

Supplemental Material-I

High-pressure Limit and Pressure-dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal-alkyl Cyclohexanes

Combustion. 1. Concerted HO₂ Elimination Reaction Class and β -Scission

Reaction Class

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15. Cartesian coordinates for all reactants, transition states and products in the class of β -scission

1. Detailed description of the master equation method

The time evolution of the population of the species in the system is described by the master equation [1]:

$$\frac{d\rho_i^\alpha}{dt} = \omega \sum_j P_{ij}^\alpha \rho_j^\alpha - \omega \sum_j P_{ji}^\alpha \rho_i^\alpha - k_i^\alpha \rho_i^\alpha + \sum_\beta k_l^\beta \rho_l^\beta + R_i \quad (1)$$

In Eq. (1), ρ_i^α is the molecular population of the isomer α at energy level E_i , ρ_j^α is the molecular population of the isomer α at energy level E_j , P_{ij}^α is the collision energy transfer probability from energy level j to energy level i of isomer α , ω is the collision frequency, which is proportional to the concentration of the third body M, hence, it is pressure dependent, k_i^α is the sum of rates for all the decomposition and isomerization channels from energy level E_i , k_l^β is the rate of isomerization from isomer β at energy level E_l to isomer α at energy level E_i , and R_i is the chemical activation flux, which is assumed to be constant. Index l for isomer β corresponds to the same energy as i for α , i.e. $E_l=E_i$. The master equation can be written in the matrix form:

$$\frac{d\rho}{dt} = B\rho + R \quad (2)$$

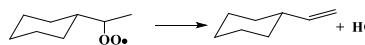
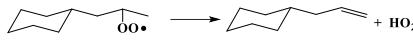
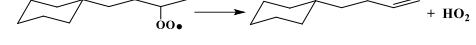
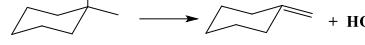
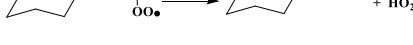
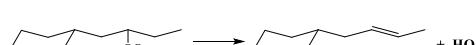
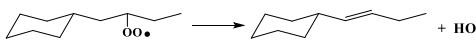
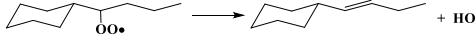
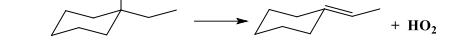
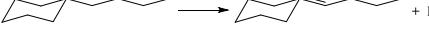
For the single-reaction channel case, the overall pressure-dependent thermal rate constant $k_{\text{uni}}(T,P)$ is equal to the negative of the largest eigenvalue of the matrix B. This eigenvalue is the chemically significant eigenvalue, which corresponds to the slow mode describing the “chemical reaction”, and for the multi-reaction channels case, there is one chemically significant eigenvalue for each reaction channel. All calculations are carried out with a series of energy grain sizes and variations in the

maximum system energy to ensure that the results have converged.

[1] R.G. Gilbert, S.C. Smith, Theory of unimolecular and recombination reactions, Blackwell, Oxford, 1990.

2. A list of reactions

Table S1. A list of reactions of concerted elimination class in this study.

No.	Reactions
R1	
R2	
R3	
R4	
R5	
R6	
R7	
R8	
R9	
R10	
R11	
R12	
R13	
R14	
R15	
R16	
R17	
R18	

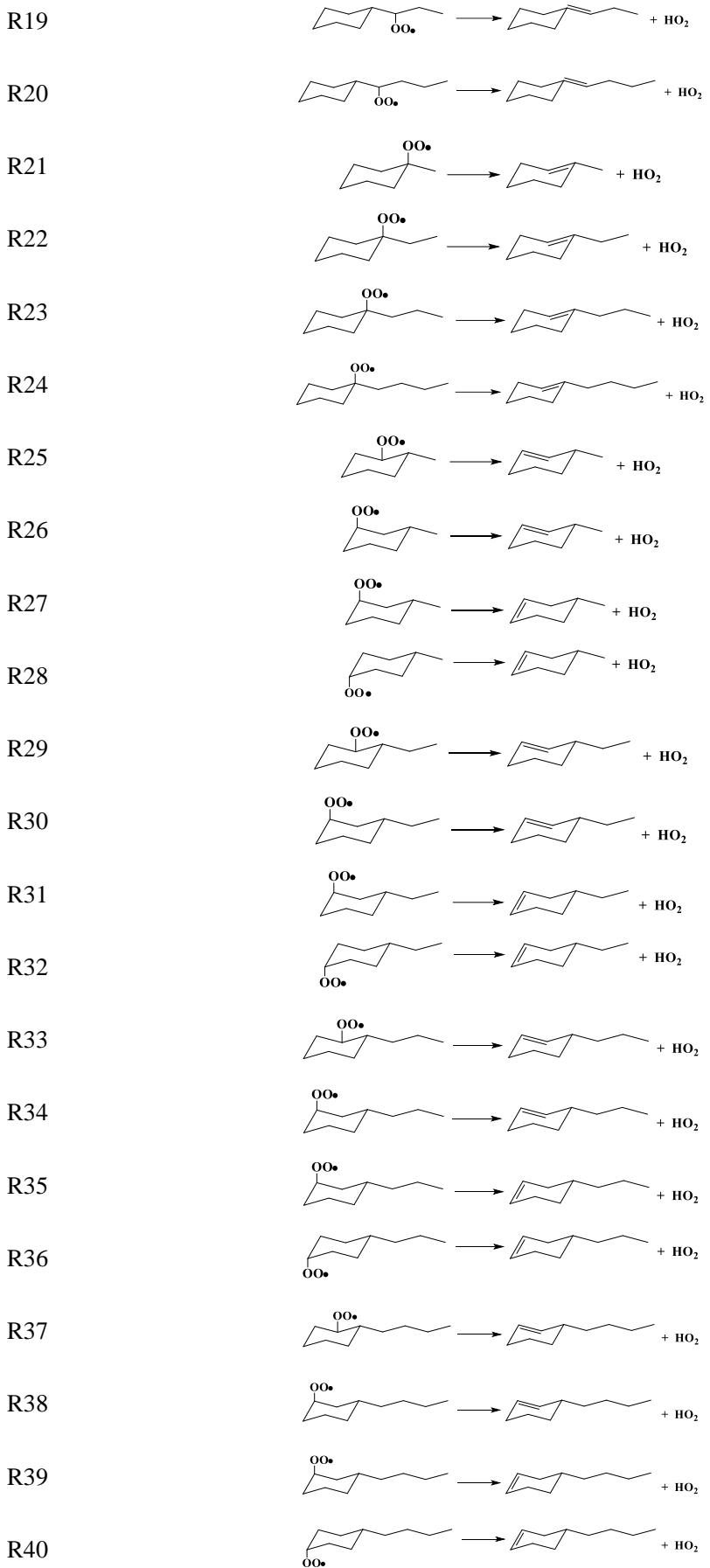
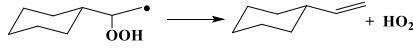
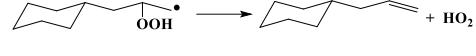
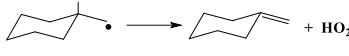
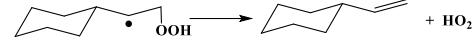
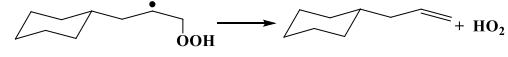
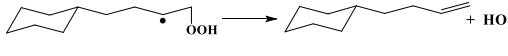
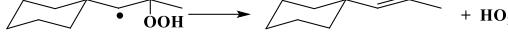
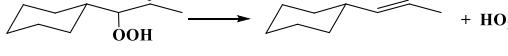
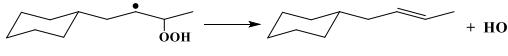
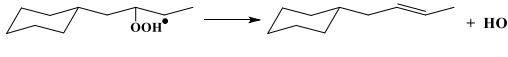
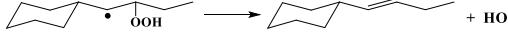
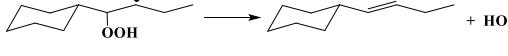
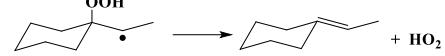
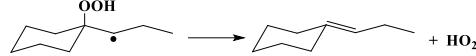
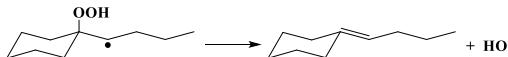
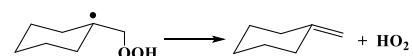
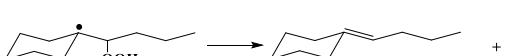
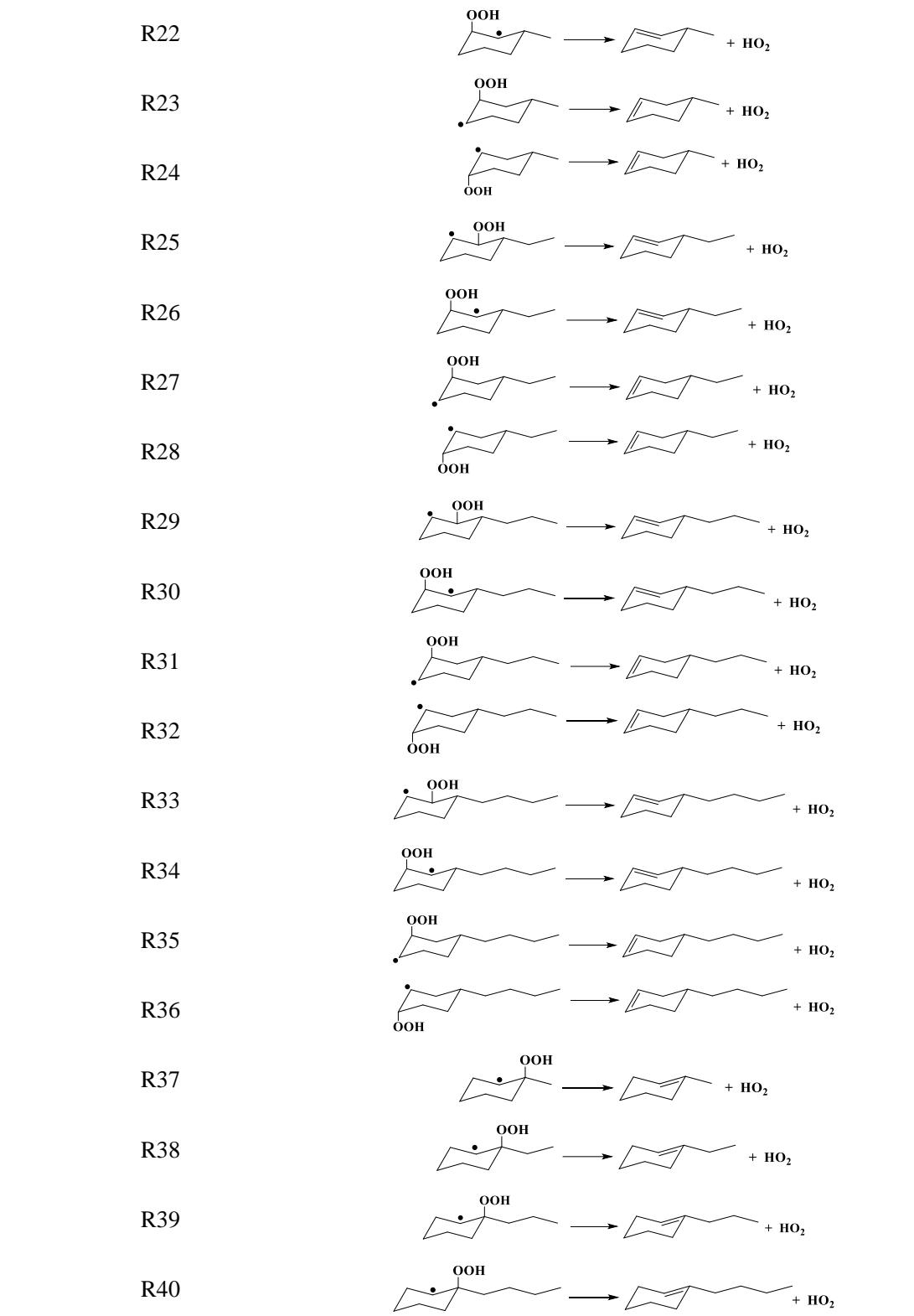


Table S2. A list of reactions of β -scission class in this study.

No.	Reactions
R1	
R2	
R3	
R4	
R5	
R6	
R7	
R8	
R9	
R10	
R11	
R12	
R13	
R14	
R15	
R16	
R17	
R18	
R19	
R20	
R21	



3. T₁ diagnostic values for some representative species in this work

Table S3. T₁ diagnostic value for reactants, transition states, and products.

Reaction class	Species	T ₁ ^a
Concerted elimination	R26	0.023
	TS26	0.026

	P26	0.009
	R27	0.023
	TS27	0.026
	P27	0.009
β -scission	R21	0.012
	TS21	0.015
	P21	0.009
	R23	0.012
	TS23	0.015
	P23	0.009

^aT₁ diagnostic value are calculated at the CCSD(T)/cc-pVTZ level.

4. Lennard-Jones parameters used in this study

The collision frequency between the reactant and bath gas (Ar) is estimated by using the Lennard-Jones (L-J) parameters σ (\AA) and ϵ (K). The L-J parameters for species were estimated using the method proposed by Wang and co-workers [2].

Table S4. Lennard-Jones parameters σ (\AA) and ϵ (K) used in this study.

Reactant ^a	σ	ϵ	Reactant ^b	σ	ϵ
C ₇ H ₁₃ O ₂	6.25	622.44	C ₇ H ₁₂ OOH	6.25	622.4
C ₈ H ₁₅ O ₂	6.46	660.78	C ₈ H ₁₄ OOH	6.46	660.8
C ₉ H ₁₇ O ₂	6.67	697.56	C ₉ H ₁₆ OOH	6.67	697.56
C ₁₀ H ₁₉ O ₂	6.86	732.99	C ₁₀ H ₁₈ OOH	6.86	732.99
Ar	3.47	114			

^aRepresents the reactants in the class of concerted elimination.

^bRepresents the reactants in the class of β -scission.

[2] Wang, M. Frenklach, Transport properties of polycyclic aromatic hydrocarbons for flame modeling, Combust. Flame 96 (1994) 163-170.

5. The calculated values of the barrier width L for all studied reactions

Table S5. Calculated barrier width L (\AA) for the class of concerted elimination.

Reaction	Barrier width L	Reaction	Barrier width L	Reaction	Barrier width L
R1	1.45	R15	1.47	R29	1.83
R2	1.51	R16	1.47	R30	1.69
R3	1.48	R17	1.78	R31	1.69

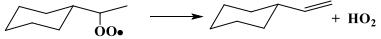
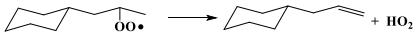
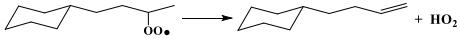
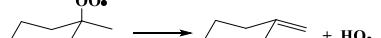
R4	1.39	R18	1.63	R32	1.71
R5	1.64	R19	1.64	R33	1.83
R6	1.69	R20	1.62	R34	1.69
R7	1.68	R21	1.61	R35	1.70
R8	1.51	R22	1.66	R36	1.71
R9	1.62	R23	1.65	R37	1.83
R10	1.55	R24	1.65	R38	1.69
R11	1.64	R25	1.83	R39	1.69
R12	1.53	R26	1.69	R40	1.69
R13	1.57	R27	1.70		
R14	1.52	R28	1.70		

Table S6. Calculated barrier width L (\AA) for the class of β -scission.

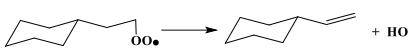
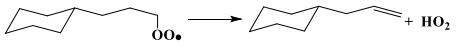
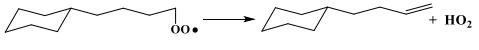
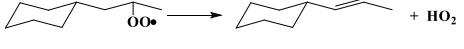
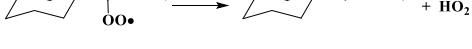
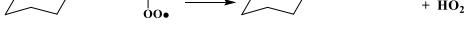
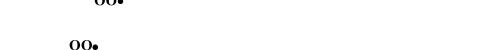
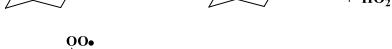
Reaction	Barrier width L	Reaction	Barrier width L	Reaction	Barrier width L
R1	1.09	R15	1.27	R29	1.10
R2	1.10	R16	1.27	R30	1.04
R3	1.12	R17	0.94	R31	1.03
R4	1.26	R18	1.04	R32	1.04
R5	0.95	R19	1.02	R33	1.10
R6	0.97	R20	1.01	R34	1.03
R7	0.97	R21	1.12	R35	1.03
R8	1.07	R22	1.04	R36	1.04
R9	1.08	R23	1.03	R37	1.03
R10	1.09	R24	1.04	R38	1.00
R11	1.07	R25	1.11	R39	0.99
R12	1.07	R26	1.04	R40	0.99
R13	1.07	R27	1.04		
R14	1.27	R28	1.04		

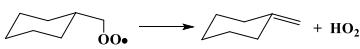
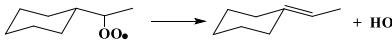
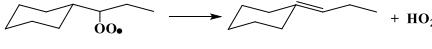
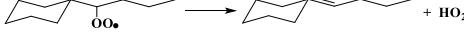
6. Energy barriers for the class of concerted elimination

Table S7. Energy barriers for the reaction center of concerted elimination class occurs on the alkyl side chain (kcal mol $^{-1}$).

Subclass	Reaction	Energy barrier
Eli-p-SC	R1 	30.3
	R2 	31.3
	R3 	31.4
	R4 	31.2

31.1^a,1.1^b

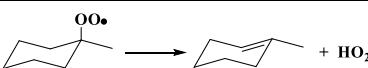
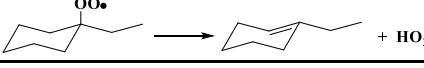
Eli-s-SC			
	R5		29.5
	R6		30.1
	R7		30.4
	R8		29.6
	R9		29.8
	R10		30.2
	R11		30.7
	R12		29.6
	R13		29.4
	R14		30.9
	R15		30.8
	R16		30.8
			30.2^a,1.5^b

Eli-t-SC			
	R17		30.1
	R18		30.0
	R19		29.9
	R20		29.5
			29.9^a,0.6^b

^aThe average energy barrier of reactions in each subclass.

^bThe maximum deviation of energy barriers in each subclass.

Table S8. Energy barriers for the reaction center of concerted elimination class occurs on cycle (kcal mol⁻¹).

Subclass		Reaction	Energy barrier
Eli-s-CY	R21		31.6
	R22		31.8

Reaction	Chemical Reaction Diagram	Energy barrier (kcal mol ⁻¹)
R23		31.9
R24		32.0
R25		32.7
R26		32.2
R27		31.9
R28		32.0
R29		32.5
R30		31.9
R31		31.9
R32		32.0
R33		32.5
R34		31.9
R35		31.9
R36		32.0
R37		32.5
R38		31.9
R39		31.9
R40		31.8
		32.0^a,1.1^b

^aThe average energy barrier of reactions in each subclass.

^bThe maximum deviation of energy barriers in each subclass.

7. Energy barriers for the class of β -scission

Table S9. Energy barriers for the reaction center of β -scission class occurs on the alkyl side chain (kcal mol⁻¹).

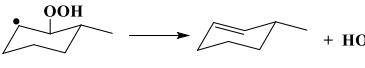
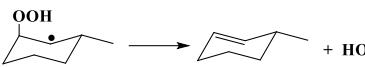
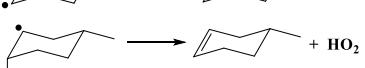
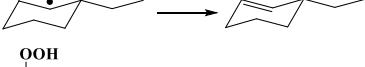
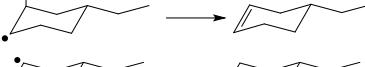
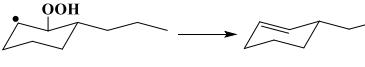
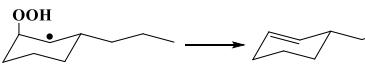
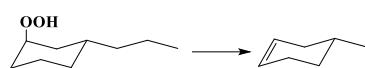
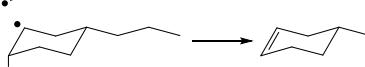
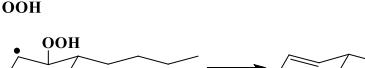
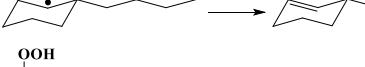
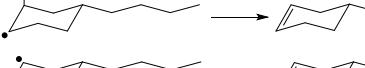
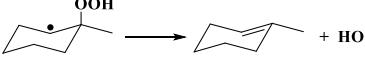
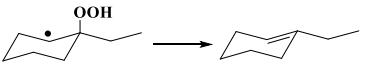
Subclass	Reaction	Energy barrier
Sci-p-SC	R1	16.0

	R2		15.9
	R3		16.2
	R4		16.0
			16.0^a,0.3^b
Sci-s-SC	R5		15.6
	R6		16.1
	R7		16.0
	R8		15.3
	R9		15.3
	R10		16.3
	R11		15.6
	R12		15.7
	R13		15.2
	R14		16.6
	R15		16.5
	R16		16.4
			15.9^a,1.4^b
Sci-t-SC	R17		14.4
	R18		14.1
	R19		14.0
	R20		13.9
			14.1^a,0.2^b

^aThe average energy barrier of reactions in each subclass.

^bThe maximum deviation of energy barriers in each subclass.

Table S10. Energy barriers for the reaction center of β -scission class occurs on the cycle (kcal mol⁻¹).

Subclass		Reaction	Energy barrier
Sci-s-CY	R21		15.6
	R22		15.2
	R23		15.0
	R24		15.1
	R25		15.6
	R26		15.1
	R27		14.9
	R28		15.1
	R29		15.7
	R30		15.1
	R31		15.0
	R32		15.1
	R33		15.6
	R34		15.0
	R35		15.0
	R36		15.1
	R37		15.3
	R38		15.2
	R39		15.1
	R40		15.2
			15.2^a,0.8^b

^aThe average energy barrier of reactions in each subclass.

^bThe maximum deviation of energy barriers in each subclass.

8. Pre-exponential factors for the class of concerted elimination

Table S11. Pre-exponential factor (s^{-1}) ($T=298$ K) for concerted elimination class.

	Reaction	<i>A</i> ^a (s^{-1})	<i>f</i> ^b
Eli-p-SC subclass	R1	1.69E+13	3.8
	R2	2.16E+13	
	R3	2.45E+13	
	R4	6.44E+12	
Eli-s-SC subclass	R5	9.91E+12	5.6
	R6	4.87E+12	
	R7	2.06E+13	
	R8	5.34E+12	
	R9	2.45E+13	
	R10	1.32E+13	
	R11	1.53E+13	
	R12	9.48E+12	
	R13	1.37E+13	
	R14	2.72E+13	
	R15	2.07E+13	
	R16	2.62E+13	
Eli-t-SC rate rule	R17	1.08E+13	2.9
	R18	1.44E+13	
	R19	1.19E+13	
	R20	5.04E+12	
Eli-s-CY subclass	R21	5.14E+13	5.5
	R22	4.94E+13	
	R23	5.43E+13	
	R24	2.08E+13	
	R25	3.12E+13	
	R26	3.41E+13	
	R27	2.90E+13	
	R28	3.57E+13	
	R29	3.61E+13	
	R30	5.11E+13	
	R31	3.67E+13	
	R32	3.05E+13	
	R33	6.21E+13	

R34	2.19E+13
R35	4.66E+13
R36	1.15E+14
R37	3.78E+13
R38	2.41E+13
R39	2.55E+13
R40	3.05E+13

^aPre-exponential factors are calculated at T=298 K.

^b $f = A_{\max}/A_{\min}$ for each subclass.

9. Pre-exponential factors for the class of β -scission

Table S12. Pre-exponential factor (s⁻¹) (T=298 K) for β -scission class.

	Reaction	<i>A</i> ^a (s ⁻¹)	<i>f</i> ^b
Sci-p-SC subclass	R1	6.96E+13	3.6
	R2	4.75E+13	
	R3	9.89E+13	
	R4	2.78E+13	
Sci-s-SC subclass	R5	9.40E+13	9.4
	R6	2.03E+14	
	R7	2.19E+14	
	R8	1.26E+14	
	R9	2.73E+13	
	R10	2.82E+13	
	R11	8.16E+13	
	R12	1.79E+14	
	R13	2.32E+13	
	R14	2.90E+13	
	R15	2.73E+13	
	R16	2.76E+13	
Sci-t-SC rate rule	R17	8.04E+13	5.0
	R18	3.05E+13	
	R19	3.38E+13	
	R20	1.60E+13	
Sci-s-CY subclass	R21	1.08E+14	8.0
	R22	1.10E+14	

R23	1.41E+14
R24	1.21E+14
R25	1.88E+14
R26	9.41E+13
R27	1.79E+14
R28	9.70E+13
R29	3.07E+14
R30	1.61E+14
R31	1.79E+14
R32	8.15E+13
R33	1.01E+14
R34	2.19E+14
R35	2.29E+14
R36	3.32E+14
R37	8.21E+13
R38	4.48E+13
R39	5.80E+13
R40	4.13E+13

^aPre-exponential factor (s^{-1}) is calculated at $T=298 \text{ K}$.

^b $f = A_{\max}/A_{\min}$ for each subclass.

10. High-pressure limit rate constants of the class of concerted elimination

Table S13. Calculated rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in each subclass for the reaction center of concerted elimination occurring on the alkyl side chain at high pressure.

Reaction	Modified Arrhenius parameters			$T=800 \text{ K}$	
	$A (\text{s}^{-1})$	n	$E (\text{cal mol}^{-1})$	$k (\text{s}^{-1})$	k/k_{ave}^e
R1	2.05E+08	1.43	28588.6	4.5E+04	1.5
R2	5.73E+07	1.63	29378.4	3.0E+04	1.0
R3	2.32E+08	1.47	29678.5	3.3E+04	1.1
R4	1.22E+08	1.41	29626.9	1.3E+04	0.4
Eli-p-SC rate rule	4.38E+08	1.36	29567.6	3.0E+04	3.6[#]
R5	1.49E+08	1.43	28016	4.5E+04	0.8
R6	1.28E+06	1.94	27923.5	1.3E+04	0.2
R7	3.07E+08	1.41	28894.2	4.9E+04	0.8
R8	3.07E+08	1.41	28894.2	4.9E+04	0.8
R9	4.03E+10	0.81	29029.2	1.1E+05	1.8
R10	7.17E+09	0.95	29261.9	4.2E+04	0.7
R11	8.07E+09	0.96	29744.5	3.6E+04	0.6
R12	6.25E+09	0.96	28783.5	5.4E+04	0.9
R13	1.01E+11	0.62	28903.8	8.3E+04	1.4

R14	3.60E+09	1.22	29854	8.5E+04	1.4
R15	6.29E+59	-14.41	48554.4	6.6E+04	1.1
R16	5.21E+09	1.15	29782.7	8.3E+04	1.4
Eli-s-SC rate rule	6.13E-25	11.30	14517.3	5.9E+04	8.3[#]
R17	2.02E+08	1.38	28615.3	3.2E+04	0.7
R18	4.00E+09	1.09	29106.3	6.5E+04	1.4
R19	2.76E+09	1.10	28933.7	5.5E+04	1.2
R20	9.96E+08	1.15	28577.4	3.3E+04	0.7
Eli-t-SC rate rule	1.39E+09	1.17	28851.4	4.6E+04	2.0[#]

[#]The uncertainty factor values of the high-pressure limit rule at 800 K for each subclass in our study (The ratios of the largest rate constant of a reaction to the smallest rate constant at 800 K for each subclass).

^e k_{ave} is the average rate constants at 800 K for each reaction subclass.

Table S14. Calculated rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in each subclass for the reaction center of concerted elimination occurring on the cycle.

Reaction	Modified Arrhenius parameters			<i>T=800 K</i>	
	A (s ⁻¹)	n	E (cal mol ⁻¹)	k (s ⁻¹)	k/k _{ave} ^e
R21	8.12E+09	1.18	30590.8	9.4E+04	1.6
R22	6.93E+09	1.22	30843.1	9.0E+04	1.5
R23	9.84E+09	1.17	30916.4	8.6E+04	1.5
R24	3.85E+09	1.15	30984.9	3.0E+04	0.5
R25	1.99E+09	1.30	31577.2	2.7E+04	0.5
R26	1.03E+09	1.37	30906	3.5E+04	0.6
R27	9.60E+08	1.38	30694.2	3.9E+04	0.7
R28	1.08E+09	1.37	30725.9	4.2E+04	0.7
R29	8.28E+09	1.14	31614.3	3.8E+04	0.7
R30	5.73E+09	1.19	30793.8	6.4E+04	1.1
R31	3.61E+09	1.21	30793.7	4.6E+04	0.8
R32	3.38E+09	1.19	30893.8	3.5E+04	0.6
R33	2.98E+09	1.35	31363.7	6.5E+04	1.1
R34	6.73E+08	1.37	30597	2.8E+04	0.5
R35	1.19E+09	1.40	30594.8	5.9E+04	1.0
R36	3.20E+08	1.38	30669.4	1.3E+05	2.3
R37	9.07E+09	1.12	31586.3	3.9E+04	0.7
R38	7.42E+08	1.37	30614.3	3.1E+04	0.5
R39	5.08E+08	1.43	30579.7	3.3E+04	0.6
R40	3.31E+08	1.67	29897.8	1.6E+05	2.8
Eli-s-CY rate rule	2.17E+09	1.33	30793.8	5.9E+04	6.0[#]

[#]The uncertainty factor values of the high-pressure limit rule at 800 K for each class in our study (The ratios of the largest rate constant of a reaction to the smallest rate constant at 800 K for each subclass).

^e k_{ave} is the average rate constants at 800 K for each reaction subclass.

11. High-pressure limit rate constants of the class of β -scission

Table S15. Calculated rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in each subclass for the reaction center of β -scission occurring on the alkyl side chain at high pressure.

Reaction	Modified Arrhenius parameters			T=800 K	
	A (s ⁻¹)	n	E (cal mol ⁻¹)	k (s ⁻¹)	k/k _{ave} ^e
R1	1.65E+09	1.03	13609.5	3.1E+08	1.1
R2	5.92E+08	1.12	13450.3	2.2E+08	0.7
R3	6.34E+10	0.55	14151.2	3.4E+08	1.1
R4	1.72E+09	1.07	14070.9	3.2E+08	1.1
Sci-p-SC rate rule	2.92E+09	0.96	13794.3	3.0E+08	1.1[#]
R5	5.76E+07	1.39	12418.6	3.1E+08	0.8
R6	6.94E+07	1.44	12809.7	2.2E+08	0.5
R7	1.23E+10	0.88	13078.8	3.4E+08	0.9
R8	4.26E+10	0.76	13479.0	1.4E+09	3.7
R9	7.37E+10	0.47	13767.8	2.9E+08	0.7
R10	5.57E+09	0.82	14378.8	1.6E+08	0.4
R11	1.77E+10	0.78	13602.4	6.3E+08	1.6
R12	1.10E+10	0.76	12805.5	5.5E+08	1.4
R13	6.68E+10	0.45	13744.2	2.3E+08	0.6
R14	1.44E+10	0.79	15301.0	1.9E+08	0.5
R15	5.50E+09	0.85	15121.5	1.2E+08	0.3
R16	1.10E+12	0.22	15693.4	2.5E+08	0.6
Sci-s-SC rate rule	5.68E+09	0.87	13510.6	3.9E+08	5.3[#]
R17	1.93E+09	1.02	12021.8	9.3E+08	0.7
R18	1.19E+11	0.58	13004.3	1.6E+09	1.2
R19	2.15E+10	0.83	12621.5	1.9E+09	1.4
R20	6.45E+10	0.56	12711.4	9.1E+08	0.7
Sci-t-SC rate rule	2.51E+10	0.75	12625.4	1.4E+09	2.1[#]

[#]The uncertainty factor values of the high-pressure limit rule at 800 K for each subclass in our study (The ratios of the largest rate constant of a reaction to the smallest rate constant at 800 K for each subclass).

^ek_{ave} is the average rate constants at 800 K for each reaction subclass.

Table S16. Calculated rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in each subclass for the reaction center of β -scission occurring on cycle at high pressure.

Reaction	Modified Arrhenius parameters			T=800K	
	A (s ⁻¹)	n	E (cal mol ⁻¹)	k (s ⁻¹)	k/k _{ave} ^e
R21	3.15E+11	0.50	14236.3	1.1E+09	0.6
R22	1.42E+11	0.59	13623.7	1.3E+09	0.8
R23	1.78E+11	0.58	13390.9	1.8E+09	1.0
R24	1.61E+11	0.59	13550.6	1.6E+09	0.9
R25	8.55E+11	0.43	14295.2	1.9E+09	1.1

R26	2.55E+10	0.79	13232.7	1.2E+09	0.7
R27	5.96E+10	0.78	13113.5	2.8E+09	1.6
R28	4.29E+10	0.72	13309	1.2E+09	0.7
R29	9.25E+10	0.76	13809.4	2.5E+09	1.4
R30	4.81E+10	0.78	13238.7	2.1E+09	1.2
R31	2.39E+11	0.57	13391.6	2.3E+09	1.3
R32	1.15E+11	0.57	13535.1	1.1E+09	0.6
R33	5.91E+10	0.68	13866.5	9.2E+08	0.5
R34	2.69E+10	0.90	13029.3	3.1E+09	1.8
R35	5.25E+10	0.79	13052.5	2.9E+09	1.6
R36	4.48E+10	0.89	13143.9	4.4E+09	2.5
R37	1.24E+11	0.55	13618.9	9.5E+08	0.5
R38	1.24E+11	0.47	13563.3	5.6E+08	0.3
R39	1.81E+11	0.48	13543.7	8.7E+08	0.5
R40	1.15E+11	0.49	13615.4	5.6E+08	0.3
Sci-s-CY rate rule	6.34E+10	0.72	13371.0	1.8E+09	8.0[#]

[#]The uncertainty factor values of the high-pressure limit rule at 800 K for each subclass in our study (The ratios of the largest rate constant of a reaction to the smallest rate constant at 800 K for each subclass).

^e k_{ave} is the average rate constants at 800 K for each reaction subclass.

12. Pressure-dependent rate constants of the concerted elimination

Table S17. Calculated rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in each subclass for the reaction center of concerted elimination occurring on the alkyl side chain at different pressures.

Reaction	Pressure (atm)	Modified Arrhenius parameters			T=800 K	
		A (s ⁻¹)	n	E (cal mol ⁻¹)	k (s ⁻¹)	k/k _{ave} ^e
R1	0.01	4.65E+54	-12.93	46051.0	3.7E+04	1.5
	0.1	1.99E+48	-10.94	43743.4	4.0E+04	1.5
	1	6.41E+35	-7.00	39478.1	4.7E+04	1.5
	10	1.63E+22	-2.79	34336.9	4.9E+04	1.6
	100	2.86E+12	0.19	30353.9	4.9E+04	1.6
R2	0.01	7.97E+54	-12.92	47481.2	2.6E+04	1.0
	0.1	6.03E+48	-11.02	45206.7	2.7E+04	1.0
	1	2.56E+35	-6.84	40439.4	3.0E+04	1.0
	10	2.12E+21	-2.49	35014.1	3.1E+04	1.0
	100	4.99E+11	0.45	31052.5	3.1E+04	1.0
R3	0.01	1.76E+55	-13.00	47791.7	2.8E+04	1.1
	0.1	1.92E+49	-11.15	45549.1	2.9E+04	1.1
	1	4.88E+35	-6.91	40636.6	3.2E+04	1.1
	10	3.50E+21	-2.54	35162.4	3.3E+04	1.1
	100	1.16E+12	0.35	31253.5	3.3E+04	1.1
R4	0.01	7.93E+48	-11.18	45387.2	1.1E+04	0.4

	0.1	1.54E+43	-9.40	43282.0	1.1E+04	0.4
	1	1.40E+30	-5.34	38530.6	1.2E+04	0.4
	10	2.24E+17	-1.40	33496.5	1.3E+04	0.4
	100	1.70E+10	0.77	30543.1	1.3E+04	0.4
Eli-p-SC rate rule	0.01	1.94E+53	-12.47	46379.1	2.5E+04	3.5[#]
	0.1	1.95E+47	-10.61	44165.5	2.7E+04	3.5 [#]
	1	2.34E+34	-6.56	39602.9	3.0E+04	3.8 [#]
	10	6.24E+20	-2.37	34403.6	3.1E+04	3.9 [#]
	100	3.30E+11	0.47	30596.7	3.2E+04	3.9 [#]
R5	0.01	9.89E+52	-12.45	44886.0	3.8E+04	0.8
	0.1	5.61E+46	-10.50	42617.8	4.1E+04	0.8
	1	2.15E+34	-6.59	38355.9	5.1E+04	0.8
	10	1.01E+21	-2.47	33298.5	5.5E+04	0.8
	100	6.57E+11	0.34	33298.5	5.0E+03	0.1
R6	0.01	4.55E+44	-9.90	43149.5	1.3E+04	0.3
	0.1	5.86E+39	-8.39	41277.1	1.4E+04	0.3
	1	4.34E+26	-4.32	36303.8	1.5E+04	0.2
	10	1.40E+14	-0.49	31314.1	1.4E+04	0.2
	100	7.18E+07	1.42	28685.6	1.4E+04	0.2
R7	0.01	3.20E+54	-12.81	46583.5	3.8E+04	0.8
	0.1	3.21E+48	-10.95	44336.0	3.9E+04	0.8
	1	1.62E+35	-6.80	39578.6	4.6E+04	0.8
	10	2.25E+21	-2.52	34244.4	4.9E+04	0.7
	100	1.10E+12	0.32	30413.8	4.6E+04	0.8
R8	0.01	3.20E+54	-12.81	46583.5	3.8E+04	0.8
	0.1	3.21E+48	-10.95	44336.0	3.9E+04	0.8
	1	1.62E+35	-6.80	39578.6	4.6E+04	0.8
	10	2.25E+21	-2.52	34244.4	4.9E+04	0.7
	100	1.10E+12	0.32	30413.8	4.6E+04	0.8
R9	0.01	5.35E+58	-14.15	46781.1	7.5E+04	1.6
	0.1	6.62E+51	-11.99	44303.1	8.3E+04	1.7
	1	1.41E+40	-8.27	40557.7	1.1E+05	1.8
	10	6.49E+26	-4.12	35685.4	1.3E+05	1.9
	100	8.82E+15	-0.79	31306.0	1.2E+05	2.0
R10	0.01	5.92E+55	-13.21	46713.8	4.7E+04	1.0
	0.1	4.34E+49	-11.30	44430.1	5.0E+04	1.0
	1	4.48E+36	-7.23	39858.6	6.0E+04	1.0
	10	1.00E+23	-3.01	34649.1	6.3E+04	0.9
	100	4.40E+13	-0.15	30812.8	6.1E+04	1.0
R11	0.01	3.43E+54	-12.81	46961.0	3.3E+04	0.7
	0.1	5.18E+48	-11.00	44774.1	3.5E+04	0.7
	1	2.63E+35	-6.85	39977.5	4.0E+04	0.7
	10	5.88E+21	-2.64	34695.5	4.2E+04	0.6
	100	1.09E+13	0.02	31095.5	4.0E+04	0.7

R12	0.01	4.86E+54	-12.90	45918.4	5.0E+04	1.1
	0.1	4.39E+48	-11.02	43666.3	5.2E+04	1.1
	1	5.48E+35	-6.98	39113.6	6.3E+04	1.0
	10	1.85E+22	-2.81	33964.4	6.6E+04	1.0
	100	1.73E+13	-0.06	30259.3	6.4E+04	1.0
R13	0.01	5.62E+71	-18.23	51470.4	5.9E+04	1.3
	0.1	1.52E+72	-18.34	51758.9	6.2E+04	1.2
	1	3.40E+73	-18.73	52439.0	6.5E+04	1.1
	10	6.20E+73	-18.81	52567.8	6.6E+04	1.0
	100	6.58E+73	-18.82	52580.8	6.6E+04	1.1
R14	0.01	8.91E+60	-14.79	48616.4	5.2E+04	1.1
	0.1	1.03E+54	-12.62	46174.1	5.9E+04	1.2
	1	5.48E+42	-9.01	42694.5	8.2E+04	1.3
	10	1.84E+29	-4.80	37881.2	9.7E+04	1.4
	100	1.19E+17	-1.06	33016.9	9.6E+04	1.6
R15	0.01	6.29E+59	-14.41	48554.4	4.9E+04	1.1
	0.1	1.49E+53	-12.35	46142.7	5.4E+04	1.1
	1	6.66E+40	-8.44	42037.2	6.9E+04	1.1
	10	8.68E+26	-4.12	36919.1	7.8E+04	1.2
	100	3.43E+15	-0.63	32311.6	7.6E+04	1.2
R16	0.01	1.97E+61	-14.84	49065.4	6.5E+04	1.4
	0.1	2.11E+54	-12.67	46522.8	7.0E+04	1.4
	1	6.91E+41	-8.71	42386.3	9.1E+04	1.5
	10	6.11E+27	-4.34	37206.2	1.0E+05	1.5
	100	1.22E+16	-0.76	32478.7	9.9E+04	1.6
Eli-s-SC rate rule	0.01	1.90E+56	-13.40	46574.4	4.7E+04	5.7[#]
	0.1	2.41E+50	-11.55	44448.4	5.0E+04	6.1[#]
	1	6.25E+37	-7.60	40091.8	6.2E+04	7.6[#]
	10	2.27E+24	-3.43	35056.6	6.7E+04	8.8[#]
	100	2.24E+14	-0.37	31073.1	6.1E+04	8.9[#]
R17	0.01	1.08E+52	-12.16	45022.1	2.8E+04	0.7
	0.1	2.73E+43	-9.46	42026.8	3.2E+04	0.8
	1	4.12E+30	-5.42	37600.4	3.7E+04	0.8
	10	8.02E+17	-1.51	32643.1	3.8E+04	0.8
	100	4.12E+10	0.71	29630.4	3.8E+04	0.8
R18	0.01	3.09E+56	-13.48	46574.2	4.5E+04	1.2
	0.1	1.21E+50	-11.47	44274.0	5.0E+04	1.2
	1	1.12E+38	-7.67	40281.0	6.0E+04	1.2
	10	2.10E+27	-4.31	36479.3	6.4E+04	1.3
	100	1.25E+16	-0.88	31883.8	6.4E+04	1.3
R19	0.01	3.11E+55	-13.15	46366.2	4.5E+04	1.2
	0.1	1.55E+49	-11.19	44050.7	4.9E+04	1.2
	1	3.14E+36	-7.20	39663.1	5.6E+04	1.2
	10	8.19E+22	-2.99	34513.0	5.8E+04	1.2

	100	2.22E+13	-0.07	30601.3	5.9E+04	1.2
R20	0.01	3.65E+51	-11.96	45047.6	3.4E+04	0.9
	0.1	1.06E+46	-10.24	42955.6	3.6E+04	0.9
	1	7.48E+32	-6.14	38162.4	3.9E+04	0.8
	10	4.31E+19	-2.06	33007.0	4.0E+04	0.8
	100	4.66E+11	0.37	29713.6	4.0E+04	0.8
Eli-t-SC rate rule	0.01	9.38E+53	-12.71	45771.3	3.8E+04	1.6[#]
	0.1	1.82E+47	-10.61	43330.9	4.2E+04	1.5[#]
	1	4.93E+34	-6.66	38986.5	4.8E+04	1.6[#]
	10	2.49E+22	-2.85	34353.6	5.0E+04	1.7[#]
	100	1.30E+13	-0.02	30547.6	5.0E+04	1.7[#]

[#]The uncertainty factor values of the high-pressure limit rule at 800 K for each subclass in our study (The ratios of the largest rate constant of a reaction to the smallest rate constant at 800 K for each subclass).

^e k_{ave} is the average rate constants at 800 K for each reaction subclass.

Table S18. Calculated rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in each class for the reaction center of concerted elimination occurring on the cycle at different pressures.

Reaction	Pressure (atm)	Modified Arrhenius parameters			T=800K	
		A (s ⁻¹)	n	E (cal mol ⁻¹)	k (s ⁻¹)	k/k _{ave} ^e
R21	0.01	9.50E+61	-15.12	49043.5	4.7E+04	1.3
	0.1	7.76E+54	-12.88	46694.3	5.6E+04	1.3
	1	8.08E+44	-9.63	43944.6	8.6E+04	1.5
	10	7.05E+31	-5.53	39425.7	1.1E+05	1.6
	100	1.14E+19	-1.60	34386.4	1.1E+05	1.6
R22	0.01	2.02E+63	-15.46	50249.0	4.8E+04	1.3
	0.1	1.16E+56	-13.19	47743.5	5.5E+04	1.3
	1	8.02E+44	-9.60	44385.6	7.9E+04	1.4
	10	1.56E+31	-5.31	39511.9	9.4E+04	1.4
	100	2.48E+18	-1.38	34418.5	9.3E+04	1.4
R23	0.01	1.56E+64	-15.69	50869.5	5.4E+04	1.4
	0.1	7.73E+56	-13.41	48274.8	6.1E+04	1.4
	1	1.11E+45	-9.63	44557.0	8.4E+04	1.5
	10	1.02E+31	-5.24	39503.3	9.8E+04	1.5
	100	1.67E+18	-1.32	34389.3	9.6E+04	1.5
R24	0.01	1.41E+57	-13.53	49371.4	2.4E+04	0.7
	0.1	1.38E+51	-11.66	47111.4	2.5E+04	0.6
	1	2.58E+37	-7.38	42147.9	3.0E+04	0.5
	10	1.25E+23	-2.96	36606.8	3.1E+04	0.5
	100	2.70E+13	-0.02	32623.0	2.9E+04	0.4
R25	0.01	1.98E+59	-14.24	50178.7	1.8E+04	0.5
	0.1	5.04E+52	-12.17	47873.5	2.0E+04	0.5
	1	2.68E+40	-8.28	43830.5	2.6E+04	0.5

	10	1.96E+26	-3.89	38559.8	2.9E+04	0.4
	100	1.22E+15	-0.46	34018.7	2.8E+04	0.4
R26	0.01	2.11E+59	-14.28	49483.9	2.3E+04	0.6
	0.1	4.14E+52	-12.16	47159.1	2.6E+04	0.6
	1	5.46E+40	-8.39	43343.3	3.5E+04	0.6
	10	5.84E+26	-4.04	38194.9	4.0E+04	0.6
	100	1.80E+15	-0.52	33551.4	3.9E+04	0.6
	0.01	1.25E+59	-14.22	49149.8	2.5E+04	0.7
R27	0.1	2.39E+52	-12.10	46823.4	2.8E+04	0.7
	1	3.91E+40	-8.35	43056.0	3.8E+04	0.7
	10	4.97E+26	-4.03	37945.3	4.3E+04	0.7
	100	1.64E+15	-0.51	33316.5	4.2E+04	0.6
	0.01	9.16E+59	-14.48	49369.3	2.7E+04	0.7
R28	0.1	1.41E+53	-12.33	47031.3	3.2E+04	0.8
	1	4.51E+41	-8.66	43439.8	4.4E+04	0.8
	10	6.70E+27	-4.35	38406.5	5.0E+04	0.8
	100	9.08E+15	-0.71	33642.3	4.9E+04	0.8
	0.01	1.04E+62	-15.03	51001.9	2.8E+04	0.8
R29	0.1	1.36E+55	-12.87	48562.4	3.2E+04	0.8
	1	6.16E+42	-8.96	44526.2	4.2E+04	0.7
	10	3.26E+28	-4.52	39253.8	4.7E+04	0.7
	100	4.11E+16	-0.88	34448.9	4.6E+04	0.7
	0.01	6.78E+61	-15.01	49945.1	4.0E+04	1.1
R30	0.1	6.21E+54	-12.80	47474.8	4.5E+04	1.1
	1	1.08E+43	-9.05	43763.0	6.1E+04	1.1
	10	1.23E+29	-4.71	38698.4	7.1E+04	1.1
	100	8.75E+16	-0.99	33822.5	6.9E+04	1.1
	0.01	9.49E+60	-14.75	49819.7	3.5E+04	0.9
R31	0.1	1.17E+54	-12.58	47375.2	3.9E+04	0.9
	1	9.40E+41	-8.74	43464.2	5.2E+04	0.9
	10	8.32E+27	-4.37	38298.9	5.9E+04	0.9
	100	1.41E+16	-0.77	33553.1	5.7E+04	0.9
	0.01	4.01E+58	-14.03	49369.7	2.5E+04	0.7
R32	0.1	1.14E+52	-11.98	47010.8	2.7E+04	0.6
	1	1.97E+39	-7.96	42670.2	3.4E+04	0.6
	10	1.44E+25	-3.58	37341.1	3.7E+04	0.6
	100	3.21E+14	-0.32	33001.0	3.6E+04	0.6
	0.01	1.30E+65	-15.94	51936.0	4.5E+04	1.2
R33	0.1	6.30E+57	-13.65	49334.9	5.0E+04	1.2
	1	4.98E+45	-9.79	45499.2	6.9E+04	1.2
	10	2.38E+31	-5.32	40324.8	8.0E+04	1.2
	100	1.83E+18	-1.30	35076.5	7.8E+04	1.2
	0.01	6.07E+56	-13.45	48988.0	2.3E+04	0.6
R34	0.1	3.77E+50	-11.52	46686.5	2.4E+04	0.6

	1	1.27E+37	-7.30	41894.0	2.8E+04	0.5
	10	6.76E+22	-2.90	36403.6	3.0E+04	0.5
	100	8.24E+12	0.13	32328.7	2.8E+04	0.4
R35	0.01	1.99E+61	-14.82	50170.8	3.8E+04	1.0
	0.1	2.47E+54	-12.66	47671.4	4.2E+04	1.0
	1	4.72E+41	-8.64	43425.2	5.4E+04	0.9
	10	1.96E+27	-4.17	38083.5	6.0E+04	0.9
	100	2.90E+15	-0.55	33292.5	5.8E+04	0.9
R36	0.01	1.26E+52	-12.04	47719.0	7.1E+04	1.9
	0.1	3.79E+46	-10.33	45630.8	8.2E+04	1.9
	1	8.12E+32	-6.08	40562.7	1.2E+05	2.1
	10	1.64E+19	-1.87	35164.7	1.5E+05	2.2
	100	1.40E+11	0.59	31813.4	1.5E+05	2.3
R37	0.01	1.44E+61	-14.71	51151.5	3.0E+04	0.8
	0.1	4.30E+54	-12.68	48728.1	3.2E+04	0.8
	1	1.15E+41	-8.43	43964.8	3.9E+04	0.7
	10	2.36E+26	-3.88	38383.5	4.2E+04	0.6
	100	1.82E+15	-0.49	33838.9	4.0E+04	0.6
R38	0.01	5.18E+57	-13.70	49435.1	2.7E+04	0.7
	0.1	3.35E+51	-11.78	47117.1	2.8E+04	0.7
	1	6.64E+37	-7.50	42207.0	3.3E+04	0.6
	10	2.22E+23	-3.03	36635.3	3.5E+04	0.5
	100	1.46E+13	0.08	32448.2	3.3E+04	0.5
R39	0.01	1.48E+59	-14.14	49922.4	3.1E+04	0.8
	0.1	5.61E+52	-12.14	47531.2	3.2E+04	0.8
	1	1.42E+39	-7.88	42729.6	3.9E+04	0.7
	10	3.56E+24	-3.37	37157.5	4.1E+04	0.6
	100	5.47E+13	-0.07	32728.1	3.9E+04	0.6
R40	0.01	8.30E+65	-16.22	50733.0	9.1E+04	2.4
	0.1	1.30E+58	-13.78	47967.4	1.0E+05	2.5
	1	8.65E+46	-10.18	44661.0	1.5E+05	2.6
	10	1.86E+33	-5.89	39910.9	1.8E+05	2.8
	100	2.69E+19	-1.64	34450.6	1.8E+05	2.8
Eli-s-CY rate rule	0.01	4.96E+60	-14.66	49617.3	3.8E+04	5.1[#]
	0.1	1.25E+54	-12.59	47300.9	4.2E+04	5.1[#]
	1	3.69E+42	-8.92	43659.2	4.8E+04	5.6[#]
	10	9.67E+28	-4.68	38754.7	5.0E+04	6.3[#]
	100	6.64E+16	-0.96	33771.6	5.0E+04	6.5[#]

[#]The uncertainty factor values of the high-pressure limit rule at 800 K for each subclass in our study (The ratios of the largest rate constant of a reaction to the smallest rate constant at 800 K for each subclass).

