

Reactions between hydroxyl-substituted alkylperoxy radicals and Criegee intermediates: Correlations of the electronic characteristics of methyl substituents and the reactivity

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(Electronic Supplementary Information)

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Fig.S1 Plots of the total energy against the internal torsion angles of O-C-C-O(1), C-C-O-O(2) and H-O-C-C(3) in $\text{HO}(\text{CH}_3)_2\text{CCH}_2\text{OO}$ using M06-2X/6-311+G(d,p)

Fig.S2 The diagram for the conformations transitions of $\text{HO}(\text{CH}_3)_2\text{CCH}_2\text{OO}$. The values under the conformation denote the relative energies and that on the two sides of arrows denote the energies barriers

Fig.S3 Optimized geometries of the transition states

Table S1 Y/X (Y=DFT, CCSD(T), X=aug-cc-pVTZ, 6-311+(d,p), cc-pVTZ, def2-TZVP, ma-TZVP) calculated electronic-energy barrier (ΔE , kcal/mol) for the formation of $\text{HOCH}_2(\text{CH}_3)\text{CHOOCH}_2\text{OO}$ based on the optimized geometries at M06-2X/6-311+(d,p)

Table S2 Spin contamination at M06-2X/6-311+G(d,p)^a and M06-2X/ma-TZVP^b, as well as values of the T_1 diagnostic calculated at CCSD(T)/cc-pVTZ and for some species of the C+b and C+d reactions.

Table S3 Selected geometrical parameters of the transition states in the addition reactions

Table S4 Relative energies $\Delta E(\Delta \text{ (ESP+scaled ZPE) in kcal/mol})$ and Gibbs free energy $\Delta G(\text{kcal/mol})$ for selected stationary points in the reactions of $\text{HO}(\text{CH}_3)_2\text{CCH}_2\text{OO}(\text{A})$ with different SCI(a, b, c, d)

Table S5 Relative energies $\Delta E(\Delta \text{ (ESP+scaled ZPE) in kcal/mol})$ and Gibbs free energy $\Delta G(\text{kcal/mol})$ for selected stationary points in the reactions of $\text{HOCH}_2(\text{CH}_3)_2\text{COO}(\text{B})$ with different SCI(a, b, c, d)

Table S6 Relative energies $\Delta E(\Delta \text{ (ESP+scaled ZPE) in kcal/mol})$ and Gibbs free energy $\Delta G(\text{kcal/mol})$ for selected stationary points in the reactions of $\text{HO}(\text{CH}_3)\text{CHCH}_2\text{OO}(\text{C})$ with different SCI(a, b, c, d)

Table S7 Relative energies $\Delta E(\Delta \text{ (ESP+scaled ZPE) in kcal/mol})$ and Gibbs free energy $\Delta G(\text{kcal/mol})$ for selected stationary points in the reactions of $\text{HOCH}_2(\text{CH}_3)\text{CHOO}(\text{D})$ with different SCI(a, b, c, d)

Table S8 The Cartesian coordinates of the stationary points for the relative reactions.

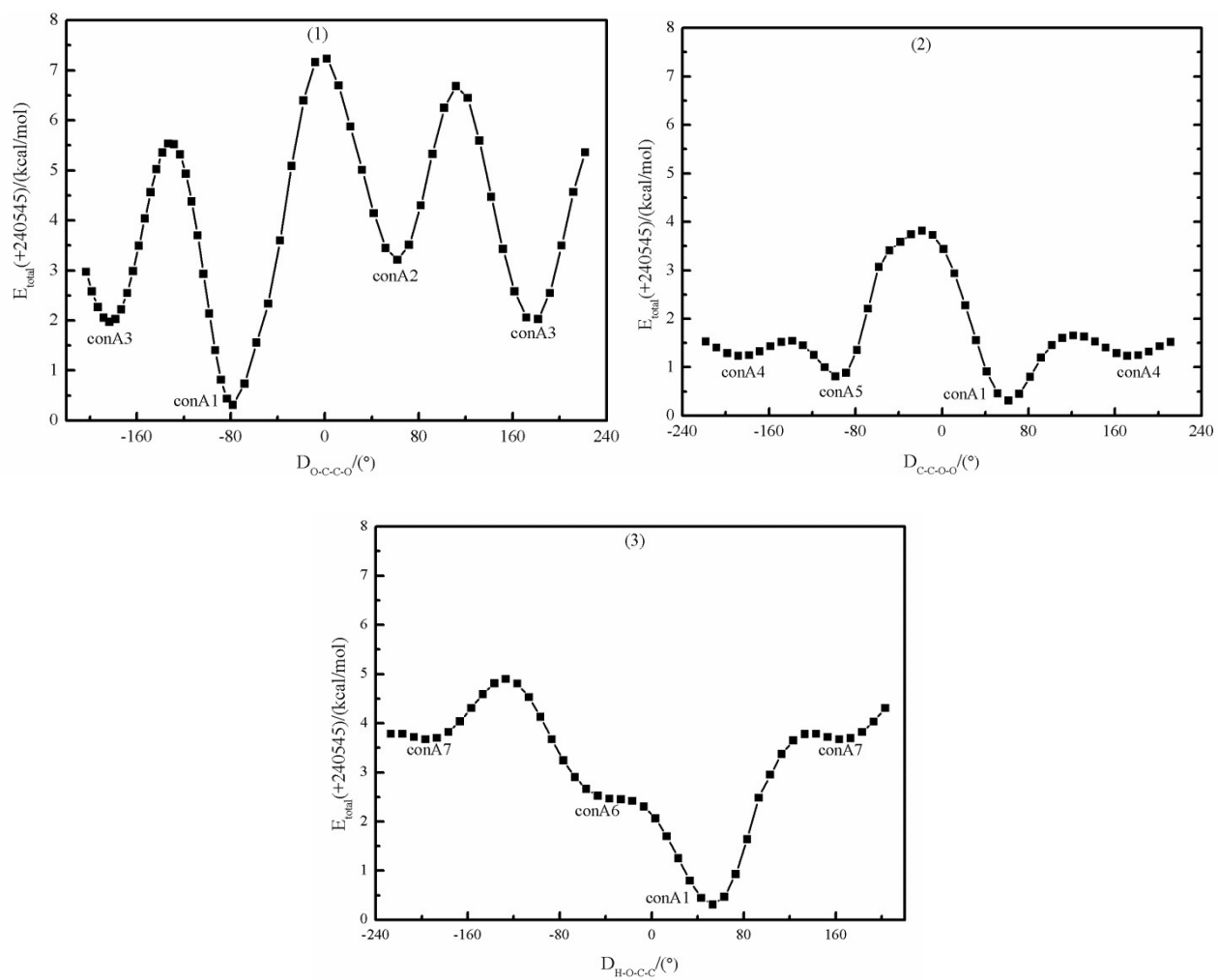


Fig.S1 Plots of the total energy against the internal torsion angles of O-C-C-O(1), C-C-O-O(2) and H-O-C-C(3) in $\text{HO}(\text{CH}_3)_2\text{CCH}_2\text{OO}$ using M06-2X/6-311+G(d,p)

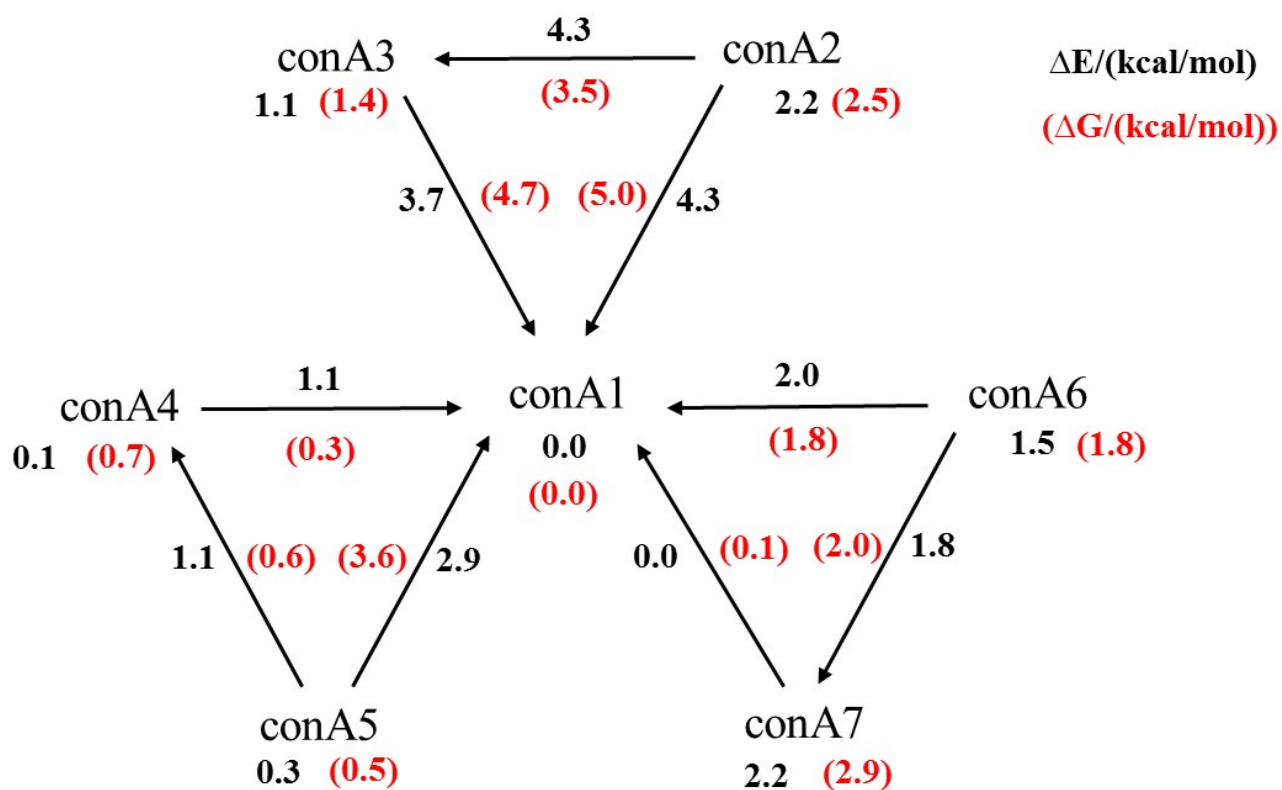


Fig.S2 The diagram for the conformations transitions of $\text{HO}(\text{CH}_3)_2\text{CCH}_2\text{OO}$. The values under the conformation denote the relative energies and that on the two sides of arrows denote the energies barriers

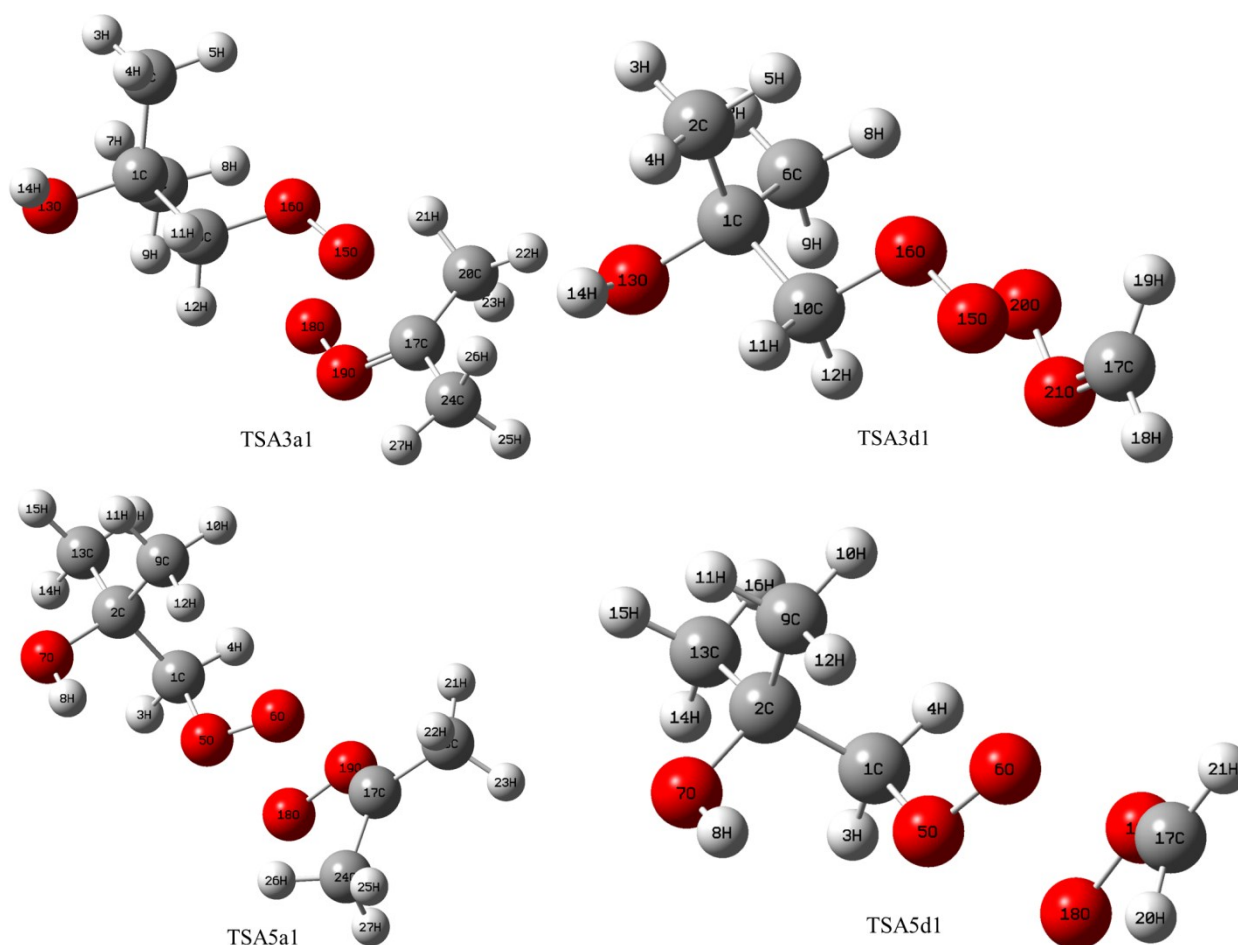


Fig.S3 Optimized geometries of the transition states.

Discussions

By rotating the internal dihedrals of O-C-C-O, C-C-O-O and H-O-C-C of the RO₂, we can obtain many conformations. Taking the conformations of HO(CH₃)₂CCH₂OO(A) as example (shown as Fig.S1), one can see that the conformation conA1 is one of the most stable conformation and this is the one that we used to do our calculations in our work.

To make a comparison, the stable conformations have been selected and the energy barriers (Fig.S2) of the conformation transition between them were calculated at M06-2X/ma-TZVP// M06-2X/6-311+G(d,p). The relative energies of conformations were calculated by the difference with respect to conformation (1). The energy barriers of the conformation transition were obtained by the energy difference between the relevant transition state and the conformation acting as a reactant.

The most stable conformations are conA1 and conA5, especially conA1, which are similar as the most stable conformations of HOCH₂CH₂OO (ref.51). In addition, conA3 is a stable conformation. Due to the difference between the conformations, the product composition would be changed, but the channel of addition reaction is a favorable pathway, from the point of the structures of RO₂. In addition, as mentioned in the paper, we focused on the addition reaction to form the oligomers. Thus, the addition reactions of (CH₃)₂COO(a) and CH₂OO(d) with conA3 and conA5 were calculated, respectively. The geometries for the transition states marked as TSA3a, TSA3d, TSA5a and TSA5d are shown in Fig.S3 and the selected geometric parameters are given in Table S3. And the Gibbs free energy barriers of the reactions are 9.3, 8.7, 6.3 and 6.1kcal/mol, while that for the addition reactions involving conA1 are 8.5 and 5.9kcal/mol as presented in our work (Entry Aa1 and Ad1). The results support the proposed SCI+RO₂ reaction as a source of low-volatility.

The energy barriers of the addition reactions involving conA3 and conA5 are close to (or higher than) that involving conA1, as well as the conformation transition barriers. From the point of energy barriers, conA3 and conA5 tend to isomerize to conA1 and then involve in the reactions. Thus, the conformations used in our work could reflect the reaction characteristics of RO₂ radicals and the general conclusion are reasonable.

Table S1.Y/X (Y=DFT, CCSD(T), X=aug-cc-pVTZ, 6-311+(d,p), cc-pVTZ, def2-TZVP, ma-TZVP) calculated electronic-energy barrier(ΔE , kcal/mol) for the formation of $\text{HOCH}_2(\text{CH}_3)\text{CHOOCH}_2\text{OO}$ based on the optimized geometries at M06-2X/6-311+(d,p)

Y	X	ΔE
CCSD(T)	aug-cc-pVTZ	2.9
	cc-pVTZ	3.4
M06-2X	aug-cc-pVTZ	1.4
	def2-TZVP	1.5
	ma-TZVP	1.6
	6-311+(d,p)	1.5
B3LYP	aug-cc-pVTZ	-0.4
	def2-TZVP	-0.4
	ma-TZVP	-0.3
BP86	aug-cc-pVTZ	-4.2
	def2-TZVP	-4.2
	ma-TZVP	-4.1
MPW1PW91	aug-cc-pVTZ	-0.4
	def2-TZVP	-0.4
	ma-TZVP	-0.3
M06-L	aug-cc-pVTZ	-2.5
	def2-TZVP	-2.6
	ma-TZVP	-2.6
TPSSH	aug-cc-pVTZ	-2.1
	def2-TZVP	-2.1
	ma-TZVP	-2.0
B97-D	aug-cc-pVTZ	-3.0
	def2-TZVP	-3.1
	ma-TZVP	-3.0
M05-2X	aug-cc-pVTZ	0.8
	def2-TZVP	1.0
	ma-TZVP	1.1
CAM-B3LYP	aug-cc-pVTZ	1.0
	def2-TZVP	1.0
	ma-TZVP	1.1
ω B97X	aug-cc-pVTZ	1.5
	def2-TZVP	1.4
	ma-TZVP	1.5

Table S2. Spin contamination at M06-2X/6-311+G(d,p)^a and M06-2X/ma-TZVP^b, as well as values of the T_1 diagnostic calculated at CCSD(T)/cc-pVTZ and for some species of the C+b and C+d reactions

Species	$\langle S^2 \rangle^a$	$\langle S^2 \rangle^b$	T_1 value	Species	$\langle S^2 \rangle^a$	$\langle S^2 \rangle^b$	T_1 value
CRCd1	0.7501	0.7500	0.030	CRCd3	0.7500	0.7500	0.028
TSCd1	0.7504	0.7505	0.032	TSCd3	0.7503	0.7503	0.038
CPCd1	0.7500	0.7500	0.019	CPCd3	0.7500	0.7500	0.025
CRCd2	0.7500	0.7500	0.028	CRCd4	0.7500	0.7500	0.028
TSCd2	0.7504	0.7504	0.031	TSCd4	0.7501	0.7501	0.034
CPCd2	0.7500	0.7500	0.019	CPCd4	0.7500	0.7500	0.017
CRCb1	0.7501	0.7501	0.029	CRCb2	0.7500	0.7500	0.027
TSCb1	0.7504	0.7505	0.029	TSCb2	0.7504	0.7504	0.030
CPCb1	0.7500	0.7500	0.018	CPCb2	0.7500	0.7500	0.018

Table S3 Selected geometrical parameters for the structures of the transition states in the addition reactions of conA3+a, conA3+d, conA5+a and conA3+d

Parameter	TSA3a1	TSA3d1	Parameter	TSA5a1	TSA5d1
H14-O13-C1-C10(°)	75.2	76.6	H8-O7-C2-C1(°)	60.1	61.9
O13-C1-C10-O16(°)	-178.6	-178.8	O7-C2-C1-O6(°)	-59.4	-60.4
C1-C10-O16-O15(°)	173.8	172.2	C2-C1-O5-O6(°)	-90.1	-91.1
O16-O15-C17(°)	104.6	102.9	O5-O6-C17(°)	103.1	101.1
O15-C17(Å)	2.145	2.226	O6-C17(Å)	2.167	2.249

Table S4 Relative energies $\Delta E(\Delta$ (ESP+scaled ZPE) in kcal/mol) and Gibbs free energy $\Delta G(\text{kcal/mol})$ for selected stationary points in the reactions of $\text{HO}(\text{CH}_3)_2\text{CCH}_2\text{OO}(\text{A})$ with different SCI(a, b, c, d)

Entry	Energy	Species				Entry	Energy	Species			
Aa1		A+a	CRAa1	TSaA1	CPAa1	Ab1		A+b	CRAb1	TSAb1	CPAb1
	ΔE	0.0	-7.3	-3.9	-40.5		ΔE	0.0	-6.2	-3.7	-42.7
	ΔG	0.0	3.4	8.5	-28.1		ΔG	0.0	4.3	8.3	-30.8
Aa2		A+a	CRAa2	TSaA2	CPAa2	Ab2		A+b	CRAb2	TSAb2	CPAb2
	ΔE	0.0	-13.4	-0.1	-41.8		ΔE	0.0	--	-1.0	-34.0
	ΔG	0.0	-2.3	12.1	-28.9		ΔG	0.0	--	10.9	-22.3
Aa3		A+a	CRAa3	TSaA3	CPAa3	Ab3		A+b	CRAb3	TSAb3	CPAb3
	ΔE	0.0	-12.3	26.0	-48.8		ΔE	0.0	-12.4	23.1	-48.6
	ΔG	0.0	-1.9	37.3	-38.5		ΔG	0.0	-1.2	34.9	-38.7
Aa4		A+a	CRAa4	TSaA4	CPAa4	Ab4		A+b	CRAb4	TSAb4	CPAb4
	ΔE	0.0	-14.6	2.8	-25.2		ΔE	0.0	-12.8	1.5	-29.1
	ΔG	0.0	-2.8	16.3	-11.7		ΔG	0.0	-1.4	14.9	-16.1
Aa5		A+a	CRAa5	TSaA5	CPAa5	Ab5		A+b	CRAb5	TSAb5	CPAb5
	ΔE	0.0	-9.3	2.7	-34.3		ΔE	0.0	-9.6	3.8	-41.4
	ΔG	0.0	0.0	15.1	-21.2		ΔG	0.0	0.9	15.7	-29.5
Aa6		A+a	CRAa6	TSaA6	CPAa6	Ab6		A+b	CRAb6	TSAb6	CPAb6
	ΔE	0.0	-9.3	13.7	-68.5		ΔE	0.0	-5.3	8.1	-2.7
	ΔG	0.0	1.9	26.3	-58.1		ΔG	0.0	4.2	20.9	10.0
Aa7		A+a	CRAa7	TSaA7	CPAa7						
	ΔE	0.0	-6.9	8.7	1.4						
	ΔG	0.0	2.7	22.2	14.8						
Ac1		A+c	CRAc1	TSAc1	CPAc1	Ad1		A+d	CRAd1	TSAd1	CPAd1
	ΔE	0.0	-7.0	-5.6	-48.0		ΔE	0.0	-5.9	-5.3	-50.5
	ΔG	0.0	2.7	6.0	-36.2		ΔG	0.0	3.5	5.9	-39.2
Ac2		A+c	CRAc2	TSAc2	CPAc2	Ad2		A+d	CRAd2	TSAd2	CPAd2
	ΔE	0.0	-13.0	-2.3	-47.5		ΔE	0.0	-10.3	-2.9	-50.5
	ΔG	0.0	-2.1	9.8	-35.2		ΔG	0.0	0.3	8.9	-39.2
Ac3		A+c	CRAc3	TSAc3	CPAc3	Ad3		A+d	CRAd3	TSAd3	CPAd3
	ΔE	0.0	-12.6	21.1	-51.6		ΔE	0.0	-11.4	17.9	-51.2
	ΔG	0.0	-1.6	32.5	-41.9		ΔG	0.0	-1.0	29.5	-41.6
Ac4		A+c	CRAc4	TSAc4	CPAc4	Ad4		A+d	CRAd4	TSAd4	CPAd4
	ΔE	0.0	-14.6	-1.5	-32.3		ΔE	0.0	-12.4	-2.1	-36.4
	ΔG	0.0	-3.1	11.7	-19.2		ΔG	0.0	-1.3	10.8	-23.9
Ac5		A+c	CRAc5	TSAc5	CPAc5	Ad5		A+d	CRAd5	TSAd5	CPAd5
	ΔE	0.0	-11.9	-4.9	-43.3		ΔE	0.0	-7.3	-0.6	-48.7
	ΔG	0.0	-1.2	7.3	-31.0		ΔG	0.0	2.5	11.0	-36.7
Ac6		A+c	CRAc6	TSAc6	CPAc6	Ad6		A+d	CRAd6	TSAd6	CPAd6
	ΔE	0.0	-6.8	5.1	-5.3		ΔE	0.0	-5.8	5.7	-8.3
	ΔG	0.0	2.9	17.9	7.3		ΔG	0.0	3.7	17.8	3.9

Table S5 Relative energies $\Delta E(\Delta$ (ESP+scaled ZPE) in kcal/mol) and Gibbs free energy $\Delta G(\text{kcal/mol})$ for selected stationary points in the reactions of $\text{HOCH}_2(\text{CH}_3)_2\text{COO}(\text{B})$ with different SCI(a, b, c, d)

Entry	Energy	Species				Entry	Energy	Species			
Ba1		B+a	CRBa1	TSBa1	CPBa1	Bb1		B+b	CRBb1	TSBb1	CPBb1
	ΔE	0.0	-8.3	-3.2	-39.2		ΔE	0.0	-7.0	-3.2	-41.4
	ΔG	0.0	3.0	9.6	-26.2		ΔG	0.0	4.1	9.2	-29.0
Ba2		B+a	CRBa2	TSBa2	CPBa2	Bb2		B+b	CRBb2	TSBb2	CPBb2
	ΔE	0.0	-13.8	-2.8	-41.5		ΔE	0.0	-12.2	-3.3	-44.8
	ΔG	0.0	-1.9	10.2	-28.3		ΔG	0.0	-1.1	9.2	-32.1
Ba3		B+a	CRBa3	TSBa3	CPBa3	Bb3		B+b	CRBb3	TSBb3	CPBb3
	ΔE	0.0	-12.8	27.7	-41.1		ΔE	0.0	-7.0	26.6	-45.8
	ΔG	0.0	-1.5	39.0	-31.8		ΔG	0.0	4.1	38.4	-35.8
Ba4		B+a	CRBa4	TSBa4	CPBa4	Bb4		B+b	CRBb4	TSBb4	CPBb4
	ΔE	0.0	-13.8	-3.1	-24.4		ΔE	0.0	-12.2	-3.8	-28.8
	ΔG	0.0	-1.9	10.5	-10.9		ΔG	0.0	-1.1	9.3	-15.8
Ba5		B+a	CRBa5	TSBa5	CPBa5	Bb5		B+b	CRBb5	TSBb5	CPBb5
	ΔE	0.0	-10.8	1.0	-37.4		ΔE	0.0	-10.0	0.5	-41.1
	ΔG	0.0	0.0	12.9	-25.0		ΔG	0.0	0.5	12.6	-28.8
Ba6		B+a	CRBa6	TSBa6	CPBa6	Bb6		B+b	CRBb6	TSBb6	CPBb6
	ΔE	0.0	-8.3	19.1	11.1		ΔE	0.0	-7.0	17.1	1.7
	ΔG	0.0	3.0	32.8	25.2		ΔG	0.0	4.0	30.1	14.5
Bc1		B+c	CRBc1	TSBc1	CPBc1	Bd1		B+d	CRBd1	TSBd1	CPBd1
	ΔE	0.0	-7.9	-5.5	-46.8		ΔE	0.0	-6.6	-4.8	-48.4
	ΔG	0.0	2.4	6.7	-34.6		ΔG	0.0	3.3	7.0	-37.3
Bc2		B+c	CRBc2	TSBc2	CPBc2	Bd2		B+d	CRBd2	TSBd2	CPBd2
	ΔE	0.0	-12.6	-5.7	-47.2		ΔE	0.0	-11.1	-8.4	-50.1
	ΔG	0.0	-1.9	6.9	-34.4		ΔG	0.0	-0.7	3.4	-38.1
Bc3		B+c	CRBc3	TSBc3	CPBc3	Bd3		B+d	CRBd3	TSBd3	CPBd3
	ΔE	0.0	-7.9	24.2	15.7		ΔE	0.0	-11.5	19.2	-49.5
	ΔG	0.0	2.4	35.9	27.9		ΔG	0.0	-0.8	30.0	-39.5
Bc4		B+c	CRBc4	TSBc4	CPBc4	Bd4		B+d	CRBd4	TSBd4	CPBd4
	ΔE	0.0	-12.6	-6.7	-31.9		ΔE	0.0	-10.7	-7.3	-36.5
	ΔG	0.0	-1.9	6.5	-18.7		ΔG	0.0	-0.5	5.3	-24.0
Bc5		B+c	CRBc5	TSBc5	CPBc5	Bd5		B+d	CRBd5	TSBd5	CPBd5
	ΔE	0.0	-13.6	-8.1	-47.3		ΔE	0.0	-10.8	-0.8	-47.6
	ΔG	0.0	-2.3	4.3	-35.3		ΔG	0.0	0.4	10.6	-36.4
Bc6		B+c	CRBc6	TSBc6	CPBc6	Bd6		B+d	CRBd6	TSBd6	CPBd6
	ΔE	0.0	-13.9	5.4	1.8		ΔE	0.0	-6.3	7.9	-5.8
	ΔG	0.0	-2.6	19.1	14.6		ΔG	0.0	3.3	20.0	6.4

Table S6 Relative energies ΔE (Δ (ESP+scaled ZPE) in kcal/mol) and Gibbs free energy ΔG (kcal/mol) for selected stationary points in the reactions of $\text{HO}(\text{CH}_3)\text{CHCH}_2\text{OO}(\text{C})$ with different SCI(a, b, c, d)

Entry	Energy	Species				Entry	Energy	Species			
Ca1		C+a	CRCa1	TSCa1	CPCa1	Cb1		C+b	CRCb1	TSCb1	CPCb1
	ΔE	0.0	-7.4	-3.9	-40.5		ΔE	0.0	-6.3	-3.7	-42.6
	ΔG	0.0	3.5	8.6	-28.0		ΔG	0.0	4.2	8.4	-30.7
Ca2		C+a	CRCa2	TSCa2	CPCa2	Cb2		C+b	CRCb2	TSCb2	CPCb2
	ΔE	0.0	-12.5	-0.7	-40.6		ΔE	0.0	-10.6	-1.0	-43.8
	ΔG	0.0	-1.3	11.9	-28.7		ΔG	0.0	0.4	11.3	-32.2
Ca3		C+a	CRCa3	TSCa3	CPCa3	Cb3		C+b	CRCb3	TSCb3	CPCb3
	ΔE	0.0	-12.0	25.9	-46.8		ΔE	0.0	-12.5	23.3	-48.4
	ΔG	0.0	-1.1	37.3	-37.2		ΔG	0.0	-1.2	34.7	-39.0
Ca4		C+a	CRCa4	TSCa4	CPCa4	Cb4		C+b	CRCb4	TSCb4	CPCb4
	ΔE	0.0	-14.3	3.2	-24.5		ΔE	0.0	-12.5	2.2	-28.4
	ΔG	0.0	-2.3	16.9	-11.0		ΔG	0.0	-1.0	15.6	-15.4
Ca5		C+a	CRCa5	TSCa5	CPCa5	Cb5		C+b	CRCb5	TSCb5	CPCb5
	ΔE	0.0	-13.8	0.3	-36.9		ΔE	0.0	-9.3	3.0	-44.2
	ΔG	0.0	-2.0	13.3	-23.9		ΔG	0.0	1.2	14.7	-31.7
Ca6		C+a	CRCa6	TSCa6	CPCa6	Cb6		C+b	CRCb6	TSCb6	CPCb6
	ΔE	0.0	-8.1	13.6	-33.5		ΔE	0.0	-5.4	8.2	-2.4
	ΔG	0.0	3.5	26.0	-20.1		ΔG	0.0	4.2	20.9	10.2
Ca7		C+a	CRCa7	TSCa7	CPCa7						
	ΔE	0.0	-7.0	8.9	1.8						
	ΔG	0.0	2.9	22.4	15.0						
Cc1		C+c	CRCc1	TSCc1	CPCc1	Cd1		C+d	CRCd1	TSCd1	CPCd1
	ΔE	0.0	-7.2	-5.7	-47.9		ΔE	0.0	-5.9	-5.3	-50.3
	ΔG	0.0	2.5	6.1	-36.0		ΔG	0.0	3.4	6.1	-39.0
Cc2		C+c	CRCc2	TSCc2	CPCc2	Cd2		C+d	CRCd2	TSCd2	CPCd2
	ΔE	0.0	-13.6	-7.4	-48.3		ΔE	0.0	-9.7	-2.9	-49.8
	ΔG	0.0	-2.6	4.7	-35.4		ΔG	0.0	0.9	9.0	-38.7
Cc3		C+c	CRCc3	TSCc3	CPCc3	Cd3		C+d	CRCd3	TSCd3	CPCd3
	ΔE	0.0	-13.4	20.9	-52.1		ΔE	0.0	-11.3	17.8	-51.7
	ΔG	0.0	-2.7	32.0	-42.1		ΔG	0.0	-0.3	29.0	-42.6
Cc4		C+c	CRCc4	TSCc4	CPCc4	Cd4		C+d	CRCd4	TSCd4	CPCd4
	ΔE	0.0	-14.3	-0.2	-31.6		ΔE	0.0	-10.0	-1.1	-32.7
	ΔG	0.0	-2.9	13.0	-18.5		ΔG	0.0	0.7	12.1	-20.3
Cc5		C+c	CRCc5	TSCc5	CPCc5	Cd5		C+d	CRCd5	TSCd5	CPCd5
	ΔE	0.0	-12.1	-5.2	-44.9		ΔE	0.0	-10.0	-2.5	-50.7
	ΔG	0.0	-1.4	7.2	-32.4		ΔG	0.0	0.7	9.1	-39.3
Cc6		C+c	CRCc6	TSCc6	CPCc6	Cd6		C+d	CRCd6	TSCd6	CPCd6
	ΔE	0.0	-7.0	5.2	-4.9		ΔE	0.0	-5.9	5.7	-7.9
	ΔG	0.0	2.9	17.9	7.7		ΔG	0.0	4.0	17.7	4.2

Table S7 Relative energies $\Delta E(\Delta$ (ESP+scaled ZPE) in kcal/mol) and Gibbs free energy ΔG (kcal/mol) for selected stationary points in the reactions of $\text{HOCH}_2(\text{CH}_3)\text{CHOO}(\text{D})$ with different SCI(a, b, c, d)

Entry	Energy	Species				Entry	Energy	Species			
Da1		D+a	CRDa1	TSDa1	CPDa1	Db1		D+b	CRDb1	TSDb1	CPDb1
	ΔE	0.0	-7.7	-2.6	-39.5		ΔE	0.0	-5.9	-2.7	-41.8
	ΔG	0.0	3.3	9.9	-26.4		ΔG	0.0	4.7	9.4	-29.6
Da2		D+a	CRDa2	TSDa2	CPDa2	Db2		D+b	CRDb2	TSDb2	CPDb2
	ΔE	0.0	-13.9	-3.1	-42.0		ΔE	0.0	-12.3	-3.6	-45.2
	ΔG	0.0	-2.1	9.8	-28.8		ΔG	0.0	-1.2	8.9	-32.5
Da3		D+a	CRDa3	TSDa3	CPDa3	Db3		D+b	CRDb3	TSDb3	CPDb3
	ΔE	0.0	-13.9	26.5	-47.3		ΔE	0.0	-11.0	24.5	-40.9
	ΔG	0.0	-2.1	37.9	-36.8		ΔG	0.0	0.0	35.3	-32.0
Da4		D+a	CRDa4	TSDa4	CPDa4	Db4		D+b	CRDb4	TSDb4	CPDb4
	ΔE	0.0	-13.9	-2.9	-24.6		ΔE	0.0	-12.3	-3.5	-28.8
	ΔG	0.0	-2.1	10.7	-11.1		ΔG	0.0	-1.2	9.6	-15.9
Da5		D+a	CRDa5	TSDa5	CPDa5	Db5		D+b	CRDb5	TSDb5	CPDb5
	ΔE	0.0	-11.1	0.7	-37.7		ΔE	0.0	-10.4	0.2	-41.4
	ΔG	0.0	-0.1	12.6	-25.5		ΔG	0.0	0.1	12.5	-29.1
Da6		D+a	CRDa6	TSDa6	CPDa6	Db6		D+b	CRDb6	TSDb6	CPDb6
	ΔE	0.0	-7.7	16.6	5.7		ΔE	0.0	-6.7	14.2	2.0
	ΔG	0.0	3.3	29.8	18.9		ΔG	0.0	2.7	26.8	14.4
Dc1		D+c	CRDc1	TSDc1	CPDc1	Dd1		D+d	CRDd1	TSDd1	CPDd1
	ΔE	0.0	-7.4	-4.7	-47.1		ΔE	0.0	-6.0	-4.4	-49.7
	ΔG	0.0	2.8	7.2	-34.8		ΔG	0.0	3.9	7.1	-38.0
Dc2		D+c	CRDc2	TSDc2	CPDc2	Dd2		D+d	CRDd2	TSDd2	CPDd2
	ΔE	0.0	-12.6	-5.8	-47.7		ΔE	0.0	-11.9	-7.9	-50.0
	ΔG	0.0	-1.6	6.7	-35.0		ΔG	0.0	-1.2	3.6	-37.7
Dc3		D+c	CRDc3	TSDc3	CPDc3	Dd3		D+d	CRDd3	TSDd3	CPDd3
	ΔE	0.0	-7.4	23.7	15.1		ΔE	0.0	-11.9	18.9	-49.8
	ΔG	0.0	2.8	35.6	27.2		ΔG	0.0	-1.2	29.6	-39.7
Dc4		D+c	CRDc4	TSDc4	CPDc4	Dd4		D+d	CRDd4	TSDd4	CPDd4
	ΔE	0.0	-12.6	-6.4	-32.0		ΔE	0.0	-10.7	-6.9	-36.6
	ΔG	0.0	-1.6	6.8	-18.9		ΔG	0.0	-0.5	5.7	-24.1
Dc5		D+c	CRDc5	TSDc5	CPDc5	Dd5		D+d	CRDd5	TSDd5	CPDd5
	ΔE	0.0	-13.7	-8.1	-47.3		ΔE	0.0	-10.9	-0.9	-47.8
	ΔG	0.0	-2.4	3.8	-35.3		ΔG	0.0	0.3	10.4	-36.7
Dc6		D+c	CRDc6	TSDc6	CPDc6	Dd6		D+d	CRDd6	TSDd6	CPDd6
	ΔE	0.0	-7.8	8.1	-4.8		ΔE	0.0	-6.3	6.8	-6.1
	ΔG	0.0	2.3	20.8	8.0		ΔG	0.0	3.7	18.6	5.8

Table S8 The Cartesian coordinates of the stationary points for the relative reactions.

