Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Unravelling the Catalytic Influence of Naturally Occurring Salts on Biomass Pyrolysis Chemistry Using Glucose as a Model Compound: A Combined Experimental and DFT Study

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Supporting Information

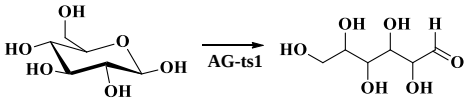
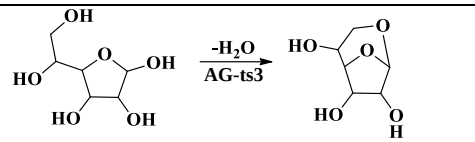
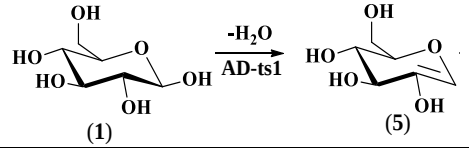
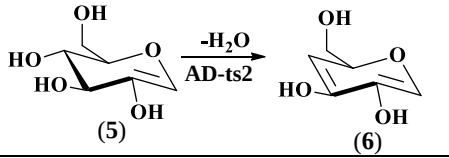
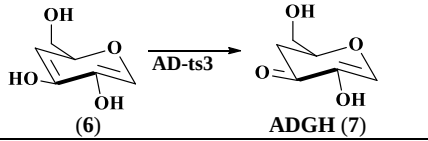
Contents

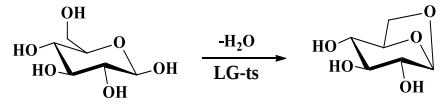
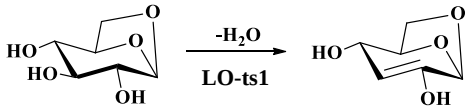
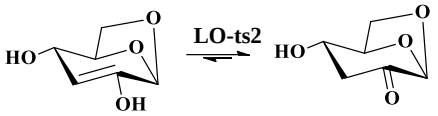
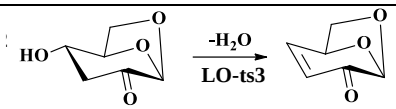
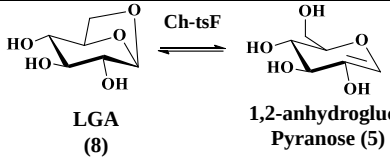
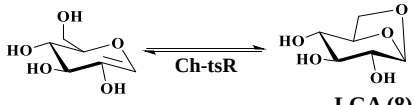
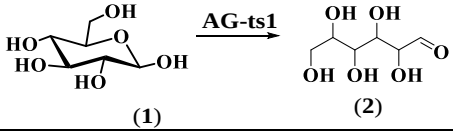
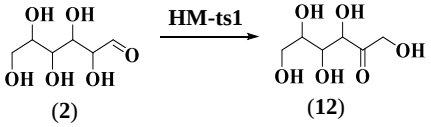
Table S1: Product distribution of glucose thin-film pyrolysis in the presence and absence of alkali and alkaline-earth metal salts at 200 ºC

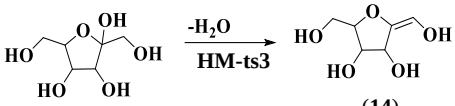
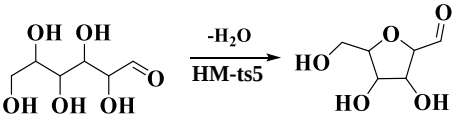
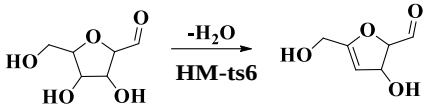
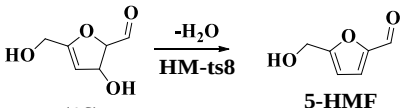
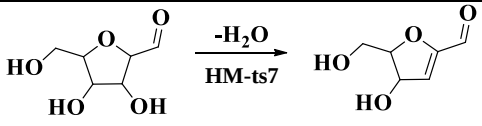
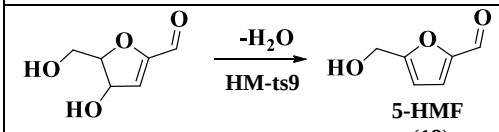
Pyrolysis products	Glucose	Glucose + NaCl	Glucose + KCl	Glucose + $CaCl_2$	Glucose + $MgCl_2$
	Product yield (%C basis)				
Furan	0.10 ± 0.02	0.068 ± 0.01	0.17 ± 0.15	0.092 ± 0.015	0.47 ± 0.024
Furfural	2.56 ± 0.14	3.01 ± 0.03	3.97 ± 0.08	5.41 ± 0.72	7.05 ± 0.54
CPD	0.55 ± 0.08	0.22 ± 0.03	1.76 ± 1.4	0.349 ± 0.2	0.11 ± 0.01
5-methylfurfural	0.095 ± 0.03	0.058 ± 0.028	0.23 ± 0.24	0.2 ± 0.08	0.58 ± 0.03
LGO	ND	ND	ND	3.81 ± 0.18	1.05 ± 0.04
DHMDHP	8.09 ± 0.43	2.69 ± 0.15	2.88 ± 0.32	1.35 ± 0.13	1.51 ± 0.23
DAGP	ND	ND	ND	0.46 ± 0.40	0.20 ± 0.06
5-HMF	0.19 ± 0.13	0.216 ± 0.13	0.13 ± 0.09	0.19 ± 0.08	0.023 ± 0.01
ADGH	1.22 ± 0.10	0.56 ± 0.25	0.63 ± 0.33	0.24 ± 0.15	0.12 ± 0.08
LGA	6.91 ± 0.64	4.86 ± 0.08	5.8 ± 1.23	5.76 ± 0.3	8.08 ± 0.5
AGF	1.21 ± 0.02	3.58 ± 0.35	3.47 ± 1.08	2.63 ± 1.5	1.14 ± 0.34
Char	61.71 ± 1.05	70.1 ± 0.60	71.11 ± 1.58	60.51 ± 1.52	62.0 5± 2.09
Total	**82.64 ± 0.94**	**85.38 ± 0.3**	**90.17 ± 1.54**	**81 ± 1.93**	**82.39 ± 2.68**

ND: Not detected; **CPD** : 1,2-cyclopentanedione; **LGO**: Levoglucosenone; **DHMDHP**: 2,3-dihydro-3,5-dihydroxy-6-methyl-4HPyran-4-one; **DAGP**: 1,4;3,6-dianhydroglucopyranose; **5-HMF**: 5-hydroxymethylfurfural; **ADGH**: 1,5-anhydro-4-deoxy-D-glycerohex-1-en-3-ulose; **LGA**: levoglucosan; **AGF**: 1,6-anhydroglucofuranose

Table S2: Activation enthalpies and free energies of activation (written in parenthesis) of all the transition states involving bio-oil formation and char. The M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent) were employed.