^a k_{ave} is the average rate constants at 800 K for each reaction subclass.

13. Pressure-dependent rate constants of the β -scission class

Table S19. Calculated rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in each subclass for the reaction center of β -scission occurring on the alkyl side chain at different pressures.

Reaction	Pressure (atm)	Modified Arrhenius parameters			T=800 K	
		A (s ⁻¹)	n	E (cal mol ⁻¹)	k (s ⁻¹)	k/k _{ave} ^e
R1	0.01	1.05E+13	-1.32	8704.0	6.6E+06	0.9
	0.1	6.91E+11	-0.67	9672.0	1.8E+07	1.0
	1	1.33E+17	-1.95	13362.9	6.4E+07	1.0
	10	1.57E+21	-2.89	16764.4	1.7E+08	1.0
	100	1.05E+19	-2.03	17136.2	2.7E+08	1.0
R2	0.01	1.32E+14	-1.62	9326.3	7.3E+06	1.0
	0.1	1.01E+12	-0.71	9881.1	1.7E+07	1.0
	1	5.43E+17	-2.13	13863.5	6.0E+07	0.9
	10	1.46E+21	-2.88	16990.6	1.4E+08	0.9
	100	5.22E+17	-1.66	16715.1	2.2E+08	0.8
R3	0.01	2.14E+13	-1.38	8717.1	8.8E+06	1.2
	0.1	1.50E+13	-1.05	10165.5	2.3E+07	1.2
	1	1.85E+17	-1.97	13346.4	7.9E+07	1.2
	10	5.81E+21	-3.04	16928.6	2.0E+08	1.2
	100	1.12E+20	-2.33	17476.9	3.3E+08	1.2
R4	0.01	2.61E+13	-1.45	9126.7	5.3E+06	0.8
	0.1	2.99E+12	-0.87	10171.5	1.5E+07	0.8
	1	5.38E+17	-2.13	13804.2	5.9E+07	0.9
	10	1.03E+22	-3.13	17309.3	1.6E+08	1.0
	100	4.50E+20	-2.50	18122.5	2.8E+08	1.0
Sci-p-SC rate rule	0.01	2.84E+13	-1.43	8935.6	7.0E+06	1.6[#]
	0.1	2.48E+12	-0.83	9962.3	1.8E+07	1.5[#]
	1	7.91E+16	-1.88	13299.4	6.5E+07	1.3[#]
	10	1.83E+18	-2.02	15376.7	1.7E+08	1.3[#]
	100	9.61E+16	-1.43	16176.7	2.8E+08	1.2[#]
R5	0.01	1.20E+12	-1.05	8021.0	6.6E+06	0.8
	0.1	5.25E+10	-0.36	8887.9	1.8E+07	0.8
	1	8.09E+15	-1.61	12523.7	6.4E+07	0.8
	10	2.61E+19	-2.40	15630.6	1.7E+08	0.9
	100	2.07E+16	-1.27	15499.1	2.7E+08	0.8
R6	0.01	1.59E+12	-1.07	8027.0	7.3E+06	0.9
	0.1	1.98E+23	-4.12	14410.9	1.7E+07	0.8
	1	3.00E+29	-5.83	17350.0	6.0E+07	0.8
	10	8.18E+27	-5.05	18470.0	1.4E+08	0.7
	100	1.90E+26	-4.29	19504.6	2.2E+08	0.6
R7	0.01	4.89E+10	-0.63	6568.8	8.8E+06	1.1
	0.1	1.29E+29	-5.87	16102.1	2.3E+07	1.0
	1	1.39E+13	-0.75	10203.6	7.9E+07	1.0

	10	1.76E+20	-2.60	14783.2	2.0E+08	1.0
	100	1.06E+22	-2.89	17048.1	3.3E+08	0.9
R8	0.01	3.18E+10	-0.58	6573.0	1.0E+07	1.3
	0.1	3.98E+31	-6.63	17189.4	4.6E+07	2.1
	1	1.27E+36	-7.67	20214.6	2.1E+08	2.7
	10	2.07E+20	-2.61	14626.4	5.4E+08	2.8
	100	3.85E+21	-2.73	16734.8	1.2E+09	3.4
	0.01	3.79E+12	-1.17	8270.0	8.2E+06	1.0
R9	0.1	1.63E+12	-0.78	9592.0	2.2E+07	1.0
	1	3.94E+16	-1.79	12833.7	7.6E+07	1.0
	10	7.45E+20	-2.80	16263.4	1.9E+08	1.0
	100	1.28E+19	-2.08	16732.5	3.1E+08	0.9
	0.01	3.75E+16	-2.32	10878.1	7.3E+06	0.9
R10	0.1	3.37E+13	-1.14	11020.0	1.6E+07	0.7
	1	8.32E-07	5.04	3652.2	3.6E+07	0.5
	10	3.22E-02	3.88	6925.3	7.3E+07	0.4
	100	1.14E+10	0.62	13558.2	1.5E+08	0.4
	0.01	7.77E+11	-0.97	7638.7	9.9E+06	1.2
R11	0.1	1.11E+20	-3.12	12739.0	3.1E+07	1.4
	1	2.88E+15	-1.44	11941.3	1.1E+08	1.4
	10	5.85E+20	-2.75	15827.6	3.0E+08	1.5
	100	1.26E+21	-2.63	17382.3	5.4E+08	1.5
	0.01	2.49E+11	-0.83	7205.4	1.1E+07	1.3
R12	0.1	5.79E+18	-2.75	11923.2	3.3E+07	1.5
	1	4.44E+14	-1.22	11286.3	1.1E+08	1.4
	10	3.05E+19	-2.40	14894.5	2.8E+08	1.5
	100	6.82E+18	-2.00	15890.8	4.8E+08	1.4
	0.01	5.54E+13	-1.50	8974.0	8.7E+06	1.1
R13	0.1	5.35E+11	-0.62	9551.2	2.0E+07	0.9
	1	5.47E+14	-1.35	11396.8	5.2E+07	0.7
	10	5.97E+12	-0.51	11987.8	1.1E+08	0.6
	100	4.20E+15	-1.13	14836.4	2.0E+08	0.6
	0.01	1.31E+17	-2.50	11497.7	5.1E+06	0.6
R14	0.1	5.27E+14	-1.50	11938.2	1.3E+07	0.6
	1	5.39E+20	-2.99	16122.9	4.5E+07	0.6
	10	1.50E+24	-3.73	19343.4	1.1E+08	0.6
	100	7.92E+20	-2.55	19239.2	1.8E+08	0.5
	0.01	1.33E+19	-3.07	12643.8	5.6E+06	0.7
R15	0.1	4.36E+15	-1.76	12579.1	1.2E+07	0.5
	1	1.27E+31	-6.16	20578.0	3.9E+07	0.5
	10	4.45E+26	-4.59	19953.4	7.4E+07	0.4
	100	5.60E+24	-3.79	20686.4	1.2E+08	0.3
	0.01	1.74E+16	-2.22	10728.1	7.2E+06	0.9
R16	0.1	1.05E+14	-1.27	11277.5	1.7E+07	0.8

	1	1.45E+20	-2.80	15509.2	6.1E+07	0.8
	10	1.80E+24	-3.75	18994.6	1.5E+08	0.8
	100	6.71E+21	-2.82	19240.7	2.4E+08	0.7
Sci-s-SC rate rule	0.01	1.51E+13	-1.35	8641.5	8.0E+06	2.1[#]
	0.1	5.38E+15	-1.83	11214.1	2.2E+07	3.9[#]
	1	5.75E+16	-1.85	12815.0	7.8E+07	5.8[#]
	10	7.34E+16	-1.63	14130.8	2.0E+08	7.3[#]
	100	2.05E+17	-1.54	15732.5	3.5E+08	9.7[#]
R17	0.01	2.15E+09	-0.27	5881.8	8.7E+06	0.8
	0.1	2.56E+21	-3.59	12500.1	3.6E+07	0.9
	1	1.14E+12	-0.48	9290.1	1.3E+08	0.8
	10	1.09E+17	-1.70	12792.0	4.1E+08	0.8
	100	2.80E+18	-1.88	14828.8	8.5E+08	0.8
R18	0.01	9.22E+09	-0.44	6194.7	1.0E+07	0.9
	0.1	2.38E+10	-0.24	7686.9	3.8E+07	1.0
	1	9.85E+12	-0.73	9659.8	1.7E+08	1.1
	10	6.63E+18	-2.20	13471.3	5.7E+08	1.1
	100	2.47E+20	-2.42	15630.9	1.3E+09	1.2
R19	0.01	2.05E+10	-0.53	6193.6	1.2E+07	1.1
	0.1	6.44E+12	-0.97	8576.4	4.6E+07	1.1
	1	3.15E+12	-0.57	9299.3	2.0E+08	1.2
	10	1.66E+17	-1.71	12611.9	6.6E+08	1.3
	100	1.88E+20	-2.37	15440.6	1.5E+09	1.4
R20	0.01	1.10E+11	-0.73	6718.3	1.2E+07	1.1
	0.1	7.86E+15	-1.89	10240.6	4.0E+07	1.0
	1	1.54E+13	-0.78	10109.3	1.4E+08	0.9
	10	4.07E+18	-2.14	13877.8	4.1E+08	0.8
	100	1.08E+19	-2.05	15401.7	7.5E+08	0.7
Sci-t-SC rate rule	0.01	1.66E+10	-0.51	6269.3	1.1E+07	1.4[#]
	0.1	3.27E+14	-1.49	9473.7	4.0E+07	1.3[#]
	1	4.44E+12	-0.63	9547.6	1.6E+08	1.5[#]
	10	2.28E+17	-1.77	12866.5	5.1E+08	1.6[#]
	100	1.75E+17	-1.50	14152.5	1.1E+09	2.0[#]

[#]The uncertainty factor values of the high-pressure limit rule at 800 K for each subclass in our study (The ratios of the largest rate constant of a reaction to the smallest rate constant at 800 K for each subclass).

^e k_{ave} is the average rate constants at 800 K for each reaction subclass.

Table S20. Calculated rate constants, rate rules, ratios of rate constants of reactions to the average value of the reactions and uncertainty factor values of the rate rule in each subclass for the reaction center of β -scission occurring on the cycle at different pressures.

Reaction	Pressure (atm)	Modified Arrhenius parameters			<i>T=800K</i>	
		A (s ⁻¹)	n	E (cal mol ⁻¹)	k (s ⁻¹)	k/k _{ave} ^e
R21	0.01	3.37E+10	-0.61	6975.4	7.0E+06	0.7

	0.1	1.14E+19	-2.86	12097.7	2.8E+07	0.7
	1	1.48E+14	-1.08	10918.5	1.1E+08	0.7
	10	4.82E+19	-2.43	14746.3	3.9E+08	0.7
	100	8.18E+21	-2.84	17282.0	8.6E+08	0.7
R22	0.01	1.08E+10	-0.47	6522.4	7.7E+06	0.8
	0.1	8.04E+21	-3.72	13071.0	3.3E+07	0.9
	1	1.78E+13	-0.81	10177.7	1.3E+08	0.8
	10	4.14E+18	-2.13	13875.9	4.4E+08	0.8
	100	1.04E+21	-2.59	16449.4	9.8E+08	0.8
R23	0.01	5.65E+09	-0.39	6211.2	8.3E+06	0.8
	0.1	1.18E+26	-4.99	14643.1	4.0E+07	1.0
	1	9.66E+12	-0.74	9748.9	1.5E+08	1.0
	10	8.04E+18	-2.22	13608.5	5.4E+08	1.0
	100	6.15E+20	-2.53	15947.5	1.3E+09	1.0
R24	0.01	7.70E+09	-0.43	6363.0	8.0E+06	0.8
	0.1	2.72E+24	-4.49	14050.1	3.7E+07	1.0
	1	7.22E+12	-0.70	9838.8	1.4E+08	0.9
	10	2.53E+19	-2.37	14008.9	5.0E+08	0.9
	100	1.12E+21	-2.60	16257.0	1.1E+09	0.9
R25	0.01	1.83E+10	-0.52	6578.3	8.9E+06	0.9
	0.1	1.23E+18	-2.56	11333.9	3.6E+07	0.9
	1	1.38E+14	-1.06	10564.8	1.5E+08	1.0
	10	2.27E+20	-2.62	14636.4	5.5E+08	1.0
	100	2.25E+22	-2.95	17099.3	1.3E+09	1.0
R26	0.01	1.57E+10	-0.50	6476.8	9.2E+06	0.9
	0.1	4.59E+15	-1.83	10220.9	3.5E+07	0.9
	1	1.03E+14	-1.03	10470.4	1.4E+08	0.9
	10	9.63E+19	-2.53	14451.6	4.8E+08	0.9
	100	1.54E+24	-3.55	17766.9	1.1E+09	0.9
R27	0.01	5.24E+09	-0.37	5988.3	1.0E+07	1.0
	0.1	2.04E+12	-0.82	8387.6	4.3E+07	1.1
	1	3.00E+12	-0.57	9276.9	1.9E+08	1.2
	10	6.10E+19	-2.48	13674.5	7.2E+08	1.3
	100	1.60E+26	-4.15	17928.4	1.8E+09	1.5
R28	0.01	1.92E+10	-0.53	6583.6	9.0E+06	0.9
	0.1	1.60E+13	-1.09	9249.6	3.2E+07	0.8
	1	2.73E+13	-0.86	10350.5	1.3E+08	0.8
	10	9.54E+18	-2.23	14181.9	4.2E+08	0.8
	100	8.91E+22	-3.19	17389.0	8.9E+08	0.7
R29	0.01	2.46E+10	-0.55	6500.0	1.1E+07	1.1
	0.1	2.78E+11	-0.54	8359.2	3.9E+07	1.0
	1	6.38E+13	-0.94	10316.2	1.8E+08	1.1
	10	7.76E+21	-3.08	15190.2	6.4E+08	1.2
	100	2.34E+27	-4.46	19111.3	1.5E+09	1.2

R30	0.01	1.87E+10	-0.52	6284.0	1.1E+07	1.1
	0.1	1.26E+12	-0.74	8435.9	4.3E+07	1.1
	1	1.17E+13	-0.73	9757.4	1.9E+08	1.2
	10	7.05E+20	-2.78	14449.7	6.6E+08	1.2
	100	7.69E+25	-4.04	18134.9	1.6E+09	1.3
R31	0.01	1.68E+10	-0.50	6184.7	1.2E+07	1.2
	0.1	1.24E+13	-1.05	8758.7	4.5E+07	1.2
	1	5.01E+12	-0.63	9477.3	2.0E+08	1.2
	10	2.33E+20	-2.64	14093.4	7.0E+08	1.3
	100	4.32E+25	-3.97	17864.3	1.7E+09	1.3
R32	0.01	4.62E+10	-0.63	6706.4	1.0E+07	1.0
	0.1	4.05E+27	-5.42	15565.0	4.1E+07	1.1
	1	3.24E+13	-0.87	10413.1	1.4E+08	0.9
	10	3.76E+20	-2.70	14939.0	4.5E+08	0.8
	100	1.30E+23	-3.22	17518.9	9.2E+08	0.7
R33	0.01	2.08E+11	-0.81	7102.8	1.1E+07	1.1
	0.1	8.96E+17	-2.50	11458.0	3.7E+07	1.0
	1	1.50E+14	-1.05	10937.5	1.4E+08	0.9
	10	4.90E+21	-3.01	15720.6	4.6E+08	0.8
	100	3.53E+24	-3.62	18489.9	9.6E+08	0.8
R34	0.01	1.15E+11	-0.75	6414.6	1.4E+07	1.4
	0.1	1.69E+09	0.14	7009.6	5.2E+07	1.4
	1	1.27E+13	-0.73	9479.6	2.4E+08	1.5
	10	6.52E+21	-3.07	14475.9	8.9E+08	1.6
	100	7.19E+27	-4.63	18572.9	2.2E+09	1.8
R35	0.01	1.08E+11	-0.74	6489.4	1.3E+07	1.3
	0.1	4.29E+14	-1.51	9402.1	4.9E+07	1.3
	1	5.89E+12	-0.64	9542.6	2.0E+08	1.3
	10	4.47E+20	-2.72	14284.2	7.0E+08	1.3
	100	1.40E+25	-3.82	17721.0	1.6E+09	1.3
R36	0.01	1.04E+11	-0.73	6341.6	1.4E+07	1.4
	0.1	7.72E+09	-0.06	7202.6	5.6E+07	1.5
	1	4.43E+12	-0.59	9156.6	2.6E+08	1.7
	10	1.99E+21	-2.91	14071.3	1.0E+09	1.9
	100	1.62E+29	-5.03	18941.4	2.7E+09	2.1
R37	0.01	2.27E+10	-0.56	6796.7	7.4E+06	0.7
	0.1	7.81E+18	-2.81	11915.2	2.9E+07	0.8
	1	7.34E+13	-1.00	10665.2	1.1E+08	0.7
	10	1.69E+19	-2.32	14407.3	3.7E+08	0.7
	100	1.63E+23	-3.27	17611.9	7.9E+08	0.6
R38	0.01	1.17E+11	-0.75	7229.6	8.2E+06	0.8
	0.1	1.10E+16	-1.94	10864.2	2.7E+07	0.7
	1	7.05E+14	-1.28	11449.6	9.8E+07	0.6
	10	8.96E+19	-2.53	15167.9	2.8E+08	0.5

	100	6.12E+20	-2.57	16899.0	5.2E+08	0.4
R39	0.01	8.83E+10	-0.71	6965.1	9.9E+06	1.0
	0.1	5.85E+23	-4.26	14051.2	3.6E+07	0.9
	1	1.48E+14	-1.07	10903.2	1.2E+08	0.8
	10	5.27E+19	-2.45	14789.9	3.7E+08	0.7
	100	9.70E+21	-2.91	17187.5	7.1E+08	0.6
R40	0.01	6.58E+11	-0.95	7533.7	1.0E+07	1.0
	0.1	1.72E+20	-3.18	12735.4	3.2E+07	0.8
	1	1.75E+15	-1.38	11735.1	1.1E+08	0.7
	10	2.83E+20	-2.67	15541.4	2.9E+08	0.5
	100	4.22E+20	-2.51	16962.0	5.2E+08	0.4
Sci-s-SC rate rule	0.01	3.10E+10	-0.59	6542.3	1.0E+07	2.0[#]
	0.1	1.07E+16	-1.94	10316.5	3.9E+07	2.1[#]
	1	1.72E+13	-0.79	10001.2	1.6E+08	2.7[#]
	10	1.88E+17	-1.73	12917.2	5.4E+08	3.6[#]
	100	4.58E+19	-2.21	15331.9	1.3E+09	5.2[#]

[#]The uncertainty factor values of the high-pressure limit rule at 800 K for each subclass in our study (The ratios of the largest rate constant of a reaction to the smallest rate constant at 800 K for each subclass).

^e*k_{ave}* is the average rate constants at 800 K for each reaction subclass.

14. Cartesian coordinates for all reactants, transition states and products in the class of concerted elimination

HO₂

O	0.05528900	-0.60941600	0.00000000
H	-0.88463000	-0.87113300	0.00000000
O	0.05528900	0.71830800	0.00000000

Eli-R1

C	-0.61754600	1.09998400	-0.53284900
C	-2.14765800	1.21275300	-0.45373000
C	-2.82400100	-0.16314500	-0.49957000
C	-2.27528100	-1.08600500	0.59632800
C	-0.74692100	-1.20360100	0.52125100
C	-0.05786700	0.17457100	0.56660600
H	-3.90866500	-0.05604000	-0.39759700
H	-2.42526200	1.72038600	0.47950200
H	-2.51343900	1.84383600	-1.26984500
H	-0.33093700	0.70322000	-1.51290600
H	-0.17349000	2.09668300	-0.45560100
H	-2.56048600	-0.68826100	1.57924000
H	-2.72897900	-2.07920800	0.52040300
H	-0.37748500	-1.82734100	1.34304800
H	-0.46431600	-1.71155400	-0.40782200
H	-0.28991600	0.63118900	1.53986900

H	-2.64569000	-0.62134600	-1.48078500
C	1.46888700	0.03375500	0.54059500
C	2.26953900	1.30696300	0.76790800
H	1.77991900	-0.73396900	1.25437700
H	3.33565800	1.08228200	0.71238600
H	2.03496600	2.06818500	0.02179800
H	2.05198100	1.71149000	1.75991100
O	1.81920400	-0.51786900	-0.78595300
O	3.03094900	-1.03103200	-0.80469800

Eli-TS1

C	-2.12705000	1.52276900	-0.03101900
H	-2.97770700	0.56111500	-0.43358200
C	-1.20447200	0.66962600	0.56267100
H	-1.30963800	0.43843600	1.61904800
O	-2.44299500	-1.20347900	0.12975300
O	-3.38657400	-0.63839600	-0.51483300
H	-2.77745900	2.11026600	0.61300700
H	-1.85371000	2.00185400	-0.96967500
C	0.08842900	0.25560500	-0.07839300
C	1.15794000	1.35114100	0.18948100
C	0.59949400	-1.11393300	0.40624300
H	-0.06741100	0.20949900	-1.16485100
C	2.51612900	0.98550700	-0.42739000
H	1.27214100	1.47737700	1.27400600
H	0.80747200	2.31061600	-0.20195400
C	1.95965500	-1.47243400	-0.20839100
H	0.69187900	-1.08697900	1.50054700
H	-0.13655400	-1.88475800	0.17239900
C	3.00947200	-0.38501000	0.05249100
H	3.24906100	1.76205100	-0.18567600
H	2.42277400	0.97446200	-1.52086800
H	2.30177300	-2.43408400	0.18681600
H	1.84156400	-1.60822600	-1.29133300
H	3.95332900	-0.63992600	-0.43985800
H	3.22145000	-0.33633000	1.12845800

Eli-P1

C	-1.36277600	1.35554600	0.26413900
C	0.13798600	1.16573500	-0.00225900
C	0.62758700	-0.21704300	0.45403300
C	-0.21913000	-1.33279700	-0.20301900
C	-1.72007900	-1.14460600	0.05769400
C	-2.19961500	0.24445100	-0.38451200
H	0.33029100	1.27788500	-1.07694900
H	0.71068000	1.95044700	0.50242300

H	-1.54024900	1.35520200	1.34756200
H	-1.68533800	2.33575700	-0.10160200
H	-0.02881800	-1.32460400	-1.28387200
H	0.10883000	-2.31168700	0.16333700
H	-2.28953800	-1.92503000	-0.45756900
H	-1.91864600	-1.27099600	1.12993600
H	-2.11844200	0.32293800	-1.47646800
H	-3.25890200	0.37564900	-0.14072200
H	0.45274200	-0.28843300	1.53980300
C	2.09754000	-0.47282100	0.23464200
H	2.44263600	-1.44230500	0.59400600
C	2.98187600	0.33384500	-0.34623200
H	4.01946600	0.03901800	-0.45727600
H	2.71494900	1.31229300	-0.72952300

Eli-R2

C	-3.41285600	0.33399500	0.16672700
C	-2.34471300	1.35167900	0.58889800
C	-1.03365100	0.66120100	0.99329000
C	-0.49577600	-0.26073000	-0.11740400
C	-1.57717500	-1.27641000	-0.52962400
C	-2.89020200	-0.59398800	-0.93785900
H	-0.28933600	1.41880600	1.25905600
H	-2.14690000	2.03593700	-0.24604100
H	-2.71200700	1.96859500	1.41532400
H	-3.70249800	-0.26802200	1.03800700
H	-4.31776300	0.85084100	-0.16856800
H	-0.27285000	0.36004200	-0.99520200
H	-1.20581600	-1.89795000	-1.35176100
H	-1.76881200	-1.95585500	0.31290300
H	-2.72170000	-0.00871300	-1.85082300
H	-3.64282300	-1.34881000	-1.18755300
H	-1.20458300	0.06083900	1.89801200
C	0.80215200	-0.98130900	0.28770600
H	1.02646400	-1.76937900	-0.44090900
H	0.65882700	-1.48408100	1.25166000
C	2.03540400	-0.09354100	0.39954800
H	1.83619400	0.81827800	0.96592500
C	3.27077400	-0.79601800	0.93916100
H	3.48397400	-1.70293500	0.36720000
H	3.11667700	-1.07350600	1.98505700
O	2.31548800	0.36407000	-0.97988800
O	3.13525900	1.39305100	-1.00460300
H	4.13323600	-0.13032600	0.88099000

Eli-TS2

C	-1.92902300	-0.93304200	0.03967600
C	-3.24042000	-1.00633700	0.49223400
H	-3.41840200	-0.95089300	1.56488400
H	-3.59936800	0.22648200	0.07443100
H	-3.94391700	-1.62434400	-0.06066400
O	-2.19470900	1.13783200	-0.87873900
O	-3.39987200	1.33345400	-0.50927600
H	-1.70417500	-1.29775400	-0.95639500
C	-0.76699900	-0.60774100	0.92917900
H	-0.48350300	-1.54273900	1.43974400
H	-1.10972500	0.06660800	1.72242400
C	0.48659700	-0.02365500	0.25252600
C	1.49949600	0.44024800	1.31586200
C	1.15515900	-1.01587600	-0.71746400
H	0.17576800	0.85685800	-0.32127000
C	2.77486400	1.02258200	0.69177500
H	1.76609400	-0.41432600	1.95402300
H	1.03066100	1.18225000	1.97163400
C	2.42940700	-0.43619500	-1.34918700
H	1.40865600	-1.93364900	-0.16811200
H	0.45859100	-1.30951300	-1.50922700
C	3.42771000	0.03315000	-0.28272800
H	3.48215400	1.30412800	1.47861500
H	2.52326200	1.94578600	0.15448600
H	2.89434200	-1.18176200	-2.00234800
H	2.15860700	0.41256800	-1.98997800
H	4.30318200	0.48853500	-0.75680900
H	3.79367200	-0.83732900	0.27745100

Eli-P2

C	1.55267400	1.50267000	-0.22705700
C	0.15319100	1.03615400	0.19891300
C	-0.14843900	-0.39782200	-0.27080500
C	0.95125300	-1.36042400	0.21178500
C	2.35396300	-0.90122600	-0.21149500
C	2.64270200	0.53364400	0.25105000
H	0.07898700	1.06885900	1.29506500
H	-0.60849500	1.72329900	-0.18106500
H	1.59078700	1.57658400	-1.32180000
H	1.74502100	2.50965400	0.15754000
H	0.90775200	-1.42762100	1.30764200
H	0.75470300	-2.36914300	-0.16861700
H	3.10930600	-1.58768100	0.18502000
H	2.43380500	-0.94998000	-1.30532000

H	2.68910000	0.55640900	1.34772900
H	3.62480600	0.85770000	-0.10861300
H	-0.13094100	-0.40037900	-1.37127300
C	-1.54551700	-0.87981800	0.17550900
H	-1.64301300	-1.93881300	-0.10041000
H	-1.61662700	-0.83401900	1.26876500
C	-2.68490900	-0.11732500	-0.43996300
H	-2.71744500	-0.11819800	-1.52947600
C	-3.63192400	0.53551100	0.22783800
H	-3.64301400	0.56668200	1.31344000
H	-4.43268800	1.05844900	-0.28327600

Eli-R3

C	-3.59852400	-0.86525500	-0.58467200
C	-2.12351900	-1.27756000	-0.48304000
C	-1.17035800	-0.06748000	-0.45801800
C	-1.58092900	0.90525800	0.66462000
C	-3.05545300	1.32364900	0.56418700
C	-3.98996100	0.10754400	0.53582000
H	-1.97312900	-1.86274200	0.43436000
H	-1.85928900	-1.93723400	-1.31709000
H	-3.77340700	-0.38534200	-1.55648000
H	-4.23846200	-1.75329700	-0.55860100
H	-1.40738400	0.41676500	1.63341900
H	-0.94704300	1.79714000	0.65031300
H	-3.31394700	1.98197200	1.39995300
H	-3.20211800	1.91201000	-0.35100100
H	-3.93472200	-0.41253900	1.50094000
H	-5.02938700	0.42932500	0.41428700
H	-1.28298800	0.46241100	-1.41658300
C	0.29169500	-0.53191800	-0.34319500
H	0.47259800	-1.30229600	-1.10365700
H	0.44022500	-1.01917200	0.62685500
C	1.33622100	0.57841800	-0.51606700
H	1.21708000	1.34906800	0.25224500
H	1.19234800	1.07662700	-1.48194000
C	2.77574100	0.08293000	-0.46369800
H	2.92050500	-0.79101200	-1.10449900
C	3.82334900	1.14478100	-0.75647900
H	3.68933700	2.01188200	-0.10447200
H	4.82254300	0.73579100	-0.59967200
H	3.74267100	1.47531600	-1.79514400
O	2.97588900	-0.41118500	0.91617700
O	4.05098600	-1.16217400	1.02382600

Eli-TS3

C	2.64735200	-0.83205900	0.51663000
C	3.79132000	-1.30619800	-0.11208400
H	3.67823300	-1.82441100	-1.06280600
H	4.25164900	-0.09450200	-0.49607300
H	4.61496200	-1.65328200	0.50724600
O	3.15064900	1.35713300	0.12770800
O	4.21552000	1.16914500	-0.54895800
H	2.68820800	-0.60793500	1.57829400
C	1.28558300	-0.84404100	-0.10906500
H	0.89269100	-1.86187100	0.03057000
H	1.38162700	-0.71044700	-1.19290300
C	0.29415400	0.17452000	0.47063600
H	0.21811900	0.02617800	1.55611400
H	0.70218900	1.17800300	0.32448300
C	-1.11631300	0.11446100	-0.14175700
C	-1.85554200	-1.19981400	0.17301000
C	-1.96015100	1.31797800	0.31968400
H	-1.01145100	0.18599400	-1.23520500
C	-3.27668300	-1.22509000	-0.41025800
H	-1.90997900	-1.31940400	1.26419800
H	-1.29263200	-2.05895700	-0.20538700
C	-3.38079500	1.29961700	-0.26220600
H	-2.01936300	1.30840000	1.41684700
H	-1.45282200	2.24924600	0.04583900
C	-4.10169300	-0.01747900	0.05291800
H	-3.77838400	-2.15770600	-0.13211300
H	-3.21528600	-1.22067000	-1.50632800
H	-3.95440000	2.14890500	0.12306300
H	-3.32654500	1.43005400	-1.35084500
H	-5.09105300	-0.03124600	-0.41582000
H	-4.26849600	-0.08794500	1.13577300

Eli-P3

C	-2.24313600	1.44554000	0.21793700
C	-0.79352400	1.11330700	-0.16686800
C	-0.37648300	-0.29975800	0.28339700
C	-1.37856200	-1.34099800	-0.25017400
C	-2.82854600	-1.01567400	0.13532300
C	-3.22762400	0.39608500	-0.31427800
H	-0.68372600	1.18049900	-1.25834500
H	-0.12115300	1.86399000	0.25916800
H	-2.32322100	1.49225300	1.31186900
H	-2.50990000	2.44012400	-0.15435600
H	-1.29642100	-1.38209300	-1.34507900

H	-1.10629700	-2.33657200	0.11765500
H	-3.50738900	-1.75855900	-0.29628100
H	-2.93781900	-1.09116100	1.22509400
H	-3.23930500	0.43566300	-1.41137800
H	-4.24551200	0.62726300	0.01640800
H	-0.42501900	-0.32736500	1.38288300
C	1.06027700	-0.66110800	-0.13078400
H	1.23906300	-1.71505700	0.11676800
H	1.15468300	-0.58553300	-1.22128100
C	2.16277100	0.18973300	0.52844900
H	2.06722900	1.23867400	0.23327900
H	2.02417500	0.15412700	1.61804300
C	3.54519900	-0.29545200	0.19307700
H	3.77417500	-1.31722700	0.49502500
C	4.47718700	0.41033800	-0.44067100
H	5.45589800	-0.00252500	-0.65849500
H	4.29518200	1.43143500	-0.76343400

Eli-R4

C	-0.63918300	0.36132000	0.26074100
C	0.37096500	1.43660200	-0.15320200
C	1.64143700	0.86320900	-0.79726300
C	2.28647200	-0.21133700	0.08724400
C	1.28413600	-1.32516100	0.41639300
C	0.01102200	-0.76786000	1.06844500
H	1.38691300	0.42864200	-1.76942700
H	-0.12164500	2.14035700	-0.83127300
H	0.63488600	1.99949000	0.74974400
H	3.16716300	-0.62991400	-0.40938100
H	1.73759800	-2.06489900	1.08306600
H	-0.72993600	-1.55740800	1.21430300
H	0.24931000	-0.36217100	2.05877600
H	2.34840100	1.67564700	-0.99126500
H	2.64142900	0.24740000	1.01986600
H	1.01535500	-1.85601700	-0.50297400
O	-1.09281200	-0.19857800	-1.05865700
O	-1.94970100	-1.18707200	-0.93850700
C	-1.86722800	0.94316600	0.94920000
H	-1.58947900	1.36811400	1.91668300
H	-2.61300100	0.16339800	1.11065700
H	-2.31261400	1.73293200	0.33918000

Eli-TS4

C	1.43942100	-0.34398100	-1.27748800
C	0.36835100	0.75825600	-1.25707000

C	-0.41227200	0.84468800	0.02905200
C	0.36798800	0.66935900	1.30639300
C	1.43975200	-0.43126700	1.25078100
C	2.30372800	-0.31402000	-0.01086700
H	0.86377400	1.73495400	-1.38159700
H	-0.31776200	0.65672000	-2.10225700
H	0.94769700	-1.31686500	-1.35968200
H	2.06354900	-0.22320500	-2.16826600
H	0.86287900	1.63527500	1.49869300
H	-0.31845500	0.50905900	2.14217400
H	2.06385600	-0.37155600	2.14772000
H	0.94839300	-1.40768700	1.26610200
H	2.87660200	0.62272700	0.02138600
H	3.03691400	-1.12580200	-0.03895600
C	-1.70951400	1.35198300	0.04640600
H	-2.08010000	1.83673800	-0.85517400
H	-2.35167200	0.17611500	0.00528600
H	-2.08047500	1.77286900	0.97935500
O	-1.20773700	-1.37523200	-0.04736500
O	-2.45475300	-1.08844900	-0.03738800

Eli-P4

C	-1.02041500	-1.26825400	-0.30049600
C	0.34520200	-1.26902300	0.41644000
C	1.11528300	0.00002900	0.13174000
C	0.34518800	1.26904400	0.41642000
C	-1.02043400	1.26824700	-0.30049400
C	-1.82234900	-0.00002300	0.02202700
H	0.16915400	-1.34293700	1.49924500
H	0.93227200	-2.14535600	0.12873100
H	-0.85326500	-1.32627500	-1.38278200
H	-1.58888500	-2.16080400	-0.01992200
H	0.16913000	1.34295000	1.49922400
H	0.93224000	2.14540300	0.12873400
H	-1.58892900	2.16077500	-0.01990200
H	-0.85330900	1.32627500	-1.38278200
H	-2.08568500	-0.00002600	1.08795900
H	-2.76687200	-0.00001800	-0.53152500
C	2.35263900	-0.00000600	-0.36305800
H	2.88176800	0.92444000	-0.57124500
H	2.88169200	-0.92450600	-0.57120700

Eli-R5

C	-3.06673700	0.47814900	-0.11574200
C	-1.94573500	1.51942800	-0.00292100

C	-0.71500600	0.95109400	0.71957800
C	-0.19566500	-0.33750900	0.05396600
C	-1.33039500	-1.37208300	-0.05815400
C	-2.56309100	-0.81042700	-0.77982100
H	0.07100600	1.71233200	0.75293300
H	-1.65282800	1.84629600	-1.00874000
H	-2.30594300	2.41103600	0.52017900
H	-3.44435200	0.24365200	0.88811700
H	-3.91124100	0.88962900	-0.67772300
H	0.12610200	-0.08557300	-0.96518100
H	-0.96514900	-2.26435900	-0.57828000
H	-1.61807700	-1.69636300	0.95176100
H	-2.30237700	-0.59943800	-1.82481200
H	-3.35842400	-1.56223900	-0.80367400
H	-0.97929300	0.72830900	1.76297300
C	1.01257400	-0.94265300	0.79117600
H	1.23164900	-1.93415900	0.37934500
H	0.76084200	-1.09690100	1.84778400
C	2.28754800	-0.12007400	0.73882900
H	2.15554700	0.91605600	1.05375400
O	2.74076400	-0.08918200	-0.65290100
O	3.78417400	0.69767000	-0.81003500
H	3.09207100	-0.57172800	1.32359200

Eli-TS5

H	1.91185900	-0.55174000	0.46339700
C	2.10880900	1.36875600	0.00661700
H	2.02143100	1.65022200	-1.03621900
H	2.87887300	1.87761900	0.57162700
O	3.54104500	-0.23160800	-0.53210800
O	2.92894600	-1.20678000	0.00160800
C	1.17103000	0.54782000	0.61989300
H	1.13466800	0.59195800	1.71116300
C	-0.16182800	0.21730200	-0.05164800
C	-0.71913700	-1.14285200	0.41037200
C	-1.20080900	1.33210200	0.19166700
H	0.01867400	0.15569900	-1.13439500
C	-2.07927400	-1.46265200	-0.22564000
H	-0.82542700	-1.12714800	1.50385100
H	-0.00139100	-1.93653700	0.17880500
C	-2.56087000	1.01275100	-0.44527300
H	-1.32857400	1.46302800	1.27485400
H	-0.81379000	2.28246400	-0.19074200
C	-3.10002200	-0.34474300	0.02451600
H	-2.45636300	-2.41541900	0.15957400

H	-1.94834700	-1.59589600	-1.30738700
H	-3.27668100	1.80820900	-0.21383000
H	-2.45371400	0.99965600	-1.53773200
H	-4.04433400	-0.57323200	-0.47993600
H	-3.32419500	-0.29268200	1.09793900

Eli-P5

C	-1.36277600	1.35554600	0.26413900
C	0.13798600	1.16573500	-0.00225900
C	0.62758700	-0.21704300	0.45403300
C	-0.21913000	-1.33279700	-0.20301900
C	-1.72007900	-1.14460600	0.05769400
C	-2.19961500	0.24445100	-0.38451200
H	0.33029100	1.27788500	-1.07694900
H	0.71068000	1.95044700	0.50242300
H	-1.54024900	1.35520200	1.34756200
H	-1.68533800	2.33575700	-0.10160200
H	-0.02881800	-1.32460400	-1.28387200
H	0.10883000	-2.31168700	0.16333700
H	-2.28953800	-1.92503000	-0.45756900
H	-1.91864600	-1.27099600	1.12993600
H	-2.11844200	0.32293800	-1.47646800
H	-3.25890200	0.37564900	-0.14072200
H	0.45274200	-0.28843300	1.53980300
C	2.09754000	-0.47282100	0.23464200
H	2.44263600	-1.44230500	0.59400600
C	2.98187600	0.33384500	-0.34623200
H	4.01946600	0.03901800	-0.45727600
H	2.71494900	1.31229300	-0.72952300

Eli-R6

C	3.22902700	-1.08884800	0.05571300
C	1.73050100	-1.36403800	-0.13066300
C	0.84781900	-0.22963000	0.42279100
C	1.27151600	1.11763400	-0.19329100
C	2.77010800	1.39969000	-0.00697200
C	3.63587300	0.25836900	-0.55588100
H	1.51539400	-1.48840000	-1.20077200
H	1.45981600	-2.31030600	0.35088900
H	3.46477100	-1.08378900	1.12793400
H	3.81647100	-1.90007700	-0.38646800
H	1.03574300	1.10210800	-1.26631600
H	0.68937200	1.93722400	0.23930100
H	3.03427800	2.34466200	-0.49264600
H	2.98208500	1.53081000	1.06220000

H	3.52039400	0.20966800	-1.64642700
H	4.69496200	0.45869700	-0.36387200
H	1.02550300	-0.17170200	1.50786100
C	-0.64183600	-0.54575900	0.20644600
H	-0.83402700	-1.57053700	0.54928900
H	-0.86164000	-0.53643400	-0.86712700
C	-1.61281700	0.39652000	0.93054700
H	-1.48463600	1.42826200	0.58998000
H	-1.39995300	0.39488700	2.00628100
C	-3.07136800	0.01369300	0.75663400
H	-3.26544900	-1.03578000	0.99055000
O	-3.42135500	0.21082500	-0.65062700
O	-4.65397600	-0.17341600	-0.90612700
H	-3.74338600	0.64564100	1.34142600

Eli-TS6

C	-1.85651700	0.32443200	0.89393300
H	-2.00500700	-0.65228400	-0.00724400
C	-3.15284800	0.79246700	0.72013500
H	-3.97471100	0.43094100	1.32440600
H	-3.37021500	1.64034300	0.08137900
O	-3.72079600	-0.60093700	-0.90137700
O	-2.64990200	-1.28076300	-0.93736400
C	-0.65670100	1.13281200	0.40085900
H	-0.98435000	1.76310200	-0.43423200
H	-0.33859200	1.82007000	1.19607600
H	-1.68881800	-0.27545200	1.78879400
C	0.56231800	0.30998700	-0.05436700
C	1.64079000	1.22707000	-0.65975900
C	1.16614100	-0.54074600	1.07914800
H	0.22837200	-0.37593900	-0.84640700
C	2.87954900	0.44796100	-1.12379100
H	1.94130100	1.96682400	0.09510200
H	1.21729700	1.79248300	-1.49730000
C	2.40523700	-1.32452100	0.62061500
H	1.44352800	0.12378100	1.90962100
H	0.42008400	-1.23756100	1.47383300
C	3.46804700	-0.40169700	0.01069800
H	3.63411600	1.13975100	-1.51206100
H	2.60056400	-0.20810800	-1.95837700
H	2.82555400	-1.88430100	1.46241100
H	2.10186900	-2.06845400	-0.12709800
H	4.31586500	-0.98959800	-0.35558600
H	3.86263500	0.26141400	0.79178900

Eli-P6

C	1.55267400	1.50267000	-0.22705700
C	0.15319100	1.03615400	0.19891300
C	-0.14843900	-0.39782200	-0.27080500
C	0.95125300	-1.36042400	0.21178500
C	2.35396300	-0.90122600	-0.21149500
C	2.64270200	0.53364400	0.25105000
H	0.07898700	1.06885900	1.29506500
H	-0.60849500	1.72329900	-0.18106500
H	1.59078700	1.57658400	-1.32180000
H	1.74502100	2.50965400	0.15754000
H	0.90775200	-1.42762100	1.30764200
H	0.75470300	-2.36914300	-0.16861700
H	3.10930600	-1.58768100	0.18502000
H	2.43380500	-0.94998000	-1.30532000
H	2.68910000	0.55640900	1.34772900
H	3.62480600	0.85770000	-0.10861300
H	-0.13094100	-0.40037900	-1.37127300
C	-1.54551700	-0.87981800	0.17550900
H	-1.64301300	-1.93881300	-0.10041000
H	-1.61662700	-0.83401900	1.26876500
C	-2.68490900	-0.11732500	-0.43996300
H	-2.71744500	-0.11819800	-1.52947600
C	-3.63192400	0.53551100	0.22783800
H	-3.64301400	0.56668200	1.31344000
H	-4.43268800	1.05844900	-0.28327600

Eli-R7

C	-3.78959100	-0.59926700	-0.84189200
C	-2.49808600	-1.26875900	-0.35089100
C	-1.33273900	-0.27099300	-0.20886400
C	-1.75302000	0.90730300	0.68924500
C	-3.04317000	1.58315500	0.20040300
C	-4.19207200	0.57634200	0.05783100
H	-2.68313700	-1.73794600	0.62543800
H	-2.21036900	-2.07674800	-1.03272900
H	-3.63934900	-0.23432500	-1.86620400
H	-4.59860500	-1.33545300	-0.89062800
H	-1.90546600	0.53292900	1.71137400
H	-0.95144100	1.64980800	0.74614000
H	-3.32632900	2.38877100	0.88564900
H	-2.85501000	2.05542000	-0.77258100
H	-4.46325500	0.19478900	1.05094300
H	-5.08411700	1.07101400	-0.33997900
H	-1.11866800	0.13220900	-1.21021800

C	-0.06180800	-0.98079900	0.29009000
H	0.10074300	-1.87432400	-0.32594200
H	-0.23444900	-1.34516300	1.31224500
C	1.21423800	-0.13064100	0.26067100
H	1.10417000	0.74117800	0.91482300
H	1.37042800	0.25826800	-0.75121900
C	2.45844800	-0.91601800	0.69487500
H	2.33037000	-1.28236000	1.72024500
H	2.58547300	-1.80252400	0.06364300
C	3.74047000	-0.10483400	0.65859100
H	3.65734200	0.84461000	1.19287200
H	4.59999200	-0.66056100	1.03979800
O	4.02848400	0.21501200	-0.74029700
O	5.07972400	0.99842200	-0.85645600

Eli-TS7

C	2.58682200	-0.78246000	0.56007800
H	2.94874900	0.50117500	0.45355200
C	3.72186100	-1.24150000	-0.09464000
H	4.62267800	-1.50500900	0.44413700
H	3.70774200	-1.49481800	-1.14804400
O	4.57087400	0.74786400	-0.57207000
O	3.69831400	1.45894100	0.01394100
C	1.20710100	-0.85056700	-0.09294500
H	1.31361300	-0.68387800	-1.17153700
H	0.81366200	-1.86565600	0.02542200
H	2.58771800	-0.88200100	1.64741400
C	0.21094300	0.16510500	0.48405300
H	0.12387700	0.01153700	1.56821700
H	0.62266600	1.17306500	0.35244000
C	-1.19561700	0.12586500	-0.13878500
C	-1.94865600	-1.18403800	0.16191700
C	-2.03216300	1.33344500	0.32519900
H	-1.08179800	0.20322300	-1.23090100
C	-3.36600200	-1.19213600	-0.43100900
H	-2.01157200	-1.31032800	1.25190100
H	-1.38942400	-2.04439100	-0.21815600
C	-3.44897400	1.33216200	-0.26631900
H	-2.09891400	1.31692400	1.42189200
H	-1.51533100	2.26264100	0.06120400
C	-4.18364800	0.01942400	0.03481900
H	-3.87790100	-2.12213700	-0.16273100
H	-3.29732500	-1.18094500	-1.52662200
H	-4.01757300	2.18395800	0.12090500
H	-3.38607500	1.46951200	-1.35364300

H	-5.16988400	0.01772700	-0.44066700
H	-4.35841700	-0.05683900	1.11603400

Eli-P7

C	-2.24313600	1.44554000	0.21793700
C	-0.79352400	1.11330700	-0.16686800
C	-0.37648300	-0.29975800	0.28339700
C	-1.37856200	-1.34099800	-0.25017400
C	-2.82854600	-1.01567400	0.13532300
C	-3.22762400	0.39608500	-0.31427800
H	-0.68372600	1.18049900	-1.25834500
H	-0.12115300	1.86399000	0.25916800
H	-2.32322100	1.49225300	1.31186900
H	-2.50990000	2.44012400	-0.15435600
H	-1.29642100	-1.38209300	-1.34507900
H	-1.10629700	-2.33657200	0.11765500
H	-3.50738900	-1.75855900	-0.29628100
H	-2.93781900	-1.09116100	1.22509400
H	-3.23930500	0.43566300	-1.41137800
H	-4.24551200	0.62726300	0.01640800
H	-0.42501900	-0.32736500	1.38288300
C	1.06027700	-0.66110800	-0.13078400
H	1.23906300	-1.71505700	0.11676800
H	1.15468300	-0.58553300	-1.22128100
C	2.16277100	0.18973300	0.52844900
H	2.06722900	1.23867400	0.23327900
H	2.02417500	0.15412700	1.61804300
C	3.54519900	-0.29545200	0.19307700
H	3.77417500	-1.31722700	0.49502500
C	4.47718700	0.41033800	-0.44067100
H	5.45589800	-0.00252500	-0.65849500
H	4.29518200	1.43143500	-0.76343400

Eli-R8

C	-3.41285600	0.33399500	0.16672700
C	-2.34471300	1.35167900	0.58889800
C	-1.03365100	0.66120100	0.99329000
C	-0.49577600	-0.26073000	-0.11740400
C	-1.57717500	-1.27641000	-0.52962400
C	-2.89020200	-0.59398800	-0.93785900
H	-0.28933600	1.41880600	1.25905600
H	-2.14690000	2.03593700	-0.24604100
H	-2.71200700	1.96859500	1.41532400
H	-3.70249800	-0.26802200	1.03800700
H	-4.31776300	0.85084100	-0.16856800