HO(CH ₃) ₂ CCH ₂ OO				(CH ₃) ₂ COO			
C	-0.695514	-0.044106	-0.024207	C	-0.372188	0.019353	-0.000002
C	-0.656753	-0.877078	1.256320	C	-1.755491	-0.526938	0.000000
H	-1.483667	-1.588370	1.240089	H	-2.292115	-0.164160	-0.880647
H	0.277559	-1.436610	1.332333	H	-1.737825	-1.614967	-0.000028
H	-0.750719	-0.244583	2.142681	H	-2.292090	-0.164209	0.880683
C	-2.040265	0.654780	-0.186489	C	-0.054208	1.460564	0.000000
H	-2.813960	-0.103119	-0.316569	H	-0.956741	2.067772	-0.000002
H	-2.280271	1.258880	0.690575	H	0.578374	1.674247	0.867311
H	-2.036402	1.291232	-1.073949	H	0.578378	1.674247	-0.867308
C	0.392774	1.035559	-0.016946	O	1.842628	-0.332221	0.000001
H	0.522666	1.446377	-1.020283	O	0.559039	-0.816630	-0.000001
H	0.166402	1.826534	0.698452				
O	-0.557618	-0.875469	-1.165480				
H	0.347412	-1.206210	-1.191111				
O	2.137534	-0.396144	-0.345540				
O	1.676276	0.539231	0.426735				
CRAa1				TSAa1			
C	-2.412428	-0.018453	-0.102586	C	2.324017	0.077013	-0.081860
C	-2.979678	-0.441781	1.251837	C	2.844313	0.302561	1.336841
H	-3.973140	-0.867734	1.103926	H	3.761955	0.891065	1.291042
H	-2.347220	-1.198130	1.721105	H	2.112008	0.847720	1.935534
H	-3.056783	0.410886	1.931138	H	3.056110	-0.646839	1.835267
C	-3.341278	0.964214	-0.805308	C	3.373552	-0.602404	-0.952753
H	-4.282998	0.459626	-1.026817	H	4.229539	0.065946	-1.058425
H	-3.543790	1.832856	-0.176013	H	3.709732	-1.539764	-0.505244
H	-2.901615	1.297170	-1.747491	H	2.971942	-0.802522	-1.948253
C	-1.048039	0.658024	0.048750	C	1.069870	-0.801699	-0.081365
H	-0.545504	0.761924	-0.912649	H	0.585976	-0.782886	-1.058875
H	-1.112601	1.628950	0.537426	H	1.292875	-1.828666	0.207952
O	-2.314228	-1.141889	-0.968149	O	2.050008	1.323776	-0.708789
H	-1.567735	-1.681098	-0.684633	H	1.238218	1.674996	-0.325484
O	0.214862	-1.218352	0.390902	O	-0.419782	0.796517	0.595190
O	-0.169598	-0.097208	0.921032	O	0.108014	-0.374775	0.905433
C	2.660737	-0.083968	-0.196028	C	-2.391383	0.240903	-0.162335
C	3.012736	-1.313306	-0.951555	C	-2.658747	1.549883	-0.813380
H	2.600487	-2.175659	-0.421851	H	-2.350837	2.352738	-0.142532
H	2.611524	-1.272777	-1.962184	H	-2.118973	1.624585	-1.755682
H	4.099752	-1.425706	-0.981835	H	-3.732987	1.649930	-0.996215
C	3.045156	0.153396	1.207805	C	-2.944666	-0.147478	1.153858
H	3.618778	-0.680953	1.604899	H	-3.258386	0.735528	1.706350
H	3.603059	1.093261	1.259848	H	-3.796871	-0.813632	0.978422
H	2.130731	0.324904	1.783573	H	-2.203519	-0.723401	1.707434
O	1.647463	1.922190	-0.121151	O	-1.731179	-1.886284	-0.391968
O	2.001979	0.783225	-0.815876	O	-1.906877	-0.661417	-0.933032
CPAa1				CRAa2			

C	-2.238911	-0.044663	-0.078846
C	-2.621839	-0.922308	1.110182
H	-3.475865	-1.544477	0.837552
H	-1.789468	-1.570008	1.392618
H	-2.887515	-0.314816	1.979103
C	-3.414233	0.805285	-0.544246
H	-4.201572	0.148795	-0.917623
H	-3.813900	1.406595	0.274862
H	-3.107794	1.466097	-1.358230
C	-1.080608	0.891228	0.282083
H	-0.668336	1.344289	-0.624213
H	-1.422499	1.676100	0.962019
O	-1.893940	-0.855128	-1.198541
H	-1.068488	-1.304622	-0.992383
O	0.566886	-0.718545	0.207545
O	-0.039635	0.272645	1.034568
C	1.907822	-0.370932	-0.033774
C	2.447650	-1.481814	-0.907391
H	2.386211	-2.428894	-0.372093
H	1.866558	-1.545133	-1.828026
H	3.488029	-1.272158	-1.155110
C	2.692883	-0.116750	1.231683
H	2.726217	-1.047631	1.798679
H	3.708677	0.187380	0.977523
H	2.225633	0.659613	1.830274
O	1.955149	1.941545	-0.281178
O	1.896231	0.806807	-0.907780
TSAa2			
C	2.102630	0.126765	-0.025013
C	2.461984	-0.126522	1.438865
H	3.167108	0.640519	1.763014
H	1.577717	-0.074255	2.075168
H	2.923445	-1.109194	1.567984
C	3.362899	0.193636	-0.884901
H	3.935200	1.075687	-0.595213
H	3.982924	-0.695049	-0.750385
H	3.099376	0.294166	-1.940479
C	1.227748	-1.001239	-0.597236
H	0.678956	-0.618993	-1.464538
H	1.828832	-1.866576	-0.880611
O	1.483147	1.386035	-0.195720
H	0.609012	1.410994	0.216333
O	-0.473012	-0.629103	0.884336
O	0.277212	-1.562386	0.326770
C	-2.206807	-0.083024	-0.185751
C	-2.412520	-1.304377	-1.009598
H	-3.460997	-1.364196	-1.315299

C	-2.191963	-0.084849	-0.087944
C	-2.153312	-0.958696	1.167024
H	-2.633085	-1.914389	0.947746
H	-1.120672	-1.154617	1.463235
H	-2.682528	-0.483095	1.997114
C	-3.627439	0.147758	-0.550811
H	-4.081544	-0.817229	-0.779777
H	-4.222932	0.645663	0.218252
H	-3.637260	0.751165	-1.461098
C	-1.576293	1.291374	0.187263
H	-1.503272	1.876268	-0.729033
H	-2.120468	1.833293	0.965144
O	-1.510553	-0.694268	-1.155088
H	-0.697490	-1.132626	-0.819253
O	0.665448	1.761495	-0.001509
O	-0.226964	1.126564	0.691318
C	2.486763	-0.239757	-0.093423
C	3.424588	0.650203	-0.822127
H	4.452372	0.339840	-0.616125
H	3.229365	0.624017	-1.891992
H	3.294727	1.665754	-0.441583
C	2.494494	-0.404869	1.372545
H	3.248497	0.229689	1.832481
H	1.492682	-0.174525	1.744182
H	2.662206	-1.461802	1.599950
O	0.791550	-1.714414	-0.121304
O	1.677815	-0.883677	-0.796467
CPAa2			
C	2.131894	0.022226	0.087470
C	2.392566	-1.194439	0.972835
H	3.160440	-0.943024	1.706449
H	1.484245	-1.487982	1.501256
H	2.733577	-2.046819	0.379499
C	3.416302	0.507898	-0.574629
H	4.091900	0.880566	0.196651
H	3.910158	-0.300169	-1.118247
H	3.203037	1.328498	-1.263473
C	1.119884	-0.304892	-1.017079
H	0.731617	0.624130	-1.445824
H	1.593337	-0.901980	-1.800972
O	1.677537	1.121407	0.868342
H	0.758304	0.963014	1.106914
O	-0.629501	-0.534659	0.482649
O	0.044918	-1.152241	-0.614081
C	-1.932955	-0.192088	0.113207
C	-2.679067	-1.285509	-0.615753
H	-3.701706	-0.959247	-0.805789

H	-1.781122	-1.279453	-1.896899	H	-2.190669	-1.517446	-1.559582
H	-2.175096	-2.187863	-0.414928	H	-2.695406	-2.178892	0.008946
C	-2.963771	0.201827	1.055334	C	-2.595858	0.289881	1.385820
H	-3.398562	-0.714936	1.448100	H	-2.690412	-0.544232	2.080479
H	-2.312160	0.670361	1.791788	H	-2.000280	1.079948	1.842085
H	-3.747692	0.927981	0.813975	H	-3.586568	0.678716	1.149261
O	-1.469934	2.026876	-0.111915	O	-1.216450	1.935214	-0.391401
O	-1.612404	0.884629	-0.799497	O	-1.866275	0.913586	-0.856619
CRAa3				TSAa3			
C	-2.186934	0.122263	-0.082701	C	2.253282	0.211298	-0.063048
C	-3.140296	-0.912379	-0.668722	C	2.433089	1.151137	1.130187
H	-3.806993	-0.418488	-1.377447	H	2.956285	2.050551	0.801184
H	-2.580426	-1.681784	-1.201818	H	1.464176	1.441763	1.540738
H	-3.741214	-1.381715	0.114009	H	3.015054	0.674049	1.923033
C	-2.951133	1.207314	0.680974	C	3.597458	-0.166489	-0.669223
H	-3.643945	1.696915	-0.005243	H	4.092189	0.736799	-1.030167
H	-3.519661	0.793280	1.518109	H	4.241468	-0.646842	0.070483
H	-2.257820	1.961650	1.062879	H	3.455922	-0.840185	-1.516462
C	-1.213966	-0.524716	0.903739	C	1.515271	-1.059414	0.347441
H	-0.499429	0.205540	1.284745	H	1.290513	-1.662909	-0.533917
H	-1.741661	-1.025568	1.720061	H	2.076531	-1.643636	1.082104
O	-1.484724	0.683041	-1.167372	O	1.518838	0.858974	-1.092267
H	-0.762111	1.244711	-0.823816	H	0.582983	0.851443	-0.855978
O	0.739976	-1.689191	0.706741	O	-0.698226	-1.567443	0.705961
O	-0.447071	-1.544502	0.214314	O	0.267722	-0.650947	0.934107
C	2.492374	0.241127	-0.197666	C	-2.509328	0.570257	-0.211876
C	3.208649	-0.794713	-0.982336	C	-2.339997	1.971434	0.244610
H	2.761100	-0.909849	-1.967109	H	-1.685988	2.521904	-0.434650
H	4.263800	-0.523494	-1.068788	H	-3.304577	2.478719	0.291619
H	3.143631	-1.738828	-0.435022	H	-1.889172	2.006656	1.246147
C	2.870359	0.631299	1.174839	C	-3.578272	-0.368330	0.190493
H	3.766898	0.106529	1.496791	H	-4.444424	0.193502	0.538908
H	2.996457	1.716656	1.208599	H	-3.869738	-1.006249	-0.648720
H	2.026870	0.402154	1.831564	H	-3.239122	-1.033819	0.994023
O	0.810837	1.730296	-0.030414	O	-1.273061	-1.236967	-0.820827
O	1.521005	0.786746	-0.764053	O	-1.436663	0.098744	-0.886954
CPAa3				CRAa4			
C	-2.117010	0.306095	0.102953	O	0.767727	-1.915019	-0.296926
C	-1.783609	1.542591	-0.728336	C	1.965850	0.192090	0.065083
H	-2.047577	2.439644	-0.165221	C	3.048912	-0.536707	0.848659
H	-0.714090	1.573805	-0.943781	H	2.619620	-1.373566	1.401105
H	-2.337447	1.543039	-1.670670	H	3.829869	-0.912104	0.183017
C	-3.606730	0.230319	0.410810	H	3.496889	0.155634	1.563039
H	-3.915309	1.140014	0.927813	C	2.535743	1.382152	-0.708654
H	-4.196085	0.128601	-0.503857	H	3.005113	2.069622	-0.002692
H	-3.811992	-0.619862	1.064716	H	3.285927	1.064703	-1.437603
C	-1.715373	-0.967742	-0.646847	H	1.733518	1.913719	-1.227438

H	-2.009369	-1.853981	-0.076714	C	1.302036	-0.746017	-0.954282
H	-2.176525	-1.015289	-1.637280	H	0.479078	-0.243771	-1.466384
O	-1.447932	0.341548	1.348402	H	2.029319	-1.137731	-1.667737
H	-0.536351	0.636055	1.211127	O	1.001019	0.623135	0.997924
O	0.266873	-1.781912	0.219767	O	-0.468601	-1.771966	0.059377
O	-0.312451	-1.035435	-0.898168	H	0.346938	1.182709	0.518705
C	2.262644	0.809976	0.128723	C	-2.345792	0.225594	0.056811
C	2.339976	0.950105	-1.369760	O	-0.892172	1.894395	-0.433757
H	1.539509	1.590454	-1.734766	O	-1.772231	0.890587	-0.835248
H	3.313516	1.336800	-1.677804	C	-2.129443	0.506883	1.488760
H	2.221079	-0.048821	-1.799518	H	-2.141071	1.587392	1.646922
C	3.484783	0.266059	0.823186	H	-2.871488	-0.008107	2.095293
H	4.258884	1.039520	0.828811	H	-1.122389	0.159103	1.751770
H	3.241018	-0.012954	1.846130	C	-3.262005	-0.840999	-0.419468
H	3.879230	-0.593010	0.277106	H	-2.955401	-1.786744	0.033625
O	1.490254	-1.901343	0.049252	H	-4.277089	-0.617636	-0.079988
O	1.266183	1.113587	0.746940	H	-3.236593	-0.920251	-1.504060
TSAa4				CPAa4			
O	0.221767	-1.697927	-0.268673	O	0.083258	-1.406783	-0.389352
C	1.856842	0.062380	0.065837	C	2.028523	0.021789	0.082727
C	2.809693	-0.840224	0.839735	C	2.474424	-0.985294	1.139105
H	2.246526	-1.598424	1.385790	H	1.609616	-1.331128	1.705085
H	3.522939	-1.332068	0.173687	H	2.949891	-1.848934	0.668452
H	3.360750	-0.235715	1.561725	H	3.182969	-0.512440	1.820544
C	2.606128	1.124905	-0.755309	C	3.238210	0.639366	-0.658958
H	3.237641	1.706387	-0.081979	H	3.859465	1.193202	0.044639
H	3.238734	0.658385	-1.514719	H	3.826607	-0.171755	-1.091687
H	1.894222	1.798722	-1.235921	H	2.905803	1.312515	-1.450296
C	1.034739	-0.774161	-0.978090	C	1.096440	-0.602436	-0.965397
H	0.432318	-0.106820	-1.591317	H	0.659412	0.184363	-1.588246
H	1.683406	-1.402725	-1.588447	H	1.650848	-1.306421	-1.591650
O	0.977340	0.645039	0.951251	O	1.422520	1.118682	0.669416
O	-0.623306	-1.107760	0.573639	O	-0.607532	-0.642406	0.591138
H	0.264649	1.331207	0.429513	H	-0.192960	1.814201	-0.049939
C	-1.903352	0.046577	-0.020946	C	-1.846981	-0.161092	0.067194
O	-0.679298	1.980299	-0.196242	O	-1.123416	2.025158	-0.252106
O	-1.363979	0.903421	-0.834643	O	-1.596169	0.848667	-0.888036
C	-2.298038	0.488151	1.354205	C	-2.585199	0.347168	1.292233
H	-2.961451	1.348173	1.235251	H	-3.437743	0.941138	0.962272
H	-2.813949	-0.318744	1.871414	H	-2.933291	-0.500999	1.881583
H	-1.426274	0.806226	1.921031	H	-1.937814	0.972814	1.903286
C	-2.768221	-0.934360	-0.761483	C	-2.605176	-1.230601	-0.696132
H	-2.964947	-1.809093	-0.145135	H	-2.643440	-2.139259	-0.095040
H	-3.713011	-0.436672	-0.993992	H	-3.617719	-0.877422	-0.890717
H	-2.288487	-1.233016	-1.693251	H	-2.112370	-1.449829	-1.641401
CRAa5				TSAa5			
C	1.410763	0.922588	-0.065366	C	0.895650	0.946160	-0.002890

C	1. 071050	1. 093014	1. 415494
H	0. 185980	1. 726626	1. 509656
H	0. 851123	0. 125272	1. 870777
H	1. 895355	1. 562884	1. 958025
C	1. 655241	2. 266270	-0. 740204
H	0. 757057	2. 880182	-0. 651476
H	2. 488224	2. 797916	-0. 274706
H	1. 869782	2. 124326	-1. 801584
C	2. 671897	0. 068661	-0. 237272
H	2. 867340	-0. 120518	-1. 293311
H	3. 532720	0. 531581	0. 249561
O	0. 335873	0. 309711	-0. 748389
H	0. 058790	-0. 494354	-0. 250947
O	2. 066330	-2. 123332	-0. 394618
O	2. 516015	-1. 207660	0. 411815
C	-2. 633345	-0. 089207	-0. 025438
C	-3. 555492	1. 044685	0. 243097
H	-3. 300946	1. 866320	-0. 432295
H	-4. 581328	0. 742473	0. 018885
H	-3. 476629	1. 373826	1. 276967
C	-2. 529395	-0. 745101	-1. 343293
H	-1. 570004	-0. 456978	-1. 789127
H	-2. 490783	-1. 826846	-1. 197197
H	-3. 350255	-0. 441740	-1. 990018
O	-1. 020395	-1. 484956	0. 704631
O	-1. 932915	-0. 463316	0. 940897

CPAa5

C	0. 841381	0. 967989	0. 042346
C	0. 750796	0. 999712	1. 571277
H	-0. 165864	1. 469618	1. 920076
H	0. 800056	0. 000863	2. 004241
H	1. 595927	1. 580994	1. 949406
C	0. 839496	2. 381139	-0. 542218
H	-0. 032029	2. 942159	-0. 204927
H	1. 731097	2. 927261	-0. 223735
H	0. 824676	2. 333661	-1. 632751
C	2. 152643	0. 290665	-0. 365681
H	2. 234443	0. 212448	-1. 449570
H	3. 012989	0. 803620	0. 067583
O	-0. 124048	0. 146008	-0. 621912
H	-0. 074340	-1. 778797	0. 838322
O	1. 950506	-1. 957614	-0. 735528
O	2. 176406	-1. 048831	0. 167582
C	-1. 474793	0. 013174	-0. 227729
C	-2. 225575	1. 326490	-0. 051936
H	-2. 128671	1. 917111	-0. 963638
H	-3. 280144	1. 110031	0. 119478

C	0. 771372	1. 050756	1. 518568
H	-0. 207249	1. 447948	1. 792957
H	0. 880970	0. 070593	1. 984959
H	1. 536738	1. 723509	1. 913032
C	0. 680803	2. 297655	-0. 675726
H	-0. 280704	2. 717019	-0. 374984
H	1. 459760	3. 006758	-0. 385410
H	0. 690120	2. 184826	-1. 761931
C	2. 291174	0. 444307	-0. 391513
H	2. 372367	0. 322663	-1. 471968
H	3. 066154	1. 109740	-0. 005365
O	-0. 030920	0. 016612	-0. 548786
H	-0. 062221	-0. 907711	0. 073476
O	2. 300647	-1. 825231	-0. 595049
O	2. 549608	-0. 836385	0. 211707
C	-1. 972078	-0. 178093	-0. 074578
C	-2. 641527	1. 154364	-0. 009027
H	-2. 396033	1. 727291	-0. 902554
H	-3. 723256	0. 991791	0. 003169
H	-2. 351914	1. 696902	0. 888466
C	-2. 202989	-1. 020950	-1. 287923
H	-2. 024302	-0. 435322	-2. 186872
H	-1. 582382	-1. 910592	-1. 280755
H	-3. 258460	-1. 314501	-1. 255626
O	-0. 737778	-1. 733045	0. 921907
O	-1. 713311	-0. 696464	1. 073715

CRAa6

C	1. 355770	-0. 795849	-0. 023334
C	2. 651142	-1. 163911	-0. 742750
H	2. 483242	-2. 054445	-1. 350610
H	2. 981315	-0. 354281	-1. 397463
H	3. 449978	-1. 370720	-0. 026694
C	0. 837055	-1. 950280	0. 824973
H	0. 525884	-2. 761473	0. 163776
H	1. 621531	-2. 321683	1. 487217
H	-0. 015307	-1. 631883	1. 427839
C	1. 544943	0. 407292	0. 905152
H	2. 201970	0. 155057	1. 737921
O	0. 335545	-0. 518101	-0. 987769
H	0. 583531	0. 300472	-1. 435081
O	1. 557651	1. 998576	-0. 736000
O	2. 234529	1. 502898	0. 253694
C	-2. 268325	0. 036118	-0. 223956
C	-2. 763047	-0. 984174	-1. 182344
H	-2. 028047	-1. 075078	-1. 986065
H	-2. 884494	-1. 946627	-0. 689263
H	-3. 710799	-0. 657038	-1. 616617

H	-1.855557	1.903381	0.794058	C	-2.076620	1.457942	-0.575519
C	-2.109489	-0.850661	-1.305028	H	-2.339261	1.642123	-1.615423
H	-2.168508	-0.283495	-2.234510	H	-2.684731	2.063436	0.103704
H	-1.511307	-1.744014	-1.470213	H	-1.040050	1.738498	-0.372087
H	-3.112002	-1.141939	-0.989848	O	-1.521003	0.562277	1.834041
O	-1.024219	-1.917176	0.982700	O	-2.032503	-0.362167	0.936744
O	-1.543334	-0.600382	1.050888	H	0.575977	0.762956	1.269834
TSAa6				CPAa6			
C	1.927171	0.050688	0.180326	C	2.076291	0.205346	0.228321
C	2.822167	-1.193671	0.116889	C	2.510119	-0.545132	1.476868
H	3.483203	-1.196978	0.985997	H	2.942255	0.154487	2.194183
H	2.210960	-2.098698	0.137657	H	1.653323	-1.047697	1.933616
H	3.427942	-1.199523	-0.792215	H	3.245649	-1.307904	1.221046
C	2.746202	1.332651	0.156357	C	3.229870	0.958104	-0.427707
H	3.398209	1.350222	1.031370	H	3.613438	1.700504	0.274211
H	3.363140	1.392604	-0.742774	H	4.028055	0.265475	-0.698356
H	2.083623	2.199066	0.200652	H	2.889278	1.477156	-1.326779
C	0.992374	0.057514	-1.045005	C	1.514147	-0.757048	-0.818869
H	1.520364	0.229541	-1.984709	H	0.771184	-0.301810	-1.507091
O	1.207998	0.058618	1.399363	O	1.087119	1.188728	0.537013
H	0.558857	-0.653436	1.319246	H	0.399440	0.753518	1.057819
O	-0.457039	-1.475299	-0.149906	O	-1.013786	-0.805970	0.609157
O	0.223696	-1.052979	-1.244022	O	1.863421	-1.897596	-0.938245
C	-2.107124	0.121638	0.254509	C	-2.139549	-0.182943	0.165802
C	-2.618438	-0.635569	1.423395	C	-3.206345	-0.303170	1.264842
H	-2.476752	-1.698877	1.226285	H	-3.393823	-1.354737	1.473660
H	-2.100070	-0.338023	2.332678	H	-2.863457	0.198311	2.169591
H	-3.690852	-0.440999	1.521799	H	-4.116502	0.179477	0.909852
C	-2.651153	-0.083551	-1.108496	C	-2.575107	-0.848990	-1.147188
H	-3.154665	-1.045352	-1.161234	H	-2.877148	-1.875888	-0.948173
H	-3.361934	0.731662	-1.288059	H	-3.412620	-0.277614	-1.548749
H	-1.874017	-0.013923	-1.863872	H	-1.760844	-0.838097	-1.868200
O	-0.859982	1.830945	-0.552277	O	-1.143752	1.481006	-1.115064
O	-1.385293	1.116439	0.552740	O	-1.955300	1.218262	0.020815
H	0.109748	1.062712	-0.837861	H	-0.276410	1.642384	-0.698460
CRAa7				TSAa7			
C	2.382934	0.074615	0.060453	C	-2.163330	0.056572	-0.035220
C	3.058545	-1.288096	-0.093295	C	-2.436774	0.194409	1.462366
H	3.994945	-1.284611	0.466542	H	-3.469767	-0.095959	1.659884
H	2.425793	-2.085466	0.301998	H	-1.775020	-0.459885	2.031855
H	3.273887	-1.507159	-1.142283	H	-2.288995	1.223713	1.801241
C	3.301275	1.199874	-0.402135	C	-3.147563	0.886653	-0.853312
H	4.171432	1.232702	0.255326	H	-4.146883	0.470143	-0.719597
H	3.638759	1.037941	-1.427739	H	-3.153799	1.930252	-0.531322
H	2.786574	2.160359	-0.337976	H	-2.900248	0.835754	-1.916049
C	1.098409	0.160068	-0.768602	C	-0.751118	0.541176	-0.384950
H	0.492254	1.030449	-0.500235	H	-0.469145	0.188112	-1.380369

H	1.315452	0.153750	-1.837131	H	-0.692389	1.629038	-0.314910
O	2.113748	0.336568	1.430007	O	-2.341955	-1.281353	-0.455856
H	1.354717	-0.193631	1.695467	H	-1.570939	-1.777567	-0.146853
O	-0.195362	-1.131918	0.608283	O	0.227361	-1.314182	0.566537
O	0.257809	-1.015144	-0.600579	O	0.235447	0.058543	0.557176
C	-2.691723	0.007701	-0.026255	C	1.996903	0.477779	-0.006862
C	-3.216354	-1.282965	-0.540173	C	1.975944	1.950934	-0.253617
H	-4.282490	-1.366885	-0.316959	H	3.008880	2.308164	-0.273437
H	-3.045097	-1.368946	-1.611264	H	1.500823	2.184576	-1.205107
H	-2.696807	-2.091553	-0.017768	H	1.461272	2.453939	0.565991
C	-2.808455	0.439572	1.379232	C	2.699150	-0.060711	1.191228
H	-3.349574	-0.293293	1.973423	H	2.625299	0.651867	2.011299
H	-1.797052	0.603411	1.763822	H	2.286941	-1.027332	1.468355
H	-3.290107	1.421568	1.403846	H	3.748967	-0.196810	0.914024
O	-1.547870	1.911988	-0.375687	O	2.015440	-1.566870	-0.893224
O	-2.095883	0.734351	-0.852577	O	1.963172	-0.220997	-1.109983
CPAa7							
C	-2.134200	-0.014348	-0.060695				
C	-2.300524	0.615583	1.323342				
H	-3.323193	0.447568	1.663912				
H	-1.614399	0.147500	2.030878				
H	-2.110903	1.693097	1.299917				
C	-3.155401	0.542743	-1.048880				
H	-4.148280	0.222523	-0.730751				
H	-3.129725	1.634225	-1.082228				
H	-2.978221	0.143614	-2.050185				
C	-0.747438	0.293645	-0.631135				
H	-0.507181	-0.367498	-1.464280				
H	-0.675645	1.344738	-0.906833				
O	-2.350766	-1.405009	-0.009466				
H	-1.551921	-1.772834	0.406874				
O	0.226835	-1.313377	0.807627				
O	0.273400	0.077053	0.399154				
C	1.656485	0.469538	0.077334				
C	1.675378	1.934315	-0.305079		syn-CH ₃ CH00		
H	2.708433	2.279437	-0.273537	C	0.473119	0.704225	0.000000
H	1.295368	2.090812	-1.313736	C	1.350949	-0.473954	0.000000
H	1.088918	2.511681	0.410970	H	2.400443	-0.192055	-0.000001
C	2.504704	0.129750	1.273888	H	1.098664	-1.092353	0.868261
H	2.189981	0.761324	2.105511	H	1.098662	-1.092354	-0.868260
H	2.384279	-0.915577	1.536415	O	-1.273766	-0.677214	0.000000
H	3.545700	0.344081	1.029753	O	-0.769918	0.584421	0.000000
O	2.567816	-1.409482	-0.892883	H	0.807295	1.737472	0.000000
O	2.011811	-0.248191	-1.108848				
TSAb1					CRAb1		
C	2.106537	0.034278	0.039109	C	2.155898	0.075771	0.016217
C	3.115560	1.175565	0.073645	C	3.050752	1.308371	-0.031822

H	4.051432	0.804837	0.494537	H	4.045724	1.032981	0.321150
H	3.307239	1.562268	-0.929141	H	3.130279	1.697584	-1.048582
H	2.753355	1.986328	0.709096	H	2.659861	2.089499	0.623161
C	0.757543	0.612127	-0.398827	C	0.731271	0.521551	-0.321967
H	0.337426	1.245008	0.384296	H	0.298500	1.112170	0.485580
H	0.836798	1.169212	-1.332239	H	0.677751	1.076918	-1.257189
O	2.025151	-0.448670	1.373467	O	2.221959	-0.395433	1.355252
H	1.248214	-1.015172	1.440302	H	1.509557	-1.029670	1.492105
O	-0.571143	-1.082247	0.376869	O	-0.380486	-1.288728	0.527966
O	-0.202248	-0.421989	-0.705008	O	-0.145241	-0.609984	-0.554580
C	-2.559407	-0.219197	0.715588	C	-2.875835	-0.168663	0.651165
C	-3.216683	-0.905510	-0.410287	C	-3.342550	-0.787225	-0.595848
H	-3.446032	-1.934552	-0.145773	H	-3.820337	-1.744529	-0.406699
H	-4.132321	-0.356561	-0.657730	H	-4.020363	-0.086876	-1.095466
H	-2.571988	-0.854097	-1.288747	H	-2.482520	-0.890281	-1.265261
O	-2.153628	1.509392	-0.626682	O	-2.089973	1.537959	-0.553954
O	-2.156898	0.985971	0.613726	O	-2.298066	0.938756	0.657786
H	-2.564518	-0.569296	1.740913	H	-2.994561	-0.596735	1.642117
C	2.563951	-1.080333	-0.900431	C	2.647698	-1.001226	-0.950043
H	2.628068	-0.725704	-1.932286	H	2.596402	-0.655622	-1.985612
H	3.547662	-1.431024	-0.584685	H	3.682887	-1.248184	-0.710017
H	1.869786	-1.922479	-0.870298	H	2.047862	-1.909289	-0.861258
TSAb2				CPAb1			
C	-1.941438	0.105387	0.122393	C	2.034772	0.048014	0.027134
C	-2.893217	0.222296	1.306662	C	3.146249	1.041448	-0.286494
H	-3.691889	0.919196	1.048532	H	4.015513	0.807762	0.329916
H	-3.333801	-0.745110	1.554814	H	3.434380	0.990544	-1.338437
H	-2.369099	0.612926	2.181462	H	2.825910	2.058781	-0.050718
C	-0.751079	-0.748928	0.562829	C	0.769781	0.491579	-0.715141
H	-0.141863	-0.219872	1.294669	H	0.365763	1.400327	-0.259238
H	-1.076118	-1.702047	0.981650	H	0.991585	0.677275	-1.769465
O	-1.512703	1.435007	-0.154789	O	1.841670	0.132815	1.435439
H	-0.849004	1.378576	-0.850944	H	1.057795	-0.378161	1.659333
O	0.527607	-0.147428	-1.261527	O	-0.707526	-0.765957	0.532571
O	0.100073	-1.160173	-0.532950	O	-0.244695	-0.506912	-0.793787
C	2.496334	0.401212	-0.546300	C	-2.058066	-0.422695	0.612801
C	2.095716	1.624479	0.184814	C	-2.934123	-1.054000	-0.438584
H	1.963426	2.447109	-0.515304	H	-2.855319	-2.136633	-0.339730
H	1.183236	1.471586	0.756305	H	-3.969440	-0.751754	-0.279966
H	2.892061	1.866569	0.898613	H	-2.618610	-0.753581	-1.433516
O	2.263809	-0.820192	1.298662	O	-2.322050	1.561172	-0.533774
O	2.723610	-0.705910	0.046956	O	-2.170424	1.026934	0.641362
H	2.904382	0.411766	-1.549520	H	-2.331095	-0.709153	1.629577
C	-2.644808	-0.493791	-1.093813	C	2.428737	-1.372793	-0.368514
H	-2.978314	-1.514313	-0.890128	H	2.577981	-1.454414	-1.448178
H	-3.512941	0.118725	-1.342173	H	3.355914	-1.643095	0.139430
H	-1.978298	-0.519491	-1.958307	H	1.649716	-2.081627	-0.080697

CRAb3				CPAb2			
C	1. 647212	-0. 270298	0. 133484	C	2. 133163	-0. 020427	-0. 004069
C	2. 961692	-0. 540368	0. 862556	C	3. 380213	0. 535179	-0. 679561
H	3. 037338	-1. 607590	1. 076762	H	4. 227759	0. 431865	-0. 000607
H	3. 824702	-0. 240902	0. 262088	H	3. 599839	-0. 002819	-1. 603869
H	2. 980507	-0. 000865	1. 811637	H	3. 252469	1. 596704	-0. 904086
C	1. 585402	1. 231473	-0. 172564	C	0. 926071	0. 275735	-0. 901644
H	1. 633660	1. 818776	0. 744501	H	0. 714273	1. 350477	-0. 890894
H	2. 357183	1. 532741	-0. 883492	H	1. 124822	-0. 050097	-1. 926322
O	0. 581273	-0. 562350	1. 010644	O	2. 023100	0. 692118	1. 224253
H	-0. 072744	-1. 160541	0. 583016	H	1. 210902	0. 411320	1. 657129
O	-0. 532867	2. 062519	0. 008514	O	-0. 658294	-0. 063185	0. 735196
O	0. 328198	1. 543362	-0. 810630	O	-0. 247307	-0. 457517	-0. 574287
C	-2. 443563	0. 191912	-0. 258425	C	-1. 968794	0. 414066	0. 671735
C	-2. 571358	0. 198081	1. 204588	C	-2. 194001	1. 535663	-0. 311270
H	-3. 149664	1. 056511	1. 536109	H	-1. 572318	2. 380643	-0. 013370
H	-3. 013222	-0. 750642	1. 521681	H	-1. 940323	1. 221304	-1. 320456
H	-1. 560099	0. 230253	1. 629465	H	-3. 241117	1. 837553	-0. 288123
O	-1. 472212	-1. 830688	-0. 148889	O	-3. 167060	-0. 903648	-0. 790967
O	-1. 936910	-0. 754686	-0. 891167	O	-2. 860878	-0. 709915	0. 456819
H	-2. 781539	0. 998222	-0. 903075	H	-2. 177954	0. 700792	1. 703630
C	1. 554959	-1. 085969	-1. 154865	C	2. 258722	-1. 518564	0. 258314
H	2. 409426	-0. 875636	-1. 802624	H	2. 345864	-2. 075502	-0. 677853
H	1. 553300	-2. 150789	-0. 913773	H	3. 146203	-1. 704009	0. 865504
H	0. 635236	-0. 863788	-1. 698720	H	1. 380849	-1. 890974	0. 790171
CPAb3				TSAb3			
C	-1. 702510	-0. 199393	-0. 120365	C	2. 025834	-0. 161317	0. 068646
C	-3. 038655	0. 106435	-0. 787713	C	3. 532976	0. 038455	0. 185671
H	-3. 589366	-0. 826488	-0. 915318	H	3. 974790	-0. 857239	0. 624396
H	-3. 637994	0. 791280	-0. 184009	H	3. 986484	0. 214926	-0. 791828
H	-2. 877185	0. 544388	-1. 774824	H	3. 755269	0. 882815	0. 842200
C	-0. 935177	1. 123493	0. 008222	C	1. 423591	1. 156699	-0. 430188
H	-0. 735949	1. 518218	-0. 991620	H	1. 487216	1. 919661	0. 348721
H	-1. 493626	1. 846704	0. 611242	H	1. 949773	1. 491781	-1. 327290
O	-1. 005833	-1. 064248	-0. 996237	O	1. 583173	-0. 455940	1. 383859
H	-0. 302725	-1. 513159	-0. 501557	H	0. 634154	-0. 625793	1. 355374
O	1. 084996	2. 061113	0. 719249	O	-0. 805583	1. 249764	0. 148568
O	0. 304438	0. 832232	0. 653502	O	0. 058985	1. 072521	-0. 872183
C	2. 244044	-1. 598334	0. 250939	C	-2. 976013	-0. 589943	-0. 559650
C	2. 497516	-0. 717017	-0. 930846	C	-3. 797802	0. 223984	0. 355449
H	3. 222695	-1. 214225	-1. 583142	H	-4. 809667	0. 303578	-0. 038296
H	1. 575675	-0. 511894	-1. 473466	H	-3. 833142	-0. 227088	1. 354124
H	2. 954216	0. 218719	-0. 599317	H	-3. 378496	1. 228503	0. 474108
O	1. 514482	2. 396817	-0. 408208	O	-1. 197208	-0. 233741	0. 766848
O	1. 187625	-2. 125340	0. 500032	O	-1. 728489	-0. 962734	-0. 231854
H	3. 106038	-1. 775523	0. 921282	H	-3. 292669	-1. 056075	-1. 479525
C	-1. 904354	-0. 852493	1. 246149	C	1. 692296	-1. 308708	-0. 882506

H	-2.437749	-0.181232	1.923616	H	2.042150	-1.093148	-1.895462
H	-2.489751	-1.765625	1.123871	H	2.177535	-2.220028	-0.528612
H	-0.945132	-1.111906	1.698232	H	0.614293	-1.475873	-0.924348
TSAb4				CRAb4			
O	0.220195	-1.629754	-0.768843	O	0.771573	-1.873871	-0.494517
C	1.570671	0.156711	0.186173	C	1.611727	0.339604	0.138610
C	2.279446	1.441789	-0.272757	C	2.040663	1.670597	-0.479972
H	2.757031	1.902313	0.593364	H	2.361000	2.343743	0.317230
H	3.044830	1.223066	-1.021460	H	2.870675	1.538134	-1.178587
H	1.552142	2.143139	-0.686183	H	1.200688	2.132984	-1.005443
C	0.965070	-0.469097	-1.121306	C	1.154985	-0.578846	-1.004439
H	0.339047	0.265109	-1.623032	H	0.295580	-0.155430	-1.527570
H	1.743079	-0.853875	-1.780305	H	1.971632	-0.785506	-1.698502
O	0.540999	0.435042	1.058626	O	0.541079	0.532138	1.037389
O	-0.774941	-1.404237	0.076867	O	-0.490340	-1.958296	-0.217599
H	-0.170113	1.123106	0.602303	H	-0.142802	1.076246	0.588575
C	-2.078297	-0.280935	-0.306491	C	-2.566537	-0.246518	-0.155105
H	-2.562461	-0.949841	-1.018134	H	-3.025995	-1.075400	-0.687656
O	-1.148031	1.792197	-0.054522	O	-1.466736	1.709102	-0.353293
O	-1.644860	0.771723	-0.923054	O	-2.106794	0.619477	-0.923586
C	-2.634474	-0.189432	1.077125	C	-2.514207	-0.149706	1.308747
H	-3.050037	-1.150228	1.374934	H	-3.184543	-0.874827	1.763486
H	-1.864540	0.123714	1.778417	H	-1.480493	-0.343934	1.624201
H	-3.417362	0.571841	1.057935	H	-2.747168	0.876391	1.603934
C	2.529441	-0.818513	0.855900	C	2.744334	-0.301472	0.928843
H	3.355817	-1.084438	0.192380	H	3.607677	-0.497011	0.288403
H	2.935356	-0.351603	1.754539	H	3.045142	0.374533	1.730529
H	1.999183	-1.725208	1.150780	H	2.412561	-1.240272	1.374140
CRAb5				CPAb4			
C	-1.646182	-0.510666	-0.188275	O	-0.055692	-1.315497	0.905805
C	-1.807036	-1.132477	1.197887	C	-1.784619	0.078246	-0.153441
H	-1.561237	-2.194799	1.147262	C	-2.960053	0.999880	0.251907
H	-1.131495	-0.659414	1.914258	H	-3.462389	1.371842	-0.640855
H	-2.833051	-1.025583	1.558367	H	-3.668060	0.414448	0.841221
C	-2.579305	-1.161323	-1.202265	H	-2.604689	1.845704	0.841883
H	-2.377018	-2.232826	-1.238020	C	-1.005895	-0.285131	1.117880
H	-3.627569	-1.010107	-0.933390	H	-0.523016	0.609189	1.522866
H	-2.402769	-0.746323	-2.196900	H	-1.678856	-0.715583	1.864005
C	-1.961928	0.989945	-0.148156	O	-1.015902	0.887766	-0.971354
H	-1.834790	1.440010	-1.133181	O	0.773256	-0.963929	-0.196025
H	-2.961762	1.178964	0.248116	H	0.646407	1.636848	-0.413277
O	-0.325296	-0.683028	-0.657365	C	1.994778	-0.448026	0.296233
H	0.290858	-0.639298	0.107763	H	2.305763	-1.039700	1.160578
O	-0.057650	2.210431	0.135256	O	1.589650	1.768301	-0.204371
O	-1.060674	1.665396	0.752180	O	1.816002	0.833903	0.840921
C	3.031367	-0.466061	-0.533604	C	2.974882	-0.507289	-0.853520
C	2.502513	0.856598	-0.877419	H	3.205011	-1.547340	-1.081574

H	1.469025	0.738332	-1.232902
H	2.415737	1.453244	0.036093
H	3.115855	1.336629	-1.635537
O	1.619410	-0.574840	1.202117
O	2.622154	-1.132887	0.437173
H	3.818084	-0.975498	-1.085826

CPAb5

C	0.995095	0.778093	0.073713
C	0.977718	0.662379	1.599124
H	0.302068	1.392939	2.045566
H	0.671961	-0.329968	1.925341
H	1.982510	0.864926	1.977515
C	1.367785	2.192250	-0.367451
H	0.603340	2.895677	-0.029016
H	2.323879	2.501039	0.060920
H	1.425856	2.248445	-1.456199
C	2.005602	-0.205271	-0.515895
H	1.906699	-0.256571	-1.600441
H	3.022871	0.050440	-0.216416
O	-0.233335	0.409699	-0.563145
H	-1.056527	-1.818717	0.139940
O	0.933965	-2.211358	-0.693802
O	1.781428	-1.526941	0.012866
C	-1.453115	0.693048	0.064459
C	-2.511997	0.814046	-1.007958
H	-2.303371	1.687895	-1.625764
H	-2.506938	-0.076247	-1.634062
H	-3.492372	0.920053	-0.543123
O	-1.957285	-1.534619	0.365921
O	-1.746062	-0.297789	1.028727
H	-1.396187	1.600883	0.675257

TSAb6

C	2.012517	-0.024181	0.041090
C	2.300376	1.381445	-0.485504
H	3.300534	1.396121	-0.921046
H	1.580185	1.655753	-1.257973
H	2.253319	2.124230	0.315648
C	3.072096	-0.463997	1.046172
H	4.026006	-0.557238	0.525291
H	3.180220	0.262281	1.854494
H	2.819817	-1.440188	1.466144
C	0.653888	-0.083448	0.747588
H	0.338076	-1.122698	0.866257
H	0.687889	0.434730	1.709160
O	2.058766	-0.971051	-1.009007
H	1.248267	-0.867874	-1.525648
O	-0.534690	0.046511	-1.221423

H	2.556801	-0.025533	-1.735353
H	3.885988	0.016828	-0.565524
C	-2.275842	-1.152774	-0.910187
H	-2.882230	-1.785581	-0.258070
H	-2.875292	-0.841373	-1.766689
H	-1.423459	-1.733521	-1.262253

TSAb5

C	0.871810	0.859440	0.048430
C	0.781117	0.770571	1.571769
H	-0.048967	1.376822	1.939260
H	0.620832	-0.260068	1.892034
H	1.703426	1.143978	2.022690
C	0.914919	2.305059	-0.430913
H	-0.003039	2.816818	-0.133491
H	1.758593	2.838674	0.011515
H	0.995551	2.346946	-1.519125
C	2.129681	0.150695	-0.461991
H	2.116784	0.080965	-1.550369
H	3.027088	0.661906	-0.109231
O	-0.248882	0.244020	-0.586415
H	-0.436497	-0.721154	-0.194194
O	1.561835	-2.045237	-0.635353
O	2.237478	-1.183053	0.066223
C	-2.115307	0.448871	0.086966
C	-2.695910	0.045893	-1.222001
H	-2.411488	0.762218	-1.989804
H	-2.392560	-0.959988	-1.494715
H	-3.783943	0.076750	-1.092574
O	-1.377819	-1.569025	0.614056
O	-1.952422	-0.338634	1.074373
H	-2.225171	1.488404	0.401370

CRAb6

C	-2.159900	-0.127392	-0.000396
C	-2.456751	0.420260	-1.396297
H	-3.531503	0.580469	-1.493436
H	-1.951498	1.374746	-1.557462
H	-2.131048	-0.277756	-2.171826
C	-2.946966	-1.405073	0.266810
H	-4.011326	-1.165270	0.273205
H	-2.756141	-2.154179	-0.503948
H	-2.683870	-1.817828	1.242678
C	-0.674738	-0.456323	0.166562
H	-0.410743	-0.619469	1.211431
H	-0.371256	-1.320317	-0.423607
O	-2.581030	0.797237	0.992398
H	-1.960437	1.534338	1.003432
O	0.052080	1.708564	0.338551

O	-0.373260	0.615132	0.003617	O	0.182245	0.604426	-0.330356
C	-2.094143	0.312975	0.843100	C	3.029941	-0.033179	-0.718468
C	-2.878325	1.229287	-0.015757	C	3.359467	0.883276	0.379777
H	-2.729799	2.258171	0.305213	H	3.936980	1.732912	0.025465
H	-2.589883	1.091201	-1.056581	H	2.425546	1.213424	0.847446
H	-3.932777	0.954094	0.085536	H	3.891681	0.318147	1.151784
O	-2.379209	-1.332875	-0.610087	O	2.078728	-1.399086	0.766429
O	-2.113612	-0.966553	0.674868	O	2.440062	-1.114509	-0.520659
H	-1.844267	0.569611	1.869633	H	3.270611	0.138311	-1.763986
CPAb6							
C	-1.991961	-0.065260	-0.019332				
C	-2.202357	1.443161	-0.157745				
H	-3.206230	1.688906	0.191203				
H	-1.478168	1.980193	0.457015				
H	-2.101745	1.769779	-1.196944				
C	-3.057022	-0.847161	-0.782468				
H	-4.021029	-0.665235	-0.305855				
H	-3.114379	-0.534228	-1.827318				
H	-2.854921	-1.919497	-0.734021				
C	-0.634726	-0.479807	-0.588709				
H	-0.353108	-1.476160	-0.247674				
H	-0.614596	-0.400539	-1.678290				
O	-2.094320	-0.464270	1.328350				
H	-1.271657	-0.166478	1.753584				
O	0.501823	0.380223	1.326625		anti-CH3CHOO		
O	0.399926	0.445669	-0.119526	C	-0.371228	0.403123	-0.000001
C	1.702624	0.280994	-0.730332	C	-1.765058	-0.095145	0.000000
C	2.633236	1.334479	-0.211149	H	-2.291086	0.283295	-0.880345
H	2.232743	2.311483	-0.480814	H	-1.780189	-1.183377	-0.000017
H	2.711781	1.252321	0.868731	H	-2.291073	0.283265	0.880366
H	3.610130	1.199754	-0.676173	O	1.843381	0.073213	0.000001
O	2.850602	-1.222182	0.557772	O	0.566391	-0.409372	-0.000001
O	2.122935	-1.061033	-0.515928	H	-0.098112	1.458224	0.000000
H	1.514677	0.334008	-1.803378				
CRAc1					TSAc1		
C	-2.193158	-0.021718	-0.128773	C	-2.056989	-0.088736	-0.170513
C	-3.158925	1.056800	-0.604829	C	-3.006194	0.601602	-1.142036
H	-4.082559	0.579158	-0.935313	H	-3.846674	-0.063794	-1.345321
H	-3.390546	1.759613	0.197672	H	-3.387123	1.535139	-0.723577
H	-2.734609	1.602305	-1.449958	H	-2.500185	0.810726	-2.086746
C	-0.853350	0.654328	0.171228	C	-0.812072	0.791258	-0.024330
H	-0.352598	0.980017	-0.739952	H	-0.224108	0.784860	-0.942879
H	-0.953647	1.494466	0.856935	H	-1.063122	1.814083	0.255016
O	-2.058853	-0.925646	-1.217310	O	-1.714498	-1.326814	-0.780060
H	-1.293306	-1.487871	-1.055506	H	-0.961820	-1.695726	-0.304466
O	0.465331	-1.215074	0.122433	O	0.610496	-0.803342	0.787294
O	0.052925	-0.236886	0.870061	O	0.039035	0.348060	1.055086

