000
H	-2.05269300	-1.86349500	-0.88802800
H	-3.35528200	-1.05363100	-0.00180200

J1

C	0.89989800	-1.18700800	-0.00002200
C	1.71062100	-0.02579400	-0.00006200
C	1.08941600	1.24092700	-0.00029600
C	-0.28169200	1.34688000	-0.00033100
C	-1.14202700	0.19183400	-0.00010400
C	-0.46743200	-1.08216100	-0.00007000
C	-2.54301600	0.31298800	0.00006500
C	-3.36433400	-0.83065900	0.00033800
N	3.12007200	-0.13189600	0.00007700
N	-4.07050800	-1.77018400	-0.00034800
O	3.81031700	0.91544100	0.00007100
O	3.64381800	-1.27084900	0.00023200
C	-3.23547500	1.66068000	0.00036000
H	1.38697600	-2.15549500	0.00004800
H	1.71935600	2.12342900	-0.00047300
H	-0.72816700	2.33677300	-0.00061100
H	-1.07432500	-1.98355800	-0.00007300
H	-2.97909500	2.26802300	-0.88267800
H	-2.97764300	2.26838500	0.88273000
H	-4.32288500	1.53415100	0.00124900

J2

C	0.48747600	-1.08268800	0.00015300
C	1.40989500	-0.00961600	0.00009100
C	0.91947600	1.31632500	0.00000100
C	-0.43212600	1.55556600	-0.00001200
C	-1.40219200	0.49214400	0.00005800

C	-0.86408200	-0.84328700	0.00013700
C	-2.77410800	0.77150700	0.00003700
C	-3.78184600	-0.20558600	-0.00010200
N	2.80082400	-0.25736100	0.00010200
N	-4.63549600	-1.01329700	-0.00021700
O	3.59281700	0.71538300	-0.00021900
O	3.20869700	-1.44288100	-0.00008100
H	0.87648700	-2.09464400	0.00021200
H	1.63555300	2.13030400	-0.00004900
H	-0.79485900	2.58191200	-0.00007500
H	-1.56056000	-1.67750500	0.00018500
H	-3.10099100	1.80833600	0.00074300

J3

C	-0.87521200	-1.12497600	0.00003300
C	-1.83216500	-0.07501900	0.00000700
C	-1.33670100	1.25471100	-0.00000700
C	0.01460500	1.51495900	0.00000000
C	1.00066400	0.46956700	0.00002000
C	0.47644600	-0.86920200	0.00003600
C	2.37419500	0.76543300	0.00002200
C	3.38902200	-0.20039100	-0.00001600
C	-3.22330600	-0.34161600	0.00000200
N	4.24854700	-1.00398900	-0.00004900
N	-4.37433500	-0.55942400	-0.00004600
H	-1.22757100	-2.15448300	0.00004500
H	-2.04615800	2.07987700	-0.00002300
H	0.35948400	2.54783900	-0.00001400
H	1.18140000	-1.69663000	0.00005200
H	2.68806900	1.80649100	0.00002600

J4

C	1.29207300	-1.20823700	-0.00001800
C	2.13333600	-0.06140100	0.00001200
C	1.50012300	1.20502700	0.00003600
C	0.12643000	1.32468500	0.00001800
C	-0.74444500	0.18048600	-0.00005900
C	-0.07729000	-1.09478400	-0.00002500
C	-2.14890800	0.31187200	-0.00002100
C	-2.97629200	-0.82401200	-0.00016100
C	3.54533200	-0.17883100	-0.00005400
N	-3.68373000	-1.76448500	0.00015000
N	4.71280100	-0.27463500	0.00004200
C	-2.82339000	1.66772500	0.00000000
H	1.75035900	-2.19502800	0.00000500
H	2.11781100	2.10107200	0.00008900
H	-0.30927900	2.31956900	0.00007800
H	-0.68898900	-1.99314000	0.00000700
H	-2.56129500	2.27577500	0.88251200
H	-2.56124600	2.27591600	-0.88238600
H	-3.91267600	1.55449700	-0.00002200

J5

C	0.13503100	-1.02424900	-0.04677900
C	1.04629600	0.05333000	-0.05532100
C	0.51519600	1.35858200	-0.02881800
C	-0.84736900	1.57649600	-0.00761700
C	-1.79820800	0.50151800	-0.00337300
C	-1.22828900	-0.81628000	-0.02556400
C	-3.18492300	0.75123000	0.01677800
C	-4.16577900	-0.24664400	0.01922500
C	2.50090300	-0.17928800	0.00070900
F	3.01467800	-0.29003400	1.27449600
F	3.22571300	0.82727600	-0.57190400
F	2.88206700	-1.33414200	-0.62068800
N	-4.99889800	-1.07926300	0.02129000
H	0.51876600	-2.04209100	-0.06800100
H	1.19396400	2.20884800	-0.03567500
H	-1.22434800	2.59834400	0.00154700
H	-1.90364700	-1.66822200	-0.03005100
H	-3.53170500	1.78189500	0.03058000

J6

C	-1.94027700	-1.39811300	0.00019100
C	-2.85683600	-0.33180600	-0.00023800
C	-2.33650500	0.96670000	-0.00042300
C	-0.96497300	1.20329800	-0.00012100
C	-0.00971900	0.13747900	0.00040800
C	-0.57247700	-1.18022400	0.00050100
C	1.39525600	0.38026100	0.00008000
C	2.30976500	-0.67860400	0.00073200
N	3.09078700	-1.56395300	-0.00109800
C	1.94500800	1.78895500	0.00016300
H	-2.30866300	-2.42510200	0.00034700

H	-3.93009300	-0.51043500	-0.00045400
H	-3.01622600	1.82067000	-0.00077300
H	-0.61053700	2.23100000	-0.00028400
H	0.10893800	-2.02795800	0.00079600
H	1.63205600	2.37913400	-0.88132200
H	1.63251000	2.37933900	0.88172400
H	3.04105000	1.77334200	-0.00010500

K1

C	2.19312100	-0.81801600	-0.60585000
C	3.15502400	0.00652900	0.00875800
C	2.75587900	1.23177200	0.57401800
C	1.43422100	1.61142700	0.52371400
C	0.42359200	0.80108200	-0.09202300
C	0.87057300	-0.43683900	-0.65905300
C	-0.90580400	1.28336300	-0.10048700
S	-2.28931600	0.50063700	-0.68037600
O	-3.40959600	1.45943300	-0.76554700
O	-2.02225500	-0.43620400	-1.79267600
N	4.52250000	-0.39342000	0.05926200
O	5.34947900	0.36179900	0.61042700
O	4.84939300	-1.48468100	-0.44847700
C	-2.87473900	-0.67429800	0.67053900
F	-3.99443500	-1.32244800	0.30157700
F	-1.93261800	-1.59489000	0.94677500
F	-3.14251100	-0.00311900	1.80723600
H	2.51661700	-1.75776600	-1.03846700
H	3.50406400	1.85865000	1.04522900
H	1.13576800	2.55941600	0.96572900
H	0.14694400	-1.07952700	-1.14540100
H	-1.15312600	2.21419400	0.39628500

K2

C	2.54733700	-0.76278300	-0.74468400
C	3.54240500	-0.10337500	0.01390500
C	3.14373000	1.00379300	0.79600300
C	1.82814700	1.41845000	0.81615600
C	0.80591500	0.76637800	0.05824800
C	1.23101200	-0.34777800	-0.72960900
C	-0.52005800	1.27235300	0.13575600
S	-1.90734400	0.63232900	-0.57093200
O	-3.02466700	1.59442500	-0.46503600
O	-1.65575300	-0.07927200	-1.84450300
C	-2.51151800	-0.78302500	0.51882400
F	-3.63528800	-1.34305300	0.03156400
F	-2.77863100	-0.35066600	1.76755100
F	-1.57593200	-1.74870800	0.61154000
C	4.89640900	-0.53617300	-0.00814700
N	6.01060600	-0.88965000	-0.02379300
H	2.83114500	-1.61649800	-1.35546400
H	3.88738100	1.53039800	1.38946900
H	1.55057700	2.27284900	1.42986600
H	0.49753400	-0.87092100	-1.33132100
H	-0.75163200	2.08804100	0.81061800

K3

C	-1.85185200	-0.55466100	0.78346500
C	-2.81104100	0.13100500	0.01935100
C	-2.37486000	1.19296000	-0.78827800
C	-1.03936200	1.55230800	-0.82361000
C	-0.04479100	0.87531700	-0.05636400
C	-0.51481400	-0.19771000	0.75742100
C	1.30695900	1.32465000	-0.14590700
S	2.66506800	0.63090400	0.55301200
O	3.83121800	1.53120200	0.41766200
O	2.39692600	-0.04761200	1.84254700
C	-4.22904900	-0.30161700	0.00442400
F	-5.09103100	0.72715600	-0.23436900
F	-4.61932200	-0.87395100	1.17650300
F	-4.51351300	-1.23318800	-0.95970400
C	3.19770900	-0.83526100	-0.50958200
F	3.46789500	-0.44452300	-1.77254800
F	4.30390800	-1.43427900	-0.02516100
F	2.22188600	-1.76426200	-0.57141200
H	-2.16802500	-1.37742000	1.41986600
H	-3.09599000	1.74325600	-1.38763800
H	-0.72999300	2.38331400	-1.45436600
H	0.19602100	-0.73543500	1.37350800
H	1.56995000	2.10858100	-0.84652100

K4

C	3.05585000	-1.14648000	-0.79610500
C	4.09403700	-0.64731700	-0.00049000
C	3.81799300	0.44825000	0.82351100
C	2.55006200	1.01861500	0.85237200

C	1.48012000	0.53015300	0.05278100
C	1.78573000	-0.58067900	-0.78076800
C	0.20574800	1.19507800	0.13099100
S	-1.23937100	0.71581300	-0.55088700
O	-2.26231300	1.77906200	-0.41361200
O	-1.09007900	-0.00335200	-1.84012600
C	-2.01073100	-0.65279100	0.50290900
F	-3.19425700	-1.07858600	0.01112200
F	-1.19328800	-1.72535000	0.57787200
F	-2.23256200	-0.22817000	1.76687600
H	3.24024100	-1.99878300	-1.44997400
H	5.08467100	-1.09629900	-0.02377500
H	4.60116900	0.86399600	1.45765000
H	2.36168800	1.86853800	1.50684200
H	1.00612200	-0.98474800	-1.41654500
H	0.06329900	1.98859000	0.85587100

K5

C	-2.75977600	-0.85118100	-0.77227900
C	-3.76695000	-0.27877100	0.01764300
C	-3.38597600	0.79761700	0.83236600
C	-2.08007300	1.27057000	0.85385100
C	-1.05154200	0.70153400	0.05354000
C	-1.44898100	-0.38584800	-0.76869900
C	0.27064300	1.26852700	0.12420800
S	1.67149500	0.67472000	-0.55909300
O	2.77297900	1.65863700	-0.43667000
O	1.46055500	-0.04516000	-1.83947300
C	-5.19394800	-0.77407400	-0.02589600
C	2.34129900	-0.73870100	0.50502100
F	2.59824400	-0.31915900	1.76373000
F	3.48799600	-1.25902000	0.01471600
F	1.44547000	-1.74520800	0.59382300
H	-3.01112300	-1.69296800	-1.41901400
H	-4.13058800	1.27465600	1.47182100
H	-1.82767100	2.10336800	1.50900000
H	-0.70845000	-0.85863300	-1.40406400
H	0.47557400	2.05341100	0.84354300
H	-5.25676700	-1.75622900	-0.51056500
H	-5.86113600	-0.09848100	-0.58511300
H	-5.62560500	-0.87600500	0.98006000

L1

C	0.22168500	-0.27998200	0.02036000
S	1.84469600	0.08954600	-0.29265000
C	2.76228600	0.46796500	1.27749700
C	2.60889600	-1.53345400	-0.62978400
C	-0.68658100	0.80139800	-0.24080700
O	-0.36186400	1.92045800	-0.62186800
O	-2.03216400	0.56849200	-0.05692700
C	-4.03333500	-0.68629600	0.21691600
C	-2.51472200	-0.73510500	0.26847100
H	-0.00279900	-1.16774000	0.59745500
H	3.82825800	0.59078100	1.06153000
H	2.34586800	1.40820500	1.64396800
H	2.60173600	-0.32687900	2.01098900
H	2.18972700	-1.89452700	-1.57020700
H	3.69060200	-1.40585700	-0.72234900
H	2.37964800	-2.23770900	0.17453900
H	-4.45518700	-1.66518800	0.47216000
H	-4.37425300	-0.40926800	-0.78552400
H	-4.41794500	0.05424900	0.92529700
H	-2.12182400	-1.47168900	-0.44515800
H	-2.17612200	-1.02587400	1.27413800

L2

C	-0.77393800	-0.00139600	0.67447000
S	0.52960400	0.00001100	-0.38421300
C	1.66861100	1.38220700	0.06503600
C	1.66973600	-1.38125800	0.06425800
C	-2.06949500	-0.00038700	0.13621600
N	-3.15605800	0.00055700	-0.30100700
H	-0.60197900	-0.00216400	1.74504800
H	1.13449200	2.30766000	-0.15656800
H	1.90996400	1.33524100	1.13045000
H	2.57909500	1.31602200	-0.53778200
H	1.13749300	-2.30706000	-0.16041400
H	1.90877100	-1.33628400	1.13028400
H	2.58142500	-1.31247500	-0.53645000

L3

C	2.59925700	-0.56214000	-0.06354800
C	1.71310500	0.51535300	-0.30219500
S	4.23501500	-0.08732000	-0.30544700

C	4.85154000	0.82739400	1.18184000
C	5.12315900	-1.65843500	-0.06741700
C	0.22902000	0.28393000	-0.20260300
O	2.13814300	1.66157400	-0.58813300
C	-0.60674800	1.40746400	-0.15634100
C	-1.99063400	1.27203100	-0.05657500
C	-2.53210200	-0.00975300	-0.00818200
C	-1.73420400	-1.14894500	-0.06497500
C	-0.35124100	-0.99123600	-0.16407800
H	2.39733300	-1.45863700	0.50902900
H	5.91068400	1.06857700	1.04994000
H	4.68722800	0.23415400	2.08488100
H	4.25256700	1.73944100	1.20500800
H	6.19684100	-1.45902200	-0.09658100
H	4.84972800	-2.11492900	0.88751600
H	4.84392800	-2.31868400	-0.89059200
H	-0.14542100	2.38844600	-0.20450000
H	-2.63320300	2.14476400	-0.01770900
H	-2.17935700	-2.13743900	-0.04092000
H	0.27529300	-1.87520700	-0.23693200
Br	-4.48936900	-0.22059800	0.13621500

L4

C	-1.04523700	0.57109700	-0.03709600
C	-0.07064900	-0.42736200	-0.28283900
S	-2.62761900	-0.01724000	-0.36592000
C	-3.22713200	-1.05509500	1.04783700
C	-3.64682600	1.46501000	-0.08409900
C	1.38594200	-0.09511400	-0.10571500
O	-0.40323000	-1.58528600	-0.63754800
C	2.29905000	-1.15674200	-0.04643900
C	3.66025500	-0.91319400	0.12425500
C	4.12912000	0.39852600	0.23320000
C	3.22867500	1.46409100	0.16418400
C	1.86624800	1.21839500	-0.00533400
H	-0.93725600	1.44580900	0.59208600
H	-4.25722900	-1.37247800	0.85957000
H	-3.14662600	-0.49836000	1.98483000
H	-2.55678900	-1.91609800	1.05181200
H	-4.69956200	1.18355000	-0.15988500
H	-3.44054800	1.89290700	0.90040900
H	-3.39616700	2.18636100	-0.86390400
H	1.91152700	-2.16588100	-0.14156800
H	4.35793100	-1.74568400	0.17153100
H	5.19108200	0.59018100	0.36497200
H	3.58921500	2.48738300	0.23408900
H	1.17548600	2.05277000	-0.08656400

L5

C	-1.91110000	0.56258000	-0.04896800
C	-0.94673700	-0.44586800	-0.30574600
S	-3.50322400	-0.02198100	-0.32318200
C	-4.07853500	-1.02597500	1.12657900
C	-4.50627700	1.47225200	-0.04592400
C	0.51121500	-0.11941200	-0.17852200
O	-1.29846500	-1.60745400	-0.63129700
C	1.42735700	-1.17565900	-0.15908700
C	2.79817600	-0.95104100	-0.03532400
C	3.27523100	0.36182000	0.06811100
C	2.36976700	1.43385400	0.03878800
C	1.00886800	1.19147400	-0.08409700
H	-1.78169100	1.44264800	0.56892000
H	-5.11598700	-1.33717700	0.97047500
H	-3.96979200	-0.45156700	2.05003800
H	-3.41622700	-1.89319800	1.13169200
H	-5.56243300	1.19650700	-0.08871500
H	-4.27215200	1.91863500	0.92409600
H	-4.27100800	2.17611600	-0.84621100
H	1.03926400	-2.18535100	-0.24718200
H	3.47857300	-1.79516400	-0.02093400
H	2.76143200	2.44441500	0.10454300
H	0.32500800	2.03393600	-0.13282300
O	4.59158600	0.70367700	0.19523000
C	5.55575700	-0.33589200	0.21843800
H	5.54532600	-0.91875000	-0.71218600
H	6.52457300	0.15621900	0.32434200
H	5.39938400	-1.01415600	1.06789100

L6

C	-2.24235000	0.56287200	-0.07370200
C	-1.34195600	-0.51362100	-0.29948300
S	-3.86835800	0.06119500	-0.29624700
C	-4.48607000	-0.83960700	1.20530700
C	-4.77858000	1.62297600	-0.07569000
C	0.13094800	-0.27061200	-0.21580000

O	-1.77249000	-1.66474000	-0.56415700
C	0.99356100	-1.37410600	-0.17217100
C	2.37035000	-1.22211900	-0.08355400
C	2.95964000	0.06397400	-0.04808900
C	2.08803700	1.17730600	-0.09209700
C	0.71171000	1.00420300	-0.17895600
H	-2.05057500	1.45361500	0.51221300
H	-5.54204800	-1.09522400	1.07390600
H	-4.33236900	-0.23212500	2.10091100
H	-3.87592400	-1.74352800	1.24355900
H	-5.84979000	1.40894100	-0.09144200
H	-4.50369000	2.09878000	0.86938600
H	-4.51510500	2.27479800	-0.91050400
H	0.55189600	-2.36507700	-0.20739800
H	2.99046900	-2.10998800	-0.04168400
H	2.48513500	2.18535200	-0.06859700
H	0.07993400	1.88632200	-0.23969400
N	4.33865600	0.22791100	0.01380800
C	4.88827600	1.54730700	0.27048500
H	4.55909100	1.96866700	1.23437400
H	5.97843600	1.48511200	0.27916300
H	4.60470100	2.25292900	-0.51988500
C	5.18306200	-0.92804500	0.25923400
H	5.05965300	-1.67924400	-0.52986900
H	6.22898700	-0.61415500	0.25335100
H	4.97448600	-1.41492300	1.22585700

M1

C	0.78793500	0.68588700	-0.00021800
C	0.29774100	-0.61163600	-0.00063900
S	-1.50841000	-0.46915100	0.00009200
N	-1.56986100	1.16533500	0.00009400
C	-0.32935000	1.72397400	-0.00012600
O	-0.06150500	2.93116900	-0.00028300
O	-2.03158000	-1.05858600	1.25309000
C	2.15954500	0.91886000	0.00033300
C	3.02408500	-0.18082300	0.00032100
C	2.51748400	-1.48753700	-0.00012500
C	1.13602900	-1.71853400	-0.00063500
O	-2.03250300	-1.05869300	-1.25234100
H	2.52510200	1.94221600	0.00050800
H	4.10143200	-0.02529900	0.00071900
H	3.20517400	-2.33112500	0.00009100
H	0.73577000	-2.72900300	-0.00064700

M2

C	0.66530900	-1.24371400	0.00000000
C	-0.66553800	-1.24326600	0.00000000
C	-1.09812500	0.23293900	0.00000000
N	0.00000000	1.04319100	0.00000000
C	1.09832300	0.23343600	0.00000000
O	2.29219700	0.56079600	0.00000000
O	-2.29207400	0.56001200	0.00000000
H	1.36845000	-2.07298600	0.00000000
H	-1.36924400	-2.07217500	0.00000000