H	-0.27285000	0.36004200	-0.99520200
H	-1.20581600	-1.89795000	-1.35176100
H	-1.76881200	-1.95585500	0.31290300
H	-2.72170000	-0.00871300	-1.85082300
H	-3.64282300	-1.34881000	-1.18755300
H	-1.20458300	0.06083900	1.89801200
C	0.80215200	-0.98130900	0.28770600
H	1.02646400	-1.76937900	-0.44090900
H	0.65882700	-1.48408100	1.25166000
C	2.03540400	-0.09354100	0.39954800
H	1.83619400	0.81827800	0.96592500
C	3.27077400	-0.79601800	0.93916100
H	3.48397400	-1.70293500	0.36720000
H	3.11667700	-1.07350600	1.98505700
O	2.31548800	0.36407000	-0.97988800
O	3.13525900	1.39305100	-1.00460300
H	4.13323600	-0.13032600	0.88099000

Eli-TS8

C	3.12657800	-1.58276200	0.38597400
C	1.95940300	-0.88294100	-0.23035900
H	2.93260300	-2.66309300	0.41943500
H	3.30212700	-1.24547000	1.40996600
C	0.94500000	-0.26298200	0.49387000
H	0.96220400	-0.43123300	1.57454100
H	1.50369900	0.94728100	0.42888800
O	3.06556400	1.03135000	-0.70339000
O	2.34905400	1.81994900	-0.00481900
H	1.82562600	-1.01993400	-1.29951900
H	4.03834800	-1.43168300	-0.19558700
C	-0.44939200	-0.06085400	-0.10049700
C	-1.29933100	-1.34437800	0.00633200
C	-1.18833600	1.12388300	0.55138200
H	-0.32477100	0.17070100	-1.16797800
C	-2.71330800	-1.15810300	-0.56217500
H	-1.36752700	-1.63440200	1.06370100
H	-0.78846300	-2.16596600	-0.50719500
C	-2.60232400	1.31178900	-0.01565900
H	-1.25311400	0.94714000	1.63385900
H	-0.60638500	2.04164800	0.41971900
C	-3.43428100	0.02695400	0.09410300
H	-3.29294700	-2.07752300	-0.43015500
H	-2.64671800	-0.98515900	-1.64414800
H	-3.10506500	2.13552300	0.50117200
H	-2.53057700	1.60589200	-1.07080700

H	-4.41901000	0.17216400	-0.36163000
H	-3.61103000	-0.19990600	1.15358400

Eli-P8

C	1.91360300	1.35313600	-0.22318100
C	0.39994400	1.16865800	-0.03833000
C	-0.07093300	-0.21184800	-0.52224700
C	0.73680800	-1.32957400	0.17903400
C	2.25052000	-1.14803300	0.00026000
C	2.71099000	0.23901300	0.46841900
H	0.15113400	1.28106900	1.02482100
H	-0.14088900	1.95687100	-0.57204800
H	2.14934700	1.35330200	-1.29535200
H	2.21930300	2.33191700	0.16066800
H	0.48789800	-1.32130400	1.24792100
H	0.42562200	-2.30722600	-0.20488000
H	2.78827900	-1.93099800	0.54497500
H	2.50644900	-1.27463000	-1.05982000
H	2.57173600	0.31727300	1.55454800
H	3.78229900	0.36685100	0.28185500
H	0.16691700	-0.28087400	-1.59628100
C	-1.55233200	-0.46393000	-0.38644300
H	-1.88068300	-1.43172700	-0.76901700
C	-2.47033100	0.34151600	0.14591500
H	-2.17092600	1.31177200	0.53565300
C	-3.93308100	0.01859800	0.25632400
H	-4.26550000	0.03613800	1.30053400
H	-4.54359400	0.75529600	-0.27831600
H	-4.15851500	-0.96894200	-0.15377200

Eli-R9

C	-2.60263000	0.77234500	0.85352200
C	-1.10604100	1.06220400	0.67043200
C	-0.28944400	-0.23021200	0.47784400
C	-0.85850000	-1.06688800	-0.68518300
C	-2.35780200	-1.34823200	-0.50402800
C	-3.16179800	-0.05646600	-0.31005000
H	-0.96622300	1.71051700	-0.20166200
H	-0.72122100	1.61771000	1.53231700
H	-2.75459900	0.22418000	1.79260400
H	-3.15323900	1.71325300	0.95051600
H	-0.69974300	-0.52292900	-1.62311200
H	-0.31884800	-2.01410700	-0.77543600
H	-2.73540200	-1.90555400	-1.36718900
H	-2.50062400	-1.99673900	0.37045100

H	-3.11765500	0.53855500	-1.23114900
H	-4.21767100	-0.28921100	-0.13859400
H	-0.38596300	-0.82335500	1.39963600
C	1.21443000	0.06418400	0.34757500
H	1.52489800	0.74939100	1.14039900
C	2.12884400	-1.15789900	0.30093200
H	1.94113800	-1.70927300	-0.62483900
H	1.84147600	-1.82171800	1.12360600
C	3.61485900	-0.80294400	0.40305800
H	3.91257000	-0.13018300	-0.40417700
H	3.84001300	-0.30742500	1.35212300
O	1.45411800	0.80796500	-0.90602300
O	1.64389800	2.09832500	-0.71385200
H	4.23545000	-1.69997700	0.33888600

Eli-TS9

C	2.03603800	-0.91409300	-0.31404900
H	2.58870600	0.22761600	-0.68723900
C	1.00660300	-0.31529600	0.40871400
H	1.13078000	-0.18055300	1.48059400
O	1.84965500	1.80505800	0.15194500
O	2.79475400	1.50617200	-0.64831000
C	-0.37269300	-0.08300000	-0.13641700
C	-1.20972400	-1.38292600	0.01914800
C	-1.10434100	1.09879200	0.52780400
H	-0.28429600	0.12008200	-1.21256100
C	-2.63739600	-1.20997700	-0.51962600
H	-1.25145200	-1.65319600	1.08235700
H	-0.70741700	-2.20821500	-0.49432100
C	-2.53229600	1.26613000	-0.00899000
H	-1.14212500	0.92442200	1.61173400
H	-0.53263600	2.01581400	0.37694200
C	-3.35319800	-0.02178300	0.13543300
H	-3.20432200	-2.13293100	-0.36023200
H	-2.59475700	-1.05346800	-1.60503400
H	-3.02766800	2.09281600	0.50994400
H	-2.48771900	1.54945200	-1.06862400
H	-4.34802500	0.10857900	-0.30233000
H	-3.50648900	-0.23556900	1.20118800
H	1.75322400	-1.32179900	-1.28729800
C	3.17474500	-1.64502600	0.38919600
H	4.07288500	-1.67664900	-0.23284000
H	3.43868700	-1.14545000	1.32509800
H	2.90094100	-2.67771700	0.62626100

Eli-P9

C	1.91360300	1.35313600	-0.22318100
C	0.39994400	1.16865800	-0.03833000
C	-0.07093300	-0.21184800	-0.52224700
C	0.73680800	-1.32957400	0.17903400
C	2.25052000	-1.14803300	0.00026000
C	2.71099000	0.23901300	0.46841900
H	0.15113400	1.28106900	1.02482100
H	-0.14088900	1.95687100	-0.57204800
H	2.14934700	1.35330200	-1.29535200
H	2.21930300	2.33191700	0.16066800
H	0.48789800	-1.32130400	1.24792100
H	0.42562200	-2.30722600	-0.20488000
H	2.78827900	-1.93099800	0.54497500
H	2.50644900	-1.27463000	-1.05982000
H	2.57173600	0.31727300	1.55454800
H	3.78229900	0.36685100	0.28185500
H	0.16691700	-0.28087400	-1.59628100
C	-1.55233200	-0.46393000	-0.38644300
H	-1.88068300	-1.43172700	-0.76901700
C	-2.47033100	0.34151600	0.14591500
H	-2.17092600	1.31177200	0.53565300
C	-3.93308100	0.01859800	0.25632400
H	-4.26550000	0.03613800	1.30053400
H	-4.54359400	0.75529600	-0.27831600
H	-4.15851500	-0.96894200	-0.15377200

Eli-R10

C	-3.59852400	-0.86525500	-0.58467200
C	-2.12351900	-1.27756000	-0.48304000
C	-1.17035800	-0.06748000	-0.45801800
C	-1.58092900	0.90525800	0.66462000
C	-3.05545300	1.32364900	0.56418700
C	-3.98996100	0.10754400	0.53582000
H	-1.97312900	-1.86274200	0.43436000
H	-1.85928900	-1.93723400	-1.31709000
H	-3.77340700	-0.38534200	-1.55648000
H	-4.23846200	-1.75329700	-0.55860100
H	-1.40738400	0.41676500	1.63341900
H	-0.94704300	1.79714000	0.65031300
H	-3.31394700	1.98197200	1.39995300
H	-3.20211800	1.91201000	-0.35100100
H	-3.93472200	-0.41253900	1.50094000
H	-5.02938700	0.42932500	0.41428700
H	-1.28298800	0.46241100	-1.41658300

C	0.29169500	-0.53191800	-0.34319500
H	0.47259800	-1.30229600	-1.10365700
H	0.44022500	-1.01917200	0.62685500
C	1.33622100	0.57841800	-0.51606700
H	1.21708000	1.34906800	0.25224500
H	1.19234800	1.07662700	-1.48194000
C	2.77574100	0.08293000	-0.46369800
H	2.92050500	-0.79101200	-1.10449900
C	3.82334900	1.14478100	-0.75647900
H	3.68933700	2.01188200	-0.10447200
H	4.82254300	0.73579100	-0.59967200
H	3.74267100	1.47531600	-1.79514400
O	2.97588900	-0.41118500	0.91617700
O	4.05098600	-1.16217400	1.02382600

Eli-TS10

C	4.05534000	-0.92317100	0.73106400
C	2.83292800	-0.81820000	-0.12148900
H	4.29204700	-1.98095600	0.90731100
H	3.90817300	-0.44968200	1.70439500
C	1.55092900	-0.60254800	0.37308000
H	1.45209900	-0.64887700	1.46075100
H	1.60799200	0.72672600	0.18600000
O	3.18483700	1.32569000	-0.74672300
O	2.11051800	1.81488800	-0.26586700
H	2.94900200	-1.09879100	-1.16446100
H	4.92292300	-0.47013200	0.24694200
C	0.31849000	-1.06062500	-0.41071900
H	0.39969200	-0.71330000	-1.44858700
H	0.31446800	-2.15667700	-0.45553600
C	-1.03131800	-0.60619800	0.17127200
C	-1.21946300	0.92241300	0.15416800
C	-2.19451400	-1.29407200	-0.56813600
H	-1.06825400	-0.93469100	1.22145700
C	-2.59377000	1.34747800	0.69303400
H	-1.10543300	1.28120600	-0.87773500
H	-0.43418300	1.41217600	0.73700900
C	-3.56815200	-0.87347800	-0.02796500
H	-2.13352900	-1.03968400	-1.63528000
H	-2.08201800	-2.38212600	-0.50278800
C	-3.73941000	0.65114000	-0.05234700
H	-2.69961400	2.43483100	0.62351700
H	-2.65530900	1.09781300	1.76040300
H	-4.36198000	-1.35535300	-0.60806500
H	-3.67634800	-1.23202600	1.00401800

H	-4.70342400	0.93237500	0.38393000
H	-3.75549200	0.99611000	-1.09433500
Eli-P10			
C	-2.10950200	1.51949900	0.19155000
C	-0.80887600	1.05068600	-0.47823600
C	-0.34279200	-0.31966900	0.04682800
C	-1.47555100	-1.35371000	-0.08916500
C	-2.77662200	-0.89143100	0.58207900
C	-3.22712300	0.47721200	0.05412300
H	-0.96675900	0.97781100	-1.56364800
H	-0.02685700	1.80073500	-0.32645000
H	-1.91872000	1.70476600	1.25661800
H	-2.42712200	2.47586000	-0.23695300
H	-1.66390300	-1.53436600	-1.15667400
H	-1.15382900	-2.31169200	0.33455700
H	-3.56413800	-1.63661600	0.42811400
H	-2.61902300	-0.82526800	1.66645500
H	-3.50393100	0.38235100	-1.00409600
H	-4.12613700	0.81149600	0.58237200
H	-0.11462100	-0.20917000	1.11659000
C	0.94237400	-0.82388800	-0.64895500
H	1.15665900	-1.83867300	-0.29519700
H	0.73740000	-0.90672200	-1.72589100
C	2.15878900	0.03472900	-0.43631200
H	2.13729500	1.03222200	-0.87344500
C	3.24500900	-0.33618600	0.24028000
H	3.27373600	-1.33652800	0.67255900
C	4.46279700	0.51271700	0.46247000
H	5.35833000	0.03919800	0.04386400
H	4.35432100	1.49769700	0.00177300
H	4.65628400	0.65715400	1.53148200

Eli-R11

C	3.74288000	0.29895300	-0.36767000
C	2.63942200	1.29038000	-0.75992300
C	1.30390200	0.57935400	-1.02443300
C	0.85967800	-0.28496500	0.17076100
C	1.97706700	-1.27239700	0.55587600
C	3.31316200	-0.56631100	0.82419600
H	0.53802500	1.32285400	-1.26671800
H	2.50367200	2.01964100	0.04890400
H	2.93869700	1.86187200	-1.64450700
H	3.96604800	-0.35087700	-1.22411500
H	4.66863300	0.83468700	-0.13423400

H	0.69794600	0.38145500	1.02824400
H	1.67276800	-1.84673100	1.43785900
H	2.10864400	-1.99946200	-0.25800900
H	3.21143800	0.06910600	1.71324400
H	4.08709600	-1.30483500	1.05704000
H	1.40636200	-0.06536500	-1.90884900
C	-0.45713300	-1.03524200	-0.09319600
H	-0.62285300	-1.76888100	0.70465200
H	-0.37461700	-1.60672800	-1.02570900
C	-1.70358800	-0.15979600	-0.18615400
H	-1.56739000	0.68821600	-0.85922100
C	-2.97472000	-0.93338100	-0.53520500
H	-3.12316500	-1.71324100	0.21987200
H	-2.79041800	-1.45022300	-1.48378000
C	-4.22881800	-0.06366100	-0.65112000
H	-4.11785500	0.69125000	-1.43460300
H	-5.09940400	-0.67683000	-0.89689800
H	-4.43827200	0.45843800	0.28435500
O	-1.88618200	0.44113200	1.15128400
O	-2.17587800	1.72612300	1.10417500

Eli-TS11

C	-2.94125400	-0.43545200	0.63306500
H	-3.10870600	0.77443100	0.11399400
C	-1.63481800	-0.57277300	0.17157200
H	-1.47047700	-1.09690300	-0.76436200
O	-1.68124700	1.36669700	-1.04664800
O	-2.81913100	1.77896900	-0.64645500
H	-3.04459600	-0.20756200	1.69642900
C	-4.08166300	-1.24723200	0.02970400
H	-5.04497600	-0.75234700	0.17689200
H	-3.93984800	-1.38048700	-1.04614600
H	-4.14860800	-2.24061800	0.48409800
C	-0.43001900	-0.25550400	1.00484400
H	-0.68266800	0.56024100	1.69214200
H	-0.24183200	-1.13212200	1.64681400
C	0.87064100	0.08217600	0.25340300
C	1.94702200	0.56712400	1.24231300
C	1.40532300	-1.10462000	-0.57014700
H	0.65344400	0.90528000	-0.43685500
C	3.27152300	0.90464300	0.54401300
H	2.12311200	-0.21683300	1.99251300
H	1.57822800	1.44228700	1.78865600
C	2.72873700	-0.77079100	-1.27473800
H	1.55853600	-1.96214600	0.10053600

H	0.66717000	-1.41970000	-1.31449800
C	3.79063700	-0.27963500	-0.28219000
H	4.01865500	1.20820300	1.28449400
H	3.12006800	1.76735400	-0.11712400
H	3.09347000	-1.64841800	-1.81826800
H	2.54885100	0.00819200	-2.02641300
H	4.70630900	-0.00042600	-0.81334200
H	4.06010800	-1.10137900	0.39422300

Eli-P11

C	-2.10950200	1.51949900	0.19155000
C	-0.80887600	1.05068600	-0.47823600
C	-0.34279200	-0.31966900	0.04682800
C	-1.47555100	-1.35371000	-0.08916500
C	-2.77662200	-0.89143100	0.58207900
C	-3.22712300	0.47721200	0.05412300
H	-0.96675900	0.97781100	-1.56364800
H	-0.02685700	1.80073500	-0.32645000
H	-1.91872000	1.70476600	1.25661800
H	-2.42712200	2.47586000	-0.23695300
H	-1.66390300	-1.53436600	-1.15667400
H	-1.15382900	-2.31169200	0.33455700
H	-3.56413800	-1.63661600	0.42811400
H	-2.61902300	-0.82526800	1.66645500
H	-3.50393100	0.38235100	-1.00409600
H	-4.12613700	0.81149600	0.58237200
H	-0.11462100	-0.20917000	1.11659000
C	0.94237400	-0.82388800	-0.64895500
H	1.15665900	-1.83867300	-0.29519700
H	0.73740000	-0.90672200	-1.72589100
C	2.15878900	0.03472900	-0.43631200
H	2.13729500	1.03222200	-0.87344500
C	3.24500900	-0.33618600	0.24028000
H	3.27373600	-1.33652800	0.67255900
C	4.46279700	0.51271700	0.46247000
H	5.35833000	0.03919800	0.04386400
H	4.35432100	1.49769700	0.00177300
H	4.65628400	0.65715400	1.53148200

Eli-R12

C	3.74288000	0.29895300	-0.36767000
C	2.63942200	1.29038000	-0.75992300
C	1.30390200	0.57935400	-1.02443300
C	0.85967800	-0.28496500	0.17076100
C	1.97706700	-1.27239700	0.55587600

C	3.31316200	-0.56631100	0.82419600
H	0.53802500	1.32285400	-1.26671800
H	2.50367200	2.01964100	0.04890400
H	2.93869700	1.86187200	-1.64450700
H	3.96604800	-0.35087700	-1.22411500
H	4.66863300	0.83468700	-0.13423400
H	0.69794600	0.38145500	1.02824400
H	1.67276800	-1.84673100	1.43785900
H	2.10864400	-1.99946200	-0.25800900
H	3.21143800	0.06910600	1.71324400
H	4.08709600	-1.30483500	1.05704000
H	1.40636200	-0.06536500	-1.90884900
C	-0.45713300	-1.03524200	-0.09319600
H	-0.62285300	-1.76888100	0.70465200
H	-0.37461700	-1.60672800	-1.02570900
C	-1.70358800	-0.15979600	-0.18615400
H	-1.56739000	0.68821600	-0.85922100
C	-2.97472000	-0.93338100	-0.53520500
H	-3.12316500	-1.71324100	0.21987200
H	-2.79041800	-1.45022300	-1.48378000
C	-4.22881800	-0.06366100	-0.65112000
H	-4.11785500	0.69125000	-1.43460300
H	-5.09940400	-0.67683000	-0.89689800
H	-4.43827200	0.45843800	0.28435500
O	-1.88618200	0.44113200	1.15128400
O	-2.17587800	1.72612300	1.10417500

Eli-TS12

C	2.86744400	-1.11659500	0.58132800
C	1.65961300	-0.55331300	-0.10552300
H	2.61538800	-2.14933200	0.86836500
H	3.03263700	-0.58302400	1.52353900
C	0.55969500	-0.02016500	0.55964000
H	0.55924800	-0.13861200	1.64733500
H	0.97795800	1.24032000	0.45820700
O	2.55040000	1.48808900	-0.63748700
O	1.71900900	2.19836400	0.01791100
H	1.58018900	-0.74369700	-1.17306400
C	-0.82907500	-0.00992300	-0.08174400
C	-1.52222800	-1.38004000	0.06693300
C	-1.72219300	1.10750300	0.49122400
H	-0.69752900	0.18505700	-1.15565700
C	-2.93130500	-1.39152100	-0.54266700
H	-1.58636100	-1.62768000	1.13528400
H	-0.90175000	-2.15600500	-0.39401300

C	-3.13188200	1.09681100	-0.11747000
H	-1.79712400	0.97686800	1.57963300
H	-1.24936700	2.08093800	0.32625000
C	-3.80627400	-0.27246700	0.03794700
H	-3.40170100	-2.36663500	-0.37905600
H	-2.85508400	-1.26202500	-1.63012900
H	-3.74410800	1.87737500	0.34537000
H	-3.06476500	1.34683500	-1.18419000
H	-4.78821200	-0.26897900	-0.44606800
H	-3.98427000	-0.46896600	1.10327400
C	4.14575200	-1.13036800	-0.26243800
H	4.95951000	-1.62012700	0.27807600
H	3.99252500	-1.67685300	-1.19784900
H	4.46026600	-0.11660600	-0.51206900

Eli-P12

C	2.29218500	1.45588200	-0.18816500
C	0.80994300	1.12680700	0.04404500
C	0.44323600	-0.26589600	-0.49198900
C	1.37509400	-1.33838800	0.12054100
C	2.85794000	-1.01262200	-0.10588300
C	3.21343000	0.38658300	0.41473100
H	0.59732100	1.16521900	1.12021100
H	0.17927200	1.88734900	-0.42755600
H	2.48153800	1.52864200	-1.26705100
H	2.52619500	2.43878000	0.23367600
H	1.17169900	-1.40318000	1.19708300
H	1.13546000	-2.32080900	-0.30069200
H	3.48525700	-1.76880100	0.37742600
H	3.07896900	-1.06515300	-1.17997300
H	3.11394300	0.40015100	1.50794800
H	4.26039600	0.61936600	0.19447000
H	0.64114000	-0.26213400	-1.57625700
C	-1.00317400	-0.65682000	-0.31472200
H	-1.26082700	-1.62939600	-0.73735700
C	-1.96563500	0.03209100	0.29761400
H	-1.74011000	1.00633700	0.72781300
C	-3.39317600	-0.42162600	0.43816300
H	-3.64620800	-0.49424800	1.50405300
H	-3.50040400	-1.42963200	0.02418800
C	-4.39331200	0.52872400	-0.24046500
H	-5.42229800	0.18879000	-0.09335800
H	-4.31537300	1.54095400	0.16790800
H	-4.20516500	0.58936300	-1.31575300

Eli-R13

C	-3.08916100	0.40893300	0.91446500
C	-1.66632200	0.95162900	0.72015100
C	-0.65098500	-0.17729300	0.45762700
C	-1.10052800	-1.05135800	-0.72988300
C	-2.52830600	-1.58488200	-0.53756700
C	-3.52993200	-0.45267000	-0.27532300
H	-1.65639100	1.64839400	-0.12524900
H	-1.35946900	1.52900300	1.59885000
H	-3.12726700	-0.19444800	1.83099200
H	-3.78578100	1.24028600	1.06122200
H	-1.05401900	-0.45325100	-1.64699300
H	-0.41259400	-1.89091500	-0.86674000
H	-2.82779600	-2.16265700	-1.41779200
H	-2.54257800	-2.28197600	0.31067400
H	-3.60430400	0.17815800	-1.17023700
H	-4.52902600	-0.86380200	-0.09857400
H	-0.62398000	-0.81403500	1.35462900
C	0.77882900	0.37082200	0.31331500
H	0.98867100	1.06712600	1.12903600
C	1.88385800	-0.67568000	0.19712000
H	1.78502500	-1.19681800	-0.76064100
H	1.72321500	-1.42738400	0.97902600
C	3.29583400	-0.08981800	0.32004100
H	3.42518700	0.69274100	-0.43390800
H	3.39837600	0.40201700	1.29460900
O	0.85978500	1.19361800	-0.91137200
O	0.82215300	2.48858800	-0.66765900
C	4.39287000	-1.14532400	0.16001100
H	5.38659900	-0.70046700	0.25577900
H	4.30536800	-1.92915900	0.91902900
H	4.33832300	-1.62661800	-0.82121100

Eli-TS13

C	1.74207600	-0.54691300	-0.18914000
H	2.15874800	0.64822000	-0.59125100
C	0.61897700	-0.06064800	0.47471000
H	0.68660300	0.13107200	1.54300600
O	1.18977600	2.14414700	0.15793700
O	2.19425000	1.93968000	-0.59920300
C	-0.76027300	-0.03420300	-0.11797400
C	-1.42196400	-1.42748600	0.07101900
C	-1.66129300	1.06460300	0.47691100
H	-0.66489600	0.13693200	-1.19903700
C	-2.84378200	-1.46693500	-0.50788100

H	-1.45831100	-1.66063200	1.14318900
H	-0.80022600	-2.19705900	-0.39607500
C	-3.08331300	1.01876200	-0.09868300
H	-1.70652900	0.92982600	1.56624100
H	-1.21122600	2.04282500	0.30030900
C	-3.72903000	-0.36113000	0.08089500
H	-3.28807900	-2.45058600	-0.32421400
H	-2.79124800	-1.34706300	-1.59758100
H	-3.69841100	1.79078500	0.37429300
H	-3.04753500	1.26472800	-1.16791600
H	-4.71974100	-0.38217200	-0.38423900
H	-3.88229000	-0.55268900	1.15091200
H	1.55185700	-1.02269800	-1.15515800
C	2.94138400	-1.10570600	0.57698100
H	3.07480700	-0.52721200	1.49766800
H	2.72234400	-2.13363300	0.88940300
C	4.24221500	-1.09208500	-0.23252400
H	5.06572600	-1.52862400	0.33850800
H	4.13793200	-1.66925600	-1.15666800
H	4.52829400	-0.07293700	-0.50714400

Eli-P13

C	2.29218500	1.45588200	-0.18816500
C	0.80994300	1.12680700	0.04404500
C	0.44323600	-0.26589600	-0.49198900
C	1.37509400	-1.33838800	0.12054100
C	2.85794000	-1.01262200	-0.10588300
C	3.21343000	0.38658300	0.41473100
H	0.59732100	1.16521900	1.12021100
H	0.17927200	1.88734900	-0.42755600
H	2.48153800	1.52864200	-1.26705100
H	2.52619500	2.43878000	0.23367600
H	1.17169900	-1.40318000	1.19708300
H	1.13546000	-2.32080900	-0.30069200
H	3.48525700	-1.76880100	0.37742600
H	3.07896900	-1.06515300	-1.17997300
H	3.11394300	0.40015100	1.50794800
H	4.26039600	0.61936600	0.19447000
H	0.64114000	-0.26213400	-1.57625700
C	-1.00317400	-0.65682000	-0.31472200
H	-1.26082700	-1.62939600	-0.73735700
C	-1.96563500	0.03209100	0.29761400
H	-1.74011000	1.00633700	0.72781300
C	-3.39317600	-0.42162600	0.43816300
H	-3.64620800	-0.49424800	1.50405300

H	-3.50040400	-1.42963200	0.02418800
C	-4.39331200	0.52872400	-0.24046500
H	-5.42229800	0.18879000	-0.09335800
H	-4.31537300	1.54095400	0.16790800
H	-4.20516500	0.58936300	-1.31575300

Eli-R14

C	0.39835900	-0.03582800	0.22763600
C	-0.23373100	-1.35859200	-0.21932900
C	-1.64089600	-1.19384400	-0.81398400
C	-2.56861300	-0.41175200	0.12318400
C	-1.95950800	0.94947400	0.48040600
C	-0.55864400	0.79936500	1.08849200
H	-1.56620400	-0.66819800	-1.77166700
H	0.42391600	-1.84768400	-0.94195100
H	-0.27787400	-2.01056900	0.66126100
H	-3.54976700	-0.27800100	-0.34268500
H	-2.60330800	1.48567100	1.18429500
H	-0.10227700	1.77766100	1.25662000
H	-0.63100400	0.30567500	2.06471000
H	-2.05793500	-2.18220500	-1.03065900
H	-2.73460200	-0.99018000	1.04189800
H	-1.89821300	1.56889700	-0.42075300
O	0.61491800	0.68890700	-1.07203400
O	1.11148600	1.89625700	-0.92075600
C	1.76485900	-0.19375000	0.90895000
H	1.59347100	-0.67586400	1.87732000
H	2.13392800	0.81350200	1.12102500
C	2.82304700	-0.96958700	0.11817300
H	2.98222900	-0.52617400	-0.86714400
H	2.54989600	-2.01819600	-0.02150300
H	3.77727200	-0.94855200	0.65038800

Eli-TS14

C	1.98501900	0.66098300	0.86943600
C	0.66345700	0.13736400	1.45010200
C	-0.31416400	-0.38801600	0.42701800
C	0.26595800	-1.18762000	-0.70975800
C	1.60418000	-0.65569800	-1.24904200
C	2.59288600	-0.33744700	-0.12189400
H	0.88568500	-0.70492600	2.12596000
H	0.17649400	0.89796700	2.06667000
H	1.80140900	1.61174600	0.36184900
H	2.68376400	0.86224200	1.68736100
H	0.41796200	-2.20905300	-0.32156800

H	-0.45971700	-1.28317900	-1.51973000
H	2.03101900	-1.39312100	-1.93595200
H	1.41493200	0.25067100	-1.83057800
H	2.86298100	-1.26266900	0.40530900
H	3.52081900	0.06419600	-0.54040000
C	-1.68343900	-0.37263300	0.71667300
H	-1.91845700	-0.12177900	1.75359200
H	-1.92322400	0.80277300	0.15433200
O	-0.45552800	1.63323000	-0.79043500
O	-1.69295000	1.85503100	-0.55322400
C	-2.68660200	-1.31491700	0.06093600
H	-3.70642500	-1.01497600	0.31249500
H	-2.60892400	-1.30935900	-1.02853800
H	-2.55425500	-2.34871800	0.39763500

Eli-P14

C	1.14849100	-1.42231300	0.26711600
C	-0.09863300	-1.08676400	-0.57769700
C	-0.60409000	0.30775700	-0.28166800
C	0.46270700	1.37266800	-0.42439100
C	1.70886600	1.04519400	0.42177400
C	2.24287400	-0.35868800	0.10779100
H	0.17824600	-1.14195300	-1.64050800
H	-0.87127800	-1.84057000	-0.41809300
H	0.85548700	-1.48646700	1.32199300
H	1.53233100	-2.40828300	-0.01478200
H	0.76805400	1.43543900	-1.47920200
H	0.06107500	2.35263900	-0.15188600
H	2.48659000	1.79627600	0.24843600
H	1.44249000	1.10370300	1.48409100
H	2.61840700	-0.37944300	-0.92386000
H	3.09528300	-0.59368200	0.75354000
C	-1.84803300	0.61828000	0.10034700
H	-2.05816600	1.67047300	0.29031800
C	-3.02277100	-0.29702900	0.29781300
H	-3.84859600	-0.01715100	-0.36665600
H	-2.78796400	-1.34517500	0.10914400
H	-3.40842600	-0.22044000	1.32095500

Eli-R15

C	0.00575300	0.03836300	0.14502500
C	-0.51602300	-1.31220400	-0.35908400
C	-1.98166700	-1.26672700	-0.81876100
C	-2.90048900	-0.67167400	0.25471100
C	-2.41238700	0.71855500	0.67967700

C	-0.95359200	0.68404300	1.15440100
H	-2.05125900	-0.66347200	-1.72978400
H	0.12066100	-1.66511900	-1.17393400
H	-0.40615100	-2.02989300	0.46264800
H	-3.92780500	-0.61513800	-0.11820900
H	-3.04296000	1.11910500	1.47928300
H	-0.59305400	1.69176800	1.37357000
H	-0.88259800	0.10679300	2.08361800
H	-2.30679500	-2.27701600	-1.08579400
H	-2.92179400	-1.33575700	1.12922600
H	-2.50216400	1.41016900	-0.16469000
O	0.01231000	0.88110600	-1.10028100
O	0.38020300	2.12458000	-0.88898100
C	1.43895000	-0.00490800	0.69162900
H	1.41659200	-0.57173200	1.62966200
H	1.71252600	1.02199400	0.95381500
C	2.50946500	-0.58906500	-0.23895400
H	2.47336700	-0.07061300	-1.20174900
H	2.29819600	-1.64331500	-0.44426400
C	3.91585000	-0.46646400	0.35622000
H	4.18028700	0.58046700	0.53241100
H	3.99001100	-0.99245100	1.31339500
H	4.66766700	-0.89079800	-0.31428800

Eli-TS15

C	2.40628000	0.42262700	0.97739900
C	1.01048400	0.00504200	1.46363400
C	0.03218200	-0.33422400	0.36573600
C	0.57907700	-1.11678400	-0.79941900
C	1.98897700	-0.69656300	-1.24633700
C	2.95273600	-0.56260000	-0.06206500
H	1.11044000	-0.90509600	2.07786200
H	0.57983300	0.76559500	2.12103200
H	2.34814500	1.42211000	0.53790900
H	3.08224800	0.48775000	1.83570600
H	0.60513500	-2.17161900	-0.47666700
H	-0.11298700	-1.08224500	-1.64293600
H	2.36809400	-1.42766200	-1.96719600
H	1.92182400	0.26185100	-1.76822200
H	3.10177800	-1.54534100	0.40569100
H	3.93520000	-0.23333200	-0.41399600
C	-1.33954700	-0.18706200	0.59788300
H	-1.59893000	0.02307900	1.63933500
H	-1.42507800	1.04175800	0.10268500
O	0.16616200	1.76518600	-0.72133100

O	-1.05270900	2.10129300	-0.52502300
C	-2.41293300	-0.97117700	-0.15634900
H	-2.25032500	-0.89113500	-1.23555100
H	-2.33113900	-2.03850900	0.08534300
C	-3.82796800	-0.48553100	0.17422800
H	-3.95899900	0.56550900	-0.09857400
H	-4.58053400	-1.06724700	-0.36396900
H	-4.03805800	-0.57967600	1.24411800

Eli-P15

C	-1.67766000	-1.41764600	-0.23126000
C	-0.37187200	-1.09174500	0.52393700
C	0.12468300	0.29700600	0.18726300
C	-0.91946200	1.37145400	0.40637300
C	-2.22515200	1.05530200	-0.34970100
C	-2.74870800	-0.34375900	0.00161100
H	-0.57597800	-1.13889300	1.60340900
H	0.38096500	-1.85360600	0.31561600
H	-1.45939000	-1.48661800	-1.30377600
H	-2.04982600	-2.39946700	0.07933100
H	-1.14843500	1.43555800	1.48020000
H	-0.52971300	2.34804300	0.10610300
H	-2.98188600	1.81338000	-0.12238100
H	-2.03364100	1.11174600	-1.42813500
H	-3.05269900	-0.36071300	1.05661800
H	-3.64555300	-0.57123500	-0.58381400
C	1.33805000	0.59492100	-0.29237600
H	1.54451700	1.64625600	-0.49697100
C	2.49473600	-0.32585400	-0.57146300
H	2.21218900	-1.37100400	-0.42527900
H	2.77604900	-0.23034600	-1.62841200
C	3.72608800	-0.00383200	0.29308600
H	4.56872800	-0.65231400	0.03669800
H	4.04710400	1.03250300	0.15100700
H	3.50334300	-0.13837600	1.35496100

Eli-R16

C	-0.44728900	0.10740000	0.17543800
C	-0.81848800	-1.31633400	-0.25605500
C	-2.25735000	-1.43975500	-0.78137900
C	-3.27812000	-0.86598000	0.20804400
C	-2.94153400	0.58994300	0.55278900
C	-1.51124000	0.72667400	1.09190100
H	-2.33677500	-0.90586300	-1.73393100
H	-0.11198000	-1.66014900	-1.01534900

H	-0.68495900	-1.96553100	0.61750800
H	-4.28745800	-0.93343000	-0.20944900
H	-3.64547000	0.98249700	1.29297300
H	-1.25623100	1.77699100	1.25129000
H	-1.43399800	0.22542700	2.06372000
H	-2.47480700	-2.49149500	-0.99180000
H	-3.27811400	-1.46860400	1.12612800
H	-3.05109700	1.21077200	-0.34270000
O	-0.45301100	0.86302200	-1.12533600
O	-0.20878400	2.14668500	-0.98617200
C	0.95429800	0.23441300	0.78700100
H	0.93430100	-0.26844400	1.76073800
H	1.12020800	1.29761600	0.98728800
C	2.11687000	-0.30920600	-0.05262200
H	2.08200000	0.13526400	-1.05294900
H	2.01347200	-1.39146300	-0.18878500
C	3.48284300	-0.01886800	0.58168800
H	3.59735300	1.06400600	0.70905200
H	3.51392400	-0.44914800	1.59032200
C	4.65417200	-0.56247400	-0.24104900
H	4.66712400	-0.12613000	-1.24449500
H	5.61331900	-0.33565000	0.23215800
H	4.58857700	-1.64919600	-0.35419200

Eli-TS16

C	2.92440600	0.30462600	0.85974500
C	1.51759100	0.10375800	1.44239700
C	0.45172300	-0.22597100	0.42646500
C	0.84638300	-1.17531400	-0.67458300
C	2.26930400	-0.96807800	-1.21915400
C	3.30165000	-0.83442600	-0.09479100
H	1.54606200	-0.74544800	2.14493500
H	1.20981800	0.97171900	2.03240900
H	2.95666500	1.25637900	0.32250100
H	3.64699100	0.37343900	1.67891500
H	0.77081800	-2.19004200	-0.24793000
H	0.11961400	-1.14106500	-1.48822100
H	2.52593000	-1.80476500	-1.87631400
H	2.28287600	-0.06322900	-1.83275300
H	3.36298200	-1.77787400	0.46471000
H	4.29567100	-0.65834100	-0.51723400
C	-0.88194000	0.09929700	0.69728200
H	-1.06265700	0.43703600	1.72157000
H	-0.85637200	1.27655400	0.08441200
O	0.76278500	1.72968000	-0.86990100

O	-0.39977900	2.22171200	-0.66141200
C	-2.07049300	-0.62724500	0.06981800
H	-1.95082500	-0.68151200	-1.01746600
H	-2.10226000	-1.66643300	0.42443300
C	-3.41140100	0.04826100	0.38515700
H	-3.38832600	1.08129500	0.01993700
H	-3.53615300	0.11153900	1.47286300
C	-4.60884400	-0.68520800	-0.22385100
H	-4.67584600	-1.71233100	0.14859200
H	-5.54889700	-0.18273100	0.01860100
H	-4.53041300	-0.73352300	-1.31437200

Eli-P16

C	2.07800800	1.49062500	-0.23068500
C	0.80571900	1.05386600	0.52577600
C	0.42836800	-0.37152100	0.18789500
C	1.56036400	-1.35379500	0.40332800
C	2.83321300	-0.92672100	-0.35431100
C	3.23663500	0.51109200	-0.00119500
H	1.00653500	1.11680200	1.60505700
H	-0.00963300	1.74902400	0.31957700
H	1.85297300	1.54249200	-1.30276400
H	2.36604400	2.50000200	0.08099900
H	1.79596500	-1.39984800	1.47665100
H	1.25430100	-2.35947800	0.10211300
H	3.65195700	-1.61822000	-0.12959500
H	2.64525900	-0.99734600	-1.43252800
H	3.53972100	0.55203500	1.05342100
H	4.11007200	0.81485800	-0.58741900
C	-0.75646100	-0.77072200	-0.28976700
H	-0.87254400	-1.83545900	-0.49545300
C	-1.98723300	0.04920400	-0.56353000
H	-1.78913200	1.11760600	-0.44076900
H	-2.28019000	-0.08820200	-1.61372000
C	-3.18097700	-0.34758300	0.32626200
H	-3.36984300	-1.42188900	0.21574700
H	-2.90735100	-0.19356300	1.37583100
C	-4.45669200	0.43377400	0.00078200
H	-5.28529100	0.13166500	0.64711900
H	-4.30728300	1.50986900	0.13446700
H	-4.76722100	0.27033800	-1.03606900

Eli-R17

C	-0.44001600	1.27168800	0.06878600
C	-1.97452800	1.26738700	0.02658800

C	-2.51793400	-0.00014700	-0.64705100
C	-1.97433400	-1.26754500	0.02668900
C	-0.43981900	-1.27153700	0.06899400
C	0.11576500	0.00017500	0.73880300
H	-3.61232400	-0.00021500	-0.62541300
H	-2.36574800	1.32798300	1.05064500
H	-2.33438700	2.15929800	-0.49575800
H	-0.04606500	1.33897900	-0.95136100
H	-0.07954900	2.15840100	0.60219700
H	-2.36560100	-1.32815500	1.05072500
H	-2.33396800	-2.15956300	-0.49562500
H	-0.07923000	-2.15809900	0.60257500
H	-0.04579300	-1.33893600	-0.95112700
H	-0.21772500	0.00029400	1.78707000
H	-2.22613400	-0.00016900	-1.70495500
C	1.63636800	0.00014700	0.80593200
H	2.03053500	-0.89176400	1.29906800
O	2.16765500	-0.00006900	-0.55749900
O	3.48386400	-0.00006200	-0.56742700
H	2.03082700	0.89198500	1.29892200

Eli-TS17

C	-1.56943600	-1.27010300	-0.43543400
C	-0.50470700	-1.28505000	0.67283700
C	0.33371600	0.00010100	0.67997500
C	-0.50479100	1.28521400	0.67258800
C	-1.56962000	1.26997000	-0.43561200
C	-2.43020100	-0.00011600	-0.37349600
H	-1.00497500	-1.38318500	1.64565100
H	0.14762600	-2.15719100	0.56503400
H	-1.07546700	-1.32444300	-1.41343500
H	-2.20110500	-2.16024200	-0.35496600
H	-1.00500200	1.38353000	1.64541600
H	0.14748800	2.15736900	0.56455100
H	-2.20137400	2.16004900	-0.35516200
H	-1.07574600	1.32429400	-1.41366000
H	-3.00803900	-0.00009300	0.56020400
H	-3.15885300	-0.00021000	-1.19013600
H	0.88003200	-0.00000700	-0.52843500
C	1.57800700	0.00013700	1.30091500
H	2.05385700	0.91918200	1.62080800
H	2.05380600	-0.91889800	1.62092300
O	2.81475100	-0.00005800	-0.54470200
O	1.86649200	-0.00007700	-1.38747600

Eli-P17

C	-1.02041500	-1.26825400	-0.30049600
C	0.34520200	-1.26902300	0.41644000
C	1.11528300	0.00002900	0.13174000
C	0.34518800	1.26904400	0.41642000
C	-1.02043400	1.26824700	-0.30049400
C	-1.82234900	-0.00002300	0.02202700
H	0.16915400	-1.34293700	1.49924500
H	0.93227200	-2.14535600	0.12873100
H	-0.85326500	-1.32627500	-1.38278200
H	-1.58888500	-2.16080400	-0.01992200
H	0.16913000	1.34295000	1.49922400
H	0.93224000	2.14540300	0.12873400
H	-1.58892900	2.16077500	-0.01990200
H	-0.85330900	1.32627500	-1.38278200
H	-2.08568500	-0.00002600	1.08795900
H	-2.76687200	-0.00001800	-0.53152500
C	2.35263900	-0.00000600	-0.36305800
H	2.88176800	0.92444000	-0.57124500
H	2.88169200	-0.92450600	-0.57120700

Eli-R18

C	-0.61754600	1.09998400	-0.53284900
C	-2.14765800	1.21275300	-0.45373000
C	-2.82400100	-0.16314500	-0.49957000
C	-2.27528100	-1.08600500	0.59632800
C	-0.74692100	-1.20360100	0.52125100
C	-0.05786700	0.17457100	0.56660600
H	-3.90866500	-0.05604000	-0.39759700
H	-2.42526200	1.72038600	0.47950200
H	-2.51343900	1.84383600	-1.26984500
H	-0.33093700	0.70322000	-1.51290600
H	-0.17349000	2.09668300	-0.45560100
H	-2.56048600	-0.68826100	1.57924000
H	-2.72897900	-2.07920800	0.52040300
H	-0.37748500	-1.82734100	1.34304800
H	-0.46431600	-1.71155400	-0.40782200
H	-0.28991600	0.63118900	1.53986900
H	-2.64569000	-0.62134600	-1.48078500
C	1.46888700	0.03375500	0.54059500
C	2.26953900	1.30696300	0.76790800
H	1.77991900	-0.73396900	1.25437700
H	3.33565800	1.08228200	0.71238600
H	2.03496600	2.06818500	0.02179800
H	2.05198100	1.71149000	1.75991100

O	1.81920400	-0.51786900	-0.78595300
O	3.03094900	-1.03103200	-0.80469800

Eli-TS18

C	-2.03479500	-0.97604100	0.68144100
C	-0.78786300	-0.41255600	1.37820600
C	0.17672200	0.26419300	0.39074000
C	-0.51083400	1.28907400	-0.52058600
C	-1.76806200	0.71139600	-1.19125500
C	-2.73204000	0.09424000	-0.16919700
H	-1.10422100	0.32787600	2.12576900
H	-0.26519900	-1.20530100	1.92269100
H	-1.74282600	-1.81589100	0.03914100
H	-2.72674900	-1.37876200	1.42785800
H	-0.79695600	2.16170100	0.08331400
H	0.17770500	1.65492300	-1.28626400
H	-2.27316400	1.49653900	-1.76272500
H	-1.46889000	-0.05763600	-1.91394000
H	-3.11872600	0.88442100	0.48819500
H	-3.59872400	-0.33535800	-0.68142700
H	0.47866300	-0.73155100	-0.43556400
C	1.50651200	0.42740900	0.78817700
H	1.83289100	-0.11974800	1.66762200
O	2.32944700	-1.27904300	-0.45916500
O	1.23688600	-1.60984600	-1.02467300
C	2.46935300	1.44573100	0.26886100
H	3.49931900	1.10127800	0.37464000
H	2.29307900	1.69023100	-0.77963100
H	2.36916500	2.37772500	0.84270600

Eli-P18

C	1.14849100	-1.42231300	0.26711600
C	-0.09863300	-1.08676400	-0.57769700
C	-0.60409000	0.30775700	-0.28166800
C	0.46270700	1.37266800	-0.42439100
C	1.70886600	1.04519400	0.42177400
C	2.24287400	-0.35868800	0.10779100
H	0.17824600	-1.14195300	-1.64050800
H	-0.87127800	-1.84057000	-0.41809300
H	0.85548700	-1.48646700	1.32199300
H	1.53233100	-2.40828300	-0.01478200
H	0.76805400	1.43543900	-1.47920200
H	0.06107500	2.35263900	-0.15188600
H	2.48659000	1.79627600	0.24843600
H	1.44249000	1.10370300	1.48409100
H	2.61840700	-0.37944300	-0.92386000

H	3.09528300	-0.59368200	0.75354000
C	-1.84803300	0.61828000	0.10034700
H	-2.05816600	1.67047300	0.29031800
C	-3.02277100	-0.29702900	0.29781300
H	-3.84859600	-0.01715100	-0.36665600
H	-2.78796400	-1.34517500	0.10914400
H	-3.40842600	-0.22044000	1.32095500

Eli-R19

C	-2.60263000	0.77234500	0.85352200
C	-1.10604100	1.06220400	0.67043200
C	-0.28944400	-0.23021200	0.47784400
C	-0.85850000	-1.06688800	-0.68518300
C	-2.35780200	-1.34823200	-0.50402800
C	-3.16179800	-0.05646600	-0.31005000
H	-0.96622300	1.71051700	-0.20166200
H	-0.72122100	1.61771000	1.53231700
H	-2.75459900	0.22418000	1.79260400
H	-3.15323900	1.71325300	0.95051600
H	-0.69974300	-0.52292900	-1.62311200
H	-0.31884800	-2.01410700	-0.77543600
H	-2.73540200	-1.90555400	-1.36718900
H	-2.50062400	-1.99673900	0.37045100
H	-3.11765500	0.53855500	-1.23114900
H	-4.21767100	-0.28921100	-0.13859400
H	-0.38596300	-0.82335500	1.39963600
C	1.21443000	0.06418400	0.34757500
H	1.52489800	0.74939100	1.14039900
C	2.12884400	-1.15789900	0.30093200
H	1.94113800	-1.70927300	-0.62483900
H	1.84147600	-1.82171800	1.12360600
C	3.61485900	-0.80294400	0.40305800
H	3.91257000	-0.13018300	-0.40417700
H	3.84001300	-0.30742500	1.35212300
O	1.45411800	0.80796500	-0.90602300
O	1.64389800	2.09832500	-0.71385200
H	4.23545000	-1.69997700	0.33888600

Eli-TS19

C	2.48155600	0.70819500	0.84117300
C	1.13446100	0.24920000	1.41791100
C	0.15729000	-0.20952700	0.32319100
C	0.76722800	-1.22505700	-0.65156700
C	2.12564400	-0.75529100	-1.19789900
C	3.09240900	-0.36301200	-0.07269700

H	1.31149900	-0.58784000	2.10725700
H	0.67909300	1.05108400	2.00738400
H	2.33535600	1.63221000	0.26851000
H	3.17095400	0.95060500	1.65603800
H	0.90379500	-2.18033300	-0.12504900
H	0.08511700	-1.42411900	-1.48189100
H	2.56498500	-1.54307500	-1.81793400
H	1.96904000	0.10869400	-1.85536700
H	3.33508400	-1.25247300	0.52389700
H	4.03630500	-0.00518900	-0.49589700
H	0.02974600	0.88309200	-0.41332600
C	-1.20379600	-0.24591400	0.63692600
H	-1.52077400	0.25590800	1.54751700
O	-1.72845500	1.68673400	-0.47481400
O	-0.56807400	1.90882300	-0.95254800
C	-2.24201300	-1.09723100	-0.02975100
H	-2.07446000	-1.11316700	-1.11105600
H	-2.08392100	-2.13504300	0.30414000
C	-3.68274900	-0.67659700	0.27398100
H	-4.39471100	-1.36018000	-0.19494800
H	-3.87601800	-0.68301000	1.35091400
H	-3.87903900	0.32978800	-0.09889300

Eli-P19

C	-1.67766000	-1.41764600	-0.23126000
C	-0.37187200	-1.09174500	0.52393700
C	0.12468300	0.29700600	0.18726300
C	-0.91946200	1.37145400	0.40637300
C	-2.22515200	1.05530200	-0.34970100
C	-2.74870800	-0.34375900	0.00161100
H	-0.57597800	-1.13889300	1.60340900
H	0.38096500	-1.85360600	0.31561600
H	-1.45939000	-1.48661800	-1.30377600
H	-2.04982600	-2.39946700	0.07933100
H	-1.14843500	1.43555800	1.48020000
H	-0.52971300	2.34804300	0.10610300
H	-2.98188600	1.81338000	-0.12238100
H	-2.03364100	1.11174600	-1.42813500
H	-3.05269900	-0.36071300	1.05661800
H	-3.64555300	-0.57123500	-0.58381400
C	1.33805000	0.59492100	-0.29237600
H	1.54451700	1.64625600	-0.49697100
C	2.49473600	-0.32585400	-0.57146300
H	2.21218900	-1.37100400	-0.42527900
H	2.77604900	-0.23034600	-1.62841200