C	2.889217	-0.045510	0.258509
C	3.602495	-1.151344	-0.414223
H	3.049488	-2.077142	-0.237193
H	3.683287	-0.962299	-1.482773
H	4.597391	-1.267448	0.023301
O	1.818579	1.921727	0.258707
O	2.492658	0.922962	-0.408005
H	2.676308	-0.019096	1.326697
C	-2.739920	-0.748779	1.099330
H	-2.843283	-0.067656	1.947758
H	-3.718830	-1.166109	0.858899
H	-2.080366	-1.567282	1.394886

CPAc1

C	-2.013967	-0.029625	-0.143357
C	-3.141984	0.846534	-0.672614
H	-3.906168	0.209635	-1.120493
H	-3.595125	1.431918	0.129957
H	-2.768610	1.523690	-1.444094
C	-0.877090	0.882500	0.329445
H	-0.390133	1.352020	-0.530458
H	-1.261232	1.654088	1.001863
O	-1.593517	-0.812955	-1.256314
H	-0.800072	-1.292319	-0.999097
O	0.760494	-0.747640	0.347117
O	0.095545	0.232780	1.144226
C	2.097077	-0.378347	0.255821
C	2.839156	-1.508528	-0.407857
H	2.753158	-2.409116	0.198898
H	2.418575	-1.695511	-1.396688
H	3.889524	-1.239383	-0.512541
O	2.360637	1.887031	0.063275
O	2.197814	0.783878	-0.606244
H	2.478783	-0.068512	1.230041
C	-2.494018	-0.933833	0.988960
H	-2.819004	-0.346392	1.851399
H	-3.330644	-1.538827	0.635762
H	-1.691868	-1.598236	1.316593

TSAc2

C	1.797151	0.110593	-0.147546
C	2.943986	0.096238	-1.156011
H	3.527107	1.009370	-1.032190
H	3.595024	-0.767263	-1.005371
H	2.554336	0.080796	-2.176731
C	0.896574	-1.092304	-0.480679
H	0.249708	-0.826912	-1.323518
H	1.484367	-1.980105	-0.718266
O	1.121482	1.328015	-0.384312

C	2.671515	-0.185464	0.151327
C	3.078129	-1.452242	-0.494487
H	2.685072	-2.290116	0.082635
H	2.705131	-1.494173	-1.516356
H	4.169638	-1.525981	-0.499998
O	1.961546	1.923378	0.057240
O	2.279724	0.766165	-0.577628
H	2.827729	0.043705	1.201380
C	-2.727920	-0.331146	1.180515
H	-2.993704	0.612310	1.663878
H	-3.634453	-0.918772	1.027969
H	-2.065609	-0.883463	1.850146

CRAc2

C	1.968387	0.084043	-0.096820
C	3.371147	-0.102938	-0.667342
H	3.802357	0.878802	-0.867906
H	4.020878	-0.637973	0.029686
H	3.323678	-0.652117	-1.609990
C	1.399180	-1.316167	0.173609
H	1.338352	-1.895949	-0.747034
H	1.965389	-1.842191	0.945545
O	1.198000	0.709903	-1.091325
H	0.420806	1.142557	-0.676434
O	-0.849692	-1.588621	-0.158390
O	0.052194	-1.208643	0.692133
C	-2.603821	0.217751	0.301347
C	-3.759872	-0.501961	-0.269693
H	-3.938624	-0.190538	-1.296644
H	-3.550239	-1.572742	-0.227818
H	-4.644401	-0.307962	0.342850
O	-0.961325	1.730755	0.240702
O	-2.040227	1.094488	-0.367326
H	-2.218727	0.045867	1.305474
C	2.000949	0.911503	1.188603
H	0.992435	1.044866	1.584944
H	2.626532	0.433902	1.947325
H	2.414139	1.897029	0.965422

CPAc2

C	1.910685	0.011960	0.009598
C	3.119262	0.520515	-0.767831
H	3.881079	0.850281	-0.060013
H	3.539065	-0.263587	-1.401277
H	2.840973	1.375239	-1.388686
C	0.780488	-0.257853	-0.990914
H	0.356640	0.692217	-1.330907
H	1.157892	-0.820976	-1.848653
O	1.557458	1.077481	0.883077

H	0.364212	1.437759	0.208387	H	0.692101	0.888629	1.260065
O	-0.638716	-0.550193	1.116390	O	-0.803571	-0.537646	0.674250
O	0.059967	-1.540861	0.603012	O	-0.253439	-1.116522	-0.510802
C	-2.436201	-0.042359	0.101415	C	-2.115026	-0.146613	0.430101
C	-2.735195	-1.213347	-0.753976	C	-2.988826	-1.175496	-0.237807
H	-2.355201	-1.051822	-1.762028	H	-2.628570	-1.380453	-1.243955
H	-2.269641	-2.103556	-0.322746	H	-2.963746	-2.095299	0.346097
H	-3.814063	-1.381508	-0.793598	H	-4.012556	-0.805007	-0.285744
O	-1.684791	2.029552	0.353530	O	-1.522924	2.027998	0.138298
O	-1.950414	0.993920	-0.459231	O	-2.124279	1.024855	-0.429852
H	-2.797832	0.080417	1.116481	H	-2.472475	0.174041	1.410681
C	2.332345	0.033243	1.281653	C	2.253491	-1.245819	0.804705
H	1.527706	0.144018	2.009982	H	1.405851	-1.558735	1.416610
H	2.834556	-0.920527	1.463833	H	2.516997	-2.072034	0.139379
H	3.047545	0.843499	1.431517	H	3.100330	-1.033806	1.459536
CRAc3				TSAc3			
C	1.911689	-0.073596	-0.060966	C	1.978485	0.300478	-0.021211
C	3.414707	0.087443	0.142299	C	3.492340	0.374662	0.145792
H	3.866943	-0.901679	0.226862	H	3.890048	1.102557	-0.562735
H	3.878186	0.616871	-0.693889	H	3.765304	0.680011	1.158025
H	3.611810	0.632059	1.067888	H	3.947203	-0.594286	-0.072065
C	1.313392	1.336476	-0.193010	C	1.467951	-0.814939	0.896728
H	1.515411	1.929958	0.698368	H	1.793093	-1.788809	0.524735
H	1.649876	1.840144	-1.101360	H	1.834681	-0.659628	1.914178
O	1.399346	-0.676853	1.098779	O	1.766317	-0.028019	-1.384261
H	0.526440	-1.077844	0.904346	H	0.815925	-0.071076	-1.545071
O	-0.743551	1.467269	0.794346	O	-0.555108	-1.591962	0.118499
O	-0.123018	1.239649	-0.321582	O	0.040978	-0.852629	1.070593
C	-2.609235	-0.258657	0.285636	C	-2.998725	-0.061843	-0.162591
C	-3.491767	0.620017	-0.508374	C	-3.830118	0.911331	0.576066
H	-3.294002	1.654151	-0.218110	H	-4.615284	0.385481	1.119432
H	-3.310511	0.486162	-1.572796	H	-3.218598	1.466332	1.290793
H	-4.535638	0.397814	-0.271817	H	-4.311062	1.637074	-0.091521
O	-1.036517	-1.832911	0.509859	O	-1.035462	-0.557986	-1.114877
O	-1.848757	-1.042927	-0.297783	O	-1.796478	0.389259	-0.551251
H	-2.591827	-0.278155	1.373956	H	-3.315624	-1.002002	-0.591327
C	1.609374	-0.905850	-1.307506	C	1.319631	1.635239	0.321453
H	2.050519	-0.450269	-2.197996	H	1.493137	1.901524	1.367451
H	2.030348	-1.904356	-1.177721	H	1.740141	2.415788	-0.315037
H	0.533456	-1.013681	-1.455162	H	0.241658	1.588162	0.156100
CPAc3				CRAc4			
C	-1.807472	-0.193991	-0.045904	O	-0.516293	-1.817557	0.580814
C	-3.219010	0.140120	-0.518133	C	-1.762911	0.163839	-0.149420
H	-3.783583	-0.787865	-0.616483	C	-2.422493	1.421873	0.418274
H	-3.731963	0.794741	0.189442	H	-2.874019	1.983816	-0.401089
H	-3.187184	0.623405	-1.497019	H	-3.201742	1.173733	1.143241
C	-1.018359	1.122215	0.003148	H	-1.675181	2.056181	0.903267

H	-0.875434	1.483505	-1.019263	C	-1.099048	-0.572546	1.023532
H	-1.531946	1.870174	0.614856	H	-0.304136	0.036001	1.459670
O	-1.250819	-1.043715	-1.029952	H	-1.833422	-0.865666	1.775775
H	-0.523310	-1.556924	-0.646088	O	-0.779898	0.510148	-1.101351
O	1.062391	2.049734	0.476742	O	0.725592	-1.703945	0.238720
O	0.258585	0.843470	0.582943	H	-0.187815	1.172776	-0.680770
C	1.904622	-1.210703	-0.415691	C	2.284726	0.256269	-0.461194
C	3.241849	-0.871977	0.162703	H	1.580086	0.229234	-1.292162
H	3.226093	0.171543	0.490044	O	1.011535	1.955552	0.302499
H	3.476203	-1.527321	0.999393	O	2.107247	1.105040	0.426154
H	4.006909	-0.950224	-0.614083	C	3.442164	-0.655050	-0.359876
O	1.651021	2.097037	-0.629469	H	3.078708	-1.683841	-0.414224
O	1.180944	-2.073586	0.020975	H	4.101328	-0.489164	-1.216451
H	1.582788	-0.610056	-1.285144	H	3.984818	-0.490890	0.568701
C	-1.828871	-0.876231	1.320841	C	-2.773581	-0.728614	-0.855804
H	-2.235582	-0.208542	2.084136	H	-3.557283	-1.054973	-0.168028
H	-2.454164	-1.769221	1.265675	H	-3.231317	-0.169154	-1.672984
H	-0.822364	-1.173337	1.622838	H	-2.278616	-1.606579	-1.272704
TSAc4				CPAc4			
O	0.101315	-1.558939	0.447143	O	0.226131	-1.354764	0.343389
C	-1.686188	0.009664	-0.031969	C	-1.803263	-0.005976	-0.001200
C	-2.430547	1.169467	0.648867	C	-2.946543	0.626431	0.828190
H	-3.165319	1.569633	-0.051317	H	-3.656050	1.118547	0.163271
H	-2.950787	0.828114	1.547365	H	-3.459547	-0.170059	1.370182
H	-1.726659	1.961646	0.910953	H	-2.553827	1.356801	1.536818
C	-0.699812	-0.548438	1.052696	C	-0.747573	-0.541837	0.975561
H	-0.086635	0.259791	1.444871	H	-0.272962	0.293119	1.500103
H	-1.229986	-1.074479	1.846347	H	-1.210395	-1.220474	1.696931
O	-0.946156	0.452070	-1.110462	O	-1.298787	1.067256	-0.713833
O	0.823962	-1.120301	-0.573420	O	0.780606	-0.635791	-0.753137
H	-0.246127	1.189485	-0.780146	H	0.380660	1.866685	-0.321220
C	2.054945	0.161637	-0.361858	C	2.033938	-0.083231	-0.382602
H	2.015447	0.372450	-1.430222	H	2.417088	0.269264	-1.344063
O	0.749852	2.010812	-0.247238	O	1.327750	2.090495	-0.257765
O	1.641330	1.103092	0.408489	O	1.866749	1.005225	0.480749
C	3.175169	-0.654410	0.203859	C	2.952506	-1.064647	0.307624
H	3.327152	-1.555837	-0.385528	H	2.994757	-1.986971	-0.271292
H	4.081135	-0.044853	0.172224	H	3.949197	-0.631205	0.380018
H	2.962200	-0.915836	1.240339	H	2.584200	-1.289378	1.307194
C	-2.635331	-1.080274	-0.510369	C	-2.327707	-1.086661	-0.942839
H	-3.238028	-1.471801	0.312586	H	-2.724843	-1.930137	-0.373380
H	-3.301162	-0.660857	-1.266011	H	-3.118079	-0.673475	-1.570880
H	-2.073076	-1.897209	-0.964906	H	-1.517942	-1.446567	-1.577308
CRAc5				TSAc5			
C	-1.467064	-0.542355	0.327573	C	0.968631	0.822485	0.273100
C	-2.151591	0.279509	1.409061	C	1.751939	0.280096	1.460289
H	-2.218059	-0.319594	2.318885	H	1.496889	0.862655	2.346650

H	-1.576887	1.179917	1.630233
H	-3.156591	0.574762	1.101084
C	-2.231365	-1.836963	0.046284
H	-2.282336	-2.425220	0.963706
H	-3.248442	-1.635114	-0.298547
H	-1.715135	-2.430928	-0.713171
C	-1.364827	0.227919	-0.995088
H	-0.792015	-0.350082	-1.723405
H	-2.344039	0.506011	-1.386604
O	-0.165181	-0.837754	0.803516
H	0.305837	-1.335193	0.102556
O	-1.346223	2.473131	-0.544127
O	-0.604641	1.444585	-0.828334
C	2.304633	0.295701	0.040973
C	3.211088	0.898292	1.037563
H	3.614486	1.835355	0.647141
H	2.616756	1.144033	1.922921
H	4.013869	0.214170	1.303836
O	1.559785	-1.418787	-1.197121
O	2.496660	-0.875563	-0.318852
H	1.454120	0.824369	-0.387474

CPAc5

C	0.777805	0.779012	-0.367773
C	1.336659	1.244650	0.973833
H	0.982997	2.257826	1.174433
H	1.024501	0.592160	1.791649
H	2.428264	1.243369	0.953386
C	1.184109	1.734593	-1.485498
H	0.724130	2.707030	-1.307909
H	2.268395	1.853194	-1.518179
H	0.836375	1.363052	-2.452352
C	1.300902	-0.615907	-0.750349
H	0.631370	-1.080576	-1.474239
H	2.317915	-0.547444	-1.137468
O	-0.651809	0.829627	-0.377974
H	-1.902178	-0.832484	-1.968419
O	2.491877	-1.507492	0.975601
O	1.346542	-1.534817	0.362450
C	-1.371676	0.006377	0.511283
C	-2.026286	0.814316	1.611113
H	-2.633718	0.168902	2.245691
H	-1.258960	1.295921	2.216890
H	-2.656963	1.582458	1.162032
O	-1.901155	-1.418356	-1.199878
O	-2.440035	-0.567273	-0.202373
H	-0.734559	-0.795156	0.896218

TSAc6

H	1.498432	-0.764159	1.649473
H	2.827553	0.345499	1.283932
C	1.245419	2.309954	0.053389
H	0.954304	2.862783	0.947540
H	2.305926	2.487342	-0.138292
H	0.666016	2.692520	-0.791403
C	1.325284	0.086907	-1.022325
H	0.674848	0.412015	-1.838039
H	2.374791	0.220717	-1.285605
O	-0.413941	0.663583	0.568312
H	-1.039820	1.237950	-0.097068
O	2.140349	-1.983750	-0.497776
O	1.087624	-1.331615	-0.892667
C	-1.707464	-0.687255	-0.066234
C	-1.748243	-1.762284	0.949887
H	-2.395908	-2.562623	0.579913
H	-0.744594	-2.166010	1.078226
H	-2.137683	-1.380973	1.891539
O	-2.211277	1.263876	-0.910669
O	-2.645966	0.171814	-0.083268
H	-1.148460	-0.818388	-0.986958

CRAc6

C	-2.256686	0.030762	0.078597
C	-2.710252	1.011916	-1.001937
H	-3.673483	1.436573	-0.715336
H	-1.993817	1.828322	-1.113813
H	-2.815971	0.513286	-1.968714
C	-3.298180	-1.058559	0.304636
H	-4.209196	-0.598159	0.690102
H	-3.531245	-1.579705	-0.625858
H	-2.941133	-1.780006	1.042109
C	-0.942459	-0.654695	-0.303178
H	-0.495950	-1.182502	0.538682
H	-1.063795	-1.330033	-1.149500
O	-2.122473	0.699947	1.325267
H	-1.319618	1.232008	1.300582
O	0.477568	1.070843	0.168405
O	0.042435	0.298363	-0.777152
C	2.895502	0.021030	0.448653
C	3.804704	1.118906	0.058137
H	4.615893	1.206663	0.784664
H	4.207598	0.947340	-0.938008
H	3.238735	2.054322	0.074105
O	1.767536	-1.863894	0.031986
O	2.663776	-0.896070	-0.353834
H	2.395468	-0.037783	1.414153

CPAc6

C	-1.920755	0.085716	-0.125981	C	-1.908488	-0.017847	-0.136838
C	-2.355955	0.409484	1.302874	C	-2.208111	0.676711	1.192547
H	-3.412377	0.160727	1.414193	H	-3.257881	0.516424	1.442017
H	-1.782485	-0.178655	2.021049	H	-1.591645	0.249545	1.985111
H	-2.217325	1.470119	1.530308	H	-2.021524	1.753372	1.134500
C	-2.785586	0.820209	-1.145057	C	-2.834205	0.478395	-1.243640
H	-3.803960	0.435061	-1.077457	H	-3.851282	0.166585	-1.003054
H	-2.800743	1.895280	-0.953551	H	-2.809500	1.566874	-1.331287
H	-2.421833	0.636760	-2.158496	H	-2.562641	0.029466	-2.201695
C	-0.465180	0.502197	-0.369172	C	-0.475094	0.271575	-0.586697
H	-0.086265	0.018937	-1.273801	H	-0.156932	-0.425093	-1.362514
H	-0.374766	1.589482	-0.431336	H	-0.364401	1.311185	-0.897177
O	-2.087445	-1.292227	-0.400365	O	-2.117517	-1.407183	-0.036772
H	-1.378003	-1.764726	0.055263	H	-1.366252	-1.748169	0.479438
O	0.377865	-1.210749	0.922481	O	0.385149	-1.273276	1.024311
O	0.398737	0.135994	0.729983	O	0.436607	0.098733	0.548321
C	2.280943	0.392720	0.253621	C	1.821064	0.458936	0.349485
C	2.457125	1.851423	0.049155	C	1.966660	1.940376	0.121755
H	3.517332	2.095234	0.158596	H	3.018856	2.201521	0.231765
H	2.125312	2.145161	-0.945925	H	1.649529	2.220251	-0.882648
H	1.904219	2.396118	0.815014	H	1.384128	2.487563	0.863217
O	2.145406	-1.682109	-0.482267	O	2.919577	-1.344640	-0.481729
O	2.284937	-0.347046	-0.787367	O	2.307844	-0.228715	-0.788615
H	2.511339	-0.100893	1.193778	H	2.305312	0.062249	1.238518
CH ₂ O							
C	1.057262	0.201622	-0.000006				
H	1.973759	-0.374905	0.000051				
H	0.993479	1.285792	-0.000006				
O	-1.169503	0.191938	0.000006				
O	0.005652	-0.457015	-0.000007				
CRA _d 1				TSA _d 1			
C	-3.212311	-0.640806	0.017350	C	-2.912701	-0.680257	0.407107
H	-3.639451	-1.353790	0.712385	H	-3.005283	-1.250819	1.321542
H	-2.983431	-0.843645	-1.024646	H	-3.129160	-1.053255	-0.586662
O	-2.428784	1.410637	-0.356177	O	-2.545870	1.277172	-0.569724
O	-2.978229	0.486396	0.473925	O	-2.662370	0.541908	0.553205
C	1.855523	0.112755	0.072230	C	1.786003	0.101330	0.104817
C	2.425428	-0.845993	-0.972685	C	2.409079	-0.688742	-1.044846
H	3.451159	-1.098970	-0.700615	H	3.413528	-1.003043	-0.757568
H	1.843603	-1.769011	-1.015300	H	1.819071	-1.579392	-1.270237
H	2.423961	-0.392769	-1.967217	H	2.472697	-0.082079	-1.951620
C	2.722668	1.358807	0.206921	C	2.652377	1.294820	0.488073
H	3.702258	1.064285	0.586396	H	3.607707	0.928023	0.866395
H	2.850616	1.855897	-0.756516	H	2.836783	1.940110	-0.372874
H	2.277455	2.058262	0.917200	H	2.173266	1.876452	1.278252
C	0.442130	0.568490	-0.298537	C	0.399028	0.631032	-0.271469
H	-0.054759	1.060923	0.536908	H	-0.126470	0.998269	0.611045

H	0.433657	1.218637	-1.172662	H	0.449170	1.408924	-1.032650
O	1.857907	-0.497301	1.355223	O	1.704806	-0.704912	1.272150
H	1.154174	-1.154838	1.383983	H	1.013608	-1.363015	1.139169
O	-0.664363	-1.350659	0.276218	O	-0.767597	-1.322018	-0.036136
O	-0.394015	-0.544635	-0.705637	O	-0.419922	-0.388308	-0.887855
CPAd1				CRAd2			
C	-2.274542	-0.876921	0.205093	C	-2.885611	0.232448	0.068173
H	-2.648133	-1.535036	0.988548	H	-3.474381	0.887137	-0.565261
H	-2.740256	-1.030900	-0.768543	H	-2.713344	0.394329	1.127365
O	-2.878455	1.234686	-0.382993	O	-1.624366	-1.587191	0.308606
O	-2.575819	0.465499	0.624004	O	-2.417048	-0.770507	-0.473740
C	1.744761	0.123670	0.086063	C	1.451461	-0.291302	-0.061730
C	2.316871	-1.083011	-0.653386	C	2.645882	0.416864	-0.686218
H	3.248358	-1.389010	-0.174540	H	3.144884	-0.267749	-1.373588
H	1.615437	-1.919420	-0.626366	H	2.314958	1.290409	-1.249136
H	2.517314	-0.844593	-1.700969	H	3.359140	0.733245	0.078563
C	2.743331	1.273086	0.132640	C	1.880211	-1.535806	0.717649
H	3.611564	0.965349	0.717075	H	2.384654	-2.222331	0.035650
H	3.072266	1.549620	-0.871071	H	2.565337	-1.285331	1.531525
H	2.298689	2.144949	0.617701	H	1.005884	-2.044039	1.134015
C	0.466199	0.625663	-0.592823	C	0.719846	0.633114	0.922208
H	-0.056619	1.328375	0.062964	H	-0.176634	0.145608	1.309323
H	0.703718	1.114211	-1.541483	H	1.380930	0.952645	1.730297
O	1.489072	-0.205718	1.447559	O	0.587249	-0.639015	-1.119118
H	0.779323	-0.854656	1.471165	H	-0.127717	-1.187150	-0.749527
O	-0.908458	-1.074013	0.162500	O	-0.928823	1.874323	-0.080193
O	-0.424011	-0.408429	-1.006070	O	0.316183	1.856305	0.268230
TSAd2				CPAd2			
C	2.606924	-0.420344	0.206956	C	2.274604	-0.877020	-0.204837
H	3.308074	-1.114121	-0.237679	H	2.647999	-1.535474	-0.988097
H	2.282276	-0.491503	1.239172	H	2.740162	-1.030963	0.768884
O	1.675525	1.594422	0.171658	O	2.878980	1.234523	0.382809
O	2.532376	0.704037	-0.379944	O	2.576521	0.465084	-0.624101
C	-1.503133	0.201541	-0.056456	C	-1.745003	0.123645	-0.086071
C	-2.526076	-0.779141	-0.613015	C	-2.316888	-1.082682	0.654137
H	-3.143796	-0.265308	-1.350944	H	-3.248468	-1.388944	0.175634
H	-2.021667	-1.611008	-1.106480	H	-1.615415	-1.919072	0.627358
H	-3.170218	-1.168080	0.178782	H	-2.517111	-0.843796	1.701657
C	-2.180915	1.374181	0.658457	C	-2.743679	1.272932	-0.133084
H	-2.821280	1.894631	-0.055131	H	-3.611973	0.964817	-0.717212
H	-2.792390	1.038993	1.500126	H	-3.072434	1.549944	0.870552
H	-1.431599	2.081264	1.025015	H	-2.299223	2.144618	-0.618645
C	-0.597391	-0.479769	0.983669	C	-0.466302	0.626063	0.592298
H	0.154465	0.224906	1.345831	H	0.056364	1.328442	-0.063989
H	-1.190209	-0.868241	1.812759	H	-0.703586	1.115227	1.540694
O	-0.761038	0.664482	-1.162032	O	-1.489588	-0.206579	-1.447399
H	0.009473	1.164292	-0.848285	H	-0.779839	-0.855520	-1.470772

O	0.975702	-1.348988	-0.433306	O	0.908459	-1.073668	-0.162369
O	0.079988	-1.647034	0.481021	O	0.424020	-0.407723	1.005969
CRAd3				TSAd3			
C	2.572359	0.148970	-0.734151	C	-3.363043	-0.388842	-0.378013
H	3.327504	0.926211	-0.738001	H	-3.794400	-0.819892	-1.265220
H	1.817967	0.017556	-1.507224	H	-3.844758	0.260011	0.335907
O	1.667101	-1.622294	0.294099	O	-1.562540	-0.201547	0.922711
O	2.606614	-0.622745	0.231097	O	-2.141088	-0.843539	-0.098048
C	-1.487216	-0.235217	-0.096220	C	1.631716	-0.198439	0.005350
C	-1.463662	-1.100615	1.162289	C	1.195472	-1.279557	-0.981313
H	-1.635419	-2.142908	0.885476	H	1.662925	-2.226038	-0.704327
H	-0.493796	-1.036583	1.660089	H	0.111143	-1.404590	-0.965796
H	-2.246770	-0.792899	1.859291	H	1.493754	-1.023907	-2.001389
C	-2.837328	-0.315389	-0.800614	C	3.150136	-0.062192	0.037807
H	-3.055510	-1.358052	-1.035717	H	3.580002	-0.997596	0.398549
H	-3.639812	0.078549	-0.171844	H	3.550444	0.151866	-0.955260
H	-2.806809	0.246787	-1.736142	H	3.446505	0.734226	0.724144
C	-1.231324	1.237457	0.252442	C	1.056223	1.166693	-0.385358
H	-1.275908	1.865164	-0.637332	H	1.203540	1.885270	0.423391
H	-1.910753	1.594562	1.029053	H	1.530343	1.526414	-1.301387
O	-0.497461	-0.649964	-1.014511	O	1.257145	-0.545082	1.328320
H	0.222578	-1.107470	-0.529619	H	0.301174	-0.670874	1.354411
O	0.922851	1.930423	-0.033101	O	-1.119849	1.327258	0.347052
O	0.098365	1.376812	0.799851	O	-0.341630	1.157802	-0.729268
CPAd3				CRAd4			
C	2.737884	1.361110	0.139614	O	-0.471118	1.866959	-0.456429
H	3.526867	1.471952	-0.621482	C	-1.363103	-0.352793	0.086239
H	3.039748	0.951252	1.116817	C	-2.564794	0.301396	0.753035
O	2.357514	-1.372569	0.063710	H	-2.266378	1.223351	1.253397
O	1.601091	1.676471	-0.090048	H	-3.342863	0.530175	0.021031
C	-1.576354	0.167649	0.062941	H	-2.972122	-0.381375	1.500029
C	-1.541115	1.147737	-1.107292	C	-1.741025	-1.673060	-0.586277
H	-1.899427	2.123413	-0.773373	H	-2.134743	-2.354501	0.169797
H	-0.521871	1.261600	-1.482622	H	-2.503981	-1.526310	-1.354625
H	-2.179519	0.801926	-1.924182	H	-0.860798	-2.133529	-1.043843
C	-2.994339	-0.030361	0.581529	C	-0.767357	0.559880	-0.995191
H	-3.411556	0.935079	0.871231	H	0.158275	0.138429	-1.392682
H	-3.636694	-0.475647	-0.182130	H	-1.486177	0.750383	-1.793916
H	-2.985701	-0.676569	1.461858	O	-0.399312	-0.571933	1.096280
C	-1.022640	-1.194649	-0.364685	O	0.742912	1.985725	-0.027684
H	-1.087928	-1.910101	0.460336	H	0.306930	-1.132090	0.712549
H	-1.563053	-1.596504	-1.226081	C	2.523400	0.300307	0.602451
O	-0.811036	0.655200	1.150827	H	3.202864	1.138910	0.495946
H	-0.000212	1.056798	0.808209	H	1.826686	0.180930	1.428248
O	1.154588	-1.424203	0.372757	O	1.732589	-1.634132	-0.217292
O	0.335184	-1.116413	-0.794899	O	2.588626	-0.552714	-0.289559
TSAd4				CPAd4			

O	0.123492	-1.641282	0.601694
C	-1.339681	0.181252	-0.077479
C	-2.425136	-0.773147	-0.554382
H	-1.979879	-1.688649	-0.946470
H	-3.115965	-1.025415	0.253468
H	-2.984279	-0.293789	-1.359181
C	-1.923059	1.478320	0.503638
H	-2.540422	1.951702	-0.261329
H	-2.543836	1.274711	1.379671
H	-1.115694	2.160700	0.776399
C	-0.507984	-0.455943	1.089571
H	0.225130	0.258707	1.455249
H	-1.149739	-0.823987	1.889352
O	-0.488708	0.438368	-1.136407
O	0.960188	-1.450467	-0.398250
H	0.283261	1.065832	-0.801796
C	2.304467	-0.348880	-0.290727
H	2.993736	-1.075311	0.134818
H	2.309227	-0.175727	-1.365302
O	1.409415	1.724300	-0.183947
O	2.116465	0.664281	0.469584

CRA5

C	0.933249	0.785628	0.019949
C	0.457442	0.692713	1.469541
H	-0.289904	1.468225	1.652517
H	0.002270	-0.280823	1.662735
H	1.285964	0.837665	2.167270
C	1.430459	2.185887	-0.317408
H	0.600694	2.889114	-0.227473
H	2.226898	2.496152	0.361966
H	1.799619	2.223975	-1.344704
C	2.083246	-0.193927	-0.242354
H	2.261003	-0.288364	-1.314934
H	2.990000	0.117308	0.278458
O	-0.140040	0.524901	-0.869862
H	-0.498222	-0.364172	-0.680310
O	0.931225	-2.147633	-0.423887
O	1.817057	-1.509039	0.282495
C	-2.883830	0.709856	-0.438671
H	-3.434003	1.588037	-0.118643
H	-2.509428	0.547368	-1.444225
O	-1.982348	-1.259682	0.086492
O	-2.695680	-0.147977	0.432386

CPAd5

C	1.237843	0.171662	-0.033183
C	1.244464	0.628631	1.425399
H	1.468210	1.694052	1.501852

O	0.215705	-1.510754	0.546664
C	-1.488372	0.165474	-0.043398
C	-2.164180	-0.871524	-0.936705
H	-1.409088	-1.435001	-1.484511
H	-2.750782	-1.569480	-0.334945
H	-2.821801	-0.369713	-1.647689
C	-2.528710	1.076315	0.651932
H	-3.088391	1.635556	-0.097498
H	-3.218602	0.443631	1.213223
H	-2.039909	1.776362	1.330687
C	-0.615923	-0.474561	1.044203
H	-0.017987	0.297680	1.536882
H	-1.241580	-0.988576	1.778392
O	-0.743081	1.055444	-0.796606
O	0.944466	-1.021827	-0.574657
H	1.051910	1.595954	-0.434695
C	2.233281	-0.661657	-0.147193
H	2.632969	-1.416789	0.531493
H	2.807685	-0.564782	-1.070549
O	2.022190	1.596010	-0.339231
O	2.245595	0.529987	0.572101

TSAd5

C	0.652920	0.811283	0.040494
C	0.295683	0.586526	1.508622
H	-0.546822	1.218794	1.794449
H	0.018510	-0.453997	1.686847
H	1.148127	0.840301	2.142762
C	0.809512	2.290194	-0.288415
H	-0.140963	2.803895	-0.130499
H	1.556690	2.753627	0.358397
H	1.104386	2.425393	-1.331234
C	1.962750	0.105198	-0.323372
H	2.069608	0.040294	-1.407613
H	2.812802	0.625602	0.119998
O	-0.370671	0.311315	-0.831788
H	-0.620638	-0.654147	-0.587235
O	1.203517	-2.035011	-0.346961
O	2.049891	-1.224606	0.217946
C	-2.293968	0.567354	-0.485829
H	-2.448214	1.614586	-0.234576
H	-2.406394	0.215989	-1.506479
O	-1.864240	-1.502763	0.042711
O	-2.407055	-0.248143	0.466365

CRA6

C	1.886005	0.093157	0.068051
C	2.436588	-0.844879	-1.005577
H	3.450267	-1.141726	-0.732540

H	0.294043	0.424320	1.919168	H	1.824795	-1.745469	-1.088722
H	2.034342	0.091846	1.954882	H	2.461387	-0.355653	-1.982569
C	2.549049	0.539975	-0.722883	C	2.789045	1.306398	0.254937
H	2.678062	1.623453	-0.698092	H	3.756559	0.968822	0.629596
H	3.403073	0.076733	-0.223125	H	2.939475	1.834444	-0.688610
H	2.528304	0.222408	-1.766812	H	2.359384	1.992392	0.987558
C	1.069761	-1.346302	-0.116316	C	0.490138	0.604147	-0.298196
H	1.011272	-1.674748	-1.153709	H	0.000095	1.085530	0.547443
H	1.866037	-1.861633	0.424104	H	0.512758	1.275411	-1.156153
O	0.180969	0.721984	-0.831287	O	1.857423	-0.563120	1.327952
H	-2.390413	-0.591353	-0.237886	H	1.130339	-1.195413	1.327439
O	-1.088485	-2.035168	-0.324484	O	-0.698633	-1.272856	0.228359
O	-0.160296	-1.730666	0.527501	O	-0.377001	-0.471210	-0.738332
C	-0.754195	1.592207	-0.269746	C	-3.270149	-0.586109	0.419918
H	-0.291345	2.341711	0.376298	H	-3.865916	-1.412282	0.050699
H	-1.265506	2.059419	-1.110644	H	-2.805435	-0.539544	1.399735
O	-2.665685	0.338746	-0.265453	O	-2.368575	1.412953	0.047658
O	-1.693704	0.964697	0.558015	O	-3.132399	0.368884	-0.356721
TSAd6				CPAd6			
C	-1.707480	0.039632	-0.124749	C	-1.725014	-0.095394	0.103463
C	-2.203206	-0.312489	1.277434	C	-2.122022	0.760753	-1.100026
H	-3.203380	-0.741073	1.199551	H	-3.136440	1.130501	-0.944942
H	-1.546434	-1.047482	1.745596	H	-1.449612	1.615376	-1.190894
H	-2.247400	0.572848	1.917590	H	-2.096385	0.184600	-2.029523
C	-2.677817	0.980618	-0.831404	C	-2.709504	-1.240597	0.320745
H	-3.615512	0.448977	-0.998554	H	-3.673481	-0.812888	0.598765
H	-2.877880	1.870378	-0.230819	H	-2.835981	-1.839338	-0.583867
H	-2.281214	1.280180	-1.803952	H	-2.377748	-1.882720	1.139684
C	-0.344930	0.739713	-0.073048	C	-0.346569	-0.722243	-0.106018
H	0.120661	0.723642	-1.061725	H	0.063646	-1.091814	0.834025
H	-0.437179	1.759819	0.306652	H	-0.365183	-1.495537	-0.877688
O	-1.633584	-1.117158	-0.936397	O	-1.732846	0.666809	1.288184
H	-0.864398	-1.627065	-0.651228	H	-0.949590	1.241734	1.239207
O	0.779259	-1.185457	0.505914	O	0.727392	1.386723	0.338352
O	0.562389	0.100093	0.858653	O	0.582636	0.295197	-0.612079
C	2.387429	0.833525	0.648390	C	1.878349	-0.176715	-0.971802
H	2.261705	1.882421	0.895304	H	1.743723	-0.921235	-1.755696
H	2.709886	0.085567	1.364282	H	2.444218	0.705447	-1.256647
O	2.666830	-0.748476	-0.848825	O	3.286000	-0.024938	0.783828
O	2.532252	0.589222	-0.587150	O	2.484492	-0.822409	0.120391
HOCH ₂ (CH ₃) ₂ COO							
C	-0.518883	-0.136373	0.027508				
C	-1.882537	-0.444504	-0.564051				
H	-2.203317	-1.438236	-0.247960				
H	-2.616436	0.284150	-0.216519				
H	-1.850970	-0.413971	-1.655251				
C	-0.493175	-0.233037	1.541990				

H	-1.304126	0.358517	1.970493
H	-0.614874	-1.276029	1.840644
H	0.460229	0.120833	1.932323
C	0.565893	-0.983068	-0.645180
H	0.661905	-0.649801	-1.686960
H	0.217062	-2.018408	-0.655310
O	1.805333	-0.988202	0.015185
O	-0.310818	1.279170	-0.339178
O	0.893779	1.695563	-0.112569
H	2.116390	-0.077414	0.049434

CRBa1

C	-1.777255	-0.348973	-0.162803
C	-1.887437	-1.827066	0.163737
H	-2.842419	-2.018589	0.656239
H	-1.848052	-2.419513	-0.752443
H	-1.065349	-2.121996	0.818258
C	-2.889889	0.159878	-1.062148
H	-2.980280	-0.472006	-1.947595
H	-3.832692	0.138312	-0.512058
H	-2.699475	1.189473	-1.364139
C	-1.617088	0.472508	1.118172
H	-0.659164	0.208894	1.577196
H	-2.413142	0.157787	1.797015
O	-1.772130	1.863779	0.947189
O	-0.522965	-0.283331	-0.954650
O	-0.034294	0.908318	-1.077865
H	-1.065902	2.154767	0.362981
C	2.362090	0.075613	0.004264
C	2.903010	1.437553	-0.237921
H	2.511152	1.800372	-1.191041
H	2.617201	2.114408	0.564952
H	3.992293	1.389055	-0.317188
C	2.564260	-1.059329	-0.915057
H	3.160057	-0.765876	-1.776351
H	3.029113	-1.877894	-0.357401
H	1.578470	-1.428813	-1.212895
O	1.189358	-1.342241	1.298960
O	1.711536	-0.085211	1.061992

CPBa1

C	1.728144	-0.320751	0.015980
C	2.573718	-1.139982	-0.952610
H	3.601585	-0.773955	-0.942384
H	2.573039	-2.189361	-0.655102
H	2.182132	-1.062989	-1.969314
C	2.257423	-0.398173	1.439463
H	2.289663	-1.438415	1.769075
H	3.267171	0.016799	1.475048

TSBa1

C	1.738811	-0.267140	0.146416
C	2.166317	-1.657215	-0.290788
H	3.172899	-1.616207	-0.710867
H	2.177264	-2.332969	0.566231
H	1.469280	-2.043169	-1.036628
C	2.686211	0.358181	1.158779
H	2.845976	-0.323386	1.996115
H	3.645138	0.565693	0.679561
H	2.281633	1.299965	1.529298
C	1.518139	0.625728	-1.076103
H	0.698480	0.210540	-1.668457
H	2.429987	0.568012	-1.675676
O	1.325368	1.991896	-0.781917
O	0.472582	-0.523687	0.857760
O	-0.273747	0.550265	1.027634
H	0.563433	2.039292	-0.196530
C	-2.085460	0.072967	0.041730
C	-2.670530	1.437136	0.144181
H	-2.471834	1.837368	1.139148
H	-2.248124	2.092777	-0.616183
H	-3.754407	1.376115	0.009258
C	-2.469069	-1.039424	0.941057
H	-2.879514	-0.645883	1.868628
H	-3.217048	-1.647571	0.420554
H	-1.607787	-1.679508	1.125599
O	-1.055405	-1.443873	-1.249723
O	-1.520284	-0.184909	-1.081463

CRBa2

C	1.911063	-0.048803	-0.162213
C	2.715165	-0.448870	-1.386740
H	3.482712	0.302194	-1.582608
H	3.203164	-1.411755	-1.227414
H	2.070097	-0.521188	-2.264692
C	2.711011	-0.096336	1.122344
H	3.060652	-1.110410	1.324083
H	3.577956	0.557284	1.004260