M3

C	-0.14221400	-0.69491500	-0.00004800
C	-0.14223300	0.69489200	-0.00006300
C	1.32716200	1.11395100	-0.00021200
N	2.12198600	0.00002400	0.00058200
C	1.32719800	-1.11392900	-0.00017200
O	1.67616100	-2.30009300	-0.00014500
O	1.67608400	2.30012800	-0.00010500
C	-1.32557800	-1.41777900	0.00001700
C	-2.53341800	-0.70024600	0.00006000
C	-2.53343100	0.70021100	0.00004800
C	-1.32559700	1.41775200	-0.00000700
H	-1.30889500	-2.50576100	0.00002900
H	-3.48268700	-1.23472100	0.00009900
H	-3.48271000	1.23466800	0.00007700
H	-1.30889700	2.50573400	-0.00001900

M4

C	-1.82185100	-0.30971100	0.12183400
C	-3.21458600	-0.40146500	-0.53501800
O	0.94506400	-0.14985600	-0.21522700
C	0.15426200	0.99118100	0.01738400
N	-1.15777700	0.81313200	-0.21898500
O	0.72265000	2.04889100	0.29534400
O	-1.50870700	-1.21020100	0.92087000
C	2.33313100	0.02797100	-0.00322300
C	3.00618200	-1.31814600	-0.24197000
H	-3.40462500	0.42621900	-1.22470500

H	-3.29712700	-1.35465200	-1.07381100
H	-3.98943400	-0.41097600	0.24334500
H	2.73608200	0.79504900	-0.68070400
H	2.52513700	0.38643200	1.01754300
H	4.09135600	-1.24595800	-0.08716700
H	2.60357600	-2.07276000	0.44239100
H	2.82459400	-1.66493000	-1.26594100

M5

C	-0.76161100	1.23186300	-0.00163300
C	0.76161200	1.23186300	0.00169800
C	1.11524600	-0.28952300	0.00015200
N	-0.00000300	-1.07006100	0.00036300
C	-1.11524500	-0.28952100	-0.00012400
O	-2.29308900	-0.66557500	0.00055400
O	2.29309000	-0.66557600	-0.00095100
H	-1.21506100	1.70973700	0.87660200
H	-1.21013900	1.70603100	-0.88445700
H	1.21017100	1.70605000	0.88449800
H	1.21503200	1.70971800	-0.87656100

M6

C	-1.20324300	-0.24904900	-0.05611300
C	-1.43780300	1.03605800	0.78548300
C	1.43826100	1.03585700	-0.78552800
C	1.20318000	-0.24915700	0.05601700
N	-0.00008100	-0.84272200	-0.00039200
O	2.21023800	-0.72500600	0.61008400
O	-2.21068100	-0.72476100	-0.60963900
H	-0.51995900	1.56027700	1.07162300
H	-2.10093600	1.71899400	0.24111800
H	-1.95915900	0.74855000	1.70855300
H	1.95980100	0.74818900	-1.70843700
H	0.52059600	1.56027200	-1.07184100
H	2.10140600	1.71865300	-0.24098200

M7

N	-0.74013300	1.12142000	-0.18024000
C	0.68327800	1.22090700	0.06322800
C	1.11027000	-0.27997500	0.00397500
N	0.01035900	-1.06852900	-0.03254600
C	-1.09928900	-0.26623400	-0.02969200
O	-2.28455000	-0.59245900	0.06757900
O	2.30295400	-0.60818400	0.00658000
H	-1.36828000	1.74117000	0.31920600
H	0.94281900	1.64134800	1.04971200
H	1.22109400	1.80420000	-0.69775800

M8

C	-1.09148600	-1.18252500	-0.08892600
C	0.41476700	-1.22422200	-0.46784800
C	1.21422200	-0.00003500	0.00201100
C	0.41482500	1.22409200	-0.46803000
C	-1.09139700	1.18258200	-0.08897000
N	-1.73434300	0.00005700	0.07955600
O	-1.65333600	2.28463100	0.01878500
O	-1.65352400	-2.28453000	0.01879300
C	2.62662600	-0.00011000	-0.60696700
C	1.33248600	0.00009000	1.53937800
H	0.47867500	-1.29459600	-1.56598700
H	0.82606200	-2.16063400	-0.07069900
H	0.82623400	2.16058400	-0.07117600
H	0.47861000	1.29420100	-1.56619300
H	3.19518600	0.88815600	-0.29581300
H	3.19528500	-0.88816800	-0.29540200
H	2.58319600	-0.00036700	-1.70407900
H	1.87486200	-0.88819300	1.89157900
H	0.34209700	0.00011200	2.00495700
H	1.87481700	0.88846900	1.89140500

M9

O	0.05347100	-1.12498800	-0.11787500
C	-1.28178000	-0.75791200	0.11656200
C	-1.29238200	0.77999700	-0.09342000
N	0.07765000	1.19522200	0.08272400
C	0.85096900	0.12624800	0.00480800
O	2.07204400	-0.02985500	0.01325800
H	-1.95660900	-1.29925700	-0.56768200
H	-1.58461600	-1.01798500	1.15142000
H	-1.68377100	1.02435000	-1.10761900
H	-1.98352100	1.27508800	0.61404700

M10

O	-2.80460200	0.87628300	-0.80375500
C	-1.55329100	1.25020800	-0.28948300
C	-1.14176200	0.06900100	0.64531400
N	-2.36609400	-0.65340400	0.88926300
C	-3.29285200	-0.23812100	0.03900000
O	-4.44838100	-0.59651100	-0.17554300
C	-0.08216200	-0.86198700	0.00387900
C	1.36643500	-0.40648300	-0.00381300
C	2.38763800	-1.33332400	-0.27918800
C	3.73067900	-0.96088100	-0.30618600
C	4.09638600	0.36306200	-0.04832000
C	3.10031600	1.29725600	0.23466100
C	1.75523500	0.91711100	0.25550600
H	-0.84310400	1.42007700	-1.11536700
H	-1.62807400	2.19682700	0.28093400
H	-0.70892900	0.45737900	1.58672400
H	-0.14923200	-1.82737600	0.52237300
H	-0.40133000	-1.06482000	-1.03024800
H	2.11401200	-2.36868200	-0.47558700
H	4.49442000	-1.70509200	-0.52495900
H	5.14302500	0.65957800	-0.06553500
H	3.36783000	2.33178100	0.44150300
H	0.99817600	1.66092500	0.48147800

N1

C	-0.70577100	-0.00002400	0.01759600
N	0.75230500	-0.00002700	-0.12609800
H	-1.11522000	0.88317300	-0.48490500
H	-1.11591300	-0.88019500	-0.48966600
H	-1.08591400	-0.00265600	1.05461500
H	1.14286000	-0.81233200	0.34851300
H	1.14268100	0.81234300	0.34854900

N2

C	-1.24840100	-0.23808900	-0.02741600
C	0.05052100	0.56085300	0.05391600
N	1.20806100	-0.32564900	-0.12050400
H	-2.12063900	0.41988100	0.05746900
H	-1.30833000	-0.97526500	0.78386600
H	-1.30463900	-0.77886900	-0.97757400
H	0.07531300	1.29794300	-0.75855900
H	0.06468900	1.13608400	0.99844200
H	2.06862700	0.21890600	-0.08313200
H	1.25583000	-0.97572500	0.66401700

N3

C	1.26590100	-0.69917900	-0.09563900
C	0.00002200	0.02835500	0.36381500
C	-1.26509400	-0.70051500	-0.09550900
N	-0.00069400	1.38371600	-0.21133400
H	1.30244200	-1.71678800	0.30944100
H	2.16871000	-0.17358600	0.24093600
H	1.29514700	-0.75364400	-1.18958500
H	0.00011400	0.04036500	1.47073600
H	-2.16850900	-0.17654400	0.24195000
H	-1.29996400	-1.71853800	0.30866900
H	-1.29474300	-0.75419700	-1.18949800
H	-0.81579400	1.89660100	0.12436500
H	0.81248400	1.89835500	0.12632300

N4

C	1.35920100	-0.45488000	-0.19412900
C	0.04930600	-1.00513800	0.38523300
C	-1.24945500	-0.54118200	-0.30083500
C	-1.71769400	0.87119800	0.06994900
N	1.48992800	0.99854300	-0.02079600
H	2.19720000	-1.02460100	0.24958500
H	1.38364900	-0.65946500	-1.27299300
H	0.11052700	-2.10051500	0.32248000
H	0.00171400	-0.77104300	1.46054200
H	-2.04442600	-1.25611900	-0.04668200
H	-1.11887000	-0.61068600	-1.39039900
H	-2.66139000	1.11448500	-0.43351500
H	-0.96745600	1.61559300	-0.20751700
H	-1.89176500	0.95226900	1.15124800
H	2.37201300	1.31332300	-0.42265600
H	1.54116500	1.21697200	0.97417000

N5

N	1.94552200	-0.29223800	-0.02181100
C	0.85378800	0.09983700	-0.00746800
C	-0.52869000	0.60299500	0.04687900
N	-1.48631000	-0.49233300	-0.11682400
H	-0.62860500	1.18971800	0.97719800
H	-0.66200200	1.30615000	-0.78384700

H	-2.42817600	-0.10768700	-0.14850500
H	-1.44629700	-1.11316900	0.68913500

N6

C	0.06467200	0.51805100	0.02600900
C	-1.43623200	0.43081000	0.24914300
N	-2.01244300	-0.78765500	-0.31682700
O	0.65095300	-0.69362000	0.14846500
O	0.67606400	1.54284300	-0.17764900
C	2.07801400	-0.70762800	-0.02221800
H	-1.87559400	1.30556900	-0.23762200
H	-1.59070200	0.56056200	1.33844600
H	-3.00578600	-0.82477400	-0.09708200
H	-1.58064600	-1.59978200	0.11832300
H	2.37719700	-1.74970800	0.09366500
H	2.34718300	-0.33810400	-1.01495800
H	2.56058500	-0.08136600	0.73288500

N7

C	0.53356800	0.13197400	0.03919600
C	-0.72679500	-0.71974300	0.21398400
N	-1.87392800	0.01869200	-0.29641200
N	1.70196200	-0.56455700	-0.08705000
O	0.49318100	1.35338400	0.08523500
H	-0.61914900	-1.67547700	-0.31813700
H	-0.77722000	-0.96741200	1.29136800
H	-2.72189800	-0.26500700	0.18729300
H	-1.71532200	1.00474300	-0.08962400
H	2.54511700	-0.03276300	-0.25555800
H	1.70614900	-1.54348600	-0.33206500

N8

C	0.72832200	0.50905800	0.31241800
C	-0.65978600	0.54998600	-0.31549100
N	-1.49513600	-0.56621200	0.13230500
O	1.45637400	-0.58094800	-0.23127500
H	1.23221800	1.46910700	0.10620600
H	0.62980400	0.42195500	1.40883800
H	-1.08824300	1.54978500	-0.11113900
H	-0.53749000	0.47040300	-1.40197100
H	-2.35776700	-0.58957200	-0.40786100
H	-1.77195800	-0.42143400	1.10263600
H	2.29717800	-0.64344100	0.24579400

N9

C	0.72475300	0.62800500	0.24360600
C	-0.72479800	0.62800600	-0.24358400
N	-1.40807300	-0.59212700	0.21115600
N	1.40806700	-0.59210700	-0.21115600
H	1.24299000	1.49305500	-0.18796800
H	0.73040400	0.74996000	1.34010100
H	-1.24304200	1.49303800	0.18802200
H	-0.73045500	0.74999900	-1.34007900
H	-2.41121400	-0.50170500	0.06116400
H	-1.10929000	-1.36467700	-0.38276600
H	2.41125100	-0.50147500	-0.06160900
H	1.10967500	-1.36462000	0.38300500

N10

N	1.42662800	-0.96240100	0.01144500
C	1.30433600	0.49309300	0.20033200
C	-0.01411400	1.03871700	-0.36149000
C	-1.28247200	0.45963200	0.27792600
N	-1.53612500	-0.90865700	-0.18538900
H	2.31338500	-1.28762900	0.39390400
H	1.45111200	-1.17343800	-0.98609900
H	1.33955200	0.68462500	1.28122300
H	2.14001400	1.06167400	-0.24651600
H	-0.00696900	2.12809900	-0.22041800
H	-0.05968200	0.85970800	-1.44486500
H	-2.13845900	1.07989900	-0.01922100
H	-1.19406800	0.55693400	1.37811800
H	-2.37355400	-1.27260800	0.26737600
H	-0.75135300	-1.48850900	0.11350100

N11

C	-1.95393800	-0.23016200	-0.01171800
C	-0.80647900	0.14448800	-0.00861400
C	0.58559500	0.60064600	0.04022500
N	1.52267900	-0.52246600	-0.12421900
H	-2.96623100	-0.56422600	-0.03607600
H	0.76156600	1.30371800	-0.78480800
H	0.72705700	1.17878700	0.97212700
H	2.47535600	-0.16930100	-0.04291000
H	1.39242500	-1.18154300	0.64184300

N12

C	1.52197300	-0.55574500	-0.04449400
C	0.81624000	0.57114100	0.04727900
C	-0.68577400	0.67032500	-0.03790600
N	-1.33586400	-0.64060600	-0.04281200
H	2.60591500	-0.55291000	0.03146200
H	1.03554200	-1.51170200	-0.21394300
H	1.32986300	1.52065500	0.20262500
H	-0.95410700	1.18051700	-0.97530300
H	-1.03179600	1.34318500	0.77108000
H	-2.33901200	-0.52613000	-0.17177300
H	-1.20999100	-1.08369500	0.86626500

N13

C	0.43075100	0.24620600	0.14569500
C	1.90967900	0.54294200	0.31275300
N	2.74519900	-0.47271900	-0.33895100
C	-0.48826100	1.28924500	-0.01751200
C	-1.85485500	1.02814700	-0.13403600
C	-2.32002200	-0.28694400	-0.09755600
C	-1.40973300	-1.33530200	0.05668300
C	-0.04535700	-1.07133500	0.17827800
H	2.10236800	1.57551700	-0.02927000
H	2.16377000	0.52529500	1.38233200
H	3.72814200	-0.27611800	-0.15904500
H	2.61802700	-0.42258900	-1.34890000
H	-0.13034100	2.31642100	-0.05545200
H	-2.55343000	1.85135300	-0.26116000
H	-3.38275700	-0.49410100	-0.19314000
H	-1.76406300	-2.36290100	0.08247200
H	0.66867600	-1.88159900	0.28899500

O1

C	0.93394800	0.76986300	-0.00005000
C	0.93395200	-0.76986100	0.00005000
C	-0.31810100	-0.00000300	0.00000000
C	-1.64036400	-0.00000100	0.00000000
H	1.24084600	1.27892500	-0.91281600
H	1.24066900	1.27951100	0.91243900
H	1.24085300	-1.27892200	0.91281600
H	1.24067500	-1.27950800	-0.91243900
H	-2.20982300	0.92688200	0.00019400
H	-2.20982800	-0.92688000	-0.00019400

O2

C	-0.23605100	-1.50149500	0.00000000
C	-0.23605100	-0.39004400	1.09439900
C	0.10250700	0.61527000	0.00000000
C	-0.23605100	-0.39004400	-1.09439900
C	0.63455800	1.83309500	0.00000000
H	-1.08290400	-2.19368200	0.00000000
H	0.69209800	-2.08056200	0.00000000
H	0.47808200	-0.49105200	1.91916900
H	-1.23315900	-0.22782000	1.52398400
H	0.47808200	-0.49105200	-1.91916900
H	-1.23315900	-0.22782000	-1.52398400
H	0.86374400	2.35565000	-0.92607800
H	0.86374400	2.35565000	0.92607800

O3

C	-1.42272200	-0.73073200	-0.24544100
C	-1.42432400	0.72979600	0.24252300
C	-0.01209600	1.23155000	-0.12273700
C	0.88011000	0.00017400	0.00083500
C	-0.01185100	-1.23095000	0.12653000
C	2.21342000	0.00004800	-0.00157900
H	-2.22275400	-1.33503300	0.19498300
H	-1.55365200	-0.75632500	-1.33546000
H	-2.22276700	1.33351300	-0.20156300
H	-1.56050900	0.75516800	1.33189200
H	0.32908700	2.06553000	0.50051600
H	-0.00318600	1.58911000	-1.16276900
H	0.33182200	-2.06767600	-0.49160700
H	-0.00686700	-1.58359200	1.16833300
H	2.78683000	-0.92143200	0.07109900
H	2.78677100	0.92141700	-0.07621000

O4

C	1.02044400	-1.26885400	-0.30252900
C	1.82304200	-0.00000600	0.02219200
C	1.02045500	1.26885000	-0.30252300
C	-0.34446400	1.27056300	0.41818900
C	-1.11542300	0.00000500	0.13381000
C	-0.34446800	-1.27055500	0.41819700
C	-2.35522100	-0.00000100	-0.36378700
H	1.59063000	-2.16451700	-0.02492800
H	0.85087100	-1.32330800	-1.38701900
H	2.08385800	-0.00001300	1.09128200

H	2.77143500	-0.00000900	-0.53012700
H	1.59064700	2.16450500	-0.02491200
H	0.85089300	1.32331300	-1.38701500
H	-0.16277600	1.34661800	1.50252800
H	-0.93181100	2.15088800	0.13227000
H	-0.93182200	-2.15088000	0.13229200
H	-0.16276500	-1.34660000	1.50253400
H	-2.88767000	-0.92498100	-0.57409300
H	-2.88767500	0.92497400	-0.57410500

O5

C	-1.31910900	0.02513600	0.09289300
C	-2.40358600	-0.19588200	-0.65870100
H	-2.90757000	0.60772100	-1.19114400
H	-2.83316100	-1.18966900	-0.76543200
C	-0.77152600	1.42940800	0.27521400
H	-1.20175200	1.85855800	1.19358100
H	-1.14121800	2.05492100	-0.54700300
C	0.76334800	1.56077000	0.36956300
H	1.09595000	1.31690400	1.38827400
H	1.01125100	2.62019600	0.22542600
C	1.56968800	0.70258400	-0.62341100
H	2.54658000	1.17738000	-0.78377400
H	1.07075800	0.69193100	-1.60338400
C	1.82048500	-0.73740200	-0.14043600
H	2.28912800	-0.68754000	0.85412300
H	2.56166000	-1.21029800	-0.79919900
C	0.59188000	-1.65572400	-0.06821100
H	0.90840100	-2.62111400	0.35011000
H	0.22698600	-1.86178300	-1.08341700
C	-0.59782200	-1.12514300	0.76640400
H	-0.24223900	-0.83019800	1.76438000
H	-1.30492400	-1.94949000	0.91756300

O6

C	1.41313800	-0.30395500	0.02406100
C	2.26102000	-0.24969200	1.05786100
H	2.80980900	0.65754500	1.30256400
H	2.44051800	-1.10981100	1.69883200
C	1.15871600	0.92242900	-0.84008700
H	0.83187600	0.61902800	-1.84355700
H	2.10697700	1.45705700	-0.97775400
C	0.14507200	1.93579200	-0.25755500
H	0.15063500	2.82089000	-0.90902400
H	0.52412500	2.27075100	0.71796300
C	-1.31339000	1.47516200	-0.08164900
H	-1.88454400	2.35240200	0.24880400
C	-1.52837500	0.32496100	0.93300900
H	-0.67978000	0.29479800	1.62513300
H	-2.40890900	0.54788700	1.54955700
H	-1.73779800	1.20248600	-1.05867500
C	-1.74710300	-1.07112700	0.31644800
H	-2.75396400	-1.10383100	-0.12440200
H	-1.74873400	-1.81452000	1.12661400
C	-0.75496600	-1.51213600	-0.77019500
H	-0.84820000	-0.84824100	-1.63952700
H	-1.06120500	-2.50366400	-1.12975500
C	0.72448500	-1.60274800	-0.35527400
H	1.27197400	-2.03017500	-1.21096000
H	0.83564100	-2.32471900	0.46447400