C	3.72608800	-0.00383200	0.29308600
H	4.56872800	-0.65231400	0.03669800
H	4.04710400	1.03250300	0.15100700
H	3.50334300	-0.13837600	1.35496100

Eli-R20

C	-3.08916100	0.40893300	0.91446500
C	-1.66632200	0.95162900	0.72015100
C	-0.65098500	-0.17729300	0.45762700
C	-1.10052800	-1.05135800	-0.72988300
C	-2.52830600	-1.58488200	-0.53756700
C	-3.52993200	-0.45267000	-0.27532300
H	-1.65639100	1.64839400	-0.12524900
H	-1.35946900	1.52900300	1.59885000
H	-3.12726700	-0.19444800	1.83099200
H	-3.78578100	1.24028600	1.06122200
H	-1.05401900	-0.45325100	-1.64699300
H	-0.41259400	-1.89091500	-0.86674000
H	-2.82779600	-2.16265700	-1.41779200
H	-2.54257800	-2.28197600	0.31067400
H	-3.60430400	0.17815800	-1.17023700
H	-4.52902600	-0.86380200	-0.09857400
H	-0.62398000	-0.81403500	1.35462900
C	0.77882900	0.37082200	0.31331500
H	0.98867100	1.06712600	1.12903600
C	1.88385800	-0.67568000	0.19712000
H	1.78502500	-1.19681800	-0.76064100
H	1.72321500	-1.42738400	0.97902600
C	3.29583400	-0.08981800	0.32004100
H	3.42518700	0.69274100	-0.43390800
H	3.39837600	0.40201700	1.29460900
O	0.85978500	1.19361800	-0.91137200
O	0.82215300	2.48858800	-0.66765900
C	4.39287000	-1.14532400	0.16001100
H	5.38659900	-0.70046700	0.25577900
H	4.30536800	-1.92915900	0.91902900
H	4.33832300	-1.62661800	-0.82121100

Eli-TS20

C	3.00457800	0.50855000	0.75061500
C	1.62627400	0.27976500	1.38735600
C	0.56281900	-0.11486400	0.34931700
C	0.99983000	-1.26783900	-0.56332600
C	2.39311800	-1.02980400	-1.16864900
C	3.43727900	-0.69716300	-0.09411800

H	1.70917400	-0.52339500	2.13252300
H	1.30268400	1.17566800	1.92648400
H	2.96732800	1.40141200	0.11462500
H	3.74493500	0.71081700	1.53103000
H	1.01889000	-2.19525200	0.02648900
H	0.27275300	-1.42559500	-1.36401000
H	2.70189400	-1.91243200	-1.73770800
H	2.33732700	-0.20088200	-1.88488900
H	3.57423300	-1.56803800	0.56068600
H	4.40817300	-0.50322100	-0.56088300
H	0.56003400	0.93253100	-0.45878500
C	-0.78045400	0.05510800	0.69473500
H	-0.99840200	0.65281300	1.57594100
O	-1.07127300	1.96965000	-0.53097000
O	0.09077600	1.99515800	-1.05354900
C	-1.94353500	-0.68479300	0.10694600
H	-1.82602500	-0.76746700	-0.97899700
H	-1.90859500	-1.72087300	0.48234300
C	-3.31088200	-0.07428700	0.43832400
H	-3.41643100	-0.00289700	1.52743500
H	-3.34276000	0.94901900	0.05515300
C	-4.47653000	-0.88239600	-0.13648500
H	-4.48307100	-1.90601900	0.25174200
H	-5.43689300	-0.42582200	0.11625600
H	-4.41625500	-0.94248000	-1.22757800

Eli-P20

C	2.07800800	1.49062500	-0.23068500
C	0.80571900	1.05386600	0.52577600
C	0.42836800	-0.37152100	0.18789500
C	1.56036400	-1.35379500	0.40332800
C	2.83321300	-0.92672100	-0.35431100
C	3.23663500	0.51109200	-0.00119500
H	1.00653500	1.11680200	1.60505700
H	-0.00963300	1.74902400	0.31957700
H	1.85297300	1.54249200	-1.30276400
H	2.36604400	2.50000200	0.08099900
H	1.79596500	-1.39984800	1.47665100
H	1.25430100	-2.35947800	0.10211300
H	3.65195700	-1.61822000	-0.12959500
H	2.64525900	-0.99734600	-1.43252800
H	3.53972100	0.55203500	1.05342100
H	4.11007200	0.81485800	-0.58741900
C	-0.75646100	-0.77072200	-0.28976700
H	-0.87254400	-1.83545900	-0.49545300

C	-1.98723300	0.04920400	-0.56353000
H	-1.78913200	1.11760600	-0.44076900
H	-2.28019000	-0.08820200	-1.61372000
C	-3.18097700	-0.34758300	0.32626200
H	-3.36984300	-1.42188900	0.21574700
H	-2.90735100	-0.19356300	1.37583100
C	-4.45669200	0.43377400	0.00078200
H	-5.28529100	0.13166500	0.64711900
H	-4.30728300	1.50986900	0.13446700
H	-4.76722100	0.27033800	-1.03606900

Eli-R21

C	-0.63918300	0.36132000	0.26074100
C	0.37096500	1.43660200	-0.15320200
C	1.64143700	0.86320900	-0.79726300
C	2.28647200	-0.21133700	0.08724400
C	1.28413600	-1.32516100	0.41639300
C	0.01102200	-0.76786000	1.06844500
H	1.38691300	0.42864200	-1.76942700
H	-0.12164500	2.14035700	-0.83127300
H	0.63488600	1.99949000	0.74974400
H	3.16716300	-0.62991400	-0.40938100
H	1.73759800	-2.06489900	1.08306600
H	-0.72993600	-1.55740800	1.21430300
H	0.24931000	-0.36217100	2.05877600
H	2.34840100	1.67564700	-0.99126500
H	2.64142900	0.24740000	1.01986600
H	1.01535500	-1.85601700	-0.50297400
O	-1.09281200	-0.19857800	-1.05865700
O	-1.94970100	-1.18707200	-0.93850700
C	-1.86722800	0.94316600	0.94920000
H	-1.58947900	1.36811400	1.91668300
H	-2.61300100	0.16339800	1.11065700
H	-2.31261400	1.73293200	0.33918000

Eli-TS21

C	-1.40955200	-0.98227200	0.95426900
C	0.01904500	-0.43349400	1.11326000
C	0.46782900	0.67735900	0.38447200
C	-0.35545200	1.27792900	-0.72336000
C	-1.52443200	0.39254300	-1.16402600
C	-2.29826700	-0.10402700	0.06150800
H	0.44621600	-0.53310200	2.11238100
H	0.78003400	-1.29797000	0.48560200
H	-1.37271500	-1.99516000	0.53650200

H	-1.86294300	-1.08353600	1.94473300
H	-0.74574900	2.23785000	-0.34879100
H	0.29522100	1.52781300	-1.56669100
H	-2.17943600	0.95394300	-1.83633500
H	-1.14120900	-0.46156800	-1.73300500
H	-2.64968800	0.76434700	0.63291900
H	-3.18882700	-0.66243500	-0.24087700
C	1.63811200	1.48211800	0.86789200
H	2.29091800	0.89363700	1.51527200
H	2.22861600	1.86873300	0.03449000
H	1.27741400	2.34252800	1.44726700
O	1.74433300	-0.58530400	-1.03157000
O	1.58047500	-1.71670000	-0.46187400

Eli-P21

C	1.19481600	1.29806000	-0.10242100
C	-0.31142300	1.21919100	-0.08907800
C	-1.00986500	0.08373100	0.00536900
C	-0.32670900	-1.26609900	0.08243200
C	1.15631100	-1.21455900	-0.30841600
C	1.85102500	-0.01524100	0.34452300
H	1.53814800	1.56252400	-1.11309000
H	1.52409500	2.12200500	0.54154900
H	-0.43364000	-1.66073500	1.10337100
H	-0.85982700	-1.97726900	-0.56072100
H	1.65194100	-2.14942400	-0.02902900
H	1.23920000	-1.12697400	-1.39851300
H	1.77260500	-0.10568200	1.43473000
H	2.91846700	-0.00719000	0.10377800
C	-2.51499400	0.06648600	0.04931900
H	-2.93216600	1.07542400	0.02568900
H	-2.92859100	-0.49502000	-0.79694900
H	-2.87576600	-0.42949300	0.95864900
H	-0.84943100	2.16242000	-0.15983700

Eli-R22

C	0.39835900	-0.03582800	0.22763600
C	-0.23373100	-1.35859200	-0.21932900
C	-1.64089600	-1.19384400	-0.81398400
C	-2.56861300	-0.41175200	0.12318400
C	-1.95950800	0.94947400	0.48040600
C	-0.55864400	0.79936500	1.08849200
H	-1.56620400	-0.66819800	-1.77166700
H	0.42391600	-1.84768400	-0.94195100
H	-0.27787400	-2.01056900	0.66126100

H	-3.54976700	-0.27800100	-0.34268500
H	-2.60330800	1.48567100	1.18429500
H	-0.10227700	1.77766100	1.25662000
H	-0.63100400	0.30567500	2.06471000
H	-2.05793500	-2.18220500	-1.03065900
H	-2.73460200	-0.99018000	1.04189800
H	-1.89821300	1.56889700	-0.42075300
O	0.61491800	0.68890700	-1.07203400
O	1.11148600	1.89625700	-0.92075600
C	1.76485900	-0.19375000	0.90895000
H	1.59347100	-0.67586400	1.87732000
H	2.13392800	0.81350200	1.12102500
C	2.82304700	-0.96958700	0.11817300
H	2.98222900	-0.52617400	-0.86714400
H	2.54989600	-2.01819600	-0.02150300
H	3.77727200	-0.94855200	0.65038800

Eli-TS22

C	2.03165600	0.48661000	0.91492300
C	0.50560400	0.53750200	1.10196300
C	-0.35727300	-0.32574600	0.41031600
C	0.14585100	-1.20747300	-0.70050500
C	1.56475600	-0.86257000	-1.16508100
C	2.49179400	-0.68830200	0.04152500
H	0.17261000	0.80983700	2.10525800
H	0.12756100	1.61847200	0.47082500
H	2.38143300	1.42405700	0.46690500
H	2.50768400	0.42883900	1.89831400
H	0.12679000	-2.24239900	-0.32182700
H	-0.55373000	-1.18489500	-1.53958200
H	1.93346900	-1.64883300	-1.83004300
H	1.54174800	0.06305900	-1.75093500
H	2.48257300	-1.61276100	0.63271200
H	3.52523500	-0.53141200	-0.28066300
C	-1.72389000	-0.61246900	0.98692800
H	-2.03671600	0.25117000	1.58169800
H	-1.58970000	-1.43460400	1.70739900
O	-1.06764500	1.34593800	-1.02726800
O	-0.45667000	2.31963200	-0.46805700
C	-2.83400600	-0.99304000	0.00146200
H	-2.60244400	-1.91286000	-0.54093100
H	-3.76919600	-1.16069800	0.54167500
H	-2.99974600	-0.19860300	-0.72740100

Eli-P22

C	1.31925000	1.46440600	-0.10369100
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C	-0.12638200	1.03016600	-0.09903400
C	-0.53540600	-0.23877400	-0.00370200
C	0.45611300	-1.38279100	0.08914800
C	1.88402300	-0.98261900	-0.30239900
C	2.27137900	0.34923700	0.34719600
H	1.59306200	1.80350100	-1.11329500
H	1.43798700	2.34399700	0.53997500
H	0.44626300	-1.77844600	1.11507400
H	0.11221400	-2.20987700	-0.54423600
H	2.58701000	-1.77207900	-0.01884200
H	1.94602000	-0.88198600	-1.39282000
H	2.21630600	0.24502000	1.43762700
H	3.30594300	0.61292900	0.10686400
C	-1.98888400	-0.65850600	0.02906800
H	-2.17011900	-1.32790100	-0.82349200
H	-2.13810500	-1.29021200	0.91618100
H	-0.86152700	1.82541500	-0.17999100
C	-3.03670500	0.45481800	0.02457400
H	-2.97075100	1.06611000	-0.87954800
H	-4.04319000	0.03019000	0.06310300
H	-2.92144400	1.11772200	0.88644700

Eli-R23

C	0.00575300	0.03836300	0.14502500
C	-0.51602300	-1.31220400	-0.35908400
C	-1.98166700	-1.26672700	-0.81876100
C	-2.90048900	-0.67167400	0.25471100
C	-2.41238700	0.71855500	0.67967700
C	-0.95359200	0.68404300	1.15440100
H	-2.05125900	-0.66347200	-1.72978400
H	0.12066100	-1.66511900	-1.17393400
H	-0.40615100	-2.02989300	0.46264800
H	-3.92780500	-0.61513800	-0.11820900
H	-3.04296000	1.11910500	1.47928300
H	-0.59305400	1.69176800	1.37357000
H	-0.88259800	0.10679300	2.08361800
H	-2.30679500	-2.27701600	-1.08579400
H	-2.92179400	-1.33575700	1.12922600
H	-2.50216400	1.41016900	-0.16469000
O	0.01231000	0.88110600	-1.10028100
O	0.38020300	2.12458000	-0.88898100
C	1.43895000	-0.00490800	0.69162900
H	1.41659200	-0.57173200	1.62966200
H	1.71252600	1.02199400	0.95381500

C	2.50946500	-0.58906500	-0.23895400
H	2.47336700	-0.07061300	-1.20174900
H	2.29819600	-1.64331500	-0.44426400
C	3.91585000	-0.46646400	0.35622000
H	4.18028700	0.58046700	0.53241100
H	3.99001100	-0.99245100	1.31339500
H	4.66766700	-0.89079800	-0.31428800

Eli-TS23

C	2.41466900	0.13510100	1.06306200
C	0.90550600	0.42369400	1.14091300
C	-0.02128300	-0.23544100	0.31902400
C	0.43003800	-1.11050800	-0.81954600
C	1.91969700	-0.97062100	-1.14930100
C	2.75565900	-1.03611800	0.13155900
H	0.53509300	0.67696400	2.13599100
H	0.75994200	1.59368400	0.57507500
H	2.94608300	1.03081600	0.72074700
H	2.78907600	-0.06855200	2.07069000
H	0.21737500	-2.15181200	-0.52737500
H	-0.18268700	-0.91829000	-1.70344600
H	2.21510900	-1.75830800	-1.84830900
H	2.09274900	-0.01515800	-1.65682500
H	2.54912700	-1.98527300	0.64208100
H	3.82469100	-1.02974600	-0.09991700
C	-1.46018300	-0.32948800	0.76796500
H	-1.68561400	0.53665600	1.39952800
H	-1.52301100	-1.20478300	1.43507900
O	-0.32373700	1.62523800	-1.02874400
O	0.38034200	2.44443700	-0.34497400
C	-2.53652400	-0.46395600	-0.31800400
H	-2.35829100	-1.36757000	-0.90970300
H	-2.45925700	0.38259900	-1.00462900
C	-3.94688100	-0.52350200	0.27619500
H	-4.17345600	0.38088700	0.84927200
H	-4.70188400	-0.61508700	-0.50881200
H	-4.06206700	-1.37939300	0.94911100

Eli-P23

C	1.88185800	1.45047100	-0.09866100
C	0.42804200	1.04442000	-0.10716000
C	-0.00668800	-0.21641300	-0.01560300
C	0.96228800	-1.37915400	0.08581600
C	2.40122500	-1.00667000	-0.29246500
C	2.80821800	0.31744000	0.36089100
H	2.17131300	1.78420700	-1.10570300

H	2.01153000	2.32773800	0.54610100
H	0.93545800	-1.77469900	1.11149700
H	0.60832800	-2.19937000	-0.55088400
H	3.08612500	-1.80962100	-0.00257200
H	2.47523300	-0.90726100	-1.38226200
H	2.74101700	0.21442700	1.45075800
H	3.84984000	0.56119800	0.13017400
C	-1.46774000	-0.60994000	0.00385500
H	-1.65629100	-1.27148600	-0.85450400
H	-1.63641300	-1.24483200	0.88647700
H	-0.29019000	1.85413100	-0.19484900
C	-2.50546600	0.51540500	-0.00072000
H	-2.37212300	1.13385200	-0.89496900
H	-2.33418500	1.17362800	0.85803800
C	-3.94265000	-0.01337900	0.03950900
H	-4.12083100	-0.60944600	0.94009000
H	-4.66789100	0.80473300	0.03473500
H	-4.15543900	-0.65028000	-0.82489400

Eli-R24

C	-0.44728900	0.10740000	0.17543800
C	-0.81848800	-1.31633400	-0.25605500
C	-2.25735000	-1.43975500	-0.78137900
C	-3.27812000	-0.86598000	0.20804400
C	-2.94153400	0.58994300	0.55278900
C	-1.51124000	0.72667400	1.09190100
H	-2.33677500	-0.90586300	-1.73393100
H	-0.11198000	-1.66014900	-1.01534900
H	-0.68495900	-1.96553100	0.61750800
H	-4.28745800	-0.93343000	-0.20944900
H	-3.64547000	0.98249700	1.29297300
H	-1.25623100	1.77699100	1.25129000
H	-1.43399800	0.22542700	2.06372000
H	-2.47480700	-2.49149500	-0.99180000
H	-3.27811400	-1.46860400	1.12612800
H	-3.05109700	1.21077200	-0.34270000
O	-0.45301100	0.86302200	-1.12533600
O	-0.20878400	2.14668500	-0.98617200
C	0.95429800	0.23441300	0.78700100
H	0.93430100	-0.26844400	1.76073800
H	1.12020800	1.29761600	0.98728800
C	2.11687000	-0.30920600	-0.05262200
H	2.08200000	0.13526400	-1.05294900
H	2.01347200	-1.39146300	-0.18878500

C	3.48284300	-0.01886800	0.58168800
H	3.59735300	1.06400600	0.70905200
H	3.51392400	-0.44914800	1.59032200
C	4.65417200	-0.56247400	-0.24104900
H	4.66712400	-0.12613000	-1.24449500
H	5.61331900	-0.33565000	0.23215800
H	4.58857700	-1.64919600	-0.35419200

Eli-TS24

C	2.92906900	0.08410600	0.94057400
C	1.44587500	0.46057800	1.10124900
C	0.43126600	-0.18891600	0.38126000
C	0.75725600	-1.14375900	-0.73575000
C	2.22398500	-1.09605700	-1.17466600
C	3.14511100	-1.14567200	0.04751200
H	1.15905400	0.78635700	2.10284100
H	1.32364300	1.60347300	0.48048400
H	3.48286700	0.93239300	0.52163300
H	3.35850400	-0.09420400	1.93093200
H	0.51729100	-2.15642600	-0.37265200
H	0.09123300	-0.96620600	-1.58341100
H	2.43087800	-1.92912700	-1.85252500
H	2.40581900	-0.17478500	-1.73893800
H	2.92877400	-2.05800300	0.61748400
H	4.19400200	-1.20609700	-0.25671100
C	-0.97585500	-0.18002200	0.92954900
H	-1.10683700	0.72425800	1.53357300
H	-1.03993000	-1.02065100	1.63945700
O	0.13550200	1.61265200	-1.04831500
O	0.92826200	2.42571900	-0.46118300
C	-2.13138500	-0.29660200	-0.07365300
H	-2.05499300	-1.23947500	-0.62681400
H	-2.05013400	0.50779800	-0.80999900
C	-3.50335700	-0.23225800	0.60812200
H	-3.58854400	0.71272100	1.15799700
H	-3.57583800	-1.02882500	1.35911400
C	-4.66855100	-0.35278500	-0.37795300
H	-4.63471800	-1.30500900	-0.91661100
H	-5.63256500	-0.29572200	0.13468200
H	-4.63909900	0.44888200	-1.12201600

Eli-P24

C	2.27280900	1.54209500	-0.10167800
C	0.86379900	1.00071600	-0.11252000
C	0.54992500	-0.29536400	-0.01854900
C	1.62390100	-1.36155500	0.08768300

C	3.02270900	-0.85472700	-0.28576100
C	3.29898400	0.50283400	0.36686800
H	2.53397700	1.89588900	-1.10961000
H	2.31710600	2.43103000	0.53858600
H	1.63084600	-1.75684400	1.11382400
H	1.35134100	-2.21225400	-0.54916500
H	3.77950500	-1.58870500	0.00818500
H	3.09116900	-0.75019500	-1.37542000
H	3.23460300	0.39586000	1.45650500
H	4.31444400	0.84311900	0.14185900
C	-0.86743000	-0.82563900	0.00076500
H	-0.98880200	-1.50741000	-0.85375900
H	-0.97553500	-1.46854400	0.88704500
H	0.07164200	1.73793900	-0.20389400
C	-2.00665200	0.19590300	-0.01253700
H	-1.93392300	0.81783200	-0.91264000
H	-1.90074500	0.87587200	0.84115600
C	-3.39355100	-0.45698500	0.03300400
H	-3.47034500	-1.08041900	0.93211100
H	-3.50077500	-1.13914800	-0.81914100
C	-4.53936600	0.55858600	0.01907400
H	-4.51137300	1.17441900	-0.88538000
H	-5.51348500	0.06301000	0.05274600
H	-4.48041900	1.23335900	0.87890200

Eli-R25

C	-1.22930900	1.03453300	-0.59600100
C	-2.16599700	-0.14169900	-0.28501400
C	-1.38658000	-1.45641100	-0.14774300
C	-0.26586900	-1.33947200	0.89440500
C	0.64729400	-0.14273000	0.63269000
C	-0.11097700	1.17826300	0.45298600
H	-2.05899700	-2.27417300	0.12790800
H	-2.70550200	0.06104200	0.64962800
H	-2.92515200	-0.23360000	-1.06781000
H	-0.77694300	0.89224500	-1.58409200
H	-1.79746700	1.96914100	-0.64421400
H	-0.69491300	-1.21415500	1.89582800
H	0.34856300	-2.24287900	0.92108100
H	1.41212200	-0.05648700	1.40844800
H	-0.58904000	1.36271300	1.42502700
H	-0.94990600	-1.72298700	-1.11625000
C	0.82619100	2.35423900	0.15315800
H	1.33533000	2.21751900	-0.80338700

H	1.59118300	2.46187800	0.92792600
O	1.39604900	-0.37126800	-0.62220200
O	2.31130900	-1.30760900	-0.48699600
H	0.26334300	3.29041700	0.10659800

Eli-TS25

C	-2.18233800	-0.10722500	-0.34873300
C	-1.15848300	0.95855300	-0.75817500
C	-0.21040000	-1.24831800	0.82940400
C	-1.50039400	-1.43599700	0.01218600
H	-0.56949900	0.60604200	-1.61362800
H	-1.66452600	1.87437600	-1.07872200
H	-2.74518200	0.26193200	0.51747800
H	-2.91122800	-0.26931300	-1.14813200
H	0.75064600	-1.67621100	0.06077300
H	-0.06563500	-1.94983100	1.65201200
H	-1.27646600	-1.98694000	-0.90856700
H	-2.19271300	-2.06688400	0.57702300
C	0.85085900	2.32645100	0.05569900
H	0.37407000	3.26699800	-0.23380400
H	1.50437100	2.53028700	0.90874100
H	1.47647500	1.98676300	-0.77052200
O	2.09479300	-0.34366100	-0.37570300
O	1.844485000	-1.55897000	-0.66239400
C	-0.21365800	1.27936000	0.40884800
H	-0.83325300	1.71424900	1.21379300
C	0.34187300	0.02252100	1.02005300
H	1.07104900	0.15751500	1.81263600

Eli-P25

C	-1.91554500	0.15073900	0.26135300
C	-1.01087200	1.34305300	0.07827300
C	0.28388700	1.24711300	-0.22558300
C	1.02669200	-0.06108700	-0.38594000
C	0.19875900	-1.23208500	0.17100300
C	-1.27005400	-1.14222800	-0.25772700
H	-2.16859700	0.04586100	1.32596300
H	-2.86888000	0.33102500	-0.24889700
H	1.17611300	-0.23100300	-1.46342200
H	0.63728400	-2.18222400	-0.15134600
H	0.25582200	-1.21481300	1.26718400
H	-1.32576200	-1.15749900	-1.35276500
H	-1.82839600	-2.01363500	0.09760400
H	-1.45787200	2.32649700	0.20140600
C	2.41894600	0.00630300	0.26005600
H	2.96066800	-0.93414400	0.12169200

H	3.02185600	0.80726700	-0.17795600
H	2.33989400	0.19630500	1.33496900
H	0.86699300	2.15551500	-0.36304600

Eli-R26

C	0.94908200	-0.37004700	0.71278900
C	-0.45919900	-0.95500800	0.74108500
C	-1.39422000	-0.34762900	-0.32133200
C	-1.37990200	1.18758500	-0.22961100
C	0.04163700	1.75520000	-0.34545000
C	0.97687400	1.15598800	0.71299400
H	-0.99958700	-0.62552000	-1.30662200
H	-0.39981000	-2.04141000	0.62234600
H	-0.87304400	-0.76828500	1.74009900
H	1.56590700	-0.77193400	1.51972400
H	-2.01776100	1.60947800	-1.01334400
H	0.02715100	2.84469900	-0.24741000
H	2.00879000	1.48360600	0.56591900
H	0.67392700	1.48941700	1.71286400
H	-1.82127600	1.49379300	0.72925500
H	0.43918200	1.53666000	-1.34238400
O	1.56562700	-0.88064000	-0.53315200
O	2.85719100	-0.63440700	-0.58360900
C	-2.81048300	-0.91683800	-0.19658600
H	-2.81176900	-2.00679100	-0.29030400
H	-3.25064400	-0.66457900	0.77435100
H	-3.46633900	-0.51426200	-0.97372900

Eli-TS26

C	-1.54191100	0.96906300	-0.45992500
C	-0.24056700	1.75659000	-0.65140000
C	-0.08271800	-0.81953800	0.62285000
C	-1.28206100	-0.54006200	-0.30871100
H	0.29858100	1.37323100	-1.52492400
H	-2.05239900	1.33725200	0.44026200
H	-2.22391100	1.13900700	-1.29893400
H	0.83571300	-1.36207700	-0.14771600
H	-0.21774000	-1.65131000	1.31613300
H	-1.04081100	-0.92775100	-1.30729000
O	2.49349900	-0.36238800	-0.20390100
O	1.99855900	-1.40303200	-0.74649800
C	0.64344400	1.62572900	0.59324300
H	0.21143600	2.21811400	1.41491100
C	0.74595400	0.21104700	1.07424900
H	1.36969500	0.03733700	1.94425600

H	1.64330400	2.03550000	0.42244500
H	-0.45194000	2.81128100	-0.84837300
C	-2.53299600	-1.28189700	0.17741800
H	-3.37808000	-1.10585400	-0.49463600
H	-2.36280400	-2.36157400	0.22241400
H	-2.82238900	-0.94538900	1.17830400

Eli-P26

C	-1.91554500	0.15073900	0.26135300
C	-1.01087200	1.34305300	0.07827300
C	0.28388700	1.24711300	-0.22558300
C	1.02669200	-0.06108700	-0.38594000
C	0.19875900	-1.23208500	0.17100300
C	-1.27005400	-1.14222800	-0.25772700
H	-2.16859700	0.04586100	1.32596300
H	-2.86888000	0.33102500	-0.24889700
H	1.17611300	-0.23100300	-1.46342200
H	0.63728400	-2.18222400	-0.15134600
H	0.25582200	-1.21481300	1.26718400
H	-1.32576200	-1.15749900	-1.35276500
H	-1.82839600	-2.01363500	0.09760400
H	-1.45787200	2.32649700	0.20140600
C	2.41894600	0.00630300	0.26005600
H	2.96066800	-0.93414400	0.12169200
H	3.02185600	0.80726700	-0.17795600
H	2.33989400	0.19630500	1.33496900
H	0.86699300	2.15551500	-0.36304600

Eli-R27

C	0.94908200	-0.37004700	0.71278900
C	-0.45919900	-0.95500800	0.74108500
C	-1.39422000	-0.34762900	-0.32133200
C	-1.37990200	1.18758500	-0.22961100
C	0.04163700	1.75520000	-0.34545000
C	0.97687400	1.15598800	0.71299400
H	-0.99958700	-0.62552000	-1.30662200
H	-0.39981000	-2.04141000	0.62234600
H	-0.87304400	-0.76828500	1.74009900
H	1.56590700	-0.77193400	1.51972400
H	-2.01776100	1.60947800	-1.01334400
H	0.02715100	2.84469900	-0.24741000
H	2.00879000	1.48360600	0.56591900
H	0.67392700	1.48941700	1.71286400
H	-1.82127600	1.49379300	0.72925500
H	0.43918200	1.53666000	-1.34238400

O	1.56562700	-0.88064000	-0.53315200
O	2.85719100	-0.63440700	-0.58360900
C	-2.81048300	-0.91683800	-0.19658600
H	-2.81176900	-2.00679100	-0.29030400
H	-3.25064400	-0.66457900	0.77435100
H	-3.46633900	-0.51426200	-0.97372900

Eli-TS27

C	1.42931700	1.17668800	-0.18888700
C	1.33504700	-0.35203200	-0.31731000
C	-1.01448100	1.10334500	0.57626000
C	0.04820200	1.84591800	-0.24996000
H	0.77988400	-0.58321500	-1.23594300
H	1.91323200	1.41611600	0.76740700
H	2.07244100	1.58439200	-0.97531500
H	-1.87303800	0.62987300	-0.30105300
H	-1.69990000	1.73287200	1.14412200
H	-0.27250600	1.91359800	-1.29594700
H	0.12129700	2.87723400	0.10734500
O	-2.02647100	-1.30034500	-0.28130500
O	-2.49572700	-0.32215900	-0.94880000
C	0.52906500	-0.90466800	0.86844600
H	1.14612000	-0.84733800	1.78010300
C	-0.73335100	-0.14478400	1.13620800
H	-1.35816700	-0.51064400	1.94345700
C	2.71283500	-1.01188400	-0.41134000
H	3.31731500	-0.78543800	0.47376500
H	2.62849200	-2.09991500	-0.48825000
H	3.26082700	-0.65659800	-1.28851700
H	0.30178100	-1.96639700	0.72916100

Eli-P27

C	1.29462600	-1.22880100	-0.10975700
C	1.92065000	0.14097700	-0.05216900
C	1.21312300	1.26511400	0.05644000
C	-0.29372200	1.29921800	0.10331600
C	-0.93657700	-0.02986100	-0.33123500
C	-0.18252200	-1.20605200	0.30899900
H	1.39143200	-1.63135600	-1.12808000
H	1.85693700	-1.91832600	0.53067700
H	-0.62224000	1.55189100	1.12278100
H	-0.66330300	2.11397200	-0.53133000
H	-0.81379700	-0.11329500	-1.42000100
H	-0.24847600	-1.11358100	1.40078700
H	-0.66411800	-2.15327800	0.04443500
H	3.00532900	0.19351200	-0.10122800

C	-2.43408700	-0.06306300	-0.01527600
H	-2.95667500	0.78300500	-0.47223400
H	-2.89817500	-0.98165000	-0.38647400
H	-2.60660100	-0.01549800	1.06536800
H	1.73073700	2.21941400	0.11339100

Eli-R28

C	-1.23677300	0.36356000	0.59526000
C	-0.27029100	1.54042600	0.51147900
C	0.99096300	1.20850800	-0.29896500
C	1.69152100	-0.06601600	0.20435900
C	0.69963700	-1.24220600	0.20565500
C	-0.56523100	-0.93979800	1.02005800
H	0.71936600	1.07360100	-1.35242100
H	-0.78881100	2.40449200	0.08616000
H	0.00577100	1.80978700	1.53753200
H	-2.09354600	0.58890000	1.23420300
H	1.18208900	-2.14103600	0.60315700
H	-1.294444000	-1.74907300	0.93459300
H	-0.31413800	-0.84749900	2.08355200
H	1.68208900	2.05688200	-0.26061000
H	2.00216600	0.11124800	1.24496100
H	0.41818000	-1.47154500	-0.82898800
O	-1.79948900	0.21601100	-0.76639900
O	-2.80539900	-0.63144600	-0.79826400
C	2.94412300	-0.38352000	-0.61679600
H	3.45253300	-1.27391300	-0.23537100
H	2.68698000	-0.56987100	-1.66474500
H	3.65716800	0.44578300	-0.59101300

Eli-TS28

C	-1.71122100	0.01654100	0.17488500
C	-0.90319900	1.10957000	-0.54243500
C	0.58860000	-0.80560200	1.00080300
C	-0.80696500	-1.19167900	0.48292300
H	-0.48000200	0.70174300	-1.46847300
H	-2.04611000	0.43612900	1.13428700
H	1.42578100	-1.19141600	0.06326400
H	0.97497600	-1.41488700	1.81819500
H	-0.71378700	-1.79954300	-0.42601300
H	-1.29703200	-1.83321900	1.22184300
O	2.46192800	0.25558900	-0.69999900
O	2.31538300	-0.99717700	-0.87791500
C	0.22589500	1.63070000	0.35276200
H	-0.20071000	2.23499800	1.16850700

C	1.01300800	0.52506000	0.98526600
H	1.84915800	0.81671100	1.61104200
H	0.89553500	2.29989300	-0.19560000
C	-2.95021500	-0.40394000	-0.61954000
H	-3.62532900	0.44207000	-0.77814700
H	-2.66851500	-0.79581100	-1.60256700
H	-3.51088500	-1.18582400	-0.09843700
H	-1.55698700	1.93795100	-0.83257100

Eli-P28

C	1.29462600	-1.22880100	-0.10975700
C	1.92065000	0.14097700	-0.05216900
C	1.21312300	1.26511400	0.05644000
C	-0.29372200	1.29921800	0.10331600
C	-0.93657700	-0.02986100	-0.33123500
C	-0.18252200	-1.20605200	0.30899900
H	1.39143200	-1.63135600	-1.12808000
H	1.85693700	-1.91832600	0.53067700
H	-0.62224000	1.55189100	1.12278100
H	-0.66330300	2.11397200	-0.53133300
H	-0.81379700	-0.11329500	-1.42000100
H	-0.24847600	-1.11358100	1.40078700
H	-0.66411800	-2.15327800	0.04443500
H	3.00532900	0.19351200	-0.10122800
C	-2.43408700	-0.06306300	-0.01527600
H	-2.95667500	0.78300500	-0.47223400
H	-2.89817500	-0.98165000	-0.38647400
H	-2.60660100	-0.01549800	1.06536800
H	1.73073700	2.21941400	0.11339100

Eli-R29

C	0.54742700	1.27452700	-0.65424700
C	-0.66170600	2.14842300	-0.28981700
C	-1.92870800	1.30538300	-0.09514900
C	-1.70684600	0.19324600	0.93841800
C	-0.47817800	-0.65585600	0.62016000
C	0.79679500	0.16508100	0.38684700
H	-2.76556100	1.93684500	0.21785200
H	-0.44505800	2.69946500	0.63494100
H	-0.82507400	2.90091700	-1.06752900
H	0.38387800	0.81285300	-1.63494500
H	1.43995200	1.89903600	-0.74679200
H	-1.55786400	0.62881000	1.93376400
H	-2.57532200	-0.46680500	1.00505400
H	-0.32000600	-1.41734000	1.38801600

H	0.99825700	0.65237200	1.35228200
H	-2.21674200	0.85529200	-1.05132400
C	2.00199100	-0.73643100	0.05884300
H	1.85503700	-1.18894200	-0.92670700
H	2.01636300	-1.56764800	0.77407000
O	-0.72325300	-1.41324300	-0.62706200
O	-1.61182900	-2.36933400	-0.45691600
C	3.35598600	-0.02128000	0.10666000
H	4.17191600	-0.72723100	-0.06859600
H	3.43535200	0.76104800	-0.65213900
H	3.52497000	0.44338300	1.08358500

Eli-TS29

C	-0.69092500	2.15661100	-0.34334900
C	0.47282800	1.23326700	-0.72565000
C	-1.68157000	0.09057100	0.80330800
C	-1.96345300	1.36016300	-0.01756200
H	0.19347500	0.61414600	-1.58693900
H	1.33864700	1.82717700	-1.02875200
H	-0.39576100	2.74897900	0.53160500
H	-0.89521700	2.86977800	-1.14729400
H	-1.99892500	-0.90144500	0.02375200
H	-2.38817700	-0.11933000	1.60731100
H	-2.46832100	1.09072200	-0.95246200
H	-2.66751600	1.99252900	0.53091600
C	1.99533100	-0.66765400	0.14793600
H	2.07886100	-1.36897500	0.98591400
H	1.72544300	-1.26988900	-0.72294700
O	-0.54130500	-2.12448700	-0.37205600
O	-1.76466700	-1.98207400	-0.69552500
C	0.84946200	0.31906300	0.45070900
H	1.20941200	0.97287500	1.26699900
C	-0.37091700	-0.34295400	1.02934900
H	-0.19213800	-1.05776300	1.82646400
C	3.35278000	0.00565000	-0.07681100
H	4.13279000	-0.74364100	-0.23495500
H	3.34794800	0.65799400	-0.95376800
H	3.64603900	0.61103200	0.78722700

Eli-P29

C	2.37655500	-0.18579500	-0.26435100
C	1.74222800	1.16892400	-0.07957600
C	0.45662100	1.34463000	0.22647700
C	-0.54946700	0.22529800	0.38286500
C	0.01648700	-1.09555900	-0.16988300
C	1.47333300	-1.31108800	0.25820100

H	2.59984400	-0.34264500	-1.32922300
H	3.34718500	-0.21034800	0.24455700
H	-0.73908300	0.09211200	1.46037000
H	-0.59942600	-1.93789400	0.15710900
H	-0.03766000	-1.07140300	-1.26647400
H	1.52482900	-1.33357100	1.35335300
H	1.83555600	-2.28220700	-0.09294400
H	2.38498300	2.03761300	-0.19942100
C	-1.89602000	0.61622000	-0.26188300
H	-2.19619600	1.59424300	0.13225400
H	-1.74384500	0.75672100	-1.33913600
H	0.07850300	2.35528600	0.36767200
C	-3.03106300	-0.38502200	-0.02518000
H	-3.97027300	-0.01587500	-0.44600000
H	-2.82515700	-1.35397600	-0.48688900
H	-3.19130600	-0.55371200	1.04474700

Eli-R30

C	1.42690300	-0.35968900	0.68994400
C	-0.00078700	-0.82428200	0.95563400
C	-1.03649100	-0.21925100	-0.01159500
C	-0.89786400	1.31354700	-0.04100600
C	0.53037200	1.75495100	-0.39143700
C	1.56343900	1.15522300	0.57041200
H	-0.80948600	-0.59611500	-1.01784800
H	-0.03517900	-1.91744200	0.91438600
H	-0.25293800	-0.53909500	1.98492300
H	2.12234600	-0.75786000	1.43228000
H	-1.59990700	1.74348500	-0.76054800
H	0.60488400	2.84638100	-0.37521400
H	2.58407600	1.38833200	0.25770400
H	1.43104600	1.57693000	1.57404000
H	-1.17506100	1.71517400	0.94417100
H	0.76618200	1.44199500	-1.41427100
O	1.82043400	-0.99908400	-0.58668600
O	3.10540100	-0.86170200	-0.83419900
C	-2.45337000	-0.69100700	0.35825200
H	-2.43371300	-1.78001700	0.48442900
H	-2.72143600	-0.27693600	1.33905600
C	-3.53673100	-0.33311600	-0.66462200
H	-3.66670800	0.74730700	-0.76582200
H	-3.29059000	-0.73279400	-1.65339900
H	-4.50303500	-0.75131700	-0.37029900

Eli-TS30

C	-0.95432800	1.27216900	-0.35660200
C	0.45288500	1.78967600	-0.67931600
C	0.23749500	-0.71297200	0.71001000
C	-0.97178100	-0.25154000	-0.13231100
H	0.84216900	1.27502100	-1.56489600
H	-1.31858700	1.77312500	0.55108700
H	-1.64601100	1.53755600	-1.16037700
H	0.97037300	-1.43870000	-0.10514600
H	0.01469700	-1.48353100	1.45007800
H	-0.90620600	-0.72612400	-1.12155500
O	2.77587700	-0.77229200	-0.33061800
O	2.05332600	-1.71620800	-0.78838300
C	1.39399300	1.54913200	0.50484600
H	1.14192500	2.24198500	1.32291200
C	1.27564100	0.15871200	1.04756300
H	1.92794900	-0.09972700	1.87444400
H	2.43473000	1.76100800	0.24260300
H	0.42377300	2.85577700	-0.92127900
C	-2.28096600	-0.74228600	0.51425000
H	-2.19594000	-1.82113700	0.68974400
H	-2.38099600	-0.27942900	1.50430500
C	-3.54137600	-0.47321200	-0.31332900
H	-4.42120900	-0.91018300	0.16635600
H	-3.73224800	0.59605400	-0.43403500
H	-3.45742000	-0.91176700	-1.31290200

Eli-P30

C	2.37655500	-0.18579500	-0.26435100
C	1.74222800	1.16892400	-0.07957600
C	0.45662100	1.34463000	0.22647700
C	-0.54946700	0.22529800	0.38286500
C	0.01648700	-1.09555900	-0.16988300
C	1.47333300	-1.31108800	0.25820100
H	2.59984400	-0.34264500	-1.32922300
H	3.34718500	-0.21034800	0.24455700
H	-0.73908300	0.09211200	1.46037000
H	-0.59942600	-1.93789400	0.15710900
H	-0.03766000	-1.07140300	-1.26647400
H	1.52482900	-1.33357100	1.35335300
H	1.83555600	-2.28220700	-0.09294400
H	2.38498300	2.03761300	-0.19942100
C	-1.89602000	0.61622000	-0.26188300
H	-2.19619600	1.59424300	0.13225400
H	-1.74384500	0.75672100	-1.33913600
H	0.07850300	2.35528600	0.36767200

C	-3.03106300	-0.38502200	-0.02518000
H	-3.97027300	-0.01587500	-0.44600000
H	-2.82515700	-1.35397600	-0.48688900
H	-3.19130600	-0.55371200	1.04474700

Eli-R31

C	1.42690300	-0.35968900	0.68994400
C	-0.00078700	-0.82428200	0.95563400
C	-1.03649100	-0.21925100	-0.01159500
C	-0.89786400	1.31354700	-0.04100600
C	0.53037200	1.75495100	-0.39143700
C	1.56343900	1.15522300	0.57041200
H	-0.80948600	-0.59611500	-1.01784800
H	-0.03517900	-1.91744200	0.91438600
H	-0.25293800	-0.53909500	1.98492300
H	2.12234600	-0.75786000	1.43228000
H	-1.59990700	1.74348500	-0.76054800
H	0.60488400	2.84638100	-0.37521400
H	2.58407600	1.38833200	0.25770400
H	1.43104600	1.57693000	1.57404000
H	-1.17506100	1.71517400	0.94417100
H	0.76618200	1.44199500	-1.41427100
O	1.82043400	-0.99908400	-0.58668600
O	3.10540100	-0.86170200	-0.83419900
C	-2.45337000	-0.69100700	0.35825200
H	-2.43371300	-1.78001700	0.48442900
H	-2.72143600	-0.27693600	1.33905600
C	-3.53673100	-0.33311600	-0.66462200
H	-3.66670800	0.74730700	-0.76582200
H	-3.29059000	-0.73279400	-1.65339900
H	-4.50303500	-0.75131700	-0.37029900

Eli-TS31

C	0.91806600	1.36911600	0.00565500
C	1.00456200	-0.16411600	0.08705600
C	-1.60889600	1.08862500	0.32446000
C	-0.48499100	1.84310100	-0.40345900
H	0.65949400	-0.57873500	-0.87039000
H	1.17334700	1.78212700	0.99072400
H	1.65293700	1.76485900	-0.70024700
H	-2.23339200	0.40183100	-0.60789900
H	-2.44873800	1.69598900	0.66273200
H	-0.59950300	1.72960500	-1.48772900
H	-0.58531700	2.91380100	-0.20283400
O	-2.18966500	-1.51389900	-0.33002000

O	-2.62100800	-0.69575300	-1.20606600
C	0.04301900	-0.65394500	1.18125600
H	0.46390200	-0.40427700	2.16899100
C	-1.31632900	-0.03116300	1.10614600
H	-2.04465200	-0.36607100	1.83651600
C	2.42981900	-0.68199300	0.34160700
H	2.82912000	-0.19737100	1.24216800
H	2.37376200	-1.75216600	0.57343100
H	-0.04698800	-1.74482000	1.16359600
C	3.40189600	-0.48077800	-0.82548500
H	3.55102300	0.57656500	-1.05905000
H	4.38261300	-0.90436500	-0.59327600
H	3.03489900	-0.97283800	-1.73147100

Eli-P31

C	1.94112900	-1.02486500	-0.24460400
C	2.31830300	0.43130400	-0.15589900
C	1.43505300	1.39952600	0.08500300
C	-0.04394500	1.15965400	0.25942200
C	-0.48194300	-0.24624300	-0.19228900
C	0.53319600	-1.28730600	0.30729800
H	2.00480600	-1.35602900	-1.29086200
H	2.67676400	-1.63016900	0.29791300
H	-0.31683900	1.30865300	1.31537800
H	-0.59767100	1.92497800	-0.29540100
H	-0.45792200	-0.26226000	-1.29183700
H	0.56323900	-1.25262900	1.40388900
H	0.20403500	-2.29533500	0.03399200
H	3.36638300	0.68396500	-0.29496900
C	-1.91160700	-0.59419600	0.25262600
H	-2.12659600	-1.62562700	-0.05085100
H	-1.95336900	-0.58602900	1.34961200
H	1.77722500	2.42892800	0.15745400
C	-3.00251800	0.32547000	-0.30711300
H	-3.99576200	-0.01808400	-0.00545200
H	-2.89238800	1.35407200	0.04596400
H	-2.97791100	0.34550300	-1.40149300

Eli-R32

C	-1.67016200	0.39116700	0.58307900
C	-0.61448100	1.49067900	0.59712200
C	0.65742600	1.10076900	-0.17154700
C	1.23843000	-0.24418300	0.30156800
C	0.15825700	-1.33666200	0.20166200
C	-1.11801800	-0.97674900	0.97333100

H	0.42579000	1.03070300	-1.24098900
H	-1.04527200	2.41045400	0.19088600
H	-0.36828300	1.69301200	1.64595500
H	-2.53611200	0.65377900	1.19489300
H	0.55240000	-2.28719800	0.57549200
H	-1.89962600	-1.72406200	0.81637100
H	-0.91096600	-0.95188100	2.04994300
H	1.39513400	1.90035900	-0.06278000
H	1.51188300	-0.13886100	1.36321100
H	-0.09023200	-1.49653700	-0.85424100
O	-2.17908600	0.34727400	-0.80660700
O	-3.24179600	-0.42016000	-0.92109700
C	2.50624900	-0.64927900	-0.46944600
H	2.78705900	-1.66354400	-0.16195200
H	2.26570400	-0.71286600	-1.53821700
C	3.70940100	0.27839500	-0.26776200
H	3.52115400	1.28536700	-0.64853500
H	3.96611800	0.36616000	0.79291000
H	4.58970600	-0.10663300	-0.78935900

Eli-TS32

C	-1.25882200	-0.18244500	0.32106900
C	-0.58781200	1.02033200	-0.36191100
C	1.15225300	-0.86855400	0.93069500
C	-0.24085900	-1.32863600	0.47097600
H	-0.19606100	0.71002300	-1.33824700
H	-1.55409300	0.13640500	1.33197300
H	1.95365100	-1.11120500	-0.08376000
H	1.63895600	-1.50342200	1.67147200
H	-0.16361000	-1.85624700	-0.48830400
H	-0.62612600	-2.06342500	1.18481000
O	2.82281300	0.46943400	-0.78876200
O	2.76171000	-0.77429300	-1.05750800
C	0.55635400	1.56792500	0.49876000
H	0.14063300	2.07732200	1.38214400
C	1.46887600	0.49018900	0.99588200
H	2.31876300	0.80444200	1.59146500
H	1.13303000	2.32646800	-0.03891900
C	-2.52307500	-0.66974400	-0.40692600
H	-2.26791500	-0.88744700	-1.45183700
H	-2.83025100	-1.62581600	0.03365200
H	-1.31132000	1.81740400	-0.55055300
C	-3.70863800	0.29960400	-0.35632400
H	-3.48444600	1.25049900	-0.84655000
H	-4.58186300	-0.12602700	-0.85785200

H -3.99519200 0.51786500 0.67733700

Eli-P32

C	1.94112900	-1.02486500	-0.24460400
C	2.31830300	0.43130400	-0.15589900
C	1.43505300	1.39952600	0.08500300
C	-0.04394500	1.15965400	0.25942200
C	-0.48194300	-0.24624300	-0.19228900
C	0.53319600	-1.28730600	0.30729800
H	2.00480600	-1.35602900	-1.29086200
H	2.67676400	-1.63016900	0.29791300
H	-0.31683900	1.30865300	1.31537800
H	-0.59767100	1.92497800	-0.29540100
H	-0.45792200	-0.26226000	-1.29183700
H	0.56323900	-1.25262900	1.40388900
H	0.20403500	-2.29533500	0.03399200
H	3.36638300	0.68396500	-0.29496900
C	-1.91160700	-0.59419600	0.25262600
H	-2.12659600	-1.62562700	-0.05085100
H	-1.95336900	-0.58602900	1.34961200
H	1.77722500	2.42892800	0.15745400
C	-3.00251800	0.32547000	-0.30711300
H	-3.99576200	-0.01808400	-0.00545200
H	-2.89238800	1.35407200	0.04596400
H	-2.97791100	0.34550300	-1.40149300