H	1.630162	0.179628	2.115882	H	2.113993	0.253891	1.961563
C	1.644985	1.124198	-0.493371	C	1.232932	1.307844	-0.367583
H	1.113501	1.122401	-1.452539	H	0.646962	1.274890	-1.294567
H	2.666984	1.468501	-0.674036	H	2.029200	2.053967	-0.495985
O	1.076712	2.045713	0.408843	O	0.421641	1.621375	0.726891
O	0.450990	-0.990575	-0.084960	O	0.807902	-1.034131	-0.128200
O	-0.447181	-0.431719	0.876203	O	0.412444	-1.378569	1.056475
H	0.121532	1.943189	0.376198	C	-2.123774	-0.401153	-0.143705
C	-1.690736	-0.237475	0.273891	O	-1.936712	1.833748	-0.438763
C	-2.593942	0.250020	1.386574	O	-1.915604	0.536081	-0.948481
H	-2.698068	-0.533282	2.136525	C	-2.138317	-1.765609	-0.727267
H	-2.164781	1.137021	1.854305	H	-1.423101	-2.382237	-0.179326
H	-3.573401	0.496383	0.977164	H	-3.134803	-2.194210	-0.585600
C	-2.209724	-1.436281	-0.484711	H	-1.889216	-1.737641	-1.785697
H	-2.336951	-2.250775	0.229209	C	-2.368723	-0.128713	1.285628
H	-3.173748	-1.196244	-0.934059	H	-3.149644	0.631692	1.368337
H	-1.515562	-1.739694	-1.262276	H	-2.623277	-1.045231	1.812661
O	-1.316840	0.660554	-1.858713	H	-1.456603	0.309475	1.705895
O	-1.543989	0.937460	-0.610747	H	-0.461601	1.881083	0.372941
TSBa2				CPBa2			
C	1.853907	-0.258938	-0.013278	C	1.753961	-0.353165	-0.019905
C	2.778400	-1.053822	-0.920263	C	2.597846	-1.169300	-0.991977
H	3.748364	-0.558045	-0.976588	H	3.644153	-0.872708	-0.904220
H	2.925790	-2.059670	-0.523980	H	2.516645	-2.232279	-0.760039
H	2.365663	-1.129916	-1.928917	H	2.269972	-1.007818	-2.021202
C	2.413963	-0.065399	1.383728	C	2.237639	-0.496630	1.414749
H	2.684784	-1.028625	1.820749	H	2.275504	-1.552163	1.691172
H	3.304790	0.563489	1.327753	H	3.237482	-0.067246	1.508809
H	1.681994	0.440348	2.010686	H	1.579071	0.036764	2.098077
C	1.478939	1.078054	-0.671559	C	1.723675	1.111291	-0.478863
H	0.831418	0.878457	-1.533995	H	1.151127	1.164930	-1.413615
H	2.419719	1.494024	-1.053181	H	2.752824	1.410957	-0.694933
O	0.909958	2.002398	0.205376	O	1.240125	2.024801	0.475111
O	0.675255	-1.136240	0.070308	O	0.458251	-0.971973	-0.173351
O	-0.263062	-0.665908	0.866172	O	-0.463602	-0.287148	0.685836
C	-1.940442	-0.405111	-0.048569	C	-1.730437	-0.372443	0.130441
O	-1.680944	1.786323	-0.548652	O	-1.354196	1.666245	-0.889667
O	-1.586921	0.481613	-0.925269	O	-1.776091	0.462078	-1.094184
C	-2.112423	-1.766421	-0.637222	C	-2.119305	-1.750652	-0.355610
H	-2.007661	-2.519686	0.141563	H	-2.042056	-2.451643	0.475855
H	-3.112012	-1.836717	-1.074814	H	-3.147939	-1.730129	-0.716097
H	-1.369533	-1.934217	-1.416016	H	-1.459305	-2.071973	-1.158355
C	-2.681193	0.036367	1.162271	C	-2.666049	0.226899	1.159225
H	-3.619674	0.493344	0.834990	H	-3.667533	0.302669	0.735302
H	-2.878177	-0.818069	1.806741	H	-2.692215	-0.414527	2.039633
H	-2.113427	0.801389	1.688967	H	-2.318925	1.219922	1.444148
H	-0.043234	2.080027	0.001924	H	0.281317	1.937227	0.497144

CRBa3				TSBa3			
C	-2.024218	-0.276795	0.082231	C	1.880955	0.512008	-0.115261
C	-2.950184	-0.801092	1.166604	C	2.203721	1.918308	0.367202
H	-3.935885	-0.345011	1.058368	H	3.245675	1.969816	0.686832
H	-3.057657	-1.884297	1.089196	H	2.051495	2.635136	-0.441262
H	-2.562696	-0.556329	2.157840	H	1.563843	2.198443	1.207847
C	-2.437130	-0.690557	-1.312932	C	2.819988	0.044602	-1.214053
H	-2.431726	-1.777435	-1.413965	H	2.854387	0.785723	-2.014888
H	-3.452068	-0.326215	-1.486418	H	3.824868	-0.092653	-0.809074
H	-1.774019	-0.251119	-2.054675	H	2.487238	-0.910858	-1.617099
C	-1.841335	1.243488	0.207683	C	1.864878	-0.449503	1.081682
H	-1.455269	1.459477	1.211853	H	0.994261	-0.209831	1.704820
H	-2.839593	1.689916	0.123515	H	2.766626	-0.254661	1.668007
O	-1.019136	1.773198	-0.782957	O	1.908634	-1.817096	0.754457
O	-0.713212	-0.866318	0.437958	O	0.541640	0.677745	-0.664591
O	0.040311	-1.198135	-0.559406	O	0.029829	-0.504565	-1.095323
H	-0.118467	1.877561	-0.402476	H	1.062991	-2.074618	0.373585
C	2.445026	-0.166096	0.045645	C	-2.686374	0.122474	0.187827
C	3.119039	-1.075500	-0.913980	C	-3.849795	0.510435	-0.647026
H	4.143984	-1.260889	-0.582800	H	-4.620523	0.985271	-0.036520
H	2.582660	-2.027281	-0.907372	H	-3.555319	1.224668	-1.427334
H	3.114721	-0.652279	-1.916082	H	-4.273916	-0.365988	-1.138114
C	2.294663	-0.467428	1.481602	C	-2.045048	0.947173	1.233965
H	2.740660	-1.428819	1.726094	H	-2.732709	1.727444	1.559687
H	2.746295	0.347234	2.054822	H	-1.764008	0.324470	2.089844
H	1.228119	-0.449185	1.721788	H	-1.123717	1.413062	0.862994
O	1.356562	1.755283	0.463425	O	-0.822521	-1.166742	0.142112
O	2.014946	0.909540	-0.424119	O	-2.146475	-1.062893	-0.141072
CPBa3				CRBa4			
C	1.488104	0.716858	-0.023432	C	1.911069	-0.048816	-0.162055
C	1.187941	2.094574	0.555921	C	2.715254	-0.449055	-1.386472
H	2.124411	2.598876	0.799947	H	3.482800	0.301990	-1.582409
H	0.645255	2.697618	-0.173450	H	3.203257	-1.411910	-1.226973
H	0.586754	2.012794	1.464970	H	2.070238	-0.521515	-2.264451
C	2.371392	0.793871	-1.258059	C	2.710932	-0.096159	1.122562
H	1.906612	1.434648	-2.009189	H	3.060559	-1.110205	1.324473
H	3.342642	1.211718	-0.984656	H	3.577885	0.557443	1.004439
H	2.542755	-0.196102	-1.678409	H	2.113856	0.254190	1.961689
C	2.093496	-0.170262	1.073876	C	1.232946	1.307798	-0.367668
H	1.326622	-0.352647	1.835547	H	0.647055	1.274711	-1.294697
H	2.906125	0.394244	1.538711	H	2.029219	2.053909	-0.496104
O	2.665764	-1.373254	0.612843	O	0.421557	1.621472	0.726693
O	0.155098	0.267077	-0.381019	O	-1.915514	0.535934	-0.948712
O	0.226203	-1.028117	-1.028268	O	-1.936701	1.833675	-0.439186
H	1.984329	-2.046979	0.545427	C	-2.123743	-0.401186	-0.143817
C	-2.640584	0.022005	-0.002245	O	0.412372	-1.378409	1.056726
C	-2.672681	1.530141	-0.111865	O	0.807913	-1.034145	-0.127972

H	-3.632854	1.894802	0.265443	C	-2.138205	-1.765728	-0.727180
H	-1.885005	1.973810	0.500035	H	-1.423079	-2.382282	-0.179040
H	-2.556338	1.827000	-1.152383	H	-3.134717	-2.194300	-0.585606
C	-2.477853	-0.543724	1.390263	H	-1.888943	-1.737916	-1.785575
H	-3.207991	-0.099465	2.071640	C	-2.368839	-0.128535	1.285450
H	-2.585994	-1.626256	1.367571	H	-3.149812	0.631838	1.367966
H	-1.479515	-0.286185	1.754354	H	-2.623389	-1.044984	1.812605
O	-0.063442	-1.939986	-0.219324	H	-1.456785	0.309776	1.705732
O	-2.748210	-0.688051	-0.970772	H	-0.461651	1.881136	0.372628
TSBa4				CPBa4			
C	1.875169	-0.249868	-0.017698	C	1.817612	-0.236240	0.008826
C	2.816942	-0.896916	-1.012806	C	2.785883	-0.974842	-0.905291
H	3.740712	-0.317980	-1.059639	H	3.767274	-0.499452	-0.868370
H	3.063572	-1.915583	-0.708806	H	2.885002	-2.007948	-0.569737
H	2.370195	-0.919739	-2.008228	H	2.425531	-0.975611	-1.935605
C	2.343335	-0.317499	1.422024	C	2.327062	-0.136818	1.438192
H	2.378266	-1.355164	1.761353	H	2.562571	-1.137140	1.806116
H	3.349205	0.102527	1.480001	H	3.231711	0.474153	1.470844
H	1.680253	0.259988	2.063246	H	1.578651	0.317389	2.084357
C	1.541866	1.240906	-0.429364	C	1.522555	1.170440	-0.602619
H	1.224942	1.228649	-1.481523	H	1.017543	1.034636	-1.566811
H	2.514997	1.749940	-0.348459	H	2.510682	1.639895	-0.741728
O	0.623300	1.796860	0.397769	O	0.820674	1.949165	0.266981
O	-1.615848	0.376697	-1.029530	O	-1.623212	0.459854	-0.992453
O	-1.538291	1.753600	-0.674157	O	-1.829073	1.771492	-0.492340
C	-1.856264	-0.412934	-0.027796	C	-1.614500	-0.480979	0.057492
O	-0.236912	-0.632518	0.753338	O	-0.364864	-0.429157	0.752716
O	0.622563	-0.931987	-0.197209	O	0.635196	-1.017839	-0.072682
C	-2.158272	-1.808757	-0.489052	C	-1.833947	-1.819537	-0.625977
H	-2.045469	-2.513338	0.333260	H	-1.606939	-2.624269	0.073528
H	-3.191705	-1.831801	-0.842249	H	-2.876198	-1.887723	-0.937150
H	-1.497525	-2.080123	-1.311330	H	-1.191494	-1.912252	-1.499382
C	-2.542419	0.124460	1.190392	C	-2.639792	-0.185828	1.137689
H	-3.515404	0.506230	0.872156	H	-3.595629	0.032670	0.661628
H	-2.674130	-0.670792	1.922871	H	-2.739646	-1.057877	1.783826
H	-1.979354	0.952186	1.613480	H	-2.341734	0.675238	1.732168
H	-0.379198	1.827440	-0.102018	H	-0.926330	2.042997	-0.241335
CRBa5				TSBa5			
C	-2.257463	-0.137612	-0.028638	C	-1.896008	-0.349663	-0.012608
C	-3.736472	-0.439778	-0.202735	C	-2.754806	-1.551264	-0.370568
H	-3.913297	-1.509534	-0.078052	H	-2.383576	-2.439370	0.143355
H	-4.323928	0.099552	0.541837	H	-3.786154	-1.375262	-0.062382
H	-4.076232	-0.142558	-1.196926	H	-2.741145	-1.733444	-1.447328
C	-1.760895	-0.428591	1.374751	C	-1.904427	-0.043563	1.473146
H	-2.308907	0.173353	2.102385	H	-2.932173	0.051111	1.828572
H	-1.934952	-1.484874	1.592669	H	-1.409373	-0.855265	2.009836
H	-0.695052	-0.229704	1.480059	H	-1.376390	0.884459	1.685579

C	-1.435805	-0.851680	-1.110078
H	-1.798617	-0.524639	-2.088041
H	-1.635429	-1.928316	-1.016987
O	-0.067476	-0.573294	-1.050680
O	-2.172865	1.303804	-0.319059
O	-1.146671	1.901917	0.192782
H	0.330854	-1.035901	-0.280190
C	2.804638	0.141642	0.041776
C	3.945802	0.465646	-0.852518
H	4.679896	1.060059	-0.303316
H	4.405396	-0.439660	-1.242659
H	3.574010	1.082297	-1.675430
C	1.991786	1.170935	0.711135
H	0.991529	1.169350	0.257630
H	1.849643	0.885724	1.756438
H	2.448669	2.153012	0.609997
O	1.463847	-1.411665	0.980753
O	2.560274	-1.077203	0.188507

CPBa5

C	-1.829775	0.214959	0.269137
C	-2.822275	0.539455	1.373811
H	-2.505590	1.434029	1.913046
H	-3.809400	0.719524	0.946273
H	-2.896542	-0.289469	2.080279
C	-1.762551	1.292762	-0.795888
H	-2.746867	1.449723	-1.240133
H	-1.444602	2.227726	-0.326060
H	-1.066876	1.014343	-1.585694
C	-0.464482	-0.099821	0.869854
H	-0.567673	-0.943782	1.561485
H	-0.119439	0.778396	1.430261
O	0.434680	-0.414244	-0.171371
O	-2.343602	-1.043875	-0.293672
O	-2.054605	-1.240840	-1.540730
H	1.011605	1.839084	-0.819677
C	1.810904	-0.347883	0.145258
C	2.170509	-1.085580	1.426118
H	3.254121	-1.115343	1.535802
H	1.750164	-0.589104	2.301477
H	1.788333	-2.105975	1.369474
C	2.547859	-0.882561	-1.066005
H	2.353529	-1.951231	-1.160392
H	2.207481	-0.379876	-1.968613
H	3.618204	-0.714496	-0.943548
O	1.975045	1.797849	-0.730210
O	2.147534	1.005918	0.432522

TSBa6

C	-0.484452	-0.538633	-0.572307
H	-0.541162	-0.579549	-1.663770
H	-0.100232	-1.497114	-0.194279
O	0.387542	0.507698	-0.211259
O	-2.519256	0.746240	-0.770446
O	-2.205726	1.933244	-0.355378
H	0.601840	0.375995	0.823465
C	2.306858	-0.070157	-0.226072
C	2.563751	-0.721827	-1.543548
H	3.642674	-0.766146	-1.713248
H	2.151317	-1.728928	-1.564840
H	2.121906	-0.112091	-2.332484
C	2.802369	1.322481	-0.008540
H	2.503841	1.956200	-0.841155
H	2.445006	1.727804	0.932274
H	3.895803	1.260290	0.018329
O	1.475084	-0.226207	1.834410
O	2.125870	-0.892592	0.745306

CRBa6

C	1.777434	0.348852	-0.162736
C	1.887891	1.826920	0.163864
H	2.842604	2.018093	0.657025
H	1.849341	2.419456	-0.752287
H	1.065492	2.122122	0.817882
C	2.890050	-0.160162	-1.062033
H	2.981151	0.472177	-1.947099
H	3.832682	-0.139358	-0.511609
H	2.699205	-1.189504	-1.364606
C	1.617025	-0.472638	1.118171
H	0.659208	-0.208767	1.577255
H	2.413216	-0.158249	1.797007
O	1.771606	-1.863959	0.947060
O	0.523171	0.283489	-0.954690
O	0.034234	-0.908044	-1.077947
H	1.065338	-2.154635	0.362745
C	-2.362188	-0.075507	0.004261
C	-2.903354	-1.437344	-0.237932
H	-2.511413	-1.800375	-1.190931
H	-2.617936	-2.114206	0.565076
H	-3.992608	-1.388531	-0.317463
C	-2.564212	1.059419	-0.915086
H	-3.160065	0.766032	-1.776358
H	-3.028900	1.878095	-0.357442
H	-1.578386	1.428785	-1.212909
O	-1.189245	1.342236	1.298922
O	-1.711615	0.085232	1.061987

CPBa6

C	1.299995	0.375401	0.397795
C	1.181418	0.395918	1.912169
H	2.184907	0.451251	2.342565
H	0.615811	1.252172	2.278409
H	0.716538	-0.533122	2.247317
C	1.450791	1.746386	-0.235395
H	0.618999	2.409594	0.004925
H	2.358045	2.208108	0.160029
H	1.554166	1.653194	-1.317822
C	2.480465	-0.530299	-0.004943
H	2.461690	-1.426517	0.620427
H	3.404193	0.019866	0.191907
O	2.470619	-0.855910	-1.369273
O	0.127665	-0.258145	-0.247518
O	0.032863	-1.587289	0.143221
H	1.722224	-1.449872	-1.505244
C	-1.600375	0.387269	-0.309789
C	-1.614641	1.175334	-1.581598
H	-0.923505	2.012784	-1.529518
H	-1.351910	0.528727	-2.417002
H	-2.625361	1.564809	-1.730419
C	-1.791354	1.075856	1.004838
H	-1.240236	2.012996	1.040760
H	-2.861383	1.295971	1.080807
H	-1.520800	0.424474	1.829139
O	-2.145761	-1.543385	0.651810
O	-2.179281	-0.777722	-0.477582
CRBb1			
C	-1.280291	0.515090	-0.146470
C	-1.056863	0.779186	1.330821
H	-0.129145	1.335881	1.467379
H	-1.895824	1.367381	1.708729
H	-1.023515	-0.153207	1.893088
C	-2.610570	-0.180803	-0.444028
H	-2.588575	-0.539442	-1.481732
H	-3.400464	0.569754	-0.364839
O	-2.947225	-1.211720	0.450999
O	-0.199728	-0.370337	-0.646611
O	-0.145243	-1.523410	-0.059042
H	-2.214425	-1.836129	0.470060
C	2.519254	-0.765251	0.398674
C	2.889376	-0.725356	-1.021432
H	3.218306	-1.700096	-1.371018
H	2.021678	-0.366293	-1.583696
H	3.663621	0.037491	-1.154697
O	2.020939	1.409336	0.280676
O	2.123890	0.250776	1.004578

C	1.366820	0.464509	0.104241
C	1.325867	1.341410	1.337339
H	2.349759	1.637140	1.579766
H	0.745154	2.253571	1.190072
H	0.924464	0.774341	2.179104
C	1.710260	1.181497	-1.192208
H	1.141438	2.092029	-1.358202
H	2.764471	1.461507	-1.140951
H	1.586073	0.499240	-2.033915
C	2.364517	-0.690214	0.319073
H	2.240561	-1.086587	1.328022
H	3.362663	-0.252157	0.230193
O	2.244015	-1.687487	-0.650930
O	0.037957	-0.245674	-0.088720
O	-0.050571	-1.437892	0.734199
H	1.403580	-2.125632	-0.435156
C	-1.289842	0.398612	-0.089024
C	-1.314234	1.636335	-0.955589
H	-0.750431	2.451622	-0.507175
H	-0.943092	1.418722	-1.955930
H	-2.358470	1.942416	-1.030315
C	-1.828160	0.596615	1.306217
H	-1.359654	1.471213	1.755274
H	-2.902146	0.771679	1.236957
H	-1.640911	-0.291134	1.903264
O	-2.746949	-1.395036	-0.135800
O	-2.056305	-0.557730	-0.848911
TSBb1			
C	-1.297295	0.497195	-0.130043
C	-1.042129	0.755698	1.343114
H	-0.245852	1.489831	1.462657
H	-1.963077	1.140945	1.786219
H	-0.780468	-0.162726	1.865818
C	-2.505295	-0.415731	-0.364952
H	-2.531605	-0.687499	-1.428089
H	-3.408944	0.154559	-0.136868
O	-2.531832	-1.556358	0.457820
O	-0.145446	-0.170395	-0.765612
O	0.248225	-1.262767	-0.142728
H	-1.687590	-2.011071	0.363086
C	2.248252	-0.728150	0.413849
C	2.803116	-0.747500	-0.952573
H	2.963050	-1.771538	-1.280542
H	2.129050	-0.215445	-1.624051
H	3.748698	-0.194166	-0.943259
O	1.878897	1.458890	0.202107
O	1.934045	0.364562	0.989298

H	2.562146	-1.649963	1.027151
C	-1.103508	1.759563	-0.995764
H	-1.795388	2.531206	-0.654197
H	-0.080351	2.122197	-0.882746
H	-1.303524	1.549478	-2.049086

CPBb1

C	1.334492	0.489871	0.156793
C	1.065220	0.910956	-1.278858
H	0.399290	1.775545	-1.297470
H	2.008951	1.172285	-1.762479
H	0.611684	0.101493	-1.849201
C	2.331050	-0.671668	0.251054
H	2.302658	-1.058695	1.277837
H	3.333024	-0.278547	0.063473
O	2.134463	-1.698926	-0.693361
O	0.104769	0.141160	0.834913
O	-0.443839	-1.029639	0.222828
H	1.246019	-2.043948	-0.567633
C	-1.810314	-0.833322	0.032622
C	-2.560114	-0.369731	1.255942
H	-2.421784	-1.113716	2.040482
H	-2.187282	0.592341	1.594924
H	-3.621382	-0.285119	1.021478
O	-2.098950	1.299369	-0.799127
O	-2.007433	0.041002	-1.111570
H	-2.154769	-1.799587	-0.339492
C	1.827168	1.653981	1.007770
H	2.716364	2.089350	0.549320
H	1.055608	2.422959	1.069410
H	2.074524	1.321387	2.017953

TSBb2

C	1.710865	-0.133819	-0.060451
C	2.164021	-0.430450	1.356701
H	2.561931	-1.444970	1.423649
H	2.947488	0.277540	1.634296
H	1.333069	-0.305063	2.048214
C	1.140918	1.287142	-0.196539
H	0.593519	1.360512	-1.144039
H	2.013140	1.949550	-0.264849
O	0.359394	1.684756	0.888499
O	0.688387	-1.120553	-0.448251
O	-0.328042	-1.166076	0.381809
H	-0.573669	1.735171	0.597538
C	-1.981288	-0.765756	-0.491839
C	-2.835865	-0.913907	0.709759
H	-2.899672	-1.962552	0.991753
H	-2.431420	-0.314304	1.524190

H	2.308578	-1.557152	1.109432
C	-1.417657	1.780004	-0.931854
H	-2.230861	2.386712	-0.529822
H	-0.483534	2.338185	-0.853292
H	-1.622515	1.568825	-1.983617

CRBb2

C	1.769620	0.073023	-0.068121
C	2.341100	-0.642016	1.138063
H	2.788581	-1.593606	0.845232
H	3.116991	-0.008207	1.572691
H	1.569592	-0.819073	1.884054
C	0.954330	1.308765	0.323548
H	0.517318	1.743892	-0.583419
H	1.654565	2.039572	0.749819
O	-0.040980	0.976451	1.249771
O	0.827494	-0.802107	-0.796128
O	0.235786	-1.694926	-0.069731
H	-0.898150	1.315518	0.906807
C	-2.192092	-0.674486	-0.630089
C	-2.578573	-1.044547	0.738046
H	-2.765129	-2.112998	0.807340
H	-1.754352	-0.761379	1.403883
H	-3.445168	-0.447396	1.033672
O	-2.293035	1.496218	-0.057286
O	-2.064738	0.507299	-1.003759
H	-1.991213	-1.391990	-1.420549
C	2.815124	0.419934	-1.113342
H	3.501225	1.167979	-0.712099
H	3.388785	-0.466380	-1.388775
H	2.343675	0.826539	-2.010215

CPBb2

C	1.627362	-0.248328	-0.091629
C	2.113589	-0.709953	1.273136
H	2.328658	-1.779985	1.249347
H	3.023510	-0.168495	1.540920
H	1.366198	-0.504550	2.037798
C	1.362563	1.263217	-0.133883
H	0.785535	1.485280	-1.040631
H	2.329912	1.765653	-0.218312
O	0.745575	1.791899	1.014459
O	0.449419	-0.990452	-0.475527
O	-0.591779	-0.708577	0.471067
H	-0.188429	1.560933	0.978230
C	-1.778709	-0.793671	-0.216600
C	-2.904855	-0.815537	0.785909
H	-2.828933	-1.714427	1.396161
H	-2.841145	0.065099	1.425575

H	-3.826763	-0.516977	0.471776
O	-2.083915	1.466434	-0.229166
O	-1.762568	0.391324	-1.007641
H	-1.868973	-1.553502	-1.228963
C	2.794621	-0.373207	-1.097739
H	3.663574	0.243516	-0.864515
H	3.101135	-1.420321	-1.091783
H	2.440960	-0.115691	-2.098610

CRBb3

C	-1.280156	0.515111	-0.146460
C	-1.056997	0.779254	1.330861
H	-0.129133	1.335651	1.467657
H	-1.895867	1.367725	1.708545
H	-1.024077	-0.153133	1.893179
C	-2.610498	-0.180599	-0.444205
H	-2.588364	-0.539337	-1.481873
H	-3.400263	0.570113	-0.365232
O	-2.947522	-1.211364	0.450849
O	-0.199624	-0.370485	-0.646281
O	-0.145516	-1.523569	-0.058659
H	-2.214830	-1.835893	0.470130
C	2.519263	-0.765316	0.398620
C	2.888925	-0.725557	-1.021609
H	3.217370	-1.700409	-1.371322
H	2.021118	-0.366102	-1.583475
H	3.663422	0.036994	-1.155137
O	2.021195	1.409331	0.280621
O	2.124165	0.250784	1.004568
H	2.562195	-1.650018	1.027113
C	-1.103091	1.759488	-0.995856
H	-1.794935	2.531256	-0.654500
H	-0.079903	2.122030	-0.882792
H	-1.302989	1.549269	-2.049174

CPBb3

C	1.872591	-0.019724	0.094912
C	1.569899	-0.337992	1.550042
H	1.922878	-1.341021	1.794949
H	2.069928	0.388674	2.194272
H	0.500935	-0.270671	1.750641
C	1.412485	1.393799	-0.294390
H	1.393974	1.460801	-1.388353
H	2.173182	2.090343	0.070953
O	0.190776	1.786845	0.279328
O	1.269926	-1.021965	-0.768553
O	-0.161453	-0.860245	-0.731967
H	-0.550593	1.591921	-0.312547
C	-2.650871	0.391635	0.257257

H	-3.859936	-0.811288	0.261228
O	-1.795692	1.481481	-0.488967
O	-1.930433	0.357370	-1.116915
H	-1.774522	-1.631162	-0.916229
C	2.599038	-0.623923	-1.204015
H	3.584522	-0.212734	-0.980129
H	2.683264	-1.708989	-1.279645
H	2.260723	-0.229931	-2.164749

TSBb3

C	1.766570	-0.116026	0.026366
C	1.451007	-0.221979	1.509375
H	1.542474	-1.259937	1.833865
H	2.159751	0.391222	2.071212
H	0.448902	0.138054	1.730779
C	1.601237	1.308383	-0.513996
H	1.610844	1.260040	-1.610498
H	2.469545	1.889683	-0.195091
O	0.472352	2.004647	-0.037693
O	0.929962	-1.039254	-0.735294
O	-0.326973	-0.589023	-0.906163
H	-0.309878	1.533588	-0.341012
C	-2.699095	0.554332	0.396586
C	-3.441687	-0.030461	-0.738499
H	-4.222455	0.659018	-1.055090
H	-2.779893	-0.239522	-1.584687
H	-3.898478	-0.986579	-0.453502
O	-1.286157	-1.194873	0.328599
O	-1.741934	-0.147027	1.029850
H	-2.974817	1.428185	0.967530
C	3.163449	-0.629563	-0.294628
H	3.901111	-0.091202	0.302368
H	3.232501	-1.692476	-0.057966
H	3.393504	-0.493963	-1.353517

CRBb4

C	1.769775	0.072894	-0.068065
C	2.340960	-0.642170	1.138226
H	2.788257	-1.593863	0.845445
H	3.116976	-0.008548	1.572912
H	1.569322	-0.818968	1.884142
C	0.954423	1.308713	0.323274
H	0.517488	1.743480	-0.583921
H	1.654625	2.039722	0.749272
O	-0.040906	0.976639	1.249478
O	0.827757	-0.802361	-0.796157
O	0.235162	-1.694341	-0.069454
H	-0.898064	1.315849	0.906416
C	-2.192259	-0.674402	-0.630245

C	-3.900026	-0.423751	0.360949	O	-2.292818	1.496146	-0.056928
H	-4.461698	-0.124552	1.249470	O	-2.064698	0.507459	-1.003685
H	-4.508923	-0.308516	-0.533675	C	-2.578680	-1.044593	0.737863
H	-3.613872	-1.470974	0.492950	H	-3.445979	-0.448224	1.033067
O	-0.705199	-1.771034	-0.056861	H	-2.764279	-2.113198	0.807288
O	-2.346412	1.045250	-0.710236	H	-1.754981	-0.760401	1.403875
H	-1.973825	0.368326	1.132781	H	-1.991699	-1.391755	-1.420919
C	3.349656	-0.190431	-0.236489	C	2.815404	0.419628	-1.113207
H	3.945527	0.432341	0.432685	H	3.501157	1.168105	-0.712180
H	3.647907	-1.231173	-0.102659	H	3.389448	-0.466599	-1.388125
H	3.551067	0.102476	-1.268835	H	2.344004	0.825649	-2.010372
TSBb4				CPBb4			
C	1.723973	-0.121860	-0.062350	C	1.692163	-0.172021	-0.053886
C	2.135214	-0.752724	1.252206	C	2.144219	-0.501521	1.360045
H	2.332477	-1.818509	1.117548	H	2.496531	-1.534051	1.393535
H	3.051775	-0.269048	1.594898	H	2.961039	0.160707	1.655022
H	1.358740	-0.610392	2.001289	H	1.325697	-0.377418	2.066309
C	1.167639	1.338487	0.161502	C	1.229519	1.313079	-0.185934
H	0.881820	1.739493	-0.820084	H	0.779906	1.455829	-1.175710
H	2.042098	1.890396	0.538117	H	2.148604	1.914084	-0.083911
O	0.148872	1.360831	1.061419	O	0.400278	1.665970	0.836687
O	0.605336	-0.815589	-0.652607	O	0.625248	-1.014056	-0.469255
O	-0.320101	-1.101369	0.231171	O	-0.470693	-0.858146	0.428038
H	-0.799448	1.470128	0.543077	H	-1.361500	1.745486	0.310020
C	-1.904589	-0.749064	-0.527400	C	-1.638633	-0.782856	-0.369896
O	-1.956998	1.488629	-0.159223	O	-2.198919	1.440693	-0.085769
O	-1.775511	0.410329	-1.074903	O	-1.744535	0.460332	-1.008066
C	-2.742040	-0.945628	0.692713	C	-2.797837	-1.124040	0.539390
H	-3.755129	-0.618446	0.448422	H	-3.730490	-0.922800	0.013016
H	-2.745124	-1.997037	0.975994	H	-2.746277	-2.177971	0.809989
H	-2.375550	-0.324229	1.506259	H	-2.767919	-0.515193	1.440832
H	-1.876633	-1.531996	-1.283374	H	-1.530550	-1.479709	-1.204460
C	2.797012	-0.143450	-1.131860	C	2.772577	-0.444926	-1.091410
H	3.617504	0.508039	-0.827043	H	3.680363	0.103022	-0.834229
H	3.189801	-1.152375	-1.267783	H	3.000277	-1.511521	-1.106198
H	2.401625	0.216780	-2.083060	H	2.441219	-0.145117	-2.087153
CRBb5				TSBb5			
C	-1.960057	-0.178912	0.032629	C	1.759931	-0.335580	0.048120
C	-3.026205	0.084927	-1.016731	C	2.937037	0.014380	0.941178
H	-3.517198	-0.853687	-1.279316	H	3.147533	-0.820691	1.612171
H	-3.778430	0.770987	-0.623063	H	3.824798	0.202925	0.335186
H	-2.588488	0.519844	-1.915738	H	2.720628	0.901858	1.536822
C	-2.518708	-0.768877	1.312760	C	2.039047	-1.500578	-0.880920
H	-3.312752	-0.133085	1.708408	H	2.906696	-1.283779	-1.506070
H	-2.930465	-1.758217	1.104160	H	2.249506	-2.393588	-0.289236
H	-1.727653	-0.874803	2.054049	H	1.173224	-1.696103	-1.512503
C	-0.815190	-1.006398	-0.536092	C	0.486037	-0.534783	0.861783

H	-0.334082	-0.433012	-1.337805
H	-1.249612	-1.912778	-0.978653
O	0.101759	-1.325507	0.481023
O	-1.406674	1.122089	0.472775
O	-0.936818	1.834782	-0.499623
H	0.974840	-1.427348	0.054768
C	3.181183	0.573075	0.485414
C	1.949241	1.336795	0.271120
H	1.120627	0.794552	0.747430
H	2.025043	2.340132	0.681107
H	1.711573	1.346306	-0.796554
O	2.434850	-1.037515	-0.887951
O	3.400199	-0.533371	-0.046371
H	3.998485	0.893616	1.127772

CPBb5

C	1.653383	-0.413577	0.038345
C	2.984075	-0.302563	0.764356
H	3.152022	-1.201633	1.359726
H	3.795468	-0.208115	0.040671
H	2.997585	0.567873	1.421344
C	1.575736	-1.617024	-0.880120
H	2.412157	-1.609903	-1.580663
H	1.621502	-2.530621	-0.284596
H	0.638228	-1.623161	-1.436121
C	0.493834	-0.356563	1.035343
H	0.474873	0.634447	1.500888
H	0.692658	-1.093946	1.815808
O	-0.754859	-0.706830	0.490061
O	1.535427	0.734566	-0.885492
O	1.635490	1.881017	-0.291883
H	-3.067476	-1.344853	0.760412
C	-1.397079	0.232023	-0.361363
C	-1.641503	1.575152	0.298538
H	-0.714303	2.141973	0.388126
H	-2.328849	2.143407	-0.328672
H	-2.089958	1.438532	1.282260
O	-3.434835	-0.554872	0.340164
O	-2.575231	-0.398924	-0.779028
H	-0.842528	0.341654	-1.300357

TSBb6

C	1.216478	0.491535	0.097077
C	1.045025	1.416663	1.289242
H	2.034489	1.724158	1.637063
H	0.486767	2.318601	1.040998
H	0.546784	0.883191	2.099726
C	1.445920	1.211043	-1.218938
H	0.622775	1.889188	-1.455860

H	0.310315	0.355691	1.477014
H	0.640652	-1.386005	1.535916
O	-0.589538	-0.791321	-0.002250
O	1.524003	0.790448	-0.880230
O	1.261192	1.904140	-0.277625
H	-1.472149	-1.155122	0.493961
C	-1.980042	0.519413	-0.605917
C	-1.887525	1.494004	0.510040
H	-0.914297	1.982674	0.510188
H	-2.644079	2.256892	0.290071
H	-2.117803	1.032951	1.465768
O	-2.903278	-1.072476	0.619959
O	-2.832363	-0.426242	-0.660172
H	-1.632055	0.824767	-1.592446

CRBb6

C	-1.441538	-0.510604	0.016779
C	-1.249403	-1.791483	0.808132
H	-2.142534	-1.986112	1.404430
H	-1.098111	-2.634032	0.130555
H	-0.380296	-1.696586	1.461446
C	-2.643915	-0.543667	-0.909663
H	-2.617872	-1.439838	-1.532231
H	-3.556833	-0.552491	-0.310989
H	-2.665567	0.342527	-1.543395
C	-1.435307	0.702869	0.949089
H	-0.435508	0.796262	1.385270
H	-2.134585	0.483637	1.759309
O	-1.881603	1.901338	0.357207
O	-0.234089	-0.476921	-0.846093
O	0.001327	0.676118	-1.385233
H	-1.258888	2.120756	-0.341927
C	2.527696	0.623552	-0.317130
C	2.913132	-0.682203	-0.865505
H	3.393119	-0.577185	-1.834594
H	3.564081	-1.181900	-0.140485
H	2.011304	-1.299724	-0.926422
O	1.713674	-0.426611	1.478604
O	1.976381	0.733192	0.796666
H	2.692185	1.576965	-0.810401

CPBb6

C	-1.152867	0.117050	0.539257
C	-1.396887	1.443628	1.229671
H	-2.441956	1.483591	1.546228
H	-0.780738	1.578482	2.121059
H	-1.219730	2.253610	0.519440
C	-0.977349	-1.065715	1.471714
H	-0.152325	-0.934720	2.173728

H	2.354500	1.811471	-1.140168
H	1.577890	0.490159	-2.027094
C	2.343097	-0.513930	0.386611
H	2.184645	-0.929457	1.386997
H	3.293015	0.025787	0.374045
O	2.428711	-1.524546	-0.583759
O	0.037056	-0.364107	-0.142046
O	-0.325009	-1.075511	0.968830
H	1.635713	-2.066643	-0.506853
C	-1.623791	0.313656	-0.845380
C	-1.916491	1.456548	0.054879
H	-1.390743	2.351805	-0.270113
H	-2.997210	1.627114	0.017751
H	-1.667567	1.191187	1.081597
O	-2.682432	-0.988849	0.582898
O	-2.263591	-0.799405	-0.694269
H	-1.300373	0.449695	-1.872261

CRBc1

C	-1.356641	0.468524	-0.080584
C	-1.061649	0.646242	1.397087
H	-0.161830	1.252106	1.515046
H	-1.909122	1.150789	1.865851
H	-0.936694	-0.319907	1.885467
C	-2.630537	-0.332477	-0.359816
H	-2.625700	-0.631026	-1.416729
H	-3.477825	0.339823	-0.206670
O	-2.838576	-1.434869	0.487607
O	-0.216651	-0.264893	-0.689713
O	-0.089755	-1.481833	-0.263793
H	-2.063839	-2.002282	0.421090
C	2.537563	-0.194379	-0.369486
O	1.773934	1.833681	0.195088
O	2.329306	0.621878	0.540532
C	3.120896	-1.513302	-0.047736
H	2.417282	-2.285960	-0.367855
H	4.049306	-1.649674	-0.608303
H	3.311029	-1.599546	1.020244
H	2.264541	0.120224	-1.375780
C	-1.354594	1.779545	-0.843622
H	-2.082144	2.457614	-0.394604
H	-0.361685	2.227091	-0.778356
H	-1.619604	1.624114	-1.892228

CPBc1

C	-1.464272	0.356520	-0.091730
C	-1.088337	0.804961	1.311486
H	-0.606400	1.783705	1.275641
H	-1.989945	0.869457	1.924480

H	-1.895384	-1.169568	2.054008
H	-0.819193	-1.977402	0.894074
C	-2.243419	-0.154983	-0.509554
H	-2.516316	0.788145	-0.987716
H	-3.111914	-0.545839	0.027944
O	-1.850981	-1.114517	-1.447035
O	0.105714	0.213222	-0.280265
O	-0.087793	1.067503	-1.439922
H	-1.173436	-0.678712	-1.986279
C	1.351494	0.426219	0.412674
C	2.314004	1.245680	-0.393780
H	1.899522	2.237692	-0.553471
H	3.246025	1.306274	0.171111
H	2.481406	0.774906	-1.359308
O	2.209935	-1.537012	-0.359695
O	1.869351	-0.882645	0.711915
H	1.144387	0.839855	1.399314

TSBc1

C	-1.398363	0.396756	0.045156
C	-0.855169	0.367243	1.461424
H	-0.163756	1.195806	1.611801
H	-1.696090	0.463415	2.151664
H	-0.357002	-0.577384	1.673949
C	-2.475954	-0.665984	-0.194727
H	-2.703350	-0.692071	-1.268132
H	-3.378930	-0.356788	0.337035
O	-2.140514	-1.943367	0.290414
O	-0.332620	0.127919	-0.940336
O	0.362108	-0.955966	-0.689738
H	-1.281778	-2.183502	-0.074685
C	2.362272	-0.155264	-0.342983
O	1.508960	1.881387	-0.052652
O	2.022157	0.740137	0.478850
C	2.990486	-1.388299	0.181878
H	2.620053	-2.245819	-0.380352
H	4.074470	-1.332203	0.045928
H	2.763708	-1.507430	1.240125
H	2.346892	0.120908	-1.392747
C	-1.886093	1.774464	-0.362253
H	-2.667129	2.102971	0.325617
H	-1.050057	2.473659	-0.317005
H	-2.290827	1.764061	-1.376477

CRBc2

C	-1.668800	-0.311333	0.174367
C	-2.504856	-0.405918	-1.084122
H	-2.562811	-1.439501	-1.431664
H	-3.513686	-0.057461	-0.852808

H	-0.412727	0.094423	1.785507	H	-2.085539	0.222011	-1.867121
C	-2.203477	-0.986584	-0.101031	C	-1.392978	1.146485	0.580053
H	-2.250809	-1.339516	-1.139247	H	-0.722722	1.144871	1.448978
H	-3.224992	-0.817647	0.247679	H	-2.353368	1.575486	0.890210
O	-1.659419	-1.967498	0.752723	O	-0.869956	1.901544	-0.466002
O	-0.296810	0.282482	-0.942420	O	-0.342436	-0.922306	-0.046040
O	0.571189	-0.748688	-0.464435	O	0.139086	-0.754187	-1.236772
H	-0.748951	-2.116647	0.482714	H	0.100700	1.950871	-0.339195
C	1.859660	-0.232765	-0.456117	C	2.482810	-0.218513	-0.245321
O	1.875659	1.923374	0.309009	O	1.764940	1.857095	0.189727
O	1.995970	0.677624	0.662826	O	2.063625	0.565681	0.616817
C	2.810585	-1.378537	-0.225026	C	2.809297	-1.606667	0.137907
H	2.722482	-2.097024	-1.038975	H	2.204574	-2.277708	-0.476224
H	3.831208	-1.000215	-0.182702	H	3.861930	-1.806428	-0.078327
H	2.573889	-1.870016	0.719603	H	2.601717	-1.772764	1.192781
H	2.042327	0.357254	-1.355936	H	2.598619	0.176702	-1.253120
C	-2.299594	1.403602	-0.818274	C	-2.231798	-1.104632	1.339320
H	-3.187301	1.634920	-0.227640	H	-3.181789	-0.667981	1.652272
H	-1.718800	2.317987	-0.948067	H	-2.405983	-2.142491	1.050436
H	-2.610081	1.041782	-1.800523	H	-1.545779	-1.084753	2.188712
TSBc2				CPBc2			
C	1.608491	-0.284547	-0.108618	C	1.497908	-0.373770	-0.128682
C	2.312375	-0.166672	1.229154	C	2.193446	-0.556600	1.211012
H	2.568971	-1.155922	1.613573	H	2.281719	-1.619886	1.442234
H	3.229313	0.410588	1.094998	H	3.191634	-0.115348	1.170017
H	1.679489	0.362691	1.938661	H	1.639949	-0.055705	2.003580
C	1.212300	1.090803	-0.676613	C	1.405006	1.102811	-0.539366
H	0.490932	0.940582	-1.490452	H	0.673411	1.187018	-1.353290
H	2.130460	1.499648	-1.117526	H	2.381413	1.397907	-0.932727
O	0.740735	1.979380	0.281440	O	1.120760	1.997036	0.508337
O	0.391186	-1.098994	0.060720	O	0.189544	-0.985743	-0.094771
O	-0.403200	-0.648386	1.000762	O	-0.597937	-0.290867	0.882907
H	-0.239898	2.045156	0.194672	H	0.185290	1.916045	0.720866
C	-2.139745	-0.348612	0.309792	C	-1.911332	-0.309794	0.459737
O	-1.873580	1.835350	-0.139370	O	-1.709557	1.796939	-0.395960
O	-1.939740	0.535568	-0.592744	O	-2.086207	0.590476	-0.680603
C	-2.502438	-1.706955	-0.176538	C	-2.448958	-1.646288	0.017060
H	-2.354828	-2.434946	0.618845	H	-2.299033	-2.370031	0.817893
H	-3.553975	-1.705843	-0.473551	H	-3.514118	-1.557343	-0.195420
H	-1.889995	-1.969218	-1.038729	H	-1.926548	-1.985220	-0.875344
H	-2.456843	0.034307	1.276900	H	-2.459256	0.135292	1.292960
C	2.391444	-1.085185	-1.134137	C	2.175556	-1.167221	-1.239451
H	3.365246	-0.619052	-1.289550	H	3.228335	-0.886598	-1.296826
H	2.549222	-2.105931	-0.782405	H	2.111459	-2.236313	-1.031364
H	1.864138	-1.118402	-2.090137	H	1.703162	-0.967373	-2.203718
CRBc3				TSBc3			
C	-1.356826	0.468457	-0.080434	C	1.725271	0.106584	0.166235