Reaction step	Activation enthalpies (kcal.mol^{-1})				
	No metal	**Mg(II)**	**Ca(II)**	**Na(I)**	**K(I)**
AGF formation					
 **β-D-glucopyranose (1)** **AG-ts1** **D-glucose (2)**	45.4 (45.3)	40.0 (44.7)	40.7 (38.4)	43.7 (41.7)	44.4 (41.2)
 **D-glucose (2)** **AG-ts2** **β-D-glucofuranose (3)**	38.3 (59.7)	34.8 (39.6)	34.3 (40.1)	36.2 (40.9)	35.0 (43.6)
 **β-D-glucofuranose (3)** **$-H_2O$ AG-ts3** **Anhydroglucofuranose (AGF) (4)**	54.7 (45.3)	61.9 (60.3)	56.7 (57.6)	45.4 (48.9)	44.7 (46.6)
ADGH formation	**No metal**	**Mg(II)**	**Ca(II)**	**Na(I)**	**K(I)**
 **(1)** **$-H_2O$ AD-ts1** **(5)**	60.2 (58.7)	82.5 (69.7)	77.9 (67.8)	57.1 (54.8)	57.5 (55.3)
 **(5)** **$-H_2O$ AD-ts2** **(6)**	69.9 (66.0)	56.9 (64.7)	69.4 (64.3)	73.0 (71.9)	73.5 (70.8)
 **(6)** **AD-ts3** **ADGH (7)**	50.3 (51.8)	56.1 (55.3)	53.3 (55.7)	51.9 (53.3)	53.5 (50.2)
LGA formation	**No metal**	**Mg(II)**	**Ca(II)**	**Na(I)**	**K(I)**

 β-D-glucopyranose (1) Levoglucosan (8)	47.2 (48.6)	48.2 (48.3)	52.0 (53.2)	47.1 (44.6)	48.2 (46.4)
LGO formation	**No metal**	**Mg(II)**	**Ca(II)**	**Na(I)**	**K(I)**
 LGA (8) (9)	71.5 (71.2)	70.6 (71.1)	72.1 (73.0)	75.5 (74.7)	74.4 (72.1)
 (9) (10)	57.3 (58.1)	66.3 (66.6)	63.5 (63.0)	61.0 (59.9)	60.2 (60.7)
 (10) LGO (11)	51.6 (52.9)	55.2 (52.1)	49.9 (50.6)	49.7 (49.3)	50.9 (51.0)
LGA isomerization	**No metal**	**Mg(II)**	**Ca(II)**	**Na(I)**	**K(I)**
 LGA (8) 1,2-anhydrogluco Pyranose (5)	61.0 (56.1)	76.9 (72.0)	72.1 (67.9)	60.0 (51.7)	62.1 (53.6)
 1,2-anhydrogluco Pyranose (5) LGA (8)	53.3 (52.9)	33.0 (34.4)	33.5 (43.1)	48.2 (51.1)	50.2 (51.9)
HMF formation	**No metal**	**Mg(II)**	**Ca(II)**	**Na(I)**	**K(I)**
 (1) (2)	45.4 (45.3)	39.3 (44.7)	39.5 (38.4)	42.5 (41.7)	41.8 (41.2)
 (2) (12)	39.3 (42.3)	25.9 (29.9)	29.2 (34.8)	31.9 (40.2)	38.2 (38.8)

 (12) HM-ts2 (13)	29.5 (40.3)	24.3 (32.2)	36.7 (44.0)	31.5 (41.3)	30.7 (39.1)
 (13) $-H_2O$ HM-ts3 (14)	66.5 (58.6)	38.3 (31.5)	47.9 (37.6)	62.9 (52.1)	64.9 (52.7)
 (14) HM-ts4 (15)	58.9 (61.3)	57.1 (55.7)	66.0 (63.9)	62.8 (63.7)	63.1 (63.0)
 D-glucose (2) $-H_2O$ HM-ts5 keto form (15)	78.1 (83.3)	(not computed as this route has a high activation barrier compared to "via fructose" route)			
 keto form (15) $-H_2O$ HM-ts6 (16)	73.7 (59.2)	63.1 (45.1)	64.5 (75.3)	68.7 (51.8)	68.0 (51.0)
 (16) $-H_2O$ HM-ts8 5-HMF (18)	51.1 (55.2)	42.9 (66.2)	44.3 (62.9)	47.5 (59.5)	46.9 (58.0)
 keto form (15) $-H_2O$ HM-ts7 (17)	56.7 (14.8)	44.9 (64.6)	73.7 (65.1)	51.7 (67.9)	51.4 (67.1)
 (17) $-H_2O$ HM-ts9 5-HMF (18)	55.2 (51.1)	64.5 (45.2)	63.1 (47.6)	62.5 (47.9)	58.0 (48.9)
Furfural formation	**No metal**	**Mg(II)**	**Ca(II)**	**Na(I)**	**K(I)**

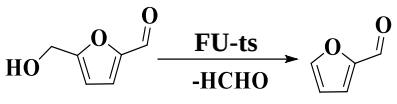
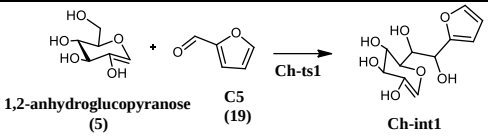
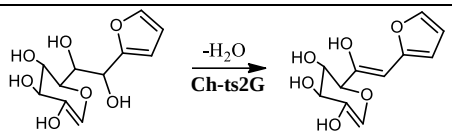
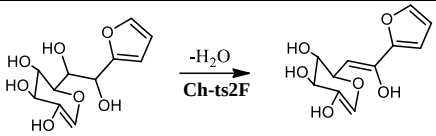
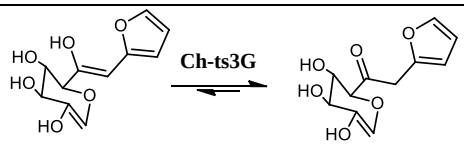
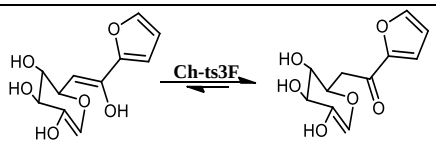
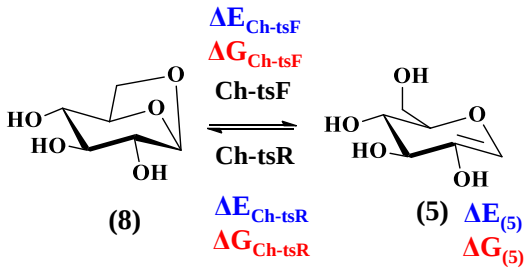
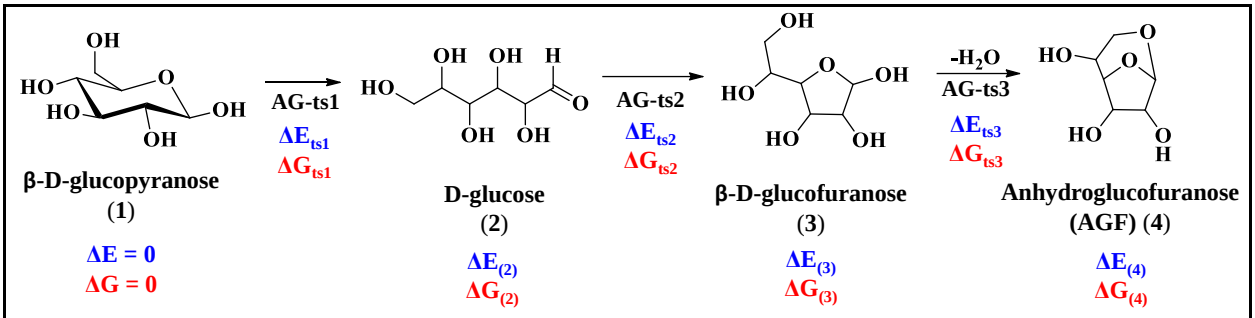
 (**18**) (**19**)	78.4 (80.1)	60.1 (57.2)	65.6 (64.7)	74.5 (68.5)	76.4 (75.6)
Char formation	**No metal**	**Mg(II)**	**Ca(II)**	**Na(I)**	**K(I)**
 **1,2-anhydroglucopyranose (5)** **C5 (19)** **Ch-ts1** **Ch-int1 (20)**	79.5 (87.4)	80.9 (83.2)	83.8 (81.8)	76.3 (84.3)	72.8 (84.7)
 **Ch-int1 (20)** **-H_2O** **Ch-ts2G** **Ch-int2G (21)**	67.5 (67.5)	64.7 (66.2)	62.5 (63.2)	66.6 (69.1)	66.5 (69.7)
 **Ch-int1 (20)** **-H_2O** **Ch-ts2F** **Ch-int2F (22)**	66.1 (65.4)	67.4 (72.8)	68.4 (70.5)	68.8 (71.3)	68.6 (71.3)
 **Ch-int2G (21)** **Ch-ts3G** **Ch-int3G (23)**	63.6 (62.6)	61.3 (60.2)	62.8 (64.2)	63.3 (64.4)	63.2 (63.3)
 **Ch-int2F (22)** **Ch-ts3F** **Ch-int3F (24)**	54.1 (57.6)	49.7 (51.8)	52.7 (53.2)	53.6 (54.6)	53.5 (56.2)

Table S3: Electronic and free energy changes (relative to levoglucosan (LGA)) involved during isomerization of LGA to 1,2-anhydroglucopyranose are calculated at M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent). All the energy values are reported in kcal.mol^{-1}.