O7

C	-1.62245900	-0.27819900	0.01006500
C	-2.32754900	-0.09214600	1.13198900
H	-2.68562700	0.88964700	1.43441300
H	-2.58392400	-0.92002000	1.78885200
C	-1.27216300	0.88131500	-0.91631100
H	-2.19567000	1.27595200	-1.36231800
H	-0.68240600	0.50494800	-1.75912800
C	-0.52168200	2.06274100	-0.25769600
H	-1.20385400	2.58029200	0.42969900
H	-0.28163100	2.78781000	-1.04846300
C	0.76070300	1.70143500	0.51501500
H	1.18303000	2.63057800	0.91827000
H	0.47750300	1.10445900	1.38905100
C	1.83956500	0.95375900	-0.31053300
H	2.71767100	1.59851900	-0.44236100
H	1.46884600	0.77024700	-1.32656800
C	2.32025300	-0.38003300	0.29766300
H	3.06676900	-0.81762800	-0.38084900
H	2.85149700	-0.17200200	1.23748400
C	1.22641300	-1.42761900	0.58798000
H	0.57530000	-1.05325200	1.38685200
H	1.71500500	-2.31863300	1.00224600
C	0.35625000	-1.82594600	-0.62996700

H	0.54119600	-2.87276500	-0.90080500
H	0.65333200	-1.24546500	-1.51147800
C	-1.16650700	-1.66444500	-0.40540100
H	-1.49783300	-2.38787900	0.35046900
H	-1.67615300	-1.93997100	-1.34219100

P1

C	-0.60149600	0.99208500	-0.00004900
C	-1.13950900	-0.27037800	0.00005200
N	-0.14652300	-1.22650000	-0.00004900
C	0.98194600	-0.55140100	0.00000800
N	0.76550900	0.79864200	0.00003600
H	-1.04097300	1.97815500	-0.00009500
H	-2.18488300	-0.54807400	0.00010300
H	1.97637600	-0.97771100	-0.00000300
H	1.47093400	1.52080200	0.00001900

P2

C	0.22598400	1.11556600	-0.00004300
C	1.50155900	0.60744200	0.00006000
N	1.47775500	-0.76912700	0.00004700
C	0.20047300	-1.08424400	-0.00004400
N	-0.61146300	0.01689900	-0.00014800
C	-2.06308600	0.02901900	0.00008800
H	-0.16063000	2.12434100	-0.00015600
H	2.43534700	1.15401700	0.00013400
H	-0.20561600	-2.08804200	-0.00009500
H	-2.42489600	-1.00172300	0.00010000
H	-2.44906000	0.53519200	-0.89101900
H	-2.44876200	0.53511400	0.89136700

P3

C	-1.84771000	1.00762700	0.48287800
C	-3.12238000	0.55705000	0.26049800
N	-3.10603900	-0.68408300	-0.34007000
C	-1.83480100	-0.98391000	-0.46954400
N	-1.00943100	0.00562600	0.01512400
C	0.41077100	0.00708000	0.01189000
C	1.11045400	1.18375900	-0.27896200
C	2.50450000	1.17808000	-0.27806600
C	3.20675900	0.00206500	-0.00745000
C	2.50436500	-1.17098700	0.27405800
C	1.11023800	-1.17149700	0.29578900
H	-1.45720700	1.89651100	0.95391800
H	-4.05330700	1.05212600	0.50233500
H	-1.43659700	-1.87608800	-0.93323800
H	0.56266800	2.08839200	-0.52373400
H	3.04187000	2.09489000	-0.50391800
H	4.29286000	0.00031900	-0.01447600
H	3.04141800	-2.08926500	0.49448700
H	0.56340300	-2.07329500	0.55270100

P4

C	1.48807700	0.63963200	-0.00002700
C	1.42817500	-0.72937800	0.00003600
N	0.11898400	-1.16169000	0.00001900
C	-0.62014900	-0.06928600	0.00003600
N	0.16903000	1.05308900	-0.00008600
C	-2.11451600	-0.02267600	-0.00002900
H	2.30973900	1.34009400	-0.00011600
H	2.25094900	-1.43163000	-0.00000800
H	-0.15291200	2.01008200	0.00061600
H	-2.51127700	0.48935000	0.88607300
H	-2.51114200	0.49003000	-0.88578400
H	-2.49097300	-1.04747200	-0.00040600

P5

C	-0.18077900	1.10807700	-0.00009600
C	0.65728700	0.01863000	0.00009100
N	-0.08614000	-1.14834000	0.00009600
C	-1.34428900	-0.76846400	0.00000800
N	-1.46320700	0.59154000	-0.00007100
C	2.15416200	-0.00912400	-0.00005500
H	0.00836400	2.17122900	0.00060000
H	-2.20508800	-1.42432600	-0.00022200
H	-2.32171100	1.12232800	0.00009700
H	2.53852300	-0.53557000	-0.88176500
H	2.56824700	1.00441300	-0.00034300
H	2.53880700	-0.53518000	0.88177000

P6

C	-0.68536300	1.23146900	0.00010900
C	-1.11059000	-0.07347300	-0.00000100
N	-0.01914800	-0.92421000	-0.00011500
C	1.05052100	-0.15381400	-0.00011300
N	0.69746200	1.16989500	-0.00008000
C	-2.51155900	-0.60063800	0.00004800
C	2.46926000	-0.62587000	0.00008000

H	-1.21781100	2.17114000	-0.00018800
H	1.32763700	1.95856800	0.00017300
H	-3.24123600	0.21580500	0.00004900
H	-2.69873700	-1.22549600	-0.88157400
H	-2.69868300	-1.22543400	0.88172500
H	3.01886500	-0.28064000	-0.88512000
H	2.47002500	-1.71767400	-0.00076500
H	3.01812800	-0.28211300	0.88633200

P7

C	-1.48249000	-1.11017400	-0.01380800
C	-2.76302300	-0.62694800	0.01652000
N	-2.76015900	0.75273900	0.01473900
C	-1.48990600	1.08329600	-0.01438700
N	-0.63822500	-0.00239900	-0.03927500
Si	1.15891800	-0.00488500	0.00383000
C	1.74378000	-1.35863200	-1.16676800
C	1.72470700	1.69371900	-0.57824000
C	1.72447700	-0.34161700	1.76826000
H	-1.09649700	-2.11928200	-0.02923400
H	-3.68895400	-1.18694300	0.03348100
H	-1.11602100	2.09878900	-0.02934100
H	1.41044100	-2.35280700	-0.84719800
H	1.37001200	-1.19162100	-2.18331400
H	2.83976100	-1.38128700	-1.21197600
H	1.39624400	2.49381100	0.09502600
H	1.35079900	1.92185700	-1.58264600
H	2.82051900	1.73059600	-0.61531500
H	1.35203600	0.42681800	2.45549900
H	1.36070800	-1.31133600	2.12736600
H	2.81951300	-0.35043500	1.83631500

SA

C	-2.49539800	-0.87502700	0.00018600
C	-1.27599900	0.08891000	-0.00015900
C	0.00000000	-0.54270100	-0.00048100
O	-1.54736700	1.30434800	0.00005500
C	1.27599900	0.08891000	-0.00015200
C	2.49539800	-0.87502700	0.00017900
O	1.54736700	1.30434800	0.00007100
H	-3.11716500	-0.66834500	0.88200400
H	-3.11995200	-0.66525900	-0.87889800
H	-2.23313100	-1.94068300	-0.00197300
H	0.00000100	-1.63137900	-0.00065200
H	3.11981200	-0.66544000	-0.87904700
H	2.23313100	-1.94068400	-0.00173600
H	3.11730400	-0.66816500	0.88185700

SB1

C	1.48997400	-1.59935800	0.40194600
P	-0.07964100	-0.59414800	0.35454500
O	0.26343800	0.87210300	-0.26334700
O	-0.63057800	-0.50237100	1.73777000
O	-1.13453100	-1.34845300	-0.62988500
C	0.29960500	1.99944300	0.57419300
C	0.62105100	3.22962900	-0.26906500
C	-2.52011900	-1.11866200	-0.54983000
C	-2.90434200	0.35826100	-0.61394100
C	2.74025200	-1.09481300	-0.34166700
N	3.68353400	-0.71413400	-0.89495200
H	1.51690900	-2.55734300	0.94141000
H	1.08599100	1.85657100	1.35270500
H	-0.68976100	2.13522300	1.06945000
H	0.67882000	4.14340100	0.36646600
H	-0.16408000	3.40095400	-1.04121600
H	1.59857000	3.11513500	-0.79144300
H	-2.98801600	-1.66738500	-1.40138200
H	-2.90669200	-1.57537300	0.39155600
H	-4.00845300	0.46751900	-0.71923300
H	-2.62066600	0.91624900	0.30554500
H	-2.43790600	0.85896700	-1.49347300

SB2

C	-0.18447500	2.40565500	0.46347500
P	0.00440900	0.62095500	0.96763300
O	0.01053800	0.53554900	2.45702600
C	-1.42586300	-0.34976600	0.33362000
C	-1.23898400	-1.55744100	-0.34640400
C	-2.33736000	-2.27861500	-0.81954100
C	-3.63220200	-1.80141000	-0.60792800
C	-3.82538700	-0.60197100	0.07991200
C	-2.72560700	0.12041600	0.54840500
C	-0.56119800	2.74611700	-0.98987900
N	-0.84331100	2.99300300	-2.08524900
C	1.58231100	-0.03499900	0.28459600

C	1.81513100	0.00881500	-1.09397000
C	3.00324400	-0.49510300	-1.62721600
C	3.96946100	-1.04658400	-0.78372800
C	3.74342300	-1.09155100	0.59299700
C	2.55361200	-0.58893900	1.12457100
H	-0.05206600	3.20853300	1.20283800
H	-0.22799300	-1.95865900	-0.51892800
H	-2.18257900	-3.22808100	-1.35735500
H	-4.49917900	-2.37203400	-0.97855000
H	-4.84680800	-0.22622200	0.25467800
H	-2.89708700	1.06439000	1.09117500
H	1.06078100	0.43240300	-1.77658200
H	3.17635000	-0.46229900	-2.71510900
H	4.90612700	-1.44740300	-1.20395000
H	4.50386200	-1.52816900	1.26074400
H	2.39470000	-0.63994900	2.21363100

SB3

C	-1.10230700	-1.05954300	-0.73276400
P	0.05755200	-0.15102300	0.40975800
O	-0.31404400	-0.43363100	1.82622400
C	1.79615600	-0.68761300	0.14503400
C	2.09187700	-1.87440800	-0.53182000
C	3.41917200	-2.27042000	-0.71269700
C	4.45909100	-1.48361300	-0.21442200
C	4.16861300	-0.29991500	0.46651800
C	2.84136400	0.09449800	0.64740500
C	-1.88632700	-2.29207300	-0.23989000
O	-1.36460100	-3.36666000	-0.45069100
O	-3.09808800	-2.20749100	0.37732200
C	-3.66174600	-0.94236900	0.60429800
C	-4.30166900	-0.37634200	-0.66011000
C	-0.06082700	1.65177300	0.05612000
C	-0.26285500	2.57706200	1.08468600
C	-0.34263000	3.94187200	0.79897400
C	-0.21874100	4.39067600	-0.51729100
C	-0.01060800	3.47120700	-1.54681500
C	0.07225200	2.10707700	-1.25941100
H	-1.12190100	-0.79830400	-1.80158700
H	1.28705300	-2.51318600	-0.92813000
H	3.64661400	-3.20759400	-1.24622500
H	5.50612800	-1.79732800	-0.35410200
H	4.98705400	0.32122500	0.86530900
H	2.63036100	1.02839600	1.19356000
H	-4.45020200	-1.07733900	1.38249700
H	-2.90552500	-0.24850500	1.03147800
H	-4.80989300	0.59113100	-0.44047800
H	-3.55256100	-0.18152900	-1.45910100
H	-5.06720900	-1.07432100	-1.07017900
H	-0.35842800	2.24375700	2.13041600
H	-0.50161700	4.66679300	1.61369100
H	-0.28106000	5.46764100	-0.74268600
H	0.09166000	3.82270900	-2.58643600
H	0.24521600	1.39684200	-2.08411800

SB4

C	0.93307700	-1.23540100	0.03147700
P	-0.54797800	-0.10586000	0.13606800
O	-1.87512100	-0.98920500	-0.19345300
O	-0.58031000	0.45657000	1.51689800
O	-0.36851200	1.05338400	-0.99228200
C	-3.02517100	-0.86243700	0.60388900
C	-4.09583200	-1.81673900	0.08256600
C	-0.63009300	2.40900300	-0.72481400
C	-2.03852700	2.67625800	-0.19974700
C	2.10618100	-0.91428600	-0.91594000
O	2.11032500	-1.51637000	-1.96896400
O	3.09746000	-0.02929600	-0.61196000
C	3.06035700	0.65054400	0.61455700
C	3.45518300	-0.25246900	1.77967000
H	0.91257900	-2.19927400	0.56270900
H	-3.40243700	0.18469800	0.55322700
H	-2.77948600	-1.11715700	1.66162200
H	-5.02984100	-1.73505900	0.68493600
H	-3.74944000	-2.87441500	0.13580600
H	-4.35326700	-1.59223200	-0.97806700
H	-0.47980700	2.95886500	-1.68408300
H	0.13173300	2.78916100	-0.00436600
H	-2.23913500	3.77238500	-0.17301400
H	-2.19292000	2.30818700	0.83804400
H	-2.80766800	2.21442100	-0.86023700
H	3.79479400	1.48718100	0.53811700
H	2.06367500	1.11785000	0.76679900
H	3.49938700	0.33140700	2.72796500
H	2.73047000	-1.07969100	1.94278700
H	4.45925800	-0.70592100	1.61487500

SB5

C	0.97617900	-0.71925900	-0.36712300
P	-0.76368700	-0.11732100	-0.07552400
C	-1.97438600	-1.35860800	-0.75956600
C	-3.27905700	-0.96759300	-1.06028400
C	-4.18505200	-1.89652800	-1.57205100
C	-3.78628800	-3.21632600	-1.78327000
C	-2.48161700	-3.60734000	-1.48255300
C	-1.57562500	-2.67842500	-0.97068800
C	-1.00492500	1.52109900	-0.93102300
C	-1.34847500	2.65123300	-0.18922600
C	-1.52910700	3.87725100	-0.82946500
C	-1.36597800	3.97311900	-2.21137900
C	-1.02242900	2.84298600	-2.95317600
C	-0.84188300	1.61692300	-2.31295500
C	-1.05147800	0.08738200	1.75471400
C	-0.26111200	0.97024500	2.49048700
C	-0.47642000	1.12331200	3.86011000
C	-1.48218300	0.39369900	4.49382600
C	-2.27254900	-0.48916500	3.75805300
C	-2.05718600	-0.64231500	2.38842800
C	2.17302800	0.12677400	0.10551200
C	6.03788400	-1.21034600	-0.54246100
C	5.05121700	-2.10422300	-0.12656000
C	3.74924000	-1.65378600	0.09177800
C	3.43405800	-0.30950200	-0.10583500
C	4.42076200	0.58437200	-0.52164200
C	5.72270300	0.13393800	-0.74007400
O	1.98430200	1.18051100	0.66522900
H	1.14803300	-1.67878700	-0.87680000
H	-3.59348300	0.07329200	-0.89386600
H	-5.21402500	-1.58824300	-1.80906100
H	-4.50074100	-3.94881900	-2.18701400
H	-2.16717300	-4.64820800	-1.64904400
H	-0.54669300	-2.98674200	-0.73353400
H	-1.47695700	2.57565900	0.90062700
H	-1.80021100	4.76850800	-0.24451600
H	-1.50826700	4.94001800	-2.71621600
H	-0.89387400	2.91858200	-4.04301900
H	-0.57092800	0.72563100	-2.89791900
H	0.53195900	1.54577100	1.99067600
H	0.14698200	1.81943400	4.44044000
H	-1.65205800	0.51456200	5.57388800
H	-3.06566700	-1.06463200	4.25785500
H	-2.68048700	-1.33854900	1.80812300
H	7.06461500	-1.56557100	-0.71461700
H	5.29982500	-3.16437200	0.02925300
H	2.97110100	-2.35870200	0.41979200
H	4.17219200	1.64455200	-0.67731100
H	6.50082000	0.83884400	-1.06816000

SB6

C	-0.12914100	-0.04983100	2.34834600
C	-1.36432200	-0.22348200	2.98760200
N	-2.40953400	-0.37836200	3.49799200
P	0.02080800	-0.00188500	0.64667400
C	1.80464900	0.11075100	0.27949900
C	2.32294900	1.06661100	-0.60438500
C	3.69665500	1.12296700	-0.84819400
C	4.55876200	0.22812700	-0.21397900
C	4.04724200	-0.72851100	0.66647400
C	2.67676500	-0.79135300	0.91262800
C	-0.80856000	1.41942700	-0.18415900
C	-1.14645300	1.40625100	-1.54712600
C	-1.75052500	2.52042500	-2.12860800
C	-2.03421200	3.64797800	-1.35310600
C	-1.71426000	3.66039000	0.00513000
C	-1.10342000	2.54979400	0.58933800
C	-0.64026900	-1.47429600	-0.23175800
C	-1.85525000	-2.03786700	0.19419600
C	-2.37037100	-3.15608200	-0.46007400
C	-1.68597300	-3.72150500	-1.53862900
C	-0.47736600	-3.16829400	-1.96241600
C	0.04611000	-2.04894600	-1.31226800
H	0.76235700	0.15317200	2.92945700
H	1.65901300	1.76989700	-1.09626800
H	4.09095800	1.87087300	-1.53043100
H	5.62761000	0.27547100	-0.40382100
H	4.71562600	-1.42683400	1.16229700
H	2.27954800	-1.53122000	1.60080600
H	-0.94952700	0.52475300	-2.15051300
H	-2.00972400	2.50527000	-3.18379000
H	-2.51378600	4.51113500	-1.80692400
H	-1.94781200	4.52964900	0.61354500
H	-0.86646500	2.54178600	1.64950300

H	-2.38815600	-1.61967900	1.04272400
H	-3.30773900	-3.58827600	-0.12138100
H	-2.09172000	-4.59388300	-2.04377900
H	0.06324200	-3.60837200	-2.79609800
H	0.99314600	-1.63225300	-1.64245900

SB7

C	0.70846200	-0.11461300	1.83073100
P	-0.14437300	-0.01174900	0.17646800
C	-1.99142400	-0.03633600	0.42605900
C	-2.83230400	-0.40287600	-0.62468200
C	-4.21448900	-0.42114700	-0.43790500
C	-4.75569200	-0.07310000	0.79961400
C	-3.91481100	0.29344000	1.85035500
C	-2.53261000	0.31180800	1.66356300
C	0.35933900	-1.46767400	-0.87284100
C	1.00060000	-1.25872400	-2.09374900
C	1.37741500	-2.34824400	-2.87899500
C	1.11315700	-3.64660900	-2.44321500
C	0.47189700	-3.85556000	-1.22230800
C	0.09498500	-2.76603100	-0.43708400
C	0.34588700	1.57084800	-0.67765700
C	1.68654500	1.81742700	-0.97316300
C	2.05339100	3.00178000	-1.61221300
C	1.07957900	3.93936000	-1.95590500
C	-0.26107900	3.69278100	-1.66040000
C	-0.62793500	2.50845800	-1.02125500
C	2.24664400	-0.11238000	1.90550300
O	2.90052200	-0.04396600	0.89208000
O	2.85881900	-0.18621800	3.09295200
C	2.09993100	-0.26561900	4.26912700
H	0.11304400	-0.17691100	2.75355000
H	-2.40547700	-0.67752300	-1.60058600
H	-4.87768600	-0.71004400	-1.26658400
H	-5.84568600	-0.08768600	0.94691800
H	-4.34164100	0.56801300	2.82627800
H	-1.86941700	0.60085000	2.49219400
H	1.20915500	-0.23478500	-2.43733800
H	1.88298700	-2.18349900	-3.84193700
H	1.41048400	-4.50578900	-3.06241400
H	0.26341300	-4.87950200	-0.87868900
H	-0.41072200	-2.93076800	0.52578900
H	2.45450700	1.07793500	-0.70226400
H	3.11069400	3.19636000	-1.84512600
H	1.36889600	4.87325900	-2.46001700
H	-1.02904600	4.43224300	-1.93136800
H	-1.68522000	2.31394300	-0.78820500
H	2.78098600	-0.31921000	5.14779700
H	1.46281600	-1.17769900	4.23806600
H	1.45385500	0.63657000	4.35520100