C	-1.061946	0.645994	1.397279
H	-0.161998	1.251643	1.515310
H	-1.909317	1.150822	1.865919
H	-0.937288	-0.320175	1.885670
C	-2.630581	-0.332740	-0.359852
H	-2.625701	-0.630977	-1.416851
H	-3.478041	0.339284	-0.206457
O	-2.838278	-1.435439	0.487263
O	-0.216818	-0.264672	-0.689770
O	-0.089237	-1.481421	-0.263488
H	-2.063305	-2.002534	0.420770
C	2.537713	-0.194390	-0.369577
C	3.121343	-1.513071	-0.047364
H	4.050320	-1.648987	-0.607116
H	3.310633	-1.599204	1.020777
H	2.418398	-2.286080	-0.368062
O	1.773716	1.833714	0.194429
O	2.329132	0.622063	0.540201
H	2.264759	0.119919	-1.375985
C	-1.355002	1.779620	-0.843238
H	-2.082870	2.457396	-0.394300
H	-0.362231	2.227432	-0.777691
H	-1.619685	1.624290	-1.891942

CPBc3

C	1.624299	0.135865	0.201028
C	1.042921	0.489192	1.559834
H	1.296670	-0.289405	2.281680
H	1.465717	1.438132	1.898931
H	-0.037698	0.594453	1.515124
C	1.299681	1.185283	-0.868274
H	1.549611	0.769337	-1.851924
H	1.950621	2.044715	-0.691725
O	-0.018069	1.684886	-0.835635
O	1.196417	-1.192462	-0.222936
O	-0.032150	-1.168343	-0.905980
H	-0.613048	0.993709	-1.145680
C	-2.554318	-0.108373	-0.207737
C	-3.078611	1.144030	0.389855
H	-3.665547	0.950254	1.296457
H	-2.253262	1.811255	0.652650
H	-3.722728	1.650959	-0.328816
O	-0.996836	-1.769625	-0.117927
O	-1.673901	-0.759323	0.615359
H	-3.112749	-0.746726	-0.884350
C	3.135391	-0.056337	0.274974
H	3.598805	0.829330	0.712601
H	3.370775	-0.917134	0.902941

C	1.174651	0.047985	1.581720
H	1.449093	-0.900944	2.045747
H	1.601530	0.866018	2.167232
H	0.092670	0.154422	1.592490
C	1.317562	1.382726	-0.576704
H	1.576405	1.260452	-1.635999
H	1.915638	2.204869	-0.176703
O	0.030696	1.766414	-0.418985
O	1.304239	-1.073144	-0.586123
O	0.055836	-0.981938	-1.066985
H	0.569631	1.092730	-0.846081
C	2.669682	-0.188330	-0.257799
C	3.392149	0.996538	0.256590
H	4.123630	0.729113	1.029060
H	2.685866	1.710157	0.688837
H	3.927334	1.481956	-0.559366
O	1.023881	-1.686597	0.050289
O	1.755623	-0.700654	0.580339
H	2.957097	-0.819086	-1.088997
C	3.241206	-0.036753	0.144183
H	3.695136	0.732482	0.770774
H	3.527149	-1.015389	0.532711
H	3.625785	0.058060	-0.873331

CRBc4

C	-1.668803	-0.311326	0.174370
C	-2.504864	-0.405904	-1.084116
H	-2.562821	-1.439484	-1.431664
H	-3.513693	-0.057447	-0.852796
H	-2.085549	0.222032	-1.867113
C	-1.392960	1.146490	0.580047
H	-0.722694	1.144874	1.448964
H	-2.353342	1.575506	0.890211
O	-0.869939	1.901536	-0.466018
O	-0.342447	-0.922317	-0.046035
O	0.139074	-0.754217	-1.236771
H	0.100717	1.950866	-0.339210
C	2.482808	-0.218517	-0.245322
C	2.809293	-1.606671	0.137909
H	3.861923	-1.806436	-0.078336
H	2.601724	-1.772761	1.192786
H	2.204560	-2.277712	-0.476213
O	1.764950	1.857097	0.189727
O	2.063633	0.565682	0.616817
H	2.598607	0.176694	-1.253124
C	-2.231810	-1.104611	1.339328
H	-3.181793	-0.667943	1.652281
H	-2.406012	-2.142468	1.050448

H	3. 552960	-0. 227906	-0. 719029
TSBc4			
C	1. 635902	-0. 284833	-0. 119747
C	2. 263388	-0. 437729	1. 250401
H	2. 289324	-1. 489786	1. 542832
H	3. 287878	-0. 063813	1. 204144
H	1. 709290	0. 140150	1. 987525
C	1. 333118	1. 228286	-0. 438889
H	0. 871903	1. 272442	-1. 434707
H	2. 329710	1. 692214	-0. 481431
O	0. 567582	1. 802763	0. 527815
O	0. 328380	-0. 900352	-0. 169339
O	0. 391940	-0. 619516	0. 887959
H	0. 455800	1. 854401	0. 199187
C	2. 077268	-0. 332568	0. 302284
C	2. 533252	-1. 706690	-0. 064252
H	3. 600152	-1. 662197	-0. 292358
H	1. 997513	-2. 051528	-0. 948254
H	2. 372809	-2. 393689	0. 764774
O	1. 758133	1. 827970	-0. 238436
O	1. 962982	0. 484102	-0. 678229
H	2. 357811	0. 111553	1. 256549
C	2. 410917	-0. 944126	-1. 242228
H	3. 357684	-0. 418753	-1. 377227
H	2. 626604	-1. 987518	-1. 006431
H	1. 851603	-0. 897255	-2. 178172

CRBc5

C	-1. 823422	-0. 135432	0. 070928
C	-2. 962538	0. 060419	-0. 913112
H	-3. 560911	-0. 851141	-0. 960664
H	-3. 606187	0. 879397	-0. 587112
H	-2. 580769	0. 284936	-1. 909561
C	-2. 293725	-0. 374809	1. 492239
H	-2. 936063	0. 443382	1. 822607
H	-2. 864065	-1. 304846	1. 529999
H	-1. 438509	-0. 466460	2. 160784
C	-0. 847751	-1. 206382	-0. 401377
H	-0. 462922	-0. 922845	-1. 389547
H	-1. 414724	-2. 139785	-0. 519245
O	0. 181160	-1. 339595	0. 540705
O	-1. 075103	1. 141605	0. 176444
O	-0. 601326	1. 556851	-0. 952737
H	0. 978390	-1. 724825	0. 109861
C	2. 120699	0. 554194	-0. 167562
C	2. 223840	1. 802779	0. 607457
H	2. 366953	2. 644893	-0. 073062
H	1. 258488	1. 954416	1. 101917

H	-1. 545788	-1. 084740	2. 188718
CPBc4			
C	1. 584310	-0. 212243	-0. 077157
C	2. 266835	-0. 032973	1. 269744
H	2. 580263	-1. 008243	1. 646585
H	3. 147340	0. 603850	1. 160636
H	1. 591406	0. 430121	1. 986273
C	1. 166624	1. 154583	-0. 704835
H	0. 544970	0. 961353	-1. 587406
H	2. 111710	1. 644447	-0. 992826
O	0. 559200	1. 955890	0. 215189
O	0. 426846	-1. 030404	0. 029713
O	-0. 483117	-0. 423011	0. 943347
H	-1. 261111	2. 005086	0. 005234
C	-1. 786917	-0. 519739	0. 388614
C	-2. 114046	-1. 895804	-0. 147888
H	-3. 182736	-1. 951688	-0. 350748
H	-1. 563879	-2. 082531	-1. 068460
H	-1. 840774	-2. 648790	0. 591053
O	-2. 174739	1. 682253	-0. 106911
O	-1. 968536	0. 389355	-0. 656431
H	-2. 413699	-0. 226676	1. 234229
C	2. 451098	-0. 968077	-1. 075001
H	3. 413874	-0. 466505	-1. 184277
H	2. 624441	-1. 981421	-0. 710550
H	1. 963548	-1. 026153	-2. 049853

TSBc5

C	-1. 726036	-0. 254020	0. 121132
C	-2. 935666	-0. 460707	-0. 773091
H	-3. 282437	-1. 492354	-0. 689135
H	-3. 746837	0. 203105	-0. 469334
H	-2. 681675	-0. 256889	-1. 814239
C	-2. 035959	-0. 399375	1. 597844
H	-2. 808931	0. 311598	1. 894489
H	-2. 398267	-1. 410476	1. 792860
H	-1. 136688	-0. 233338	2. 190729
C	-0. 556533	-1. 126679	-0. 314526
H	-0. 343438	-0. 935716	-1. 375246
H	-0. 868698	-2. 174697	-0. 223460
O	0. 573382	-0. 888913	0. 483616
O	-1. 304208	1. 159763	0. 002457
O	-0. 898075	1. 480849	-1. 183354
H	1. 423531	-1. 455784	0. 046827
C	1. 876922	0. 534334	-0. 162201
C	1. 756635	1. 772561	0. 638152
H	1. 946807	2. 633021	-0. 007862
H	0. 731342	1. 853801	1. 000069

H	3.025564	1.747621	1.340541
O	2.572483	-1.589389	-0.598456
O	2.836819	-0.417226	0.113254
H	1.419878	0.432672	-0.991641

CPBc5

C	1.675523	-0.207039	-0.236192
C	2.806096	-1.051251	0.325292
H	3.007915	-1.887863	-0.346482
H	3.713817	-0.451782	0.413346
H	2.544284	-1.441667	1.309366
C	2.013611	0.439241	-1.565407
H	2.905582	1.059914	-1.466246
H	2.207758	-0.336201	-2.308924
H	1.181264	1.051866	-1.911815
C	0.372829	-1.004195	-0.293080
H	0.124783	-1.376363	0.705900
H	0.532164	-1.860784	-0.953891
O	-0.690396	-0.249774	-0.830006
O	1.461754	0.948836	0.656632
O	1.160427	0.609730	1.869822
H	-2.661852	-1.943914	-0.444491
C	-1.536761	0.406353	0.087955
C	-1.660911	1.870369	-0.260760
H	-2.375619	2.357399	0.402205
H	-0.684549	2.342570	-0.150043
H	-1.997034	1.968772	-1.293825
O	-2.768426	-1.484202	0.398587
O	-2.831818	-0.130310	-0.021266
H	-1.173159	0.242928	1.107900

TSBc6

C	1.339405	0.281963	0.041886
C	2.312470	0.603940	1.164161
H	3.335436	0.512916	0.792807
H	2.159764	1.625123	1.517388
H	2.170566	-0.084140	1.996777
C	1.427711	1.302324	-1.080095
H	1.144584	2.294305	-0.722596
H	2.467196	1.353956	-1.409243
H	0.825423	1.026182	-1.945612
C	1.530373	-1.154602	-0.442715
H	1.489583	-1.822983	0.420052
H	2.531761	-1.209309	-0.879642
O	0.607593	-1.537446	-1.432043
O	-0.019219	0.433438	0.652368
O	-0.246934	-0.545819	1.584012
H	-0.195146	-1.831705	-0.970867
C	-1.434478	0.481057	-0.403644

H	2.455294	1.753790	1.472011
O	2.637897	-1.484850	-0.544287
O	2.872953	-0.219885	0.074375
H	1.378226	0.431551	-1.124017

CRBc6

C	1.731949	0.003507	-0.044088
C	2.785215	0.356755	0.990279
H	3.569367	-0.402336	0.979317
H	3.236624	1.322925	0.756833
H	2.350330	0.401005	1.989006
C	2.273129	-0.028442	-1.459794
H	2.741135	0.925033	-1.711505
H	3.022375	-0.818367	-1.539846
H	1.470547	-0.244718	-2.164254
C	0.989670	-1.277615	0.321041
H	0.494413	-1.130530	1.287945
H	1.739574	-2.071247	0.437587
O	0.062086	-1.606455	-0.679176
O	0.729779	1.094810	-0.089036
O	0.196809	1.349762	1.063765
H	-0.780998	-1.866563	-0.238443
C	-2.181450	0.300697	-0.523827
C	-2.278397	1.771850	-0.577929
H	-3.099241	2.044760	-1.247647
H	-2.433495	2.186687	0.414933
H	-1.351327	2.164403	-1.002689
O	-2.260870	-1.672823	0.546359
O	-2.339071	-0.284179	0.558446
H	-1.989865	-0.320477	-1.398187

CPBc6

C	1.283952	-0.306878	0.043239
C	2.117748	-1.184479	-0.872874
H	3.168622	-1.057862	-0.605241
H	1.839644	-2.230987	-0.745295
H	1.961600	-0.914054	-1.914643
C	1.552714	-0.613202	1.506252
H	1.320242	-1.657570	1.723758
H	2.616365	-0.452927	1.692558
H	1.014066	0.047790	2.183215
C	1.452748	1.163063	-0.312616
H	0.960088	1.329320	-1.275744
H	2.524367	1.345102	-0.433231
O	0.978198	2.035472	0.690620
O	-0.133753	-0.742322	-0.235776
O	-0.462038	-0.825553	-1.650438
H	0.106974	2.336968	0.417115
C	-1.258385	-0.280804	0.531155

C	-1.920860	1.888943	-0.344494
H	-2.813321	1.976072	-0.968258
H	-2.173506	2.145988	0.683476
H	-1.161884	2.569884	-0.723974
O	-1.661732	-1.619440	0.230596
O	-2.225495	-0.366332	0.201858
H	-0.941887	0.106755	-1.295239

CRBd1

C	-0.922444	0.538728	-0.090993
C	-0.398956	1.709230	-0.902113
H	-0.973781	2.603062	-0.654243
H	0.649076	1.883757	-0.652336
H	-0.495050	1.517312	-1.973475
C	-0.839187	0.773551	1.405363
H	0.180382	1.058309	1.668884
H	-1.528972	1.574863	1.677962
H	-1.131280	-0.122181	1.952997
C	-2.312421	0.113973	-0.570967
H	-2.217369	-0.286300	-1.589269
H	-2.927924	1.014864	-0.622952
O	-2.988993	-0.780691	0.275871
O	0.033572	-0.547171	-0.426074
O	-0.309459	-1.709595	0.030983
H	-2.437304	-1.563755	0.370460
C	2.683278	-1.140692	-0.147140
H	3.051950	-1.785162	-0.936824
H	2.156909	-1.482939	0.738375
O	2.426719	0.920334	0.650821
O	2.889629	0.069552	-0.299660

CPBd1

C	-1.207961	0.548119	0.047654
C	-1.563387	1.965667	-0.382273
H	-2.542417	2.234320	0.017626
H	-0.823318	2.670039	0.000093
H	-1.589729	2.044535	-1.470666
C	-1.223626	0.390612	1.560758
H	-0.578766	1.141805	2.022173
H	-2.240888	0.525071	1.934098
H	-0.899284	-0.607580	1.855154
C	-2.137809	-0.449427	-0.652291
H	-1.925956	-0.411093	-1.727947
H	-3.168702	-0.122948	-0.496212
O	-2.068553	-1.767983	-0.158591
O	0.137865	0.418381	-0.463987
O	0.606938	-0.906909	-0.209218
H	-1.181525	-2.097598	-0.327422
C	1.784034	-0.799313	0.502640

C	-2.119601	-1.466917	0.859207
H	-3.030546	-1.138913	1.359555
H	-2.365685	-1.975047	-0.073459
H	-1.567868	-2.142576	1.512139
O	-1.530861	1.731245	-0.525952
O	-2.082604	0.596837	-0.246963
H	-0.874475	0.280617	1.381168

TSBd1

C	-0.988036	0.554567	0.029130
C	-0.937671	1.996894	-0.439763
H	-1.635099	2.597880	0.146298
H	0.073958	2.382623	-0.307284
H	-1.208651	2.072588	-1.494895
C	-0.621563	0.399663	1.492907
H	0.343616	0.869815	1.682440
H	-1.387393	0.895497	2.093083
H	-0.600782	-0.649535	1.784763
C	-2.336460	-0.089929	-0.310260
H	-2.468956	-0.060748	-1.399026
H	-3.124326	0.514360	0.145587
O	-2.490004	-1.394748	0.191939
O	0.008018	-0.103708	-0.837045
O	0.310236	-1.324561	-0.471223
H	-1.758152	-1.931599	-0.131127
C	2.374925	-1.103354	0.299604
H	2.740646	-2.026745	-0.127107
H	1.918640	-1.012122	1.277321
O	2.250892	1.105420	0.181570
O	2.690773	-0.057285	-0.327712

CRBd2

C	1.402058	0.006376	-0.055858
C	2.391163	-0.604094	-1.032552
H	3.337072	-0.062138	-0.977740
H	2.574621	-1.648994	-0.778845
H	2.013987	-0.546563	-2.055937
C	1.862861	-0.062687	1.387119
H	2.059846	-1.095412	1.676116
H	2.784237	0.514173	1.490890
H	1.108731	0.373599	2.041601
C	0.987859	1.418796	-0.472964
H	0.554756	1.368281	-1.479780
H	1.899939	2.021835	-0.525642
O	0.111246	2.022298	0.433118
O	0.131066	-0.743452	-0.178665
O	0.198582	-1.982413	0.193173
H	-0.799645	1.778586	0.180909
C	-2.493851	-1.136548	-0.063085

H	2.048115	-1.816126	0.793486	H	-2.742078	-1.920766	0.643136
H	1.704120	-0.102636	1.338027	H	-2.168223	-1.301735	-1.085537
O	3.139114	0.915452	-0.122002	O	-2.284330	1.032241	-0.515775
O	2.845993	-0.332907	-0.345869	O	-2.597037	0.019835	0.355007
TSBd2				CPBd2			
C	1.275736	-0.224191	0.047041	C	1.192279	-0.316686	0.125682
C	2.424255	-1.143393	-0.341253	C	2.047386	-1.569772	0.014468
H	3.309512	-0.887692	0.243972	H	2.917243	-1.494525	0.670431
H	2.156965	-2.181362	-0.134902	H	1.467210	-2.444711	0.312756
H	2.661874	-1.042584	-1.402417	H	2.388398	-1.711560	-1.012998
C	0.954922	-0.269144	1.526811	C	0.725936	-0.056100	1.550357
H	0.882724	-1.295497	1.884434	H	0.173322	-0.911016	1.940219
H	1.758992	0.242470	2.059370	H	1.601971	0.107865	2.181645
H	0.027414	0.261680	1.739847	H	0.098452	0.833306	1.600119
C	1.508552	1.200471	-0.464801	C	1.914483	0.900124	-0.460104
H	1.422514	1.180906	-1.560316	H	2.158556	0.687780	-1.508825
H	2.538668	1.470709	-0.216164	H	2.848228	1.046383	0.086868
O	0.681141	2.162668	0.114154	O	1.172425	2.088697	-0.337334
O	0.113082	-0.686193	-0.754800	O	0.078948	-0.418187	-0.792349
O	-0.567217	-1.647368	-0.198197	O	-0.859732	-1.380921	-0.317037
H	-0.249756	1.942954	-0.078014	H	0.291716	1.931679	-0.696938
C	-2.496958	-0.854757	-0.050559	C	-2.101512	-0.807415	-0.474997
H	-2.828420	-1.622357	0.637625	H	-2.826744	-1.596747	-0.283277
H	-2.594688	-0.913505	-1.128045	H	-2.213538	-0.328822	-1.448920
O	-1.875900	1.235042	-0.421022	O	-2.002660	1.386239	0.119551
O	-2.236712	0.259646	0.466262	O	-2.336013	0.196606	0.530479
CRBd3				TSBd3			
C	1.468039	-0.131244	0.064875	C	-1.147924	0.545393	0.042410
C	2.372159	-1.079191	-0.701431	C	-1.679947	1.923353	-0.321705
H	3.328260	-0.585492	-0.883714	H	-2.553986	2.153231	0.289353
H	2.557014	-1.984016	-0.119013	H	-0.916275	2.679960	-0.134879
H	1.931350	-1.358932	-1.658276	H	-1.961921	1.965535	-1.375853
C	2.050181	0.314859	1.390470	C	-0.809555	0.433672	1.520297
H	2.327771	-0.547958	1.998803	H	-0.080081	1.198343	1.793635
H	2.941993	0.916176	1.203579	H	-1.719450	0.580014	2.106840
H	1.331039	0.933099	1.926262	H	-0.405857	-0.547519	1.760417
C	1.024442	1.051318	-0.805038	C	-2.129266	-0.535828	-0.421742
H	0.443295	0.653513	-1.646148	H	-2.134922	-0.540852	-1.519581
H	1.934197	1.512039	-1.204557	H	-3.127639	-0.251586	-0.080876
O	0.314535	2.020943	-0.094736	O	-1.889563	-1.820505	0.100228
O	0.237853	-0.858316	0.465134	O	0.073918	0.472399	-0.760107
O	-0.319760	-1.504996	-0.503662	O	0.582953	-0.766261	-0.817384
H	-0.634266	1.790564	-0.133020	H	-1.014488	-2.093073	-0.192281
C	-2.736619	-1.008608	0.189588	C	3.214203	0.407347	-0.413556
H	-2.908200	-1.723459	0.986902	H	3.670545	1.382207	-0.400722
H	-2.813307	-1.229929	-0.870073	H	3.476325	-0.431467	-1.038066
O	-2.212149	1.045283	-0.464556	O	1.674360	-0.944682	0.460765

O	-2.459024	0.139785	0.543878	O	2.318666	0.216747	0.561222
	CPBd3				CRBd4		
C	1.327121	0.029596	-0.252982	C	-1.485483	-0.059826	0.175362
C	2.068194	0.040354	-1.584581	C	-2.289329	-0.308988	1.438292
H	2.938303	0.695425	-1.509893	H	-3.116074	0.402072	1.489598
H	2.405474	-0.965186	-1.838217	H	-2.699817	-1.320045	1.441863
H	1.423443	0.407992	-2.385545	H	-1.664562	-0.177872	2.323835
C	2.167339	-0.582504	0.859277	C	-2.230300	-0.403287	-1.096687
H	2.375682	-1.631680	0.640978	H	-2.463865	-1.468992	-1.133886
H	3.115095	-0.044388	0.926593	H	-3.165864	0.160000	-1.104033
H	1.660527	-0.501981	1.819966	H	-1.643866	-0.129277	-1.971277
C	0.853422	1.443673	0.096561	C	-0.923957	1.371275	0.149613
H	0.237892	1.817428	-0.731030	H	-0.398387	1.558441	1.092910
H	1.736566	2.084404	0.181062	H	-1.781404	2.050803	0.086970
O	0.162681	1.514124	1.316099	O	-0.088364	1.589027	-0.946612
O	0.183992	-0.809098	-0.554004	O	-0.300797	-0.928058	0.336073
O	-0.469370	-1.197343	0.694849	O	0.207063	-1.362448	-0.770439
H	-0.764605	1.316392	1.135675	H	0.829314	1.459838	-0.637496
C	-2.725446	0.371204	-0.916511	C	2.594491	-0.984741	-0.222370
H	-3.782271	0.355442	-1.231963	H	2.742604	-2.012721	0.087265
H	-2.011318	-0.242522	-1.487345	H	2.570156	-0.650339	-1.255388
O	-1.439674	-1.930414	0.429635	O	2.293174	1.160591	0.310939
O	-2.372450	1.034574	0.022063	O	2.488828	-0.153924	0.684337
	TSBd4				CPBd4		
C	-1.457654	-0.062554	0.124192	C	1.432512	-0.050625	-0.081583
C	-2.387416	-0.408238	1.269251	C	2.474422	-0.451677	-1.116586
H	-3.167522	0.351886	1.334504	H	3.279384	0.284563	-1.136042
H	-2.862515	-1.377003	1.106944	H	2.894834	-1.422456	-0.851117
H	-1.844641	-0.430222	2.215760	H	2.029345	-0.524025	-2.110507
C	-2.085712	-0.167247	-1.249520	C	2.028835	0.142028	1.303701
H	-2.380512	-1.197775	-1.459018	H	2.571993	-0.760316	1.590264
H	-2.978796	0.460162	-1.265726	H	2.722507	0.985544	1.297484
H	-1.393444	0.184726	-2.011885	H	1.248943	0.340698	2.036167
C	-0.775515	1.334122	0.336982	C	0.690020	1.228103	-0.579845
H	-0.322656	1.338792	1.336934	H	0.157210	0.989026	-1.507646
H	-1.610921	2.048285	0.319145	H	1.482557	1.972112	-0.766244
O	0.124254	1.617308	-0.652031	O	-0.121954	1.739427	0.389082
O	-0.350532	-0.995865	0.265354	O	0.517636	-1.140143	-0.105847
O	0.405274	-1.041587	-0.794908	O	-0.531440	-0.887956	0.826336
H	1.091124	1.422357	-0.304371	H	-1.925882	1.385327	0.144069
C	2.116722	-1.131537	-0.202638	C	-1.730251	-1.216487	0.168422
H	2.114189	-2.162097	0.141493	H	-1.599241	-2.136794	-0.403152
H	2.508677	-0.872498	-1.183720	H	-2.464572	-1.312916	0.969462
O	2.387609	1.050214	0.217422	O	-2.706460	0.829723	-0.036600
O	2.231454	-0.274306	0.726705	O	-2.129071	-0.254652	-0.751394
	CRBd5				TSBd5		
C	-1.484633	-0.079811	0.178501	C	1.380071	0.417756	0.024535

C	-2.997143	-0.093588	0.321619	C	2.212875	1.651388	-0.283106
H	-3.323380	-1.070501	0.683811	H	1.728021	2.542591	0.119257
H	-3.321642	0.667353	1.032961	H	3.200764	1.555477	0.168940
H	-3.475100	0.098332	-0.640703	H	2.334752	1.774405	-1.360859
C	-0.773146	-0.117408	1.517517	C	1.266726	0.143622	1.512470
H	-0.972114	0.797688	2.078450	H	2.259551	0.023123	1.949083
H	-1.163562	-0.964079	2.086423	H	0.779769	0.997011	1.991243
H	0.303093	-0.246475	1.416767	H	0.696678	-0.764188	1.700790
C	-1.026652	-1.192983	-0.776581	C	0.024960	0.521509	-0.662341
H	-1.636585	-1.144433	-1.682007	H	0.172585	0.612964	-1.742719
H	-1.227680	-2.152818	-0.282420	H	-0.492839	1.425839	-0.312957
O	0.307813	-1.076287	-1.173781	O	-0.757744	-0.627068	-0.393685
O	-1.219838	1.190728	-0.519565	O	2.111720	-0.667177	-0.645091
O	-0.046604	1.689848	-0.315624	O	1.923605	-1.842340	-0.133467
C	2.389518	0.866232	-0.442586	C	-2.182849	-0.337902	1.007732
H	2.578685	1.930726	-0.354439	H	-1.686028	-0.000896	1.914396
H	2.003479	0.381175	-1.335801	H	-2.408041	-1.386008	0.840046
O	2.401891	-1.160379	0.525048	O	-3.125447	0.016010	-0.925265
O	2.638355	0.199607	0.568140	O	-2.801419	0.543574	0.359978
H	0.934207	-1.339754	-0.467605	H	-1.601630	-0.542555	-0.962727
CPBd5				CRBd6			
C	-1.451272	-0.393978	-0.016449	C	0.956829	0.520493	0.087840
C	-2.332030	-1.543655	-0.477939	C	0.632908	1.370910	1.302067
H	-1.965990	-2.486289	-0.066845	H	1.271023	2.257270	1.301622
H	-3.356662	-1.388365	-0.137869	H	-0.412352	1.679954	1.258871
H	-2.335595	-1.613370	-1.567470	H	0.810269	0.810614	2.221752
C	-1.494501	-0.187191	1.485093	C	0.628254	1.204735	-1.223489
H	-2.517706	0.017077	1.805196	H	-0.429324	1.473823	-1.239488
H	-1.151795	-1.099361	1.979305	H	1.224015	2.115949	-1.307371
H	-0.868732	0.651003	1.785983	H	0.870090	0.555520	-2.065517
C	-0.034198	-0.575086	-0.562117	C	2.385162	-0.017628	0.141558
H	-0.085045	-0.606662	-1.653200	H	2.556815	-0.489745	1.113711
H	0.371837	-1.531015	-0.211601	H	3.063795	0.832616	0.047177
O	0.815123	0.496904	-0.199830	O	2.684166	-0.899410	-0.917516
O	-2.014727	0.771867	-0.713085	O	0.042736	-0.650375	0.095612
O	-1.817002	1.905988	-0.118823	O	0.217986	-1.445349	1.103073
C	1.755356	0.202074	0.787942	H	2.226144	-1.729525	-0.759346
H	1.330423	-0.388982	1.605852	C	-2.620668	-1.154327	-0.130051
H	2.152955	1.155016	1.136650	H	-2.852906	-1.988322	-0.782458
O	3.570805	0.187433	-0.585410	H	-2.295063	-1.244565	0.901789
O	2.788318	-0.604972	0.293305	O	-2.444196	1.048417	0.132906
H	3.026044	0.220204	-1.384435	O	-2.741618	-0.030620	-0.633862
TSBd6				CPBd6			
C	0.848391	0.512022	0.215012	C	0.884265	0.582678	0.148136
C	0.128079	1.022326	1.450783	C	0.236734	1.319988	1.300258
H	0.871724	1.368415	2.173085	H	1.027175	1.795593	1.886779
H	-0.537853	1.854226	1.220584	H	-0.453636	2.094668	0.963564

H	-0.453711	0.215970	1.901295
C	1.286717	1.599165	-0.746393
H	0.440833	2.200378	-1.086003
H	1.975131	2.269494	-0.227801
H	1.802371	1.165720	-1.603999
C	2.023400	-0.385487	0.622214
H	1.684980	-1.082025	1.393786
H	2.797877	0.257971	1.046047
O	2.597507	-1.060317	-0.469589
O	-0.041835	-0.360983	-0.597073
O	-0.411675	-1.470976	0.075630
H	1.985661	-1.752360	-0.740691
C	-1.772183	0.304658	-1.143903
H	-1.540859	1.227594	-1.663760
H	-1.907069	-0.640190	-1.659158
O	-2.594135	-0.738623	0.608934
O	-2.325551	0.455737	-0.010360

CRCa1

C	2.657874	0.100237	0.260363
C	3.737204	-0.722980	-0.420880
H	4.675286	-0.167943	-0.404136
H	3.881566	-1.678315	0.086428
H	3.467044	-0.907243	-1.462913
C	1.317349	-0.610917	0.155934
H	0.904620	-0.558375	-0.851970
H	1.362047	-1.648223	0.482879
O	2.631066	1.363032	-0.376869
H	1.825402	1.822182	-0.116666
O	-0.026480	1.167259	0.673358
O	0.351671	-0.013232	1.059384
C	-2.388942	0.088828	-0.254767
C	-2.734234	1.413248	-0.831441
H	-2.391939	2.190618	-0.143877
H	-2.263397	1.544847	-1.803526
H	-3.820041	1.500645	-0.923701
C	-2.859014	-0.379006	1.062507
H	-3.491363	0.365175	1.541239
H	-3.381125	-1.330819	0.925723
H	-1.980397	-0.613137	1.671152
O	-1.307566	-1.875929	-0.421983
O	-1.657367	-0.650733	-0.953434
H	2.900275	0.220956	1.325418

CPCa1

C	2.466875	0.186286	0.309930
C	3.739204	-0.389510	-0.286304
H	4.521977	0.369006	-0.270619
H	4.080471	-1.259854	0.277308

H	-0.296045	0.611194	1.935498
C	1.389034	1.468508	-0.974899
H	0.616286	2.123046	-1.381551
H	2.170837	2.113416	-0.568844
H	1.821326	0.857237	-1.768240
C	1.989915	-0.356441	0.653628
H	1.659091	-0.817386	1.586474
H	2.866385	0.265415	0.855604
O	2.349169	-1.316574	-0.297836
O	-0.104308	-0.366117	-0.486933
O	-0.338721	-1.565770	0.296638
H	1.601736	-1.935300	-0.317246
C	-1.340795	0.100788	-0.996017
H	-1.148639	0.991847	-1.589153
H	-1.764729	-0.733120	-1.548728
O	-3.069058	-0.480191	0.336178
O	-2.218921	0.471187	0.046855

TSCa1

C	2.559410	0.118107	0.300761
C	3.745406	-0.439467	-0.466702
H	4.596598	0.231610	-0.350187
H	4.022520	-1.428920	-0.098713
H	3.506411	-0.506107	-1.530504
C	1.329688	-0.747867	0.069543
H	0.938661	-0.617142	-0.941098
H	1.529247	-1.801495	0.262913
O	2.354362	1.443409	-0.150686
H	1.489282	1.734622	0.158176
O	-0.249044	0.762155	0.750493
O	0.281462	-0.420961	1.006934
C	-2.135844	0.237752	-0.208409
C	-2.389241	1.594347	-0.759994
H	-2.159994	2.339243	0.002875
H	-1.778286	1.767059	-1.644131
H	-3.447917	1.686338	-1.021042
C	-2.781654	-0.280988	1.017617
H	-3.163247	0.541080	1.619230
H	-3.598148	-0.945464	0.713342
H	-2.071864	-0.889901	1.576824
O	-1.397010	-1.844629	-0.572146
O	-1.565918	-0.579886	-1.014836
H	2.779337	0.117075	1.377349

CRCa2

C	-1.842340	-0.338090	0.139504
C	-3.204978	-0.022940	0.725605
H	-3.473937	-0.774863	1.467733
H	-3.208584	0.962079	1.198507

H	3.568349	-0.680643	-1.325480	H	-3.956776	-0.039300	-0.067209
C	1.329569	-0.820047	0.211350	C	-1.388084	0.746766	-0.844172
H	1.009480	-0.943201	-0.827920	H	-0.527308	0.411384	-1.422784
H	1.640402	-1.786864	0.615676	H	-2.198655	1.057668	-1.504394
O	2.182850	1.377338	-0.403864	O	-1.901300	-1.560163	-0.545090
H	1.306377	1.679351	-0.147629	H	-0.990465	-1.914579	-0.548894
O	-0.412945	0.668662	0.475809	O	0.144021	1.808503	0.451556
O	0.208951	-0.488336	1.030600	O	-1.002333	1.949467	-0.136237
C	-1.709764	0.342296	0.041868	C	2.117084	-0.178320	0.014466
C	-2.272470	1.632915	-0.511254	C	2.850270	0.904923	-0.686958
H	-2.313762	2.380773	0.280099	H	3.923537	0.774287	-0.522075
H	-1.640366	1.995428	-1.322438	H	2.634553	0.893351	-1.753536
H	-3.277305	1.453295	-0.893021	H	2.557321	1.863113	-0.251975
C	-2.548953	-0.310600	1.115071	C	2.173446	-0.384216	1.473468
H	-2.676738	0.408485	1.924812	H	2.808315	0.359430	1.949350
H	-3.525806	-0.572171	0.707277	H	1.152000	-0.337699	1.860749
H	-2.067306	-1.206686	1.494955	H	2.519176	-1.403323	1.668867
O	-1.572625	-1.794984	-0.866419	O	0.767128	-1.976948	-0.057450
O	-1.565447	-0.524910	-1.132485	O	1.444498	-0.950360	-0.705458
H	2.621189	0.412878	1.373897	H	-1.087672	-0.384279	0.935623
TSCa2				CPCa2			
C	1.991794	0.162712	0.179426	C	2.313893	0.106470	0.330408
C	3.382287	-0.322206	0.543959	C	3.024065	-1.226978	0.428433
H	3.868305	0.396406	1.204137	H	3.722944	-1.220521	1.265303
H	3.331173	-1.290185	1.048469	H	2.299702	-2.030156	0.571323
H	3.988664	-0.424858	-0.359350	H	3.585190	-1.414514	-0.490429
C	1.245685	-0.864234	-0.694493	C	1.301011	0.131007	-0.812113
H	0.663342	-0.342990	-1.456898	H	0.851335	1.123779	-0.916700
H	1.916594	-1.578578	-1.173903	H	1.795608	-0.142081	-1.748375
O	2.116485	1.378522	-0.523420	O	3.298272	1.100026	0.074925
H	1.252754	1.821024	-0.489561	H	2.900809	1.969007	0.175732
O	-0.454484	-1.011067	0.841929	O	-0.468750	-0.503719	0.495591
O	0.334090	-1.707833	0.046181	O	0.280265	-0.847651	-0.670785
C	-1.913621	0.061597	-0.051454	C	-1.793827	-0.260694	0.137782
C	-2.534270	-1.001814	-0.893279	C	-2.408539	-1.332644	-0.733710
H	-3.498434	-0.646579	-1.268807	H	-3.454667	-1.091499	-0.923385
H	-1.891002	-1.242605	-1.739250	H	-1.876116	-1.406010	-1.679607
H	-2.697382	-1.894333	-0.291165	H	-2.347652	-2.288124	-0.212065
C	-2.478708	0.502854	1.247015	C	-2.520112	-0.004909	1.440232
H	-3.088016	-0.288146	1.678828	H	-2.530208	-0.920153	2.031480
H	-1.673546	0.790131	1.921784	H	-2.015674	0.784151	1.996013
H	-3.083557	1.397121	1.065100	H	-3.545256	0.298985	1.226881
O	-0.664165	1.932541	-0.045328	O	-1.350289	1.992686	-0.110827
O	-1.162699	0.877673	-0.720918	O	-1.844039	0.951500	-0.702836
H	1.398281	0.311444	1.086020	H	1.791373	0.320891	1.269092
CRCa3				TSCa3			
C	2.462047	0.093088	-0.389142	C	2.430196	0.417042	0.305956

C	3.600577	-0.440082	0.478593	C	3.862775	0.335554	-0.186479
H	4.258133	-1.053021	-0.137771	H	4.291878	1.337061	-0.223689
H	4.187224	0.368416	0.922734	H	4.471355	-0.282501	0.476555
H	3.202035	-1.069114	1.279364	H	3.888995	-0.084702	-1.194293
C	1.529473	0.922373	0.478127	C	1.769391	-0.948579	0.303294
H	1.030438	0.309344	1.230160	H	1.624779	-1.297094	-0.721904
H	2.047959	1.766213	0.939865	H	2.328475	-1.684965	0.886651
O	1.784233	-0.941039	-1.050901	O	1.728668	1.297404	-0.550190
H	1.101421	-1.320255	-0.461269	H	0.781934	1.165908	-0.418392
O	-0.564256	1.806730	0.306511	O	-0.422014	-1.640513	0.401826
O	0.488487	1.475222	-0.367715	O	0.475279	-0.761688	0.900258
C	-2.243693	-0.365675	-0.058854	C	-2.327257	0.558295	-0.106429
C	-3.070843	0.283226	-1.105866	C	-2.289409	1.821702	0.669690
H	-2.662390	0.088588	-2.095092	H	-1.643564	2.554749	0.182168
H	-4.101166	-0.073579	-1.037042	H	-3.291070	2.243578	0.762577
H	-3.070422	1.359417	-0.911276	H	-1.897812	1.650828	1.681891
C	-2.559098	-0.313029	1.381784	C	-3.348638	-0.506693	-0.016240
H	-3.497753	0.207349	1.557703	H	-4.269749	-0.094091	0.394240
H	-2.577939	-1.333876	1.772881	H	-3.548295	-0.936801	-1.001924
H	-1.729347	0.189172	1.887154	H	-3.009152	-1.328142	0.626797
O	-0.405090	-1.529220	0.511168	O	-0.936383	-0.980468	-1.034671
O	-1.225213	-0.969053	-0.459777	O	-1.186003	0.321411	-0.792775
H	2.875737	0.740829	-1.169552	H	2.413510	0.803077	1.334986
CPCa3				CRCa4			
C	1.968582	-0.492601	-0.187490	O	-0.898811	2.052831	0.077669
C	3.488668	-0.494336	-0.179388	C	-2.203356	0.015561	0.346352
H	3.843617	-1.515563	-0.042098	C	-3.006363	-1.028354	-0.423433
H	3.891689	-0.100599	-1.114029	H	-3.461438	-1.723750	0.282340
H	3.857592	0.108345	0.653780	H	-3.797199	-0.568747	-1.021254
C	1.453249	0.940991	-0.285955	H	-2.341379	-1.592833	-1.083097
H	1.536671	1.414004	0.696582	C	-1.573917	0.997133	-0.639970
H	1.990853	1.513509	-1.047477	H	-0.840607	0.498024	-1.276883
O	1.548401	-1.117572	0.999081	H	-2.331626	1.506557	-1.237532
H	0.582195	-1.118171	1.080388	O	-1.216888	-0.572234	1.152572
O	-0.566718	2.142024	-0.444601	O	0.351494	1.796617	0.292081
O	0.076304	0.845081	-0.655313	H	-0.661452	-1.141080	0.569842
C	-1.838809	-1.035663	0.144938	C	2.039591	-0.339662	-0.086151
C	-1.354994	-1.892714	-1.000426	O	0.412613	-1.845376	-0.565373
H	-0.507911	-2.500455	-0.683369	O	1.328502	-0.873846	-0.967186
H	-2.164500	-2.543525	-1.341725	C	1.941288	-0.736197	1.331273
H	-1.067796	-1.253177	-1.838151	H	1.871793	-1.824076	1.395377
C	-2.993617	-0.110341	-0.140791	H	2.782110	-0.341021	1.897458
H	-3.872347	-0.690088	-0.435451	H	1.000302	-0.333929	1.727686
H	-3.218571	0.486859	0.740651	C	2.991364	0.695175	-0.562722
H	-2.736631	0.540967	-0.980488	H	2.816023	1.613035	0.003223
O	-0.744402	2.368464	0.771521	H	4.012289	0.361815	-0.357149
O	-1.323679	-1.086932	1.238707	H	2.863529	0.881146	-1.626834

H	1.607403	-1.042642	-1.069106
TSCa4			
O	-0.265484	1.830507	0.266629
C	-2.050628	0.210136	0.395196
C	-3.030261	-0.557834	-0.500437
H	-3.654081	-1.199809	0.121267
H	-3.674367	0.127329	-1.056858
H	-2.474049	-1.185496	-1.200044
C	-1.250301	1.182331	-0.526045
H	-0.795252	0.627155	-1.344955
H	-1.876923	1.994361	-0.894512
O	-1.186700	-0.618844	1.064012
O	0.584117	0.979619	0.835512
H	-0.622407	-1.282454	0.350201
C	1.618485	-0.154115	-0.153443
O	0.158041	-1.894242	-0.480155
O	0.873889	-0.781173	-1.013973
C	2.133286	-0.891020	1.043587
H	2.664755	-1.770783	0.672871
H	2.806465	-0.253617	1.613746
H	1.309966	-1.229471	1.668268
C	2.490539	0.865338	-0.830311
H	2.874624	1.579198	-0.104599
H	3.326812	0.334584	-1.292142
H	1.931905	1.385993	-1.607821
H	-2.595079	0.817064	1.127102
CRCa5			
C	-2.116940	-0.574753	-0.250730
C	-3.331122	-0.213763	0.588001
H	-3.716005	-1.112063	1.070692
H	-3.049786	0.500877	1.363154
H	-4.120652	0.222935	-0.027600
C	-1.548546	0.632705	-0.998006
H	-0.637306	0.370283	-1.537519
H	-2.290230	1.070387	-1.668409
O	-1.148919	-1.134828	0.595582
H	-0.402811	-1.463862	0.039909
O	-0.009736	1.613645	0.374831
O	-1.224149	1.689906	-0.067855
C	2.132351	-0.082771	0.092289
C	2.906876	1.177614	-0.032466
H	2.442823	1.933361	0.605565
H	3.924283	1.008006	0.330461
H	2.927690	1.521019	-1.064412
C	1.882547	-0.737476	1.390229
H	0.821501	-0.602575	1.635925
H	2.046367	-1.812212	1.286277