	No metal		Mg(II)		Ca(II)		Na(I)		K(I)	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
Ch-tsF	60.1	56.1	76.9	72.0	72.1	68.0	60.0	51.7	62.1	53.6
Ch-tsR	59.4	57.2	51.2	43.6	48.2	5.8	60.0	51.9	62.1	53.6
(5)	3.8	4.3	18.2	9.2	14.8	48.8	11.8	0.6	11.9	1.7

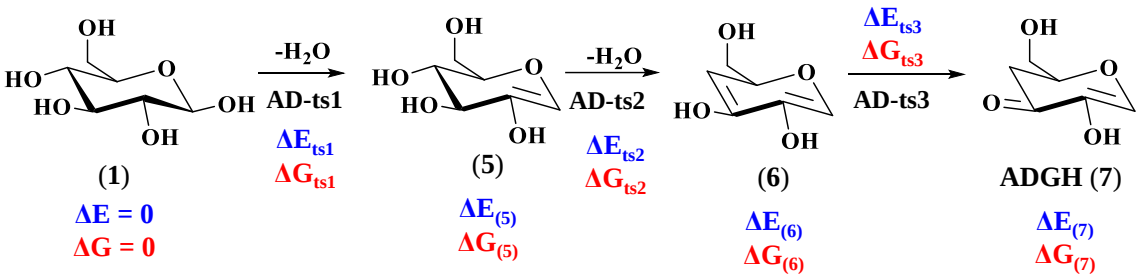
Table S4: *Electronic, free energy changes and $δE involved during 1,6-anhydroglucofuranose (AGF) formation from β-D-glucopyranose are calculated at M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent).



	No metal		Mg(II)		Ca(II)		Na(I)		K(I)	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
AG-ts1	45.4	45.3	42.9	44.7	42.9	38.4	42.9	41.7	45.6	41.2
(2)	10.3	1.8	9.8	3.6	10.8	0.5	11.0	3.5	11.5	3.6
AG-ts1	**62.3**	61.5	44.7	43.2	45.1	40.6	47.2	44.5	46.5	47.2
(3)	**7.6**	7.2	**3.1**	3.9	**4.3**	2.2	**5.9**	2.4	**6.7**	4.4
AG-ts3	51.9	52.5	**65.0**	64.2	**61.0**	59.9	**51.3**	51.4	**51.4**	51.1
AGF (4)	13.5	-9.8	9.1	-11.9	8.2	-14.3	15.5	-7.2	14.8	-8.8
$δE	54.7		62.0		56.7		45.4		44.7	

*The electronic energies of the highest and the lowest points of the catalytic cycle/ reaction mechanism are written in bold; $is energetic span of the catalytic cycle in the presence of alkali and alkaline-earth metal ions. All the energy values are reported in kcal.mol^{-1}.

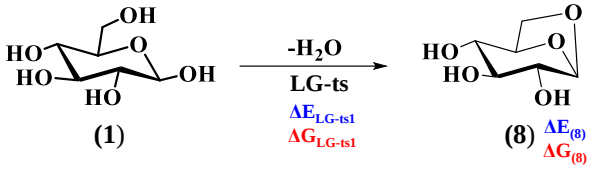
Table S5: *Electronic, free energy changes and $^{\$}\delta$E involved during 1,5-anhydro-4-deoxy-D-glycerohex-1-en-3-ulose (ADGH) formation from β-D-glucopyranose are calculated at M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent).



	No metal		Mg(II)		Ca(II)		Na(I)		K(I)	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
AD-ts1	60.2	58.7	71.0	69.7	72.3	67.9	57.1	54.8	57.5	55.3
(5)	**13.5**	-9.8	17.9	-9.8	16.6	-13.1	15.6	-15.2	15.8	-13.7
AD-ts2	**85.8**	56.3	**83.5**	54.9	**83.6**	51.2	**88.7**	56.7	**89.3**	57.1
(6)	21.0	-36.2	23.0	-32.8	22.9	-36.9	21.6	-36.4	20.0	-33.6
AD-ts3	71.4	15.5	79.2	22.5	76.3	18.8	73.6	16.9	73.5	16.6
ADGH (7)	14.0	-42.5	**6.9**	-51.4	**6.8**	-52.5	**5.3**	-51.7	**5.6**	-52.2
δE	72.3		76.6		76.7		83.4		83.7	

*The electronic energies of the highest and the lowest points of the catalytic cycle/ reaction mechanism are written in bold; $^{\$}$is energetic span of the catalytic cycle in the presence of alkali and alkaline-earth metal ions. All the energy values are reported in kcal.mol^{-1}.

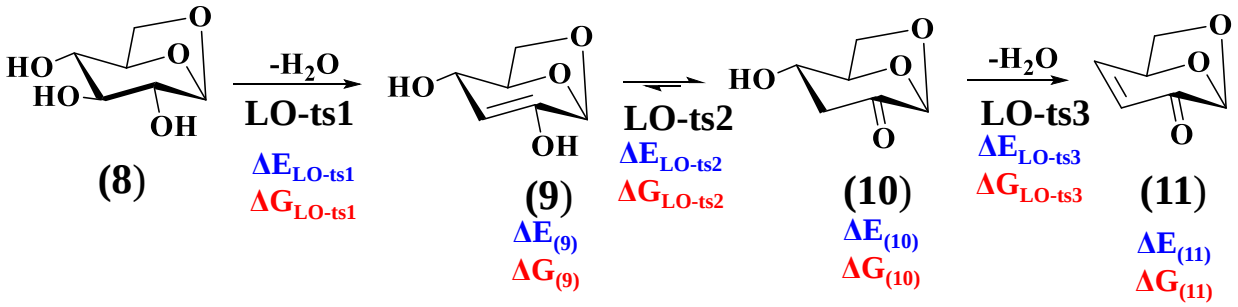
Table S6: Electronic, free energy changes and $^{\$}\delta$E involved during levoglucosan (LGA) formation from β-D-glucopyranose are calculated at M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent).



	No metal		Mg(II)		Ca(II)		Na(I)		K(I)	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
LG-ts	47.2	48.6	48.2	48.3	52.0	53.2	3.8	-15.8	48.2	46.4
(8)	9.7	-14.0	-0.3	-19.0	1.8	-18.9	47.0	44.6	4.0	-15.5
δE	37.5		48.5		50.2		43.2		44.2	

$^{\$}$is energetic span of the catalytic cycle in the presence of alkali and alkaline-earth metal ions. All the energy values are reported in kcal.mol^{-1}.