Eli-R33

C	-0.82882500	0.67908400	0.62567500
C	0.31600200	-0.31913200	0.41030600
C	-0.07599300	-1.37889600	-0.63976400
C	-1.40782000	-2.06434400	-0.30065500
C	-2.53953300	-1.04373400	-0.12713400
C	-2.17553500	0.02050900	0.91705400
H	-0.15101600	-0.89701500	-1.62161000
H	0.42626400	-0.83284700	1.37665600
H	-0.57437000	1.40601000	1.40093300
H	-1.66579600	-2.78358200	-1.08411200
H	-3.46747600	-1.54415300	0.16506600
H	-2.93711200	0.80247200	0.97089000
H	-2.11204900	-0.43498600	1.91257500
H	0.71486500	-2.12938500	-0.71844500
H	-1.29286400	-2.64187900	0.62605300
H	-2.73618500	-0.55280600	-1.08628800
O	-0.93755100	1.46882000	-0.62083100
O	-1.67629500	2.54618600	-0.45936800

C	1.64559700	0.39593800	0.10626200
H	1.77671200	1.20878500	0.83226500
H	1.58158400	0.87620000	-0.87602300
C	2.88489600	-0.50662300	0.15791800
H	2.80762200	-1.29299000	-0.59982900
H	2.92023800	-1.01801900	1.12809900
C	4.18870100	0.26794000	-0.05710500
H	4.32298800	1.03818600	0.70869600
H	4.19532300	0.76668200	-1.03107500
H	5.05710300	-0.39516800	-0.01759400

Eli-TS33

C	1.44784500	-2.06355100	-0.36659400
C	0.13943600	-1.33884400	-0.70517700
C	2.13661900	0.12708900	0.76546900
C	2.58640600	-1.07270000	-0.08522600
H	0.28581200	-0.68573000	-1.57428100
H	-0.63056800	-2.06411600	-0.97944600
H	1.28267100	-2.69220100	0.51715100
H	1.73434700	-2.73742100	-1.17932800
H	2.27173100	1.16717900	-0.00504000
H	2.82622800	0.43486100	1.55253100
H	2.99735900	-0.71749100	-1.03734900
H	3.40861100	-1.58472300	0.42294700
C	-1.62918100	0.30714000	0.22112000
H	-1.78978900	0.99797200	1.05808100
H	-1.48508500	0.93526800	-0.66262600
O	0.62922800	2.15023700	-0.34003200
O	1.84998900	2.20610600	-0.69821600
C	-0.33863000	-0.49330200	0.48657500
H	-0.56983400	-1.19578900	1.30884600
C	0.78184300	0.34670100	1.03635500
H	0.51895100	1.01666600	1.84888800
C	-2.88443200	-0.55672100	0.04821500
H	-2.76328600	-1.22781200	-0.80881300
H	-3.00559900	-1.20199400	0.92746900
C	-4.15260800	0.27944800	-0.14827400
H	-5.03419200	-0.35573600	-0.26987700
H	-4.33107700	0.93587400	0.70908500
H	-4.07380000	0.91288700	-1.03702600

Eli-P33

C	-2.88358200	-0.15031600	0.36534900
C	-2.23607400	1.19068200	0.13288300
C	-0.96841600	1.33986400	-0.25190600
C	0.00488400	0.20012800	-0.46235800

C	-0.55176900	-1.10632000	0.13288100
C	-2.03585600	-1.29562000	-0.20446200
H	-3.04335100	-0.29698900	1.44307500
H	-3.88421600	-0.15885300	-0.08228200
H	0.12391900	0.05779600	-1.54865200
H	0.02682200	-1.96220600	-0.22545600
H	-0.43112100	-1.07743000	1.22397200
H	-2.15447300	-1.32248000	-1.29426400
H	-2.39438400	-2.25775900	0.17418800
H	-2.85343600	2.07241000	0.28648400
C	1.39507500	0.56980800	0.09572300
H	1.68861900	1.54127300	-0.32232400
H	1.31372600	0.71896700	1.18042400
H	-0.58023700	2.34218300	-0.42196500
C	2.50555700	-0.44572400	-0.19978800
H	2.26833600	-1.40654700	0.26866700
H	2.54379900	-0.63292200	-1.28021500
C	3.88122000	0.02211500	0.28536800
H	3.88172700	0.19277900	1.36651400
H	4.65536700	-0.71844100	0.06627000
H	4.17267100	0.96052300	-0.19657600

Eli-R34

C	1.87809700	-0.41490400	0.68489100
C	0.42077500	-0.74945100	0.98321500
C	-0.57712800	-0.07748700	0.01983700
C	-0.30717100	1.43681200	-0.04609600
C	1.14767600	1.74590900	-0.42801200
C	2.14180900	1.07989900	0.53126800
H	-0.40072800	-0.49316500	-0.98106800
H	0.29214700	-1.83622100	0.96637000
H	0.21301500	-0.42294300	2.00996700
H	2.54970000	-0.85678700	1.42446300
H	-0.98140300	1.91037400	-0.76484900
H	1.31574600	2.82693800	-0.43808500
H	3.17337900	1.21874100	0.19892400
H	2.06216200	1.53166500	1.52747300
H	-0.53245900	1.88186600	0.93353000
H	1.33788500	1.39151400	-1.44681900
O	2.19321600	-1.11075900	-0.58387300
O	3.48086300	-1.09024100	-0.85376100
C	-2.02127400	-0.41867100	0.42485000
H	-2.09236300	-1.50309700	0.57939500
H	-2.23756900	0.04003900	1.39975500

C	-3.09981000	-0.00181400	-0.58325100
H	-3.09135400	1.08510200	-0.71502100
H	-2.85903900	-0.43105500	-1.56334800
C	-4.50548200	-0.44356800	-0.16444600
H	-4.78691800	-0.00595800	0.79848700
H	-4.56462900	-1.53165000	-0.06243500
H	-5.25515900	-0.13770800	-0.89920000

Eli-TS34

C	-0.32395400	1.44208600	-0.36490600
C	1.14073300	1.79832200	-0.64702400
C	0.60077600	-0.68630500	0.68826700
C	-0.52103100	-0.07430500	-0.17994500
H	1.48682300	1.25906200	-1.53591200
H	-0.64900800	1.96081900	0.54754100
H	-0.96113700	1.80400000	-1.17603200
H	1.26334300	-1.48602900	-0.11768200
H	0.26894000	-1.43249200	1.41221100
H	-0.47159100	-0.53058800	-1.17862100
O	3.13771900	-1.02959400	-0.29909500
O	2.32125500	-1.87919700	-0.78292200
C	2.02120900	1.42696700	0.54951400
H	1.83720900	2.13086200	1.37617500
C	1.72577000	0.05229100	1.06345900
H	2.32207700	-0.29369300	1.90069200
H	3.08511100	1.51660300	0.31103900
H	1.24152000	2.86499900	-0.86627600
C	-1.89839600	-0.43084300	0.40934500
H	-1.93935000	-1.51685200	0.56253000
H	-1.98715200	0.02024100	1.40692100
C	-3.09851800	-0.01477300	-0.44978900
H	-3.12030100	1.07442600	-0.55917500
H	-2.97437300	-0.42179700	-1.46092700
C	-4.43523300	-0.48788100	0.12951200
H	-5.27419200	-0.17791200	-0.49930900
H	-4.46712700	-1.57871600	0.21237800
H	-4.60072400	-0.07597700	1.12999400

Eli-P34

C	-2.88358200	-0.15031600	0.36534900
C	-2.23607400	1.19068200	0.13288300
C	-0.96841600	1.33986400	-0.25190600
C	0.00488400	0.20012800	-0.46235800
C	-0.55176900	-1.10632000	0.13288100
C	-2.03585600	-1.29562000	-0.20446200
H	-3.04335100	-0.29698900	1.44307500

H	-3.88421600	-0.15885300	-0.08228200
H	0.12391900	0.05779600	-1.54865200
H	0.02682200	-1.96220600	-0.22545600
H	-0.43112100	-1.07743000	1.22397200
H	-2.15447300	-1.32248000	-1.29426400
H	-2.39438400	-2.25775900	0.17418800
H	-2.85343600	2.07241000	0.28648400
C	1.39507500	0.56980800	0.09572300
H	1.68861900	1.54127300	-0.32232400
H	1.31372600	0.71896700	1.18042400
H	-0.58023700	2.34218300	-0.42196500
C	2.50555700	-0.44572400	-0.19978800
H	2.26833600	-1.40654700	0.26866700
H	2.54379900	-0.63292200	-1.28021500
C	3.88122000	0.02211500	0.28536800
H	3.88172700	0.19277900	1.36651400
H	4.65536700	-0.71844100	0.06627000
H	4.17267100	0.96052300	-0.19657600

Eli-R35

C	1.87809700	-0.41490400	0.68489100
C	0.42077500	-0.74945100	0.98321500
C	-0.57712800	-0.07748700	0.01983700
C	-0.30717100	1.43681200	-0.04609600
C	1.14767600	1.74590900	-0.42801200
C	2.14180900	1.07989900	0.53126800
H	-0.40072800	-0.49316500	-0.98106800
H	0.29214700	-1.83622100	0.96637000
H	0.21301500	-0.42294300	2.00996700
H	2.54970000	-0.85678700	1.42446300
H	-0.98140300	1.91037400	-0.76484900
H	1.31574600	2.82693800	-0.43808500
H	3.17337900	1.21874100	0.19892400
H	2.06216200	1.53166500	1.52747300
H	-0.53245900	1.88186600	0.93353000
H	1.33788500	1.39151400	-1.44681900
O	2.19321600	-1.11075900	-0.58387300
O	3.48086300	-1.09024100	-0.85376100
C	-2.02127400	-0.41867100	0.42485000
H	-2.09236300	-1.50309700	0.57939500
H	-2.23756900	0.04003900	1.39975500
C	-3.09981000	-0.00181400	-0.58325100
H	-3.09135400	1.08510200	-0.71502100
H	-2.85903900	-0.43105500	-1.56334800

C	-4.50548200	-0.44356800	-0.16444600
H	-4.78691800	-0.00595800	0.79848700
H	-4.56462900	-1.53165000	-0.06243500
H	-5.25515900	-0.13770800	-0.89920000

Eli-TS35

C	0.29210200	1.52433600	-0.02144900
C	0.54338700	0.01718500	0.15569000
C	-2.20024800	0.97918900	0.21957100
C	-1.13593000	1.81554300	-0.50840200
H	0.28651300	-0.48673100	-0.78620700
H	0.45784200	2.01722500	0.94582600
H	1.00872400	1.96028000	-0.72234800
H	-2.69758800	0.17266900	-0.69271500
H	-3.11822600	1.50398700	0.48512100
H	-1.19107400	1.63374400	-1.58801400
H	-1.36169300	2.87730100	-0.37246100
O	-2.45963400	-1.70662900	-0.29072200
O	-2.93401900	-0.99511500	-1.23504100
C	-0.40497700	-0.51333600	1.24281800
H	-0.05574000	-0.16199700	2.22761700
C	-1.82018400	-0.05269800	1.08036100
H	-2.53816100	-0.42559800	1.80249900
C	2.00381700	-0.32392500	0.49437300
H	2.31791000	0.26840200	1.36501500
H	2.05248100	-1.37383000	0.81068000
H	-0.37443500	-1.60653400	1.28914300
C	3.00328100	-0.11700600	-0.65074100
H	2.99752700	0.93035200	-0.97072200
H	2.67820000	-0.70358300	-1.51836100
C	4.43232300	-0.51724700	-0.27137500
H	5.12290300	-0.36943600	-1.10596000
H	4.79879200	0.07644300	0.57196000
H	4.48381700	-1.57097800	0.01995000

Eli-P35

C	2.44786400	-1.05449600	-0.23013200
C	2.85657400	0.39293800	-0.13692000
C	1.99215800	1.38060300	0.09305500
C	0.50600000	1.17383400	0.24868500
C	0.04211700	-0.22203900	-0.20831000
C	1.02791500	-1.28519000	0.30441900
H	2.51715000	-1.38740900	-1.27550000
H	3.16301100	-1.67589600	0.32154000
H	0.22293200	1.32956200	1.30092900
H	-0.02324000	1.95099800	-0.31347800

H	0.08067700	-0.23958400	-1.30731100
H	1.04499000	-1.25040100	1.40126900
H	0.67977000	-2.28578500	0.02742100
H	3.91168700	0.62201200	-0.26309300
C	-1.39967700	-0.53993600	0.21879200
H	-1.63254700	-1.56895300	-0.08424900
H	-1.45800800	-0.52766500	1.31603800
H	2.35603900	2.40223400	0.16978800
C	-2.47482300	0.39245100	-0.35450600
H	-2.30361400	1.41796300	-0.01060600
H	-2.38358900	0.41722200	-1.44750900
C	-3.89582600	-0.03306400	0.02806000
H	-4.02673800	-0.04084400	1.11474800
H	-4.64335100	0.64609900	-0.39101300
H	-4.11898600	-1.04014500	-0.33783500

Eli-R36

C	-2.20007600	0.39314400	0.49020100
C	-1.17492500	1.52005900	0.53599100
C	0.16510700	1.12953400	-0.10696000
C	0.73644400	-0.17584500	0.47506000
C	-0.30703200	-1.30060300	0.34328600
C	-1.65058600	-0.93913500	0.99065200
H	0.02536300	1.00497400	-1.18728000
H	-1.59200900	2.40811500	0.05234300
H	-1.02063300	1.77728500	1.59037600
H	-3.11915300	0.66043100	1.01651200
H	0.07707900	-2.22134300	0.79408000
H	-2.39900500	-1.71399500	0.80759200
H	-1.53356500	-0.85852100	2.07807300
H	0.87199300	1.95306200	0.02408500
H	0.92197200	-0.01467100	1.54847500
H	-0.46481600	-1.51704600	-0.71996000
O	-2.59201100	0.27016000	-0.93210000
O	-3.62391100	-0.53005000	-1.09425800
C	2.06963500	-0.58350400	-0.17554000
H	2.34809700	-1.57736400	0.19773700
H	1.91732800	-0.69945500	-1.25717500
C	3.24197300	0.37488900	0.07176200
H	3.01265500	1.36316500	-0.34003000
H	3.36946900	0.51556400	1.15228200
C	4.55674800	-0.12455800	-0.53532400
H	4.47008000	-0.24531300	-1.61962500
H	4.84345300	-1.09440800	-0.11715400

H 5.37533800 0.57475700 -0.34422500

Eli-TS36

C -0.75394100 -0.09386300 0.48735400
C -0.10506300 1.03992100 -0.32470700
C 1.67796300 -0.81978300 0.95320300
C 0.24070000 -1.26138500 0.63203400
H 0.19759300 0.65410300 -1.30581500
H -0.95639700 0.29820200 1.49519500
H 2.39007400 -1.15452700 -0.10033000
H 2.20242500 -1.42103700 1.69627000
H 0.22787000 -1.84958600 -0.29454300
H -0.10761700 -1.93760700 1.41900600
O 3.24657800 0.34658700 -0.97482000
O 3.12865300 -0.90912600 -1.15379200
C 1.11966000 1.60213400 0.40536500
H 0.79063900 2.18247500 1.28150800
C 2.03701300 0.52897400 0.90277500
H 2.93964700 0.85254900 1.40904600
H 1.67353300 2.30339600 -0.22589100
C -2.08647500 -0.58386000 -0.10325200
H -1.93180400 -0.85586100 -1.15601300
H -2.37388600 -1.51161200 0.40821700
H -0.81799200 1.84746400 -0.50901100
C -3.25159900 0.40830200 0.00227000
H -3.00845100 1.33231900 -0.53297000
H -3.38719600 0.69082600 1.05349400
C -4.56575400 -0.15660900 -0.54582100
H -5.38073600 0.56621200 -0.45234000
H -4.47317500 -0.41742600 -1.60464400
H -4.86140500 -1.06257500 -0.00761300

Eli-P36

C 2.44786400 -1.05449600 -0.23013200
C 2.85657400 0.39293800 -0.13692000
C 1.99215800 1.38060300 0.09305500
C 0.50600000 1.17383400 0.24868500
C 0.04211700 -0.22203900 -0.20831000
C 1.02791500 -1.28519000 0.30441900
H 2.51715000 -1.38740900 -1.27550000
H 3.16301100 -1.67589600 0.32154000
H 0.22293200 1.32956200 1.30092900
H -0.02324000 1.95099800 -0.31347800
H 0.08067700 -0.23958400 -1.30731100
H 1.04499000 -1.25040100 1.40126900
H 0.67977000 -2.28578500 0.02742100

H	3.91168700	0.62201200	-0.26309300
C	-1.39967700	-0.53993600	0.21879200
H	-1.63254700	-1.56895300	-0.08424900
H	-1.45800800	-0.52766500	1.31603800
H	2.35603900	2.40223400	0.16978800
C	-2.47482300	0.39245100	-0.35450600
H	-2.30361400	1.41796300	-0.01060600
H	-2.38358900	0.41722200	-1.44750900
C	-3.89582600	-0.03306400	0.02806000
H	-4.02673800	-0.04084400	1.11474800
H	-4.64335100	0.64609900	-0.39101300
H	-4.11898600	-1.04014500	-0.33783500

Eli-R37

C	-1.33970500	0.66002100	0.62423100
C	-0.13768100	-0.26704500	0.40249000
C	-0.47052300	-1.34729400	-0.64704000
C	-1.75611700	-2.11275900	-0.30071800
C	-2.94731200	-1.16346500	-0.11714300
C	-2.64153300	-0.07916900	0.92472900
H	-0.58073900	-0.86925200	-1.62736500
H	0.00749100	-0.77407300	1.36774400
H	-1.12517400	1.40195800	1.39736700
H	-1.97501000	-2.84531300	-1.08377400
H	-3.83977600	-1.72098600	0.18232300
H	-3.44940400	0.65436100	0.98446500
H	-2.54280600	-0.53036500	1.91934400
H	0.36461100	-2.04761800	-0.73141700
H	-1.59970100	-2.68368400	0.62403600
H	-3.18268000	-0.68596700	-1.07442500
O	-1.50360700	1.44030600	-0.62224300
O	-2.30740900	2.46957800	-0.45781100
C	1.14419000	0.52882200	0.09454400
H	1.22119900	1.35294600	0.81551400
H	1.05022000	0.99808900	-0.89055700
C	2.43784400	-0.29256000	0.15435700
H	2.41725200	-1.08425700	-0.60324300
H	2.50205300	-0.80051000	1.12605100
C	3.69767800	0.55691700	-0.05213700
H	3.73087500	1.34378400	0.71110800
H	3.62904400	1.07355200	-1.01689000
C	4.99275000	-0.25828300	-0.00013800
H	5.87036200	0.37747000	-0.14508500
H	5.10450200	-0.76285000	0.96478900

H	5.00827400	-1.02747800	-0.77860800
Eli-TS37			
C	1.79485300	-2.11286300	-0.36921400
C	0.52375800	-1.31482400	-0.68626700
C	2.62892700	0.04062100	0.73799500
C	2.99417500	-1.18894700	-0.10991800
H	0.69117900	-0.67299700	-1.55996000
H	-0.29177100	-1.99500600	-0.94420900
H	1.60944200	-2.72966700	0.51888400
H	2.02778200	-2.80347700	-1.18496800
H	2.80608400	1.06452500	-0.04431800
H	3.35039800	0.31533300	1.50856600
H	3.41281300	-0.86515400	-1.06986000
H	3.79109500	-1.74618800	0.39090700
C	-1.12969700	0.43312100	0.26761300
H	-1.22583100	1.14230800	1.09886100
H	-0.97005800	1.04053400	-0.62772200
O	1.21461600	2.13578000	-0.35554800
O	2.42871000	2.12040400	-0.73936400
C	0.11763600	-0.44020200	0.51101100
H	-0.13679200	-1.12535200	1.34096100
C	1.29433700	0.33767600	1.03365300
H	1.08531700	1.02681900	1.84580400
C	-2.43797000	-0.35615000	0.13944000
H	-2.37958900	-1.04976400	-0.70748700
H	-2.57856800	-0.97750000	1.03423500
C	-3.66514100	0.54476200	-0.04455900
H	-3.73095000	1.24130000	0.79994200
H	-3.52516300	1.16459100	-0.93808400
C	-4.97663500	-0.23631600	-0.16525500
H	-5.82994200	0.43440700	-0.29734300
H	-4.95435900	-0.91739700	-1.02183600
H	-5.16314600	-0.83805300	0.72993600
Eli-P37			
C	-3.39498500	0.32457400	-0.36472700
C	-2.86517200	-1.06643200	-0.12735400
C	-1.61442200	-1.32252600	0.25645900
C	-0.54538700	-0.27093100	0.46028200
C	-0.99083600	1.07906100	-0.13279900
C	-2.45333900	1.39402200	0.20450700
H	-3.53927600	0.48192800	-1.44309300
H	-4.39218200	0.42015000	0.08048700
H	-0.40780400	-0.13964400	1.54572800
H	-0.34178600	1.88295100	0.22557200

H	-0.87334700	1.04113500	-1.22404100
H	-2.56926400	1.43155400	1.29427100
H	-2.72826900	2.38288100	-0.17508200
H	-3.55669300	-1.89231200	-0.27504700
C	0.80470100	-0.75762500	-0.10665600
H	1.01192700	-1.75504200	0.30135800
H	0.70612000	-0.88828300	-1.19214700
H	-1.31426400	-2.35378000	0.43129900
C	1.99983700	0.15418000	0.19494100
H	1.84334900	1.14005100	-0.25759100
H	2.06226700	0.32202900	1.27848900
C	3.33395400	-0.41393000	-0.30364000
H	3.26856900	-0.59186100	-1.38389300
H	3.50185400	-1.39583000	0.15537900
C	4.52856500	0.49761400	-0.00886900
H	5.46345600	0.06145800	-0.37140400
H	4.40969000	1.47377700	-0.48949000
H	4.63815700	0.67079700	1.06634000

Eli-R38

C	2.41547900	-0.41330200	0.61314300
C	0.98612300	-0.75039600	1.02279100
C	-0.08326900	-0.08201700	0.13689100
C	0.17553200	1.43302500	0.05112900
C	1.59671700	1.74706600	-0.43826400
C	2.66301600	1.08225800	0.44110800
H	0.02043200	-0.49727400	-0.87441400
H	0.85870400	-1.83743200	1.01745400
H	0.85694800	-0.42243700	2.06188100
H	3.14314200	-0.85413400	1.29831500
H	-0.55203700	1.90364400	-0.61562000
H	1.76045100	2.82862600	-0.45848500
H	3.66563400	1.22438600	0.03071100
H	2.65894300	1.53261400	1.44113300
H	0.02182000	1.87824600	1.04453300
H	1.71072600	1.39567000	-1.46953000
O	2.63271500	-1.10801700	-0.67655800
O	3.89561900	-1.08534400	-1.04513600
C	-1.49163700	-0.43092300	0.64730300
H	-1.54815500	-1.51758300	0.79092700
H	-1.63189100	0.01285900	1.64272100
C	-2.64501200	-0.00077100	-0.26761400
H	-2.65553700	1.08995700	-0.37468900
H	-2.47739200	-0.40522700	-1.27430100

C	-4.01798700	-0.46096500	0.23748100
H	-4.18041900	-0.06773100	1.24844100
H	-4.01878100	-1.55348200	0.33336200
C	-5.17314400	-0.02749500	-0.66934000
H	-6.13573400	-0.37339600	-0.28297600
H	-5.22214800	1.06264400	-0.75410900
H	-5.05628800	-0.43193700	-1.67957800

Eli-TS38

C	0.14990400	1.43583400	-0.31692200
C	1.60113300	1.79121600	-0.66231400
C	1.12404600	-0.69055400	0.69740500
C	-0.04032400	-0.07925500	-0.11350100
H	1.91052200	1.24781500	-1.56213800
H	-0.13607600	1.96026300	0.60526600
H	-0.52160700	1.79269000	-1.10214400
H	1.75212200	-1.48157200	-0.14289300
H	0.82888800	-1.44226500	1.43146900
H	-0.04665300	-0.54217800	-1.11017800
O	3.61797700	-1.02517900	-0.39802300
O	2.78199900	-1.87135300	-0.85367700
C	2.53058200	1.42624500	0.49865700
H	2.37654500	2.13096800	1.33073000
C	2.26197900	0.05081400	1.02535300
H	2.89566600	-0.29434700	1.83495600
H	3.58366900	1.51994000	0.21759500
H	1.69162500	2.85688000	-0.89076000
C	-1.38526300	-0.42684700	0.55220600
H	-1.42019000	-1.51136600	0.71603800
H	-1.41703300	0.03285800	1.54903900
C	-2.62771600	-0.01332300	-0.24531500
H	-2.65455200	1.07611200	-0.36139300
H	-2.55942100	-0.42744100	-1.26006400
C	-3.94012300	-0.47551600	0.39926300
H	-3.92381700	-1.56666500	0.50809900
H	-4.00479800	-0.07004600	1.41628400
C	-5.18199600	-0.06068700	-0.39484200
H	-5.16215600	-0.47847800	-1.40629600
H	-6.09959700	-0.40640200	0.08887200
H	-5.24627600	1.02792700	-0.48882500

Eli-P38

C	-3.39498500	0.32457400	-0.36472700
C	-2.86517200	-1.06643200	-0.12735400
C	-1.61442200	-1.32252600	0.25645900
C	-0.54538700	-0.27093100	0.46028200

C	-0.99083600	1.07906100	-0.13279900
C	-2.45333900	1.39402200	0.20450700
H	-3.53927600	0.48192800	-1.44309300
H	-4.39218200	0.42015000	0.08048700
H	-0.40780400	-0.13964400	1.54572800
H	-0.34178600	1.88295100	0.22557200
H	-0.87334700	1.04113500	-1.22404100
H	-2.56926400	1.43155400	1.29427100
H	-2.72826900	2.38288100	-0.17508200
H	-3.55669300	-1.89231200	-0.27504700
C	0.80470100	-0.75762500	-0.10665600
H	1.01192700	-1.75504200	0.30135800
H	0.70612000	-0.88828300	-1.19214700
H	-1.31426400	-2.35378000	0.43129900
C	1.99983700	0.15418000	0.19494100
H	1.84334900	1.14005100	-0.25759100
H	2.06226700	0.32202900	1.27848900
C	3.33395400	-0.41393000	-0.30364000
H	3.26856900	-0.59186100	-1.38389300
H	3.50185400	-1.39583000	0.15537900
C	4.52856500	0.49761400	-0.00886900
H	5.46345600	0.06145800	-0.37140400
H	4.40969000	1.47377700	-0.48949000
H	4.63815700	0.67079700	1.06634000

Eli-R39

C	2.41547900	-0.41330200	0.61314300
C	0.98612300	-0.75039600	1.02279100
C	-0.08326900	-0.08201700	0.13689100
C	0.17553200	1.43302500	0.05112900
C	1.59671700	1.74706600	-0.43826400
C	2.66301600	1.08225800	0.44110800
H	0.02043200	-0.49727400	-0.87441400
H	0.85870400	-1.83743200	1.01745400
H	0.85694800	-0.42243700	2.06188100
H	3.14314200	-0.85413400	1.29831500
H	-0.55203700	1.90364400	-0.61562000
H	1.76045100	2.82862600	-0.45848500
H	3.66563400	1.22438600	0.03071100
H	2.65894300	1.53261400	1.44113300
H	0.02182000	1.87824600	1.04453300
H	1.71072600	1.39567000	-1.46953000
O	2.63271500	-1.10801700	-0.67655800
O	3.89561900	-1.08534400	-1.04513600

C	-1.49163700	-0.43092300	0.64730300
H	-1.54815500	-1.51758300	0.79092700
H	-1.63189100	0.01285900	1.64272100
C	-2.64501200	-0.00077100	-0.26761400
H	-2.65553700	1.08995700	-0.37468900
H	-2.47739200	-0.40522700	-1.27430100
C	-4.01798700	-0.46096500	0.23748100
H	-4.18041900	-0.06773100	1.24844100
H	-4.01878100	-1.55348200	0.33336200
C	-5.17314400	-0.02749500	-0.66934000
H	-6.13573400	-0.37339600	-0.28297600
H	-5.22214800	1.06264400	-0.75410900
H	-5.05628800	-0.43193700	-1.67957800

Eli-TS39

C	-0.21438400	1.54643300	-0.00223600
C	0.04606800	0.05971300	0.29441600
C	-2.70721200	0.95594200	0.02859000
C	-1.59146300	1.76957700	-0.64583600
H	-0.10904600	-0.50788700	-0.63346400
H	-0.15597600	2.10142200	0.94357600
H	0.56058300	1.95637700	-0.65494200
H	-3.10137100	0.08239700	-0.87346000
H	-3.65537600	1.47503100	0.17070300
H	-1.53472800	1.51620100	-1.71084100
H	-1.84953900	2.83188500	-0.60471700
O	-2.86667700	-1.76149400	-0.33049700
O	-3.26206300	-1.12204400	-1.35903100
C	-0.99453900	-0.42435400	1.31684100
H	-0.75212500	-0.00058900	2.30517300
C	-2.39546300	-0.01105200	0.98671200
H	-3.17436400	-0.35520600	1.65821000
C	1.47288200	-0.22416100	0.79230400
H	1.68726000	0.42480600	1.65253800
H	1.51062800	-1.25282800	1.17280200
H	-0.94751200	-1.51114400	1.43933100
C	2.57351300	-0.05546100	-0.26232700
H	2.58254700	0.97446900	-0.63777700
H	2.34378900	-0.69304300	-1.12587600
C	3.97215400	-0.40293700	0.26152300
H	4.20140500	0.23108700	1.12669400
H	3.97167300	-1.43467900	0.63336000
C	5.07030500	-0.24207200	-0.79342000
H	5.12086400	0.78857900	-1.15842700
H	6.05318500	-0.49915300	-0.38927300

H	4.88685700	-0.88919500	-1.65679200
Eli-P39			
C	3.04341200	-0.91218400	-0.33665400
C	3.34282300	0.55720300	-0.19027900
C	2.41549500	1.46254300	0.11911600
C	0.95781700	1.13316600	0.32200500
C	0.58292800	-0.27459600	-0.18040300
C	1.66935400	-1.27827900	0.24102300
H	3.09378100	-1.19158200	-1.39862200
H	3.82713600	-1.49909700	0.15654300
H	0.70836700	1.22112100	1.39059600
H	0.34700900	1.89007100	-0.18241800
H	0.57348300	-0.24132700	-1.27959600
H	1.73095200	-1.29217900	1.33668300
H	1.38801300	-2.28970300	-0.07044800
H	4.37100000	0.87427700	-0.34516400
C	-0.80956300	-0.72333500	0.29071100
H	-0.97170300	-1.75624500	-0.04293000
H	-0.82046400	-0.75445500	1.38888000
H	2.70295000	2.50515300	0.23054200
C	-1.97688400	0.14001900	-0.20365000
H	-1.87109100	1.16458300	0.17146300
H	-1.93595700	0.21039900	-1.29875700
C	-3.34948900	-0.40090200	0.21431200
H	-3.38750900	-0.48083800	1.30753800
H	-3.46642100	-1.42220300	-0.16815300
C	-4.51574400	0.46272900	-0.27443700
H	-4.52354500	0.53515000	-1.36657600
H	-5.47848000	0.04827900	0.03711100
H	-4.44840400	1.48040300	0.12284500

Eli-R40			
C	-2.68176500	0.44208900	0.49121000
C	-1.59823900	1.50898100	0.59299400
C	-0.27303500	1.07104300	-0.05027200
C	0.21902400	-0.28587100	0.48515300
C	-0.88234700	-1.34579500	0.29852600
C	-2.21211900	-0.93618700	0.94572000
H	-0.40570800	0.99665600	-1.13609300
H	-1.96008200	2.43657100	0.14009900
H	-1.44421600	1.71607100	1.65839300
H	-3.59224300	0.73873100	1.01671000
H	-0.55458700	-2.30285700	0.71687200
H	-2.99948800	-1.66105700	0.72523700

H	-2.10447400	-0.90302700	2.03653800
H	0.47613900	1.84856300	0.12101500
H	0.39983300	-0.17749100	1.56591600
H	-1.03890200	-1.51181200	-0.77391100
O	-3.06010900	0.39548800	-0.93931000
O	-4.13272700	-0.33854400	-1.14458500
C	1.53572700	-0.74103200	-0.16807400
H	1.74780100	-1.76654200	0.15994300
H	1.39242800	-0.79587800	-1.25555500
C	2.75840800	0.13225700	0.14075300
H	2.59504500	1.15329500	-0.22255000
H	2.88056400	0.21098300	1.22919800
C	4.05641700	-0.40643300	-0.47304400
H	3.93343700	-0.48832900	-1.55974900
H	4.23133900	-1.42640700	-0.10995900
C	5.27845400	0.46253700	-0.16258100
H	6.18575500	0.05241000	-0.61432900
H	5.14840700	1.47976300	-0.54517000
H	5.44849000	0.53527000	0.91624600

Eli-TS40

C	0.23463400	-0.23137700	-0.52080400
C	-0.32380900	0.99746400	0.21715100
C	-2.24791600	-0.84201100	-0.87315600
C	-0.83043300	-1.34402900	-0.55310900
H	-0.61912500	0.70568600	1.23246300
H	0.43257600	0.07116300	-1.55985600
H	-2.95098200	-1.05651400	0.21818700
H	-2.82651500	-1.46327600	-1.55725300
H	-0.82589000	-1.86114200	0.41493600
H	-0.54387400	-2.09666400	-1.29420700
O	-3.69067500	0.55340500	0.99980600
O	-3.64403000	-0.69134400	1.26681700
C	-1.53460900	1.57566500	-0.52345000
H	-1.19803300	2.06683600	-1.44976500
C	-2.52718500	0.52568700	-0.91419600
H	-3.42388500	0.86457300	-1.42104100
H	-2.02734700	2.35529200	0.06526700
C	1.55118100	-0.75629300	0.07598400
H	1.40414800	-0.94867400	1.14716200
H	1.77387000	-1.73076600	-0.37734300
H	0.43933100	1.77281400	0.32124500
C	2.76603900	0.15964200	-0.11781400
H	2.58578800	1.13113100	0.35695400
H	2.89694900	0.36328900	-1.18877000

C	4.06512100	-0.43107500	0.44341600
H	3.93364200	-0.64011900	1.51189900
H	4.25620000	-1.39999100	-0.03367800
C	5.27906100	0.48158600	0.24793100
H	6.18783600	0.03027100	0.65527800
H	5.45574000	0.68318400	-0.81331700
H	5.13471100	1.44486000	0.74714100

Eli-P40

C	3.04341200	-0.91218400	-0.33665400
C	3.34282300	0.55720300	-0.19027900
C	2.41549500	1.46254300	0.11911600
C	0.95781700	1.13316600	0.32200500
C	0.58292800	-0.27459600	-0.18040300
C	1.66935400	-1.27827900	0.24102300
H	3.09378100	-1.19158200	-1.39862200
H	3.82713600	-1.49909700	0.15654300
H	0.70836700	1.22112100	1.39059600
H	0.34700900	1.89007100	-0.18241800
H	0.57348300	-0.24132700	-1.27959600
H	1.73095200	-1.29217900	1.33668300
H	1.38801300	-2.28970300	-0.07044800
H	4.37100000	0.87427700	-0.34516400
C	-0.80956300	-0.72333500	0.29071100
H	-0.97170300	-1.75624500	-0.04293000
H	-0.82046400	-0.75445500	1.38888000
H	2.70295000	2.50515300	0.23054200
C	-1.97688400	0.14001900	-0.20365000
H	-1.87109100	1.16458300	0.17146300
H	-1.93595700	0.21039900	-1.29875700
C	-3.34948900	-0.40090200	0.21431200
H	-3.38750900	-0.48083800	1.30753800
H	-3.46642100	-1.42220300	-0.16815300
C	-4.51574400	0.46272900	-0.27443700
H	-4.52354500	0.53515000	-1.36657600
H	-5.47848000	0.04827900	0.03711100
H	-4.44840400	1.48040300	0.12284500

15. Cartesian coordinates for all reactants, transition states and products in the class of β -scission

HO₂

O	0.05528900	-0.60941600	0.00000000
H	-0.88463000	-0.87113300	0.00000000
O	0.05528900	0.71830800	0.00000000

Sci-R1

C	1.38991200	0.34603200	0.23597100
C	1.98836100	1.64830800	-0.17000200
H	2.12608000	1.86128800	-1.22493100
H	2.26926000	2.40317300	0.55259600
O	2.12041400	-0.75059800	-0.36268700
O	3.41601600	-0.83650600	0.28070100
H	3.96576000	-0.33575000	-0.33835000
H	1.43597700	0.22267400	1.32401900
C	-0.06810800	0.14516200	-0.23899900
C	-0.62722500	-1.22388800	0.19212500
C	-0.97672000	1.28194800	0.26637200
H	-0.05241500	0.18339900	-1.33730600
C	-2.08189200	-1.41371200	-0.26082400
H	-0.57632900	-1.29394400	1.28746400
H	0.00430500	-2.02228300	-0.20050300
C	-2.43209800	1.09233800	-0.18453800
H	-0.93765400	1.30746300	1.36397500
H	-0.60047900	2.24913500	-0.08089300
C	-2.98520300	-0.27647200	0.23384700
H	-2.45711600	-2.37907000	0.09392700
H	-2.11676000	-1.45252500	-1.35736300
H	-3.05414200	1.89551200	0.22360800
H	-2.48393400	1.18399900	-1.27719500
H	-4.00403400	-0.40551300	-0.14566600
H	-3.05212500	-0.31902400	1.32879500

Sci-TS1

C	1.26653100	0.66716600	0.32980700
C	1.91844600	1.80449700	-0.11431300
H	1.62790600	2.29027800	-1.03910800
H	2.80743400	2.17065700	0.38441200
O	2.32990400	-0.65804000	-0.54920800
O	3.37889900	-1.04166700	0.29053300
H	4.15240700	-0.66228700	-0.15049600
H	1.51537900	0.30432800	1.32327700
C	-0.10352600	0.27768300	-0.18426400
C	-0.51691000	-1.13818300	0.25593900
C	-1.16540300	1.30839100	0.26873600
H	-0.06133200	0.30184200	-1.28218000
C	-1.91928600	-1.50831800	-0.24549100
H	-0.50328800	-1.18100700	1.35386100
H	0.22317800	-1.85779700	-0.09643000
C	-2.56988600	0.93864900	-0.23058700
H	-1.16879300	1.35493300	1.36589200
H	-0.88858700	2.30686400	-0.08248800

C	-2.97046700	-0.48032000	0.19360300
H	-2.19095500	-2.50621000	0.11336800
H	-1.90667800	-1.56685900	-1.34171300
H	-3.29801600	1.66740200	0.14042600
H	-2.59090500	1.00790800	-1.32596300
H	-3.95145000	-0.73585700	-0.22004500
H	-3.07371700	-0.51393400	1.28600400

Sci-P1

C	-1.36188100	1.35604600	0.26389600
C	0.13867300	1.16528400	-0.00291700
C	0.62786700	-0.21797100	0.45279600
C	-0.22052300	-1.33313700	-0.20299800
C	-1.72118900	-1.14385600	0.05853900
C	-2.20003000	0.24547600	-0.38385800
H	0.33066600	1.27757000	-1.07767400
H	0.71175600	1.94974100	0.50165800
H	-1.53922700	1.35684100	1.34725100
H	-1.68366400	2.33620300	-0.10266200
H	-0.03080600	-1.32617700	-1.28386800
H	0.10664200	-2.31199600	0.16409600
H	-2.29137500	-1.92417800	-0.45600700
H	-1.91909800	-1.26958200	1.13102600
H	-2.11938300	0.32352700	-1.47587000
H	-3.25907700	0.37759800	-0.13956000
H	0.45422200	-0.28925600	1.53879600
C	2.09757100	-0.47438100	0.23236100
H	2.44160600	-1.44555200	0.58806200
C	2.98293000	0.33438400	-0.34395300
H	4.02044200	0.03951600	-0.45536300
H	2.71678000	1.31466900	-0.72308000

Sci-R2

C	-2.02985100	-0.17483300	0.43329000
C	-3.20725400	-0.94677100	0.91858100
H	-3.63367100	-1.71926800	0.28754800
H	-3.60397100	-0.81165700	1.91652400
O	-2.25505100	0.33857400	-0.89836600
O	-3.23529700	1.40204400	-0.81329400
H	-4.05108400	0.92196000	-1.01406000
H	-1.83827000	0.67762600	1.09141800
C	-0.76466500	-1.04434400	0.29707200
H	-0.59857600	-1.54146600	1.25979300
H	-0.98388700	-1.83535800	-0.42908200
C	0.51093300	-0.29506600	-0.12918600

C	1.00310100	0.70004100	0.93766000
C	1.62859300	-1.29705200	-0.47440700
H	0.27421900	0.27218000	-1.03704700
C	2.30087300	1.40569500	0.51623100
H	1.17447600	0.15722900	1.87826400
H	0.23362200	1.45002500	1.14475500
C	2.92674600	-0.59684700	-0.90053800
H	1.82938400	-1.92713200	0.40370200
H	1.28813500	-1.97089600	-1.26842600
C	3.40507900	0.40101100	0.16241300
H	2.63758900	2.07561600	1.31415400
H	2.09630300	2.03947100	-0.35604200
H	3.70487900	-1.34044600	-1.10217800
H	2.75382400	-0.06325100	-1.84389500
H	4.29990200	0.92699300	-0.18604800
H	3.69858200	-0.14757900	1.06719700

Sci-TS2

C	-2.01885000	-0.90248300	0.13763800
C	-3.27741300	-1.11071900	0.67908100
H	-4.00523200	-1.73582100	0.17744700
H	-3.60283600	-0.57041700	1.56195400
O	-2.40160200	0.43303300	-1.18038200
O	-2.47248000	1.70275500	-0.60104200
H	-3.42399600	1.87977400	-0.58934700
C	-0.91193400	-0.25891200	0.93668600
H	-1.29930800	0.68104300	1.34374600
H	-0.69495600	-0.90452000	1.79870400
C	0.39149100	0.01338300	0.16850300
C	1.31907400	0.93275500	0.98351500
C	1.13504600	-1.28097300	-0.21326700
H	0.12302700	0.53840900	-0.75539200
C	2.63856700	1.22258000	0.25446700
H	1.53711300	0.45755100	1.95055700
H	0.80027600	1.87120100	1.20655500
C	2.45134800	-0.99649100	-0.95177600
H	1.35017900	-1.85018400	0.70226200
H	0.49941400	-1.92125800	-0.83372100
C	3.36538300	-0.07108600	-0.13789000
H	3.28488300	1.84595800	0.88126600
H	2.42725000	1.80575400	-0.65090600
H	2.96581600	-1.93654800	-1.17701300
H	2.22683900	-0.52512200	-1.91707700
H	4.27364800	0.16028200	-0.70407200
H	3.68937200	-0.59389400	0.77166800

H	-1.71510400	-1.57682900	-0.65698700
Sci-P2			
C	1.55267400	1.50267000	-0.22705700
C	0.15319100	1.03615400	0.19891300
C	-0.14843900	-0.39782200	-0.27080500
C	0.95125300	-1.36042400	0.21178500
C	2.35396300	-0.90122600	-0.21149500
C	2.64270200	0.53364400	0.25105000
H	0.07898700	1.06885900	1.29506500
H	-0.60849500	1.72329900	-0.18106500
H	1.59078700	1.57658400	-1.32180000
H	1.74502100	2.50965400	0.15754000
H	0.90775200	-1.42762100	1.30764200
H	0.75470300	-2.36914300	-0.16861700
H	3.10930600	-1.58768100	0.18502000
H	2.43380500	-0.94998000	-1.30532000
H	2.68910000	0.55640900	1.34772900
H	3.62480600	0.85770000	-0.10861300
H	-0.13094100	-0.40037900	-1.37127300
C	-1.54551700	-0.87981800	0.17550900
H	-1.64301300	-1.93881300	-0.10041000
H	-1.61662700	-0.83401900	1.26876500
C	-2.68490900	-0.11732500	-0.43996300
H	-2.71744500	-0.11819800	-1.52947600
C	-3.63192400	0.53551100	0.22783800
H	-3.64301400	0.56668200	1.31344000
H	-4.43268800	1.05844900	-0.28327600

Sci-R3			
C	2.74278200	0.43910600	0.26409000
C	3.68264900	1.53767800	-0.09278600
H	3.89514600	1.73711400	-1.13765000
H	4.10211500	2.19414800	0.65860200
O	3.09273100	-0.78612000	-0.41674900
O	4.30914700	-1.30258500	0.17664900
H	4.97729500	-0.94710100	-0.42627000
H	2.77114100	0.24307300	1.34155800
C	1.29175800	0.71799000	-0.17265200
H	1.02894100	1.71604700	0.18910600
H	1.27048600	0.76417200	-1.26780400
C	0.29083300	-0.32889800	0.33480300
H	0.65429500	-1.32001200	0.04981100
H	0.27434100	-0.30907000	1.43277200
C	-1.14310900	-0.15308100	-0.19286900

C	-2.01654200	-1.36180500	0.19397000
C	-1.80880300	1.15311900	0.28176900
H	-1.09344600	-0.12124200	-1.29201200
C	-3.45944500	-1.23167300	-0.31215600
H	-2.02443800	-1.45659700	1.28864600
H	-1.56273300	-2.28087300	-0.19221500
C	-3.25311400	1.28997200	-0.22258500
H	-1.80599600	1.16918500	1.38086600
H	-1.22579900	2.02085600	-0.04266400
C	-4.10750100	0.07547100	0.16374300
H	-4.05201000	-2.09163200	0.01690000
H	-3.46058000	-1.25545900	-1.40970500
H	-3.70044800	2.20944800	0.16930400
H	-3.24435700	1.39095800	-1.31572700
H	-5.11645300	0.17348400	-0.25020100
H	-4.21956000	0.04586800	1.25551300

Sci-TS3

C	2.75494600	-0.44587600	-0.68238000
C	3.79635000	-1.34893200	-0.57320400
H	3.65269700	-2.31518400	-0.10245700
H	4.80541600	-1.07520200	-0.85602500
O	2.94993600	0.50916800	0.96833100
O	3.80989900	1.59370700	0.78982000
H	4.59998200	1.32175700	1.27846500
H	2.92445400	0.44140900	-1.28505200
C	1.31385700	-0.86696200	-0.51172500
C	0.31326600	0.29099700	-0.60973500
H	1.22195700	-1.38422300	0.44861800
H	0.46409700	0.79698500	-1.57204000
H	0.54593700	1.02670700	0.16606900
C	-1.16433200	-0.12261500	-0.50586900
C	-1.53553400	-0.67812500	0.88272500
C	-2.08651500	1.05822000	-0.86412300
H	-1.34758200	-0.91938900	-1.24370800
C	-3.02346400	-1.04535400	0.98706700
H	-1.29437300	0.08081400	1.63956700
H	-0.92546600	-1.55511500	1.11992600
C	-3.57495200	0.69646300	-0.76479900
H	-1.87030200	1.89314700	-0.18364900
H	-1.85320800	1.41442600	-1.87375200
C	-3.92797800	0.13842600	0.62028200
H	-3.25110700	-1.39819100	1.99838200
H	-3.23617500	-1.88384900	0.31088700
H	-4.19044300	1.57384200	-0.98943800

H	-3.81553100	-0.05523400	-1.52803100
H	-4.98033000	-0.16252100	0.65260500
H	-3.80663900	0.93098700	1.37018800
H	1.08406600	-1.61161300	-1.28519100

Sci-P3

C	-2.35629400	1.36534300	0.24718800
C	-0.92820000	1.14002600	-0.27222400
C	-0.34321900	-0.20859000	0.18890100
C	-1.29502300	-1.35615700	-0.19883000
C	-2.72279100	-1.13851800	0.32115200
C	-3.29038500	0.21097400	-0.13873800
H	-0.93502600	1.16249000	-1.37109000
H	-0.28743600	1.96605900	0.05090200
H	-2.33085900	1.45801300	1.34079200
H	-2.74720600	2.31427900	-0.13450100
H	-1.31830200	-1.44182900	-1.29407300
H	-0.89871600	-2.30588200	0.17702400
H	-3.37156500	-1.95642900	-0.00911600
H	-2.71584400	-1.17134300	1.41845700
H	-3.41532400	0.19709000	-1.22941200
H	-4.28673900	0.36976800	0.28663500
H	-0.28290700	-0.18754000	1.28781200
C	1.07304600	-0.46827100	-0.35305300
H	1.36505100	-1.49411500	-0.10005600
H	1.05167800	-0.41978500	-1.44996300
C	2.15963600	0.48589100	0.17872900
H	1.90643300	1.51672900	-0.09732700
H	2.17784700	0.44806300	1.27379200
C	3.52537500	0.16308300	-0.35890100
H	3.63323700	0.22202500	-1.44168300
C	4.57783900	-0.19241600	0.37215000
H	5.53668200	-0.41893800	-0.08068200
H	4.51908800	-0.26685400	1.45424700

Sci-R4

C	-1.22500600	-1.37718700	0.34707700
C	-0.01826200	-0.77265700	1.07536100
C	0.61159500	0.40158000	0.30933400
C	-0.45681700	1.45301500	-0.07212000
C	-1.66999400	0.84217000	-0.78903800
C	-2.27947000	-0.31228800	0.01748500
H	-0.32443300	-0.39876300	2.06016800
H	0.74984700	-1.53091500	1.24260000
H	-0.88160000	-1.84989600	-0.57840700

H	-1.66279400	-2.16870600	0.96354200
H	-0.77702800	1.94006200	0.85552200
H	0.01425900	2.22206500	-0.69168800
H	-2.41722700	1.62415900	-0.95983400
H	-1.36004100	0.47693300	-1.77224800
H	-2.70401200	0.08011200	0.95152100
H	-3.10970200	-0.76051600	-0.53747700
C	1.74312900	1.02516400	1.05448500
H	2.23485300	1.90035900	0.64366300
H	2.11140200	0.61027700	1.98443700
O	1.07771500	-0.03629400	-1.00912700
O	2.04967000	-1.10157000	-0.85617300
H	2.87635100	-0.60103700	-0.89489700

Sci-TS4

C	-1.09169700	-1.30098200	0.62251700
C	-0.01944700	-0.44067400	1.30602600
C	0.48853000	0.70525600	0.45435900
C	-0.56075600	1.46328100	-0.34033700
C	-1.62832500	0.56827200	-0.98876500
C	-2.20418600	-0.43987400	0.01249900
H	-0.44059200	0.00493500	2.21795800
H	0.82671900	-1.05755000	1.61798200
H	-0.62042500	-1.89832800	-0.16207800
H	-1.50870100	-2.00143100	1.35328400
H	-1.04918200	2.15499500	0.35965600
H	-0.06364600	2.08252300	-1.09260800
H	-2.42406700	1.19910200	-1.39796700
H	-1.18016600	0.02804100	-1.82613000
H	-2.73603300	0.09538200	0.81119300
H	-2.94476000	-1.07667600	-0.48159200
C	1.65034500	1.36764300	0.83166700
H	1.94091800	2.29780600	0.35805400
H	2.34720100	0.91678500	1.52921600
O	1.25511600	-0.22740800	-1.06213300
O	1.89663500	-1.40949800	-0.67415100
H	2.83194500	-1.18787600	-0.78449600