H	-2.859271	0.578988	1.016638
CPCa4			
O	0.198956	-1.536233	0.194770
C	2.201493	-0.154497	0.435494
C	3.551078	0.139517	-0.252693
H	4.151186	0.806004	0.364924
H	4.086852	-0.801024	-0.387399
H	3.384204	0.606505	-1.224457
C	1.320934	-0.997932	-0.481136
H	1.008037	-0.405350	-1.347391
H	1.865037	-1.885162	-0.815061
O	1.647935	1.085166	0.670713
O	-0.506089	-0.479798	0.833460
H	0.175039	1.670630	-0.397986
C	-1.643862	-0.096512	0.059141
O	-0.708346	1.868495	-0.759523
O	-1.217241	0.589237	-1.100682
C	-2.448514	0.776571	1.004706
H	-3.209304	1.303690	0.428655
H	-2.925010	0.148732	1.757426
H	-1.809812	1.508617	1.494679
C	-2.416021	-1.292152	-0.465739
H	-2.586378	-1.993812	0.350963
H	-3.372650	-0.950914	-0.861040
H	-1.858816	-1.793678	-1.254734
H	2.379228	-0.679153	1.382867
TSCa5			
C	-0.967234	0.948771	0.420707
C	-1.686026	2.143211	-0.193200
H	-0.955604	2.896181	-0.494063
H	-2.248563	1.826320	-1.073217
H	-2.370634	2.596955	0.527002
C	-1.930145	-0.161915	0.827445
H	-1.448478	-0.932866	1.426676
H	-2.791890	0.246856	1.357332
O	-0.047081	0.425552	-0.512210
H	0.735076	1.172583	-0.630439
O	-1.761515	-1.845746	-0.685497
O	-2.462904	-0.807925	-0.343861
C	1.614127	-0.501725	0.173188
C	1.235732	-1.524729	1.189755
H	0.429718	-2.139923	0.788130
H	2.102037	-2.166896	1.372420
H	0.940188	-1.051456	2.125164
C	1.954275	-0.970475	-1.203344
H	1.140865	-1.584474	-1.586593
H	2.156327	-0.137611	-1.868667

H	2.504756	-0.297172	2.166526	H	2.854103	-1.587920	-1.106840
O	0.972366	-1.753088	-0.910482	O	2.020078	1.634677	-0.309427
O	1.711469	-0.572895	-0.979942	O	2.072424	0.592780	0.669109
H	-2.409866	-1.290228	-1.033543	H	-0.435540	1.268717	1.330878
CPCa5				CRCa6			
C	-0.730717	0.957030	0.424667	C	-2.065740	-0.182726	0.306122
C	-1.100310	2.238791	-0.307228	C	-2.223451	-1.671721	0.058811
H	-0.202975	2.807620	-0.556268	H	-2.624788	-2.148640	0.953186
H	-1.625321	1.997892	-1.232943	H	-2.910588	-1.849718	-0.771196
H	-1.741998	2.868254	0.312362	H	-1.256049	-2.112968	-0.188576
C	-1.981066	0.165385	0.813298	C	-1.475102	0.481935	-0.936479
H	-1.761160	-0.701480	1.432364	H	-2.205102	0.499117	-1.746899
H	-2.702628	0.815024	1.311907	O	-1.216476	-0.011585	1.429161
O	0.085134	0.199038	-0.454461	H	-1.207177	0.919382	1.671089
H	1.930460	1.721964	-0.598099	O	-0.017345	2.055990	-0.155944
O	-2.246921	-1.505006	-0.698874	O	-1.203683	1.874660	-0.653756
O	-2.642377	-0.310852	-0.371856	C	1.805576	-0.263109	0.274256
C	1.152555	-0.558755	0.085021	C	1.880694	0.116873	1.707189
C	0.763569	-1.464135	1.243943	H	1.576421	1.162693	1.800960
H	-0.042104	-2.125339	0.923217	H	1.227131	-0.515907	2.302805
H	1.628303	-2.061600	1.531804	H	2.916959	0.039858	2.048640
H	0.448344	-0.886983	2.114961	C	2.547438	0.434637	-0.796040
C	1.727484	-1.339522	-1.080041	H	3.111935	1.273799	-0.395525
H	0.991155	-2.073736	-1.408526	H	3.198152	-0.292659	-1.291485
H	1.957661	-0.672216	-1.907529	H	1.838506	0.765864	-1.557625
H	2.639344	-1.847354	-0.764457	O	0.983373	-1.604159	-1.337774
O	2.668778	1.151967	-0.339201	O	1.093109	-1.253075	-0.002232
O	2.094519	0.335942	0.666900	H	-0.552059	-0.004392	-1.259783
H	-0.181238	1.196476	1.343187	H	-3.041661	0.273593	0.515610
TSCa6				CPCa6			
C	-2.133707	0.189888	0.398559	C	2.119793	0.109940	-0.471762
C	-3.194443	-0.683479	-0.245135	C	3.573429	0.008737	-0.047786
H	-3.830535	-1.106389	0.532889	H	4.100333	-0.682271	-0.705131
H	-3.816383	-0.110412	-0.935400	H	4.056267	0.986079	-0.090384
H	-2.716503	-1.503878	-0.784815	H	3.638044	-0.373310	0.973774
C	-1.236920	0.794344	-0.686160	C	1.369765	1.021452	0.434956
H	-1.800908	1.273378	-1.488017	H	1.636007	1.186696	1.473063
O	-1.435984	-0.601815	1.332320	O	1.587647	-1.230419	-0.441150
H	-0.683741	-0.064830	1.613750	H	0.774167	-1.232768	-0.960052
O	0.434412	1.329198	0.785879	O	-0.545199	0.656341	-0.811721
O	-0.316280	1.716032	-0.271274	O	0.169668	1.533635	0.098167
C	1.825774	-0.372476	0.033249	C	-1.653699	0.012864	-0.169981
C	2.449893	-0.516358	1.371512	C	-2.588751	-0.316651	-1.322734
H	2.473613	0.466900	1.842730	H	-2.966553	0.608859	-1.755072
H	1.894241	-1.225215	1.982125	H	-2.055400	-0.879934	-2.089495
H	3.479644	-0.862330	1.238786	H	-3.418088	-0.918198	-0.952112
C	2.388093	0.530324	-0.998747	C	-2.291916	0.872506	0.901681

H	3.027810	1.272250	-0.527949	H	-2.529027	1.853147	0.488757
H	2.969725	-0.099337	-1.682298	H	-3.209131	0.382451	1.229610
H	1.605663	1.009434	-1.579915	H	-1.627879	0.992464	1.753006
O	0.339914	-1.120401	-1.503213	O	-0.455135	-1.119255	1.475929
O	0.967888	-1.261203	-0.240455	O	-1.261559	-1.256615	0.313166
H	-0.505644	-0.235124	-1.197283	H	0.422602	-1.335082	1.109331
H	-2.608721	1.037607	0.919671	H	2.043554	0.489282	-1.496664
CRCa7				TSCa7			
C	2.634288	-0.310226	-0.008161	C	2.338325	0.080339	-0.333881
C	3.720302	0.676420	-0.402000	C	3.438882	0.970889	0.219600
H	4.604285	0.496400	0.209959	H	4.406464	0.545283	-0.046209
H	3.990354	0.567417	-1.453869	H	3.375073	1.982976	-0.184894
H	3.380194	1.698179	-0.220981	H	3.376625	1.012698	1.309708
C	1.356623	-0.003903	-0.776393	C	0.979245	0.591829	0.131021
H	0.844451	0.889482	-0.404916	H	0.793174	0.290857	1.166002
H	1.544701	0.073461	-1.847348	H	0.909404	1.674240	0.009723
O	2.453100	-0.193905	1.388522	O	2.585428	-1.225317	0.127284
H	1.629510	-0.631938	1.626784	H	1.794013	-1.744622	-0.071725
O	-0.034240	-1.282730	0.516242	O	-0.051303	-1.311995	-0.659696
O	0.415941	-1.111178	-0.687229	O	-0.086127	0.059566	-0.693393
C	-2.419949	0.119587	-0.024776	C	-1.785329	0.468912	0.028796
C	-3.042230	-1.061207	-0.675531	C	-1.769448	1.950466	0.221511
H	-4.115327	-1.077031	-0.471635	H	-2.801790	2.290183	0.338824
H	-2.859567	-1.050775	-1.748126	H	-1.201996	2.226562	1.108940
H	-2.601247	-1.960580	-0.235498	H	-1.354768	2.432735	-0.664507
C	-2.530036	0.415466	1.415891	C	-2.596193	-0.123457	-1.071542
H	-3.148680	-0.320807	1.923905	H	-2.618010	0.558846	-1.919913
H	-1.517064	0.444937	1.828984	H	-2.197472	-1.093941	-1.354896
H	-2.921004	1.430229	1.535187	H	-3.610065	-0.263101	-0.684338
O	-1.102989	1.937670	-0.160491	O	-1.675450	-1.541738	0.984604
O	-1.743685	0.869664	-0.763757	O	-1.629103	-0.187850	1.147795
H	2.950386	-1.331963	-0.262917	H	2.348898	0.112086	-1.432511
CPCa7							
C	2.306681	0.060186	-0.287897				
C	3.431518	0.880543	0.325480				
H	4.383300	0.503176	-0.047747				
H	3.345741	1.938408	0.068843				
H	3.429218	0.770382	1.412623				
C	0.980516	0.503409	0.315936				
H	0.826425	0.063691	1.302632				
H	0.910889	1.590047	0.333710				
O	2.572542	-1.289934	-0.025884				
H	1.758538	-1.758446	-0.278841				
O	-0.038599	-1.396177	-0.671836				
O	-0.116874	0.046634	-0.544034				
C	-1.483990	0.442343	-0.157934				
C	-1.546135	1.949524	-0.031819				

H	-2.595306	2.241843	0.002872
H	-1.066224	2.295504	0.882762
H	-1.079740	2.415666	-0.900552
C	-2.418835	-0.133869	-1.187780
H	-2.218044	0.353711	-2.142375
H	-2.265254	-1.203658	-1.278496
H	-3.443363	0.078720	-0.880647
O	-2.209468	-1.263055	1.208478
O	-1.689975	-0.066163	1.163217
H	2.254281	0.247693	-1.370223

CRCb1

C	2.388087	-0.113560	-0.283635
C	3.423143	0.978935	-0.078701
H	4.408188	0.523778	0.025097
H	3.438969	1.669346	-0.923651
H	3.205535	1.535255	0.835632
C	0.993233	0.492084	-0.324885
H	0.654762	0.800583	0.664953
H	0.917243	1.326572	-1.019923
O	2.529983	-1.027913	0.785760
H	1.764722	-1.612610	0.795506
O	-0.190035	-1.442278	-0.013867
O	0.033353	-0.466014	-0.841268
H	2.569074	-0.621345	-1.241315
C	-2.601079	-0.313526	0.634597
C	-3.171763	-0.459503	-0.710103
H	-3.711510	-1.397125	-0.810038
H	-3.816809	0.403551	-0.906460
H	-2.354804	-0.385010	-1.434941
O	-1.749968	1.650613	0.001327
O	-1.943606	0.696660	0.962350
H	-2.702921	-1.038118	1.437080

CPCb1

C	-2.258275	-0.247215	0.231463
C	-3.473009	0.659547	0.140561
H	-4.338876	0.074478	-0.169582
H	-3.689602	1.126728	1.103072
H	-3.304349	1.439304	-0.606003
C	-1.014353	0.562042	0.568336
H	-0.712955	1.182922	-0.281114
H	-1.196813	1.197005	1.439178
O	-2.141737	-0.900988	-1.020032
H	-1.302176	-1.369590	-1.040820
O	0.553038	-0.984821	-0.126207
O	0.083457	-0.241981	0.999280
H	-2.401970	-0.986530	1.031435
C	1.862593	-0.595371	-0.410648

TSCb1

C	2.330230	-0.161251	-0.284988
C	3.472521	0.790782	0.023836
H	4.396728	0.221602	0.124810
H	3.596637	1.528212	-0.771110
H	3.285594	1.307956	0.967630
C	1.012339	0.598252	-0.332230
H	0.693208	0.898713	0.667529
H	1.063009	1.465629	-0.989653
O	2.325962	-1.149972	0.726307
H	1.498635	-1.640271	0.668493
O	-0.394694	-1.194900	-0.114076
O	-0.031370	-0.212014	-0.916868
H	2.489464	-0.626862	-1.267445
C	-2.293760	-0.413034	0.647703
C	-3.052281	-0.610109	-0.599925
H	-3.343595	-1.651922	-0.705996
H	-3.936078	0.037114	-0.568382
H	-2.448348	-0.277296	-1.445147
O	-1.820838	1.659573	-0.012340
O	-1.807912	0.724599	0.956343
H	-2.278719	-1.109000	1.477970

CRCb2

C	-1.430374	-0.488875	0.235391
C	-2.747314	-0.346872	0.974137
H	-2.778725	-1.038735	1.815975
H	-2.879856	0.672505	1.344401
H	-3.571873	-0.589743	0.299610
C	-1.310754	0.534900	-0.899843
H	-0.476314	0.294942	-1.558627
H	-2.237444	0.614462	-1.469256
O	-1.340353	-1.776330	-0.314006
H	-0.391197	-1.996793	-0.359237
O	0.120837	2.004179	0.079322
O	-1.087679	1.862618	-0.366253
H	-0.592015	-0.308838	0.920933
C	2.269107	0.336902	-0.272548

C	2. 809178	-0. 656499	0. 760466
H	2. 829605	-1. 682936	1. 126594
H	3. 809407	-0. 369414	0. 435533
H	2. 482666	0. 008550	1. 554691
O	1. 935289	1. 700227	-0. 199519
O	1. 834883	0. 715010	-1. 041402
H	2. 148828	-1. 255115	-1. 231026

TSCb2

C	-1. 654216	0. 239756	-0. 284085
C	-3. 008427	-0. 228479	-0. 780564
H	-3. 312632	0. 356495	-1. 648726
H	-2. 969520	-1. 284273	-1. 059837
H	-3. 757358	-0. 096675	0. 004080
C	-1. 155889	-0. 616665	0. 893217
H	-0. 563027	-0. 005126	1. 575486
H	-1. 971735	-1. 086646	1. 443990
O	-1. 770512	1. 579852	0. 138760
H	-0. 871867	1. 942904	0. 178704
O	0. 614807	-1. 392865	-0. 353168
O	-0. 333013	-1. 737526	0. 493465
H	-0. 915330	0. 161595	-1. 086401
C	2. 118882	-0. 251495	0. 320332
C	2. 754283	-0. 146053	-1. 009843
H	3. 259445	-1. 075938	-1. 259474
H	1. 999526	0. 101200	-1. 755941
H	3. 466977	0. 684289	-0. 980919
O	1. 118345	1. 718583	-0. 025949
O	1. 479306	0. 741408	0. 831031
H	2. 436271	-0. 955830	1. 081581

CRCb3

C	-1. 606763	-0. 477650	0. 127055
C	-2. 959810	-1. 111617	-0. 172179
H	-2. 843615	-2. 192981	-0. 245907
H	-3. 689916	-0. 890821	0. 610313
H	-3. 338950	-0. 744995	-1. 128933
C	-1. 751941	1. 034874	0. 219027
H	-1. 991504	1. 466670	-0. 753615
H	-2. 477304	1. 329789	0. 978917
O	-0. 679201	-0. 762366	-0. 890665
H	0. 009930	-1. 361489	-0. 525491
O	0. 202282	2. 091878	-0. 333821
O	-0. 493466	1. 601986	0. 646225
H	-1. 227663	-0. 844033	1. 090153
C	2. 133383	0. 240618	0. 360397
C	2. 408793	0. 138316	-1. 078433
H	2. 971285	1. 002692	-1. 421697
H	2. 924528	-0. 805101	-1. 274366

C	2. 514660	0. 362478	1. 174435
H	2. 947553	1. 310327	1. 481787
H	1. 567175	0. 174283	1. 687002
H	3. 161773	-0. 483158	1. 429580
O	1. 413085	-1. 716477	-0. 042465
O	1. 764156	-0. 647452	-0. 845318
H	2. 518613	1. 147253	-0. 951837

CPCb2

C	-2. 064705	0. 075593	-0. 393074
C	-2. 908418	-1. 161289	-0. 168666
H	-3. 562749	-1. 330861	-1. 024130
H	-2. 268827	-2. 033724	-0. 027063
H	-3. 528640	-1. 027946	0. 721175
C	-1. 106487	0. 330200	0. 768306
H	-0. 561773	1. 270156	0. 630878
H	-1. 665862	0. 371661	1. 706822
O	-2. 947119	1. 185335	-0. 494902
H	-2. 456608	1. 949747	-0. 808435
O	0. 658905	-0. 786813	-0. 181693
O	-0. 185544	-0. 733531	0. 969842
H	-1. 481006	-0. 032707	-1. 313970
C	1. 951837	-0. 542875	0. 238970
C	2. 880086	-0. 850268	-0. 907626
H	2. 815109	-1. 909993	-1. 150613
H	2. 595100	-0. 257252	-1. 776097
H	3. 903009	-0. 605627	-0. 622003
O	1. 823980	1. 681770	-0. 297216
O	2. 090557	0. 850908	0. 663324
H	2. 172144	-1. 082972	1. 161122

TSCb3

C	-2. 002282	-0. 302653	0. 251240
C	-3. 498072	-0. 325698	0. 523153
H	-3. 833001	-1. 358894	0. 612209
H	-3. 742924	0. 208145	1. 443131
H	-4. 036062	0. 134311	-0. 309708
C	-1. 543294	1. 137009	0. 036521
H	-1. 801709	1. 472025	-0. 971391
H	-1. 998396	1. 795142	0. 779716
O	-1. 787406	-1. 109291	-0. 888740
H	-0. 837346	-1. 222953	-1. 001205
O	0. 594374	0. 965577	-0. 809188
O	-0. 139756	1. 352085	0. 251981
H	-1. 457093	-0. 705263	1. 115827
C	2. 629945	-0. 276324	0. 896227
C	3. 568045	-0. 011808	-0. 211428
H	4. 536798	0. 274424	0. 194761
H	3. 690978	-0. 900836	-0. 841581

H	1.443203	0.089027	-1.597502	H	3.198849	0.790417	-0.858081
O	1.378018	-1.877176	0.366497	O	0.994095	-0.622164	-0.606080
O	1.662786	-0.695726	1.034618	O	1.402372	-0.781412	0.665664
H	2.314686	1.135219	0.950090	H	2.844433	-0.248037	1.952949
CPCb3				CRCb4			
C	1.779149	-0.501263	-0.178120	O	-0.956151	1.997524	-0.113906
C	3.270943	-0.453429	0.112268	C	-1.835546	-0.197490	0.460060
H	3.659882	-1.470246	0.160414	C	-2.501105	-1.438564	-0.124933
H	3.812081	0.097050	-0.659670	H	-2.758572	-2.123763	0.683142
H	3.445197	0.023431	1.079642	H	-3.411960	-1.186363	-0.672981
C	1.224544	0.919480	-0.232916	H	-1.807837	-1.948141	-0.800105
H	1.255425	1.350060	0.772185	C	-1.487334	0.773446	-0.665822
H	1.776871	1.539903	-0.945247	H	-0.737266	0.350155	-1.337053
O	1.154473	-1.234615	0.848549	H	-2.376710	1.079667	-1.218986
H	0.341111	-1.621776	0.492823	O	-0.689268	-0.518994	1.204861
O	-0.763415	2.116639	-0.537280	O	0.334968	1.997018	-0.023971
O	-0.133654	0.807138	-0.657407	H	-0.115732	-1.087819	0.644268
H	1.602890	-0.979033	-1.150069	C	2.257304	0.133797	-0.360049
C	-2.179416	-1.482959	-0.400342	H	2.688627	0.966839	-0.909303
C	-2.464205	-0.547791	0.731826	O	1.016012	-1.741868	-0.500424
H	-3.282356	-0.964091	1.328202	O	1.636467	-0.655035	-1.098007
H	-1.580197	-0.396463	1.349463	H	-2.518934	0.310364	1.146840
H	-2.811806	0.409609	0.335646	C	2.409493	-0.050417	1.088283
O	-0.983199	2.410786	0.660236	H	3.186179	0.603751	1.476538
O	-1.150897	-2.097166	-0.541622	H	1.447634	0.186432	1.562238
H	-2.991639	-1.614932	-1.139491	H	2.611477	-1.104909	1.291748
TSCb4				CPCb4			
O	-0.273756	1.883946	-0.212124	O	-0.183186	1.651810	-0.220425
C	-1.754184	0.110860	0.511573	C	-1.960139	0.110419	0.449894
C	-2.742698	-0.917355	-0.051416	C	-3.291548	-0.484461	-0.055231
H	-3.170076	-1.485613	0.774561	H	-3.760277	-1.076873	0.729034
H	-3.551681	-0.428865	-0.599526	H	-3.957730	0.334091	-0.330701
H	-2.215832	-1.607151	-0.714163	H	-3.114515	-1.118718	-0.925023
C	-1.232375	0.947338	-0.696315	C	-1.252792	0.845068	-0.683664
H	-0.797397	0.287998	-1.444748	H	-0.903555	0.125548	-1.431217
H	-2.014882	1.575733	-1.120433	H	-1.929460	1.566729	-1.148093
O	-0.699094	-0.472718	1.167957	O	-1.231626	-0.975823	0.884253
O	0.769230	1.333250	0.391017	O	0.680305	0.862881	0.588997
H	-0.164021	-1.146053	0.489240	H	0.290742	-1.632872	-0.082102
C	1.805713	0.161500	-0.418291	C	1.794737	0.462887	-0.183830
H	2.289567	0.899278	-1.058534	H	2.099353	1.295391	-0.822570
O	0.598015	-1.780124	-0.418349	O	1.192818	-1.751852	-0.431045
O	1.128386	-0.669300	-1.145256	O	1.433651	-0.528846	-1.111488
H	-2.261327	0.792964	1.202257	H	-2.158400	0.793973	1.285209
C	2.523559	-0.298281	0.808691	C	2.863535	0.039485	0.798084
H	3.126887	0.512355	1.212680	H	3.225192	0.912775	1.339519
H	1.815317	-0.651385	1.554748	H	2.465518	-0.686521	1.504453

H	3.161110	-1.134054	0.512498
CRCb5			
C	1.750214	-0.736542	-0.213733
C	2.687441	-1.707417	0.486445
H	2.369769	-2.729934	0.283219
H	3.718386	-1.584445	0.147119
H	2.647768	-1.546038	1.566374
C	2.206697	0.696357	0.041692
H	2.169614	0.934684	1.105818
H	3.199846	0.882336	-0.371697
O	0.448073	-0.921231	0.282011
H	-0.203670	-0.681085	-0.415475
O	0.413198	2.100952	0.140469
O	1.328852	1.615414	-0.639645
C	-2.839516	-0.456589	0.531275
C	-2.189296	0.745614	1.059455
H	-1.143815	0.499807	1.293598
H	-2.128540	1.496331	0.265565
H	-2.704093	1.110384	1.944501
O	-1.597149	-0.309049	-1.328062
O	-2.565600	-0.948328	-0.580965
H	-3.609133	-1.018511	1.056141
H	1.771638	-0.914138	-1.296426
CPCb5			
C	-1.104259	0.813585	-0.306758
C	-1.741532	2.180917	-0.107556
H	-1.033495	2.962558	-0.387497
H	-2.637548	2.292926	-0.721763
H	-2.006620	2.322327	0.942244
C	-2.047114	-0.298270	0.118360
H	-2.188721	-0.309117	1.199712
H	-2.999232	-0.236116	-0.410201
O	0.067176	0.700170	0.485315
H	1.022404	-1.873893	-0.053063
O	-0.831522	-2.132490	0.710680
O	-1.469369	-1.561378	-0.265008
C	1.275265	0.802502	-0.223039
C	2.384452	1.051257	0.770340
H	2.244572	2.030592	1.227948
H	2.365056	0.286697	1.544367
H	3.346891	1.019145	0.259772
O	1.866835	-1.433751	-0.237410
O	1.482794	-0.328774	-1.040668
H	1.210586	1.603285	-0.971815
H	-0.852067	0.651448	-1.361047
TSCb6			
C	-2.197548	-0.125919	-0.309839

H	3.684679	-0.419270	0.247635
TSCb5			
C	-0.797173	0.941475	-0.283701
C	-0.787667	2.447560	-0.082760
H	0.197078	2.855058	-0.316709
H	-1.517972	2.934502	-0.731533
H	-1.018485	2.689008	0.957125
C	-2.168066	0.374848	0.059452
H	-2.373566	0.473261	1.126675
H	-2.943571	0.857849	-0.536976
O	0.179598	0.359593	0.562594
H	0.314839	-0.648909	0.257054
O	-1.825550	-1.786828	0.676255
O	-2.250378	-1.019638	-0.283037
C	2.034995	0.379245	-0.217861
C	2.665155	-0.011944	1.070645
H	2.472360	0.753243	1.819995
H	2.315076	-0.983166	1.405226
H	3.743820	-0.057268	0.881692
O	1.109067	-1.591171	-0.582944
O	1.723390	-0.428844	-1.150370
H	2.207282	1.390500	-0.589941
H	-0.569340	0.683921	-1.327236
CRCb6			
C	-2.370311	-0.052207	-0.323584
C	-3.260119	-1.257032	-0.070287
H	-4.299595	-0.975543	-0.239128
H	-3.003699	-2.083410	-0.735302
H	-3.159238	-1.586134	0.966208
C	-0.926717	-0.395209	0.011267
H	-0.747463	-0.431726	1.086342
H	-0.602443	-1.330269	-0.443556
O	-2.861579	1.002645	0.479133
H	-2.208516	1.710459	0.486866
O	-0.155077	1.761234	-0.017626
O	-0.011520	0.585161	-0.546199
C	2.838933	-0.158816	-0.639840
C	3.123834	0.892854	0.343582
H	3.751600	1.671542	-0.081211
H	2.171665	1.306107	0.693781
H	3.583491	0.427816	1.221688
O	1.744997	-1.282885	0.946355
O	2.201102	-1.187888	-0.338860
H	3.154982	-0.139661	-1.679156
H	-2.417883	0.227153	-1.385774
CPCb6			
C	-2.175904	0.070615	-0.292466

C	-3.376640	-0.734330	0.431593	C	-3.344277	-0.879536	-0.080217
H	-4.299521	-0.302687	0.044408	H	-4.273230	-0.322273	-0.199039
H	-3.412231	-1.817842	0.303008	H	-3.331240	-1.701783	-0.798506
H	-3.313901	-0.498348	1.496519	H	-3.321787	-1.283974	0.934432
C	-0.892240	-0.624441	0.297715	C	-0.873179	-0.665363	-0.019741
H	-0.675981	-0.092282	1.227863	H	-0.690119	-0.771705	1.050170
H	-0.912367	-1.705801	0.451980	H	-0.834419	-1.625991	-0.538418
O	-2.314137	1.272783	-0.205283	O	-2.342651	1.157888	0.575849
H	-1.477003	1.653518	-0.502514	H	-1.492508	1.631443	0.568605
O	0.358625	0.912028	-0.878714	O	0.321695	1.395359	0.109985
O	0.215945	-0.413807	-0.612030	O	0.235968	0.116975	-0.573699
C	1.873507	-0.848906	0.285722	C	1.524842	-0.545870	-0.565696
C	2.765943	-0.680133	-0.883686	C	2.543737	0.340193	-1.215201
H	2.700495	-1.552879	-1.530016	H	2.240837	0.515052	-2.247290
H	2.501470	0.230983	-1.417695	H	2.599600	1.284256	-0.681605
H	3.787138	-0.570751	-0.505524	H	3.509683	-0.165222	-1.199178
O	2.043641	1.307160	0.761210	O	2.513505	-0.042888	1.435733
O	1.778475	0.048212	1.209391	O	1.813999	-0.926538	0.773708
H	1.620919	-1.834237	0.669704	H	1.354485	-1.491488	-1.081832
H	-2.217542	-0.438303	-1.363347	H	-2.152748	0.405083	-1.340024
CRCc1				TSCc1			
C	-2.443470	-0.200777	0.201828	C	-2.315153	-0.166115	0.191527
C	-3.565045	0.700855	-0.284011	C	-3.432322	0.405199	-0.663888
H	-4.477435	0.113362	-0.387405	H	-4.275682	-0.285502	-0.661215
H	-3.746389	1.516241	0.418250	H	-3.765598	1.371600	-0.281778
H	-3.314209	1.117968	-1.261699	H	-3.092259	0.524844	-1.694993
C	-1.136436	0.575717	0.251008	C	-1.089354	0.733306	0.121877
H	-0.726157	0.758846	-0.742201	H	-0.593543	0.653308	-0.846940
H	-1.226427	1.515937	0.792622	H	-1.328022	1.773678	0.339005
O	-2.369614	-1.293933	-0.692669	O	-2.036064	-1.464049	-0.297563
H	-1.541506	-1.761681	-0.540891	H	-1.210269	-1.764853	0.097000
O	0.279654	-1.217007	0.393120	O	0.449906	-0.767347	0.902189
O	-0.137184	-0.153631	1.010384	O	-0.133918	0.382888	1.148267
H	-2.668236	-0.558511	1.216435	H	-2.639611	-0.219898	1.239835
C	2.645065	0.056504	0.196947	C	2.427678	-0.136072	0.068096
C	3.390696	-1.112685	-0.313960	C	2.835342	-1.434296	-0.511006
H	2.898212	-2.019614	0.045691	H	2.520373	-2.237884	0.155776
H	3.415671	-1.106946	-1.401801	H	2.389183	-1.568073	-1.494929
H	4.407890	-1.103956	0.085875	H	3.925454	-1.470574	-0.595627
O	1.459538	1.936197	-0.081564	O	1.631421	1.934451	-0.127444
O	2.161875	0.872489	-0.603096	O	1.945971	0.743048	-0.697715
H	2.479579	0.257757	1.254855	H	2.654314	0.179298	1.082348
CPCc1				CRCc2			
C	-2.256388	-0.239534	0.203191	C	1.981325	0.134410	0.178129
C	-3.492094	0.394479	-0.410565	C	3.498535	0.092101	0.275337
H	-4.256856	-0.368778	-0.554758	H	3.856999	1.041448	0.672725
H	-3.894015	1.179216	0.233005	H	3.839879	-0.716402	0.925605

H	-3.249391	0.821533	-1.386541	H	3.931740	-0.041857	-0.719051
C	-1.138225	0.785226	0.327015	C	1.474677	-1.190957	-0.383859
H	-0.741427	1.047294	-0.658788	H	1.757069	-1.291501	-1.432316
H	-1.500200	1.686320	0.828667	H	1.797587	-2.050258	0.206031
O	-1.892015	-1.320913	-0.637269	O	0.025725	-1.206335	-0.401944
H	-1.040463	-1.658612	-0.344914	O	-0.470719	-1.418518	0.775506
O	0.617253	-0.706081	0.542481	O	1.610456	1.191938	-0.662769
O	-0.076722	0.364236	1.183054	H	-2.302074	0.266452	1.447141
H	-2.486026	-0.607249	1.212646	C	-2.439050	0.270722	0.367312
C	1.910876	-0.272344	0.279252	C	-3.413215	-0.581772	-0.342507
C	2.701270	-1.459746	-0.203913	H	1.539480	0.259712	1.175439
H	2.729347	-2.221406	0.574326	H	-4.418217	-0.394774	0.043251
H	2.235514	-1.872948	-1.099368	H	-3.376505	-0.398875	-1.414283
H	3.716729	-1.145659	-0.442339	O	-1.722304	1.043529	-0.281332
O	1.963647	1.921164	-0.372852	O	-0.793927	1.775854	0.450139
O	1.864121	0.696471	-0.799643	H	-3.161990	-1.624315	-0.130017
H	2.323878	0.252794	1.142019	H	0.728551	1.511605	-0.377799
TSCc2				CPCc2			
C	1.889088	0.085467	0.318598	C	-1.820429	-0.140241	-0.387011
C	3.270062	-0.213731	0.877478	C	-3.302162	-0.393452	-0.590959
H	3.650394	0.671848	1.386239	H	-3.578475	-0.154458	-1.618042
H	3.243367	-1.045022	1.584990	H	-3.550982	-1.438722	-0.395511
H	3.957802	-0.458534	0.064481	H	-3.884449	0.245054	0.076940
C	1.365074	-1.139700	-0.420799	C	-1.411789	-0.433573	1.048314
H	1.966358	-1.310891	-1.315722	H	-1.988983	0.191925	1.734973
H	1.331115	-2.028773	0.209882	H	-1.544751	-1.488161	1.304838
O	0.029741	-0.923402	-0.929627	O	-0.069490	-0.041332	1.310386
O	-0.891130	-1.366448	-0.105527	O	0.802903	-0.983019	0.693685
O	2.000574	1.176104	-0.557886	O	-1.562937	1.212184	-0.706698
H	-1.488901	0.176783	1.469923	H	0.767072	0.053971	-1.094288
C	-2.074112	0.177899	0.554953	C	1.464187	-0.357691	-0.360737
C	-3.382983	-0.501256	0.419207	C	2.447996	-1.351700	-0.917909
H	1.190410	0.319113	1.132618	H	-1.251492	-0.804174	-1.054946
H	-4.121050	0.002618	1.049493	H	2.998467	-0.896319	-1.740291
H	-3.710684	-0.475360	-0.618611	H	3.144704	-1.652506	-0.135451
O	-1.785592	1.079828	-0.291671	O	2.211431	0.773405	0.145727
O	-0.633096	1.750183	-0.050590	O	1.544683	1.883535	0.032003
H	-3.288585	-1.534960	0.750690	H	1.913868	-2.229114	-1.281417
H	1.103015	1.500993	-0.728194	H	-0.704524	1.474260	-0.347828
CRCc3				TSCc3			
C	-1.961611	0.326725	-0.112012	C	1.813453	0.433690	-0.290152
C	-3.347439	0.582076	0.463841	C	3.172023	1.116546	-0.300273
H	-3.516097	1.656412	0.534800	H	3.486354	1.278461	-1.331088
H	-4.130327	0.142548	-0.158714	H	3.137967	2.077439	0.216347
H	-3.413588	0.161090	1.469883	H	3.914879	0.477586	0.184000
C	-1.730135	-1.176919	-0.231466	C	1.411594	0.120513	1.148414
H	-1.719507	-1.650372	0.751130	H	1.947263	-0.761795	1.507910

H	-2.454911	-1.649061	-0.896947	H	1.616292	0.975694	1.795876
O	-0.987985	0.884739	0.730124	O	1.942804	-0.733394	-1.075268
H	-0.308374	1.340672	0.174436	H	1.066117	-1.115462	-1.194659
O	0.481933	-1.674001	0.027887	O	-0.385584	-1.304618	0.940017
O	-0.443217	-1.415622	-0.840563	O	0.002005	-0.084541	1.342665
H	-1.885921	0.761542	-1.116411	H	1.053737	1.102638	-0.716520
C	2.097020	0.327301	0.465037	C	-2.691285	0.015044	-0.292079
C	3.206422	-0.631606	0.639802	C	-3.235126	1.359185	-0.006974
H	3.883392	-0.251065	1.410342	H	-4.302459	1.291183	0.199648
H	2.798302	-1.581743	0.987942	H	-2.740231	1.806518	0.864105
H	3.744639	-0.771239	-0.295278	H	-3.086644	2.031973	-0.855673
O	0.966466	1.862918	-0.737312	O	-0.836830	-1.185395	-0.671453
O	1.988665	0.932566	-0.612508	O	-1.451431	-0.004026	-0.817350
H	1.369949	0.550944	1.246585	H	-3.084936	-0.938304	0.027553
CPCc3				CRCc4			
C	1.940116	0.312620	0.306615	O	-0.609842	2.014137	-0.208256
C	3.450427	0.218176	0.176688	C	-1.990376	0.108350	0.413640
H	3.883668	1.209360	0.310250	C	-2.903124	-0.970236	-0.161203
H	3.872178	-0.455620	0.924750	H	-3.344577	-1.540779	0.656218
H	3.717797	-0.137784	-0.820882	H	-3.707183	-0.539527	-0.762469
C	1.300345	-1.046709	0.047535	H	-2.321617	-1.654753	-0.785645
H	1.351713	-1.267366	-1.022357	C	-1.357876	0.894910	-0.732311
H	1.773747	-1.842658	0.629182	H	-0.673394	0.265683	-1.305645
O	1.491798	1.265820	-0.623145	H	-2.115430	1.345394	-1.375373
H	0.522930	1.266719	-0.679412	O	-0.998183	-0.438172	1.244712
O	-0.833519	-1.869019	-0.351219	O	0.637852	1.741963	-0.007740
O	-0.065647	-0.913781	0.437595	H	-0.529081	-1.121420	0.715078
H	1.679964	0.616302	1.331764	C	2.003421	-0.451455	0.331971
C	-2.217839	1.144811	-0.263027	H	1.385791	-0.436381	1.229800
C	-2.011293	1.324821	1.208400	O	0.476795	-1.917272	-0.453738
H	-2.705525	2.082237	1.582348	O	1.647124	-1.178057	-0.608574
H	-2.243757	0.380922	1.707961	H	-2.566954	0.803379	1.030797
H	-0.982276	1.611106	1.421705	C	3.246554	0.334288	0.198939
O	-2.041331	-1.752449	-0.077677	H	3.016229	1.384129	0.393871
O	-1.350788	1.260136	-1.093167	H	3.958873	0.002902	0.959618
H	-3.245076	0.888816	-0.581668	H	3.675775	0.215435	-0.793705
TSCc4				CPCc4			
O	-0.119088	-1.732140	-0.105352	O	-0.144334	-1.483225	0.083320
C	1.873171	-0.416286	0.245743	C	1.980555	-0.293562	0.315360
C	2.883515	0.450310	-0.514428	C	3.286593	-0.000596	-0.452814
H	3.632086	0.818938	0.186642	H	3.990483	0.525885	0.189880
H	3.385509	-0.123926	-1.296732	H	3.728286	-0.947536	-0.765818
H	2.369452	1.304929	-0.959266	H	3.077437	0.612022	-1.330952
C	0.874683	-0.986372	-0.804988	C	0.957805	-0.933024	-0.617658
H	0.429157	-0.173979	-1.375977	H	0.622167	-0.200277	-1.359098
H	1.347202	-1.721898	-1.455194	H	1.394796	-1.799463	-1.120628
O	1.186859	0.288634	1.206611	O	1.556459	0.935843	0.770484

O	-0.808508	-1.006974	0.762663	O	-0.693252	-0.483450	0.934482
H	0.651754	1.090353	0.733009	H	0.024023	1.814124	0.036573
C	-1.763172	0.415335	0.249167	C	-1.839322	0.091132	0.327809
H	-1.772314	0.774371	1.277969	H	-2.254853	0.683154	1.147685
O	-0.140323	1.982566	0.027335	O	-0.880312	2.107581	-0.178550
O	-1.125772	1.148995	-0.591925	O	-1.477244	0.941434	-0.723996
H	2.375597	-1.259656	0.730198	H	2.195075	-0.958884	1.161407
C	-2.964117	-0.275256	-0.318111	C	-2.808170	-0.924616	-0.231451
H	-3.324619	-1.039788	0.366432	H	-3.002288	-1.688906	0.520695
H	-3.743327	0.476386	-0.463480	H	-3.739023	-0.423666	-0.494216
H	-2.720318	-0.720771	-1.282555	H	-2.391404	-1.397914	-1.118915
CRCc5				TSCc5			
C	-1.664414	-0.366398	0.577181	C	-1.168655	0.735428	-0.521930
C	-2.592807	-1.570859	0.481578	C	-1.601551	2.195756	-0.539459
H	-2.592417	-2.103399	1.432667	H	-1.262848	2.663074	-1.463867
H	-3.616690	-1.270161	0.247741	H	-2.688130	2.284817	-0.479210
H	-2.244344	-2.258337	-0.294858	H	-1.157522	2.736552	0.301138
C	-1.643498	0.373612	-0.754599	C	-1.628286	0.071104	0.768078
H	-1.186850	-0.237926	-1.535678	H	-1.115141	0.484891	1.639237
H	-2.637462	0.714627	-1.048532	H	-2.710285	0.142078	0.888258
O	-0.359886	-0.743763	0.958136	O	0.231692	0.647557	-0.690799
H	0.011230	-1.295343	0.237533	H	0.774189	1.303837	-0.018065
O	-1.290067	2.469253	0.072125	O	-1.940729	-2.004441	-0.117051
O	-0.787835	1.537964	-0.680278	O	-1.277793	-1.333256	0.774792
C	2.100434	0.198132	-0.061314	C	1.540546	-0.582532	0.144530
C	3.123406	0.768012	0.836401	C	1.715304	-1.725037	-0.778490
H	3.557964	1.659462	0.378486	H	2.316819	-2.487488	-0.274816
H	2.619571	1.086851	1.754062	H	0.737678	-2.153746	-0.998735
H	3.895431	0.037310	1.067463	H	2.213343	-1.405435	-1.691323
O	1.135665	-1.498465	-1.164142	O	1.867920	1.453298	0.866305
O	2.179465	-0.995625	-0.387683	O	2.426662	0.329875	0.165618
H	1.257265	0.771538	-0.444251	H	0.912118	-0.674666	1.024460
H	-2.021153	0.325475	1.344613	H	-1.626394	0.193510	-1.354369
CPCc5				CRCc6			
C	0.887797	0.854946	0.414127	C	-2.493438	-0.251637	0.236652
C	1.199261	2.323686	0.647398	C	-3.674910	0.655474	-0.060375
H	0.642129	2.678353	1.513927	H	-4.565389	0.045439	-0.212776
H	2.265289	2.468957	0.828247	H	-3.856814	1.347378	0.763752
H	0.901435	2.918080	-0.219748	H	-3.490015	1.225040	-0.973715
C	1.581761	0.369764	-0.853859	C	-1.219900	0.573305	0.346941
H	1.028533	0.672353	-1.744697	H	-0.861110	0.922510	-0.621251
H	2.610309	0.730781	-0.895020	H	-1.330531	1.411682	1.033471
O	-0.521477	0.756525	0.334448	O	-2.417078	-1.195000	-0.814372
H	-2.522141	1.321442	-0.853773	H	-1.562273	-1.636274	-0.769186
O	2.424394	-1.565693	-0.016950	O	0.277067	-1.141263	0.151244
O	1.637907	-1.074290	-0.924913	O	-0.152128	-0.208843	0.942325
C	-1.090144	-0.528235	0.131314	C	2.621844	-0.071402	-0.478912