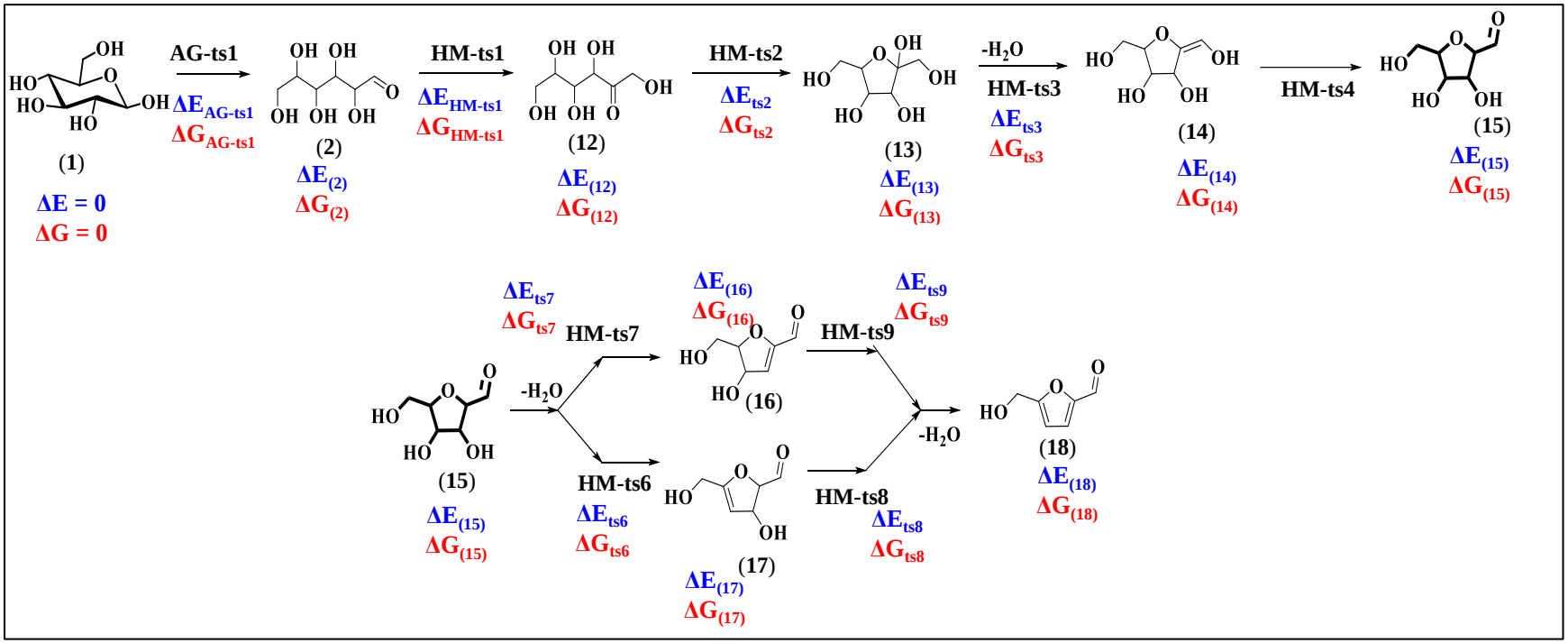
Table S7: *Electronic, free energy changes and $^{\$}\delta$E involved during levoglucosenone (LGO) formation from levoglucosan (LGA) are calculated at M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent).



	No metal		Mg(II)		Ca(II)		Na(I)		K(I)	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
LO-ts1	**71.5**	71.2	70.6	71.1	72.1	73.0	**75.5**	74.7	**74.4**	72.1
(9)	3.4	-22.8	17.6	-13.5	14.2	-16.4	10.4	-21.2	10.3	-22.7
LO-ts2	60.7	35.4	**83.9**	53.1	**77.7**	46.7	71.4	38.8	70.5	38.1
(10)	**-7.4**	-33.1	**9.5**	-21.5	**4.4**	-26.4	**-0.4**	-31.5	**-0.6**	-31.7
LO-ts3	44.2	19.8	64.7	30.6	54.4	24.2	49.3	17.8	50.3	19.3
LGO (11)	1.8	-51.5	25.9	-34.0	17.7	-43.8	10.8	-51.8	11.0	-50.7
δE	78.9		74.5		73.2		75.9		75.1	

*The electronic energies of the highest and the lowest points of the catalytic cycle/ reaction mechanism are written in bold; $^{\$}$is energetic span of the catalytic cycle in the presence of alkali and alkaline-earth metal ions. All the energy values are reported in kcal.mol^{-1}.

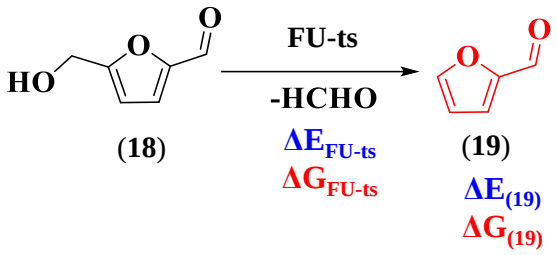
Table S8: *Electronic, free energy changes and $^{\$}\delta$E involved during 5-hydroxymethylfurfural (5-HMF) formation from β-D-glucopyranose are calculated at M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent).



	No metal		Mg(II)		Ca(II)		Na(I)		K(I)	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
AG-ts1	45.4	45.3	42.9	44.7	42.9	38.4	42.9	41.7	45.6	41.2
(2)	10.3	1.8	9.8	3.6	10.8	0.5	11.0	3.5	11.5	3.6
HM-TS1	49.6	44.2	35.8	33.5	40.0	35.3	48.7	43.7	49.7	42.4
(12)	10.2	3.1	6.6	2.4	7.6	0.2	8.8	0.7	9.6	1.6
HM-TS2	39.7	43.4	31.0	34.6	44.4	44.3	40.4	42.0	40.4	40.8
(13)	**3.9**	3.7	**0.1**	3.4	**0.9**	1.8	**1.4**	2.7	**1.9**	2.7
HM-TS3	70.4	62.3	38.4	35.0	48.7	39.5	64.3	54.8	66.9	55.5
(14)	21.2	-10.7	23.2	-7.6	22.3	-10.0	21.1	-12.5	21.1	-13.0
HM-TS4	80.2	50.6	**80.3**	48.1	**88.4**	53.9	**83.9**	51.2	**84.3**	50.1
(15)	15.0	-15.6	10.7	-14.5	13.2	-14.8	14.8	-13.5	14.6	-14.0
HM-TS6	71.7	43.5	55.7	30.6	86.9	60.6	66.5	38.3	66.0	37.1
(17)	18.5	-41.3	14.2	-40.5	15.7	-42.9	17.3	-40.8	17.4	-41.9
HM-TS7	**88.6**	58.3	73.8	50.1	77.8	50.3	83.5	54.4	82.6	53.2
(16)	18.4	-41.0	13.7	-41.3	14.6	-43.0	16.0	-41.9	15.3	-43.0
HM-TS8	6.5	-63.6	78.2	24.9	77.7	19.9	78.5	17.6	77.6	15.0
HM-TS9	9.8	-64.2	57.1	4.6	60.0	4.8	64.8	7.2	64.3	7.0
(18)	6.3	-79.9	8.7	-74.6	2.6	-81.5	5.3	-75.8	5.1	-81.1
δE	84.7		80.2		87.5		82.5		82.4	

*The electronic energies of the highest and the lowest points of the catalytic cycle/ reaction mechanism are written in bold; $^{\$}$is energetic span of the catalytic cycle in the presence of alkali and alkaline-earth metal ions. All the energy values are reported in kcal.mol^{-1}.