Sci-P4

C	-1.02042800	-1.26871000	-0.30004100
C	0.34535100	-1.26901700	0.41631100
C	1.11520900	0.00003000	0.13143300
C	0.34533500	1.26903500	0.41629400
C	-1.02044500	1.26870400	-0.30004000
C	-1.82249200	-0.00002200	0.02141900
H	0.16961600	-1.34279800	1.49911600

H	0.93236600	-2.14516300	0.12805300
H	-0.85383800	-1.32821400	-1.38228800
H	-1.58881500	-2.16079500	-0.01797100
H	0.16958400	1.34280500	1.49909700
H	0.93233100	2.14520900	0.12806100
H	-1.58886100	2.16076600	-0.01795400
H	-0.85388500	1.32820700	-1.38228900
H	-2.08734400	-0.00002300	1.08702200
H	-2.76642100	-0.00001500	-0.53310700
C	2.35274900	-0.00000400	-0.36301200
H	2.88183000	0.92447900	-0.57098300
H	2.88175600	-0.92454100	-0.57094200

Sci-R5

C	1.89233600	1.56758700	-0.09917500
C	0.62623000	0.95680300	0.51686400
C	0.31163600	-0.44462900	-0.08177600
C	1.54068200	-1.36925900	0.07009600
C	2.80880700	-0.75288200	-0.53725100
C	3.10295800	0.63620000	0.04523500
H	0.75980300	0.85119300	1.60133300
H	-0.23505300	1.61150400	0.36658400
H	1.71432400	1.76923200	-1.16329800
H	2.10009500	2.53553100	0.36879200
H	1.70488000	-1.56300400	1.13853700
H	1.33172800	-2.33855800	-0.39381500
H	3.66068200	-1.42159300	-0.37580500
H	2.68266300	-0.66848200	-1.62441100
H	3.35618800	0.53580600	1.10877500
H	3.97981400	1.07348800	-0.44322300
H	0.12290200	-0.29878500	-1.15507000
C	-0.91368000	-1.03698600	0.52939800
H	-0.84419800	-1.43981300	1.53623800
C	-2.26102400	-0.88091700	-0.07543800
H	-2.23438100	-1.02028300	-1.16280500
H	-2.98844700	-1.57809800	0.35564800
O	-2.69307600	0.47640300	0.18957300
O	-3.95666800	0.66747500	-0.51474400
H	-4.56072600	0.74533900	0.23616000

Sci-TS5

C	-0.97920000	-0.98529600	-0.36776300
H	-4.52327800	0.41314300	-0.38798600
C	-2.10724400	-1.19737800	0.40084800
H	-2.96306600	-1.69873600	-0.03622900

H	-2.00367000	-1.30733500	1.47537300
O	-2.93309100	0.50478100	0.59492300
O	-3.66457000	0.83165100	-0.55098600
H	-1.07063600	-1.04566900	-1.45041400
C	0.32105600	-0.47911100	0.16861500
C	1.51602400	-1.33041600	-0.31955200
C	0.53237900	1.00802100	-0.21802100
H	0.28846000	-0.53515600	1.26517500
C	2.85630900	-0.78634000	0.19549600
H	1.52160400	-1.33387900	-1.41760500
H	1.38209800	-2.37017100	-0.00437000
C	1.87243800	1.54606600	0.30119200
H	0.50298400	1.09417500	-1.31219600
H	-0.30427000	1.59676800	0.16502700
C	3.05281800	0.68963500	-0.17654800
H	3.67861700	-1.39149100	-0.20005400
H	2.89156600	-0.89086000	1.28762300
H	2.00251100	2.58492200	-0.01910200
H	1.85537200	1.55952700	1.39865700
H	3.99075300	1.06436000	0.24595800
H	3.14476100	0.77786400	-1.26695300

Sci-P5

C	-1.36188100	1.35604600	0.26389600
C	0.13867300	1.16528400	-0.00291700
C	0.62786700	-0.21797100	0.45279600
C	-0.22052300	-1.33313700	-0.20299800
C	-1.72118900	-1.14385600	0.05853900
C	-2.20003000	0.24547600	-0.38385800
H	0.33066600	1.27757000	-1.07767400
H	0.71175600	1.94974100	0.50165800
H	-1.53922700	1.35684100	1.34725100
H	-1.68366400	2.33620300	-0.10266200
H	-0.03080600	-1.32617700	-1.28386800
H	0.10664200	-2.31199600	0.16409600
H	-2.29137500	-1.92417800	-0.45600700
H	-1.91909800	-1.26958200	1.13102600
H	-2.11938300	0.32352700	-1.47587000
H	-3.25907700	0.37759800	-0.13956000
H	0.45422200	-0.28925600	1.53879600
C	2.09757100	-0.47438100	0.23236100
H	2.44160600	-1.44555200	0.58806200
C	2.98293000	0.33438400	-0.34395300
H	4.02044200	0.03951600	-0.45536300
H	2.71678000	1.31466900	-0.72308000

Sci-R6

C	-1.60554800	-1.19370200	0.73462100
H	-1.46752000	-1.31737800	1.80450800
C	-2.91791000	-0.70956800	0.23843000
H	-3.20798400	-1.20848700	-0.69463800
H	-3.71486900	-0.84743400	0.97764900
O	-2.76750400	0.70208100	-0.04377100
O	-3.99999800	1.14310000	-0.68849100
H	-4.35900300	1.71653900	0.00221400
C	-0.44020600	-1.42660600	-0.16576200
H	-0.69844700	-1.13945400	-1.19163200
H	-0.21878400	-2.50691600	-0.19487700
C	0.85719100	-0.69901000	0.25930100
C	2.05599200	-1.15856500	-0.58860100
C	0.71104300	0.83135400	0.19595100
H	1.06280400	-0.97545300	1.30441400
C	3.35563800	-0.44301000	-0.19160900
H	1.83971700	-0.95513500	-1.64636100
H	2.18208500	-2.24364700	-0.50024000
C	2.00596700	1.54971200	0.60047400
H	0.43964100	1.11643900	-0.82915600
H	-0.12147100	1.15573200	0.82677600
C	3.20013000	1.08311900	-0.24342400
H	4.17440300	-0.76439500	-0.84383500
H	3.63480100	-0.74237900	0.82711700
H	1.87693700	2.63306900	0.50849000
H	2.21456100	1.35097400	1.66015200
H	4.12062600	1.56921500	0.09628600
H	3.04874100	1.39490800	-1.28504600

Sci-TS6

C	1.59129800	0.33837100	-0.37613300
H	5.39684500	0.28219200	-0.47376100
C	2.58240000	0.97136000	0.34691900
H	3.19762700	1.72144800	-0.13632600
H	2.46744200	1.08441000	1.41977900
O	3.96286200	-0.31941100	0.56770800
O	4.73616200	-0.41697200	-0.59152800
C	0.56148800	-0.56633600	0.21810200
H	0.81912100	-1.60271800	-0.04657500
H	0.60137900	-0.51125500	1.31231200
C	-0.87973200	-0.29008500	-0.26412000
C	-1.84826800	-1.38122700	0.22427000
C	-1.37659100	1.10043100	0.16798400

H	-0.87393600	-0.31782000	-1.36405000
C	-3.29307200	-1.11988900	-0.22645400
H	-1.81282700	-1.42115700	1.32168500
H	-1.51334700	-2.36154900	-0.13226100
C	-2.81893700	1.36836400	-0.28525100
H	-1.32216700	1.16787800	1.26368600
H	-0.70700000	1.87409000	-0.22162000
C	-3.77663000	0.27233200	0.20156300
H	-3.95621300	-1.89270200	0.17575000
H	-3.34956700	-1.20115600	-1.31977800
H	-3.14925600	2.34850900	0.07397500
H	-2.85003100	1.41340300	-1.38175600
H	-4.78767900	0.45529400	-0.17657500
H	-3.84136700	0.31071100	1.29682300
H	1.63705300	0.38156800	-1.46201800

Sci-P6

C	1.55267400	1.50267000	-0.22705700
C	0.15319100	1.03615400	0.19891300
C	-0.14843900	-0.39782200	-0.27080500
C	0.95125300	-1.36042400	0.21178500
C	2.35396300	-0.90122600	-0.21149500
C	2.64270200	0.53364400	0.25105000
H	0.07898700	1.06885900	1.29506500
H	-0.60849500	1.72329900	-0.18106500
H	1.59078700	1.57658400	-1.32180000
H	1.74502100	2.50965400	0.15754000
H	0.90775200	-1.42762100	1.30764200
H	0.75470300	-2.36914300	-0.16861700
H	3.10930600	-1.58768100	0.18502000
H	2.43380500	-0.94998000	-1.30532000
H	2.68910000	0.55640900	1.34772900
H	3.62480600	0.85770000	-0.10861300
H	-0.13094100	-0.40037900	-1.37127300
C	-1.54551700	-0.87981800	0.17550900
H	-1.64301300	-1.93881300	-0.10041000
H	-1.61662700	-0.83401900	1.26876500
C	-2.68490900	-0.11732500	-0.43996300
H	-2.71744500	-0.11819800	-1.52947600
C	-3.63192400	0.53551100	0.22783800
H	-3.64301400	0.56668200	1.31344000
H	-4.43268800	1.05844900	-0.28327600

Sci-R7

C	-3.01165900	0.84145300	1.22769800
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C	-1.52469900	0.63921500	0.89939000
C	-1.28338400	-0.59561200	0.01013400
C	-2.15663500	-0.51358100	-1.25603200
C	-3.64448900	-0.31548000	-0.93289100
C	-3.86862200	0.91399800	-0.04211600
H	-1.14437600	1.52745200	0.37641400
H	-0.95378500	0.55939100	1.82933700
H	-3.36022600	0.00704300	1.85041300
H	-3.14168400	1.74923400	1.82593000
H	-1.80572300	0.32412700	-1.87404200
H	-2.01989700	-1.41959000	-1.85677300
H	-4.22097900	-0.22455000	-1.85939500
H	-4.02317300	-1.20768900	-0.41710000
H	-3.60569100	1.81964300	-0.60421400
H	-4.92809900	1.00626600	0.21868400
H	-1.60446900	-1.48386600	0.57609000
C	0.19709300	-0.78419100	-0.36350900
H	0.27497000	-1.59899200	-1.09308500
H	0.57330600	0.11492900	-0.86255100
C	1.12791200	-1.11283400	0.83379300
H	1.10905700	-0.28493200	1.54925800
H	0.72058800	-1.99388700	1.34860800
C	2.53570400	-1.37841400	0.42199800
H	2.75985900	-2.30404600	-0.09944700
C	3.58355200	-0.32704600	0.46962100
H	4.59106300	-0.74397200	0.35984100
H	3.53508700	0.24840100	1.40202600
O	3.32339400	0.58112900	-0.62818700
O	4.26333500	1.68981600	-0.49772600
H	4.82170800	1.53243600	-1.27118900

Sci-TS7

C	2.40879400	-0.70646200	0.37050900
H	6.02097300	0.48597800	0.36601000
C	3.51514300	-0.99545100	-0.40295500
H	4.34313700	-1.54059700	0.03501100
O	4.43699100	0.65432900	-0.61677500
O	5.18598700	0.95143800	0.52481000
H	3.39824000	-1.11017900	-1.47555600
C	1.13345100	-0.14226700	-0.16494800
H	1.08195500	0.91828900	0.11637800
H	1.14576500	-0.16958800	-1.26021400
C	-0.11767000	-0.87230100	0.36345200
H	-0.12958300	-0.82173700	1.46012100
H	-0.03263600	-1.93507800	0.10822100

C	-1.45430400	-0.33906000	-0.18033600
C	-2.61380100	-1.27575800	0.20879600
C	-1.76091700	1.09907900	0.27882500
H	-1.39042800	-0.33228800	-1.27915000
C	-3.97024200	-0.78096000	-0.31265700
H	-2.65403800	-1.35296100	1.30414400
H	-2.41312300	-2.28584300	-0.16529000
C	-3.11605900	1.60101600	-0.24236600
H	-1.76368400	1.12398600	1.37760500
H	-0.96966200	1.78187000	-0.04486500
C	-4.26009500	0.65483100	0.14463700
H	-4.76767700	-1.45419900	0.01865300
H	-3.96952500	-0.81660100	-1.40987200
H	-3.31153200	2.60909500	0.13749100
H	-3.07196200	1.68504200	-1.33602600
H	-5.20509100	1.00649500	-0.28210000
H	-4.38617500	0.66788300	1.23517800
H	2.50541100	-0.76171400	1.45224300

Sci-P7

C	-2.35629400	1.36534300	0.24718800
C	-0.92820000	1.14002600	-0.27222400
C	-0.34321900	-0.20859000	0.18890100
C	-1.29502300	-1.35615700	-0.19883000
C	-2.72279100	-1.13851800	0.32115200
C	-3.29038500	0.21097400	-0.13873800
H	-0.93502600	1.16249000	-1.37109000
H	-0.28743600	1.96605900	0.05090200
H	-2.33085900	1.45801300	1.34079200
H	-2.74720600	2.31427900	-0.13450100
H	-1.31830200	-1.44182900	-1.29407300
H	-0.89871600	-2.30588200	0.17702400
H	-3.37156500	-1.95642900	-0.00911600
H	-2.71584400	-1.17134300	1.41845700
H	-3.41532400	0.19709000	-1.22941200
H	-4.28673900	0.36976800	0.28663500
H	-0.28290700	-0.18754000	1.28781200
C	1.07304600	-0.46827100	-0.35305300
H	1.36505100	-1.49411500	-0.10005600
H	1.05167800	-0.41978500	-1.44996300
C	2.15963600	0.48589100	0.17872900
H	1.90643300	1.51672900	-0.09732700
H	2.17784700	0.44806300	1.27379200
C	3.52537500	0.16308300	-0.35890100
H	3.63323700	0.22202500	-1.44168300

C	4.57783900	-0.19241600	0.37215000
H	5.53668200	-0.41893800	-0.08068200
H	4.51908800	-0.26685400	1.45424700

Sci-R8

C	-0.85797200	-0.74607900	-0.44684400
H	-3.32296900	1.95956200	0.00784600
C	-2.11913400	-0.64749600	0.33983800
O	-2.29862900	0.67254000	0.92674900
O	-2.42436000	1.64429800	-0.15600200
C	-3.36366200	-1.09704400	-0.41786700
H	-3.50641200	-0.48310400	-1.30903000
H	-3.26087900	-2.13898400	-0.73146300
H	-4.24943400	-1.01277500	0.21603400
H	-2.02449600	-1.22564800	1.27262700
H	-0.91586300	-1.03459700	-1.49323000
C	0.46437400	-0.33108200	0.10676300
C	1.53643800	-1.43372000	-0.07122700
C	0.95915500	0.99301900	-0.53481400
H	0.34327300	-0.14299300	1.18198100
C	2.90561300	-1.00252300	0.47415000
H	1.62640000	-1.66763900	-1.14042200
H	1.20549400	-2.35357000	0.42190100
C	2.32700500	1.42053200	0.01512300
H	1.03118100	0.84919100	-1.62117900
H	0.21291900	1.77310700	-0.36936300
C	3.37872100	0.31590200	-0.15286800
H	3.64219900	-1.79360500	0.29786400
H	2.83647800	-0.87961200	1.56281900
H	2.65696500	2.33797700	-0.48358500
H	2.22610300	1.66535800	1.08037000
H	4.33114200	0.62511800	0.29011600
H	3.56858100	0.15846100	-1.22278600

Sci-TS8

C	-0.78291200	-0.73028500	-0.34118400
H	-3.98092400	1.27107600	-0.35495800
C	-1.93036900	-0.81647200	0.43351800
H	-1.79089600	-0.89104500	1.50889700
O	-2.42081800	1.02369700	0.65423300
O	-3.05669200	1.52792300	-0.48869300
H	-0.88540600	-0.79998700	-1.42347500
C	0.56766600	-0.36074400	0.18264700
C	1.64666200	-1.37756300	-0.25986700
C	0.96491900	1.06921400	-0.26448700

H	0.52657700	-0.36511100	1.28006700
C	3.04519300	-0.98526700	0.23764800
H	1.65194600	-1.43138200	-1.35667900
H	1.38225100	-2.37697400	0.10039200
C	2.36334200	1.45545500	0.23627900
H	0.94450400	1.11397400	-1.36143200
H	0.21037000	1.77318700	0.09303400
C	3.42557200	0.43628600	-0.19770100
H	3.78444000	-1.70581400	-0.12758000
H	3.06774800	-1.04597600	1.33344400
H	2.62385800	2.45441200	-0.12832900
H	2.34962400	1.51936200	1.33204400
H	4.40393200	0.70776900	0.21192000
H	3.52631500	0.46339300	-1.29055100
C	-3.20196300	-1.41750800	-0.09941900
H	-3.13640200	-2.51013000	-0.11178000
H	-4.05416200	-1.14537700	0.52800600
H	-3.39235000	-1.08302900	-1.12195900

Sci-P8

C	1.91362600	1.35312600	-0.22318300
C	0.39995500	1.16866900	-0.03834500
C	-0.07094100	-0.21181800	-0.52227500
C	0.73678700	-1.32957300	0.17904800
C	2.25049500	-1.14804900	0.00029100
C	2.71099400	0.23899600	0.46842500
H	0.15116100	1.28107200	1.02481100
H	-0.14086500	1.95691800	-0.57203100
H	2.14937600	1.35327400	-1.29535200
H	2.21934600	2.33190400	0.16065800
H	0.48784300	-1.32126300	1.24792200
H	0.42557500	-2.30721400	-0.20486800
H	2.78825400	-1.93100800	0.54501900
H	2.50643500	-1.27466400	-1.05978400
H	2.57174700	0.31727400	1.55455200
H	3.78230500	0.36680400	0.28184900
H	0.16696700	-0.28087700	-1.59629000
C	-1.55233200	-0.46391900	-0.38650700
H	-1.88071000	-1.43163000	-0.76927300
C	-2.47032300	0.34148000	0.14594200
H	-2.17088900	1.31169300	0.53577300
C	-3.93307700	0.01861300	0.25634800
H	-4.54357600	0.75527700	-0.27835700
H	-4.15853900	-0.96895700	-0.15365100
H	-4.26553300	0.03624800	1.30055500

Sci-R9

C	-1.16335900	-0.04072600	-0.39345000
C	-2.07491300	-0.97145000	0.33391700
H	-1.79415200	-1.32195900	1.32099000
O	-1.75751100	1.28896000	-0.49456100
O	-1.82842600	1.87039000	0.83600200
H	-2.74403100	1.67064100	1.07469100
C	-3.36183400	-1.42058600	-0.26937000
H	-3.22410800	-2.31147400	-0.90340600
H	-4.10173300	-1.68888400	0.48964500
H	-3.79081500	-0.64481900	-0.91231300
H	-1.13963500	-0.29894500	-1.46366600
C	0.27458900	0.00099600	0.14535300
C	0.95746900	-1.37097300	-0.01843400
C	1.11228100	1.10177400	-0.52879700
H	0.21225900	0.23141100	1.21647500
C	2.40335200	-1.35836600	0.49944900
H	0.95906400	-1.64105200	-1.08382700
H	0.38482100	-2.14889300	0.49624400
C	2.55731300	1.11680800	-0.01004500
H	1.11852300	0.93005700	-1.61437000
H	0.63928700	2.07241000	-0.37073700
C	3.23298100	-0.25181100	-0.16512500
H	2.86774300	-2.33579900	0.33224900
H	2.39428900	-1.19948300	1.58556800
H	3.13295600	1.88597200	-0.53511300
H	2.55606400	1.40096600	1.05031500
H	4.24269500	-0.22962100	0.25789800
H	3.34699300	-0.47932500	-1.23316100

Sci-TS9

C	1.02888200	0.27103100	0.23031300
C	1.86787100	1.23092100	-0.31079400
H	1.59679200	1.67136100	-1.26767600
O	1.79565100	-1.30254600	-0.56509800
O	2.85633000	-1.75149300	0.23413000
H	3.63268800	-1.53039000	-0.29981800
H	1.24105300	-0.06095000	1.24394300
C	-0.40560300	0.11085300	-0.22640800
C	-1.05995400	-1.17060800	0.32274800
C	-1.24664100	1.34814900	0.16945700
H	-0.39707900	0.05009200	-1.32372500
C	-2.52052400	-1.30692900	-0.12688600
H	-1.02200500	-1.13974000	1.42065000

H	-0.47518300	-2.03729900	0.01241800
C	-2.70938600	1.21311200	-0.27757700
H	-1.20776600	1.46874400	1.26033500
H	-0.80242600	2.25242500	-0.25767300
C	-3.35147200	-0.07475500	0.25503600
H	-2.96020300	-2.21060400	0.30744700
H	-2.55209600	-1.44100400	-1.21611300
H	-3.27981000	2.08799600	0.05133800
H	-2.75026900	1.20945400	-1.37461900
H	-4.37499800	-0.17156200	-0.12167200
H	-3.42548800	-0.01448000	1.34873400
C	3.20615400	1.58438800	0.24808900
H	3.39861400	1.07176600	1.19236400
H	4.01227000	1.32509700	-0.45210700
H	3.29409400	2.66443700	0.42005300

Sci-P9

C	1.91362600	1.35312600	-0.22318300
C	0.39995500	1.16866900	-0.03834500
C	-0.07094100	-0.21181800	-0.52227500
C	0.73678700	-1.32957300	0.17904800
C	2.25049500	-1.14804900	0.00029100
C	2.71099400	0.23899600	0.46842500
H	0.15116100	1.28107200	1.02481100
H	-0.14086500	1.95691800	-0.57203100
H	2.14937600	1.35327400	-1.29535200
H	2.21934600	2.33190400	0.16065800
H	0.48784300	-1.32126300	1.24792200
H	0.42557500	-2.30721400	-0.20486800
H	2.78825400	-1.93100800	0.54501900
H	2.50643500	-1.27466400	-1.05978400
H	2.57174700	0.31727400	1.55455200
H	3.78230500	0.36680400	0.28184900
H	0.16696700	-0.28087700	-1.59629000
C	-1.55233200	-0.46391900	-0.38650700
H	-1.88071000	-1.43163000	-0.76927300
C	-2.47032300	0.34148000	0.14594200
H	-2.17088900	1.31169300	0.53577300
C	-3.93307700	0.01861300	0.25634800
H	-4.54357600	0.75527700	-0.27835700
H	-4.15853900	-0.96895700	-0.15365100
H	-4.26553300	0.03624800	1.30055500

Sci-R10

C	-2.43524100	1.37780400	0.86467700
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C	-1.11603900	0.83138600	0.30118500
C	-1.15281700	-0.69717900	0.12878600
C	-2.35691700	-1.10854400	-0.73624100
C	-3.68178600	-0.56469600	-0.18151400
C	-3.63523400	0.95841100	0.00418800
H	-0.91791400	1.28996000	-0.67663300
H	-0.27628200	1.11658200	0.94145700
H	-2.57599600	1.00149000	1.88661000
H	-2.38640600	2.46901200	0.94066800
H	-2.20736600	-0.72686900	-1.75541500
H	-2.40308200	-2.20059200	-0.81682800
H	-4.50807200	-0.84209800	-0.84434400
H	-3.88764400	-1.03923800	0.78686800
H	-3.55865600	1.43963400	-0.97956100
H	-4.56893700	1.31373900	0.45254700
H	-1.29010100	-1.14583500	1.12435900
C	0.16966100	-1.24860300	-0.45166700
H	0.02128500	-2.32302600	-0.65495400
H	0.36483300	-0.77798200	-1.42185800
C	1.35407500	-1.08054300	0.43761200
H	1.26690700	-1.35688300	1.48494900
C	2.64035500	-0.49884500	-0.03514600
H	2.89477100	-0.89661700	-1.02738800
C	3.80675500	-0.69815600	0.92434900
H	4.69824200	-0.19570400	0.54523000
H	3.56268200	-0.29129900	1.90973400
H	4.03629700	-1.76150300	1.03392100
O	2.35478000	0.91527400	-0.22997400
O	3.44080000	1.48407000	-1.02947500

Sci-TS10

C	1.32311100	0.15611700	-0.32905600
H	5.01894400	-0.51908900	-0.46129500
C	2.36950000	0.67006000	0.42089100
H	2.23916800	0.68403300	1.49977100
O	3.51901700	-0.85437000	0.61105500
O	4.24881200	-1.09831200	-0.55879400
C	0.23928000	-0.71338000	0.21910400
H	0.44344700	-1.75075200	-0.08538000
H	0.27208900	-0.70697700	1.31482400
C	-1.17981400	-0.34049500	-0.26122700
C	-2.20897800	-1.40124500	0.16667700
C	-1.61094800	1.05291700	0.22969300
H	-1.16364900	-0.31811300	-1.36127200
C	-3.63253800	-1.04623100	-0.28654800

H	-2.18985500	-1.49282600	1.26138200
H	-1.91952800	-2.38016600	-0.23099500
C	-3.03212800	1.41498000	-0.22458400
H	-1.56681500	1.06766900	1.32779600
H	-0.89827500	1.80818600	-0.11768600
C	-4.05017700	0.34803400	0.20095800
H	-4.33950300	-1.80151900	0.07191200
H	-3.67877200	-1.07340300	-1.38301900
H	-3.31678200	2.39299800	0.17712700
H	-3.04754600	1.51215600	-1.31800900
H	-5.04587700	0.60011100	-0.17825200
H	-4.12648200	0.33926900	1.29611800
H	1.36597800	0.26375400	-1.41175900
C	3.31015500	1.70389400	-0.13446800
H	4.21874800	1.76703800	0.46903700
H	3.58462700	1.46740000	-1.16529600
H	2.84267400	2.69378300	-0.13172400

Sci-P10

C	-2.10950200	1.51949900	0.19155000
C	-0.80887600	1.05068600	-0.47823600
C	-0.34279200	-0.31966900	0.04682800
C	-1.47555100	-1.35371000	-0.08916500
C	-2.77662200	-0.89143100	0.58207900
C	-3.22712300	0.47721200	0.05412300
H	-0.96675900	0.97781100	-1.56364800
H	-0.02685700	1.80073500	-0.32645000
H	-1.91872000	1.70476600	1.25661800
H	-2.42712200	2.47586000	-0.23695300
H	-1.66390300	-1.53436600	-1.15667400
H	-1.15382900	-2.31169200	0.33455700
H	-3.56413800	-1.63661600	0.42811400
H	-2.61902300	-0.82526800	1.66645500
H	-3.50393100	0.38235100	-1.00409600
H	-4.12613700	0.81149600	0.58237200
H	-0.11462100	-0.20917000	1.11659000
C	0.94237400	-0.82388800	-0.64895500
H	1.15665900	-1.83867300	-0.29519700
H	0.73740000	-0.90672200	-1.72589100
C	2.15878900	0.03472900	-0.43631200
H	2.13729500	1.03222200	-0.87344500
C	3.24500900	-0.33618600	0.24028000
H	3.27373600	-1.33652800	0.67255900
C	4.46279700	0.51271700	0.46247000
H	5.35833000	0.03919800	0.04386400

H	4.35432100	1.49769700	0.00177300
H	4.65628400	0.65715400	1.53148200

Sci-R11

C	1.71034900	-0.33041300	-0.08082600
C	2.99481700	-0.29921700	-0.84023700
H	3.02222400	0.19036800	-1.80793600
O	1.84272400	0.31762500	1.21838200
O	2.06711600	1.73890900	1.01224800
H	3.03135300	1.78303800	1.07210300
C	4.21384400	-0.98788600	-0.32941500
H	4.30064100	-2.01105700	-0.72976800
H	5.13189800	-0.46652200	-0.61779800
H	4.19266900	-1.07491200	0.76093400
H	1.51021100	-1.35620600	0.26166800
C	0.51818200	0.20926200	-0.87346000
H	0.75527200	1.23553600	-1.17003300
H	0.43952400	-0.37734800	-1.79798600
C	-0.83010400	0.19871900	-0.13675500
C	-1.89017200	0.96780300	-0.94730300
C	-1.33349800	-1.22221800	0.17976500
H	-0.68807500	0.72486200	0.81527700
C	-3.25940900	0.98430800	-0.25404200
H	-1.99228300	0.50051000	-1.93712200
H	-1.54567900	1.99290200	-1.12237400
C	-2.70304600	-1.21159600	0.87539000
H	-1.40819900	-1.79154500	-0.75796500
H	-0.61185300	-1.75102600	0.81026200
C	-3.74758400	-0.43554400	0.06272600
H	-3.99091500	1.50749100	-0.87884100
H	-3.18240000	1.55565600	0.67997900
H	-3.04262400	-2.23816300	1.04877800
H	-2.59827700	-0.74744500	1.86440100
H	-4.69905600	-0.39908000	0.60349400
H	-3.94342600	-0.96864300	-0.87716600

Sci-TS11

C	1.61369500	-0.49137000	-0.15262300
C	2.80770200	-1.18939600	-0.06970100
H	2.91582300	-1.93441900	0.71552400
O	1.97783100	1.04704300	0.92602200
O	2.72389500	1.98684500	0.20407800
H	3.60231500	1.91622800	0.60417600
H	1.46105600	0.11649400	-1.03971200
C	0.36880200	-0.96026800	0.56975500

H	0.39095100	-0.56356600	1.59272100
H	0.40511200	-2.05168100	0.66196300
C	4.01779500	-0.87299900	-0.88409400
H	4.83791200	-0.50394100	-0.25227300
H	4.40558000	-1.76772700	-1.38652500
H	3.80887200	-0.11579200	-1.64171500
C	-0.95473200	-0.55669000	-0.10285600
C	-2.14259000	-1.30175800	0.53280700
C	-1.20258600	0.96278700	-0.06813400
H	-0.90045700	-0.86574500	-1.15816000
C	-3.48156100	-0.92626400	-0.11805500
H	-2.17928100	-1.06023900	1.60402500
H	-1.98272700	-2.38388700	0.46402600
C	-2.53487000	1.34269800	-0.72999600
H	-1.20841100	1.29104700	0.97939900
H	-0.37605900	1.49827600	-0.54224900
C	-3.71471800	0.59067900	-0.09939400
H	-4.30301100	-1.44382300	0.38835100
H	-3.48680400	-1.27865700	-1.15783600
H	-2.69225300	2.42375900	-0.65756100
H	-2.48831800	1.10755600	-1.80164500
H	-4.64661000	0.83709900	-0.61894400

Sci-P11

C	-2.10950200	1.51949900	0.19155000
C	-0.80887600	1.05068600	-0.47823600
C	-0.34279200	-0.31966900	0.04682800
C	-1.47555100	-1.35371000	-0.08916500
C	-2.77662200	-0.89143100	0.58207900
C	-3.22712300	0.47721200	0.05412300
H	-0.96675900	0.97781100	-1.56364800
H	-0.02685700	1.80073500	-0.32645000
H	-1.91872000	1.70476600	1.25661800
H	-2.42712200	2.47586000	-0.23695300
H	-1.66390300	-1.53436600	-1.15667400
H	-1.15382900	-2.31169200	0.33455700
H	-3.56413800	-1.63661600	0.42811400
H	-2.61902300	-0.82526800	1.66645500
H	-3.50393100	0.38235100	-1.00409600
H	-4.12613700	0.81149600	0.58237200
H	-0.11462100	-0.20917000	1.11659000
C	0.94237400	-0.82388800	-0.64895500
H	1.15665900	-1.83867300	-0.29519700
H	0.73740000	-0.90672200	-1.72589100
C	2.15878900	0.03472900	-0.43631200

H	2.13729500	1.03222200	-0.87344500
C	3.24500900	-0.33618600	0.24028000
H	3.27373600	-1.33652800	0.67255900
C	4.46279700	0.51271700	0.46247000
H	5.35833000	0.03919800	0.04386400
H	4.35432100	1.49769700	0.00177300
H	4.65628400	0.65715400	1.53148200

Sci-R12

C	3.22345500	-0.90834200	0.88578700
C	1.87220800	-1.39634600	0.34417800
C	0.89982100	-0.22532400	0.05813800
C	1.57547000	0.80060200	-0.89020300
C	2.92552600	1.28635000	-0.34432200
C	3.87518900	0.11687400	-0.05157300
H	2.03135700	-1.95563300	-0.58711000
H	1.41042500	-2.09351600	1.05057700
H	3.07158200	-0.45034800	1.87182900
H	3.89207500	-1.76154100	1.04019900
H	1.72673800	0.32625500	-1.86859400
H	0.89570500	1.64132300	-1.04972000
H	3.38528200	1.97971400	-1.05630400
H	2.75837000	1.85618100	0.57906200
H	4.14207600	-0.37567700	-0.99561700
H	4.81030100	0.48613300	0.38189300
H	0.70431400	0.28966400	1.00900900
C	-0.40122800	-0.70999200	-0.48944900
H	-0.38959600	-1.29615500	-1.40513900
C	-1.71613100	-0.30008800	0.07652200
H	-1.71234100	-0.40832100	1.17043500
C	-2.89793600	-1.05654800	-0.53285800
H	-2.69286700	-2.12794600	-0.41663900
H	-2.90308000	-0.85322500	-1.60947400
C	-4.26563000	-0.72468800	0.06830300
H	-5.04758300	-1.32043400	-0.41054000
H	-4.29100600	-0.93936400	1.14085000
H	-4.50920400	0.33012300	-0.06176600
O	-1.80375600	1.13575500	-0.17910200
O	-2.67026500	1.74451700	0.83081000
H	-2.03485000	2.33559600	1.25625600

Sci-TS12

C	0.43537600	-0.54579400	0.49185100
H	3.41336300	1.78511500	0.49312000
C	1.62360400	-0.59317700	-0.22190200

H	1.54535000	-0.75771100	-1.29440500
O	1.95380300	1.27637900	-0.56942900
O	2.45734400	1.92515000	0.56653200
H	0.48656200	-0.53008500	1.58000400
C	-0.91246000	-0.33589700	-0.11965600
C	-1.92311000	-1.41066100	0.34671300
C	-1.45451900	1.08073200	0.20042200
H	-0.81317200	-0.41402300	-1.21060500
C	-3.32096000	-1.18059600	-0.24534700
H	-1.98305400	-1.38680900	1.44295100
H	-1.55563400	-2.40569700	0.07570700
C	-2.85164100	1.30475800	-0.39393100
H	-1.49745300	1.20336500	1.29078700
H	-0.74475300	1.82244900	-0.17203100
C	-3.84524400	0.22834900	0.06336400
H	-4.01455300	-1.93708500	0.13633200
H	-3.27818700	-1.31952700	-1.33338700
H	-3.21561000	2.29973900	-0.11762200
H	-2.78404300	1.29291600	-1.48949800
H	-4.81918900	0.38191000	-0.41263600
H	-4.00807900	0.32354000	1.14489900
C	2.91935700	-1.03188100	0.41690600
H	2.80095300	-2.06031300	0.77755400
H	3.08608600	-0.41943400	1.31020900
C	4.12769300	-0.95909800	-0.52108000
H	5.04828600	-1.23710100	-0.00192000
H	4.00647700	-1.64006100	-1.36866800
H	4.24890700	0.04618100	-0.93166000

Sci-P12

C	2.29218500	1.45588200	-0.18816500
C	0.80994300	1.12680700	0.04404500
C	0.44323600	-0.26589600	-0.49198900
C	1.37509400	-1.33838800	0.12054100
C	2.85794000	-1.01262200	-0.10588300
C	3.21343000	0.38658300	0.41473100
H	0.59732100	1.16521900	1.12021100
H	0.17927200	1.88734900	-0.42755600
H	2.48153800	1.52864200	-1.26705100
H	2.52619500	2.43878000	0.23367600
H	1.17169900	-1.40318000	1.19708300
H	1.13546000	-2.32080900	-0.30069200
H	3.48525700	-1.76880100	0.37742600
H	3.07896900	-1.06515300	-1.17997300
H	3.11394300	0.40015100	1.50794800

H	4.26039600	0.61936600	0.19447000
H	0.64114000	-0.26213400	-1.57625700
C	-1.00317400	-0.65682000	-0.31472200
H	-1.26082700	-1.62939600	-0.73735700
C	-1.96563500	0.03209100	0.29761400
H	-1.74011000	1.00633700	0.72781300
C	-3.39317600	-0.42162600	0.43816300
H	-3.64620800	-0.49424800	1.50405300
H	-3.50040400	-1.42963200	0.02418800
C	-4.39331200	0.52872400	-0.24046500
H	-5.42229800	0.18879000	-0.09335800
H	-4.31537300	1.54095400	0.16790800
H	-4.20516500	0.58936300	-1.31575300

Sci-R13

C	0.72861400	0.28499600	0.49132500
C	1.81342500	-0.52852100	-0.13070900
H	2.08558400	2.13200200	-1.03474100
H	1.65815400	-0.94968000	-1.11944300
O	1.09591000	1.69840800	0.51886600
O	1.13919600	2.19549100	-0.84657500
H	0.69109300	0.09557200	1.57511300
C	3.10998400	-0.76746200	0.56976400
H	3.36218400	0.11400500	1.17361300
H	2.98681200	-1.58526700	1.30110900
C	-0.66726800	0.05844200	-0.10824200
C	-1.13163200	-1.39427600	0.11692900
C	-1.70584900	1.04531800	0.45307500
H	-0.58598400	0.23119200	-1.18886200
C	-2.52866100	-1.64697300	-0.46865600
H	-1.15211500	-1.59702900	1.19693200
H	-0.41348600	-2.09791300	-0.31574600
C	-3.10267500	0.79619200	-0.13305500
H	-1.74668400	0.93658200	1.54592100
H	-1.38556100	2.06932700	0.25424800
C	-3.56105900	-0.65281300	0.07947800
H	-2.84051200	-2.67529100	-0.25814800
H	-2.48187100	-1.55304600	-1.56125600
H	-3.82236800	1.49090300	0.31198900
H	-3.08554000	1.01503500	-1.20861100
H	-4.53472800	-0.81903700	-0.39311800
H	-3.70085300	-0.83394500	1.15334500
C	4.27347600	-1.11387000	-0.36703700
H	5.19093900	-1.30437300	0.19535200

H	4.05083400	-2.00864500	-0.95575000
H	4.47311400	-0.29777600	-1.06751300
Sci-TS13			
C	-0.65189300	-0.05264500	0.33459500
C	-1.61614800	-0.94892100	-0.09767500
H	-1.43923200	-1.49151400	-1.02486300
O	-1.29537200	1.54141200	-0.52578500
O	-2.18361700	2.19510700	0.34303400
H	-3.03845700	2.06349100	-0.09100800
H	-0.77576400	0.37124100	1.32826500
C	0.76743100	-0.08612200	-0.19095200
C	1.58122500	1.15084500	0.23151900
C	1.48869400	-1.37740500	0.26423300
H	0.71166800	-0.10439000	-1.28841300
C	3.02479600	1.09265100	-0.28557900
H	1.59361400	1.20305800	1.32913800
H	1.07789200	2.05201900	-0.12056200
C	2.93461900	-1.43717000	-0.25007000
H	1.48994600	-1.41441400	1.36179200
H	0.93046400	-2.25547900	-0.07455200
C	3.73629900	-0.19327000	0.15555800
H	3.57913600	1.97094000	0.06061000
H	3.01785400	1.14418700	-1.38223400
H	3.42296100	-2.34380300	0.12212500
H	2.92247500	-1.51730900	-1.34485800
H	4.74453100	-0.23784900	-0.26912200
H	3.85732700	-0.18250100	1.24667200
C	-2.96101100	-1.11296100	0.53835800
H	-3.07799600	-0.37551400	1.33820000
H	-3.01909900	-2.10009400	1.02052300
C	-4.12271500	-0.99674700	-0.46348400
H	-5.08700200	-1.12669400	0.03475300
H	-4.12137400	-0.02073900	-0.95698300
H	-4.04481800	-1.75633100	-1.24649500

Sci-P13			
C	2.29218500	1.45588200	-0.18816500
C	0.80994300	1.12680700	0.04404500
C	0.44323600	-0.26589600	-0.49198900
C	1.37509400	-1.33838800	0.12054100
C	2.85794000	-1.01262200	-0.10588300
C	3.21343000	0.38658300	0.41473100
H	0.59732100	1.16521900	1.12021100
H	0.17927200	1.88734900	-0.42755600
H	2.48153800	1.52864200	-1.26705100

H	2.52619500	2.43878000	0.23367600
H	1.17169900	-1.40318000	1.19708300
H	1.13546000	-2.32080900	-0.30069200
H	3.48525700	-1.76880100	0.37742600
H	3.07896900	-1.06515300	-1.17997300
H	3.11394300	0.40015100	1.50794800
H	4.26039600	0.61936600	0.19447000
H	0.64114000	-0.26213400	-1.57625700
C	-1.00317400	-0.65682000	-0.31472200
H	-1.26082700	-1.62939600	-0.73735700
C	-1.96563500	0.03209100	0.29761400
H	-1.74011000	1.00633700	0.72781300
C	-3.39317600	-0.42162600	0.43816300
H	-3.64620800	-0.49424800	1.50405300
H	-3.50040400	-1.42963200	0.02418800
C	-4.39331200	0.52872400	-0.24046500
H	-5.42229800	0.18879000	-0.09335800
H	-4.31537300	1.54095400	0.16790800
H	-4.20516500	0.58936300	-1.31575300

Sci-R14

C	1.91782900	0.97238200	0.51065000
C	0.54088400	0.73383600	1.14143200
C	-0.39810900	-0.07960100	0.23416800
C	0.29292300	-1.38721400	-0.23304700
C	1.68059200	-1.14973000	-0.84843900
C	2.58537400	-0.34438100	0.09262600
H	0.65222200	0.18094500	2.08227500
H	0.05696500	1.68300100	1.37986400
H	1.80038500	1.61728500	-0.36576400
H	2.55392700	1.51309100	1.21879900
H	0.38066500	-2.03484100	0.64655600
H	-0.36004000	-1.90086600	-0.94412700
H	2.13894700	-2.11590300	-1.08453200
H	1.56597200	-0.61129600	-1.79349100
H	2.80355500	-0.94148500	0.98840500
H	3.54728000	-0.14503200	-0.39042800
C	-1.71658800	-0.34918600	0.89478600
H	-1.81181500	-0.14732200	1.95667200
O	-0.60805200	0.61112000	-1.03759300
O	-1.15014100	1.93411800	-0.79480200
H	-2.10002900	1.76228700	-0.85869000
C	-2.85025000	-1.00500400	0.18130700
H	-2.92369100	-2.07789400	0.41923000

H	-3.81354900	-0.56734500	0.46675200
H	-2.74118200	-0.92314800	-0.90324900

Sci-TS14

C	1.91009400	0.67721400	0.70748100
C	0.52581200	0.43713500	1.32441500
C	-0.45696700	-0.26267100	0.40582700
C	0.10116900	-1.38998400	-0.44336100
C	1.50417900	-1.12178700	-1.01075000
C	2.46611400	-0.59599300	0.05953600
H	0.63651700	-0.19474800	2.21688000
H	0.08865200	1.38126000	1.65899900
H	1.83293000	1.46669800	-0.04435200
H	2.59036900	1.03901500	1.48538500
H	0.13366700	-2.28645500	0.19314500
H	-0.59347300	-1.61617800	-1.25621300
H	1.89160800	-2.04419200	-1.45557900
H	1.42415700	-0.38383200	-1.81265800
H	2.62209500	-1.36484400	0.82910400
H	3.44688000	-0.39640100	-0.38378600
C	-1.80381700	-0.26228900	0.76067900
H	-2.12226500	0.47636400	1.49162400
O	-0.60817600	1.02244000	-1.07491200
O	-0.55646900	2.34674500	-0.62091000
H	-1.47915800	2.63050600	-0.68507400
C	-2.86481000	-1.09874100	0.11605700
H	-2.61739200	-2.16608800	0.12621200
H	-3.82516100	-0.97447300	0.61971600
H	-3.00291800	-0.81741000	-0.93613100

Sci-P14

C	1.70887600	1.04517900	-0.42179400
C	0.46272200	1.37270800	0.42436100
C	-0.60408100	0.30779400	0.28174100
C	-0.09864200	-1.08678000	0.57770000
C	1.14845200	-1.42233500	-0.26710800
C	2.24286100	-0.35871700	-0.10777400
H	0.76810500	1.43560100	1.47915500
H	0.06108900	2.35265600	0.15176100
H	1.44250400	1.10363600	-1.48411200
H	2.48664600	1.79622300	-0.24847600
H	0.17820400	-1.14198100	1.64051800
H	-0.87136000	-1.84050100	0.41807500
H	1.53233100	-2.40830400	0.01476100
H	0.85548200	-1.48646000	-1.32199700
H	2.61836300	-0.37945800	0.92388100

H	3.09526000	-0.59372000	-0.75353300
C	-1.84802100	0.61828000	-0.10030900
H	-2.05816200	1.67047000	-0.29032300
C	-3.02275900	-0.29703200	-0.29783400
H	-2.78802400	-1.34514800	-0.10893400
H	-3.84871500	-0.01699100	0.36639800
H	-3.40817000	-0.22060500	-1.32107600

Sci-R15

C	2.34126000	0.86120700	0.63897000
C	0.91096800	0.68760300	1.16262900
C	-0.00730700	-0.03842500	0.16410900
C	0.63847500	-1.36832300	-0.30492300
C	2.07917300	-1.19619300	-0.81013600
C	2.95815500	-0.48050600	0.22314700
H	0.92155600	0.10043700	2.08926000
H	0.46723000	1.65658700	1.39964900
H	2.32573200	1.53838400	-0.22071700
H	2.95516500	1.33993000	1.40862100
H	0.62306200	-2.05210800	0.55139300
H	0.01015200	-1.81406800	-1.08094200
H	2.49536700	-2.18050000	-1.04943300
H	2.06716300	-0.62030200	-1.74006400
H	3.07084600	-1.11877800	1.11004100
H	3.96409100	-0.32723000	-0.18045200
C	-1.38129800	-0.25123500	0.72483700
H	-1.54104400	-0.06244700	1.78264900
O	-0.08674300	0.70728500	-1.09215300
O	-0.57018600	2.05043700	-0.83526700
H	-1.51760100	1.94128700	-0.99627400
C	-2.50025000	-0.84175800	-0.06922800
H	-2.52558500	-1.93552900	0.07442100
H	-2.30900100	-0.69448600	-1.13792900
C	-3.88062000	-0.27797700	0.30420700
H	-4.67194000	-0.75324400	-0.28133200
H	-4.10046700	-0.44632400	1.36241600
H	-3.93062400	0.80025700	0.12638900

Sci-TS15

C	2.32752200	0.45582700	0.84954200
C	0.87750000	0.35899500	1.34257400
C	-0.09754800	-0.18965200	0.31860900
C	0.39962800	-1.34289000	-0.53394400
C	1.86613400	-1.21835300	-0.97587100
C	2.78714000	-0.85058500	0.19210800

H	0.83885800	-0.30994100	2.21388100
H	0.52437500	1.33650400	1.68045000
H	2.40392800	1.27357500	0.12854000
H	2.97645900	0.70904100	1.69423400
H	0.27773200	-2.25899600	0.06250500
H	-0.24595600	-1.45854700	-1.40809800
H	2.18294700	-2.16146600	-1.43292700
H	1.93771500	-0.44460500	-1.74401900
H	2.78488100	-1.65968100	0.93556800
H	3.81913300	-0.75363400	-0.15981200
C	-1.46100800	-0.04652600	0.56451100
H	-1.75748600	0.69324900	1.30574300
O	0.02576100	1.15735200	-1.10983000
O	0.18974100	2.44916400	-0.59299800
H	-0.68564200	2.84179900	-0.71737200
C	-2.55881600	-0.72990700	-0.19588200
H	-2.42842400	-1.81960300	-0.14872400
H	-2.46877800	-0.47462100	-1.26103300
C	-3.96055100	-0.36362900	0.30195400
H	-4.14079200	0.71202200	0.21561400
H	-4.73216700	-0.87779000	-0.27611100
H	-4.09080500	-0.63912100	1.35256800

Sci-P15

C	2.22515200	1.05530200	-0.34970000
C	0.91946200	1.37145400	0.40637300
C	-0.12468300	0.29700600	0.18726300
C	0.37187200	-1.09174400	0.52393700
C	1.67766000	-1.41764600	-0.23126000
C	2.74870800	-0.34375900	0.00161200
H	1.14843500	1.43555800	1.48020000
H	0.52971300	2.34804300	0.10610400
H	2.03364100	1.11174600	-1.42813500
H	2.98188600	1.81338000	-0.12238100
H	0.57597700	-1.13889200	1.60340800
H	-0.38096500	-1.85360600	0.31561600
H	2.04982500	-2.39946800	0.07933100
H	1.45938900	-1.48661800	-1.30377600
H	3.05269900	-0.36071300	1.05661800
H	3.64555300	-0.57123500	-0.58381400
C	-1.33805000	0.59492100	-0.29237600
H	-1.54451700	1.64625600	-0.49697100
C	-2.49473600	-0.32585400	-0.57146300
H	-2.21218900	-1.37100400	-0.42528000
H	-2.77605000	-0.23034500	-1.62841200

C	-3.72608800	-0.00383200	0.29308600
H	-4.56872800	-0.65231400	0.03669800
H	-3.50334200	-0.13837700	1.35496100
H	-4.04710400	1.03250300	0.15100800