SB8

C	-0.67173100	-0.90492500	-1.45334200
C	0.16209100	-1.55539800	-2.48872800
C	-2.20740500	-0.96131400	-1.55397900
O	-2.88798400	-0.43038800	-0.70888000
O	-2.78782500	-1.59836900	-2.57746300
C	-1.99794800	-2.21456000	-3.55828200
P	0.13686600	-0.01742900	-0.02750300
C	1.98992000	-0.12989200	-0.19495100
C	2.80376200	0.05806800	0.92210900
C	4.19043900	-0.02597800	0.79674100
C	4.76317400	-0.29818300	-0.44558300
C	3.94933200	-0.48614400	-1.56264300
C	2.56263700	-0.40200500	-1.43730800
C	-0.39043500	-0.80922400	1.57546600
C	-1.06425600	-0.05602600	2.53679300
C	-1.45872400	-0.64854600	3.73636300
C	-1.17955500	-1.99423100	3.97444900
C	-0.50573400	-2.74742900	3.01312400
C	-0.11117000	-2.15489100	1.81357100
C	-0.38003400	1.77344100	-0.03718000
C	-1.72868400	2.11064500	0.07650500
C	-2.11546200	3.45079500	0.06913800
C	-1.15359300	4.45364000	-0.05169200
C	0.19505800	4.11643700	-0.16537600
C	0.58184800	2.77626900	-0.15810700
H	-0.49538900	-2.02927200	-3.25157400
H	0.80714500	-0.79194100	-2.97843100
H	0.80126000	-2.33377100	-2.01505300
H	-2.65542700	-2.68843300	-4.32112700
H	-1.35289500	-1.45110300	-4.04798400
H	-1.35877900	-2.99293300	-3.08460700
H	2.35206900	0.27257100	1.90188600
H	4.83231100	0.12241700	1.67763800
H	5.85671200	-0.36462400	-0.54437400

H	4.40102800	-0.70072000	-2.54240100
H	1.92076800	-0.55025000	-2.31823200
H	-1.28456900	1.00518900	2.34895200
H	-1.98997700	-0.05453700	4.49460100
H	-1.49080200	-2.46150300	4.92037900
H	-0.28549100	-3.80866300	3.20093800
H	0.42021600	-2.74885600	1.05539200
H	-2.48723100	1.31976400	0.17196700
H	-3.17906600	3.71676600	0.15862000
H	-1.45863300	5.51048400	-0.05732600
H	0.95360700	4.90732500	-0.26076200
H	1.64543600	2.51028800	-0.24774100

SC1

C	-1.35425900	-0.05521000	0.00009500
C	0.22016000	0.00177000	-0.00003300
O	0.80882900	-1.10825800	-0.00006400
O	0.69593000	1.16599800	-0.00003500
H	-1.73299700	-1.08538300	-0.00006700
H	-1.75015300	0.47187100	0.88075500
H	-1.75032400	0.47223400	-0.88026900

SC2

C	0.28017900	0.00000000	0.00000700
C	1.83613900	0.00000000	0.00001300
O	2.36739100	1.13875900	-0.00000900
O	2.36739100	-1.13875900	-0.00000600
C	-0.43696400	-1.20252500	0.00000400
C	-1.83351800	-1.20769700	-0.00000200
C	-2.53920500	0.00000000	-0.00000400
C	-1.83351800	1.20769700	-0.00000100
C	-0.43696400	1.20252500	0.00000400
H	0.14475300	-2.12050000	0.00000600
H	-2.37790900	-2.15245000	-0.00000500
H	-3.62884200	0.00000000	-0.00000900
H	-2.37790900	2.15245000	-0.00000300
H	0.14475400	2.12050000	0.00000700

SC3

C	1.41916900	-0.00000100	0.00032100
C	2.97716000	0.00000000	0.00043400
O	3.49861400	-1.14081200	-0.00047600
O	3.49861400	1.14081300	-0.00048400
C	0.70487900	1.20736200	0.00028300
C	-0.68505900	1.22161000	0.00020600
C	-1.37021300	0.00000000	0.00017600
C	-0.68506000	-1.22161000	0.00020500
C	0.70487800	-1.20736300	0.00028300
N	-2.82499800	0.00000000	0.00011100
O	-3.41694300	-1.08769100	-0.00035000
O	-3.41694300	1.08769200	-0.00034300
H	1.28882800	2.12242400	0.00031900
H	-1.25195900	2.14540300	0.00017500
H	-1.25196000	-2.14540200	0.00017400
H	1.28882700	-2.12242500	0.00032100

SC4

C	1.42991900	-0.00017000	0.00002600
C	2.99132000	-0.00032300	-0.00003800
O	3.50263800	1.14208200	0.00059800
O	3.50242500	-1.14282200	-0.00072900
C	0.72195700	-1.20443600	-0.00000900
C	-0.67494900	-1.18621100	0.00003000
C	-1.40408100	0.00014700	-0.00000600
C	-0.67469600	1.18633000	0.00000300
C	0.72222300	1.20425300	0.00007300
N	-1.42047400	-2.45293800	0.00006800
N	-1.41991800	2.45324300	-0.00003300
O	-2.65453000	2.40214700	0.00003900
O	-0.77740600	3.50379300	-0.00016800
O	-2.65505300	-2.40152100	-0.00032500
O	-0.77820900	-3.50362500	0.00049100
H	1.28865700	-2.12823000	-0.00013000
H	-2.48414100	0.00022500	-0.00004000
H	1.28914300	2.12790800	0.00020300

SD1

C	-0.25770600	0.69195400	-0.00003000
C	-0.26874600	-0.72462200	0.00003600
N	-1.57529400	-1.20170800	-0.00004600
C	-2.31855700	-0.12653100	-0.00009100
N	-1.59665800	1.04638300	0.00009000
C	0.92485900	1.43459800	-0.00006800

C	2.11591000	0.71342800	-0.00003400
C	2.12482100	-0.69648500	0.00001700
C	0.94229300	-1.42846800	0.00005900
H	-3.40165800	-0.11752200	-0.00011300
H	-1.97507400	1.98183700	0.00045300
H	0.92279600	2.52116100	-0.00006800
H	3.06040300	1.25053700	-0.00002500
H	3.07804500	-1.21784100	0.00002500
H	0.94190400	-2.51413700	0.00008300

SD2

C	-0.15551100	-0.36007900	-0.00014100
C	0.36930800	0.95587000	0.00003300
N	-0.66221500	1.88695300	0.00051500
C	-1.75117000	1.16301500	-0.00050300
N	-1.53192500	-0.19776400	-0.00022100
C	0.65905900	-1.49492700	-0.00004100
C	2.03480200	-1.27706100	-0.00006700
C	2.57475400	0.02517200	-0.00003500
C	1.75605000	1.15014200	0.00002000
C	-2.53095800	-1.24666300	0.00034500
H	-2.76128500	1.55646300	-0.00070700
H	0.24797600	-2.50054600	0.00017700
H	2.70703300	-2.13075200	0.00004400
H	3.65429000	0.14844200	0.00006900
H	2.16647300	2.15533100	0.00019000
H	-3.52397300	-0.79115400	-0.00829200
H	-2.42942300	-1.88229600	-0.88659200
H	-2.44011800	-1.87261600	0.89538300

SD3

C	-0.21589200	0.70269500	-0.00006500
C	-0.17979600	-0.71303800	-0.00011100
N	1.13463800	-1.16459800	-0.00050100
C	1.87276600	-0.08070000	-0.00059300
N	1.11742400	1.07817500	-0.00045500
C	-1.41007300	1.42415100	0.00006000
C	-2.59018600	0.68268500	0.00025600
C	-2.57436200	-0.72593300	0.00023800
C	-1.37778200	-1.43710200	0.00002100
C	3.36658700	-0.05130300	0.00068100
H	1.47640200	2.02142700	-0.00054000
H	-1.42680200	2.51068500	0.00003300
H	-3.54346600	1.20410600	0.00043000
H	-3.51788800	-1.26477500	0.00039200
H	-1.35928300	-2.52271500	-0.00003400
H	3.73709100	-1.07768500	-0.01306600
H	3.76029000	0.45010900	0.89390000
H	3.76165800	0.47507500	-0.87733500

SD4

C	0.84836600	0.70589700	0.00028000
C	0.55561400	-0.67733700	-0.00015000
N	1.72925200	-1.42374300	-0.00025600
C	2.68628400	-0.53247500	0.00014000
N	2.23250200	0.76745400	0.00083000
C	-0.15567500	1.67657800	-0.00016200
C	-1.46901800	1.22038200	-0.00088100
C	-1.79729100	-0.15774300	-0.00096800
C	-0.77806700	-1.10767900	-0.00088300
C	-3.25047500	-0.57854900	0.00121000
H	3.74609100	-0.75595400	0.00034300
H	2.80201800	1.60037000	0.00106300
H	0.06898300	2.73975300	-0.00032600
H	-2.27689600	1.94865600	-0.00148900
H	-1.00155100	-2.17081300	-0.00150900
H	-3.34866800	-1.66826000	-0.02485200
H	-3.77252100	-0.21925100	0.89738100
H	-3.78815400	-0.17492600	-0.86614400

SD5

C	0.33019500	0.83002900	0.00008600
C	0.15852800	-0.57277200	-0.00005400
N	1.39243900	-1.21253800	0.00001600
C	2.28178300	-0.24797500	0.00013100
N	1.70423700	1.00861200	0.00022100
C	-0.75290800	1.70974000	-0.00001800
C	-2.02351000	1.14226000	-0.00023700
C	-2.23104600	-0.25783200	-0.00027300
C	-1.13223000	-1.11630900	-0.00025600
C	-3.64200200	-0.80396500	0.00030200
C	3.76366400	-0.43823600	-0.00005000
H	2.19664700	1.88947100	0.00018600
H	-0.62081200	2.78842500	-0.00006400
H	-2.89086300	1.79867700	-0.00042500
H	-1.26379400	-2.19484500	-0.00041100

H	-3.64417000	-1.89844200	-0.00684300
H	-4.20109200	-0.47638400	0.88619300
H	-4.20636800	-0.46462200	-0.87771100
H	3.97916000	-1.50811000	0.00268800
H	4.23029400	0.01426700	0.88407400
H	4.22941600	0.00940200	-0.88713300

SD6

C	-1.00406000	0.68813100	-0.00001000
C	-1.01856700	-0.72306600	0.00000900
N	-2.32561400	-1.19972600	-0.00008700
C	-3.06700900	-0.12257700	0.00003200
N	-2.34165800	1.04886500	0.00001500
C	0.18505600	1.41829100	-0.00005300
C	1.38961700	0.71465400	-0.00003100
C	1.39491300	-0.71262000	0.00001600
C	0.19524300	-1.42061000	0.00002700
C	2.69400500	1.47823100	-0.00000100
C	2.70696800	-1.46435200	0.00002400
H	-4.15001400	-0.11087600	0.00005300
H	-2.71690300	1.98546200	0.00033600
H	0.18554200	2.50558100	-0.00009300
H	0.19184400	-2.50704100	0.00001000
H	2.51862900	2.55856900	-0.00080100
H	3.30577300	1.24187200	0.88053700
H	3.30652200	1.24067100	-0.87968100
H	2.53699000	-2.54520400	0.00066400
H	3.31749800	-1.22523900	-0.88084700
H	3.31803000	-1.22426800	0.88025200

SD7

C	-1.33581200	0.66250600	0.00020100
C	-0.78898600	-0.63954500	-0.00027700
N	-1.80002000	-1.59247600	-0.00025800
C	-2.90946800	-0.89648400	0.00007800
N	-2.70878500	0.46306700	0.00043400
C	-0.52864400	1.80360600	0.00024400
C	0.84421800	1.60720500	-0.00008600
C	1.40796900	0.30763200	-0.00056600
C	0.60243800	-0.82863000	-0.00071300
O	2.77818500	0.28569200	-0.00108300
C	3.41930200	-0.97742800	0.00128700
H	-3.90756500	-1.31687400	0.00018600
H	-3.42439600	1.17419100	0.00112700
H	-0.94528400	2.80690400	0.00059200
H	1.52573000	2.45167800	0.00001500
H	1.00518400	-1.83392800	-0.00123900
H	4.49149400	-0.77100300	0.00271100
H	3.16102200	-1.56091800	0.89553700
H	3.16386400	-1.56289300	-0.89250300

SE1

C	-2.49539800	-0.87502700	0.00018600
C	-1.27599900	0.08891000	-0.00015900
C	0.00000000	-0.54270100	-0.00048100
O	-1.54736700	1.30434800	0.00005500
C	1.27599900	0.08891000	-0.00015200
C	2.49539800	-0.87502700	0.00017900
O	1.54736700	1.30434800	0.00007100
H	-3.11716500	-0.66834500	0.88200400
H	-3.11995200	-0.66525900	-0.87889800
H	-2.23313100	-1.94068300	-0.00197300
H	0.00000100	-1.63137900	-0.00065200
H	3.11981200	-0.66544000	-0.87904700
H	2.23313100	-1.94068400	-0.00173600
H	3.11730400	-0.66816500	0.88185700

SE2

C	0.00000000	1.23041700	0.05099700
C	0.00000000	0.00000000	0.71155500
C	0.00000000	-1.23041700	0.05099700
N	0.00000000	2.28500100	-0.47710800
N	0.00000000	-2.28500100	-0.47710800
H	0.00000000	0.00000000	1.79821700

SE3

C	1.30566000	0.17663100	-0.24945900
C	0.00691900	-0.37256000	-0.18955700
O	1.71179300	1.33861900	-0.20381000
C	-1.17448200	0.38949500	-0.03963100
O	-1.37009400	1.59989800	0.06301900
O	2.26403500	-0.88200000	-0.39017100
C	4.22421200	-0.29656200	0.94487600
C	3.61385600	-0.46217700	-0.44769700
O	-2.30636400	-0.48467600	-0.01065000

C	-4.63481900	-0.89745800	0.15504000
C	-3.54881200	0.17165200	0.13612300
H	-0.09029900	-1.44878300	-0.25672200
H	5.29231300	-0.04234600	0.88223900
H	4.12127800	-1.22170300	1.52500800
H	3.70286200	0.50723200	1.47221000
H	4.15027900	-1.24065800	-1.00897400
H	3.68919800	0.48573200	-0.99231100
H	-5.62891400	-0.44418100	0.26737600
H	-4.62252700	-1.47814600	-0.77481300
H	-4.47665200	-1.59487200	0.98602900
H	-3.57127300	0.76636200	1.06087900
H	-3.71643500	0.88250900	-0.68620600

SE4

C	0.32642400	0.12598200	-0.23170300
C	-0.91233600	-0.54429800	-0.08107800
O	0.61730000	1.31988400	-0.28356300
C	-2.17910600	0.07822900	0.06731900
C	-3.37688400	-0.89641600	0.21953800
O	-2.45570300	1.29325700	0.09219800
O	1.38470800	-0.84283400	-0.33790100
C	3.33061400	0.02357000	0.85831400
C	2.68110900	-0.29769300	-0.48862900
H	-0.86482900	-1.62858300	-0.07622900
H	-4.10718100	-0.69471000	-0.57566000
H	-3.10343300	-1.95846700	0.18540000
H	-3.88617100	-0.69457500	1.17164600
H	4.36227100	0.38094900	0.72611900
H	2.75132200	0.80387600	1.35988400
H	3.35178700	-0.86529700	1.50085300
H	3.27087100	-1.05548000	-1.02459100
H	2.63599600	0.61357800	-1.09586600

SE5

C	-1.30020200	-0.24396900	-0.24155600
C	-0.01510200	0.35044000	-0.11743000
O	-1.63573300	-1.42856000	-0.29392300
C	1.12979000	-0.49500900	-0.04609800
O	1.25124300	-1.71921000	-0.05338600
C	0.16916100	1.85408700	-0.07612900
O	2.31861400	0.29266700	0.04971800
C	4.67266800	0.52868800	0.19558200
C	3.51321100	-0.45810500	0.13187300
O	-2.33457000	0.74878900	-0.31395700
C	-4.25294200	-0.08456800	0.94873500
C	-3.64867300	0.23479600	-0.41895800
H	-0.79954800	2.35569400	-0.03074900
H	0.75788700	2.17496100	0.79609800
H	0.70521100	2.24633200	-0.95671800
H	5.63319200	0.00010900	0.26096700
H	4.68764400	1.16532700	-0.69672900
H	4.57734700	1.18264800	1.07030400
H	3.50493600	-1.10938200	1.01790600
H	3.61356500	-1.12596300	-0.73524900
H	-5.29710500	-0.41568000	0.85208400
H	-3.67373600	-0.88390700	1.41910000
H	-4.22850400	0.79788100	1.59988000
H	-4.23717600	1.01411000	-0.92386000
H	-3.64761900	-0.66977600	-1.03676300

SE6

C	-0.17028000	0.00041800	-0.20657500
C	-1.33867700	-0.71358200	0.10800100
O	0.00057900	1.19370800	-0.48387500
C	-2.60300200	-0.11505800	0.16742300
N	-3.68662500	0.33884200	0.23228700
O	0.96123300	-0.87512700	-0.18017300
C	2.83011200	0.37945800	0.77154200
C	2.20032300	-0.25569300	-0.46873900
H	-1.26266600	-1.77515700	0.31701600
H	3.82347100	0.79258200	0.54379000
H	2.18570100	1.18894600	1.12527800
H	2.93826400	-0.36065400	1.57386500
H	2.85047600	-1.04984200	-0.86285200
H	2.06576600	0.51031700	-1.24063100

SE7

C	1.07592800	-1.25763400	-0.09371800
C	-0.42802800	-1.24676800	-0.45717600
C	-1.20819900	-0.00006300	0.00503700
C	-0.42809700	1.24664100	-0.45734000
C	1.07573000	1.25773800	-0.09344600
C	1.71159800	0.00007500	0.05842700
O	1.62862100	-2.37634800	0.00648200
O	1.62841100	2.37647600	0.00638400
C	-2.61860800	-0.00010000	-0.61280900
C	-1.34522200	0.00004300	1.54122800

H	-0.86897400	-2.16638500	-0.04876500
H	-0.50559000	-1.32932600	-1.55422500
H	-0.50544800	1.32879300	-1.55443800
H	-0.86929200	2.16629800	-0.04929100
H	2.77479600	0.00013900	0.29318300
H	-3.18895600	-0.88823900	-0.30480500
H	-2.56924700	0.00040400	-1.70972500
H	-3.18931100	0.88752700	-0.30399700
H	-1.89214300	0.88857900	1.88630100
H	-1.89319000	-0.88785300	1.88628300
H	-0.35951200	-0.00055800	2.01533100

SE8

C	0.98634700	1.24664200	-0.08470100
O	-0.40623200	1.18336300	-0.37334200
C	-1.09112600	0.00000300	0.00743600
O	-0.40617200	-1.18346200	-0.37311600
C	0.98632700	-1.24662300	-0.08444100
C	1.61235900	0.00003700	0.14119500
O	1.47670000	2.37286900	-0.09231900
O	1.47688300	-2.37277000	-0.09239900
C	-2.39946100	-0.00012600	-0.78074100
C	-1.33972600	0.00008900	1.52693600
H	2.67662300	0.00004000	0.34300300
H	-2.98735400	-0.89339900	-0.54352300
H	-2.98747900	0.89309300	-0.54363200
H	-2.17050100	-0.00017300	-1.85027900
H	-1.90366700	-0.89318200	1.81872200
H	-0.38156200	0.00018900	2.05239800
H	-1.90381200	0.89330300	1.81861500