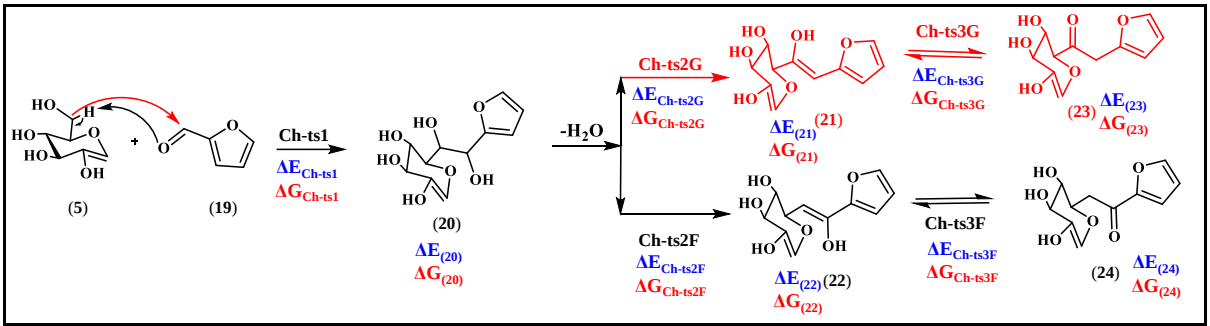
Table S9: Electronic, free energy changes and $^{\$}\delta$E involved during furfural formation from 5-hydroxymethylfurfural (5-HMF) are calculated at M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent).



	No metal		Mg(II)		Ca(II)		Na(I)		K(I)	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
FU-ts	78.0	80.1	60.1	57.2	69.3	64.7	74.5	68.5	76.4	75.6
(19)	15.0	-11.6	21.2	39.9	23.8	40.7	17.3	33.8	17.6	37.9
δE	38.9		76.6		45.5		57.2		58.8	

$^{\$}$is energetic span of the catalytic cycle in the presence of alkali and alkaline-earth metal ions. All the energy values are reported in kcal.mol^{-1}.

Table S10: Electronic, free energy changes and $^{\$}\delta$E involved during char formation furfural and 1,2-anhydroglucopyranose are calculated at M06-2X/6-311++G(2d,p) level of theory with implicit conditions (ethanol as a solvent).



	No metal		Mg(II)		Ca(II)		Na(I)		K(I)	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
Ch-ts1	**79.6**	87.4	**80.9**	83.2	**75.4**	81.8	**76.3**	84.4	**76.0**	84.7
(20)	-5.0	1.0	-1.9	1.0	-2.4	1.8	-5.9	-1.6	-6.4	-2.6
Ch-ts2G	62.6	68.5	62.7	67.1	60.1	65.0	60.7	67.5	60.1	67.1
Ch-ts2F	61.2	66.4	69.6	73.8	66.0	72.3	62.9	69.7	62.2	68.7
(21)	-3.4	-25.7	-0.3	-19.2	-2.9	-24.9	-5.4	-26.4	-6.1	-27.2
(22)	-5.3	-26.9	0.7	-21.2	-0.3	-21.4	-3.2	-23.5	-3.8	-25.4
Ch-ts3G	58.3	36.9	60.9	41.0	59.9	39.4	58.0	38.0	57.1	36.1
Ch-ts3F	50.6	30.7	50.5	30.7	52.4	31.8	50.5	31.4	49.7	30.8
(23)	-7.0	-30.1	0.1	-23.4	-3.5	-27.1	-6.7	-29.6	-7.4	-29.8
(24)	**-13.8**	-36.1	**-7.8**	-31.4	**-11.4**	-34.4	**-13.7**	-35.2	**-13.9**	-35.5
δE	93.3		88.7		86.8		90.0		89.9	

*The electronic energies of the highest and the lowest points of the catalytic cycle/ reaction mechanism are written in bold; $^{\$}$is energetic span of the catalytic cycle in the presence of alkali and alkaline-earth metal ions. All the energy values are reported in kcal.mol^{-1}.

Atomic coordinates for all structures

Cartesian Coordinates of all the reactants, transition states, intermediates, and the products optimized at M06-2X/6-311++G(2d,p) in the presence of an implicit environment of ethanol at 200ºC. Above the coordinates, the energies for the species are listed in hartrees.

Local minima

β-D-glucopyranose (**1**)

E = -686.908639
H = -686.906191
G = -687.121519

C	-0.97082100	-1.26920300	-0.38714400
C	1.16843500	-0.28189300	-0.61059900
C	-1.54027000	-0.03958400	0.30155900
C	-0.78854800	1.18944400	-0.16484200
C	0.70008200	1.00783600	0.05563900
C	2.62271300	-0.59658200	-0.32298800
O	-1.62079900	-2.37823100	0.13380500
O	0.41169700	-1.37859800	-0.10997900
O	-2.90192000	0.14679100	-0.02113200
O	-1.18209600	2.35116600	0.54086900
O	1.42954300	2.07903000	-0.50825400
O	2.85778800	-0.78088700	1.06067400
H	-1.47137100	-3.13821500	-0.43937200
H	1.03348800	-0.19176100	-1.69746100
H	-1.40495100	-0.16484600	1.38322500
H	-3.39585200	-0.61248800	0.30923800
H	-1.11654200	-1.19569700	-1.47408400
H	-0.97039000	1.32567900	-1.24000900
H	-2.12211900	2.49603400	0.38260400
H	0.89201100	0.93565500	1.13307000
H	1.03709800	2.89870400	-0.18393300
H	2.90851500	-1.48817000	-0.88909400
H	3.24146400	0.23948200	-0.64633000
H	2.26539500	-1.47864500	1.36452400

D-glucose (**2**)

E = -686.892176
H = -686.889728
G = -687.118626

C	-1.80384900	0.27371900	0.68760800
C	-0.59938200	-0.46467200	0.10423100
C	0.66806300	0.39019800	0.08712900
C	1.84682200	-0.38812900	-0.50641600
H	-0.40192100	-1.31684200	0.76272800
H	0.90071300	0.64250800	1.13120300
H	1.66735700	-0.49736800	-1.57892900
O	1.93277200	-1.69181100	0.04094100
H	2.39147200	-1.61248500	0.88811800
O	-0.97594900	-0.91191700	-1.18751800
H	-0.37572400	-1.61601600	-1.45633500
O	0.54764100	1.56405100	-0.69466800
H	-0.36459100	1.87893900	-0.62653400
C	3.15658900	0.35047500	-0.31239300
H	3.06754000	1.37135300	-0.68991800
O	3.42605800	0.33759600	1.08601400
H	4.34174800	0.59098200	1.23256100
H	3.94609100	-0.17211000	-0.85798900
C	-2.99700200	-0.65143100	0.63758500
H	-2.88793300	-1.62451700	1.14161900
O	-4.00754900	-0.34241600	0.06263100
O	-2.09641700	1.47634000	0.01556800
H	-2.93242300	1.34878900	-0.45829600
H	-1.59222600	0.49106800	1.74156000

β-D-glucofuranose (**3**)

E = -686.896571
H = -686.894122
G = -687.110024

C	1.02541200	-1.34726400	0.40295600
C	-0.24721800	0.55283700	0.87255900
C	1.11105700	1.05451000	0.39378000
C	1.64207200	-0.15636600	-0.35833200
C	-1.33396400	0.69155800	-0.20471200
H	1.78024700	-1.82445400	1.03111100
O	0.48703400	-2.33715800	-0.42135700
H	-0.43082200	-2.07931100	-0.62507700
C	-2.50802700	-0.24215600	0.03300100
H	-3.40211200	0.21490600	-0.39709100
H	-2.66696900	-0.40332500	1.10261300
O	-2.21983100	-1.47454900	-0.62467700
H	-2.84955100	-2.14167500	-0.33292500
O	3.05267200	-0.13580400	-0.35593200
H	3.37944000	-0.77936500	-0.99364600
H	1.25792400	-0.14974000	-1.38299600
O	0.96334500	2.21838000	-0.39287700
H	1.83313700	2.53156600	-0.66331800
H	1.75872200	1.24354000	1.25587600
O	-1.82520000	2.01973200	-0.19621900
H	-1.07283800	2.59846900	-0.37877000
H	-0.92531700	0.44944800	-1.19452300
O	0.01735400	-0.79692500	1.23830300
H	-0.60084300	1.07181500	1.76529600