C	-0.868715	-1.472946	1.291013	C	3.616967	-0.989030	0.114453
H	-1.445415	-2.383129	1.127666	H	4.403379	-1.206047	-0.612140
H	0.184706	-1.744871	1.368435	H	4.045639	-0.558502	1.017197
H	-1.194403	-0.997945	2.217522	H	3.114320	-1.930132	0.354067
O	-2.729044	0.419114	-1.134790	O	1.381472	1.788893	-0.463379
O	-2.468845	-0.318380	0.047705	O	2.356702	0.996365	0.093877
H	-0.738512	-0.942842	-0.819839	H	2.084351	-0.275462	-1.403619
H	1.264822	0.257316	1.253320	H	-2.653212	-0.767105	1.194093
TSCc6				CPCc6			
C	-2.115151	0.173489	0.239564	C	-2.100503	0.122579	0.196638
C	-3.115972	1.047038	-0.498611	C	-3.139782	0.885527	-0.610273
H	-4.122406	0.678778	-0.299939	H	-4.132029	0.573927	-0.284864
H	-3.050410	2.088029	-0.176262	H	-3.045460	1.964578	-0.472376
H	-2.942022	0.990442	-1.575796	H	-3.043204	0.645834	-1.671855
C	-0.694805	0.593655	-0.121632	C	-0.711963	0.465247	-0.324325
H	-0.418783	0.190559	-1.100485	H	-0.488779	-0.072770	-1.246617
H	-0.582094	1.679851	-0.091595	H	-0.586510	1.542767	-0.435113
O	-2.369491	-1.159398	-0.134664	O	-2.376601	-1.244510	0.067486
H	-1.631720	-1.693375	0.188009	H	-1.599593	-1.700513	0.435878
O	0.197453	-1.246785	0.944196	O	0.193655	-1.381674	0.899105
O	0.258420	0.108924	0.852673	O	0.281097	0.051952	0.672938
C	2.087264	0.336015	0.208153	C	1.663772	0.376346	0.401990
C	2.308391	1.799491	0.104765	C	1.881831	1.866285	0.399702
H	3.384395	1.993000	0.117892	H	2.954562	2.053725	0.439140
H	1.888420	2.189487	-0.821623	H	1.489702	2.323218	-0.508747
H	1.864792	2.297335	0.967426	H	1.410580	2.312138	1.275656
O	1.787309	-1.662200	-0.676975	O	2.575057	-1.313235	-0.808383
O	1.955866	-0.311747	-0.885345	O	2.004985	-0.136296	-0.872365
H	2.391213	-0.243700	1.075468	H	2.198053	-0.183313	1.165841
H	-2.236211	0.301117	1.324383	H	-2.143001	0.434612	1.250421
HO(CH ₃)CHCH ₂ OO							
C	-0.757950	0.063686	-0.319455				
C	-2.169437	-0.422497	-0.039430				
H	-2.881269	0.288426	-0.458603				
H	-2.345534	-1.403441	-0.484099				
H	-2.340983	-0.479361	1.037969				
C	0.254155	-0.857904	0.349588				
H	0.299234	-0.665461	1.424175				
H	0.035035	-1.907527	0.153846				
O	-0.669235	1.383114	0.174592				
H	0.250689	1.664763	0.123837				
O	2.032636	0.521534	-0.025959				
O	1.585027	-0.684992	-0.191148				
H	-0.565205	0.045639	-1.401225				
CRCa1				TSCa1			
C	-2.103585	-0.090061	0.216354	C	-2.029405	-0.047148	0.220449
C	-3.138532	0.984966	-0.067283	C	-3.062079	0.931167	-0.311539

H	-4.108606	0.514159	-0.226867	H	-4.020640	0.421744	-0.410632
H	-3.217542	1.685263	0.765971	H	-3.181499	1.781992	0.361326
H	-2.871481	1.532898	-0.973523	H	-2.764032	1.292456	-1.298309
C	-0.722283	0.536623	0.333584	C	-0.660005	0.615101	0.272994
H	-0.318063	0.832587	-0.634668	H	-0.240193	0.736222	-0.727147
H	-0.707812	1.382745	1.019374	H	-0.683669	1.572097	0.792485
O	-2.167754	-1.020393	-0.846141	O	-2.033499	-1.167502	-0.642257
H	-1.394922	-1.593467	-0.802792	H	-1.269391	-1.716587	-0.436316
O	0.489253	-1.397234	0.153644	O	0.604140	-1.283874	0.448986
O	0.216679	-0.394785	0.932278	O	0.264359	-0.173855	1.057975
H	-2.336207	-0.587155	1.168601	H	-2.298277	-0.353929	1.240600
C	3.012107	-0.522311	0.088375	C	2.666052	-0.704451	-0.319302
H	3.486298	-1.376444	-0.380223	H	2.735199	-1.501455	-1.047527
H	2.810382	-0.424221	1.150926	H	2.971729	-0.777698	0.717409
O	2.072885	1.485468	-0.132516	O	2.242095	1.429378	0.112630
O	2.685402	0.399235	-0.671387	O	2.330828	0.417995	-0.773272
CPCa1				CRCa2			
C	-1.991802	-0.113212	0.196053	C	1.184145	-0.532561	-0.183648
C	-3.117931	0.805078	-0.244906	C	2.599490	-0.399980	-0.710006
H	-4.000535	0.209159	-0.477180	H	2.765443	-1.120893	-1.510606
H	-3.372257	1.521674	0.538219	H	2.781490	0.606469	-1.093459
H	-2.827643	1.348777	-1.147071	H	3.310333	-0.608726	0.093033
C	-0.718304	0.684937	0.434561	C	0.884484	0.508301	0.900045
H	-0.300277	1.041259	-0.512277	H	-0.068945	0.306239	1.389631
H	-0.917959	1.535762	1.090978	H	1.688160	0.558009	1.635233
O	-1.827580	-1.077962	-0.828346	O	1.023430	-1.807000	0.383022
H	-1.045562	-1.602086	-0.632855	H	0.068190	-1.984573	0.395191
O	0.772721	-1.083561	0.331736	O	-0.282352	2.032952	-0.321196
O	0.273912	-0.035472	1.165156	O	0.818654	1.837964	0.330429
H	-2.258682	-0.606399	1.140730	H	0.460947	-0.381303	-0.996011
C	2.109274	-0.822343	0.103598	C	-2.412929	0.510731	-0.455839
H	2.512346	-1.715599	-0.371760	H	-2.889818	1.399334	-0.058299
H	2.628595	-0.526812	1.015473	H	-2.053141	0.407013	-1.475635
O	2.509365	1.384786	-0.267910	O	-1.704493	-1.582068	-0.171716
O	2.258401	0.245647	-0.848147	O	-2.304463	-0.444413	0.319163
TSCa2				CPCa2			
C	-1.388537	0.270212	-0.191046	C	-1.788904	0.253368	-0.290228
C	-2.802348	-0.196374	-0.477340	C	-2.740117	-0.924468	-0.279925
H	-3.238751	0.402063	-1.277174	H	-3.479541	-0.817260	-1.073871
H	-2.805884	-1.246831	-0.778510	H	-2.190279	-1.855588	-0.424594
H	-3.420059	-0.081205	0.416532	H	-3.263934	-0.966799	0.678232
C	-0.711327	-0.605080	0.878350	C	-0.713006	0.125136	0.785963
H	0.017380	-0.019507	1.440801	H	-0.081047	1.018914	0.822453
H	-1.427766	-1.053632	1.567451	H	-1.182197	-0.024356	1.762084
O	-1.438278	1.598407	0.276761	O	-2.549767	1.423260	-0.021612
H	-0.542296	1.958213	0.187682	H	-2.014176	2.198687	-0.208569
O	0.803943	-1.420444	-0.643342	O	0.841296	-0.853888	-0.589397

O	-0.014116	-1.748749	0.326728	O	0.100501	-1.029066	0.621132
H	-0.781370	0.212719	-1.098431	H	-1.301872	0.330924	-1.268625
C	2.428077	-0.311171	-0.182170	C	2.172408	-0.828293	-0.245245
H	2.922052	-1.031766	0.457617	H	2.431055	-1.611964	0.466684
H	2.586803	-0.243874	-1.251786	H	2.729312	-0.878144	-1.180481
O	1.385469	1.641645	-0.362568	O	2.432346	1.418537	-0.367971
O	1.954821	0.698928	0.423552	O	2.521922	0.397546	0.433261
CRCa3				TSCa3			
C	1.202622	-0.590538	-0.184972	C	1.561065	-0.305254	-0.277155
C	2.464418	-1.438508	-0.087598	C	3.035560	-0.340260	-0.646651
H	2.188648	-2.488578	0.013257	H	3.363617	-1.376709	-0.721915
H	3.091031	-1.328142	-0.976043	H	3.218586	0.160863	-1.598813
H	3.040154	-1.151763	0.795391	H	3.627513	0.146893	0.132345
C	1.564002	0.881022	-0.306124	C	1.118928	1.142288	-0.081644
H	2.010257	1.254936	0.616425	H	1.446458	1.511341	0.893454
H	2.201878	1.076511	-1.169584	H	1.516111	1.774012	-0.878553
O	0.400240	-0.727639	0.964388	O	1.421887	-1.070018	0.902191
H	-0.337737	-1.334803	0.750131	H	0.481718	-1.179767	1.081792
O	-0.075100	2.247327	0.527127	O	-0.953737	0.985408	0.906799
O	0.351185	1.633274	-0.534774	O	-0.299684	1.349878	-0.200498
H	0.629537	-0.879111	-1.076599	H	0.960527	-0.736364	-1.089664
C	-2.173688	0.465468	0.167256	C	-2.993616	-0.271276	-0.765213
H	-2.415338	1.417804	-0.291860	H	-3.280505	-0.290772	-1.802535
H	-1.926760	0.337327	1.218048	H	-3.599840	0.016276	0.078711
O	-1.854919	-1.740026	-0.046551	O	-1.388783	-0.637779	0.736700
O	-2.174630	-0.514042	-0.586506	O	-1.787909	-0.799835	-0.529048
CPCa3				CRCa4			
C	-1.675397	0.108186	-0.240971	O	-0.365923	1.974458	0.007419
C	-3.140204	-0.294190	-0.273831	C	-1.721257	-0.024193	0.318729
H	-3.755156	0.599651	-0.375914	C	-2.484463	-1.104930	-0.441108
H	-3.351370	-0.966791	-1.107291	H	-3.000964	-1.747964	0.271721
H	-3.410771	-0.788070	0.662207	H	-3.221329	-0.675779	-1.124140
C	-0.802553	-1.134056	-0.081223	H	-1.786868	-1.720880	-1.016121
H	-0.973752	-1.571080	0.906686	C	-0.990310	0.868158	-0.681387
H	-1.003087	-1.865050	-0.870297	H	-0.211689	0.307012	-1.201942
O	-1.490230	0.985682	0.841423	H	-1.685813	1.330330	-1.384457
H	-0.655468	1.455599	0.708591	O	-0.828188	-0.568163	1.253399
O	1.380548	-1.838583	0.148706	O	0.904927	1.826211	0.189739
O	0.545256	-0.685089	-0.176652	H	-0.244367	-1.182819	0.773743
H	-1.402465	0.599446	-1.184425	C	2.587402	-0.053610	-0.250752
C	2.010770	2.029317	-0.252846	H	2.345163	0.203484	-1.276931
H	2.342483	0.988177	-0.123469	H	3.314094	0.472474	0.358848
H	2.758844	2.770547	-0.582340	O	1.072986	-1.672228	-0.471167
O	2.578764	-1.505511	0.117294	O	2.036340	-1.022402	0.275464
O	0.872542	2.358755	-0.048336	H	-2.417582	0.598574	0.887548
TSCa4				CPCa4			
O	0.127746	1.831265	-0.114488	C	-0.450431	0.786206	-0.193108

C	-1.582597	0.190741	0.383899	C	-0.113214	2.259231	-0.339244
C	-2.568476	-0.730842	-0.343979	H	0.896030	2.369111	-0.738658
H	-3.157049	-1.267700	0.399705	H	-0.805971	2.754452	-1.022454
H	-3.244106	-0.163129	-0.987556	H	-0.158290	2.755129	0.632807
H	-2.020029	-1.460047	-0.944860	C	-1.870777	0.601995	0.311027
C	-0.793599	0.954682	-0.735546	H	-1.976514	0.996611	1.321998
H	-0.284559	0.212853	-1.352595	H	-2.601776	1.049657	-0.364447
H	-1.444609	1.610496	-1.311857	O	0.439351	0.199061	0.752642
O	-0.707728	-0.489919	1.188469	H	2.787518	0.735614	0.167995
O	1.125447	1.232828	0.507133	O	-2.258029	-1.378708	-0.724645
H	-0.187957	-1.159539	0.573980	O	-2.186977	-0.801831	0.436104
C	2.093699	0.036364	-0.316394	C	1.017192	-1.011660	0.353855
H	1.789713	0.258932	-1.338598	O	3.109043	-0.169112	0.047175
H	3.030123	0.449732	0.049120	O	2.018046	-0.801632	-0.603793
O	0.686429	-1.701027	-0.462935	H	0.300413	-1.671472	-0.143086
O	1.860474	-1.137903	0.131297	H	-0.349906	0.279667	-1.158644
H	-2.114637	0.930776	0.988974	H	1.440399	-1.465616	1.249439
CRCa5				TSCa5			
C	-1.327940	0.627442	-0.414200	C	0.830684	0.878602	0.404747
C	-1.977134	1.948400	-0.021473	C	0.970845	2.370164	0.132098
H	-2.017932	2.603853	-0.891415	H	0.591123	2.932641	0.984406
H	-2.992203	1.799185	0.353580	H	2.016171	2.639263	-0.030854
H	-1.388362	2.446518	0.754605	H	0.393671	2.654176	-0.752361
C	-1.245178	-0.288575	0.800186	C	1.310549	0.077457	-0.796595
H	-0.564872	0.115720	1.552550	H	0.607633	0.148790	-1.629915
H	-2.228936	-0.493100	1.225391	H	2.310839	0.386552	-1.102191
O	-0.049856	0.822157	-0.980862	O	-0.525046	0.593127	0.724483
H	0.530868	1.185817	-0.286081	H	-1.138634	0.802052	-0.100911
O	-1.447597	-2.281328	-0.288678	O	2.317164	-1.607396	0.353520
O	-0.652921	-1.558329	0.441064	O	1.367060	-1.334310	-0.488660
C	2.327717	-0.758069	-0.509284	C	-1.536882	-1.087047	0.563275
O	1.892024	0.884750	0.939414	O	-2.234904	0.264041	-0.995557
O	2.700511	0.310905	-0.012850	O	-2.580706	-0.493628	0.173308
H	2.984188	-1.164825	-1.271822	H	-1.576234	-1.492225	1.570798
H	-1.926027	0.125027	-1.178809	H	1.430245	0.589276	1.271188
H	1.401203	-1.218625	-0.174086	H	-0.834528	-1.470253	-0.168057
CPCa5				CRCa6			
C	-0.450431	0.786206	-0.193108	C	-2.127181	-0.087502	0.232020
C	-0.113214	2.259231	-0.339244	C	-3.187522	0.939145	-0.126552
H	0.896030	2.369111	-0.738658	H	-4.145456	0.434763	-0.253790
H	-0.805971	2.754452	-1.022454	H	-3.286013	1.693292	0.656133
H	-0.158290	2.755129	0.632807	H	-2.931746	1.429597	-1.068292
C	-1.870777	0.601995	0.311027	C	-0.761781	0.579878	0.307582
H	-1.976514	0.996611	1.321998	H	-0.362966	0.821187	-0.677856
H	-2.601776	1.049657	-0.364447	H	-0.771608	1.465649	0.941532
O	0.439351	0.199061	0.752642	O	-2.164390	-1.090821	-0.763588
H	2.787518	0.735614	0.167995	H	-1.375012	-1.636393	-0.680648

O	-2.258029	-1.378708	-0.724645	O	0.510325	-1.315097	0.229616
O	-2.186977	-0.801831	0.436104	O	0.199528	-0.289991	0.959203
C	1.017192	-1.011660	0.353855	C	3.029417	-0.608814	-0.325100
O	3.109043	-0.169112	0.047175	O	2.005156	1.356537	-0.515781
O	2.018046	-0.801632	-0.603793	O	2.860613	0.529155	0.133408
H	0.300413	-1.671472	-0.143086	H	3.700119	-1.248731	0.235739
H	-0.349906	0.279667	-1.158644	H	-2.350496	-0.523810	1.215663
H	1.440399	-1.465616	1.249439	H	2.515737	-0.890052	-1.239041
TSCa6				CPCa6			
C	1.910224	0.001242	0.232842	C	1.932345	0.005626	0.212397
C	3.051492	-0.730122	-0.454467	C	3.047124	-0.870152	-0.338009
H	3.970583	-0.160739	-0.316926	H	3.994545	-0.345806	-0.215881
H	3.189940	-1.730652	-0.040530	H	3.103322	-1.827361	0.184162
H	2.858158	-0.806079	-1.527072	H	2.895591	-1.047304	-1.405324
C	0.594196	-0.712890	-0.051405	C	0.592489	-0.663423	-0.050774
H	0.231086	-0.454901	-1.050126	H	0.281328	-0.539239	-1.088774
H	0.687250	-1.793900	0.072089	H	0.591624	-1.711856	0.255874
O	1.900916	1.318443	-0.264059	O	2.012765	1.253315	-0.419584
H	1.084618	1.737850	0.036046	H	1.189077	1.718846	-0.191445
O	-0.627865	0.999022	0.890968	O	-0.560048	1.389498	0.446025
O	-0.423763	-0.335661	0.910897	O	-0.426146	-0.018983	0.787596
C	-2.193518	-0.969927	0.315932	C	-1.719270	-0.619618	0.757354
O	-2.338459	0.949864	-0.740776	O	-2.984916	0.327020	-0.851699
O	-2.207763	-0.411565	-0.822784	O	-2.198290	-0.681474	-0.562688
H	-2.075658	-2.048250	0.294247	H	-1.606937	-1.644064	1.110653
H	2.065814	-0.001719	1.320639	H	2.041575	0.108569	1.301846
H	-2.610690	-0.432258	1.160257	H	-2.353176	0.018605	1.365883
CRDa1				TSDa1			
C	-1.688432	-0.705362	0.127909	C	-1.846114	-0.668609	0.248065
C	-2.939320	-1.031614	-0.663774	C	-2.911740	-0.714189	-0.831945
H	-2.801702	-1.944936	-1.243290	H	-2.962211	-1.707469	-1.278738
H	-3.773610	-1.174215	0.025686	H	-3.882551	-0.469785	-0.396785
H	-3.190012	-0.207584	-1.332173	H	-2.691997	0.020977	-1.606244
C	-1.793469	0.553051	0.974820	C	-1.742686	0.678756	0.953022
H	-0.801514	0.814402	1.349895	H	-0.871996	0.670612	1.612538
H	-2.418071	0.304164	1.835265	H	-2.636592	0.782395	1.572969
O	-2.423386	1.633137	0.319620	O	-1.738265	1.784772	0.074832
O	-0.572067	-0.625903	-0.829563	O	-0.579897	-1.090971	-0.344027
O	-0.306521	0.569982	-1.249033	O	-0.017531	-0.148086	-1.078662
H	-1.833454	1.909276	-0.387795	H	-1.004598	1.649270	-0.532947
C	2.220608	0.122034	0.024329	C	1.877278	0.161079	-0.150355
C	2.694471	1.407237	-0.549547	C	2.227551	1.372333	-0.939657
H	2.297748	1.494702	-1.564563	H	1.941288	1.216076	-1.980544
H	2.354093	2.247231	0.052663	H	1.722708	2.250154	-0.538309
H	3.785481	1.403953	-0.612406	H	3.309789	1.527531	-0.901694
C	2.534682	-1.196762	-0.555613	C	2.416936	-1.184515	-0.450496
H	3.202718	-1.102146	-1.408691	H	2.746228	-1.233214	-1.486302

H	2.958691	-1.828978	0.229843
H	1.590028	-1.671472	-0.838337
O	1.019054	-0.978446	1.578831
O	1.510917	0.200539	1.052779
H	-1.365610	-1.530369	0.764086

CPDa1

C	1.835890	-0.368112	-0.674625
C	2.535644	-1.361822	0.235209
H	2.421440	-2.374808	-0.152400
H	3.599179	-1.120433	0.288328
H	2.125519	-1.308841	1.242423
C	1.937808	1.077232	-0.190999
H	1.309492	1.709722	-0.828158
H	2.976384	1.394546	-0.319522
O	1.635568	1.259526	1.174873
O	0.486936	-0.765605	-0.961539
O	-0.201743	-0.929425	0.281529
H	0.678679	1.260783	1.269668
C	-1.456323	-0.326208	0.188661
C	-2.138805	-0.636868	1.503545
H	-2.282430	-1.713268	1.590539
H	-1.522742	-0.290460	2.334244
H	-3.105732	-0.135345	1.537678
C	-2.242678	-0.712374	-1.041797
H	-2.420004	-1.787451	-0.997254
H	-3.198857	-0.188453	-1.045551
H	-1.696942	-0.471218	-1.948778
O	-1.198847	1.728330	-0.912063
O	-1.219303	1.132183	0.241033
H	2.265896	-0.405922	-1.681852

TSDa2

C	1.978683	-0.614210	-0.439245
C	2.739352	-0.827800	0.853489
H	2.866090	-1.892223	1.054392
H	3.722755	-0.361119	0.772408
H	2.204553	-0.351774	1.673765
C	1.793182	0.864858	-0.789417
H	1.040578	0.960855	-1.580205
H	2.754006	1.192611	-1.204470
O	1.494575	1.663871	0.316517
O	0.711178	-1.332380	-0.394826
O	-0.057770	-0.928589	0.598263
C	-1.755668	-0.222891	-0.017268
O	-1.175026	1.962157	-0.065791
O	-1.337433	0.781458	-0.720638
C	-2.204181	-1.373738	-0.855405
H	-2.150220	-2.293542	-0.275844

H	3.258629	-1.366951	0.226704
H	1.663639	-1.940882	-0.234947
O	1.123374	-0.673016	1.789571
O	1.372626	0.399365	1.004769
H	-2.002141	-1.444345	1.000641

CRDa2

C	2.070736	-0.143477	-0.622316
C	3.070766	-0.377930	0.485884
H	3.392633	-1.419454	0.512828
H	3.940215	0.254123	0.295158
H	2.640801	-0.107659	1.448174
C	1.456412	1.251734	-0.604526
H	0.730807	1.338525	-1.421758
H	2.265400	1.970388	-0.792941
O	0.848445	1.484146	0.633783
O	0.952242	-1.091826	-0.565368
O	0.720918	-1.581296	0.612807
C	-1.915929	-0.327763	-0.023088
O	-1.647959	1.917987	-0.092538
O	-1.791396	0.691818	-0.740424
C	-2.112199	-1.608491	-0.746740
H	-1.353994	-2.316836	-0.406989
H	-3.094561	-2.010585	-0.482039
H	-2.045345	-1.460743	-1.822290
C	-1.895871	-0.223375	1.448627
H	-2.597591	0.557048	1.754110
H	-2.118814	-1.185207	1.904426
H	-0.897778	0.115431	1.748749
H	-0.063659	1.816657	0.457029
H	2.500405	-0.342509	-1.607588

CPDa2

C	1.847164	-0.667656	-0.503006
C	2.471349	-1.292123	0.732134
H	2.315742	-2.371573	0.729283
H	3.543829	-1.087366	0.743943
H	2.038396	-0.863057	1.634500
C	2.045055	0.845665	-0.587276
H	1.406946	1.239388	-1.387552
H	3.086737	1.029585	-0.863552
O	1.830873	1.527711	0.625797
O	0.472862	-1.048238	-0.649610
O	-0.230126	-0.525418	0.487761
C	-1.542069	-0.274190	0.118749
O	-0.921765	1.897882	-0.369761
O	-1.567191	0.873063	-0.819862
C	-2.207710	-1.390094	-0.654729
H	-2.171287	-2.301822	-0.057977

H	-3.239196	-1.202273	-1.163811
H	-1.577427	-1.458431	-1.742273
C	-2.290608	0.026804	1.346340
H	-3.164130	0.678635	1.251578
H	-2.567931	-0.916251	1.813021
H	-1.552536	0.558249	1.944666
H	0.549571	1.909668	0.278025
H	2.465142	-1.114685	-1.280415

CRDa3

C	2.070710	-0.143490	-0.622346
C	3.070760	-0.377964	0.485830
H	3.392603	-1.419496	0.512772
H	3.940218	0.254068	0.295079
H	2.640824	-0.107678	1.448130
C	1.456420	1.251737	-0.604543
H	0.730796	1.338545	-1.421758
H	2.265419	1.970372	-0.792977
O	0.848487	1.484163	0.633780
O	0.952181	-1.091800	-0.565365
O	0.720933	-1.581338	0.612796
H	-0.063624	1.816666	0.457046
C	-1.915927	-0.327753	-0.023066
C	-2.112237	-1.608472	-0.746723
H	-3.094599	-2.010550	-0.481998
H	-2.045409	-1.460718	-1.822274
H	-1.354038	-2.316833	-0.406996
C	-1.895830	-0.223378	1.448648
H	-2.118755	-1.185214	1.904445
H	-0.897732	0.115436	1.748748
H	-2.597548	0.557038	1.754154
O	-1.647934	1.917995	-0.092506
O	-1.791400	0.691832	-0.740397
H	2.500348	-0.342537	-1.607628

CPDa3

C	1.997353	0.026185	0.720038
C	3.087967	0.706450	-0.091296
H	3.198563	1.748118	0.212916
H	4.034553	0.189856	0.076993
H	2.859262	0.657534	-1.155285
C	1.699784	-1.399395	0.265586
H	0.884078	-1.802099	0.874300
H	2.596441	-2.001362	0.445757
O	1.394750	-1.479946	-1.103957
O	0.798141	0.820036	0.782954
O	0.439991	1.205925	-0.575597
H	0.436159	-1.411630	-1.192260
C	-2.160316	-0.493632	0.081870

H	-3.247713	-1.126284	-0.847683
H	-1.694481	-1.558420	-1.598964
C	-2.251983	0.128864	1.394020
H	-3.263788	0.456856	1.155118
H	-2.297271	-0.726479	2.067467
H	-1.713337	0.943483	1.877794
H	0.878828	1.574242	0.765110
H	2.269338	-1.111347	-1.411451

TS Da3

C	-1.917190	-0.769842	0.484347
C	-2.905642	-1.076791	-0.622678
H	-2.811792	-2.116516	-0.938343
H	-3.921137	-0.904244	-0.260907
H	-2.736634	-0.420122	-1.474450
C	-2.020602	0.659236	1.018374
H	-1.143621	0.865783	1.642840
H	-2.908553	0.703713	1.654499
O	-2.197036	1.641817	0.026654
O	-0.566563	-1.115553	0.088097
O	-0.192176	-0.487479	-1.046305
H	-1.343267	1.778168	-0.397876
C	2.422708	0.127066	0.189126
C	2.914857	-0.696052	1.321060
H	4.001999	-0.778758	1.288945
H	2.621464	-0.252968	2.274253
H	2.492689	-1.709576	1.280998
C	2.918081	0.090445	-1.204348
H	3.945400	-0.272862	-1.215634
H	2.302503	-0.569597	-1.828388
H	2.879254	1.084934	-1.657571
O	0.476041	0.956784	-0.629071
O	1.254891	0.759179	0.458858
H	-2.052833	-1.450315	1.330481

CRDa4

C	2.070332	-0.143779	-0.622357
C	3.070403	-0.378619	0.485727
H	3.392400	-1.420112	0.512201
H	3.939771	0.253646	0.295311
H	2.640423	-0.108748	1.448116
C	1.456607	1.251705	-0.604595
H	0.731048	1.338898	-1.421819
H	2.265919	1.969994	-0.792974
O	0.848734	1.484424	0.633741
O	-1.790852	0.692047	-0.740297
O	-1.647266	1.918114	-0.092252
C	-1.915574	-0.327619	-0.023108
O	0.720428	-1.581426	0.612958

C	-2.139400	-0.257585	1.569321	O	0.951423	-1.091686	-0.565178
H	-3.145292	-0.329505	1.988606	C	-2.112308	-1.608123	-0.747073
H	-1.467206	-0.962761	2.054320	H	-1.354526	-2.316958	-0.407435
H	-1.772331	0.758641	1.739446	H	-3.094907	-2.009794	-0.482563
C	-3.243316	0.202329	-0.701626	H	-2.045333	-1.460105	-1.822581
H	-4.201468	-0.279409	-0.484498	C	-1.895634	-0.223452	1.448624
H	-3.319741	1.246413	-0.391975	H	-2.597860	0.556525	1.754089
H	-3.035333	0.137488	-1.767512	H	-2.118119	-1.185460	1.904254
O	-0.640076	1.825427	-0.548044	H	-0.897798	0.115870	1.748972
O	-1.342027	-1.203744	-0.460888	H	-0.063471	1.816925	0.456999
H	2.273660	0.001021	1.780092	H	2.499759	-0.343157	-1.607662
TSDa4				CPDa4			
C	2.015155	-0.546527	-0.488120	C	1.949226	-0.594683	-0.409539
C	2.677974	-0.983577	0.798841	C	2.644764	-0.893621	0.905823
H	2.609736	-2.065990	0.919863	H	2.711690	-1.973298	1.043544
H	3.731481	-0.701966	0.760926	H	3.652882	-0.474619	0.899812
H	2.208499	-0.485710	1.645309	H	2.093155	-0.459162	1.737274
C	1.868207	1.019142	-0.581154	C	1.870255	0.925969	-0.733815
H	1.400577	1.257824	-1.545321	H	1.248891	1.066502	-1.625518
H	2.909500	1.376632	-0.584455	H	2.910350	1.236917	-0.924080
O	1.178289	1.502787	0.481404	O	1.417846	1.616175	0.351329
O	-1.414728	0.699588	-0.817124	O	-1.384248	0.788189	-0.778622
O	-1.098888	1.934839	-0.184599	O	-1.305310	1.966930	0.007098
C	-1.654841	-0.270300	0.011576	C	-1.433374	-0.356581	0.042325
O	-0.004497	-0.852106	0.484363	O	-0.130111	-0.646268	0.557524
O	0.684004	-1.042478	-0.623246	O	0.666829	-1.172430	-0.501060
C	-2.208530	-1.472688	-0.694847	C	-1.947151	-1.459076	-0.867125
H	-2.107124	-2.359383	-0.071325	H	-1.792892	-2.425464	-0.386773
H	-3.267725	-1.290876	-0.890748	H	-3.011540	-1.302302	-1.041055
H	-1.693530	-1.617678	-1.643554	H	-1.421759	-1.444669	-1.819963
C	-2.110530	0.041640	1.403516	C	-2.278724	-0.166640	1.289059
H	-3.047428	0.597629	1.320477	H	-3.225594	0.290605	1.001954
H	-2.271826	-0.882664	1.956515	H	-2.461809	-1.137790	1.748651
H	-1.388268	0.676519	1.909965	H	-1.779354	0.485572	2.002371
H	0.124655	1.753068	0.179783	H	-0.345905	2.048760	0.161666
H	2.513398	-0.924596	-1.382699	H	2.471857	-1.064025	-1.248406
CRDa5				TSDa5			
C	-2.561753	-0.303120	-0.109253	C	2.046393	0.088053	-0.768069
C	-2.107745	-0.633867	1.296756	C	2.165271	1.454933	-0.127122
H	-2.703414	-0.089760	2.030961	H	3.209893	1.765843	-0.090890
H	-2.241079	-1.705037	1.462442	H	1.592211	2.177155	-0.711055
H	-1.054729	-0.395017	1.444406	H	1.771022	1.441164	0.887861
C	-1.714669	-0.942979	-1.208754	C	0.614274	-0.411968	-0.916931
H	-2.075542	-0.592309	-2.178259	H	0.629048	-1.452078	-1.252548
H	-1.876028	-2.028642	-1.159865	H	0.121607	0.206946	-1.680614
O	-0.358159	-0.614063	-1.116592	O	-0.099016	-0.344838	0.297238
O	-2.599195	1.137629	-0.343277	O	2.821949	-0.916952	-0.051421

O	-1.618083	1.785342	0.199716	O	2.713605	-0.835864	1.239114
H	0.044149	-1.076903	-0.347918	H	-0.292208	0.689564	0.475395
C	2.443397	0.223180	0.082049	C	-2.078440	-0.201819	0.005344
C	3.596701	0.628239	-0.762137	C	-2.470216	-1.294922	-0.931509
H	4.277030	1.248090	-0.173251	H	-3.550060	-1.450493	-0.864193
H	4.118498	-0.241893	-1.154050	H	-2.202852	-1.042328	-1.955968
H	3.222125	1.243297	-1.584987	H	-1.976106	-2.217632	-0.624927
C	1.552759	1.191815	0.743017	C	-2.375587	-0.365724	1.460232
H	0.570643	1.145928	0.253864	H	-2.030479	-1.339623	1.801364
H	1.389952	0.876010	1.776440	H	-1.929313	0.429452	2.048165
H	1.958162	2.199247	0.678909	H	-3.465595	-0.318650	1.559602
O	1.156380	-1.421093	0.938079	O	-1.192750	1.821721	0.290085
O	2.259647	-1.010063	0.192827	O	-1.968703	0.954399	-0.545919
H	-3.606629	-0.584635	-0.264789	H	2.511985	0.071632	-1.756638
CPDa5				CRDa6			
C	1.978927	0.176423	-0.757954	C	-1.688562	0.705436	-0.127915
C	2.031011	1.520176	-0.062633	C	-2.939365	1.031524	0.663905
H	3.062296	1.805912	0.146210	H	-2.802276	1.945468	1.242540
H	1.592832	2.272612	-0.723491	H	-3.774010	1.172871	-0.025385
H	1.483474	1.485166	0.877854	H	-3.189270	0.207954	1.333173
C	0.571862	-0.319288	-1.041839	C	-1.793601	-0.553043	-0.974712
H	0.623372	-1.325606	-1.471212	H	-0.801657	-0.814545	-1.349688
H	0.104212	0.353923	-1.771457	H	-2.418072	-0.304130	-1.835253
O	-0.150766	-0.327535	0.170995	O	-2.423753	-1.632994	-0.319506
O	2.684219	-0.857847	-0.008660	O	-0.571972	0.626325	0.829321
O	2.628224	-0.710023	1.278249	O	-0.306486	-0.569384	1.249319
H	-0.786218	2.006405	0.218357	H	-1.833830	-1.909337	0.387826
C	-1.559414	-0.390644	0.063315	C	2.220754	-0.122021	-0.024179
C	-2.042885	-1.483345	-0.878067	C	2.694889	-1.406617	0.550847
H	-3.126391	-1.571501	-0.805047	H	2.297636	-1.493547	1.565704
H	-1.785999	-1.257802	-1.913730	H	2.355174	-2.247199	-0.050915
H	-1.586583	-2.431351	-0.589007	H	3.785856	-1.402782	0.614289
C	-2.082546	-0.559120	1.475351	C	2.534669	1.197363	0.554438
H	-1.806462	-1.547416	1.843790	H	3.202239	1.103733	1.407959
H	-1.653899	0.195771	2.130801	H	2.959245	1.828501	-0.231589
H	-3.168273	-0.458799	1.474700	H	1.589984	1.672754	0.835923
O	-1.746967	1.913050	0.295405	O	1.018960	0.976888	-1.579673
O	-2.022520	0.808627	-0.549069	O	1.511049	-0.201596	-1.052545
H	2.528392	0.197301	-1.702171	H	-1.366104	1.530499	-0.764212
TSDa6				CPDa6			
C	-1.246603	0.392074	-0.632686	C	1.297067	0.731757	0.157145
C	-1.492556	1.826204	-0.206107	C	2.057552	1.307384	-1.015219
H	-0.625893	2.469750	-0.353483	H	1.494418	2.115856	-1.482040
H	-2.307190	2.234227	-0.807046	H	3.019972	1.688819	-0.669283
H	-1.793604	1.849984	0.842582	H	2.242717	0.522708	-1.747472
C	-2.506306	-0.467569	-0.491829	C	2.072456	-0.322293	0.941855
H	-2.351032	-1.422384	-0.994652	H	1.390448	-0.846124	1.620074

H	-3.329164	0.061099	-0.978943
O	-2.861459	-0.647605	0.856270
O	-0.237812	-0.171064	0.264156
O	-0.186067	-1.548839	0.115666
H	-2.200831	-1.240478	1.235285
C	1.517005	0.403013	0.147440
C	1.615792	1.420228	1.240065
H	0.896016	2.221948	1.097637
H	1.445095	0.939106	2.201575
H	2.622234	1.846997	1.223273
C	1.642471	0.807295	-1.287845
H	1.125573	1.745502	-1.480482
H	2.710843	0.949282	-1.477660
H	1.291063	0.017026	-1.946182
O	1.986965	-1.690556	-0.441883
O	2.074918	-0.725949	0.516003
H	-0.874291	0.312581	-1.657835

CRDb1

C	1.357043	0.506175	0.656171
C	1.125680	1.529320	-0.435567
H	0.163620	2.018605	-0.286743
H	1.926855	2.269948	-0.394308
H	1.159886	1.053843	-1.415544
C	2.714094	-0.188401	0.602289
H	2.709140	-1.032947	1.302825
H	3.466985	0.526031	0.942072
O	3.099420	-0.591983	-0.689224
O	0.302174	-0.513604	0.631529
O	0.296995	-1.212935	-0.460993
H	2.397655	-1.145849	-1.047107
H	1.207485	0.940239	1.646602
C	-2.355996	-0.458506	-0.691020
C	-2.784053	-1.129403	0.542659
H	-3.056257	-2.164445	0.355206
H	-1.968612	-1.049871	1.268324
H	-3.616021	-0.561902	0.972829
O	-1.999734	1.395692	0.502419
O	-2.000255	0.737260	-0.698722
H	-2.320139	-0.924202	-1.671419

CPDb1

C	1.378768	0.425978	0.819840
C	1.164535	1.674152	-0.015891
H	0.365760	2.283094	0.408239
H	2.087392	2.257352	-0.039809
H	0.906425	1.414424	-1.042142
C	2.535756	-0.447718	0.339690
H	2.502094	-1.398728	0.885004

H	2.804315	0.219745	1.548610
O	2.778118	-1.210188	0.127435
O	0.056008	0.150256	-0.429755
O	0.231859	-1.248896	-0.758019
H	2.088455	-1.621585	-0.419466
C	-1.236368	0.358863	0.246722
C	-1.482647	1.847594	0.381538
H	-0.912921	2.285757	1.198779
H	-1.246700	2.353762	-0.555425
H	-2.542837	1.986159	0.594721
C	-1.331738	-0.447927	1.513599
H	-0.688026	0.000292	2.272242
H	-2.361564	-0.426448	1.871719
H	-1.034029	-1.474921	1.315811
O	-2.582229	-1.282179	-0.646399
O	-2.167516	-0.055020	-0.760915
H	0.957893	1.511921	0.839109

TSDb1

C	-1.375015	0.558511	-0.668955
C	-1.123816	1.552893	0.445176
H	-0.255933	2.168733	0.215402
H	-2.007829	2.185362	0.549205
H	-0.969162	1.037601	1.392433
C	-2.647997	-0.265544	-0.490836
H	-2.670261	-1.051467	-1.255743
H	-3.502920	0.393798	-0.656549
O	-2.798685	-0.801406	0.801882
O	-0.255252	-0.361298	-0.851585
O	-0.008198	-1.076605	0.229267
H	-1.999142	-1.297192	1.009427
H	-1.403467	1.052880	-1.642380
C	2.011128	-0.498717	0.714538
C	2.644032	-1.165505	-0.438052
H	2.698248	-2.238309	-0.271125
H	2.082010	-0.931331	-1.342718
H	3.646924	-0.744048	-0.568158
O	1.944311	1.391411	-0.460991
O	1.794717	0.756867	0.718694
H	1.916403	-0.937617	1.700848

CRDb2

C	1.971521	0.185621	-0.502578
C	2.797981	-0.290191	0.669936
H	3.280013	-1.242897	0.447674
H	3.569465	0.456275	0.868133
H	2.174986	-0.397522	1.555334
C	1.139160	1.428145	-0.203144
H	0.532377	1.674167	-1.082060

H	3.472736	0.054870	0.589793	H	1.836859	2.257555	-0.027806
O	2.563985	-0.653253	-1.055440	O	0.331089	1.206597	0.919320
O	0.174373	-0.340599	0.973872	O	1.040549	-0.843766	-0.972158
O	-0.161260	-0.888289	-0.306317	O	0.626759	-1.650599	-0.046828
H	1.733322	-1.067793	-1.305679	H	-0.591438	1.448041	0.678909
H	1.573463	0.691585	1.864457	H	2.586084	0.365632	-1.388116
C	-1.523621	-0.701755	-0.531754	C	-1.932181	-0.823655	-0.355112
C	-2.419866	-1.154903	0.592832	C	-2.081118	-1.014605	1.093644
H	-2.236932	-2.215476	0.765584	H	-2.171267	-2.070873	1.333113
H	-2.212296	-0.595686	1.500406	H	-1.191322	-0.592990	1.576981
H	-3.462074	-1.009684	0.308120	H	-2.937647	-0.430739	1.440640
O	-2.053600	1.456693	0.087621	O	-2.124729	1.397579	-0.070703
O	-1.753893	0.682019	-0.912041	O	-1.957321	0.297194	-0.899024
H	-1.700154	-1.241039	-1.463844	H	-1.791063	-1.634585	-1.064128
TSDb2				CPDb2			
C	1.907014	-0.257671	-0.488936	C	1.779412	-0.373570	-0.576880
C	2.589503	-0.723302	0.780592	C	2.451113	-1.159824	0.534384
H	2.901266	-1.764546	0.691058	H	2.514230	-2.214866	0.265921
H	3.469714	-0.103238	0.959870	H	3.458767	-0.773284	0.699999
H	1.912246	-0.604872	1.624711	H	1.895135	-1.052519	1.464688
C	1.449416	1.202281	-0.426194	C	1.689282	1.126313	-0.294987
H	0.771166	1.408058	-1.261816	H	1.017489	1.583537	-1.031375
H	2.355194	1.802222	-0.577635	H	2.685954	1.552072	-0.437233
O	0.883544	1.547107	0.803044	O	1.307965	1.446566	1.022204
O	0.806227	-1.153334	-0.824909	O	0.509218	-0.938754	-0.926967
O	-0.082329	-1.240610	0.140995	O	-0.346184	-0.816244	0.220728
H	-0.078593	1.667903	0.679011	H	0.360236	1.292798	1.098293
H	2.547741	-0.387917	-1.364482	H	2.317535	-0.506427	-1.521814
C	-1.825750	-0.645032	-0.420973	C	-1.626222	-0.671632	-0.257930
C	-2.497848	-0.885883	0.876675	C	-2.582595	-0.842168	0.895484
H	-2.594856	-1.955138	1.050905	H	-2.503854	-1.855995	1.285446
H	-1.932727	-0.409007	1.676573	H	-2.335144	-0.129132	1.682284
H	-3.481661	-0.409075	0.842634	H	-3.601244	-0.662077	0.552973
O	-1.725477	1.542169	0.091025	O	-1.454653	1.604547	-0.049380
O	-1.598104	0.549708	-0.835367	O	-1.799290	0.656859	-0.860748
H	-1.874391	-1.347065	-1.246124	H	-1.811493	-1.332616	-1.106298
CRDb3				TSDb3			
C	1.813325	0.539561	0.003477	C	1.694504	-0.613413	-0.624552
C	2.344710	-0.183597	-1.213164	C	1.593399	-1.516040	0.591871
H	2.537462	0.516203	-2.026513	H	0.852485	-2.297612	0.419949
H	3.273438	-0.693816	-0.953319	H	2.566059	-1.978454	0.774027
H	1.621130	-0.930432	-1.543152	H	1.313702	-0.949086	1.477543
C	1.582862	-0.353131	1.216225	C	2.646374	0.565523	-0.443089
H	1.023006	0.230007	1.960879	H	2.524584	1.245401	-1.295294
H	2.561255	-0.579173	1.649068	H	3.669591	0.183332	-0.458665
O	0.964782	-1.572572	0.921330	O	2.499949	1.245042	0.783125
O	0.528538	1.102721	-0.427103	O	0.394183	-0.162777	-1.071738