TSa/A

C	-0.13784800	0.14947000	0.44179000
C	-0.13209400	1.65409000	-1.01346500
C	1.44180100	-1.34429100	-0.88443900
C	2.61980700	-2.07548300	-0.95474600
C	3.49413000	-2.08551200	0.14036700
C	3.20414200	-1.34858100	1.29075700
C	2.03072500	-0.60206300	1.34173600
C	-1.47975600	-0.41230100	0.24600200
C	-1.73560000	-1.63428400	-0.41173600
C	-3.02781900	-2.13168500	-0.51786800
C	-4.09429300	-1.41230800	0.03234200
C	-3.87100800	-0.20267600	0.70439900
C	-2.57758900	0.28169100	0.80690400
C	1.11172100	-0.60670600	0.27172500
C	0.85310700	2.52025400	-0.55525900
C	2.29030100	2.29297600	-0.87140400
C	0.50522200	3.67418100	0.32867500
H	1.80610000	-0.03615400	2.24227200
H	3.89060000	-1.35731600	2.13022000
H	2.87015100	-2.63383700	-1.85016500
H	0.79046500	-1.32583400	-1.75270400
H	-0.10510900	0.81633100	1.30079100
H	-2.40733100	1.21637000	1.33605800
H	-4.70350500	0.33577500	1.14359900
H	-3.21298600	-3.07950600	-1.01104900
H	-0.92116900	-2.22843400	-0.80602300
H	-1.16912800	1.95365500	-0.90234200
H	0.07873800	1.00912000	-1.86108500
H	2.82589200	3.24159600	-0.98625300
H	2.76123600	1.77658800	-0.01750300
H	2.44308600	1.67482000	-1.75831800
H	1.26888900	3.79904400	1.10773700
C	0.41807600	5.00282600	-0.48486100
H	-0.46093100	3.50703700	0.81948000
C	0.07392700	6.19151200	0.41659800
H	1.37401100	5.18128800	-0.99125800
H	-0.33958500	4.89054000	-1.26933100
H	0.01423900	7.10993400	-0.17568500
H	-0.89254100	6.05084500	0.91335500
H	0.83495400	6.34048000	1.19060600
Cl	-5.70842000	-2.03292700	-0.09996300
Cl	4.96325500	-3.00878000	0.05481500

TSe/A

C	1.70932400	-1.29077000	1.34978800
C	0.84430700	-1.06929200	0.25988000
C	1.02620600	-1.85705100	-0.89530800
C	2.00060900	-2.84511200	-0.93352300
C	2.83290000	-3.09857400	0.17277700
C	2.67118700	-2.29786100	1.31054800
C	-0.19963900	-0.03883300	0.41165800
C	-1.63771700	-0.29460000	0.21786500
C	-2.15731200	-1.40164500	-0.48229300
C	-3.53000400	-1.59100300	-0.58741200
C	-4.44125100	-0.69576300	-0.00523700

C	-3.92358900	0.40566000	0.70049600
C	-2.55647600	0.60072200	0.81112200
C	-5.92627000	-0.92507600	-0.09771600
C	3.85902200	-4.20090500	0.12850900
C	0.13634500	1.38388500	-0.99260900
C	1.30818800	2.00110800	-0.55820300
C	2.64394300	1.43855600	-0.89125700
C	1.25444500	3.19791800	0.33328200
H	1.60271000	-0.69042900	2.25034500
H	3.30889500	-2.45917500	2.17531300
H	2.12597900	-3.43298900	-1.83901900
H	0.42412800	-1.67871200	-1.78135800
H	-0.02916800	0.58341100	1.28875900
H	-2.18376700	1.45793100	1.36804200
H	-4.60603400	1.10798800	1.17136100
H	-3.90526200	-2.45891800	-1.12267600
H	-1.49278900	-2.13997500	-0.91323300
H	-0.79263900	1.93273000	-0.87557600
H	0.17768000	0.72863700	-1.85777900
H	3.41852600	2.21160200	-0.90127600
H	2.92035400	0.72476500	-0.09448500
H	2.65421800	0.88708900	-1.83395100
H	2.03510000	3.12973200	1.10266400
C	1.48246800	4.51237400	-0.47596600
H	0.28175200	3.26455300	0.83435200
H	-6.47486400	0.02023000	-0.15763300
H	-6.18696500	-1.53366500	-0.96836600
H	-6.28994600	-1.45414200	0.79334400
H	4.61349100	-4.08211700	0.91118900
H	3.38141000	-5.17833600	0.27554900
H	4.36902700	-4.23505200	-0.83996800
C	1.45937000	5.74281400	0.43514200
H	2.44308400	4.45353400	-1.00122200
H	0.70566200	4.59594900	-1.24514300
H	1.61422900	6.65229200	-0.15380400
H	0.49878800	5.83945500	0.95333600
H	2.25007000	5.69430700	1.19198400

TSf/A

C	1.59953400	0.25819900	-0.53010800
C	2.34845700	-0.84815400	0.91210500
C	1.73399200	2.40197300	0.85152100
C	2.14392400	3.72721600	0.97327300
C	2.86792900	4.33884900	-0.05496200
C	3.19444800	3.61171700	-1.19983400
C	2.79622000	2.27957500	-1.31752800
C	0.18318400	-0.13258100	-0.53929000
C	-0.85325800	0.63491000	0.03353500
C	-2.17698900	0.22594000	-0.02791100
C	-2.50370800	-0.98356700	-0.66524300
C	-1.48766200	-1.76335100	-1.25521000
C	-0.17715700	-1.33968400	-1.18960700
C	2.03956200	1.66081500	-0.30529900
C	3.73168000	-0.83371900	0.69724100
C	4.58672300	0.26089200	1.22651100
C	4.37886400	-1.87480200	-0.15314200
H	3.04909300	1.72186500	-2.21615800
H	3.76215600	4.07636500	-2.00030700
H	1.90184500	4.28398600	1.87361100
H	1.19214900	1.94001400	1.67181800
H	2.13313300	-0.19855700	-1.36257300
H	0.59574400	-1.94677000	-1.65613100
H	-1.76459600	-2.68173700	-1.76175100
H	-2.95982500	0.84258800	0.39746200
H	-0.63183900	1.58898200	0.49576000
H	1.82944600	-1.77585400	0.68979900
H	1.95752900	-0.30461500	1.76789700
H	5.59455500	-0.09881700	1.46047700
H	4.70507300	1.01967000	0.43328000
H	4.15673000	0.76127500	2.09614600
H	5.17137400	-1.42478000	-0.76528900
C	5.01940900	-2.99666800	0.72431700
H	3.64621200	-2.33936200	-0.82338000
C	5.71922300	-4.05052100	-0.13837900
H	5.73599000	-2.54666900	1.42147000
H	4.23593500	-3.46390600	1.33238600
H	6.15134600	-4.83106300	0.49568600
H	5.01881700	-4.53118700	-0.83049900
H	6.53048100	-3.60958900	-0.72798100
H	3.18306800	5.37330100	0.04268100
O	-3.75641200	-1.46815100	-0.78545800
C	-4.84033400	-0.80161400	-0.18911800
C	-5.12722700	-1.03060000	1.15436500
C	-5.64612500	0.00340400	-0.98870600
C	-6.25364500	-0.42266900	1.71193300
H	-4.48894300	-1.68405300	1.74103000
C	-6.77034200	0.60355200	-0.41782300
H	-5.39924000	0.14216000	-2.03644800

C	-7.07323100	0.39383100	0.92928000
H	-6.49368100	-0.59618700	2.75673900
H	-7.41099500	1.23093800	-1.03030100
H	-7.95107400	0.85955900	1.36671300

TSg/A

C	1.61014100	-2.09316400	1.43088500
C	0.93953200	-1.62003300	0.28768300
C	0.94678000	-2.41766800	-0.87195900
C	1.57514100	-3.66027800	-0.87354500
C	2.20959800	-4.13158600	0.28019200
C	2.22694500	-3.34472200	1.43190800
C	0.24913200	-0.30703700	0.38987200
C	-1.19557600	-0.15510400	0.17483600
C	-1.99155800	-1.06601400	-0.56071700
C	-3.35044100	-0.87066900	-0.70187600
C	-3.97804700	0.25037500	-0.11820000
C	-3.20750400	1.16693800	0.62497500
C	-1.84504700	0.95526100	0.75887500
O	-5.29957400	0.34507700	-0.31649600
C	-6.02654000	1.43882600	0.25461000
C	1.02273900	0.88974700	-0.97296500
C	2.33567100	1.11571900	-0.54536100
C	3.43415500	0.17145800	-0.87951400
C	2.65549900	2.27221300	0.34186100
H	1.62240600	-1.48923700	2.33507700
H	2.72316000	-3.69935400	2.33019900
H	2.69532600	-5.10264400	0.27545000
H	1.57363400	-4.26179600	-1.77759300
H	0.48049600	-2.06192700	-1.78616700
H	0.56930100	0.24252300	1.27388700
H	-1.26255100	1.66710600	1.34000200
H	-3.66716500	2.02477800	1.10055000
H	-3.96648300	-1.57779500	-1.24713300
H	-1.54816000	-1.95591400	-0.98968100
H	0.32659600	1.71729700	-0.87443000
H	0.86772100	0.26941100	-1.85133300
H	4.39300800	0.69308100	-0.97094400
H	3.54639200	-0.53813800	-0.04119800
H	3.24004400	-0.41432400	-1.77992700
H	3.40127200	1.97946700	1.09241400
C	3.23574900	3.46625300	-0.48050600
H	1.75656800	2.61926200	0.86496600
H	-7.06277500	1.28609200	-0.04528700
H	-5.95349700	1.42848900	1.34760100
H	-5.66614600	2.39590300	-0.13827600
C	3.59394700	4.64782600	0.42504500
H	4.12441000	3.13093400	-1.02812500
H	2.49807600	3.77376400	-1.23096900
H	3.99183300	5.47423100	-0.17225100
H	2.71617400	5.01829900	0.96617300
H	4.35505700	4.36983300	1.16237800

TSh/A

C	0.39012900	-0.07637700	-0.35392600
C	0.99968500	1.25033000	0.97444000
C	-1.59504400	-0.84429300	1.05671200
C	-2.94630900	-1.10458400	1.16843200
C	-3.81582200	-0.85483300	0.08374300
C	-3.29898200	-0.30659100	-1.10070600
C	-1.93756000	-0.02813700	-1.18915700
C	1.42196300	-1.13128100	-0.20423300
C	1.23210700	-2.32563500	0.51503500
C	2.24060600	-3.28146500	0.57949900
C	3.47289200	-3.09304400	-0.06365700
C	3.65974800	-1.90320300	-0.78917600
C	2.65854800	-0.94663200	-0.85930900
C	-1.04639300	-0.31759900	-0.13674400
C	0.46246600	2.46058300	0.52295400
C	-0.93993000	2.83561600	0.83702600
C	1.25058200	3.35757400	-0.37133900
H	-1.55028300	0.38597300	-2.11723200
H	-3.94271400	-0.09495300	-1.94596300
H	-3.36990200	-1.50190700	2.08487300
H	-0.95839000	-1.02976500	1.91662800
H	0.56361300	0.49494600	-1.26531100
H	2.82954900	-0.03880300	-1.43460100
H	4.59942600	-1.73503700	-1.30851900
H	2.06385800	-4.19994100	1.13265900
H	0.28435000	-2.53457800	0.99536000
H	2.07285900	1.12200900	0.87408100
H	0.57249000	0.79410000	1.86298800
H	-1.11932000	3.90745800	0.71681500
H	-1.59347700	2.31209600	0.11408100
H	-1.25636900	2.50993700	1.83142600
H	0.60268600	3.77610100	-1.15308200
C	1.86701800	4.54420300	0.43429900
H	2.06530500	2.80669300	-0.85513200

C	2.64955800	5.49347300	-0.47735500
H	1.06578700	5.09072200	0.94577100
H	2.52314400	4.14038200	1.21422800
H	3.07967800	6.31137600	0.10914400
H	3.47201200	4.97568000	-0.98334500
H	2.00299400	5.93412900	-1.24435200
C	-6.05864300	-0.94527300	-0.75135200
H	-7.01479700	-1.27657600	-0.34720400
H	-6.11932000	0.11643500	-1.01622500
H	-5.80760500	-1.53885700	-1.63756100
O	-5.10652600	-1.15946900	0.29493600
C	4.54925500	-4.14544000	-0.01229900
H	4.50159000	-4.79081700	-0.89950700
H	5.54769800	-3.69693100	0.00707100
H	4.44210300	-4.78847800	0.86609700

TSj/A

C	2.07062900	-0.57481800	1.20871600
C	1.19125700	-0.50543900	0.11307600
C	1.60383800	-1.11565800	-1.09283100
C	2.80788200	-1.78924300	-1.18008400
C	3.65610100	-1.88654900	-0.05701200
C	3.27906000	-1.26621600	1.14336700
C	-0.11271400	0.17737700	0.29996300
C	-1.40193400	-0.53575300	0.12892900
C	-1.57345600	-1.68390600	-0.67565400
C	-2.80349800	-2.30580200	-0.77732600
C	-3.92081400	-1.80219000	-0.08150100
C	-3.77126400	-0.66347500	0.73145100
C	-2.52895300	-0.05137500	0.82257100
O	-5.06768500	-2.48139700	-0.25005500
C	-6.24702400	-2.05150800	0.43486000
C	-0.24779600	1.59874000	-0.95439900
C	0.64314300	2.58922800	-0.50075000
C	2.09259400	2.50662800	-0.80547700
C	0.17023100	3.68163600	0.39460400
H	1.78885300	-0.10873700	2.15019400
H	3.91282200	-1.31450000	2.02069400
O	4.79603800	-2.57522800	-0.24766500
H	3.12697300	-2.25375500	-2.10725400
H	0.98557300	-1.04648400	-1.98320800
H	-0.12276700	0.73643400	1.23605700
H	-2.42733300	0.82565500	1.45873500
H	-4.60736800	-0.26600000	1.29410000
H	-2.93246200	-3.19925100	-1.37909700
H	-0.72975600	-2.11992200	-1.19606800
H	-1.30395700	1.83897200	-0.87297300
H	0.01239400	1.06950000	-1.86761700
H	2.60238600	3.46404700	-0.66778200
H	2.53882800	1.79156500	-0.08844600
H	2.29747900	2.10813400	-1.80273300
H	0.91406200	3.87773000	1.17837200
C	-0.04378200	5.00428300	-0.40974700
H	-0.77744400	3.41054800	0.87370600
H	-7.02772200	-2.75154000	0.13820500
H	-6.10817200	-2.09437600	1.52106900
H	-6.52946800	-1.03648700	0.13313000
C	5.70767700	-2.73153300	0.84226500
H	6.53131600	-3.32819600	0.45078300
H	6.08682700	-1.76061600	1.18166500
H	5.23500600	-3.26046700	1.67774600
C	-0.49697500	6.14571900	0.50482600
H	0.89056500	5.27610800	-0.91473100
H	-0.78903100	4.82730500	-1.19398900
H	-0.64623300	7.05970700	-0.07859000
H	-1.44336900	5.90819800	1.00319400
H	0.24995400	6.35856300	1.27751400

TSa/B

C	1.40291000	2.21166200	0.99433700
C	0.04426900	1.70666300	1.00928600
C	-0.99623900	2.59507700	0.53900100
C	-0.69324600	3.75476300	-0.12502100
C	0.66063800	4.14851600	-0.29658100
C	1.68087600	3.36700700	0.27634000
C	0.98252200	5.40107800	-1.05396400
C	2.46721000	1.51445000	1.78096200
C	-0.09647000	0.27937200	-0.31439300
C	-1.48467400	-0.25394100	-0.16745000
C	-2.31888700	-0.21126500	-1.29827500
C	-3.60519400	-0.74319300	-1.26748000
C	-4.08619200	-1.30124900	-0.08170000
C	-3.28889200	-1.32838900	1.06645300
C	-1.99884300	-0.80935300	1.01724700
C	1.06200600	-0.63965600	-0.22436600
C	1.07704200	-1.81005500	0.56043700
C	2.17077100	-2.66860800	0.54663000

C	3.27064500	-2.37319500	-0.26482100
C	3.28088000	-1.22335100	-1.06275900
C	2.18783900	-0.36856000	-1.03086700
H	-4.23222600	-0.72054000	-2.15206000
H	-1.95228600	0.22356300	-2.22444400
H	-3.67884500	-1.74855000	1.98710200
H	-1.40538500	-0.82494400	1.92721500
H	-0.01055800	0.90686300	-1.19995400
H	2.19987100	0.52310600	-1.65263900
H	4.13229300	-1.01288800	-1.70066900
H	2.16872600	-3.57145700	1.14746600
H	0.21947700	-2.07829700	1.16513200
H	-2.02979900	2.28495300	0.65347100
H	-0.20749500	1.07989200	1.86299300
H	2.70759700	3.71639500	0.20810600
H	-1.48469300	4.38691700	-0.51696300
H	0.40607200	6.24845300	-0.66339400
H	2.04537900	5.64883800	-1.01111600
H	0.69762400	5.29152200	-2.10904700
H	3.47148600	1.80067500	1.45870500
H	2.36516800	1.79033700	2.84065200
H	2.36918700	0.42549000	1.73173200
Cl	4.63526900	-3.44915300	-0.29086000
Cl	-5.69970500	-1.95419800	-0.02504600

TSb/B

C	1.45389300	2.15624000	0.43349200
C	0.49588700	1.45931500	-0.32975500
C	-0.34801300	2.19970100	-1.18491600
C	-0.23522700	3.58193500	-1.28194000
C	0.71531900	4.25889100	-0.51139900
C	1.55579700	3.54252500	0.34476900
C	0.37541000	-0.01732500	-0.34919100
C	1.58753900	-0.87372200	-0.17066500
C	2.00044600	-1.63758800	-1.27661200
C	3.15941500	-2.41019300	-1.21619500
C	3.90726400	-2.45792600	-0.03912600
C	3.49107000	-1.72743600	1.07721300
C	2.34307400	-0.94066100	1.01302000
C	-0.88279100	-0.62189700	1.02954800
C	-1.03802900	-2.00356200	0.63554800
C	-2.16935500	-2.43526900	-0.00706200
C	-3.25010900	-1.54225600	-0.22967700
C	-3.17048000	-0.22966500	0.26999100
C	-2.05661200	0.22365300	0.96440400
C	-4.46876500	-2.01363800	-0.96468600
H	3.47166100	-2.97937800	-2.08653700
H	1.42255900	-1.60888700	-2.19687200
H	4.80380300	-3.06809400	0.01356000
H	4.05981400	-1.77287700	2.00104200
H	2.03050300	-0.39756000	1.90070900
H	-0.20876000	-0.33766900	-1.21023300
H	-1.08848500	1.67858500	-1.78707000
H	-0.88081200	4.13163500	-1.96010200
H	0.80612100	5.33849100	-0.58473200
H	2.30443800	4.06363500	0.93360800
H	2.14244700	1.61735000	1.07287900
H	-0.20390300	-2.68043200	0.78892700
H	-0.21215700	-0.42758900	1.86412200
C	-2.06849700	1.54073900	1.67369300
H	-4.03215600	0.42370800	0.16295800
H	-2.25214700	-3.46498700	-0.34232500
H	-4.83276800	-2.96012300	-0.54767300
H	-5.27806600	-1.28068300	-0.93468200
H	-4.22475400	-2.21010300	-2.01753800
H	-2.87772100	2.18767200	1.32590500
H	-2.21754900	1.36613700	2.74907400
H	-1.11549000	2.06998700	1.57225300

TSc/B

C	1.77585600	1.53936000	0.97682300
C	0.33466900	1.36050000	1.00233100
C	-0.47283400	2.48317100	0.56726300
C	0.08535600	3.55179500	-0.08205800
C	1.49184100	3.61867700	-0.27242600
C	2.30784400	2.60933200	0.27126200
C	2.08828100	4.77368500	-1.01735700
C	2.65542300	0.60039900	1.73856400
C	-0.14408500	0.04815100	-0.30938400
C	-1.62091000	-0.15218600	-0.16092500
C	-2.42375000	0.07916300	-1.29254100
C	-3.79740500	-0.14452100	-1.26177500
C	-4.37649500	-0.57852500	-0.07336500
C	-3.61980300	-0.78965300	1.07735800
C	-2.24564900	-0.57649000	1.02549900
C	0.76016900	-1.12858000	-0.25196600
C	0.50522200	-2.27538500	0.52761300
C	1.35622300	-3.37407700	0.48593700