Anhydroglucofuranose (**4**)

E = -610.487037
H = -610.484588
G = -610.673969

C	0.69181500	-1.24910300	-0.02211200

O	0.03196200	-0.80218200	-1.17796200
C	-0.40405700	0.51156400	-0.80972900
C	0.85714900	1.11926600	-0.14598900
C	1.66575100	-0.12449500	0.30278200
H	1.43545200	1.64233200	-0.91195200
H	1.88884300	-0.08689600	1.37064300
C	-1.61647600	0.37222600	0.11789800
H	-1.57846600	1.13521100	0.89569700
O	-2.78732300	0.52984300	-0.67038600
H	-3.54812200	0.60482500	-0.08484100
O	0.49896700	2.00014500	0.89573300
H	1.27668100	2.50497400	1.15513600
O	2.82830600	-0.33523600	-0.47241700
H	3.46210500	0.36450800	-0.28372000
H	1.15863500	-2.21152300	-0.22965800
C	-1.55572300	-1.03148600	0.72615100
H	-1.96258300	-1.74232300	0.00290800
H	-2.12767900	-1.09679900	1.65010200
O	-0.21435100	-1.36006600	1.06721000
H	-0.69610000	1.03784400	-1.71574600

1,2-anhydroglucopyranose (**5**)

E = -610.487037
H = -610.484588
G = -610.673969

C	-0.75788000	-1.69457200	0.02032800
C	1.04937900	-0.30961700	-0.61305000
C	-1.61444400	-0.68376700	-0.06926400
C	-1.17014500	0.73829700	-0.24477200
C	0.31285300	0.84199000	0.05384000
C	2.54650800	-0.26403300	-0.39254900
O	0.60420500	-1.54844700	-0.06148000
O	-2.97793700	-0.79880200	-0.02260000
O	-1.83929800	1.61463400	0.64743800
O	0.85542500	2.05091700	-0.43377600
O	2.87768100	-0.27298800	0.98352100
H	0.83764000	-0.30222200	-1.69049400
H	-3.23667500	-1.71292000	0.14270900
H	-1.06087100	-2.72417100	0.16237800
H	-1.34978400	1.05934000	-1.27916800
H	-2.78833900	1.53159700	0.49887700
H	0.44959700	0.76283100	1.13871400
H	0.34901400	2.77730700	-0.05202000
H	3.00320800	-1.11323700	-0.91001900
H	2.94304000	0.65834300	-0.81315600
H	2.49491700	-1.06917800	1.37016200

(**6**)

E = -534.07489
H = -534.072442
G = -534.253103

C	0.59245200	-1.52487900	-0.10039800
C	-1.12877700	-0.12549800	0.69445600
C	1.48498700	-0.53933300	0.00464000
C	1.00700500	0.84358500	0.07740600
C	-0.27959100	1.06476200	0.34271500
C	-2.60333700	0.08537500	0.42305600
O	-0.75012800	-1.27396400	-0.08394200
O	2.84679300	-0.66793300	-0.03921600
O	1.89942900	1.82830000	-0.19094000
O	-2.85629000	0.40666000	-0.93078400
H	-1.00482100	-0.39675500	1.75459400
H	3.09725500	-1.52761100	-0.39675100
H	0.84752900	-2.56004300	-0.28712900
H	2.75606900	1.42233000	-0.38211800
H	-0.70298100	2.06015600	0.34625900
H	-3.15056700	-0.81477200	0.71932200
H	-2.95905600	0.92198100	1.02538200
H	-2.43828800	-0.27386000	-1.47175100

ADGH (**7**)

E = -534.086048
H = -534.0836
G = -534.262997

C	-0.90321200	-1.50925100	0.07749600
C	1.07003100	-0.27801800	-0.23595600
C	-1.66437900	-0.41354700	-0.07388000
C	-1.08167500	0.91611200	0.07388800
C	0.39590900	0.94107300	0.36516200
C	2.52682700	-0.40845800	0.15369200
O	0.43751900	-1.48926300	0.19447200
O	-3.01339400	-0.49628900	-0.24215700
O	-1.79228300	1.90560700	0.03819800
O	3.19442200	0.72617700	-0.36580800
H	0.98230700	-0.23832500	-1.32887600
H	-3.34549200	0.41425100	-0.21614700
H	-1.32389500	-2.50625300	0.12462400
H	0.83887800	1.85418600	-0.02971100
H	0.51900900	0.94514200	1.45473300
H	2.60542900	-0.45361200	1.24495400
H	2.92473500	-1.33604700	-0.26688900
H	4.12790200	0.66333100	-0.14273900

Levoglucosan (**8**)

E = -610.493056
H = -610.492088
G = -610.680776

C	0.55702600	-1.21361200	-0.26309100
C	-0.89199200	-1.21734200	0.24995500
C	1.19078000	0.12594900	0.08593100
O	-1.06008100	-0.21308600	1.22244600
O	-1.78101600	-0.87929800	-0.80515300
C	0.23533400	1.27372400	-0.20959700
C	-1.14272700	0.96487700	0.40781500
C	-2.15392600	0.49201200	-0.62561000
H	0.54216600	-1.34435600	-1.34967000
H	-1.15853200	-2.18319600	0.67781400
H	1.39294800	0.12757100	1.15947900
H	0.14190300	1.37869100	-1.29704500
H	-1.48110100	1.79379500	1.02419100
H	-3.17121800	0.54958900	-0.23606500

H	-2.08527700	1.01343700	-1.57875100
O	1.24971500	-2.28159400	0.35519300
H	2.15489900	-2.28052600	0.02333900
O	2.39726100	0.30840900	-0.64242800
H	3.13588100	0.37326000	-0.03090900
O	0.71740500	2.48437100	0.34409100
H	1.57509200	2.66766900	-0.05799600

(9)

E = -534.087546
H = -534.085098
G = -534.253951

C	-0.96657000	-0.89961300	-0.02159200
C	-1.01826500	0.44603900	0.68151000
C	0.16803600	-1.30720900	-0.58143700
O	0.23351900	0.73301600	1.24062800
O	-1.23605000	1.46778900	-0.26831100
C	1.39705800	-0.44181400	-0.49148900
C	1.02461600	0.93092500	0.06287100
C	0.05328300	1.70560700	-0.85232000
H	-1.78845200	0.49692100	1.45179300
H	0.22799100	-2.25720000	-1.09824000
H	1.84175500	-0.30801900	-1.48044500
H	1.91367500	1.49393600	0.33519800
H	0.23848900	2.77745700	-0.83615500
H	0.07884300	1.33789000	-1.87927500
O	-2.11983000	-1.60435900	-0.12515800
H	-2.80808500	-1.22215800	0.43113000
O	2.41329700	-1.05172600	0.29589300
H	2.01935100	-1.28019400	1.14631900

(10)