Sci-R16

C	2.83414000	0.84288700	0.49203300
C	1.43344800	0.74113600	1.10672800
C	0.44014700	-0.02232500	0.21235400
C	1.02746200	-1.39755400	-0.20157100
C	2.43868200	-1.29641500	-0.80060700
C	3.39460800	-0.53834300	0.12941000
H	1.48496600	0.21360600	2.06716400
H	1.02616800	1.73436300	1.30577900
H	2.78400500	1.46444400	-0.40751400
H	3.50303400	1.35298700	1.19262500
H	1.04935500	-2.02026700	0.69983100
H	0.34315800	-1.87892600	-0.90578900
H	2.81785900	-2.30474200	-0.99792800
H	2.38365400	-0.78198800	-1.76432600
H	3.54821500	-1.12123500	1.04783600
H	4.37696200	-0.43750200	-0.34298900
C	-0.90035300	-0.16124600	0.86768800
H	-0.97586900	0.05087300	1.93038000
O	0.30772200	0.64031900	-1.08330200
O	-0.13539400	2.00946300	-0.88931700
H	-1.07912400	1.92468400	-1.08142600
C	-2.11119300	-0.66949900	0.15757700
H	-2.30203500	-1.71974500	0.43758100
H	-1.93053700	-0.67782200	-0.92309500
C	-3.38951100	0.13683900	0.46387000
H	-3.55673700	0.14355600	1.54695000
H	-3.23138200	1.18385900	0.17931300
C	-4.62940100	-0.41176900	-0.24620700
H	-4.83068900	-1.44474300	0.05398600
H	-5.51729000	0.18151700	-0.01208400
H	-4.50052300	-0.40343700	-1.33300100

Sci-TS16

C	2.84499200	0.32110900	0.75638600
C	1.41760700	0.37994400	1.31653500
C	0.34888400	-0.11576600	0.36116700
C	0.69644400	-1.34668700	-0.45574600
C	2.14582800	-1.38116900	-0.96571700
C	3.15192000	-1.04896600	0.14133900

H	1.35997900	-0.24774700	2.21702900
H	1.17178000	1.39868000	1.62645700
H	2.96114900	1.09740600	-0.00406300
H	3.55417000	0.54771300	1.55918600
H	0.51874300	-2.21997100	0.18894800
H	0.00222500	-1.43982300	-1.29470100
H	2.35213300	-2.36993000	-1.38836600
H	2.25157300	-0.65410200	-1.77453500
H	3.11369700	-1.82159200	0.92179500
H	4.16992500	-1.06296000	-0.26085200
C	-0.98193300	0.16808300	0.65783500
H	-1.17190400	0.96159200	1.37806500
O	0.52903200	1.15234700	-1.13216700
O	0.83530800	2.44355100	-0.68261300
H	-0.00577400	2.91036900	-0.78524800
C	-2.17365200	-0.43531700	-0.02344900
H	-2.16243400	-1.52926400	0.08918000
H	-2.09986900	-0.25649100	-1.10611400
C	-3.51294100	0.10901100	0.48977100
H	-3.53177100	1.19714900	0.35628600
H	-3.58237400	-0.06723200	1.56957000
C	-4.72244500	-0.51383300	-0.21061800
H	-5.66030800	-0.10363600	0.17297200
H	-4.69411800	-0.32774700	-1.28874100
H	-4.74976500	-1.59806500	-0.06364300

Sci-P16

C	-2.83324500	-0.92677300	-0.35428000
C	-1.56033100	-1.35382300	0.40323800
C	-0.42837800	-0.37148400	0.18782700
C	-0.80576300	1.05391700	0.52565600
C	-2.07813700	1.49060700	-0.23066300
C	-3.23670800	0.51101600	-0.00107400
H	-1.79585800	-1.39997700	1.47657400
H	-1.25422500	-2.35946800	0.10193200
H	-2.64538000	-0.99733100	-1.43251700
H	-3.65195100	-1.61831100	-0.12953200
H	-1.00643200	1.11690100	1.60496300
H	0.00956300	1.74906400	0.31930800
H	-2.36620400	2.49997300	0.08103700
H	-1.85322700	1.54247800	-1.30276800
H	-3.53968000	0.55191600	1.05357200
H	-4.11021000	0.81475200	-0.58721600
C	0.75649300	-0.77063100	-0.28976200
H	0.87263200	-1.83536300	-0.49544500

C	1.98724300	0.04938200	-0.56338600
H	1.78916800	1.11774000	-0.44018400
H	2.28009400	-0.08763900	-1.61365300
C	3.18110100	-0.34774600	0.32613800
H	2.90756600	-0.19415300	1.37579200
H	3.36995700	-1.42200400	0.21515500
C	4.45676500	0.43377400	0.00083500
H	5.28546400	0.13138800	0.64691900
H	4.76714700	0.27080300	-1.03613700
H	4.30735400	1.50980600	0.13502800

Sci-R17

C	-1.94168500	1.25883000	0.26451000
C	-0.40368800	1.26761400	0.17499100
C	0.20178100	-0.07099900	0.46613100
C	-0.43688200	-1.27732500	-0.15338200
C	-1.97480900	-1.25073200	-0.05631000
C	-2.54391900	0.09270100	-0.52969800
H	-0.10961500	1.57184800	-0.84546900
H	0.01540500	2.02988200	0.84089900
H	-2.24011000	1.16829800	1.31608500
H	-2.33878800	2.21319800	-0.09561000
H	-0.15382600	-1.32263400	-1.21929200
H	-0.03762400	-2.19413900	0.29385400
H	-2.39634100	-2.07341900	-0.64249700
H	-2.27323700	-1.41947500	0.98558400
H	-2.32217000	0.22604900	-1.59676500
H	-3.63460500	0.09503800	-0.43468600
H	3.48160900	0.91534300	-0.79295900
C	1.58758500	-0.17910200	0.99319800
H	1.90578900	0.74250200	1.49492600
H	1.69121800	-1.01963200	1.69145300
O	2.57341600	-0.53721500	-0.00748500
O	2.61183400	0.53986800	-0.98653500

Sci-TS17

C	1.55242400	0.59721000	-1.12315300
C	0.91271400	1.51058800	-0.05054700
C	-0.07312400	0.73828800	0.77865700
C	0.46302100	-0.51677900	1.40612600
C	1.11593000	-1.42929000	0.33942300
C	2.15507100	-0.66371400	-0.49006700
H	1.71209700	1.89479400	0.60045100
H	0.43381000	2.37418000	-0.51893100
H	0.77517800	0.31223100	-1.83929000

H	2.31705000	1.15460400	-1.67365000
H	1.22862200	-0.24746300	2.14920000
H	-0.32650800	-1.05440600	1.93691100
H	1.57741300	-2.29234400	0.83019100
H	0.32684600	-1.81015900	-0.31562800
H	2.99982300	-0.38008400	0.15206400
H	2.56222400	-1.31528100	-1.26992600
H	-3.10146700	-1.26853400	-0.20916300
C	-1.42246500	1.04055100	0.76872300
H	-2.08325100	0.54878800	1.47457900
H	-1.74465600	2.02089700	0.43517000
O	-2.12664200	0.21878900	-0.80877700
O	-2.23568400	-1.16858200	-0.63209200

Sci-P17

C	-1.02042800	-1.26871000	-0.30004100
C	0.34535100	-1.26901700	0.41631100
C	1.11520900	0.00003000	0.13143300
C	0.34533500	1.26903500	0.41629400
C	-1.02044500	1.26870400	-0.30004000
C	-1.82249200	-0.00002200	0.02141900
H	0.16961600	-1.34279800	1.49911600
H	0.93236600	-2.14516300	0.12805300
H	-0.85383800	-1.32821400	-1.38228800
H	-1.58881500	-2.16079500	-0.01797100
H	0.16958400	1.34280500	1.49909700
H	0.93233100	2.14520900	0.12806100
H	-1.58886100	2.16076600	-0.01795400
H	-0.85388500	1.32820700	-1.38228900
H	-2.08734400	-0.00002300	1.08702200
H	-2.76642100	-0.00001500	-0.53310700
C	2.35274900	-0.00000400	-0.36301200
H	2.88183000	0.92447900	-0.57098300
H	2.88175600	-0.92454100	-0.57094200

Sci-R18

C	2.05735800	1.32249300	0.25441800
C	0.54258800	1.12990900	0.46891700
C	-0.01336000	-0.00883000	-0.33235300
C	0.76988700	-1.28901200	-0.32956000
C	2.27953800	-1.06602800	-0.54102900
C	2.82482500	0.00454000	0.41163300
H	0.36105700	0.92465200	1.53901400
H	0.01573600	2.06318400	0.25416900
H	2.22913700	1.71962000	-0.75356700

H	2.43506400	2.07198500	0.95731000
H	0.62308900	-1.79320100	0.64115500
H	0.37429900	-1.98095700	-1.08069400
H	2.81555900	-2.01057600	-0.40370600
H	2.45630500	-0.74965100	-1.57636000
H	2.73205200	-0.34898700	1.44698500
H	3.89263600	0.16508500	0.23044000
H	-3.12081300	-0.22985400	1.56650900
C	-1.44592100	-0.07684200	-0.76117700
H	-1.50555400	-0.64580200	-1.69922900
O	-2.21435200	-0.98345600	0.09287300
O	-2.18841800	-0.45635000	1.45288100
C	-2.17931900	1.24915900	-0.93023900
H	-1.65540300	1.89362900	-1.64076100
H	-2.25750700	1.78047800	0.01942900
H	-3.18706100	1.06650800	-1.31037500

Sci-TS18

C	-1.64422700	-0.85792200	-1.11774600
C	-0.66480400	-1.56590400	-0.15153800
C	0.09246200	-0.56174200	0.67109800
C	-0.77021000	0.42576300	1.40758300
C	-1.76543500	1.12660400	0.45319100
C	-2.56816100	0.10698900	-0.36472900
H	-1.24908100	-2.20960100	0.52344400
H	0.00602300	-2.22217900	-0.70785600
H	-1.05770100	-0.30171700	-1.85621200
H	-2.22953200	-1.60682900	-1.66108100
H	-1.34643300	-0.10850500	2.17884400
H	-0.15452700	1.16687400	1.92303600
H	-2.43861400	1.76663600	1.03303700
H	-1.19728600	1.77610400	-0.21871000
H	-3.22405800	-0.46607400	0.30459500
H	-3.22276300	0.62724300	-1.07150700
H	2.16057900	2.45008100	-0.12990200
C	1.47333300	-0.40658500	0.61965000
H	1.89386600	0.27784600	1.35243900
O	1.70822600	0.78862100	-0.87950300
O	1.35840400	2.10758700	-0.55092300
C	2.42846700	-1.45724000	0.11695500
H	2.12676000	-1.84242700	-0.85843700
H	3.42881700	-1.03577800	0.01189900
H	2.48235900	-2.30111800	0.81304200

Sci-P18

C	1.70887600	1.04517900	-0.42179400
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C	0.46272200	1.37270800	0.42436100
C	-0.60408100	0.30779400	0.28174100
C	-0.09864200	-1.08678000	0.57770000
C	1.14845200	-1.42233500	-0.26710800
C	2.24286100	-0.35871700	-0.10777400
H	0.76810500	1.43560100	1.47915500
H	0.06108900	2.35265600	0.15176100
H	1.44250400	1.10363600	-1.48411200
H	2.48664600	1.79622300	-0.24847600
H	0.17820400	-1.14198100	1.64051800
H	-0.87136000	-1.84050100	0.41807500
H	1.53233100	-2.40830400	0.01476100
H	0.85548200	-1.48646000	-1.32199700
H	2.61836300	-0.37945800	0.92388100
H	3.09526000	-0.59372000	-0.75353300
C	-1.84802100	0.61828000	-0.10030900
H	-2.05816200	1.67047000	-0.29032300
C	-3.02275900	-0.29703200	-0.29783400
H	-2.78802400	-1.34514800	-0.10893400
H	-3.84871500	-0.01699100	0.36639800
H	-3.40817000	-0.22060500	-1.32107600

Sci-R19

C	2.29920300	1.35669700	0.52542300
C	0.85278100	0.91070000	0.81749900
C	0.30765100	-0.00466700	-0.23805900
C	1.20447900	-1.11427200	-0.70415200
C	2.64536300	-0.64351700	-0.98013600
C	3.20486200	0.16384100	0.19742500
H	0.83622300	0.37611500	1.78392700
H	0.21415800	1.78689300	0.95417200
H	2.29626800	2.04959300	-0.32489100
H	2.69266600	1.91140200	1.38329400
H	1.23492800	-1.89614900	0.07414300
H	0.78245200	-1.60039300	-1.59021300
H	3.28281900	-1.50848800	-1.18958200
H	2.65505500	-0.01813900	-1.88133500
H	3.28335600	-0.48567400	1.07915000
H	4.21906100	0.50952200	-0.02785600
H	-2.44651900	-1.23362800	1.82062900
C	-1.15635700	-0.13387700	-0.52259700
H	-1.28781100	-0.40869600	-1.57921500
O	-1.70722300	-1.34601900	0.08766300
O	-1.52439800	-1.24598700	1.53251100

C	-2.03077900	1.08202700	-0.21019000
H	-1.56035100	1.96666700	-0.65221600
H	-2.03830800	1.24188600	0.87159300
C	-3.46330600	0.93965000	-0.73162900
H	-3.93973000	0.04103000	-0.33272300
H	-4.07291600	1.80162800	-0.44861800
H	-3.48176500	0.86299300	-1.82316400

Sci-TS19

C	-1.91429300	-1.01751800	-1.10224500
C	-0.83766200	-1.59953900	-0.15546200
C	-0.20201300	-0.50729200	0.65791000
C	-1.17145500	0.35205200	1.42057700
C	-2.26648700	0.92428400	0.48922500
C	-2.94306400	-0.18412400	-0.32786300
H	-1.32652800	-2.31186900	0.52613500
H	-0.09830300	-2.16381600	-0.72573200
H	-1.41597400	-0.38625300	-1.84478300
H	-2.40739600	-1.83239800	-1.64219700
H	-1.65857900	-0.25902500	2.19611100
H	-0.64879700	1.16395400	1.93202400
H	-3.00734800	1.46564000	1.08673200
H	-1.79906300	1.64849400	-0.18369100
H	-3.51045900	-0.84168500	0.34465200
H	-3.66904500	0.25334100	-1.02086000
H	1.47347800	2.75915400	-0.18336900
C	1.14377900	-0.17013700	0.56489100
H	1.49823700	0.55990800	1.28988500
O	1.14784100	1.06353500	-0.92420700
O	0.68293200	2.33336100	-0.54646300
C	2.20928000	-1.08837900	0.00813900
H	1.98266500	-1.29727900	-1.04225400
H	2.16143000	-2.05128700	0.53110500
C	3.62147100	-0.50889200	0.12095000
H	3.89594900	-0.33290900	1.16589500
H	4.36117700	-1.19130500	-0.30517300
H	3.68503800	0.43944000	-0.41584300

Sci-P19

C	2.22515200	1.05530200	-0.34970000
C	0.91946200	1.37145400	0.40637300
C	-0.12468300	0.29700600	0.18726300
C	0.37187200	-1.09174400	0.52393700
C	1.67766000	-1.41764600	-0.23126000
C	2.74870800	-0.34375900	0.00161200
H	1.14843500	1.43555800	1.48020000

H	0.52971300	2.34804300	0.10610400
H	2.03364100	1.11174600	-1.42813500
H	2.98188600	1.81338000	-0.12238100
H	0.57597700	-1.13889200	1.60340800
H	-0.38096500	-1.85360600	0.31561600
H	2.04982500	-2.39946800	0.07933100
H	1.45938900	-1.48661800	-1.30377600
H	3.05269900	-0.36071300	1.05661800
H	3.64555300	-0.57123500	-0.58381400
C	-1.33805000	0.59492100	-0.29237600
H	-1.54451700	1.64625600	-0.49697100
C	-2.49473600	-0.32585400	-0.57146300
H	-2.21218900	-1.37100400	-0.42528000
H	-2.77605000	-0.23034500	-1.62841200
C	-3.72608800	-0.00383200	0.29308600
H	-4.56872800	-0.65231400	0.03669800
H	-3.50334200	-0.13837700	1.35496100
H	-4.04710400	1.03250300	0.15100800

Sci-R20

C	-2.45080700	-1.53823300	0.64079900
C	-1.11472600	-0.81653900	0.90820900
C	-0.70218500	0.07167100	-0.22748600
C	-1.76259200	0.95689700	-0.81487500
C	-3.08822200	0.21320700	-1.06692200
C	-3.53885800	-0.56281100	0.17645000
H	-1.22497200	-0.19402200	1.81380400
H	-0.33786200	-1.54746800	1.14577900
H	-2.29825000	-2.30095000	-0.13268000
H	-2.77035500	-2.06579500	1.54528400
H	-1.95638400	1.79052700	-0.11794700
H	-1.40288700	1.42440500	-1.73764000
H	-3.85973900	0.92647500	-1.37420500
H	-2.95578600	-0.48788100	-1.90008600
H	-3.76118600	0.14523200	0.98563500
H	-4.46829900	-1.10342000	-0.03028900
H	1.76678800	1.88665200	1.76175600
C	0.72600900	0.42362600	-0.50495700
H	0.83249400	0.64074500	-1.57745600
O	1.05337200	1.75222700	0.01959000
O	0.86100000	1.72654100	1.46617400
C	1.78231000	-0.60365800	-0.09458700
H	1.46595600	-1.58892700	-0.45594100
H	1.80927400	-0.66778400	0.99780400

C	3.18226800	-0.28492800	-0.63201600
H	3.46107300	0.72941200	-0.32910900
H	3.15369200	-0.27444900	-1.72831800
C	4.24534300	-1.28010700	-0.15909600
H	4.00616200	-2.29909100	-0.47919300
H	5.23151800	-1.02990700	-0.55923800
H	4.32254900	-1.28864300	0.93280300

Sci-TS20

C	-2.14875500	-1.24175000	-1.09175500
C	-1.02281400	-1.62512600	-0.10196400
C	-0.57536600	-0.42582100	0.68569700
C	-1.67915300	0.31472800	1.38794000
C	-2.81747900	0.68804200	0.40951300
C	-3.30640000	-0.53735700	-0.37327500
H	-1.41745200	-2.38079500	0.59408600
H	-0.19264300	-2.09003600	-0.63596000
H	-1.72866900	-0.57356800	-1.85032700
H	-2.50500900	-2.13955400	-1.60720300
H	-2.09678600	-0.32983600	2.17687400
H	-1.29196600	1.21165200	1.87728000
H	-3.64428700	1.14071400	0.96668100
H	-2.43973300	1.44475200	-0.28384600
H	-3.79028600	-1.24354300	0.31505400
H	-4.06973000	-0.23741700	-1.09854700
H	0.64959600	3.00940300	-0.23648900
C	0.71357300	0.09173200	0.62317200
H	0.93515000	0.89048000	1.32803300
O	0.60759100	1.25805300	-0.91505200
O	-0.05323000	2.45947200	-0.61288300
C	1.91596700	-0.68807400	0.14077100
H	1.77919500	-0.93455900	-0.91816900
H	1.96622000	-1.64525000	0.67571900
C	3.23849300	0.06618800	0.31836000
H	3.38359000	0.29521300	1.38134800
H	3.16192300	1.02437300	-0.20372400
C	4.44665200	-0.71436100	-0.20427800
H	5.37428200	-0.15367200	-0.06157700
H	4.55583000	-1.67313600	0.31276300
H	4.34757900	-0.92462900	-1.27360700

Sci-P20

C	-2.83324500	-0.92677300	-0.35428000
C	-1.56033100	-1.35382300	0.40323800
C	-0.42837800	-0.37148400	0.18782700
C	-0.80576300	1.05391700	0.52565600

C	-2.07813700	1.49060700	-0.23066300
C	-3.23670800	0.51101600	-0.00107400
H	-1.79585800	-1.39997700	1.47657400
H	-1.25422500	-2.35946800	0.10193200
H	-2.64538000	-0.99733100	-1.43251700
H	-3.65195100	-1.61831100	-0.12953200
H	-1.00643200	1.11690100	1.60496300
H	0.00956300	1.74906400	0.31930800
H	-2.36620400	2.49997300	0.08103700
H	-1.85322700	1.54247800	-1.30276800
H	-3.53968000	0.55191600	1.05357200
H	-4.11021000	0.81475200	-0.58721600
C	0.75649300	-0.77063100	-0.28976200
H	0.87263200	-1.83536300	-0.49544500
C	1.98724300	0.04938200	-0.56338600
H	1.78916800	1.11774000	-0.44018400
H	2.28009400	-0.08763900	-1.61365300
C	3.18110100	-0.34774600	0.32613800
H	2.90756600	-0.19415300	1.37579200
H	3.36995700	-1.42200400	0.21515500
C	4.45676500	0.43377400	0.00083500
H	5.28546400	0.13138800	0.64691900
H	4.76714700	0.27080300	-1.03613700
H	4.30735400	1.50980600	0.13502800

Sci-R21

C	-2.16939500	-0.54341700	-0.23863200
C	-1.44159100	0.75635300	-0.60442100
C	-0.03967400	-1.33374500	0.84095100
C	-1.18155000	-1.71342500	-0.04479900
H	-0.96121000	0.65142000	-1.58381900
H	-2.16388800	1.57463600	-0.69378200
H	-2.72995900	-0.39357300	0.69175400
H	-2.90099000	-0.80086900	-1.01079200
H	2.33514600	-1.67253000	-0.80832600
H	0.40243900	-2.06195000	1.51098000
H	-0.80021600	-2.00438400	-1.03925700
H	-1.69863600	-2.59413400	0.34731900
C	0.30573700	2.47082000	0.13877000
H	-0.43286500	3.27716000	0.10801900
H	1.04316400	2.72080800	0.90720700
H	0.82412900	2.44027700	-0.82074600
O	1.43653600	-0.02461200	-0.58505900
O	2.59654000	-0.86078900	-0.35226700

C	-0.37728300	1.13308400	0.44340300
H	-0.88641000	1.22200500	1.41254700
C	0.63525000	-0.01798200	0.63447800
H	1.31572400	0.21422200	1.45900000

Sci-TS21

C	-2.30045500	-0.23570900	-0.28651300
C	-1.35090000	0.91632100	-0.63997300
C	-0.28687000	-1.36047300	0.75233400
C	-1.53484600	-1.54913800	-0.05669600
H	-0.82187500	0.69218600	-1.57340000
H	-1.91982000	1.83616200	-0.80929600
H	-2.85198600	0.02350900	0.62516800
H	-3.04696700	-0.37412200	-1.07432300
H	2.79552000	-1.74240500	-0.55292500
H	0.18518400	-2.24292800	1.17434600
H	-1.25584600	-1.98584100	-1.02875100
H	-2.18150500	-2.29418000	0.42095700
C	0.64412500	2.30304300	0.16832700
H	0.08752800	3.23516600	0.03346400
H	1.35190600	2.45226700	0.98923100
H	1.22029200	2.10155500	-0.73452900
O	1.54089500	-0.36556200	-0.70892500
O	2.78825600	-0.82114300	-0.25736600
C	-0.31745800	1.14920600	0.47420300
H	-0.87331300	1.42135900	1.38537900
C	0.38879400	-0.14957800	0.81654700
H	1.22333100	-0.07111500	1.50563900

Sci-P21

C	-1.26992500	-1.14245000	-0.25761400
C	0.19881900	-1.23180900	0.17167600
C	1.02663300	-0.06096900	-0.38574500
C	0.28389000	1.24719800	-0.22481600
C	-1.01097400	1.34291300	0.07847700
C	-1.91587900	0.15068900	0.26053800
H	0.63758100	-2.18207600	-0.15004100
H	-1.82832300	-2.01377000	0.09791800
H	-1.45826000	2.32632000	0.20114400
H	-2.86876000	0.33082100	-0.25066600
C	2.41936200	0.00623800	0.25933300
H	0.86679900	2.15577600	-0.36193200
H	3.02194500	0.80718100	-0.17916200
H	2.34099300	0.19621900	1.33430100
H	2.96081200	-0.93428100	0.12052800
H	1.17530600	-0.23105800	-1.46331700

H	0.25553700	-1.21381600	1.26785600
H	-1.32513600	-1.15829200	-1.35265000
H	-2.17004600	0.04612300	1.32493500

Sci-R22

C	-1.69139300	0.88284600	-0.28619900
C	-0.49623400	1.82076200	-0.49311600
C	-0.10968300	-0.80704500	0.67374700
C	-1.26659400	-0.60361300	-0.25617500
H	-0.04824300	1.63761200	-1.47553800
H	-0.83206400	2.86244600	-0.48973100
H	-2.18522200	1.12511100	0.66392400
H	-2.43541300	1.03110600	-1.07586700
H	2.08692700	-1.82358500	-0.97276500
H	-0.00974200	-1.74827800	1.20417000
H	-0.92523800	-0.84644200	-1.27975300
O	1.89495800	-0.01007600	-0.47606700
O	2.58169600	-1.27959800	-0.34502200
C	0.56538900	1.61700200	0.59536100
H	0.15280300	1.89712900	1.57103600
C	1.02965900	0.15777000	0.69009600
H	1.65868600	0.00948800	1.57233400
H	1.43913900	2.24999900	0.41820900
C	-2.44412000	-1.53048000	0.07049700
H	-3.26087300	-1.39568700	-0.64414800
H	-2.14180500	-2.58135400	0.03981100
H	-2.83433700	-1.32360500	1.07178100

Sci-TS22

C	-1.77300700	0.83616200	-0.32951300
C	-0.57934400	1.78419200	-0.49328200
C	-0.13398500	-0.85033900	0.56178500
C	-1.33725200	-0.64122100	-0.31570500
H	-0.07802300	1.58289800	-1.44597900
H	-0.92088600	2.82309100	-0.52768800
H	-2.28849500	1.06114900	0.61344300
H	-2.50266800	0.99350200	-1.13036500
H	2.70920800	-1.74751600	-0.83987300
H	0.09461300	-1.86974400	0.86243100
H	-1.03688500	-0.90593400	-1.34369100
O	2.05098800	-0.02129500	-0.56044900
O	2.96849300	-1.02918000	-0.24568500
C	0.42693600	1.60161900	0.64967200
H	0.00454000	1.99123800	1.58576500
C	0.77972200	0.14990500	0.86289800

H	1.52534400	-0.05964600	1.62176800
C	-2.49102000	-1.57745700	0.07543500
H	-3.34182700	-1.44992500	-0.59976300
H	-2.18350200	-2.62644800	0.03252400
H	-2.83358600	-1.36984400	1.09376300
H	1.34402100	2.16381100	0.45899000

Sci-P22

C	-1.26992500	-1.14245000	-0.25761400
C	0.19881900	-1.23180900	0.17167600
C	1.02663300	-0.06096900	-0.38574500
C	0.28389000	1.24719800	-0.22481600
C	-1.01097400	1.34291300	0.07847700
C	-1.91587900	0.15068900	0.26053800
H	0.63758100	-2.18207600	-0.15004100
H	-1.82832300	-2.01377000	0.09791800
H	-1.45826000	2.32632000	0.20114400
H	-2.86876000	0.33082100	-0.25066600
C	2.41936200	0.00623800	0.25933300
H	0.86679900	2.15577600	-0.36193200
H	3.02194500	0.80718100	-0.17916200
H	2.34099300	0.19621900	1.33430100
H	2.96081200	-0.93428100	0.12052800
H	1.17530600	-0.23105800	-1.46331700
H	0.25553700	-1.21381600	1.26785600
H	-1.32513600	-1.15829200	-1.35265000
H	-2.17004600	0.04612300	1.32493500

Sci-R23

C	1.50491200	1.16864800	-0.14971200
C	1.41151800	-0.35623300	-0.31857300
C	-0.88695800	1.18126800	0.64151000
C	0.12314400	1.84655800	-0.23499000
H	0.98252500	-0.56180700	-1.30740500
H	1.95574100	1.39175700	0.82600400
H	2.17116700	1.59093800	-0.90929700
H	-3.00813600	0.16370000	-1.10162100
H	-1.69865900	1.75776400	1.07020400
H	-0.21340400	1.80621300	-1.28627900
H	0.20101700	2.91061800	0.00899000
O	-1.56525000	-0.88347800	-0.47495500
O	-2.97403900	-0.54520400	-0.44506200
C	0.45824800	-0.94508000	0.73566200
H	0.88217900	-0.78928300	1.73526000
C	-0.93681100	-0.30824200	0.71422500

H	-1.52572200	-0.64289900	1.57289500
C	2.78977600	-1.02026300	-0.24813200
H	3.25973400	-0.84822600	0.72645300
H	2.71619400	-2.10164600	-0.39572100
H	3.46040500	-0.62290200	-1.01563700
H	0.34829300	-2.02470500	0.59634000

Sci-TS23

C	1.66158000	1.05901500	-0.19672200
C	1.38939700	-0.45001000	-0.29726500
C	-0.74728700	1.32763300	0.51810400
C	0.36973400	1.88370000	-0.31156600
H	0.88659400	-0.63911500	-1.25415200
H	2.14174000	1.26871500	0.76787700
H	2.36931900	1.36830500	-0.97264500
H	-3.37670300	0.05168700	-1.00269300
H	-1.60396600	1.96500000	0.71620300
H	0.04826100	1.91520100	-1.36487300
H	0.55431300	2.92821600	-0.03502800
O	-1.77517900	-0.79962900	-0.55241400
O	-3.14796500	-0.62217200	-0.34710000
C	0.42254300	-0.87850900	0.81929100
H	0.93922400	-0.83289600	1.78881800
C	-0.80650700	-0.00607200	0.89545700
H	-1.55791800	-0.29389100	1.62214800
H	0.10952700	-1.91634200	0.67837600
C	2.68180800	-1.26919700	-0.26062000
H	2.47435900	-2.34050800	-0.33790200
H	3.34687900	-0.99750100	-1.08561200
H	3.22590400	-1.10182000	0.67552800

Sci-P23

C	-0.18306100	-1.20600900	0.30904600
C	-0.93625700	-0.02938300	-0.33112300
C	-0.29335700	1.29936200	0.10447800
C	1.21341800	1.26509400	0.05610700
C	1.92058200	0.14070100	-0.05282800
C	1.29404000	-1.22922600	-0.10918400
H	-0.66483800	-2.15297700	0.04373500
H	3.00521800	0.19285900	-0.10343700
H	1.85622500	-1.91811400	0.53210100
H	1.73119200	2.21939200	0.11179800
H	-0.62119800	1.55058200	1.12449600
H	-0.81260100	-0.11221500	-1.41980800
H	-0.24945300	-1.11413400	1.40079500
H	1.39149300	-1.63281500	-1.12703000

H	-0.66354500	2.11484200	-0.52883700
C	-2.43392500	-0.06281200	-0.01608200
H	-2.95623900	0.78348700	-0.47275800
H	-2.89771600	-0.98121100	-0.38805100
H	-2.60717200	-0.01605500	1.06452000

Sci-R24

C	-1.76022000	-0.06400500	0.21723000
C	-1.03429900	1.17308400	-0.33602800
C	0.50826100	-0.91309400	0.95701100
C	-0.78209500	-1.26067000	0.28998800
H	-0.73385900	0.98174800	-1.37274000
H	-2.07380700	0.16456700	1.24524100
H	2.58357000	-1.38484800	-1.04633600
H	1.03117400	-1.65271300	1.55202900
H	-0.59010400	-1.59327400	-0.74656600
H	-1.25771600	-2.10949500	0.79187700
O	1.83038100	0.31257500	-0.69371600
O	2.94943300	-0.60435900	-0.60836800
C	0.20297200	1.53686200	0.49506000
H	-0.10197800	1.82139600	1.50819800
C	1.19178800	0.36978900	0.61946300
H	1.97734300	0.60383200	1.34332800
H	0.72709100	2.39329600	0.06201400
H	-1.72198800	2.02523600	-0.35993900
C	-3.00826200	-0.41109400	-0.59789700
H	-3.52326800	-1.28379400	-0.18502600
H	-3.71761900	0.42153400	-0.60766500
H	-2.74622300	-0.63844400	-1.63671000

Sci-TS24

C	-1.82822000	-0.04208100	0.17644400
C	-1.02464900	1.16703600	-0.32685600
C	0.41800700	-1.00720000	0.87111100
C	-0.91887700	-1.28330800	0.25166400
H	-0.65555900	0.95946900	-1.33799800
H	-2.16191800	0.18378500	1.19883200
H	3.10357600	-1.24280000	-1.01690300
H	1.00492000	-1.85349700	1.21584000
H	-0.76604800	-1.67593500	-0.76752600
H	-1.42279100	-2.08947700	0.79847100
O	1.99584900	0.24145100	-0.76756100
O	3.22382000	-0.39713200	-0.56235600
C	0.16608400	1.47705600	0.58919300
H	-0.19332000	1.87200100	1.54896600

C	1.00147400	0.25163000	0.86805300
H	1.89179700	0.39879100	1.46899700
H	0.80471000	2.24763800	0.15109000
C	-3.06828100	-0.30813700	-0.68086000
H	-3.74105500	0.55434100	-0.68151700
H	-2.78817600	-0.51304600	-1.71966500
H	-3.63166400	-1.17055800	-0.31144000
H	-1.67504700	2.04476500	-0.40030100

Sci-P24

C	-0.18306100	-1.20600900	0.30904600
C	-0.93625700	-0.02938300	-0.33112300
C	-0.29335700	1.29936200	0.10447800
C	1.21341800	1.26509400	0.05610700
C	1.92058200	0.14070100	-0.05282800
C	1.29404000	-1.22922600	-0.10918400
H	-0.66483800	-2.15297700	0.04373500
H	3.00521800	0.19285900	-0.10343700
H	1.85622500	-1.91811400	0.53210100
H	1.73119200	2.21939200	0.11179800
H	-0.62119800	1.55058200	1.12449600
H	-0.81260100	-0.11221500	-1.41980800
H	-0.24945300	-1.11413400	1.40079500
H	1.39149300	-1.63281500	-1.12703000
H	-0.66354500	2.11484200	-0.52883700
C	-2.43392500	-0.06281200	-0.01608200
H	-2.95623900	0.78348700	-0.47275800
H	-2.89771600	-0.98121100	-0.38805100
H	-2.60717200	-0.01605500	1.06452000

Sci-R25

C	-0.46473900	2.25394100	-0.24230100
C	0.62653800	1.26076100	-0.66394300
C	-1.65208400	0.34635500	0.88078500
C	-1.81322900	1.54776700	0.00785200
H	0.36973400	0.81489600	-1.63162300
H	1.56997600	1.79605000	-0.80308700
H	-0.15341800	2.76201300	0.67823400
H	-0.58853900	3.02927500	-1.00489700
H	-2.57223000	-1.87688000	-0.74685500
H	-2.42478600	0.07284600	1.58982100
H	-2.22582800	1.24548900	-0.97063600
H	-2.54025000	2.24342600	0.43739200
C	1.95154100	-0.84144400	0.03147200
H	1.89377400	-1.69262300	0.71964500

H	1.78603000	-1.25384300	-0.96748700
O	-0.75626000	-1.37514800	-0.59139200
O	-1.82398400	-2.31636200	-0.32002100
C	0.81274600	0.13743800	0.37360500
H	1.05629300	0.61077900	1.33567100
C	-0.52427400	-0.59713400	0.62145600
H	-0.41013900	-1.31383000	1.44021900
C	3.35134900	-0.22415000	0.12083900
H	4.11955200	-0.97594800	-0.07922400
H	3.49255800	0.58323400	-0.60255500
H	3.54212800	0.18598900	1.11809900

Sci-TS25

C	0.53122500	-2.31634400	-0.28798800
C	-0.56974900	-1.31893500	-0.67370600
C	1.71346700	-0.35367400	0.77791000
C	1.87055100	-1.61051600	-0.02324700
H	-0.29493200	-0.79809600	-1.59829700
H	-1.50020800	-1.85675000	-0.87400200
H	0.22303400	-2.85444200	0.61643600
H	0.65701000	-3.06958800	-1.07154900
H	2.30441600	2.65050400	-0.54547300
H	2.60355700	0.08396700	1.22056400
H	2.34647700	-1.35437100	-0.98309700
H	2.57235100	-2.28816700	0.47654600
C	-1.89243200	0.75355900	0.12317500
H	-1.86806600	1.52712700	0.89942500
H	-1.65212100	1.26200200	-0.81268700
O	0.82848700	1.51490400	-0.70634900
O	1.38598100	2.71767500	-0.24874100
C	-0.79019600	-0.27599500	0.43580600
H	-1.11010400	-0.81952800	1.34029800
C	0.53029000	0.37129000	0.81121000
H	0.46980600	1.20820700	1.49932700
C	-3.30180500	0.15580400	0.06009900
H	-4.04646600	0.93928000	-0.10424200
H	-3.40677900	-0.56555000	-0.75474300
H	-3.56182200	-0.35635800	0.99266900

Sci-P25

C	-1.47411400	-1.31077000	-0.25840900
C	-0.01702600	-1.09615700	0.16893700
C	0.54992400	0.22522800	-0.38224400
C	-0.45643700	1.34469100	-0.22728800
C	-1.74221600	1.16912900	0.07813800
C	-2.37619300	-0.18535000	0.26552200

H	0.59830100	-1.93858900	-0.15911100
H	-1.83620600	-2.28189900	0.09285400
H	-2.38512700	2.03794000	0.19636900
H	-3.34831200	-0.21056900	-0.24052600
C	1.89564000	0.61490100	0.26470100
H	-0.07842700	2.35518800	-0.36966800
H	2.19489700	1.59486900	-0.12537100
H	1.74256700	0.75070300	1.34238700
H	0.74106500	0.09279400	-1.45959400
H	0.03712700	-1.07319100	1.26555200
H	-1.52644100	-1.33258900	-1.35349300
H	-2.59638200	-0.34133600	1.33120100
C	3.03168800	-0.38407600	0.02379600
H	3.97022800	-0.01634200	0.44736200
H	2.82614900	-1.35573300	0.48002200
H	3.19296600	-0.54681600	-1.04690500

Sci-R26

C	-1.04226400	1.32243500	-0.14532300
C	0.31450500	1.92525600	-0.53011400
C	0.18736000	-0.64024100	0.80458600
C	-0.98425700	-0.21976800	-0.03036700
H	0.59955800	1.58251100	-1.53041500
H	0.23620100	3.01577200	-0.58210000
H	-1.36320800	1.73268500	0.82148500
H	-1.79894600	1.61250200	-0.87953300
H	1.87904400	-2.25355000	-0.95162400
H	0.11502200	-1.54053400	1.40609500
H	-0.82441900	-0.60111200	-1.05728200
O	2.18694400	-0.42497400	-0.58562100
O	2.55796800	-1.81615900	-0.42006900
C	1.40815100	1.53367900	0.47103200
H	1.18044700	1.96013400	1.45438300
C	1.51902900	0.01312700	0.63857100
H	2.18652300	-0.23735700	1.46790000
H	2.38270600	1.92392400	0.16514200
C	-2.29748500	-0.83861200	0.48620000
H	-2.13879700	-1.91469400	0.62295500
H	-2.50875800	-0.43334300	1.48314800
C	-3.50949200	-0.62695000	-0.42597600
H	-4.38622900	-1.14985900	-0.03478100
H	-3.77446400	0.42922200	-0.51837200
H	-3.31724700	-1.01079200	-1.43313300

Sci-TS26

C	-1.16415100	1.25485900	-0.21569600
C	0.18463100	1.91235500	-0.53194000
C	0.16225800	-0.68432700	0.67994400
C	-1.05053800	-0.27938100	-0.11186100
H	0.55310800	1.54927500	-1.49730300
H	0.06362000	2.99578600	-0.62597300
H	-1.54287800	1.64583900	0.73826700
H	-1.89957400	1.52360100	-0.97876100
H	2.63541700	-2.23719500	-0.85205500
H	0.20341300	-1.71124800	1.03466800
H	-0.91638900	-0.67266300	-1.13508600
O	2.36857800	-0.39854200	-0.65131400
O	3.08392600	-1.55723300	-0.32981500
C	1.22252600	1.59310300	0.55019200
H	0.96647900	2.11596500	1.48164100
C	1.28535400	0.11442200	0.84201900
H	2.03338500	-0.20698300	1.55817600
C	-2.32288200	-0.94229200	0.45812000
H	-2.13346400	-2.01671900	0.56620700
H	-2.49562600	-0.56025300	1.47156600
H	2.21638600	1.93862600	0.25641900
C	-3.58042100	-0.74128500	-0.39263800
H	-4.42638800	-1.29039500	0.02924500
H	-3.87093900	0.31047900	-0.45214800
H	-3.42723800	-1.10263100	-1.41467100

Sci-P26

C	-1.47411400	-1.31077000	-0.25840900
C	-0.01702600	-1.09615700	0.16893700
C	0.54992400	0.22522800	-0.38224400
C	-0.45643700	1.34469100	-0.22728800
C	-1.74221600	1.16912900	0.07813800
C	-2.37619300	-0.18535000	0.26552200
H	0.59830100	-1.93858900	-0.15911100
H	-1.83620600	-2.28189900	0.09285400
H	-2.38512700	2.03794000	0.19636900
H	-3.34831200	-0.21056900	-0.24052600
C	1.89564000	0.61490100	0.26470100
H	-0.07842700	2.35518800	-0.36966800
H	2.19489700	1.59486900	-0.12537100
H	1.74256700	0.75070300	1.34238700
H	0.74106500	0.09279400	-1.45959400
H	0.03712700	-1.07319100	1.26555200
H	-1.52644100	-1.33258900	-1.35349300
H	-2.59638200	-0.34133600	1.33120100

C	3.03168800	-0.38407600	0.02379600
H	3.97022800	-0.01634200	0.44736200
H	2.82614900	-1.35573300	0.48002200
H	3.19296600	-0.54681600	-1.04690500

Sci-R27

C	0.99926000	1.33317300	0.04226100
C	1.05534300	-0.20317000	0.00023600
C	-1.47607300	1.18939700	0.50200300
C	-0.40781400	1.87131600	-0.28740200
H	0.78632200	-0.52705300	-1.01417900
H	1.28638800	1.67000500	1.04700700
H	1.72162500	1.76603500	-0.65512400
H	-3.23816000	-0.16059700	-1.41396500
H	-2.38543000	1.72014600	0.75971500
H	-0.58784900	1.71717900	-1.36630700
H	-0.44930100	2.95420200	-0.13377600
O	-1.81719700	-1.01094900	-0.50368700
O	-3.23922400	-0.80659300	-0.69464700
C	0.01092400	-0.78663900	0.96887500
H	0.27494700	-0.51070700	1.99712400
C	-1.41421200	-0.28735400	0.70241800
H	-2.08978200	-0.60796800	1.50048200
C	2.45416700	-0.75971800	0.31736400
H	2.76468400	-0.40211300	1.30795600
H	2.37988000	-1.85034500	0.39953600
H	0.00882800	-1.87953000	0.91811000
C	3.53364700	-0.41581700	-0.71451100
H	3.71689700	0.65997800	-0.77652900
H	4.48329700	-0.89326000	-0.45836000
H	3.24757000	-0.76276000	-1.71247800

Sci-TS27

C	1.11663400	1.33856800	-0.03530700
C	1.06110600	-0.19628800	0.04140400
C	-1.38597900	1.33798700	0.32082000
C	-0.24057700	1.94245000	-0.43122300
H	0.73150600	-0.57400300	-0.93590400
H	1.41389300	1.72934700	0.94666400
H	1.87923900	1.66526300	-0.74722500
H	-3.59128300	-0.49238300	-1.31075300
H	-2.33675100	1.86278300	0.31718600
H	-0.40565200	1.79458800	-1.51045100
H	-0.23265400	3.02913400	-0.28722000
O	-1.96772200	-1.03039200	-0.55734300

O	-3.36717400	-1.04000000	-0.54518700
C	0.00279600	-0.61835200	1.07533200
H	0.36344800	-0.38082500	2.08647000
C	-1.32627900	0.06691000	0.87341200
H	-2.13066000	-0.23708500	1.53387900
H	-0.15236700	-1.69989600	1.04296400
C	2.42185000	-0.83535000	0.36418300
H	2.26390700	-1.90358500	0.55362400
H	2.79998900	-0.41428800	1.30515200
C	3.48300100	-0.68162700	-0.73050300
H	3.74587900	0.36477700	-0.90604300
H	4.40283000	-1.20603500	-0.45776200
H	3.13253100	-1.10043700	-1.67904700

Sci-P27

C	0.53220600	-1.28741000	0.30741300
C	-0.48212200	-0.24500200	-0.19120800
C	-0.04252000	1.16058900	0.26021100
C	1.43650100	1.39910100	0.08463200
C	2.31862000	0.42997500	-0.15654700
C	1.94006500	-1.02589000	-0.24506000
H	0.20198500	-2.29492300	0.03338100
H	3.36685300	0.68157600	-0.29644300
H	2.67556100	-1.63188700	0.29689700
H	1.77960200	2.42823700	0.15669300
H	-0.31416300	1.30993300	1.31648800
H	-0.45849400	-0.26088200	-1.29077500
H	0.56278700	-1.25361300	1.40397800
H	2.00270000	-1.35696400	-1.29142000
H	-0.59616900	1.92650300	-0.29400100
C	-1.91174100	-0.59230500	0.25429600
H	-2.12587000	-1.62481800	-0.04624500
H	-1.95392200	-0.58096000	1.35127400
C	-3.00313800	0.32451900	-0.30887800
H	-3.99624500	-0.01928600	-0.00696700
H	-2.89434300	1.35428200	0.04124800
H	-2.97750800	0.34134000	-1.40326100

Sci-R28

C	-1.30292600	-0.23588200	0.31871000
C	-0.68497600	1.06922700	-0.21064600
C	1.05518200	-0.95785400	0.91382100
C	-0.24223700	-1.36263600	0.29481600
H	-0.41764100	0.93873500	-1.26590800
H	-1.58331900	-0.07264900	1.36958500

H	3.06921800	-1.19202200	-1.18802900
H	1.65833600	-1.68957600	1.43870900
H	-0.08130800	-1.64343700	-0.76221900
H	-0.63509400	-2.26022900	0.78338600
O	2.21912300	0.43165900	-0.72632700
O	3.40010800	-0.40822300	-0.72870200
C	0.56229300	1.48075000	0.58391200
H	0.28440600	1.69895300	1.62103100
C	1.63363300	0.38373400	0.61226900
H	2.43172700	0.63915000	1.31496600
H	1.00580900	2.39053200	0.16978300
H	-1.41702500	1.88070100	-0.16880800
C	-2.56679000	-0.66178200	-0.44657500
H	-2.85843000	-1.66245800	-0.10535600
H	-2.31892100	-0.76497500	-1.51076600
C	-3.76377700	0.28157100	-0.28672100
H	-3.56088900	1.27510900	-0.69420200
H	-4.64152500	-0.11083600	-0.80724600
H	-4.03160500	0.40274000	0.76778200

Sci-TS28

C	1.36652500	0.25003500	0.28871300
C	0.67792300	-1.04802100	-0.16558100
C	-0.98450200	1.07596200	0.81280100
C	0.35833100	1.41543900	0.24063500
H	0.34005400	-0.93092600	-1.20198100
H	1.66800700	0.11865700	1.33832800
H	-3.56746400	0.97793400	-1.21617300
H	-1.65058000	1.89477600	1.06866400
H	0.22956700	1.73281800	-0.80769700
H	0.77040600	2.29065100	0.75746800
O	-2.37609700	-0.40144800	-0.80356400
O	-3.65387900	0.16054000	-0.70568200
C	-0.52751800	-1.38986600	0.71943100
H	-0.18430900	-1.68746500	1.71943600
C	-1.46974200	-0.22210300	0.87295500
H	-2.37581200	-0.39961900	1.44125500
H	-1.08045300	-2.23892900	0.31070800
C	2.62732000	0.58709100	-0.52429300
H	2.36060700	0.63383500	-1.58789200
H	2.95736000	1.59668500	-0.25065200
H	1.38378700	-1.88289700	-0.15354300
C	3.79738700	-0.38286300	-0.32945400
H	3.55301500	-1.39396300	-0.66470000
H	4.67389200	-0.05527700	-0.89492700

H	4.08738400	-0.44305200	0.72442100
Sci-P28			
C	0.53220600	-1.28741000	0.30741300
C	-0.48212200	-0.24500200	-0.19120800
C	-0.04252000	1.16058900	0.26021100
C	1.43650100	1.39910100	0.08463200
C	2.31862000	0.42997500	-0.15654700
C	1.94006500	-1.02589000	-0.24506000
H	0.20198500	-2.29492300	0.03338100
H	3.36685300	0.68157600	-0.29644300
H	2.67556100	-1.63188700	0.29689700
H	1.77960200	2.42823700	0.15669300
H	-0.31416300	1.30993300	1.31648800
H	-0.45849400	-0.26088200	-1.29077500
H	0.56278700	-1.25361300	1.40397800
H	2.00270000	-1.35696400	-1.29142000
H	-0.59616900	1.92650300	-0.29400100
C	-1.91174100	-0.59230500	0.25429600
H	-2.12587000	-1.62481800	-0.04624500
H	-1.95392200	-0.58096000	1.35127400
C	-3.00313800	0.32451900	-0.30887800
H	-3.99624500	-0.01928600	-0.00696700
H	-2.89434300	1.35428200	0.04124800
H	-2.97750800	0.34134000	-1.40326100

Sci-R29			
C	-0.84638600	0.64023900	0.62540700
C	0.32551500	-0.33919600	0.38925600
C	-0.06318900	-1.40191000	-0.65794000
C	-1.33401000	-2.16283000	-0.25745000
C	-2.52115200	-1.20685800	-0.01742600
C	-2.13839900	-0.06674100	0.86852200
H	-0.21340600	-0.91130600	-1.62643800
H	0.45743300	-0.85446000	1.35144800
H	-0.60410600	1.31880500	1.44865800
H	-1.59729900	-2.89360700	-1.02852900
H	-3.37662300	-1.74893400	0.39615100
H	-2.59181500	2.29717400	-0.75528000
H	-2.84907300	0.34536400	1.57538000
H	0.75864700	-2.11169300	-0.78775100
H	-1.14107100	-2.72801700	0.66215000
H	-2.85143700	-0.82258500	-0.99834000
O	-0.90944400	1.45150000	-0.58595400
O	-1.77618700	2.58195600	-0.32070400

C	1.63681500	0.40065700	0.06821800
H	1.72845700	1.25630100	0.74884900
H	1.57760400	0.82615700	-0.93828700
C	2.89836600	-0.46290500	0.19626600
H	2.84962500	-1.30625600	-0.50095400
H	2.93714300	-0.89993300	1.20205100
C	4.18456300	0.32699200	-0.06453700
H	4.28796400	1.15774900	0.64046400
H	5.07006700	-0.30668800	0.03574700
H	4.19020900	0.74959200	-1.07395400