C	2.46959000	-3.33250000	-0.35115600
C	2.75443700	-2.22151700	-1.14482800
C	1.90142400	-1.12834100	-1.08300500
H	-4.41886400	0.01622700	-2.13604600
H	-1.96669000	0.41855700	-2.21827600
H	-4.11074300	-1.11073800	1.98965000
H	-1.66826700	-0.72667800	1.93351300
H	0.07552200	0.63888900	-1.19761100
H	2.11457400	-0.25810400	-1.69873700
H	3.62237200	-2.23469800	-1.79515200
H	1.16259400	-4.26438800	1.07434200
H	-0.37873900	-2.33001700	1.15110200
H	-1.54886600	2.42182300	0.69323500
H	-0.04199100	0.81085000	1.86387500
H	3.38688400	2.71044300	0.19219400
H	-0.53980500	4.36056500	-0.44900100
H	1.71962800	5.72537200	-0.61599100
H	3.17972700	4.77281400	-0.97773800
H	1.78317300	4.74244700	-2.07217700
H	3.69633200	0.65117200	1.40958700
H	2.62755900	0.87322300	2.80366500
H	2.30480100	-0.43432900	1.67247600
F	-5.69654300	-0.78485400	-0.02807500
F	3.28414100	-4.38827700	-0.40015700

TSd/B

C	0.83277200	-1.94999000	0.97417500
C	1.22432100	-0.55117100	0.99675200
C	2.57083900	-0.24064900	0.55774300
C	3.33790800	-1.16856500	-0.09545500
C	2.85525800	-2.49100800	-0.28336900
C	1.61219300	-2.85416000	0.26702900
C	3.68457300	-3.48735300	-1.03517800
C	-0.37290700	-2.39663900	1.73637800
C	0.20055000	0.39110000	-0.30812900
C	0.59448200	1.83278100	-0.16566400
C	1.08107800	2.48349700	-1.31175200
C	1.40900100	3.83856700	-1.27683300
C	1.28181100	4.55900800	-0.08874300
C	0.82318100	3.91729200	1.06427300
C	0.48096500	2.56654400	1.02690300
C	-1.23607100	0.02667800	-0.24068400
C	-2.18020500	0.69955500	0.55946300
C	-3.52514800	0.34810600	0.51735200
C	-3.98969300	-0.67300700	-0.32691800
C	-3.04815700	-1.34413400	-1.12506700
C	-1.70211000	-1.00721600	-1.07908800
H	1.76984800	4.32703400	-2.17701500
H	1.18505800	1.93018900	-2.24175900
H	0.73395800	4.46805800	1.99584500
H	0.14089200	2.08763100	1.94143400
H	0.65165300	-0.04407300	-1.19897300
H	-0.99664100	-1.54412500	-1.70931800
H	-3.37967700	-2.13452500	-1.79320800
C	-5.45501900	-1.01439400	-0.40048200
H	-4.23334300	0.88738200	1.14074900
H	-1.87313500	1.52039800	1.19689300
H	2.92981800	0.77567600	0.68275300
H	0.86704800	0.00862400	1.85993900
H	1.28865600	-3.88864200	0.18993700
H	4.32391800	-0.90468500	-0.46655300
H	4.71676600	-3.49291300	-0.66560900
H	3.27843300	-4.49897900	-0.96643700
H	3.73529100	-3.21128600	-2.09735500
H	-0.69571600	-3.39913300	1.44499300
H	-0.13014700	-2.41884800	2.80862200
H	-1.20965000	-1.69964900	1.62072300
H	-5.95997100	-0.82997300	0.55260100
H	-5.95584700	-0.39767500	-1.15856300
H	-5.61144600	-2.06108500	-0.67861300
H	1.54650200	5.61154300	-0.05731500

TSe/B

C	1.68086000	1.70444700	0.94677000
C	0.25849500	1.39355900	0.97843700
C	-0.64664900	2.45227200	0.56435500
C	-0.19034600	3.57158900	-0.07739100
C	1.20309800	3.76115000	-0.28062000
C	2.10928200	2.82353100	0.24799100
C	1.68986800	4.96835100	-1.02237400
C	2.64730300	0.84191500	1.69131100
C	-0.11890200	0.07459000	-0.29777000
C	-1.58099600	-0.23833500	-0.15641600
C	-2.38640100	-0.11511500	-1.29953900
C	-3.73807000	-0.45133400	-1.26321300
C	-4.34472800	-0.89307500	-0.08050000
C	-3.54258800	-0.99113000	1.06706400
C	-2.18818100	-0.67168700	1.03374100

C	0.85827500	-1.04673800	-0.23479900
C	0.70832100	-2.17203400	0.59766500
C	1.62795900	-3.21486700	0.55420300
C	2.72349800	-3.18967700	-0.32331500
C	2.87345200	-2.06643200	-1.15291100
C	1.96586700	-1.01576000	-1.10550800
H	-4.33104400	-0.36451800	-2.16987900
H	-1.94737500	0.22392300	-2.23481300
C	-5.81592700	-1.22224000	-0.02938200
H	-3.98639000	-1.32294900	2.00219500
H	-1.61382300	-0.75173700	1.95324200
H	0.05692700	0.65822700	-1.20121300
H	2.10751600	-0.15951200	-1.76139000
H	3.70874000	-2.02126700	-1.84671800
C	3.68788200	-4.34509200	-0.39634400
H	1.48597000	-4.07415400	1.20426800
H	-0.14195500	-2.25104600	1.26496200
H	-1.71179000	2.29313000	0.69615500
H	-0.05796100	0.82754300	1.85426700
H	3.17435000	3.02078900	0.16228600
H	-0.88684200	4.32642900	-0.43047900
H	1.24124500	5.88188900	-0.61389600
H	2.77743900	5.06331000	-0.99021400
H	1.38139000	4.91458200	-2.07533900
H	3.68365100	1.05752700	1.42029700
H	2.53404900	1.02448800	2.76961100
H	2.44624300	-0.22304600	1.53353700
H	-6.01362200	-2.06665900	0.63872400
H	-6.39567300	-0.36897400	0.34614200
H	-6.20552200	-1.47202900	-1.02056500
H	3.77437700	-4.85857500	0.56611300
H	3.34622000	-5.08621200	-1.13100500
H	4.68566400	-4.01848600	-0.70500200

TSa/C

C	-3.21239400	3.55446100	-0.39260100
C	-2.45888100	2.29277700	-0.86712000
C	-1.00664300	2.60825600	-0.68238800
C	-0.87316300	3.86498500	0.13448500
C	-2.28627400	4.13648700	0.69262100
C	0.04800900	1.83836900	-1.13197300
C	0.27115500	0.36434500	0.42471400
C	-0.85777000	-0.55345800	0.25360500
C	-1.80117900	-0.63424800	1.30112500
C	-2.85707400	-1.53910400	1.25620300
C	-3.01022000	-2.35229300	0.13068100
C	-2.11699000	-2.26001800	-0.94609600
C	-1.05351900	-1.37163200	-0.88038300
C	1.67849800	0.01102700	0.24492500
C	2.12118000	-1.18568900	-0.36051300
C	3.47458900	-1.47844400	-0.45819900
C	4.41659600	-0.57593900	0.04880400
C	4.00868900	0.61197700	0.67190000
C	2.65618200	0.89158100	0.76739000
H	-0.38955000	-1.29221600	-1.73528600
H	-2.26577900	-2.87858600	-1.82438000
H	-3.55895200	-1.61123400	2.07968700
H	-1.68217800	-0.00786100	2.18149400
H	0.12644200	1.06221300	1.24612800
H	2.34216000	1.81044100	1.25668300
H	4.74824000	1.29254500	1.07895800
H	3.80530900	-2.40690500	-0.91048000
H	1.40806700	-1.91747700	-0.71801100
H	1.05251000	2.24414000	-1.07175400
H	-0.11835000	1.11391000	-1.92292400
H	-0.58175300	4.66881500	-0.56245000
H	-0.07211900	3.81538500	0.88199200
H	-2.68971200	1.43870000	-0.20232600
H	-2.69863000	1.95381700	-1.88087600
H	-2.42608900	3.60053900	1.63958800
H	-2.46333500	5.19685500	0.88737800
H	-4.21738000	3.33016900	-0.02718700
H	-3.31413100	4.26073100	-1.22482900
Cl	-4.33362700	-3.47308900	0.05025900
Cl	6.10718600	-0.93953600	-0.07464000

TSb/C

C	3.97077900	-1.51124400	-0.34651200
C	2.77900600	-0.67198100	-0.85717300
C	1.57980500	-1.55755900	-0.70723200
C	1.95523300	-2.76576100	0.10854100
C	3.33357600	-2.42866600	0.71483900
C	0.31431600	-1.28458200	-1.18194900
C	-0.50819200	-0.05327600	0.41029500
C	0.15091100	1.24655400	0.26296700
C	0.97777700	1.67775500	1.32368300
C	1.56879400	2.93977500	1.30039900

C	1.38078100	3.77491200	0.19833500
C	0.60342800	3.34301900	-0.88393600
C	-0.00659900	2.09495000	-0.85465800
H	1.84888000	4.75427600	0.17219700
C	-1.93426300	-0.31209800	0.21250900
C	-2.82443100	0.60870900	-0.38278200
C	-4.17845900	0.30971000	-0.49020000
C	-4.67392400	-0.90559100	-0.00932300
C	-3.81001600	-1.82376400	0.60018000
C	-2.45962700	-1.52800600	0.71254000
H	-5.73264300	-1.13152600	-0.09415400
H	-0.58056400	1.76355400	-1.71424500
H	0.47944100	3.98252800	-1.75242200
H	2.17916800	3.26542500	2.13694300
H	1.12128900	1.03301500	2.18718800
H	-0.09106400	-0.65051700	1.21770900
H	-1.79191900	-2.23975000	1.19256000
H	-4.19586200	-2.75961900	0.99201000
H	-4.85342900	1.03269400	-0.93748100
H	-2.46964900	1.57470400	-0.71854100
H	-0.44147000	-2.06175400	-1.14109200
H	0.17903400	-0.53540300	-1.95554700
H	2.04870600	-3.61062100	-0.59420200
H	1.18281300	-3.06088100	0.82881700
H	2.61901900	0.20435500	-0.20097800
H	2.88784200	-0.26855000	-1.86985400
H	3.20536300	-1.88552500	1.65936300
H	3.92780400	-3.32051500	0.92770300
H	4.78090400	-0.89333600	0.04830900
H	4.38296000	-2.10969000	-1.16743100

TSd/C

C	4.20092100	-1.77327600	-0.39973900
C	3.05682500	-0.85415400	-0.88030200
C	1.80362800	-1.64801700	-0.68324600
C	2.11360300	-2.86688600	0.14196800
C	3.53514600	-2.63041500	0.69417500
C	0.54250000	-1.28830600	-1.12131600
C	-0.15184900	-0.00502400	0.41237700
C	0.62056000	1.23880300	0.26801200
C	1.44864600	1.61917000	1.34493700
C	2.14919100	2.82432700	1.31645300
C	2.06693300	3.65056000	0.19507100
C	1.28408400	3.26645100	-0.90010400
C	0.56715800	2.07562000	-0.86641200
C	-1.59775100	-0.11606200	0.22445100
C	-2.39371900	0.87141300	-0.39529200
C	-3.76880000	0.70872700	-0.49819300
C	-4.41251300	-0.43306800	0.00655700
C	-3.62217700	-1.41469000	0.63429900
C	-2.25133800	-1.25885800	0.74511700
H	-0.01262600	1.78085800	-1.73571700
H	1.23826300	3.89709700	-1.78271200
H	2.76220100	3.11191200	2.16504000
H	1.51245500	0.98188500	2.22348600
H	0.19778900	-0.62171300	1.23764900
H	-1.66492200	-2.02999400	1.24005100
H	-4.09723000	-2.30182900	1.04398100
H	-4.36117700	1.48863000	-0.96850300
H	-1.94565700	1.78714900	-0.76010600
H	-0.25570300	-2.02043000	-1.05565800
H	0.44411400	-0.56083400	-1.92097300
H	2.11465900	-3.72740700	-0.54829300
H	1.34574700	-3.08914100	0.89285800
H	2.97873000	0.03425100	-0.22506000
H	3.16140800	-0.46362000	-1.89841600
H	3.48360300	-2.07151000	1.63669300
H	4.06727000	-3.56327000	0.89523300
H	5.06658800	-1.21203200	-0.03981700
H	4.54022800	-2.40816300	-1.22662800
C	-5.90663100	-0.58681400	-0.08204400
H	-6.19440400	-1.63347900	-0.22262200
H	-6.38268300	-0.24278000	0.84609800
H	-6.32520900	0.00298200	-0.90246000
H	2.62005800	4.58443600	0.16526100

TSe/C

C	-3.49370600	2.89333000	-0.35616400
C	-2.59652700	1.74330400	-0.86423500
C	-1.19342800	2.23018400	-0.69428300
C	-1.20152600	3.49132900	0.12285500
C	-2.62375000	3.57731900	0.71580000
C	-0.05277700	1.57819300	-1.13630200
C	0.32731400	0.21305700	0.36964000
C	-0.67663500	-0.85209600	0.22541100
C	-1.57583700	-1.05515200	1.29249200
C	-2.50024000	-2.09641600	1.26487900
C	-2.59135900	-2.95216300	0.15941100

C	-1.72789700	-2.71812400	-0.92750800
C	-0.78947100	-1.69623900	-0.89951400
C	-3.57545600	-4.09227800	0.13056100
C	1.77478200	0.01899200	0.20671400
C	2.35809100	-1.09967900	-0.42200500
C	3.73981300	-1.22944700	-0.49490100
C	4.59799300	-0.25875300	0.04528400
C	4.01708900	0.85157300	0.68587900
C	2.64120100	0.98700600	0.76560400
C	6.09370100	-0.39377900	-0.05774100
H	-0.16074500	-1.53612700	-1.77024300
H	-1.80065100	-3.34878400	-1.80958900
H	-3.16434600	-2.24205300	2.11234700
H	-1.52266700	-0.41207500	2.16791000
H	0.10910400	0.87071700	1.20907600
H	2.21941700	1.85120800	1.27447000
H	4.65751400	1.60658700	1.13371800
H	4.16434600	-2.11065500	-0.96776000
H	1.73660600	-1.89493500	-0.81418300
H	0.88902600	2.11585500	-1.09714500
H	-0.13887200	0.85353700	-1.94014200
H	-1.03439100	4.32577700	-0.57973800
H	-0.38051100	3.54420900	0.84780400
H	-2.70365100	0.85406300	-0.21313200
H	-2.80786100	1.39088200	-1.87989200
H	-2.67052600	3.01741600	1.65789400
H	-2.92827400	4.60477200	0.92862800
H	-4.45268400	2.53837200	0.02884000
H	-3.70499000	3.59027700	-1.17564800
H	-4.01679000	-4.21641100	-0.86369600
H	-3.07639500	-5.03726000	0.38228400
H	-4.38434600	-3.94612400	0.85197700
H	6.39365300	-1.42770500	-0.24952300
H	6.47987800	0.22038500	-0.88224700
H	6.58989900	-0.05289900	0.85674700

TSf/C

C	-5.34410300	2.63046000	-0.20638000
C	-4.49747000	1.45611000	-0.74401500
C	-3.07811300	1.90938800	-0.63467800
C	-3.01994500	3.16318700	0.18936600
C	-4.41715700	3.29012800	0.83276000
C	-1.96699400	1.23267200	-1.12685600
C	-1.51384300	-0.11278300	0.30035600
C	-2.58157400	-1.14211400	0.27165300
C	-3.32635800	-1.34328500	1.44984700
C	-4.29890000	-2.34095100	1.51980500
C	-4.56618800	-3.13354800	0.40327000
C	-3.85943800	-2.92194600	-0.78501900
C	-2.87773900	-1.93736500	-0.85246600
H	-5.32835700	-3.90532000	0.45218700
C	-0.10764400	-0.40975000	0.02150700
C	0.33914300	-1.55807300	-0.67499300
C	1.68583000	-1.78828000	-0.87871100
C	2.64298200	-0.87294700	-0.39903600
C	2.22710800	0.27394400	0.30416700
C	0.87500300	0.48716000	0.50381700
O	3.93012500	-1.18572100	-0.64802200
H	-2.35708900	-1.77473600	-1.79167200
H	-4.07756700	-3.52396400	-1.66196200
H	-4.84849300	-2.49311500	2.44374200
H	-3.11929400	-0.73397800	2.32634900
H	-1.61365600	0.55021700	1.15823700
H	0.56226800	1.37218800	1.05392900
H	2.96074700	0.97085900	0.69135800
H	2.03350100	-2.67780400	-1.39313900
H	-0.37217700	-2.29731000	-1.02160800
H	-1.02378300	1.76995200	-1.14445500
H	-2.10886400	0.53369900	-1.94581700
H	-2.84876200	3.99699700	-0.51341300
H	-2.17224800	3.18448700	0.88519800
H	-4.59792800	0.57598100	-0.08067600
H	-4.75919600	1.10069200	-1.74679000
H	-4.44576500	2.73181600	1.77636400
H	-4.68439300	4.32593700	1.05486800
H	-6.29745000	2.30142600	0.21384400
H	-5.56602600	3.33247700	-1.01869900
C	4.96691300	-0.34477200	-0.20732700
C	5.42881900	0.65660400	-1.05706300
C	5.55508100	-0.59295500	1.02979200
C	6.51010700	1.43840000	-0.64554900
H	4.95883700	0.80452800	-2.02435500
C	6.63554500	0.19698700	1.42798800
H	5.18038700	-1.39705400	1.65532100
C	7.11144300	1.21155700	0.59443700
H	6.88581600	2.21943000	-1.29987500
H	7.10818400	0.01233900	2.38806500
H	7.95525500	1.81905500	0.90714900

TSg/C

C	4.44525300	-1.94410400	-0.44763000
C	3.32956800	-0.97663100	-0.89818200
C	2.05041700	-1.70709200	-0.64859800
C	2.32716700	-2.91751900	0.19678600
C	3.78109100	-2.74846500	0.68678500
C	0.78576800	-1.29364300	-1.05103200
C	0.17035600	-0.00353300	0.38175600
C	1.03311200	1.19724300	0.27601400
C	1.79186100	1.55695800	1.40658700
C	2.56987500	2.71484200	1.40687700
C	2.62969200	3.51476800	0.26535600
C	1.91162600	3.14993600	-0.87814600
C	1.12120700	2.00414300	-0.87520500
H	3.24127500	4.41191600	0.25969100
C	-1.27703300	0.02895000	0.17356200
C	-1.95858000	1.05515800	-0.52659800
C	-3.33131900	1.03500500	-0.66016400
C	-4.09038600	-0.01690100	-0.10344500
C	-3.43583900	-1.04561900	0.60419500
C	-2.05750000	-1.00952200	0.73166700
O	-5.41375500	0.06125500	-0.28968300
H	0.59123300	1.72632000	-1.78153400
H	1.97172200	3.75889200	-1.77514300
H	3.13113000	2.98615800	2.29582400
H	1.74574100	0.94145800	2.30179200
H	0.43374200	-0.62049100	1.23932700
H	-1.56482200	-1.80633300	1.28475400
H	-3.99652200	-1.85446000	1.05690900
H	-3.85817100	1.83008400	-1.17695600
H	-1.41030800	1.89622900	-0.93210600
H	-0.02450400	-2.01168200	-0.96924000
H	0.70766500	-0.61145600	-1.89229500
H	2.24897000	-3.79478900	-0.46819900
H	1.57809100	-3.07543800	0.98267300
H	3.31226500	-0.08280400	-0.24566100
H	3.41558400	-0.59481300	-1.92130500
H	3.79707000	-2.17329800	1.62054300
H	4.27142100	-3.70507600	0.88219300
H	5.35103200	-1.42108000	-0.13183500
H	4.71879500	-2.60804800	-1.27603900
C	-6.27039100	-0.94713600	0.25954200
H	-7.28071200	-0.65473900	-0.02452800
H	-6.03833000	-1.93055100	-0.16361300
H	-6.18800800	-0.97707400	1.35144300