E = -534.104736
H = -534.102288
G = -534.270379

C	1.14288200	0.82406000	-0.09189900
C	1.07580300	-0.53568400	0.60802800
C	-0.01773100	1.07091100	-1.02809300
O	-0.15601100	-0.59773300	1.28668700
O	1.04376300	-1.55491200	-0.36435000
C	-1.33800100	0.50742700	-0.46955200
C	-1.08999600	-0.83062700	0.22094400
C	-0.33559700	-1.83909800	-0.64305000
H	1.90178900	-0.68227900	1.30143100
H	-0.10898500	2.13450200	-1.24168900
H	-2.05313300	0.37537500	-1.28228200
H	-2.00752200	-1.22056200	0.65535600
H	-0.54972000	-2.86468300	-0.34636700
H	-0.53109000	-1.71363700	-1.70856100
O	2.04224200	1.60085300	0.10416500
H	0.22792200	0.55550900	-1.96251600
O	-1.93902800	1.40718600	0.44140800
H	-1.43114400	1.39069700	1.26308200

(11)

E = -457.689975
H = -457.687527
G = -457.83666

C	1.35475300	-0.03906400	0.00926300
C	0.21407400	-0.97650300	0.41646000
C	0.91852100	1.34433100	-0.25930800
O	-0.65252300	-0.30203500	1.28152600
O	-0.53872800	-1.25791800	-0.75689700
C	-0.37191300	1.64379900	-0.09820700
C	-1.32782400	0.58899600	0.38804600
C	-1.67295100	-0.38541800	-0.74913300
H	0.58187000	-1.89418200	0.87162400
H	-0.76656400	2.62317900	-0.34255900
H	-2.19584400	1.00310700	0.89216400
H	-2.57034500	-0.95462600	-0.50641900
H	-1.77121700	0.09305400	-1.72139700
O	2.48851700	-0.43827400	-0.12874300
H	1.65600900	2.05844900	-0.60321800

(12)

E = -686.892415
H = -686.889967
G = -687.116646

C	1.81779400	0.71976100	-0.30696900
C	3.24647400	0.21986500	-0.24637300
C	0.70496700	-0.29038100	-0.04474100
C	-0.65087900	0.39327200	0.05614900
C	-1.75141100	-0.62130600	0.36651100
H	0.67765100	-0.97443500	-0.90116400
H	-0.86305000	0.85342600	-0.91586900
H	-1.55182400	-1.05593800	1.34745200
H	3.66414100	0.55915800	0.70787300
O	-1.72133600	-1.67884700	-0.57660400
O	1.60050100	1.88817000	-0.52956800
H	-2.18375100	-1.36088200	-1.36342300
O	3.26888400	-1.19193300	-0.35398400
H	4.16867500	-1.50289500	-0.21233400
O	0.97912600	-0.99410200	1.15257000
H	1.75690200	-1.54313300	0.98597100
O	-0.67949800	1.36773300	1.08286800
H	-0.09173300	2.08290900	0.81131800
C	-3.12357700	0.02238600	0.38251500
H	-3.13699300	0.86088100	1.08118200
O	-3.38738300	0.45743500	-0.94847500
H	-4.32404600	0.65543500	-1.03549500
H	-3.85924600	-0.72385700	0.69342200
H	3.80072000	0.70010000	-1.05594600

(13)

E = -686.902421
H = -686.899972
G = -687.115617

C	1.06334700	-0.46346300	0.28442200

C	-1.22011000	-0.97113300	0.46146600
C	-0.96888900	0.39475600	1.15451000
C	0.36519100	0.86064300	0.57197000
H	0.94238900	1.46845600	1.26840600
C	-2.24924100	-0.94656500	-0.65327600
H	-2.39664300	-1.96875100	-1.00764300
H	-3.19700300	-0.59505000	-0.23152300
O	-1.87426000	-0.17034800	-1.77296300
H	-1.28623500	0.54265000	-1.48568800
C	2.05197200	-0.41044700	-0.87232300
H	1.49303700	-0.30926700	-1.80422700
H	2.60966500	-1.34851000	-0.90161800
O	2.98647300	0.63591500	-0.70997700
H	2.52315000	1.46252400	-0.89100500
O	0.17328000	1.54877800	-0.65413400
H	-0.33917500	2.34534400	-0.46175600
O	0.04886000	-1.37173400	-0.06973500
H	-1.54408100	-1.71036300	1.19865400
O	-1.94665400	1.37711300	0.89021800
H	-2.65495700	1.31064700	1.53763600
H	-0.85071000	0.24293600	2.22801400
O	1.66895100	-0.83073300	1.49892000
H	1.99374100	-1.73529400	1.41150900

(14)

E = -610.474664
H = -610.472216
G = -610.675486

C	-1.00170700	-0.60924500	-0.24757700
C	1.21142300	-0.28102800	-0.68477700
C	0.71132800	0.96319200	0.03964300
C	-0.79266100	0.88316700	-0.19046200
H	-1.02089500	1.33919800	-1.16289300
C	2.54087100	-0.81215200	-0.21702300
H	2.74662600	-1.75413600	-0.73395800
H	3.30959700	-0.08489600	-0.49837600
O	2.50180100	-1.00042300	1.18618500
H	3.33246100	-1.39711300	1.46425400
C	-2.15181300	-1.24951000	-0.10804900
H	-2.24071200	-2.32795300	-0.13821800
O	-3.31233800	-0.50851200	0.02459100
H	-3.93523400	-0.98559900	0.58266200
O	-1.49998800	1.53520000	0.84077300
H	-2.42024800	1.24503700	0.78541800
O	0.18772500	-1.25960200	-0.46665700
H	1.28311500	-0.06118000	-1.75712000
O	1.34495000	2.10084100	-0.49484900
H	1.16139300	2.85520600	0.07452900
H	0.90203700	0.86485900	1.11283000

(15)

E = -610.484654
H = -610.482206
G = -610.683350

C	1.07678000	-1.78915500	-0.25021400
C	0.07514500	1.10442000	-0.30370700
C	1.20544300	0.63023900	0.60606600
C	0.77038400	-0.81358000	0.87436100
C	-1.14021200	0.41900300	0.31010900
C	-2.16917500	-0.04112900	-0.69534500
H	0.40030300	-2.66093600	-0.29133200
H	0.64789900	2.90459300	-0.74089500
H	0.25683700	0.73068000	-1.32143300
H	1.19975800	-1.22175600	1.79357500
H	-1.60384600	1.08824000	1.04031300
H	-2.56475400	0.82412000	-1.23016300
H	-1.69348600	-0.71021400	-1.42298500
O	-0.11723300	2.49786100	-0.31864300
O	-3.26159400	-0.68058200	-0.06467500
O	1.96260200	-1.64967400	-1.05618200
O	-0.63973100	-0.73351200	1.02313900
H	-2.91139300	-1.43074600	0.42981500
O	2.50188900	0.82312200	0.10908200
H	2.65504400	0.17074600	-0.58895700
H	1.13597200	1.18876100	1.54267400

(16)

E = -534.079101
H = -534.076653
G = -534.260618

C	-2.32018800	-0.96051900	-0.23168600
C	0.55247000	1.38850000	0.34767500
C	-0.87224000	0.95786300	0.57594800
C	-1.07233400	-0.17929200	-0.08353300
C	1.14400100	0.14266300	-0.32489300
C	1.99661400	-0.67909800	0.61872000
H	-2.24229400	-1.86366700	-0.85835900
H	0.32152200	3.27778300	-0.10744400
H	1.08120600	1.61859200	1.27755800
H	1.69582700	0.40284000	-1.22786900
H	2.87596000	-0.10013400	0.90303400
H	1.42049000	-0.90241200	1.52493300
O	0.65452300	2.48817500	-0.54801900
O	2.45631000	-1.86548500	0.00471300
O	-3.35542700	-0.63776300	0.29256400
O	0.02149400	-0.68340500	-0.72210600
H	1.68246400	-2.37097800	-0.26992800
H	-1.62032600	1.50509100	1.12746600

(17)