Sci-TS29

C	1.48517700	-2.15965800	-0.30165800
C	0.17742800	-1.44451600	-0.66536800
C	2.19724200	0.02032800	0.75813800
C	2.62822600	-1.16252400	-0.05503400
H	0.30999300	-0.87264200	-1.59117800
H	-0.60584200	-2.18316800	-0.85533200
H	1.32554600	-2.75596600	0.60460000
H	1.76892200	-2.86174400	-1.09137300
H	2.03576000	3.10047800	-0.54360800
H	2.96871500	0.64939200	1.19259400
H	3.01341800	-0.79937100	-1.02105500
H	3.47772400	-1.65989200	0.42710600
C	-1.57572900	0.26706300	0.15744600
H	-1.70799700	1.04647400	0.91842900
H	-1.48336600	0.79463000	-0.79518600
O	0.88140600	1.63862600	-0.70191400
O	1.13101500	2.93939600	-0.24095800
C	-0.26257700	-0.48097500	0.45204000
H	-0.43497300	-1.08401200	1.35879100
C	0.87917300	0.45190100	0.81266100
H	0.63803400	1.25026100	1.50693200
C	-2.82262300	-0.62613400	0.14960400
H	-2.73175000	-1.39168900	-0.62863200
H	-2.89067700	-1.16605300	1.10267400
C	-4.11365600	0.16597100	-0.07890400
H	-4.98966800	-0.48863800	-0.08228000
H	-4.26132000	0.91596100	0.70450400
H	-4.08785200	0.69306300	-1.03755800

Sci-P29

C	-2.03689100	-1.29529600	-0.20363700
C	-0.55192500	-1.10765600	0.13004300
C	0.00556100	0.19987200	-0.46295000
C	-0.96871600	1.33937000	-0.25465200

C	-2.23583300	1.19084500	0.13210800
C	-2.88226400	-0.14995000	0.36911400
H	0.02486500	-1.96362900	-0.23102500
H	-2.39460100	-2.25752500	0.17522400
H	-2.85304100	2.07289200	0.28389700
H	-3.88485800	-0.15883400	-0.07399300
C	1.39400900	0.56889300	0.09894000
H	-0.58124100	2.34135700	-0.42788600
H	1.68565000	1.54489800	-0.30977000
H	1.31202100	0.70803700	1.18494000
H	0.12761000	0.05865300	-1.54906000
H	-0.42839200	-1.08123400	1.22091800
H	-2.15858200	-1.32109800	-1.29312600
H	-3.03706400	-0.29598500	1.44759800
C	2.50662200	-0.44128100	-0.20622200
H	2.26800100	-1.40874200	0.24766600
H	2.54842900	-0.61361500	-1.28898800
C	3.88030900	0.02026700	0.28980400
H	4.65573900	-0.71591200	0.06116200
H	4.17236100	0.96651000	-0.17629200
H	3.87788600	0.17384200	1.37344400

Sci-R30

C	-0.37622700	1.52422200	-0.15830800
C	1.05827800	1.93301300	-0.51575100
C	0.55092200	-0.60416700	0.78147100
C	-0.53892300	-0.01186700	-0.06080400
H	1.30970700	1.56158600	-1.51474100
H	1.13493700	3.02408600	-0.55760400
H	-0.65148000	1.96633800	0.80841200
H	-1.07230800	1.92547200	-0.89999500
H	2.03604300	-2.41809800	-0.96311200
H	0.34616500	-1.49799200	1.36164400
H	-0.42183100	-0.40165000	-1.09022000
O	2.58821900	-0.65401000	-0.56875800
O	2.75908600	-2.08491000	-0.41446200
C	2.06769400	1.38307600	0.49894000
H	1.88176900	1.82623700	1.48365800
C	1.96318100	-0.13962600	0.64846400
H	2.57257500	-0.48914500	1.48670600
H	3.09267800	1.63743300	0.21560500
C	-1.93142800	-0.44435000	0.43699100
H	-1.92934100	-1.53436200	0.56443600
H	-2.09519500	-0.02282300	1.43728000

C	-3.10130900	-0.06134700	-0.47708800
H	-3.15840900	1.02755100	-0.57595500
H	-2.91284000	-0.45059500	-1.48534100
C	-4.44680700	-0.58943200	0.03020800
H	-5.26465100	-0.30425100	-0.63699100
H	-4.44214700	-1.68154800	0.10270400
H	-4.67640200	-0.19400100	1.02453800

Sci-TS30

C	-0.49161200	1.49748100	-0.22491500
C	0.94369300	1.95329200	-0.51398000
C	0.52240000	-0.62494400	0.66265400
C	-0.60416000	-0.03813600	-0.14355000
H	1.26956300	1.55001700	-1.47867000
H	0.98456900	3.04368200	-0.59581600
H	-0.82317200	1.92685200	0.73012600
H	-1.16817600	1.88081100	-0.99339700
H	2.74764800	-2.50468300	-0.86295600
H	0.40620700	-1.65027600	1.00491400
H	-0.50604100	-0.43205000	-1.17054200
O	2.76996800	-0.65046800	-0.63228300
O	3.28951500	-1.91214100	-0.32299900
C	1.90694700	1.47353200	0.57767200
H	1.71662300	2.01852500	1.51217000
C	1.74770500	-0.00143000	0.85144300
H	2.42843400	-0.43660900	1.57462800
C	-1.96866400	-0.51898000	0.39368700
H	-1.93695400	-1.61147500	0.49363000
H	-2.10881900	-0.12530200	1.40877600
H	2.94513000	1.67222000	0.30160300
C	-3.17577800	-0.14090000	-0.47294600
H	-3.26092500	0.94852600	-0.53977400
H	-3.00986400	-0.49851100	-1.49671800
C	-4.49152300	-0.71482900	0.06152800
H	-5.33674700	-0.42978500	-0.57056900
H	-4.45997700	-1.80804500	0.10151500
H	-4.69740600	-0.35354000	1.07377800

Sci-P30

C	-2.03689100	-1.29529600	-0.20363700
C	-0.55192500	-1.10765600	0.13004300
C	0.00556100	0.19987200	-0.46295000
C	-0.96871600	1.33937000	-0.25465200
C	-2.23583300	1.19084500	0.13210800
C	-2.88226400	-0.14995000	0.36911400
H	0.02486500	-1.96362900	-0.23102500

H	-2.39460100	-2.25752500	0.17522400
H	-2.85304100	2.07289200	0.28389700
H	-3.88485800	-0.15883400	-0.07399300
C	1.39400900	0.56889300	0.09894000
H	-0.58124100	2.34135700	-0.42788600
H	1.68565000	1.54489800	-0.30977000
H	1.31202100	0.70803700	1.18494000
H	0.12761000	0.05865300	-1.54906000
H	-0.42839200	-1.08123400	1.22091800
H	-2.15858200	-1.32109800	-1.29312600
H	-3.03706400	-0.29598500	1.44759800
C	2.50662200	-0.44128100	-0.20622200
H	2.26800100	-1.40874200	0.24766600
H	2.54842900	-0.61361500	-1.28898800
C	3.88030900	0.02026700	0.28980400
H	4.65573900	-0.71591200	0.06116200
H	4.17236100	0.96651000	-0.17629200
H	3.87788600	0.17384200	1.37344400

Sci-R31

C	0.38421200	1.49074700	0.03450900
C	0.59703900	-0.03283100	0.04568200
C	-2.07508000	1.11217900	0.44721300
C	-1.06173400	1.87288300	-0.34230700
H	0.39119300	-0.41389100	-0.96336200
H	0.61238500	1.88639800	1.03287900
H	1.07572600	1.97246900	-0.66207600
H	-3.64863100	-0.46080300	-1.45921100
H	-3.03748400	1.55747300	0.67184400
H	-1.19948200	1.66749400	-1.41879200
H	-1.21464600	2.95043100	-0.22619500
O	-2.17027000	-1.13891800	-0.49650300
O	-3.60079700	-1.08524800	-0.72263700
C	-0.41006100	-0.68930200	1.00774000
H	-0.20146500	-0.35867400	2.03248300
C	-1.87094400	-0.34422100	0.69458100
H	-2.53008700	-0.70813900	1.48783700
C	2.03466400	-0.43409400	0.41881200
H	2.28187000	-0.00952800	1.40169200
H	2.06755000	-1.52390200	0.54399000
H	-0.30202800	-1.77791800	0.99153900
C	3.11232000	-0.03045400	-0.59561700
H	3.14790500	1.05962300	-0.69392800
H	2.83627200	-0.41805900	-1.58388300

C	4.50516400	-0.54414700	-0.21822300
H	4.51939300	-1.63656700	-0.15273900
H	5.25453900	-0.24593200	-0.95652300
H	4.82205100	-0.15170300	0.75321600

Sci-TS31

C	0.46325300	1.55210200	-0.04424500
C	0.60632900	0.02623600	0.08632400
C	-2.02610600	1.23531000	0.26029300
C	-0.95051600	1.95817900	-0.49086300
H	0.35394700	-0.42324100	-0.88326600
H	0.68187100	2.01014000	0.92921700
H	1.19503400	1.95258100	-0.75078400
H	-3.92896300	-0.90788500	-1.35719900
H	-3.03644700	1.63135400	0.21870700
H	-1.06666000	1.75117900	-1.56670600
H	-1.08827400	3.04089000	-0.38880900
O	-2.27693900	-1.21861100	-0.54055800
O	-3.66471500	-1.39695900	-0.56522300
C	-0.41465500	-0.49716800	1.11180600
H	-0.11332100	-0.18394100	2.12177800
C	-1.81566000	0.00226000	0.85995700
H	-2.58945200	-0.38092700	1.51575200
H	-0.42687400	-1.59023700	1.11324500
C	2.02969900	-0.41680200	0.46328000
H	2.00549000	-1.48517300	0.71301600
H	2.33447500	0.10136800	1.38319300
C	3.09225700	-0.19639600	-0.62101700
H	3.16126500	0.86809200	-0.86955300
H	2.77586500	-0.70497100	-1.53970900
C	4.47708000	-0.70452200	-0.20808000
H	4.45607800	-1.77675600	0.01060700
H	5.21476700	-0.54131600	-0.99851900
H	4.83433900	-0.19179200	0.69054800

Sci-P31

C	1.02730300	-1.28528100	0.30433300
C	0.04181800	-0.22117400	-0.20716900
C	0.50719800	1.17478800	0.24904100
C	1.99334100	1.38028500	0.09304600
C	2.85689300	0.39195500	-0.13707700
C	2.44714900	-1.05508600	-0.23088200
H	0.67846600	-2.28541800	0.02653800
H	3.91218100	0.62026500	-0.26320400
H	3.16229500	-1.67731800	0.31986800
H	2.35815000	2.40156400	0.17015400

H	0.22458000	1.33148300	1.30131700
H	0.07938800	-0.23882200	-1.30619300
H	1.04510000	-1.25157500	1.40115800
H	2.51525700	-1.38738300	-1.27650900
H	-0.02159600	1.95228800	-0.31323800
C	-1.39970200	-0.53815800	0.22137000
H	-1.63111600	-1.56931900	-0.07532300
H	-1.45833300	-0.51902600	1.31849200
C	-2.47539500	0.38932600	-0.35854400
H	-2.30299700	1.41768200	-0.02379800
H	-2.38501200	0.40463600	-1.45177300
C	-3.89621800	-0.03186800	0.02912000
H	-4.02655000	-0.02898800	1.11590900
H	-4.64365100	0.64356500	-0.39609700
H	-4.12048600	-1.04236300	-0.32673600

Sci-R32

C	-0.79524300	-0.16558300	0.49248000
C	-0.18941200	1.09790600	-0.14078300
C	1.58566500	-0.92239600	0.93974400
C	0.23487500	-1.32010000	0.44127600
H	-0.00624300	0.91384600	-1.20587900
H	-0.99160100	0.05030800	1.55268800
H	3.41759000	-1.30268400	-1.30343600
H	2.21109200	-1.64628600	1.44921400
H	0.30687600	-1.65281200	-0.61045400
H	-0.13960300	-2.18386100	1.00013500
O	2.64680400	0.36206700	-0.84884100
O	3.80298300	-0.50996000	-0.90610900
C	1.12420900	1.51088100	0.53790700
H	0.93222000	1.77901200	1.58277100
C	2.16915200	0.38844900	0.53237800
H	3.02640300	0.65312200	1.15779900
H	1.55480800	2.39084500	0.05202100
H	-0.89691100	1.92962500	-0.08129200
C	-2.12218400	-0.59178900	-0.15749300
H	-2.40809200	-1.57311900	0.24316600
H	-1.96072000	-0.74047900	-1.23393300
C	-3.29285000	0.37756400	0.05138900
H	-3.05339000	1.35375000	-0.38269500
H	-3.43134600	0.54649200	1.12637400
C	-4.60324900	-0.13166800	-0.55696500
H	-4.89844700	-1.08949800	-0.11741800
H	-5.42075900	0.57544200	-0.39212000

H	-4.50595800	-0.28015100	-1.63693600
Sci-TS32			
C	-0.85375800	0.22036300	-0.47035200
C	-0.19106500	-1.05954500	0.06634900
C	1.52476600	1.05944200	-0.82241400
C	0.13756500	1.39690100	-0.36655700
H	0.06480200	-0.91433600	1.12244200
H	-1.06753300	0.06379800	-1.53772400
H	3.93642700	1.02930600	1.40551200
H	2.20209000	1.87986200	-1.04102600
H	0.17890400	1.73692700	0.68175800
H	-0.23896900	2.25702800	-0.93333600
O	2.80179800	-0.37550900	0.92440200
O	4.07463200	0.20578900	0.91669500
C	1.08254700	-1.40841900	-0.71430000
H	0.82136700	-1.73090500	-1.73124600
C	2.02427600	-0.23470200	-0.81892900
H	2.97273200	-0.41431800	-1.31246300
H	1.60899300	-2.24294900	-0.24503600
C	-2.17842600	0.56172400	0.23143100
H	-2.00473800	0.61185700	1.31499600
H	-2.48511700	1.57154300	-0.07179000
H	-0.88614900	-1.90222300	0.02038600
C	-3.33693900	-0.40205200	-0.05515500
H	-3.07309900	-1.41372200	0.27026700
H	-3.49373300	-0.46097600	-1.13919600
C	-4.64314000	0.01722700	0.62606700
H	-4.96190000	1.01073000	0.29528500
H	-5.45262100	-0.68270900	0.40168600
H	-4.52784000	0.05319400	1.71385900
Sci-P32			
C	1.02730300	-1.28528100	0.30433300
C	0.04181800	-0.22117400	-0.20716900
C	0.50719800	1.17478800	0.24904100
C	1.99334100	1.38028500	0.09304600
C	2.85689300	0.39195500	-0.13707700
C	2.44714900	-1.05508600	-0.23088200
H	0.67846600	-2.28541800	0.02653800
H	3.91218100	0.62026500	-0.26320400
H	3.16229500	-1.67731800	0.31986800
H	2.35815000	2.40156400	0.17015400
H	0.22458000	1.33148300	1.30131700
H	0.07938800	-0.23882200	-1.30619300
H	1.04510000	-1.25157500	1.40115800

H	2.51525700	-1.38738300	-1.27650900
H	-0.02159600	1.95228800	-0.31323800
C	-1.39970200	-0.53815800	0.22137000
H	-1.63111600	-1.56931900	-0.07532300
H	-1.45833300	-0.51902600	1.31849200
C	-2.47539500	0.38932600	-0.35854400
H	-2.30299700	1.41768200	-0.02379800
H	-2.38501200	0.40463600	-1.45177300
C	-3.89621800	-0.03186800	0.02912000
H	-4.02655000	-0.02898800	1.11590900
H	-4.64365100	0.64356500	-0.39609700
H	-4.12048600	-1.04236300	-0.32673600

Sci-R33

C	-1.34698300	0.62035900	0.62563200
C	-0.12835800	-0.29594300	0.37315600
C	-0.47287100	-1.37709700	-0.67062800
C	-1.69812700	-2.20312900	-0.25759900
C	-2.93026900	-1.30956400	-0.00296900
C	-2.59704100	-0.15369500	0.88241600
H	-0.65847100	-0.89505700	-1.63728800
H	0.04240400	-0.80421500	1.33290300
H	-1.13024600	1.30897900	1.44769900
H	-1.93179600	-2.94559900	-1.02708300
H	-3.75262500	-1.89585300	0.41738400
H	-3.19452000	2.18486900	-0.72742600
H	-3.31920900	0.21792900	1.59996500
H	0.38400700	-2.04245000	-0.80959700
H	-1.46649500	-2.75872300	0.65892400
H	-3.28931300	-0.94019800	-0.97945500
O	-1.46727300	1.42969500	-0.58264100
O	-2.38930100	2.51209100	-0.30345700
C	1.13763400	0.51306900	0.03668300
H	1.17844500	1.38565800	0.70037700
H	1.05259400	0.91519100	-0.97751200
C	2.44635900	-0.27349600	0.18075500
H	2.44510300	-1.13829100	-0.49345100
H	2.51526900	-0.68076200	1.19846000
C	3.69188700	0.57379200	-0.10555300
H	3.69966500	1.44072100	0.56625300
H	3.62484300	0.97969600	-1.12198300
C	5.00247800	-0.20259800	0.04960600
H	5.86918700	0.43145100	-0.15637800
H	5.11217300	-0.59434900	1.06580200

H	5.04331300	-1.05348300	-0.63779700
Sci-TS33			
C	1.78013400	-2.23570400	-0.30175600
C	0.52929600	-1.42103300	-0.65775200
C	2.66768900	-0.11665800	0.74960200
C	2.99943600	-1.33071900	-0.06376900
H	0.69877200	-0.86346300	-1.58625900
H	-0.31076300	-2.09657100	-0.83954300
H	1.58027200	-2.81677100	0.60647600
H	2.00288900	-2.95870600	-1.09217500
H	2.73134700	2.97128000	-0.55682400
H	3.48885800	0.45099300	1.17753700
H	3.40581500	-1.00002800	-1.03276800
H	3.81024200	-1.89255400	0.41412900
C	-1.07792300	0.42527700	0.17470400
H	-1.14465700	1.20805700	0.94067200
H	-0.94735100	0.94889800	-0.77548200
O	1.47580200	1.59449700	-0.70826000
O	1.81781000	2.87616500	-0.25268700
C	0.17432100	-0.42433900	0.46049900
H	-0.03849600	-1.01052800	1.36964300
C	1.38798600	0.41717000	0.81078500
H	1.21451300	1.23422900	1.50354700
C	-2.39045100	-0.36778000	0.16779800
H	-2.36748600	-1.12989100	-0.62014800
H	-2.49539000	-0.91260600	1.11597000
C	-3.62485800	0.51779300	-0.04082400
H	-3.66105500	1.27728100	0.74953000
H	-3.51721000	1.06734300	-0.98354500
C	-4.93923700	-0.26774600	-0.05434900
H	-5.09086200	-0.80210800	0.88896100
H	-5.79825600	0.39240200	-0.20300700
H	-4.94844600	-1.01011200	-0.85875600
Sci-P33			
C	-2.45377500	1.39364900	0.20472200
C	-0.99156700	1.07925600	-0.13438200
C	-0.54516900	-0.27015400	0.45870000
C	-1.61371700	-1.32265700	0.25595800
C	-2.86523800	-1.06703200	-0.12565300
C	-3.39604900	0.32359300	-0.36245800
H	-0.34225000	1.88326700	0.22311900
H	-2.72970300	2.38222700	-0.17498600
H	-3.55650700	-1.89326700	-0.27270100
H	-4.39251600	0.41892600	0.08440700

C	0.80496700	-0.75675100	-0.10814600
H	-1.31261500	-2.35382800	0.42987100
H	1.01356800	-1.75285700	0.30252400
H	0.70556300	-0.89065500	-1.19318000
H	-0.40708600	-0.13842900	1.54404800
H	-0.87518300	1.04077200	-1.22570200
H	-2.56833500	1.43177600	1.29461500
H	-3.54207100	0.48040000	-1.44069900
C	1.99949300	0.15685800	0.19039900
H	1.84528900	1.13965100	-0.26960100
H	2.05865300	0.33220200	1.27297200
C	3.33481100	-0.41552600	-0.30023800
H	3.50036500	-1.39467300	0.16535800
H	3.27263600	-0.59999600	-1.37958200
C	4.52914500	0.49699800	-0.00718400
H	4.63783300	0.67343800	1.06760200
H	5.46442200	0.05989700	-0.36758400
H	4.41053300	1.47174900	-0.49078100

Sci-R34

C	-2.49049100	-0.15204600	0.58230400
C	-2.61322700	1.36615100	0.39974300
C	-1.54394900	1.92184400	-0.54862400
C	-0.13076900	1.54272800	-0.08801000
C	0.04820500	0.01070000	0.04145800
C	-1.08273700	-0.58376300	0.82569700
H	-1.71830300	1.53404800	-1.55780300
H	-2.50888000	1.82865400	1.38759000
H	-3.15299900	-0.50082600	1.37950700
H	0.60769800	1.94570800	-0.78652800
H	-2.39605600	-2.45484700	-0.98810900
H	-0.89944700	-1.45361600	1.44789000
H	0.07120600	2.00150300	0.88895700
H	-0.00287600	-0.39464500	-0.98728100
O	-3.01374000	-0.69733400	-0.66865300
O	-3.16699600	-2.12904700	-0.50403100
H	-3.61961200	1.59466100	0.03833900
C	1.41450000	-0.39715000	0.62503200
H	1.41674600	-1.48559400	0.76463200
H	-1.63615000	3.01078400	-0.61004000
H	1.51477100	0.03709600	1.62818300
C	2.62955500	-0.00971400	-0.22558600
H	2.69041900	1.08036100	-0.32056900
H	2.49719800	-0.39798100	-1.24430400

C	3.95478500	-0.53149400	0.34269700
H	4.08289900	-0.15270600	1.36395400
H	3.90527900	-1.62379600	0.42858800
C	5.17073600	-0.14088900	-0.50210700
H	5.26950300	0.94675900	-0.57428000
H	6.09767400	-0.53003400	-0.07218000
H	5.08716600	-0.53268600	-1.52070400

Sci-TS34

C	0.02582600	1.52170900	-0.16958800
C	1.45282400	1.94101000	-0.54328800
C	1.04066200	-0.60878400	0.69737500
C	-0.11530500	-0.00962700	-0.05618000
H	1.71686200	1.51542400	-1.51722300
H	1.51246600	3.02879400	-0.64554300
H	-0.24452900	1.97341900	0.79430600
H	-0.68302500	1.90771400	-0.90697800
H	3.15108800	-2.56371600	-0.90720200
H	0.92159500	-1.62585700	1.06257400
H	-0.08265200	-0.42215200	-1.07995200
O	3.21048200	-0.70552900	-0.71808700
O	3.73021800	-1.96790300	-0.41138600
C	2.46336500	1.45672800	0.50278000
H	2.33532100	2.02008500	1.43702300
C	2.28747000	-0.00995400	0.80889100
H	2.99756000	-0.44925900	1.50066700
C	-1.45873700	-0.45192400	0.56190000
H	-1.44297700	-1.54298300	0.67871900
H	-1.53551700	-0.03895200	1.57591300
H	3.48907500	1.62804500	0.16810000
C	-2.70134200	-0.06257000	-0.24717500
H	-2.77688000	1.02835400	-0.31850800
H	-2.59187700	-0.42933600	-1.27648500
C	-4.00388600	-0.61146200	0.34743800
H	-3.93904100	-1.70446900	0.41108900
H	-4.10803700	-0.25337400	1.37883400
C	-5.24740400	-0.22024000	-0.45598100
H	-6.15741500	-0.62800500	-0.00751500
H	-5.36049400	0.86727500	-0.50564200
H	-5.18796000	-0.59286500	-1.48342700

Sci-P34

C	-2.45377500	1.39364900	0.20472200
C	-0.99156700	1.07925600	-0.13438200
C	-0.54516900	-0.27015400	0.45870000
C	-1.61371700	-1.32265700	0.25595800

C	-2.86523800	-1.06703200	-0.12565300
C	-3.39604900	0.32359300	-0.36245800
H	-0.34225000	1.88326700	0.22311900
H	-2.72970300	2.38222700	-0.17498600
H	-3.55650700	-1.89326700	-0.27270100
H	-4.39251600	0.41892600	0.08440700
C	0.80496700	-0.75675100	-0.10814600
H	-1.31261500	-2.35382800	0.42987100
H	1.01356800	-1.75285700	0.30252400
H	0.70556300	-0.89065500	-1.19318000
H	-0.40708600	-0.13842900	1.54404800
H	-0.87518300	1.04077200	-1.22570200
H	-2.56833500	1.43177600	1.29461500
H	-3.54207100	0.48040000	-1.44069900
C	1.99949300	0.15685800	0.19039900
H	1.84528900	1.13965100	-0.26960100
H	2.05865300	0.33220200	1.27297200
C	3.33481100	-0.41552600	-0.30023800
H	3.50036500	-1.39467300	0.16535800
H	3.27263600	-0.59999600	-1.37958200
C	4.52914500	0.49699800	-0.00718400
H	4.63783300	0.67343800	1.06760200
H	5.46442200	0.05989700	-0.36758400
H	4.41053300	1.47174900	-0.49078100

Sci-R35

C	2.40823500	-0.34113600	0.62871200
C	0.97446700	-0.67670500	1.05690400
C	-0.10132200	-0.02811000	0.16649500
C	0.11395400	1.49433100	0.12142800
C	1.52788600	1.86687900	-0.36925600
C	2.59674700	1.11160800	0.34922700
H	0.02679700	-0.42136500	-0.85072500
H	0.84618200	-0.33194900	2.09015200
H	3.12493800	-0.69808600	1.37377800
H	-0.62754500	1.97030900	-0.52585500
H	1.69234800	2.94511200	-0.27830500
H	4.01488700	-0.49035500	-1.65424400
H	3.57382800	1.55700200	0.49705900
H	-0.03619800	1.90214900	1.12963900
H	1.58192900	1.64799700	-1.45052600
O	2.61353900	-1.15104000	-0.57182500
O	4.02261800	-1.10457300	-0.90763100
H	0.86201000	-1.76497000	1.06323700

C	-1.50717000	-0.42081800	0.65279500
H	-1.53435600	-1.50988000	0.78430700
H	-1.67338700	0.00819800	1.65061700
C	-2.65934700	-0.01385800	-0.27430000
H	-2.69512400	1.07694900	-0.37690500
H	-2.46930200	-0.40949000	-1.28056900
C	-4.02723500	-0.50931500	0.21087000
H	-4.21304100	-0.12260200	1.22026100
H	-4.00196100	-1.60171300	0.30469800
C	-5.18056600	-0.10314100	-0.71083700
H	-6.13941300	-0.47426200	-0.33872000
H	-5.25619800	0.98560600	-0.79428000
H	-5.03954200	-0.50216100	-1.72019400

Sci-TS35

C	-0.07163000	1.59412000	-0.01850100
C	0.10660400	0.08468600	0.21712300
C	-2.56730500	1.20620800	0.10073400
C	-1.45566300	1.92403000	-0.60086800
H	-0.05183100	-0.43009100	-0.73986600
H	0.05247600	2.11633100	0.93919600
H	0.70288600	1.97779000	-0.68781900
H	-4.25270700	-1.10343400	-1.53589400
H	-3.58268600	1.56110700	-0.04907200
H	-1.47614100	1.65416200	-1.66884600
H	-1.63476700	3.00517800	-0.57334600
O	-2.66367100	-1.29619700	-0.57111300
O	-4.03659400	-1.53618000	-0.69791000
C	-0.97925500	-0.41219400	1.18780100
H	-0.77398500	-0.02523900	2.19629900
C	-2.36913100	0.01819000	0.78896500
H	-3.18376800	-0.35656500	1.39854200
H	-0.95679300	-1.50272800	1.25903900
C	1.50675100	-0.28639900	0.73332800
H	1.49432100	-1.34080200	1.03710000
H	1.71600100	0.28841800	1.64611300
C	2.64838200	-0.08348600	-0.27060100
H	2.71907200	0.97282900	-0.55499800
H	2.41811200	-0.63328800	-1.19248000
C	4.01099300	-0.54311700	0.26193100
H	3.95034700	-1.60223200	0.54004200
H	4.23870600	0.00064300	1.18688600
C	5.15127700	-0.34362500	-0.74047000
H	5.26124600	0.71152500	-1.01018800
H	6.10711500	-0.68250800	-0.33157100

H	4.96837900	-0.90255800	-1.66359900
Sci-P35			
C	1.66888000	-1.27815600	0.24218200
C	0.58311300	-0.27360000	-0.17866600
C	0.95924400	1.13332100	0.32392200
C	2.41689400	1.46193600	0.11826500
C	3.34302200	0.55583800	-0.19269200
C	3.04212300	-0.91348100	-0.33810200
H	1.38621700	-2.28955000	-0.06821800
H	4.37107700	0.87198700	-0.35026200
H	3.82634200	-1.50103400	0.15351100
H	2.70503400	2.50447000	0.22850900
H	0.71187000	1.22081500	1.39300000
H	0.57400500	-0.23980300	-1.27789500
H	1.73206000	-1.29128900	1.33777700
H	3.08980400	-1.19313400	-1.40015500
H	0.34794700	1.89058500	-0.17920000
C	-0.80980100	-0.72197500	0.29169900
H	-0.97317000	-1.75370600	-0.04512300
H	-0.82067500	-0.75695200	1.38977000
C	-1.97691700	0.14364700	-0.19957400
H	-1.87424900	1.16583200	0.18279900
H	-1.93325600	0.22152400	-1.29406400
C	-3.34969500	-0.40251100	0.21109800
H	-3.39080300	-0.48889200	1.30374400
H	-3.46300700	-1.42180500	-0.17768100
C	-4.51630700	0.46160900	-0.27594000
H	-4.52200100	0.53949200	-1.36772700
H	-5.47907700	0.04423700	0.03161000
H	-4.45145400	1.47746800	0.12645700

Sci-R36			
C	-2.69559400	0.11918400	0.57295300
C	-2.09023100	1.52347600	0.45712600
C	-0.76024200	1.52814400	-0.30734400
C	0.27483100	0.57580500	0.31496700
C	-0.30797000	-0.85672900	0.38622400
C	-1.68120700	-0.89760200	0.97476600
H	-0.93938300	1.23882500	-1.34932100
H	-1.93488600	1.90193300	1.47355300
H	-3.54928300	0.12029800	1.25649300
H	0.35724800	-1.51886700	0.94681000
H	-3.43204600	-1.99463400	-1.09360200
H	-1.99430200	-1.75523400	1.55895100

H	-0.32999200	-1.25527000	-0.64505100
O	-3.22613300	-0.14500700	-0.76314200
O	-4.03078300	-1.34847600	-0.69511300
H	-2.82049600	2.17978600	-0.02438100
H	-0.35617800	2.54585400	-0.32908200
H	0.45616200	0.90846800	1.34740000
C	1.61155600	0.63359000	-0.44227700
H	1.90840900	1.68611400	-0.53359600
H	1.45535000	0.27366900	-1.46831900
C	2.76624500	-0.14542600	0.20021500
H	2.52817100	-1.21492100	0.23338600
H	2.88132000	0.17434200	1.24433400
C	4.10101900	0.03898400	-0.53207400
H	4.35355100	1.10586200	-0.55795900
H	3.98384600	-0.27006700	-1.57786700
C	5.25381200	-0.74273900	0.10420900
H	5.04778600	-1.81773400	0.10966400
H	6.18985200	-0.58765900	-0.43922300
H	5.41688500	-0.43302500	1.14126400

Sci-TS36

C	-0.32590100	0.36105200	-0.47960300
C	0.25107500	-0.98701200	-0.01565000
C	2.10147700	1.07972600	-0.74998100
C	0.72979400	1.46841900	-0.28872500
H	0.49420900	-0.92426500	1.05158300
H	-0.53035300	0.28409800	-1.55743100
H	4.49565700	0.76434400	1.48821700
H	2.82781300	1.87090700	-0.91149400
H	0.77535500	1.73707100	0.77996000
H	0.41173000	2.38370900	-0.80242200
O	3.26442000	-0.52407700	0.92539800
O	4.57749300	-0.04137500	0.95877300
C	1.51756500	-1.36083700	-0.79723400
H	1.25683300	-1.60653500	-1.83554400
C	2.52576000	-0.23921800	-0.81759100
H	3.47089400	-0.44402000	-1.30771600
H	1.98751500	-2.25074700	-0.37188600
C	-1.64012600	0.73736600	0.22466700
H	-1.47891400	0.71858400	1.31100800
H	-1.88406900	1.77798000	-0.02622400
H	-0.49063200	-1.78255900	-0.12663700
C	-2.84566700	-0.14254300	-0.12799300
H	-2.64838800	-1.18322700	0.15355300
H	-2.98593200	-0.14227100	-1.21698300

C	-4.14536800	0.31384800	0.54591000
H	-4.35262200	1.35308500	0.26299000
H	-4.00488100	0.31801600	1.63361700
C	-5.35078800	-0.56125100	0.19099200
H	-5.18890100	-1.60011100	0.49520900
H	-6.26008100	-0.20893500	0.68562800
H	-5.53746100	-0.55879900	-0.88754700

Sci-P36

C	1.66888000	-1.27815600	0.24218200
C	0.58311300	-0.27360000	-0.17866600
C	0.95924400	1.13332100	0.32392200
C	2.41689400	1.46193600	0.11826500
C	3.34302200	0.55583800	-0.19269200
C	3.04212300	-0.91348100	-0.33810200
H	1.38621700	-2.28955000	-0.06821800
H	4.37107700	0.87198700	-0.35026200
H	3.82634200	-1.50103400	0.15351100
H	2.70503400	2.50447000	0.22850900
H	0.71187000	1.22081500	1.39300000
H	0.57400500	-0.23980300	-1.27789500
H	1.73206000	-1.29128900	1.33777700
H	3.08980400	-1.19313400	-1.40015500
H	0.34794700	1.89058500	-0.17920000
C	-0.80980100	-0.72197500	0.29169900
H	-0.97317000	-1.75370600	-0.04512300
H	-0.82067500	-0.75695200	1.38977000
C	-1.97691700	0.14364700	-0.19957400
H	-1.87424900	1.16583200	0.18279900
H	-1.93325600	0.22152400	-1.29406400
C	-3.34969500	-0.40251100	0.21109800
H	-3.39080300	-0.48889200	1.30374400
H	-3.46300700	-1.42180500	-0.17768100
C	-4.51630700	0.46160900	-0.27594000
H	-4.52200100	0.53949200	-1.36772700
H	-5.47907700	0.04423700	0.03161000
H	-4.45145400	1.47746800	0.12645700

Sci-R37

C	1.78391300	0.85024500	-0.77500500
C	0.47385900	1.36756400	-0.28204000
C	-0.58037800	0.43292100	0.22934700
C	0.03700900	-0.70237800	1.06823700
C	1.26334600	-1.33498100	0.39996100
C	2.33995800	-0.28408600	0.10728300

H	1.65074500	0.46105800	-1.79933300
H	2.50816800	1.66675000	-0.85831100
H	0.32378500	-0.28911100	2.04191900
H	-0.73768600	-1.44953900	1.25895700
H	1.66807200	-2.12355000	1.04218900
H	0.96212100	-1.81567000	-0.53816400
H	2.69676100	0.13910700	1.05404000
H	3.20505800	-0.74353600	-0.38044200
C	-1.69246100	1.16627400	0.97634600
H	-2.11861700	1.94449800	0.33902500
H	-2.48712500	0.47053700	1.24878300
H	-1.30253900	1.63128600	1.88545200
O	-1.11855400	-0.10994500	-1.02780000
O	-2.19637600	-1.06151300	-0.73507500
H	0.18079700	2.38840100	-0.50322800
H	-1.78157000	-1.88191700	-1.03265600

Sci-TS37

C	1.83116600	0.72472600	-0.87147100
C	0.52692000	1.31186600	-0.43205600
C	-0.40218000	0.62118000	0.35004700
C	0.07310200	-0.57857800	1.14566900
C	1.23297500	-1.32610400	0.47851700
C	2.35357100	-0.35826300	0.08492800
H	1.68935400	0.28929900	-1.87429300
H	2.57415500	1.51953200	-1.00189400
H	0.38051700	-0.22321500	2.13892400
H	-0.77854100	-1.24364900	1.32202900
H	1.61409100	-2.09999900	1.15194500
H	0.86350200	-1.83132000	-0.42030900
H	2.75333900	0.11909700	0.98769200
H	3.18383100	-0.89782400	-0.38008000
C	-1.58300500	1.36093000	0.92334200
H	-1.88148700	2.18823700	0.27762500
H	-2.43219200	0.68358000	1.03561900
H	-1.33494700	1.76230000	1.91266800
O	-1.30596000	-0.29092400	-1.12212500
O	-2.33529400	-1.09543200	-0.60514800
H	0.22342500	2.25835900	-0.87011100
H	-1.92031600	-1.96808500	-0.53548000

Sci-P37

C	1.19481600	1.29806000	-0.10242100
C	-0.31142300	1.21919100	-0.08907800
C	-1.00986500	0.08373100	0.00536900
C	-0.32670900	-1.26609900	0.08243200

C	1.15631100	-1.21455900	-0.30841600
C	1.85102500	-0.01524100	0.34452300
H	1.53814800	1.56252400	-1.11309000
H	1.52409500	2.12200500	0.54154900
H	-0.43364000	-1.66073500	1.10337100
H	-0.85982700	-1.97726900	-0.56072100
H	1.65194100	-2.14942400	-0.02902900
H	1.23920000	-1.12697400	-1.39851300
H	1.77260500	-0.10568200	1.43473000
H	2.91846700	-0.00719000	0.10377800
C	-2.51499400	0.06648600	0.04931900
H	-2.93216600	1.07542400	0.02568900
H	-2.92859100	-0.49502000	-0.79694900
H	-2.87576600	-0.42949300	0.95864900
H	-0.84943100	2.16242000	-0.15983700

Sci-R38

C	-1.76194800	-1.21405900	-0.79367700
C	-0.35053300	-1.30941600	-0.31674700
C	0.36743800	-0.10140300	0.20483800
C	-0.56473300	0.75890600	1.08073600
C	-1.94248400	0.98665700	0.44681200
C	-2.63599100	-0.34207000	0.12797800
H	-1.77018900	-0.76881800	-1.80336800
H	-2.19347500	-2.21378500	-0.90349200
H	-0.68426900	0.25483500	2.04654000
H	-0.06322500	1.70926400	1.28125700
H	-2.56334400	1.58644000	1.11994500
H	-1.82897200	1.56639800	-0.47678000
H	-2.82413000	-0.88388400	1.06269000
H	-3.60990000	-0.16720500	-0.33934900
C	1.66883700	-0.44382100	0.95307100
H	2.06405100	0.48619400	1.37096700
H	1.40385600	-1.08367200	1.80222600
O	0.67790700	0.61607500	-1.03953700
O	1.41612500	1.84659900	-0.72721300
H	0.22525800	-2.20171800	-0.53012600
H	0.76954200	2.50622200	-1.01065500
C	2.75408300	-1.11038400	0.10382000
H	3.65170100	-1.27971300	0.70468200
H	2.43781400	-2.08047300	-0.28876900
H	3.02500800	-0.47793200	-0.74275400

Sci-TS38

C	-1.74642400	-1.17629500	-0.87893500
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C	-0.31213800	-1.24880800	-0.45689200
C	0.30650900	-0.27538000	0.33341900
C	-0.57615900	0.64624700	1.15431300
C	-1.94037100	0.92058500	0.51137900
C	-2.62505300	-0.38730700	0.10258900
H	-1.78521700	-0.69571000	-1.87030900
H	-2.14198800	-2.18696500	-1.02953200
H	-0.71724200	0.18470200	2.14116700
H	-0.03277800	1.57823500	1.33995000
H	-2.57188700	1.48412000	1.20515700
H	-1.80006500	1.54440800	-0.37809800
H	-2.80544200	-0.99583300	0.99687300
H	-3.60259900	-0.18853000	-0.34649600
C	1.68882200	-0.50211600	0.91429300
H	2.13298000	0.48523900	1.07279900
H	1.56170500	-0.94229000	1.91283500
O	0.78811000	0.92686900	-1.12507400
O	1.39742200	2.07910500	-0.59652800
H	0.30357000	-2.01132400	-0.92061700
H	0.66540300	2.71163300	-0.54631600
C	2.64284400	-1.35970400	0.08216100
H	3.63738300	-1.36363500	0.53535200
H	2.31343100	-2.40011800	0.01397800
H	2.73029600	-0.95506000	-0.92788800

Sci-P38

C	1.31835200	1.46463400	-0.10369800
C	-0.12696000	1.02946100	-0.09830000
C	-0.53527900	-0.23977200	-0.00313900
C	0.45674100	-1.38338100	0.08882100
C	1.88423700	-0.98172500	-0.30327900
C	2.27067600	0.34986400	0.34742200
H	1.59191900	1.80316000	-1.11358100
H	1.43678900	2.34460100	0.53948400
H	0.44801700	-1.77906400	1.11480800
H	0.11306100	-2.21060200	-0.54447800
H	2.58804500	-1.77092100	-0.02104900
H	1.94496000	-0.87978300	-1.39361000
H	2.21478600	0.24510700	1.43774700
H	3.30528900	0.61397700	0.10784500
C	-1.98895200	-0.65913000	0.03057200
H	-2.17047100	-1.33049900	-0.82036600
H	-2.13880200	-1.28843400	0.91932300
H	-0.86320300	1.82385400	-0.17825800
C	-3.03558000	0.45537000	0.02307900

H	-2.96750500	1.06469200	-0.88218700
H	-4.04270300	0.03235400	0.06170800
H	-2.91960500	1.11963800	0.88375200

Sci-R39

C	-2.02132600	-1.34332100	-0.82844400
C	-0.57510500	-1.25234000	-0.46975300
C	-0.01028600	0.00676500	0.11637900
C	-0.97756900	0.60535700	1.15813100
C	-2.42839600	0.66257300	0.66485000
C	-2.93261500	-0.72340800	0.24919900
H	-2.19067700	-0.80542600	-1.77679500
H	-2.30072500	-2.38406900	-1.01881400
H	-0.92202700	-0.00786200	2.06481700
H	-0.61590100	1.60102800	1.42748900
H	-3.06830300	1.07882800	1.44941800
H	-2.49690800	1.34373100	-0.19145900
H	-2.94921500	-1.38028300	1.12726200
H	-3.96027700	-0.66486500	-0.12240300
C	1.39797000	-0.17469500	0.70965000
H	1.67314800	0.76021800	1.20797100
H	1.33353600	-0.94044600	1.49221100
O	0.04804300	0.88320500	-1.06194800
O	0.59667800	2.18918300	-0.67647300
H	0.10845100	-2.02488700	-0.80003300
H	-0.17724700	2.74759300	-0.82748200
C	2.49849700	-0.54022300	-0.29259900
H	2.25731300	-1.48278500	-0.79581100
H	2.53324500	0.22390500	-1.07273500
C	3.87141600	-0.66603000	0.37544100
H	3.87252000	-1.44483900	1.14509100
H	4.64544900	-0.91990600	-0.35398400
H	4.16433200	0.27289400	0.85550800

Sci-TS39

C	-1.98858800	-1.36002600	-0.87410000
C	-0.53495300	-1.19937800	-0.55483800
C	-0.03435900	-0.17682200	0.25781300
C	-0.99871900	0.52596600	1.19519000
C	-2.43311200	0.59448200	0.65991200
C	-2.91387600	-0.78838400	0.21000700
H	-2.18567200	-0.84701000	-1.82977500
H	-2.21386900	-2.41621200	-1.05993400
H	-0.98694000	-0.01118300	2.15341400
H	-0.60939300	1.52584000	1.41140900

H	-3.09774200	1.00036900	1.42884300
H	-2.46800400	1.28108400	-0.19306300
H	-2.92363300	-1.46595000	1.07237800
H	-3.94105800	-0.73867100	-0.16314000
C	1.40630200	-0.18297300	0.72929400
H	1.68373200	0.85939200	0.91947300
H	1.43779200	-0.68821800	1.70529000
O	0.11451000	1.16928900	-1.14540000
O	0.54103600	2.38472000	-0.57953900
H	0.16464600	-1.81334600	-1.11068900
H	-0.28796900	2.86714100	-0.44368400
C	2.43814300	-0.81187500	-0.21124500
H	2.24620700	-1.88499200	-0.32092300
H	2.32159500	-0.36223000	-1.20119600
C	3.87298600	-0.61138800	0.28595600
H	4.59524300	-1.07189800	-0.39350600
H	4.11847600	0.45213000	0.36076200
H	4.01927900	-1.05592500	1.27592700

Sci-P39

C	1.88114100	1.45080000	-0.09844000
C	0.42754400	1.04395300	-0.10587400
C	-0.00654300	-0.21718200	-0.01450800
C	0.96311000	-1.37954300	0.08572700
C	2.40132000	-1.00561900	-0.29409400
C	2.80790700	0.31795900	0.36054300
H	2.17003000	1.78420700	-1.10577100
H	2.01083600	2.32824500	0.54604000
H	0.93795800	-1.77490600	1.11157100
H	0.60900100	-2.20003000	-0.55052600
H	3.08720800	-1.80849200	-0.00634400
H	2.47322200	-0.90446600	-1.38382300
H	2.74056500	0.21403100	1.45030300
H	3.84945200	0.56217100	0.13003700
C	-1.46757500	-0.61091100	0.00654800
H	-1.65591900	-1.27577300	-0.84928600
H	-1.63620300	-1.24245800	0.89163200
H	-0.29158900	1.85306600	-0.19234800
C	-2.50497100	0.51457200	-0.00255500
H	-2.37056700	1.12979700	-0.89888300
H	-2.33398000	1.17573000	0.85399700
C	-3.94271300	-0.01250600	0.03857900
H	-4.12258900	-0.60487500	0.94122800
H	-4.66674600	0.80668800	0.03029800
H	-4.15600700	-0.65208000	-0.82368400

Sci-R40

C	-0.45812800	0.11252600	0.14220100
C	-0.84785800	-1.27579500	-0.41134900
C	-2.30960900	-1.35725100	-0.87234800
C	-3.27815800	-0.95443800	0.24389200
C	-2.96321200	0.46463800	0.75802400
C	-1.51246000	0.63585000	1.07047700
H	-2.45110700	-0.70038000	-1.73663500
H	-0.66829800	-2.00755900	0.38445100
H	-4.31327100	-1.00231600	-0.10813400
H	-3.57233100	0.70411100	1.63493400
H	-0.95181900	2.70499900	-0.78479600
H	-1.20809000	1.27185000	1.89459100
H	-2.52610800	-2.37570100	-1.21040400
H	-3.19114200	-1.66324600	1.07617600
H	-3.26828700	1.18293500	-0.02398200
O	-0.42927800	0.91533800	-1.09471400
O	-0.07996900	2.28734200	-0.77845900
C	0.92627900	0.13196600	0.81091600
H	1.10879700	1.15705000	1.14771400
H	-0.17699000	-1.52543600	-1.23675700
H	0.86838400	-0.48848200	1.71354200
C	2.09945300	-0.32120600	-0.06417500
H	1.98002600	-1.37422800	-0.34447400
H	2.09053000	0.25225500	-0.99634000
C	3.45474100	-0.14593600	0.63195100
H	3.45673100	-0.70872200	1.57380500
H	3.58358600	0.90764600	0.90724100
C	4.63701100	-0.59430400	-0.23180000
H	5.58879900	-0.45293400	0.28780800
H	4.55633400	-1.65394200	-0.49432600
H	4.67988500	-0.02563900	-1.16576600

Sci-TS40

C	-2.21033100	-1.56138400	-0.84815500
C	-0.80424500	-1.21641900	-0.46801800
C	-0.46780200	-0.09871900	0.30249400
C	-1.55569400	0.54031700	1.14563500
C	-2.95665000	0.41199800	0.53754700
C	-3.25310800	-1.04039100	0.15163700
H	-2.40997800	-1.12901300	-1.84240500
H	-2.30487100	-2.64525500	-0.97880900
H	-1.53633400	0.06396300	2.13534100
H	-1.29409600	1.58919400	1.31734400

H	-3.70480600	0.78145200	1.24568900
H	-3.01968400	1.04050700	-0.35744500
H	-3.23432200	-1.66485900	1.05299800
H	-4.25697700	-1.13084800	-0.27362700
C	0.93566600	0.08667700	0.84487000
H	1.08324900	1.16284900	0.98470900
H	0.96691800	-0.35704500	1.85025300
O	-0.39205000	1.17601100	-1.17193800
O	-0.13107000	2.46111700	-0.66249600
H	-0.00951300	-1.77666900	-0.94745600
H	-1.01368200	2.85471900	-0.59535700
C	2.08226700	-0.47103100	-0.00252700
H	2.02092200	-1.56479700	-0.05417300
H	1.97366900	-0.09535500	-1.02480500
C	3.46101100	-0.08206600	0.54458300
H	3.53554100	1.01093000	0.58357200
H	3.55493700	-0.43158100	1.58044000
C	4.61705500	-0.64239400	-0.28855000
H	5.58631000	-0.34242500	0.11932900
H	4.59257000	-1.73652200	-0.31532800
H	4.56609900	-0.28579100	-1.32188700

Sci-P40

C	2.27207400	1.54229700	-0.10089500
C	0.86329700	1.00032000	-0.11011100
C	0.54977500	-0.29590600	-0.01635600
C	1.62454200	-1.36145400	0.08849400
C	3.02228100	-0.85438000	-0.28833600
C	3.30021000	0.50319100	0.36379200
H	2.53084200	1.89839400	-1.10865000
H	2.31694800	2.42999200	0.54102500
H	1.63391000	-1.75573000	1.11500800
H	1.35101100	-2.21270300	-0.54708700
H	3.78001600	-1.58824400	0.00346600
H	3.08769400	-0.74954000	-1.37813100
H	3.23986200	0.39616000	1.45366100
H	4.31475200	0.84395300	0.13534300
C	-0.86751300	-0.82654100	0.00333300
H	-0.98912800	-1.50850700	-0.85094100
H	-0.97588600	-1.46902000	0.88981300
H	0.07125200	1.73773800	-0.20004400
C	-2.00681900	0.19534500	-0.01039200
H	-1.93242600	0.81857900	-0.90947200
H	-1.90191700	0.87405300	0.84443800
C	-3.39388600	-0.45703900	0.03177800

H	-3.47287600	-1.08131700	0.93010800
H	-3.49979200	-1.13819600	-0.82132800
C	-4.53906800	0.55930900	0.01635100
H	-4.50874300	1.17568700	-0.88787000
H	-5.51380600	0.06434400	0.04781400
H	-4.48106200	1.23350600	0.87689600