TSh/C

C	1.97892600	-1.11299200	-0.57914200
C	1.44252700	-0.01627300	0.13683000
C	2.35427400	0.87887700	0.73849900
C	3.72639200	0.71137700	0.64013200
C	4.23696900	-0.38397700	-0.08368100
C	3.34301800	-1.29483000	-0.68546800
C	0.00641100	0.23363400	0.31506900
C	-1.02063300	-0.82883500	0.20954100
C	-1.84121700	-1.06256700	1.32929800
C	-2.77779800	-2.09462300	1.33205000
C	-2.95533600	-2.91296500	0.20969700
C	-2.16611200	-2.65078700	-0.92456600
C	-1.21865300	-1.63501600	-0.92899700
H	-0.64906400	-1.45508300	-1.83623000
H	-2.30276300	-3.25310600	-1.81893400
H	-3.38277400	-2.26179800	2.21905400
H	-1.72215600	-0.44936900	2.21965100
H	-0.16940800	0.87296800	1.17907900
H	1.97263400	1.72606000	1.30444000
H	4.38979300	1.41509000	1.12829200
O	5.53971300	-0.65429600	-0.24684000
H	3.75702500	-2.14550000	-1.21633000
H	1.32156900	-1.85098600	-1.02180100
H	0.55871300	2.11092000	-1.10338300
C	-0.37755700	1.56143200	-1.11876500
H	-0.47959400	0.86357500	-1.94474800
C	-1.51533100	2.23437500	-0.68021400
C	-1.50238400	3.49689800	0.13126000
C	-2.92286100	1.76102700	-0.83501300
C	-2.92011000	3.60603000	0.73147400
H	-1.32565400	4.32585900	-0.57615800
H	-0.67549500	3.54049000	0.85051600
C	-3.80474700	2.92399100	-0.32979500
H	-3.03025600	0.87952800	-0.17340700
H	-3.14592700	1.39787800	-1.84444600
H	-2.96779800	3.05420800	1.67813000
H	-3.21036600	4.63897200	0.93747600
H	-4.76433500	2.58138200	0.06462000
H	-4.01474100	3.61701400	-1.15293800
C	6.52051100	0.20354700	0.34626500

H	7.48420900	-0.22654800	0.07522700
H	6.44510100	1.22050900	-0.05434500
H	6.41778000	0.21994800	1.43685400
C	-3.95293800	-4.04272500	0.21117100
H	-4.49833400	-4.09722300	-0.73695200
H	-3.44524800	-5.00649800	0.34649300
H	-4.68072000	-3.93751300	1.02067000

TSe/D

C	3.17982300	-1.86734200	0.39913600
C	3.05403200	-0.46535300	0.57386700
C	4.13254000	0.36661000	0.18229700
C	5.28417400	-0.17642000	-0.37114300
C	5.38338200	-1.56092100	-0.54363300
C	4.33040700	-2.40342800	-0.15684400
C	1.88958400	0.15209300	1.13949400
C	0.67196500	-0.43872000	1.44518900
C	-0.47805400	0.02714200	-0.25059600
C	-0.74813400	1.46995700	-0.16563100
C	-1.50120800	2.08274600	0.85680400
C	-1.73440600	3.45175700	0.84326700
C	-1.23552700	4.26893900	-0.18614600
C	-0.46458900	3.66323100	-1.18921200
C	-0.21016600	2.29625500	-1.17224800
C	-1.49153100	-1.02597900	-0.17795200
C	-2.81230300	-0.82679700	0.27796300
C	-3.72480900	-1.87352500	0.28108400
C	-3.37067400	-3.15748000	-0.16492100
C	-2.05718000	-3.35654300	-0.62995400
C	-1.14216100	-2.31753900	-0.64105100
C	-4.37442000	-4.27860000	-0.18584200
H	0.39166700	1.85521800	-1.96317600
H	-0.05384500	4.27209700	-1.99010100
C	-1.52860000	5.74652500	-0.21265900
H	-2.30827100	3.90116300	1.64929300
H	-1.87795500	1.49562700	1.68905600
H	0.29925400	-0.20884600	-0.97418700
H	-0.13581300	-2.49401900	-1.01458200
H	-1.76235900	-4.33697500	-0.99419400
H	-4.73931500	-1.69163900	0.62492600
H	-3.14036000	0.15636500	0.59099500
H	0.57623000	-1.51886000	1.44397700
H	0.01009000	0.07931900	2.13024700
H	1.95164000	1.23267200	1.26675500
H	4.04961800	1.44139100	0.32075600
H	6.10431300	0.47029700	-0.66628200
H	6.28482600	-1.98861300	-0.97254800
H	4.42268100	-3.47761500	-0.28322700
H	2.38095100	-2.52935200	0.71811200
H	-3.90620900	-5.24041900	0.04674600
H	-5.18683600	-4.10646800	0.52590700
H	-4.82535800	-4.37183300	-1.18299300
H	-0.75852200	6.30062300	-0.75746100
H	-2.48648100	5.93996100	-0.71352100
H	-1.60281100	6.16026300	0.79789000

TSg/D

C	0.13271200	0.52334100	0.24206800
C	-0.72139000	-0.36927400	-1.43440700
C	-4.28419700	-0.82073900	-0.28314100
C	-5.17861200	-1.71452300	0.28997100
C	-4.77195600	-3.02561100	0.55832100
C	-3.46907200	-3.44333600	0.24836400
C	-2.08375300	-0.25306800	-1.19190000
C	-2.96133500	-1.21971800	-0.59938700
C	-2.57285200	-2.55628100	-0.32635500
C	-0.31671900	1.93374700	0.22429800
C	-0.02840100	2.83820700	-0.81530600
C	-0.46467400	4.15870400	-0.74574300
C	-1.19327000	4.60211300	0.36199200
C	-1.49965600	3.71231400	1.39284300
C	-1.07977900	2.38559400	1.31694300
C	1.52055500	0.10770700	0.12811300
C	2.56395400	0.93610200	-0.36107000
C	3.86512800	0.48503600	-0.41294900
C	4.18914900	-0.82061900	0.01843100
C	3.17211200	-1.66078500	0.51819900
C	1.87100900	-1.19266000	0.56635900
H	-1.32337300	1.69748500	2.12256300
H	-2.07039500	4.04811300	2.25338100
H	-0.24047600	4.84236500	-1.55900600
H	0.51245400	2.50614400	-1.69683700
H	-0.42247500	-0.08216900	0.95558300
H	1.09489700	-1.84464700	0.96102600
H	3.39921000	-2.65844200	0.87408200
H	4.66886100	1.12200700	-0.76661200
H	2.35273100	1.95466500	-0.66185900
H	-0.24096100	-1.34010500	-1.37521200

H	-0.27213400	0.31880000	-2.14247800
H	-2.53218400	0.71907600	-1.39405000
H	-4.59419800	0.19901500	-0.49541200
H	-6.18937300	-1.39758600	0.52647600
H	-5.47094800	-3.72804700	1.00270200
H	-3.16690500	-4.46643800	0.44936900
H	-1.57512000	-2.89700300	-0.58508200
C	5.91466200	-2.45148900	0.35900300
H	6.98943600	-2.47018800	0.18195500
H	5.71356300	-2.59322000	1.42629300
H	5.43044500	-3.24136600	-0.22526900
O	5.48049700	-1.15632100	-0.07422900
H	-1.52871400	5.63351800	0.41433100

TSh/D

C	-0.15887600	0.27544000	-0.20920100
C	0.52323400	-0.75977600	1.41736500
C	3.97947300	-1.77899600	0.29541000
C	4.72004600	-2.80110600	-0.28214500
C	4.10413800	-4.02241800	-0.57510700
C	2.74618000	-4.22263300	-0.28481300
C	1.89195200	-0.86719300	1.18802700
C	2.60437200	-1.95718600	0.59206600
C	2.00265000	-3.20740100	0.29514300
C	0.48723600	1.60533500	-0.16388100
C	0.32203400	2.53396700	0.88108000
C	0.94620200	3.77549200	0.83398500
C	1.75484800	4.14680000	-0.25282900
C	1.93809300	3.21162700	-1.28092800
C	1.33079900	1.96029800	-1.23228300
C	-1.59937300	0.06357500	-0.11325100
C	-2.51314100	1.01360200	0.40909200
C	-3.86650000	0.75222000	0.44884700
C	-4.37376500	-0.47623300	-0.02816800
C	-3.48720600	-1.43296600	-0.56294600
C	-2.13143700	-1.15442500	-0.59820300
H	1.49424100	1.25621500	-2.04463700
H	2.56915400	3.46437700	-2.12885600
H	0.80925300	4.47003600	1.65861200
H	-0.27059200	2.27950700	1.75521900
H	0.29739000	-0.37760300	-0.95096900
H	-1.45651800	-1.89558900	-1.02063300
H	-3.85382800	-2.37344600	-0.95612300
H	-4.57070100	1.48450600	0.82928800
H	-2.15912700	1.97931100	0.74745600
H	-0.10195800	-1.64386900	1.35031700
H	0.19401300	-0.02924000	2.14899500
H	2.49017900	0.01774400	1.40239600
H	4.45118100	-0.82754400	0.52617600
H	5.77225100	-2.65379800	-0.50380500
H	4.68224700	-4.82496300	-1.02372700
H	2.28128900	-5.17848000	-0.50533400
H	0.95895000	-3.38003300	0.53824500
C	-6.31235400	-1.83335600	-0.41517700
H	-7.37907100	-1.70905500	-0.23163900
H	-6.13555400	-1.96545400	-1.48816100
H	-5.94176300	-2.70324900	0.13805800
O	-5.70142400	-0.62782800	0.05875300
C	2.39438700	5.51057200	-0.31378400
H	3.30144000	5.50309900	-0.92560100
H	1.70602400	6.24095400	-0.75897100
H	2.65492700	5.87777000	0.68387800

TSi/D

C	1.08034500	-0.00994200	-0.25900900
C	1.64463700	-1.06331000	1.32659600
C	5.11712400	-2.23117500	0.40022400
C	5.84538200	-3.29112100	-0.12095000
C	5.19623100	-4.49088600	-0.43196900
C	3.81692500	-4.63156800	-0.21573300
C	3.02349600	-1.22510200	1.16552800
C	3.72073200	-2.34894000	0.62315600
C	3.08504100	-3.57911200	0.30926700
C	1.60423400	1.35929900	-0.07873400
C	1.24701600	2.21421100	0.98825700
C	1.75618700	3.49638500	1.08056300
C	2.64701900	3.98196600	0.10204400
C	3.03486100	3.14077300	-0.95275200
C	2.52730000	1.84627200	-1.02021800
C	-0.35161300	-0.33221000	-0.33709200
C	-1.38340400	0.52002500	0.10938900
C	-2.71947800	0.16636700	-0.01084700
C	-3.06441200	-1.07034700	-0.58219300
C	-2.05353100	-1.93442200	-1.04790600
C	-0.72981100	-1.56537900	-0.92495500
H	2.83642200	1.20793300	-1.84453800
H	3.72456000	3.48290100	-1.71512500
H	1.48855800	4.15080200	1.90352300

H	0.58211300	1.86498700	1.77316400
H	1.64333400	-0.55891100	-1.01237600
H	0.04190700	-2.23609300	-1.29649500
H	-2.34286000	-2.87343000	-1.50772600
H	-3.49628100	0.84672900	0.31757600
H	-1.14508900	1.49503200	0.51635600
H	1.00378800	-1.93509000	1.24726400
H	1.31886400	-0.34196700	2.06924500
H	3.64223400	-0.35690900	1.39194800
H	5.61440500	-1.29630500	0.64476500
H	6.91343700	-3.19035600	-0.28545500
H	5.76451800	-5.32287800	-0.83738800
H	3.32571400	-5.57064400	-0.45059600
H	2.02304600	-3.70550200	0.49405100
O	3.07414300	5.24663300	0.27953100
C	3.97428100	5.81856400	-0.67110100
H	4.15985100	6.83473400	-0.32346100
H	4.91940700	5.26408400	-0.70389900
H	3.52533900	5.84852100	-1.67059300
C	-5.41414600	-0.75603900	-0.26543200
C	-5.78637200	-0.88083100	1.07108100
C	-6.13690800	0.02701200	-1.16083600
C	-6.91294100	-0.19000700	1.52114400
H	-5.21205000	-1.51895200	1.73559700
C	-7.26231700	0.71124100	-0.69711000
H	-5.82570800	0.08454200	-2.19903600
C	-7.64942500	0.60572300	0.64055700
H	-7.21823700	-0.28214200	2.55927500
H	-7.83806100	1.32274500	-1.38547400
H	-8.52788800	1.13660800	0.99464000
O	-4.33164800	-1.50602200	-0.75216300

TSj/D

C	1.54108800	-2.18511000	0.52040200
C	2.78475000	-2.78427600	0.51451800
C	3.89063200	-2.13540300	-0.07406600
C	3.71468200	-0.87159200	-0.66967500
C	2.45873400	-0.28464100	-0.65742500
C	1.34032700	-0.91268300	-0.06589100
C	0.04653000	-0.21705100	-0.12207900
C	-1.26045200	-0.89694900	-0.01269300
C	-1.64285000	-1.72649200	1.06564400
C	-2.87309500	-2.35667600	1.08416700
C	-3.77848300	-2.18530300	0.01721200
C	-3.42987000	-1.34510700	-1.05201100
C	-2.19432700	-0.70401000	-1.04578200
C	0.18364900	1.01829000	1.42781700
C	-0.68973800	2.06061600	1.10669000
C	-0.36840500	3.33409600	0.54131600
H	-1.93872200	-0.05851900	-1.88280500
H	-4.10820400	-1.18652700	-1.88184500
O	-4.94241000	-2.85244600	0.12849000
H	-3.16972200	-2.98816900	1.91502600
H	-0.98182100	-1.86249100	1.91664400
H	0.04373800	0.52567400	-0.91818000
H	2.33264400	0.68790200	-1.12836900
H	4.54189500	-0.36063700	-1.14751600
O	5.05174700	-2.80612900	-0.02603700
H	2.93640000	-3.76875300	0.94441900
H	0.70676000	-2.72758800	0.94682600
H	1.24898900	1.22076200	1.45993500
H	-0.15287500	0.30474100	2.17311600
H	-1.75408200	1.84937300	1.20892100
C	-1.43272700	4.17574400	0.12694000
C	-1.17836200	5.42333300	-0.42493800
C	0.14297100	5.85836400	-0.57440400
C	1.21108000	5.04512000	-0.16638600
C	0.96392500	3.80012600	0.38870200
H	-2.45649200	3.83153900	0.24736300
H	-2.00051200	6.05935400	-0.73718700
H	0.34434100	6.83612000	-1.00216300
H	2.23181400	5.39795900	-0.27577500
H	1.79560500	3.18829900	0.72308800
C	6.22259100	-2.23368200	-0.61620100
H	7.01739000	-2.96015900	-0.44931000
H	6.08379500	-2.07993400	-1.69215900
H	6.48247700	-1.28574000	-0.13186600
C	-5.91316100	-2.73976200	-0.91377000
H	-6.74547700	-3.37340100	-0.60788600
H	-6.25961600	-1.70516000	-1.02037200
H	-5.50995700	-3.09776500	-1.86805800

TSz1/SA

C	0.31133200	-0.36341500	0.19675400
C	0.25310200	-1.76854800	-1.54880800
C	2.66975500	0.18160800	0.71871500
C	1.36332000	0.58512200	0.17252400
C	1.29899300	1.85991800	-0.53093900

O	2.08080900	2.82271800	0.04205300
C	-1.14570800	-0.08316300	0.25284700
C	-1.89463700	-0.83514300	1.18836700
C	-3.25798200	-0.64147700	1.35998100
C	-3.90586000	0.31804900	0.57939900
C	-3.20439600	1.06662200	-0.36928000
C	-1.83952700	0.86462700	-0.53036500
O	0.62345100	2.11491000	-1.53026100
O	3.75973600	0.65412100	0.42809100
C	2.20495500	4.05711700	-0.67234000
C	3.75999000	-1.57600600	1.90218000
C	1.09498900	5.03458300	-0.30201900
C	4.53841300	-0.95187800	3.05443100
H	0.56611200	-1.23376800	0.78991100
H	-1.38721700	-1.59135100	1.77816400
H	-3.82463200	-1.21628400	2.08217100
H	-3.73650400	1.79510200	-0.96924600
H	-1.28890800	1.43599300	-1.26608800
H	3.18629800	4.44854100	-0.38483400
H	2.19847200	3.85880600	-1.74799000
H	3.42041100	-2.58594400	2.14994400
H	4.36772800	-1.62498300	0.99540600
H	1.25460000	6.00069600	-0.79820200
H	0.12600300	4.63720700	-0.61601000
H	1.07246200	5.20227800	0.78057000
H	5.40797700	-1.57274700	3.30786700
H	4.88823600	0.04483700	2.77311500
H	3.90740100	-0.86551000	3.94684500
H	-2.60072600	-3.63270000	-1.07187000
C	-1.97113200	-2.97759300	-1.68031200
C	-0.59498900	-2.82983800	-1.01712400
H	-2.46455600	-2.00695900	-1.80859700
H	-1.86201600	-3.41969700	-2.68041300
O	2.55711900	-0.84860300	1.61947400
O	-0.29004400	-3.57622000	-0.08414400
C	1.70206800	-1.91644600	-1.69038500
H	-0.20825700	-1.15287500	-2.32003400
C	2.33824100	-0.98652000	-2.72636100
O	2.40679800	-2.68961400	-1.04258700
H	3.42379300	-0.98983400	-2.60239100
H	1.95281700	0.03375300	-2.62644600
H	2.09061400	-1.33259900	-3.74007300
N	-5.33570700	0.53561600	0.75241300
O	-5.88973400	1.38171800	0.04067300
O	-5.93135000	-0.13490100	1.60391700

TSz2/SA

C	0.02509800	-0.33316000	0.23503400
C	-0.13879600	-1.76547000	-1.49184400
C	2.42299400	0.11501400	0.66156000
C	1.11407000	0.56922700	0.16238400
C	1.07647300	1.84182300	-0.54685500
O	1.91912300	2.77393700	-0.00887000
C	-1.41654400	0.01130800	0.34028600
C	-2.16110200	-0.69236600	1.31320900
C	-3.50813300	-0.43629200	1.53034100
C	-4.16853000	0.54121300	0.76622000
C	-3.44677800	1.23721400	-0.22047600
C	-2.09862200	0.97483400	-0.43088200
O	0.37554800	2.12114200	-1.52170400
O	3.51969000	0.53666600	0.32183200
C	2.06768000	3.99844800	-0.73496400
C	3.48095900	-1.68061100	1.81659600
C	1.01524600	5.02372400	-0.32771800
C	4.33903400	-1.08294500	2.92555500
H	0.26379700	-1.20821100	0.82795100
H	-1.66538100	-1.46199200	1.89594400
H	-4.05600900	-0.98878300	2.28787400
H	-3.95391900	1.98490300	-0.82372500
H	-1.55322200	1.51087700	-1.19665000
H	3.07516600	4.34936500	-0.48842000
H	2.01042500	3.79590700	-1.80832200
H	3.10536400	-2.67063500	2.09116100
H	4.04388100	-1.76820400	0.88425300
H	1.19520800	5.97999100	-0.83589500
H	0.01910600	4.66541100	-0.60092300
H	1.04232500	5.19714600	0.75383700
H	5.18910000	-1.74191800	3.14689500
H	4.72192400	-0.10660300	2.61720300
H	3.75388100	-0.95835300	3.84432700
H	-3.06223400	-3.47320700	-0.88377100
C	-2.41916500	-2.87079900	-1.53142000
C	-1.01611500	-2.77659800	-0.91515200
H	-2.86600600	-1.88032900	-1.67663100
H	-2.36470900	-3.34981300	-2.51903500
O	2.30230400	-0.89954100	1.57852100
O	-0.71718400	-3.52302300	0.02046200
C	1.29645400	-1.97591300	-1.67115200

H	-0.59665200	-1.14057400	-2.25777800
C	1.94135300	-1.08354400	-2.73499800
O	1.98867700	-2.76984300	-1.03376400
H	3.02912600	-1.14938400	-2.65621500
H	1.62043500	-0.04281700	-2.61782100
H	1.63101000	-1.41067000	-3.73759200
C	-5.55539700	0.81974200	0.98350200
N	-6.68413300	1.04915600	1.16087700