O	-0.004633	1.888699	0.453208
H	0.214230	-1.442364	0.308449
H	2.427103	1.395960	0.294780
C	-2.278705	0.429320	-0.247916
C	-2.283952	-0.073491	1.134251
H	-2.829672	0.598335	1.791192
H	-2.715499	-1.079968	1.130542
H	-1.253570	-0.196461	1.481129
O	-1.131997	-1.384613	-0.873236
O	-1.755067	-0.200473	-1.184910
H	-2.741306	1.359642	-0.564610

CPDb3

C	1.554135	0.051822	0.864937
C	2.507363	1.068790	0.262862
H	2.262533	2.071612	0.614355
H	3.528665	0.827639	0.562706
H	2.463713	1.047700	-0.826226
C	1.754466	-1.368965	0.351041
H	1.016498	-2.025219	0.828196
H	2.748310	-1.709500	0.650102
O	1.709492	-1.478339	-1.054740
O	0.177610	0.460084	0.741037
O	-0.098416	0.731910	-0.672565
H	0.825034	-1.259851	-1.362728
H	1.657401	0.033813	1.955620
C	-2.602050	-0.324478	0.593416
C	-2.180837	-1.474597	-0.280673
H	-2.872245	-2.309024	-0.130545
H	-2.187449	-1.175622	-1.328084
H	-1.189068	-1.820134	0.021842
O	-0.260245	1.954864	-0.864010
O	-3.020068	0.718812	0.172858
H	-2.518831	-0.495496	1.684621

TSDb4

C	1.927023	-0.176028	-0.508609
C	2.569333	-0.857916	0.677896
H	2.715837	-1.921083	0.480636
H	3.542869	-0.398362	0.855688
H	1.949581	-0.725891	1.562891
C	1.475226	1.294141	-0.183740
H	1.020530	1.719035	-1.087282
H	2.420397	1.816858	0.025841
O	0.644960	1.322334	0.893393
O	0.733174	-0.832861	-0.947010
O	-0.049785	-1.124393	0.066268
H	-0.383546	1.459118	0.565144
H	2.551437	-0.181321	-1.403692

O	-0.131561	0.753291	-0.224035
H	1.592784	1.562296	0.831325
H	2.021168	-1.185210	-1.498384
C	-2.810427	-0.401535	-0.354233
C	-3.293650	0.952158	-0.020727
H	-4.217393	1.151094	-0.561673
H	-3.479827	1.047122	1.055817
H	-2.552336	1.712676	-0.285511
O	-0.998748	-0.049380	0.928021
O	-1.760927	-0.946848	0.288936
H	-3.295185	-1.126339	-0.989233

CRDb4

C	1.971640	0.185566	-0.502464
C	2.797902	-0.290262	0.670186
H	3.279948	-1.242978	0.447991
H	3.569372	0.456183	0.868514
H	2.174759	-0.397585	1.555480
C	1.139270	1.428118	-0.203179
H	0.532599	1.674114	-1.082179
H	1.836972	2.257518	-0.027800
O	0.331063	1.206657	0.919203
O	1.040751	-0.843821	-0.972196
O	0.626617	-1.650491	-0.046879
H	-0.591442	1.448074	0.678670
H	2.586351	0.365558	-1.387902
C	-1.932292	-0.823702	-0.355032
O	-2.124684	1.397592	-0.070958
O	-1.957391	0.297064	-0.899115
C	-2.081156	-1.014426	1.093761
H	-2.937643	-0.430473	1.440715
H	-2.171344	-2.070654	1.333395
H	-1.191316	-0.592777	1.576988
H	-1.791281	-1.634750	-1.063935

CPDb4

C	1.883280	-0.321438	-0.480028
C	2.537471	-0.863861	0.777258
H	2.770174	-1.920141	0.638752
H	3.462734	-0.321545	0.981325
H	1.873746	-0.751454	1.632480
C	1.570788	1.200948	-0.405945
H	0.998442	1.491181	-1.293752
H	2.553780	1.699327	-0.389801
O	0.934841	1.496202	0.764372
O	0.721772	-1.033198	-0.847441
O	-0.218535	-0.936033	0.220755
H	-0.883991	1.725081	0.562835
H	2.525207	-0.465823	-1.354100

C	-1.721551	-0.696329	-0.410848
O	-1.647197	1.513946	0.091515
O	-1.642981	0.492626	-0.902473
C	-2.363944	-0.950437	0.912172
H	-3.392890	-0.589311	0.849085
H	-2.352929	-2.016765	1.132181
H	-1.857884	-0.385885	1.691599
H	-1.835300	-1.430210	-1.206864

CRDb5

C	2.198379	-0.133814	0.279267
C	2.982216	-0.716769	-0.875182
H	3.788652	-0.046098	-1.172757
H	3.412653	-1.672760	-0.572049
H	2.318502	-0.892748	-1.721355
C	1.032636	-0.996117	0.726276
H	0.431347	-0.435076	1.451228
H	1.445500	-1.876536	1.236630
O	0.265165	-1.366050	-0.393136
O	1.688094	1.151243	-0.201915
O	1.213128	1.881521	0.756957
H	-0.651902	-1.478865	-0.078960
C	-2.826657	0.585611	-0.613665
C	-1.602040	1.326856	-0.299830
H	-0.748662	0.776316	-0.719105
H	-1.631038	2.336121	-0.701021
H	-1.446194	1.322398	0.783164
O	-2.184214	-1.067533	0.759231
O	-3.089615	-0.531992	-0.127163
H	-3.598314	0.933519	-1.296805
H	2.831789	0.101618	1.138046

CPDb5

C	1.876566	-0.516058	0.302492
C	1.876860	-1.774583	-0.535813
H	2.766165	-1.815533	-1.164589
H	1.868101	-2.646182	0.120671
H	0.986808	-1.818724	-1.164059
C	0.656224	-0.368233	1.204154
H	0.639702	0.641910	1.625543
H	0.762142	-1.077418	2.027520
O	-0.556981	-0.696044	0.570418
O	1.930472	0.596785	-0.643331
O	2.169307	1.727319	-0.055566
H	-2.936992	-1.139874	0.691179
C	-1.056312	0.208218	-0.405521
C	-1.244372	1.619379	0.116763
H	-0.286058	2.126832	0.232299
H	-1.837887	2.174566	-0.609999

C	-1.478012	-0.673323	-0.372116
O	-1.794404	1.519040	0.281873
O	-1.566980	0.651390	-0.819815
C	-2.519620	-1.062537	0.652725
H	-3.497384	-0.729530	0.305582
H	-2.519943	-2.145042	0.774377
H	-2.309357	-0.588703	1.609493
H	-1.550409	-1.251301	-1.296513

TSDb5

C	1.964405	-0.398994	0.320847
C	2.315392	-1.543848	-0.601965
H	3.251574	-1.343069	-1.122971
H	2.428452	-2.458221	-0.017004
H	1.517204	-1.697281	-1.327625
C	0.642995	-0.574777	1.048464
H	0.428286	0.331671	1.627142
H	0.742276	-1.409361	1.753036
O	-0.366432	-0.852183	0.112751
O	1.866337	0.784869	-0.531590
O	1.847158	1.882232	0.157431
H	-1.318447	-1.089171	0.561874
C	-1.587857	0.485875	-0.749974
C	-1.496232	1.573310	0.256354
H	-0.490188	1.989874	0.284182
H	-2.170463	2.358748	-0.106066
H	-1.832443	1.245275	1.235306
O	-2.735151	-0.879486	0.556045
O	-2.512294	-0.390555	-0.774890
H	-1.141388	0.647404	-1.730798
H	2.755976	-0.184285	1.042584

CRDb6

C	1.212926	0.259469	0.537381
C	2.394743	0.674797	1.383247
H	2.214081	1.642509	1.851994
H	2.546170	-0.068918	2.167297
H	3.301411	0.725742	0.780112
C	1.412015	-1.044610	-0.219171
H	0.539891	-1.226771	-0.853749
H	1.467696	-1.855518	0.507974
O	2.612800	-1.063096	-0.964379
O	1.035553	1.335929	-0.446649
O	-0.105986	1.272108	-1.055172
H	2.537021	-0.429848	-1.683466
C	-2.496158	-0.143337	-0.600430
C	-2.902447	0.929770	0.317489
H	-3.463647	1.701280	-0.202816
H	-3.481635	0.485440	1.133451

H	-1.773996	1.605518	1.069056
O	-3.199167	-0.361277	0.180644
O	-2.243299	-0.370877	-0.869013
H	-0.422252	0.195487	-1.299742
H	2.777814	-0.426175	0.914452

TSDb6

C	-1.155505	0.535507	-0.428511
C	-1.494650	1.715828	0.459273
H	-0.637034	2.368670	0.631019
H	-2.273042	2.311257	-0.020860
H	-1.876118	1.358485	1.416587
C	-2.345474	-0.396725	-0.649821
H	-2.065786	-1.162813	-1.375826
H	-3.172563	0.191260	-1.054100
O	-2.789589	-0.966571	0.557824
O	-0.137778	-0.234914	0.271171
O	0.208258	-1.351669	-0.441579
H	-2.118980	-1.596524	0.843577
C	1.546061	0.665145	0.538533
C	1.746391	1.293223	-0.791632
H	1.184061	2.221329	-0.876047
H	2.815856	1.499881	-0.895939
H	1.479310	0.584276	-1.576332
O	2.557557	-1.137189	-0.228323
O	2.205482	-0.400393	0.856034
H	1.278707	1.240510	1.418843
H	-0.746788	0.831697	-1.398993

CRDc1

C	-1.140272	0.621539	-0.224701
C	-1.049039	1.015056	1.234007
H	-0.036570	1.347831	1.461239
H	-1.739398	1.839853	1.419809
H	-1.337626	0.182319	1.875678
C	-2.538749	0.257704	-0.704934
H	-2.464244	-0.218989	-1.690427
H	-3.095906	1.189047	-0.825746
O	-3.274725	-0.533338	0.197548
O	-0.226699	-0.507233	-0.474874
O	-0.617138	-1.617509	0.070981
H	-2.767979	-1.334896	0.362875
H	-0.697599	1.389591	-0.860615
C	2.398685	-0.242155	-0.390914
O	1.705834	1.884221	-0.423077
O	2.209071	0.793593	0.262199
C	2.809466	-1.480509	0.300132
H	1.982932	-2.195347	0.214584
H	3.681545	-1.916964	-0.190690

H	-2.003390	1.345219	0.781167
O	-1.536112	-1.196201	1.119891
O	-1.875549	-1.150001	-0.207359
H	-2.710116	-0.158962	-1.665445
H	0.280393	0.193395	1.101747

CPDb6

C	1.238567	0.644255	0.430920
C	1.623230	1.734950	-0.545059
H	0.799424	2.418970	-0.754697
H	2.444233	2.315926	-0.120285
H	1.956322	1.278378	-1.477008
C	2.305947	-0.432744	0.578462
H	2.009205	-1.130693	1.363375
H	3.225882	0.074580	0.883220
O	2.547708	-1.086786	-0.634327
O	0.022776	-0.011281	-0.136253
O	-0.050437	-1.448242	0.041852
H	1.740164	-1.605267	-0.790443
C	-1.231849	0.610030	0.233584
C	-1.788722	0.082498	1.524385
H	-1.088899	0.303055	2.331517
H	-2.734411	0.586230	1.727298
H	-1.933674	-0.990306	1.451976
O	-2.849418	-0.611833	-0.823380
O	-2.075143	0.433723	-0.898711
H	-1.026019	1.680583	0.240865
H	0.960843	1.029962	1.416969

TSDc1

C	1.486083	-0.811895	-0.170691
C	0.980163	-0.999257	1.244122
H	0.171413	-1.727692	1.260569
H	1.807688	-1.352712	1.862623
H	0.635932	-0.051975	1.657973
C	2.700530	0.107144	-0.280927
H	2.906906	0.295820	-1.341489
H	3.559887	-0.415539	0.144798
O	2.564061	1.309835	0.437992
O	0.449055	-0.299726	-1.063830
O	-0.042755	0.848771	-0.660306
H	1.743439	1.728900	0.156677
H	1.716478	-1.770372	-0.640030
C	-2.161506	0.384066	-0.274173
O	-1.691884	-1.792604	-0.280535
O	-1.954203	-0.653635	0.412069
C	-2.515876	1.635843	0.430877
H	-2.006994	2.473037	-0.047828
H	-3.594166	1.804635	0.356624

H	3.018086	-1.286329	1.350372	H	-2.230397	1.573574	1.479765
H	2.205477	-0.183802	-1.460852	H	-2.240749	0.245787	-1.348050
CPDc1				CRDc2			
C	1.535165	0.722224	0.472404	C	-1.755892	-0.540631	0.631031
C	1.197189	1.461295	-0.809152	C	-2.740050	-0.989331	-0.424379
H	0.506541	2.279895	-0.604514	H	-2.714368	-2.072892	-0.548552
H	2.112553	1.864517	-1.247218	H	-3.742569	-0.696914	-0.106347
H	0.745052	0.788744	-1.537341	H	-2.516533	-0.505121	-1.372689
C	2.544050	-0.408854	0.285796	C	-1.623042	0.982007	0.738567
H	2.598786	-0.983206	1.218459	H	-0.841846	1.220239	1.470216
H	3.525665	0.032610	0.099881	H	-2.577491	1.358307	1.124845
O	2.276465	-1.244104	-0.819341	O	-1.361433	1.568567	-0.497870
O	0.362490	0.266512	1.163819	O	-0.416729	-1.076699	0.379859
O	-0.250357	-0.760252	0.376340	O	-0.090806	-1.106383	-0.875006
H	1.403560	-1.626304	-0.691577	H	-0.398359	1.744305	-0.543349
H	1.942761	1.413073	1.218118	H	-1.985117	-0.957825	1.614840
C	-1.610807	-0.490626	0.325060	C	2.257290	-0.116430	-0.329391
O	-2.010488	1.742094	0.024804	O	1.324123	1.918122	-0.278492
O	-1.838683	0.609126	-0.590360	O	1.820904	0.797867	0.383080
C	-2.296421	-1.704533	-0.246803	C	2.791006	-1.337114	0.307058
H	-2.130249	-2.560385	0.406129	H	2.224422	-2.190943	-0.071428
H	-3.365380	-1.512000	-0.329478	H	3.836870	-1.470659	0.018800
H	-1.896455	-1.921488	-1.238184	H	2.701622	-1.276597	1.389534
H	-1.973299	-0.159502	1.299805	H	2.229031	0.045307	-1.405754
TSDc2				CPDc2			
C	1.683869	-0.632286	-0.552622	C	-1.543262	-0.669418	0.598002
C	2.589768	-0.912411	0.627595	C	-2.364484	-1.288463	-0.518466
H	2.686427	-1.985793	0.795043	H	-2.241665	-2.372035	-0.520933
H	3.577255	-0.495042	0.422699	H	-3.419990	-1.049343	-0.373871
H	2.192772	-0.425858	1.516835	H	-2.059697	-0.884622	-1.482845
C	1.504722	0.864349	-0.835842	C	-1.699278	0.848222	0.701262
H	0.672210	1.003984	-1.536105	H	-0.917468	1.238288	1.364244
H	2.424138	1.177645	-1.345627	H	-2.667537	1.051734	1.165806
O	1.351112	1.626777	0.317996	O	-1.710282	1.517332	-0.537460
O	0.391829	-1.285097	-0.363230	O	-0.169079	-1.073220	0.524840
O	-0.198647	-0.910369	0.747751	O	0.363581	-0.526406	-0.691890
H	0.400581	1.861985	0.413775	H	-0.806551	1.539749	-0.869440
H	2.030781	-1.129159	-1.461836	H	-1.821241	-1.102581	1.565076
C	-1.930033	-0.178350	0.377438	C	1.696402	-0.238407	-0.479530
O	-1.296488	1.973499	0.316339	O	1.197206	1.952783	-0.073644
O	-1.653711	0.830022	-0.357398	O	1.827372	0.924454	0.399065
C	-2.585046	-1.326349	-0.303399	C	2.519408	-1.329633	0.155043
H	-2.487860	-2.221223	0.308174	H	2.421722	-2.237258	-0.440153
H	-3.644753	-1.097550	-0.441310	H	3.565739	-1.026316	0.183145
H	-2.127583	-1.491279	-1.278490	H	2.169549	-1.524543	1.166905
H	-2.056413	0.033932	1.436163	H	2.054040	0.073574	-1.463095
CRDc3				TSDc3			

C	1.140603	-0.621613	-0.224760
C	1.049339	-1.015116	1.233964
H	0.037086	-1.348793	1.460834
H	1.740390	-1.839265	1.420054
H	1.337028	-0.182039	1.875600
C	2.538961	-0.257371	-0.704940
H	2.464373	0.219184	-1.690495
H	3.096430	-1.188547	-0.825618
O	3.274630	0.534012	0.197494
O	0.226714	0.506927	-0.474945
O	0.616645	1.617213	0.071277
H	2.767368	1.335185	0.363110
H	0.698185	-1.389775	-0.860713
C	-2.398817	0.242007	-0.390876
C	-2.810026	1.480329	0.299969
H	-3.682046	1.916486	-0.191239
H	-3.018958	1.286260	1.350160
H	-1.983654	2.195358	0.214579
O	-1.705341	-1.884139	-0.423041
O	-2.209029	-0.793662	0.262264
H	-2.205521	0.183729	-1.460802

CPDc3

C	1.890993	0.095223	0.328696
C	1.282735	0.466385	1.667827
H	1.418385	-0.350437	2.377537
H	1.786931	1.355636	2.054283
H	0.222101	0.686121	1.575405
C	1.686661	1.150283	-0.756640
H	2.007429	0.738422	-1.720186
H	2.333546	1.997863	-0.520572
O	0.376678	1.670443	-0.825199
O	1.512221	-1.228895	-0.112345
O	0.322243	-1.206502	-0.862900
H	-0.205602	0.985153	-1.170933
H	2.970678	-0.049836	0.441431
C	-2.203728	-0.077290	-0.286130
C	-2.723574	1.193705	0.274961
H	-3.342269	1.024930	1.165272
H	-1.895102	1.850936	0.552697
H	-3.335478	1.699936	-0.471808
O	-0.692055	-1.773217	-0.113680
O	-1.370134	-0.736234	0.578966
H	-2.750774	-0.713322	-0.974147

TSDc4

C	-1.727965	-0.571714	0.593755
C	-2.534357	-1.065973	-0.585282
H	-2.439173	-2.147570	-0.694171

C	2.009821	0.088659	0.232746
C	1.457435	0.038129	1.645127
H	1.680805	-0.927408	2.099811
H	1.925900	0.825730	2.240134
H	0.381728	0.199746	1.652911
C	1.669046	1.368860	-0.524366
H	1.982026	1.254761	-1.568850
H	2.250002	2.182686	-0.084965
O	0.314723	1.759604	-0.435120
O	1.651401	-1.091557	-0.525652
O	0.416986	-1.012663	-1.051073
H	-0.204823	1.087753	-0.888736
H	3.099672	-0.008678	0.252776
C	-2.310225	-0.173253	-0.287388
C	-3.008170	1.032575	0.211598
H	-3.744643	0.789876	0.987352
H	-2.286629	1.736856	0.634344
H	-3.533361	1.518189	-0.610625
O	-0.695966	-1.700408	0.041877
O	-1.420073	-0.704280	0.563208
H	-2.594688	-0.794899	-1.126381

CRDc4

C	-1.755978	-0.540486	0.631030
C	-2.740052	-0.989344	-0.424390
H	-2.714304	-2.072914	-0.548466
H	-3.742605	-0.696955	-0.106434
H	-2.516514	-0.505205	-1.372732
C	-1.623104	0.982169	0.738291
H	-0.842005	1.220527	1.470002
H	-2.577598	1.358574	1.124355
O	-1.361299	1.568460	-0.498233
O	-0.416796	-1.076605	0.380081
O	-0.090802	-1.106657	-0.874757
H	-0.398223	1.744236	-0.543589
H	-1.985302	-0.957496	1.614895
C	2.257273	-0.116489	-0.329295
C	2.791008	-1.337096	0.307285
H	3.836930	-1.470540	0.019183
H	2.701473	-1.276530	1.389746
H	2.224573	-2.191003	-0.071239
O	1.324188	1.918107	-0.278615
O	1.820924	0.797903	0.383077
H	2.228989	0.045120	-1.405678

CPDc4

C	-1.678928	-0.583849	0.500741
C	-2.567058	-0.803202	-0.710034
H	-2.689684	-1.873102	-0.881320

H	-3.584096	-0.823845	-0.411988	H	-3.548938	-0.357485	-0.539266
H	-2.202896	-0.569521	-1.495481	H	-2.127486	-0.345583	-1.594245
C	-1.634186	0.994254	0.644720	C	-1.499879	0.916489	0.871067
H	-1.034106	1.271888	1.520404	H	-0.750263	1.000414	1.665781
H	-2.673042	1.319322	0.801510	H	-2.488797	1.249942	1.225428
O	-1.133996	1.486018	-0.521609	O	-1.188591	1.643085	-0.240818
O	-0.363511	-1.011906	0.553790	O	-0.416650	-1.202660	0.377936
O	0.161295	-0.835285	-0.635616	O	0.239215	-0.639740	-0.757448
H	-0.089812	1.728754	-0.398500	H	0.603246	2.034419	-0.369073
H	-2.078967	-0.956883	1.552805	H	-2.089396	-1.077310	1.386808
C	1.838631	-0.215494	-0.377954	C	1.590585	-0.388481	-0.399602
C	2.551214	-1.409981	0.165359	C	2.251066	-1.547188	0.313910
H	3.616618	-1.176398	0.216945	H	3.324873	-1.370159	0.357721
H	2.190053	-1.632890	1.168961	H	1.861225	-1.638994	1.326140
H	2.404147	-2.268803	-0.487115	H	2.053109	-2.470199	-0.230653
O	1.247300	1.948502	-0.208411	O	1.569117	1.900484	-0.363456
O	1.714783	0.764509	0.438443	O	1.701389	0.730148	0.429482
H	1.924271	0.054691	-1.429721	H	2.041547	-0.165094	-1.369388
CRDc5				TSDc5			
C	-2.057538	-0.080699	-0.251247	C	-1.957752	-0.443971	-0.199627
C	-2.769081	-0.305777	1.063758	C	-2.451237	-0.781303	1.189123
H	-3.408351	0.542782	1.308784	H	-3.312855	-0.167238	1.452264
H	-3.388760	-1.200783	0.987677	H	-2.746916	-1.831062	1.222802
H	-2.038511	-0.459896	1.857596	H	-1.652911	-0.624657	1.914852
C	-1.095163	-1.195273	-0.623379	C	-0.697279	-1.185811	-0.602931
H	-0.566573	-0.919808	-1.544501	H	-0.391250	-0.860346	-1.605791
H	-1.692309	-2.091529	-0.839674	H	-0.937470	-2.254766	-0.661592
O	-0.212776	-1.400995	0.445685	O	0.320497	-0.965096	0.339008
O	-1.296115	1.160497	-0.071943	O	-1.674655	0.992663	-0.165240
O	-0.799410	1.604445	-1.182329	O	-1.259064	1.454227	-1.301836
H	0.637931	-1.763035	0.107047	H	1.257668	-1.405469	-0.063088
C	1.824260	0.541738	-0.058066	C	1.544439	0.627644	-0.009875
C	1.877801	1.794599	0.715119	C	1.234887	1.753306	0.897946
H	2.597500	1.726168	1.527850	H	1.803629	1.664678	1.821102
H	2.115261	2.624964	0.046366	H	1.473028	2.690645	0.388306
H	0.871280	1.978071	1.105121	H	0.164317	1.753705	1.103276
O	2.285433	-1.610203	-0.438814	O	2.520678	-1.265658	-0.523928
O	2.489210	-0.441709	0.296319	O	2.577781	-0.065948	0.247859
H	1.208413	0.428480	-0.948777	H	1.151242	0.596446	-1.024614
H	-2.748287	0.110778	-1.075941	H	-2.728726	-0.582634	-0.962249
CPDc5				CRDc6			
C	1.864138	-0.596753	0.016331	C	1.315934	-0.398771	-0.306679
C	2.372900	-0.382322	-1.391503	C	1.773867	-1.593667	0.494019
H	3.339408	0.121651	-1.377651	H	0.903219	-2.147144	0.843745
H	2.487635	-1.347015	-1.888591	H	2.371401	-2.243185	-0.148253
H	1.659568	0.214940	-1.960156	H	2.392409	-1.280987	1.335956
C	0.481305	-1.230788	0.082606	C	2.430658	0.507870	-0.803418

H	0.147984	-1.286827	1.123307	H	1.991226	1.361304	-1.330417
H	0.552600	-2.246326	-0.315473	H	3.040431	-0.055521	-1.512120
O	-0.452435	-0.532660	-0.711398	O	3.295192	0.930463	0.229983
O	1.807072	0.732494	0.617484	O	0.475103	0.384804	0.610940
O	1.558068	0.687450	1.889261	O	-0.185910	1.319994	0.003688
H	-2.675759	-1.712349	0.020867	H	2.802327	1.502031	0.825342
C	-1.189782	0.487671	-0.073132	C	-2.477360	0.059291	0.358280
C	-1.064477	1.787220	-0.832109	C	-3.354071	1.200206	0.021368
H	-1.363110	1.630016	-1.869371	H	-2.809513	2.124589	0.229522
H	-1.699656	2.550066	-0.382476	H	-3.644363	1.164937	-1.026701
H	-0.025924	2.117154	-0.798640	H	-4.241634	1.183673	0.658858
O	-2.721303	-1.015235	0.688341	O	-1.343906	-1.800089	-0.160992
O	-2.553258	0.149487	-0.104160	O	-2.183067	-0.766821	-0.518813
H	-0.872293	0.574575	0.971702	H	-2.055790	-0.111416	1.348262
H	2.559887	-1.178346	0.627109	H	0.656827	-0.694665	-1.124064
TSDc6				CPDc6			
C	-1.045150	0.216421	-0.695055	C	-0.889735	-0.752572	0.187511
C	-1.255337	1.716134	-0.752427	C	-0.985217	-1.623033	-1.047308
H	-0.332607	2.260310	-0.962273	H	-0.031199	-2.066842	-1.330208
H	-1.962772	1.947602	-1.550316	H	-1.668329	-2.444630	-0.825062
H	-1.672978	2.063647	0.193809	H	-1.400854	-1.046014	-1.875258
C	-2.320640	-0.547094	-0.350828	C	-2.239772	-0.177716	0.621734
H	-2.147935	-1.616708	-0.473695	H	-2.156700	0.209299	1.637019
H	-3.099703	-0.232455	-1.049022	H	-2.960890	-0.998819	0.609843
O	-2.772683	-0.241979	0.947342	O	-2.688779	0.807445	-0.269351
O	-0.072817	-0.022466	0.371880	O	-0.054182	0.432664	-0.148700
O	0.028412	-1.351752	0.641780	O	-0.225449	1.507536	0.819293
H	-2.172218	-0.673829	1.564748	H	-2.114014	1.569570	-0.099086
C	1.677277	0.499383	-0.170336	C	1.330175	0.230354	-0.460272
C	2.059148	1.594907	0.757835	C	1.991328	1.544168	-0.753296
H	1.255645	2.327733	0.817722	H	1.410244	2.077446	-1.504861
H	2.257206	1.185512	1.747165	H	2.030391	2.140800	0.154175
H	2.958086	2.090061	0.381503	H	2.994605	1.347941	-1.132277
O	1.739039	-1.597570	-0.802059	O	1.947376	-1.673079	0.601224
O	2.265370	-0.627684	0.015118	O	1.983789	-0.371790	0.663048
H	1.338715	0.696463	-1.184359	H	1.357404	-0.487382	-1.277424
H	-0.611804	-0.195238	-1.612902	H	-0.403368	-1.250772	1.028817
CRDd1				TSDd1			
C	0.796748	-0.580884	-0.334227	C	-1.034180	0.751464	-0.475124
C	0.697384	-1.234830	1.027261	C	-0.562486	1.346599	0.834753
H	-0.342824	-1.481483	1.238379	H	0.389103	1.857223	0.696500
H	1.286662	-2.153628	1.024291	H	-1.314224	2.058354	1.181673
H	1.100947	-0.577644	1.797609	H	-0.462858	0.572175	1.594590
C	2.216312	-0.272244	-0.793144	C	-2.418770	0.111390	-0.407116
H	2.170980	0.388469	-1.668063	H	-2.607863	-0.424342	-1.345345
H	2.672027	-1.213265	-1.108403	H	-3.155492	0.912932	-0.319962
O	3.048498	0.256764	0.211238	O	-2.601438	-0.724649	0.709923

O	0.000244	0.654053	-0.332381	O	-0.094862	-0.243718	-0.991680
O	0.519733	1.596936	0.392803	O	0.078261	-1.249588	-0.168589
H	2.629342	1.056938	0.544327	H	-1.899328	-1.384093	0.704448
H	0.271146	-1.166579	-1.089187	H	-1.019201	1.491970	-1.277235
C	-2.706485	0.957267	-0.048475	C	2.249964	-1.087046	0.270407
H	-3.063193	1.674221	0.681915	H	2.220858	-1.765818	1.112475
H	-2.393820	1.196626	-1.059645	H	2.401827	-1.382514	-0.760360
O	-2.202140	-1.155251	-0.536866	O	2.340110	0.999118	-0.475160
O	-2.660713	-0.219941	0.331491	O	2.282930	0.135046	0.559969
CPDd1				CRDd2			
C	1.100616	0.710953	0.626689	C	-1.604198	-0.526485	0.273195
C	0.606625	1.594148	-0.503870	C	-2.475471	-0.527752	-0.961434
H	-0.264580	2.167413	-0.185249	H	-2.593499	-1.536779	-1.357487
H	1.400536	2.283037	-0.799430	H	-3.460161	-0.134716	-0.702255
H	0.340937	0.996963	-1.375650	H	-2.039970	0.121449	-1.720591
C	2.359591	-0.083563	0.286663	C	-1.345782	0.866700	0.843728
H	2.538053	-0.811791	1.086944	H	-0.604945	0.779842	1.646627
H	3.205128	0.607321	0.260769	H	-2.287128	1.216510	1.279942
O	2.325405	-0.704663	-0.979241	O	-0.944654	1.778694	-0.136743
O	0.066658	-0.142868	1.140419	O	-0.320401	-1.094430	-0.148817
O	-0.262776	-1.106361	0.131910	O	0.399163	-1.487458	0.850697
H	1.579053	-1.310477	-0.989943	H	0.028614	1.735008	-0.197580
H	1.314618	1.310382	1.517963	H	-1.975587	-1.191160	1.057196
C	-1.638838	-1.149206	0.047949	C	2.637227	-0.689038	-0.157443
H	-1.876980	-2.037826	-0.535295	H	2.909929	-1.509281	-0.812329
H	-2.107412	-1.123751	1.032180	H	2.807306	-0.666818	0.914240
O	-2.577233	0.921525	0.067186	O	1.743247	1.321774	0.125236
O	-2.139219	-0.032041	-0.704883	O	2.115743	0.287094	-0.702377
TSDd2				CPDd2			
C	1.489500	-0.614957	-0.083186	C	1.469502	-0.606201	-0.146904
C	2.216491	-0.133662	1.151912	C	2.394780	-0.481594	1.049604
H	2.338394	-0.946701	1.867644	H	2.346193	-1.381353	1.662308
H	3.201288	0.240968	0.868478	H	3.419583	-0.344670	0.700389
H	1.658831	0.677517	1.619913	H	2.119612	0.381802	1.656079
C	1.293376	0.451700	-1.153256	C	1.429329	0.651201	-1.007275
H	0.635600	0.044673	-1.932115	H	0.809498	0.468723	-1.894961
H	2.269603	0.622383	-1.614397	H	2.437971	0.878982	-1.358318
O	0.845330	1.684133	-0.665386	O	0.976434	1.773591	-0.285541
O	0.205916	-1.116779	0.415637	O	0.175656	-0.839603	0.428697
O	-0.570321	-1.567490	-0.535268	O	-0.713171	-1.291411	-0.588478
H	0.054287	1.549795	-0.113415	H	0.206094	1.523190	0.241780
H	1.977139	-1.482068	-0.539134	H	1.731482	-1.473517	-0.760995
C	-2.181097	-0.172333	-0.611520	C	-1.660004	-0.306201	-0.806215
H	-2.916856	-0.913214	-0.892649	H	-2.354748	-0.727598	-1.531716
H	-1.599062	0.405874	-1.321151	H	-1.232763	0.647397	-1.122301
O	-1.327802	1.133427	0.971322	O	-1.931878	0.965282	1.043785
O	-2.219229	0.193744	0.592835	O	-2.417612	-0.047382	0.385598

CRDd3				TSDd3			
C	-1.604206	-0.526520	0.272990	C	1.188800	0.726089	0.616683
C	-2.475451	-0.527653	-0.961659	C	0.913619	1.573960	-0.611863
H	-2.593409	-1.536628	-1.357866	H	0.053946	2.221902	-0.437615
H	-3.460171	-0.134718	-0.702440	H	1.789634	2.191658	-0.821575
H	-2.039973	0.121689	-1.720708	H	0.720464	0.949236	-1.481697
C	-1.345848	0.866600	0.843709	C	2.336487	-0.264362	0.442089
H	-0.605051	0.779663	1.646635	H	2.336390	-0.952985	1.295909
H	-2.287225	1.216342	1.279911	H	3.273442	0.296707	0.460814
O	-0.944682	1.778720	-0.136631	O	2.320289	-0.959875	-0.782855
O	-0.320376	-1.094361	-0.149059	O	-0.009716	0.052908	1.079372
O	0.399094	-1.487668	0.850412	O	-0.325923	-0.994204	0.299990
H	0.028588	1.735036	-0.197425	H	1.497088	-1.456430	-0.823389
H	-1.975589	-1.191311	1.056895	H	1.410275	1.361535	1.479186
C	2.637286	-0.688983	-0.157215	C	-3.110712	-0.153273	0.366956
H	2.910162	-1.509111	-0.812174	H	-3.729738	0.539286	0.910944
H	2.807122	-0.666935	0.914510	H	-3.236005	-1.221014	0.285556
O	1.743178	1.321751	0.125597	O	-1.328598	-0.434821	-0.940052
O	2.115894	0.287223	-0.702105	O	-2.166634	0.432944	-0.375370
CPDd3				CRDd4			
C	1.422903	-0.016335	0.726314	C	-1.637394	-0.133366	0.632406
C	2.502447	0.562734	-0.173207	C	-2.596933	-0.605411	-0.434690
H	2.680347	1.611023	0.069832	H	-2.787544	-1.675760	-0.347136
H	3.429552	0.006491	-0.024165	H	-3.539593	-0.070338	-0.305481
H	2.217315	0.472940	-1.220733	H	-2.198521	-0.386578	-1.423409
C	1.025060	-1.443037	0.361220	C	-1.168871	1.312579	0.443067
H	0.231269	-1.773497	1.040681	H	-0.473763	1.571605	1.248649
H	1.895971	-2.086991	0.516688	H	-2.053035	1.953715	0.526703
O	0.633491	-1.574652	-0.981605	O	-0.583709	1.499111	-0.811014
O	0.271067	0.842577	0.807582	O	-0.424747	-0.953969	0.679900
O	-0.138750	1.182292	-0.556204	O	-0.075905	-1.445849	-0.464999
H	-0.308130	-1.368904	-1.028648	H	0.381678	1.412734	-0.692744
H	1.754002	-0.005078	1.770799	H	-2.042803	-0.260183	1.639260
C	-2.657583	-0.361127	0.571712	C	2.361081	-0.960567	-0.319109
H	-2.079631	0.263994	1.270573	O	2.024658	1.226420	-0.041441
H	-3.756988	-0.343979	0.658147	O	2.332726	-0.015800	0.474528
O	-1.128614	1.933600	-0.504973	H	2.184342	-0.773258	-1.374128
O	-2.114778	-1.037494	-0.260976	H	2.597753	-1.930660	0.102461
TSDd4				CPDd4			
C	-1.618351	-0.157867	0.597458	C	-1.614104	-0.181777	0.517970
C	-2.511534	-0.468610	-0.581016	C	-2.485690	-0.265213	-0.721327
H	-2.774613	-1.527331	-0.602210	H	-2.955158	-1.248153	-0.769971
H	-3.427368	0.116061	-0.480802	H	-3.265467	0.497836	-0.682227
H	-2.014685	-0.188990	-1.508244	H	-1.890318	-0.106571	-1.618588
C	-1.016633	1.283608	0.540315	C	-0.952481	1.211289	0.715613
H	-0.370958	1.422904	1.415805	H	-0.249791	1.159281	1.554307
H	-1.887099	1.948362	0.628828	H	-1.782965	1.900265	0.940481

O	-0.360082	1.492719	-0.640606	O	-0.371429	1.629303	-0.446902
O	-0.469417	-1.026608	0.662753	O	-0.629008	-1.193199	0.565108
O	0.094475	-1.172610	-0.505371	O	0.218602	-1.041292	-0.573301
H	0.671340	1.387391	-0.487125	H	1.474677	1.418287	-0.517152
H	-2.097787	-0.326964	1.563144	H	-2.192598	-0.385795	1.423794
C	1.883543	-1.090270	-0.230325	C	1.537699	-1.165381	-0.101113
O	2.064507	1.140467	-0.215072	O	2.322152	0.948513	-0.410828
O	2.093473	-0.084350	0.515732	O	1.987242	-0.030931	0.562606
H	2.080024	-0.982453	-1.294693	H	2.132187	-1.350862	-0.996855
H	2.015345	-2.047075	0.267213	H	1.596412	-1.976946	0.625894
CRDd5				TSDd5			
C	-1.773773	-0.132159	0.342964	C	-1.505976	0.219517	0.795969
C	-0.999800	-0.128647	1.643932	C	-1.488717	1.555550	0.083051
H	-1.199027	0.783716	2.207607	H	-2.499401	1.955823	-0.001017
H	-1.330166	-0.982177	2.239234	H	-0.885688	2.257878	0.663271
H	0.073315	-0.224247	1.485924	H	-1.076133	1.451100	-0.918920
C	-1.390703	-1.253422	-0.625718	C	-0.144790	-0.438080	0.924590
H	-2.058428	-1.216845	-1.488700	H	-0.256000	-1.431876	1.367327
H	-1.554145	-2.208662	-0.110008	H	0.488882	0.161541	1.592836
O	-0.085575	-1.131085	-1.112959	O	0.457430	-0.557746	-0.351257
O	-1.643974	1.131489	-0.378560	O	-2.412111	-0.724607	0.154859
O	-0.473334	1.672645	-0.290545	O	-2.441616	-0.626973	-1.138094
C	1.975198	0.896725	-0.574592	C	1.873976	0.833189	-0.726666
H	2.139150	1.968140	-0.530209	H	1.412082	1.811728	-0.618954
H	1.542137	0.374316	-1.424224	H	1.944922	0.342111	-1.691623
O	2.113563	-1.098259	0.448591	O	2.899907	-0.916826	0.068800
O	2.311949	0.268316	0.435166	O	2.630672	0.476821	0.211320
H	0.590700	-1.355463	-0.439941	H	1.322825	-1.087656	-0.216961
H	-2.850083	-0.178610	0.527262	H	-1.932703	0.312936	1.797350
CPDd5				CRDd6			
C	-1.596451	0.387170	0.695537	C	0.895770	0.021511	0.756256
C	-1.742270	1.455838	-0.366252	C	2.055021	0.864742	1.245682
H	-2.796217	1.647426	-0.569883	H	1.701260	1.674958	1.883935
H	-1.284049	2.379794	-0.006940	H	2.739633	0.235645	1.817303
H	-1.264942	1.147283	-1.294850	H	2.604774	1.277842	0.399990
C	-0.160225	-0.016932	1.003009	C	1.298479	-1.162428	-0.114797
H	-0.171788	-0.857024	1.700556	H	0.401716	-1.542873	-0.612923
H	0.360229	0.818673	1.484440	H	1.671748	-1.943124	0.551079
O	0.522288	-0.433322	-0.165480	O	2.340935	-0.879880	-1.021411
O	-2.335357	-0.822087	0.352765	O	-0.040054	0.891768	0.031157
O	-2.365199	-1.079039	-0.918047	O	0.351018	1.180247	-1.170396
C	1.455660	0.477103	-0.663188	H	2.013341	-0.215327	-1.635018
H	1.082904	1.506559	-0.649647	C	-2.727112	0.552565	-0.502504
H	1.708167	0.147544	-1.670809	H	-3.399074	1.396224	-0.394788
O	3.309486	-0.691046	-0.046740	H	-2.108714	0.357881	-1.373701
O	2.605206	0.526750	0.135712	O	-1.846544	-1.288696	0.386199
H	2.802962	-1.313086	0.494268	O	-2.682966	-0.223621	0.460416

H	-2.068936	0.693702	1.632552	H	0.263247	-0.338104	1.568570
	TSDd6				CPDd6		
C	0.743675	0.494980	0.457203	C	0.809959	0.587296	0.472285
C	1.299198	1.835898	0.027857	C	1.507577	1.774971	-0.153417
H	0.512150	2.519935	-0.294196	H	0.810729	2.522961	-0.534590
H	1.815800	2.297120	0.871089	H	2.123727	2.256909	0.608071
H	2.010152	1.696668	-0.787228	H	2.152210	1.430472	-0.962259
C	1.823899	-0.534342	0.769596	C	1.766160	-0.534312	0.857563
H	1.365383	-1.428337	1.193627	H	1.221033	-1.298934	1.412216
H	2.491039	-0.094961	1.514805	H	2.525649	-0.093842	1.509581
O	2.602533	-0.837080	-0.363866	O	2.409183	-1.066801	-0.267068
O	-0.046251	0.013085	-0.682547	O	-0.098278	0.032040	-0.584409
O	-0.342948	-1.298817	-0.569272	O	-0.280786	-1.412232	-0.538191
H	2.071508	-1.403340	-0.933652	H	1.714184	-1.566359	-0.726344
C	-1.844118	0.761957	-0.666102	C	-1.380622	0.637277	-0.675053
H	-1.683671	1.828096	-0.783819	H	-1.234758	1.710349	-0.786765
H	-2.071636	0.102925	-1.496835	H	-1.885253	0.149132	-1.503330
O	-2.364944	-0.957820	0.598279	O	-2.910736	-0.585648	0.449206
O	-2.186465	0.400966	0.502121	O	-2.096854	0.438508	0.522327
H	0.057957	0.568270	1.307159	H	0.173813	0.850976	1.320223