TSz3/SA

C	-0.17782800	-0.46218900	-0.36666600
C	-0.13969900	-1.86065100	1.40887900
C	-2.41435600	0.59836300	-0.45646600
C	-0.97117500	0.69588900	-0.18670800
C	-0.48964300	1.92282900	0.43504500
O	-1.12404100	3.04129700	-0.03007600
C	1.27008000	-0.51321300	-0.70916500
C	1.63899400	-1.40207900	-1.73992400
C	2.95966800	-1.50895600	-2.16898200
C	3.96334800	-0.73857700	-1.58105400
C	3.59686500	0.12629000	-0.55209500
C	2.28640800	0.25233200	-0.10456800
O	0.39955400	2.01597000	1.28303500
O	-3.29476300	1.31211700	0.00451100
C	-0.82070300	4.27101400	0.63658200
C	-4.07557300	-0.88203900	-1.30946200
C	0.40256300	4.95190300	0.03237400
C	-4.91236600	-0.11496800	-2.32695300
H	-0.72384700	-1.25470200	-0.86424500
H	0.87341500	-2.02278100	-2.19414100
H	3.21333400	-2.20169700	-2.96784000
H	2.03818600	0.92880700	0.70246800
H	-1.71734000	4.88662300	0.50887300
H	-0.66489100	4.08010900	1.70233100
H	-4.02080000	-1.94623200	-1.55674900
H	-4.48761100	-0.78032800	-0.30260800
H	0.56798700	5.92985300	0.50315100
H	1.29051500	4.33402600	0.19021400
H	0.26714600	5.10556400	-1.04413700
H	-5.93075700	-0.52382400	-2.36958900
H	-4.96837100	0.93970400	-2.04489100
H	-4.47105700	-0.18942000	-3.32793400
H	2.09678900	-4.30159700	0.47392200
C	1.76301800	-3.51037600	1.15120600
C	0.33948800	-3.07776300	0.76953100
H	2.46372400	-2.66848000	1.10689400
H	1.77977400	-3.89330900	2.18112900
O	-2.71202400	-0.44062000	-1.30428500
O	-0.29394200	-3.74844000	-0.05040800
C	-1.52941200	-1.67257600	1.81385000
H	0.58437700	-1.36244200	2.05239000
C	-1.73868100	-0.61038300	2.89841700
O	-2.50172100	-2.26995500	1.34947800
H	-2.79884400	-0.35132500	2.95435600
H	-1.14478500	0.28670200	2.69400800
H	-1.41408200	-1.00410600	3.87244300
H	4.99739300	-0.80994900	-1.90192700
Cl	4.86348700	1.10275100	0.22063500

TSz4/SA

C	0.42573700	-0.14721200	-0.34304700
C	1.22371100	-1.33248500	1.39404700
C	-2.01280800	-0.56945900	-0.48806600
C	-0.89671700	0.33207400	-0.16760000
C	-1.22583200	1.59406900	0.48088700
O	-2.37954200	2.15419300	-0.00196800
C	1.63707800	0.67031200	-0.63172500
C	2.43692800	0.24641300	-1.71251900
C	3.57974800	0.94853400	-2.09324800
C	3.96517800	2.09315700	-1.39401100
C	3.19468800	2.51575900	-0.30833600
C	2.04862200	1.81743200	0.07289400
O	-0.57948500	2.16509600	1.36081400
O	-3.15418300	-0.50863400	-0.04968100
C	-2.86505900	3.30809800	0.68828200
C	-2.49302900	-2.71662900	-1.40282700
C	-2.25714000	4.59205200	0.13328700
C	-3.60641200	-2.55158300	-2.43129000
H	0.44524700	-1.08628300	-0.88330500
H	2.15414100	-0.65385400	-2.25064500
H	4.17172200	0.59481300	-2.93480600
H	4.85804300	2.64283400	-1.68478000
H	3.48968200	3.39919200	0.25487600
H	1.46068400	2.14946400	0.91861400
H	-3.94997600	3.29046500	0.53858200
H	-2.64833400	3.21400300	1.75644600
H	-1.82797700	-3.54559200	-1.66215900
H	-2.90062400	-2.89772000	-0.40531700

H	-2.69972300	5.46978000	0.62261900
H	-1.17827600	4.59938300	0.31026700
H	-2.43706200	4.67029200	-0.94486600
H	-4.19768700	-3.47414300	-2.50632900
H	-4.26747800	-1.73254300	-2.13615300
H	-3.19043500	-2.32978900	-3.42133700
H	4.46237200	-2.03962700	0.46754400
C	3.73107000	-1.57722500	1.13656700
C	2.31930100	-2.03969500	0.74485300
H	3.82311900	-0.48618100	1.08314600
H	3.95572600	-1.87404000	2.17065200
O	-1.63932000	-1.56709600	-1.35705900
O	2.19114600	-2.93931000	-0.08969300
C	-0.02300500	-1.98615900	1.77776200
H	1.52766300	-0.52693200	2.06135300
C	-0.81253900	-1.25810300	2.87156700
O	-0.47236800	-3.02558200	1.29184600
H	-1.83134900	-1.65183700	2.90832500
H	-0.83524500	-0.17823900	2.69107200
H	-0.33134100	-1.41886900	3.84727400

TSz5/SA

C	-0.13259200	-0.31042500	0.26168000
C	-0.37636100	-1.72504200	-1.47486900
C	2.29696200	0.02957600	0.62117900
C	0.99769000	0.53953500	0.16014200
C	0.99327100	1.81623700	-0.54011200
O	1.88240400	2.71599600	-0.01272800
C	-1.55238900	0.10784400	0.41811800
C	-2.29350300	-0.54349800	1.42449600
C	-3.62187300	-0.21398400	1.68378300
C	-4.27878900	0.77614800	0.94453300
C	-3.55303800	1.40921100	-0.07276600
C	-2.22230900	1.08818800	-0.33724500
O	0.28556800	2.13105000	-1.49854300
O	3.40420700	0.41828800	0.27252700
C	2.06140700	3.93491300	-0.73781400
C	3.31139800	-1.83176300	1.71045600
C	1.05464900	4.99708100	-0.30852000
C	4.21165600	-1.29627900	2.81831400
H	0.08242300	-1.19849900	0.84395000
H	-1.81692500	-1.33207300	1.99961700
H	-4.15811700	-0.74207400	2.47096500
H	-1.69034200	1.58711400	-1.13685000
H	3.08561800	4.25011100	-0.51104000
H	1.97516000	3.73921400	-1.81070600
H	2.90671600	-2.81589800	1.96458000
H	3.85479700	-1.91312500	0.76596200
H	1.25786200	5.94801000	-0.81859400
H	0.04173300	4.67318300	-0.56225600
H	1.10904100	5.16655000	0.77279000
H	5.04276400	-1.98977700	3.00434600
H	4.62137600	-0.32510300	2.52857600
H	3.64894700	-1.17728300	3.75187200
H	-3.36864300	-3.30000600	-0.83321300
C	-2.72885800	-2.65926700	-1.44663100
C	-1.29457700	-2.69622600	-0.89665300
H	-3.12837200	-1.63831100	-1.45086900
H	-2.74911200	-3.02241800	-2.48373700
O	2.15885700	-1.00362200	1.51805900
O	-1.01214900	-3.50401200	-0.00758500
C	1.03792700	-2.00747900	-1.69496300
H	-0.81857500	-1.05702400	-2.21296300
C	1.70361300	-1.12803300	-2.75932300
O	1.70733400	-2.85095300	-1.09570100
H	2.78871300	-1.24415500	-2.70145900
H	1.43285500	-0.07536400	-2.62440400
H	1.36223800	-1.42831400	-3.76051100
H	-4.04171200	2.17041700	-0.68007200
C	-5.71014400	1.15949300	1.24303400
H	-5.76822500	1.96867900	1.98553100
H	-6.22734900	1.51247700	0.34303000
H	-6.27746500	0.31230600	1.64619500

TSz6/SA

C	0.14918800	-0.37213100	0.25392000
C	0.14874400	-1.79745400	-1.48105700
C	2.50333800	0.29543400	0.65286200
C	1.15480600	0.62662000	0.17028100
C	0.98791500	1.88760100	-0.53510500
O	1.75633500	2.89694600	-0.01502500
C	-1.31718100	-0.15678800	0.38654500
C	-1.98123100	-0.91214700	1.37805100
C	-3.34174200	-0.77383000	1.62091800
C	-3.47338500	0.87004700	-0.14085000
C	-2.10226300	0.72517100	-0.37254700
O	0.24373000	2.10709800	-1.49380300
O	3.55561800	0.82378100	0.31804100

C	1.77997200	4.12278200	-0.74897700
C	3.73528100	-1.41852200	1.75969300
C	0.64516600	5.05217700	-0.33046200
C	4.55564900	-0.76702500	2.86753600
H	0.47480000	-1.21899300	0.84615500
H	-1.41020400	-1.62866500	1.96118800
H	-3.83776900	-1.35834200	2.39056700
H	-1.62922200	1.30248400	-1.15635900
H	2.75497400	4.56786600	-0.52283200
H	1.72265400	3.91012500	-1.82062000
H	3.45539400	-2.44361900	2.02015600
H	4.28924100	-1.43933200	0.81804700
H	0.72950100	6.01835600	-0.84546300
H	-0.31775700	4.60197200	-0.58635500
H	0.67272500	5.23325200	0.75000100
H	5.46653700	-1.34926000	3.06185200
H	4.84146000	0.24615600	2.57306300
H	3.97803700	-0.71409700	3.79815500
H	-2.59035100	-3.78694100	-0.86831100
C	-2.03478900	-3.07867100	-1.48951000
C	-0.61974200	-2.89884300	-0.91822600
H	-2.57305900	-2.12481600	-1.53082200
H	-1.98291600	-3.46945700	-2.51556100
O	2.48888900	-0.74283000	1.55494300
O	-0.23071800	-3.65783600	-0.02654300
C	1.59120300	-1.86651600	-1.68991700
H	-0.37987300	-1.19944200	-2.22241900
C	2.12879400	-0.89033800	-2.74284600
O	2.37234100	-2.60891600	-1.09231500
H	3.21269600	-0.79982700	-2.63678500
H	1.65994700	0.09446500	-2.64644800
H	1.89860300	-1.26788700	-3.74985300
H	-4.03671000	1.56465200	-0.75550600
C	-4.09949100	0.12598100	0.86320000
C	-6.23882900	1.08787000	0.42418800
H	-7.25175500	0.99963000	0.82592600
H	-5.90086500	2.12924900	0.52541600
H	-6.25137600	0.82595100	-0.64359900
O	-5.43908700	0.19900800	1.17523100

TSz7/SA

C	0.37253600	-0.35537900	0.20336800
C	0.39506600	-1.71235800	-1.58031300
C	2.73252300	0.17471900	0.75119900
C	1.43544900	0.58842500	0.20075300
C	1.37432600	1.86740600	-0.48718600
O	2.17033600	2.82534100	0.08752700
C	-1.08325000	-0.06537000	0.27405900
C	-1.84148800	-0.82910400	1.18126100
C	-3.20801000	-0.63873600	1.36141100
C	-3.15919100	1.08771400	-0.30520400
C	-1.79055200	0.89236700	-0.47324500
O	0.69175800	2.14224300	-1.47716400
O	3.82991900	0.65580800	0.49867200
C	2.29511800	4.05893500	-0.62218900
C	3.80885400	-1.62735400	1.88156400
C	1.19231000	5.04174900	-0.24164700
C	4.58146100	-1.04849800	3.06184700
H	0.62182800	-1.23574600	0.78361000
H	-1.34555300	-1.60886800	1.75242500
H	-3.72365300	-1.27076700	2.07566800
H	-1.25596200	1.48285900	-1.20628000
H	3.28029500	4.44742100	-0.34185800
H	2.27870400	3.86666100	-1.69914000
H	3.46716600	-2.64585300	2.08927100
H	4.42453400	-1.64527800	0.97894000
H	1.35085700	6.00898600	-0.73690000
H	0.22037200	4.64615700	-0.54851500
H	1.17863800	5.20657900	0.84170700
H	5.44877600	-1.67955600	3.29874500
H	4.93360600	-0.04260400	2.81871800
H	3.94435900	-0.99325700	3.95266600
H	-2.50303100	-3.54101100	-1.26110800
C	-1.86987500	-2.82214200	-1.78902700
C	-0.48477900	-2.77948500	-1.12448200
H	-2.34691800	-1.83528300	-1.77814900
H	-1.77909300	-3.13015700	-2.84015900
O	2.61130100	-0.88828600	1.61832800
O	-0.21040600	-3.60965300	-0.25378100
C	1.83981900	-1.87989300	-1.69961800
H	-0.03915600	-1.04617600	-2.32464100
C	2.51605200	-0.91101000	-2.67704600
O	2.52456900	-2.70025900	-1.08592200
H	3.58943300	-0.87845400	-2.47403100
H	2.09057500	0.09487500	-2.60226000
H	2.35977700	-1.26013100	-3.70833800
H	-3.64308700	1.83571200	-0.92381600
C	-3.90681500	0.34074700	0.62845800

C	-6.00271600	1.31046400	-0.19356500
H	-7.04683300	1.41782300	0.11451100
H	-5.58920400	2.31835000	-0.30405800
H	-5.98133800	0.82637200	-1.18631800
N	-5.28304000	0.56965400	0.82687200
C	-6.04777000	-0.45432000	1.51632800
H	-5.66549200	-0.60458600	2.53153700
H	-7.08685900	-0.12398700	1.60457000
H	-6.03566400	-1.43246700	1.00346100

TSz8/SA

C	0.72524900	-0.44655500	0.21380000
C	0.91068200	-1.73450500	-1.61342300
C	2.99155800	0.40940300	0.74775500
C	1.63711000	0.64414100	0.23063500
C	1.37514000	1.92552900	-0.40387000
O	2.02560300	2.96903200	0.20418100
C	-0.75578300	-0.37624900	0.31699800
C	-1.37556900	-1.26472400	1.21395700
C	-2.75078500	-1.26176800	1.42244000
C	-2.98785600	0.51941600	-0.19259800
C	-1.60566400	0.49754000	-0.38194700
O	0.64606800	2.13434800	-1.37670600
O	3.99906600	1.06034600	0.50145900
C	1.95633400	4.23381000	-0.45661700
C	4.34687000	-1.25550200	1.78325900
C	0.72407900	5.02586900	-0.03096100
C	5.05097000	-0.61750700	2.97588000
H	1.11377000	-1.29982800	0.75705900
H	-0.76350500	-1.97850800	1.75766000
H	-3.16563700	-1.96514000	2.13560900
H	-1.16584700	1.18200800	-1.09787300
H	2.87577800	4.75430100	-0.16721200
H	1.95536700	4.08274700	-1.54021200
H	4.16416100	-2.32124000	1.95038800
H	4.93800800	-1.14367400	0.87109700
H	0.73306600	6.02524900	-0.48601800
H	-0.18171800	4.50367000	-0.35066700
H	0.69704400	5.14258500	1.05837600
H	6.00664600	-1.12245400	3.17156800
H	5.24590200	0.43860300	2.77185600
H	4.43217200	-0.69399800	3.87795900
H	-1.66470000	-3.99434000	-1.28415200
C	-1.16282400	-3.17329500	-1.80403100
C	0.21543500	-2.93423800	-1.16795700
H	-1.78551400	-2.27251000	-1.75365700
H	-1.05283700	-3.43627600	-2.86554000
O	3.04748900	-0.69256300	1.57135600
O	0.63478200	-3.73202300	-0.32519300
C	2.36039300	-1.67423600	-1.76643600
H	0.36114200	-1.12570000	-2.33032000
C	2.85476700	-0.58900600	-2.73024600
O	3.17814800	-2.39279300	-1.18881000
H	3.92344600	-0.42196500	-2.57399200
H	2.30532000	0.34767700	-2.59042000
H	2.69236000	-0.91427600	-3.76827500
C	-3.59127200	-0.37638500	0.72320900
C	-5.74048100	0.76362500	0.44724600
H	-5.60825400	1.62435800	1.13270800
H	-6.80667900	0.50558000	0.45935400
N	-4.99294700	-0.40491900	0.89228400
C	-5.53445700	-1.08736200	2.04989200
H	-5.19419500	-0.66209000	3.01172600
H	-6.62681600	-1.02558900	2.01573400
H	-5.26435900	-2.14869000	2.03870300
C	-5.30750600	1.16304700	-0.96230500
H	-5.49022200	0.31483500	-1.63412300
H	-5.91809700	2.00347100	-1.31610700
C	-3.82132900	1.52923700	-0.96220600
H	-3.69816300	2.52674300	-0.51302200
H	-3.44663800	1.61639700	-1.98934700

TSz9/SA

C	-0.91540800	-0.40398500	-0.07494100
C	-1.11279100	-1.40445800	1.91897600
C	-3.21412900	0.08309700	-0.87054200
C	-1.94493600	0.55348200	-0.30318800
C	-1.89072000	1.92036400	0.18337600
O	-2.63197600	2.79367900	-0.57285200
C	0.55110300	-0.17516800	-0.11382600
C	1.32693900	-1.15016300	-0.76892200
C	2.70885200	-1.05359400	-0.90824200
C	2.62542800	1.06939900	0.27206100
C	1.24695800	0.92500100	0.41673700
O	-1.25606900	2.33189500	1.15852300
O	-4.31196300	0.61809600	-0.77816900
C	-2.77237100	4.11907700	-0.05986200
C	-4.26785000	-1.85377300	-1.77822400

C	-1.63658500	5.02640100	-0.52251700
C	-4.93620400	-1.45700200	-3.09028000
H	-1.16562100	-1.36637200	-0.50490300
H	0.82919700	-2.03051500	-1.16788900
H	0.69226100	1.68403300	0.95542100
H	-3.73583300	4.47097400	-0.44481500
H	-2.81216700	4.08805300	1.03304500
H	-3.94755000	-2.90001100	-1.79472300
H	-4.94654700	-1.71202800	-0.93350000
H	-1.80763500	6.05840600	-0.18821800
H	-0.68818700	4.67631200	-0.10611200
H	-1.56222900	5.02543000	-1.61592000
H	-5.80679800	-2.09764800	-3.28576700
H	-5.26870400	-0.41688400	-3.03898900
H	-4.23765900	-1.56288100	-3.92895000
H	1.80841700	-3.19588600	2.21224100
C	1.12650900	-2.40407700	2.53576100
C	-0.19824800	-2.52663700	1.76609000
H	1.59360200	-1.42599600	2.37153200
H	0.94980800	-2.50542100	3.61589900
O	-3.06776600	-1.10859000	-1.54777900
O	-0.39764100	-3.52613400	1.07021700
C	-2.56330300	-1.56817800	1.93377100
H	-0.74815100	-0.59972000	2.55581600
C	-3.32396700	-0.45491000	2.66426200
O	-3.19079600	-2.49145600	1.41185000
H	-4.37772200	-0.48212000	2.37575400
H	-2.90114600	0.53021800	2.44244200
H	-3.24774400	-0.60880800	3.75072700
C	3.38067700	0.07673300	-0.39297700
C	5.52863900	1.22836400	0.17289200
H	5.85886600	2.02207200	-0.52278100
H	6.44707200	0.76271200	0.56573000
N	4.76594600	0.21908800	-0.54450500
C	5.55871200	-0.73214000	-1.30270400
H	6.35429700	-0.18028700	-1.82753500
H	6.07064800	-1.44140500	-0.62383900
C	4.74144500	1.85472200	1.32435700
H	4.63957700	1.12528600	2.13798200
H	5.30517700	2.70974700	1.71813200
C	3.34782100	2.26987900	0.84158200
H	3.45470500	3.05941000	0.07994200
H	2.76380000	2.70625200	1.65968400
C	4.71856400	-1.51268800	-2.31288600
H	4.37903300	-0.83350500	-3.10551800
H	5.34542800	-2.28059100	-2.78312600
C	3.50362700	-2.13046300	-1.61353700
H	3.85026700	-2.88972000	-0.89481400
H	2.86703300	-2.65834600	-2.33305300