E = -534.078829
H = -534.076382
G = -534.261142

C	0.18368100	1.09372500	-0.87133300
C	-1.21023600	0.90571000	-0.33765300
C	-0.96346600	-0.28074200	0.62040000
C	1.03474100	0.44829000	-0.07713900
C	2.52312900	0.37399500	-0.06776600
H	0.45237700	1.72660000	-1.70198300
H	2.91614100	0.91834800	-0.92411400
H	2.89959000	0.84336400	0.84727400

O	2.97839600	-0.96449500	-0.17109700
O	0.43341600	-0.27063800	0.92502100
H	2.64671600	-1.45392800	0.58990300
O	-1.72424900	2.06276600	0.29792500
H	-1.01751100	2.46446300	0.81695700
H	-1.95095900	0.63068700	-1.08764000
C	-1.28963500	-1.59865700	-0.05642600
O	-2.39225900	-1.86435900	-0.44921100
H	-0.44134500	-2.29853500	-0.16555000
H	-1.53672300	-0.19112600	1.54355200

(18)

E = -457.698174
H = -457.696369
G = -457.859595

C	0.46505	1.57871	-0.08258
C	-0.93082	1.34003	-0.18579
C	-1.10423	0.00694	0.0367
C	1.03967	0.37591	0.20016
C	2.44986	-0.05118	0.41524
H	0.98561	2.51418	-0.20376
H	3.08446	0.83264	0.39159
H	2.54819	-0.51995	1.39879
O	2.91163	-0.92263	-0.60503
O	0.09889	-0.58652	0.27764
H	2.44992	-1.7639	-0.52313
H	-1.71393	2.04934	-0.39799
C	-2.27716	-0.84845	0.06428
O	-3.40225	-0.44239	-0.12614
H	-2.0746	-1.91179	0.27477

(19)

E = -343.215550
H = -343.213101
G = -343.343842

C	1.97138700	0.41200700	0.00013100
C	0.76964300	1.17161600	0.00019400
C	-0.25133700	0.26754100	0.00006900
C	1.58327100	-0.89059400	0.00007700
H	2.98438700	0.77653800	0.00016700
O	0.24224100	-0.99751300	-0.00000300
H	2.13323300	-1.81685700	0.00003900
H	0.66196600	2.24441200	0.00025300
C	-1.68608700	0.47203800	0.00009800
O	-2.50673500	-0.41902600	-0.00043500
H	-1.98490000	1.53257100	-0.00038000

Adduct (5) + (19)

E = -953.703925
H = -953.701476
G = -953.989867

C	-2.38589600	1.76297000	-0.68797800
C	-1.61978600	-0.58358400	0.51545300
C	-0.55327300	0.48934800	0.39675300
C	-1.18147900	1.75639800	-0.12505200
C	-2.48284000	-0.59826400	-0.73466200
C	-3.55267600	-1.66925400	-0.70891300
H	0.93577500	0.94241700	1.55853100
H	-2.85147500	2.66533900	-1.06029900
H	0.44709600	2.74057400	0.16469700
H	-0.40787600	-1.79483200	1.40384600
H	-4.78513700	-0.63498900	0.37037600
H	-2.25427500	-0.33807500	1.37555500
H	0.21820200	0.13862400	-0.30126600
H	-1.84397700	-0.74082700	-1.61672100
H	-4.11536500	-1.62623400	-1.64663100
H	-3.08070900	-2.64703600	-0.62650900
O	0.02087000	0.65224400	1.68205700
O	-0.48985400	2.92963300	0.00876200
O	-1.03606900	-1.85950000	0.67384900
O	-4.41492100	-1.52488000	0.40468300
O	-3.16909300	0.64616800	-0.85251300
C	4.07458300	-2.00104700	-0.62728600
C	4.27063600	-0.64568900	-0.99481700
C	3.34962100	0.07626900	-0.28991300
C	3.05087600	-1.99699000	0.27031700
H	4.61369700	-2.86525100	-0.97568200
O	2.59984700	-0.75108300	0.48723100
H	2.55562700	-2.78332500	0.81576300
H	4.99147600	-0.24264300	-1.68822600
C	3.06933800	1.48484600	-0.26308900
O	2.19428400	1.98673900	0.42553700
H	3.70180800	2.10166600	-0.91516200

(20)

E = -953.711818
H = -953.709369
G = -953.988296

C	-2.33113100	1.71477100	-0.15127200
C	-1.83219800	-0.99440700	-0.24308500
C	-3.22254400	-0.57261200	0.20050900
C	-3.37162500	0.91300000	0.04319500
C	-0.81080800	-0.02999600	0.34418600
C	0.61610400	-0.39972600	-0.03162700
H	-4.11749600	-1.12190100	-1.45629600
H	-2.42693300	2.78231000	-0.29437700
H	-5.25328400	0.69645500	-0.08094100
H	-2.22278600	-2.88776200	-0.07929000
H	0.49392000	0.50256500	-1.74358100
H	-1.77476500	-0.93258400	-1.33835900
H	-3.36815700	-0.86095300	1.24601000
H	-0.91331500	-0.01050600	1.43518600
H	0.80335100	-1.42640300	0.28775500
O	-4.24322300	-1.26495100	-0.50870600
O	-4.64177900	1.41516100	0.12975300
O	-1.51675400	-2.29427700	0.20307100
O	0.79467800	-0.36067300	-1.43039700
O	-1.02973100	1.28219800	-0.17064700
C	5.08474000	-0.57556000	-0.16323800

C	3.92129500	-0.74751900	0.65777400
C	3.02874600	0.18411700	0.24431600
C	4.80180300	0.44424500	-1.00460200
H	6.00399600	-1.13597600	-0.12632500
O	3.55393400	0.92169400	-0.76527400
H	5.35397300	0.93273800	-1.78902700
H	3.76957900	-1.46569600	1.44671300
C	1.63481700	0.50720600	0.67225300
O	1.45942600	0.28801600	2.05960600
H	2.10305700	0.82050700	2.53959300
H	1.42126600	1.54874500	0.40323700

(**21**)

E = -877.309270

H = -877.306822

G = -877.567761

C	2.35276200	-1.63576800	-0.24713100
C	1.68504200	1.04861400	-0.13030000
C	3.11401500	0.67752300	0.23095500
C	3.34549700	-0.78538000	-0.01777000
C	0.74463200	-0.02149100	0.41382700
C	-0.69610900	0.32370800	0.20441400
H	3.92668800	1.36621200	-1.41551700
H	2.50432700	-2.68642000	-0.45102200
H	5.20934200	-0.44752500	-0.13803100
H	1.97497600	2.94443200	0.16007700
H	1.58122300	1.06568700	-1.22480100
H	3.28174000	0.90749900	1.28760200
H	0.96531100	-0.15988800	1.48333900
H	-0.94339300	1.37023900	0.10227000
O	4.06695500	1.47006800	-0.46495000
O	4.64297500	-1.21364100	0.02749900
O	1.32000600	2.28920100	0.42875000
O	1.02842200	-1.26528400	-0.24496300
C	-5.29949000	-0.04588300	-0.23633700
C	-4.21062800	-0.96422500	-0.09798700
C	-3.09028800	-0.20458000	0.01321800
C	-4.75272400	1.19117200	-0.19793700
H	-6.34519200	-0.27734400	-0.34964600
O	-3.40790100	1.11294300	-0.04460000
H	-5.16376800	2.18393600	-0.26352600
H	-4.24689600	-2.04023200	-0.08437100
C	-1.69006700	-0.57026800	0.17727200
O	-1.54495900	-1.91534500	0.30006400
H	-0.60420000	-2.13065200	0.20588500

(**22**)

E = -877.312292

H = -877.309844

G = -877.569664

C	-2.60770800	-1.69627600	0.21826000
C	-1.55570100	0.84622600	0.13282300
C	-2.97305400	0.68005500	-0.38645000
C	-3.44026200	-0.72363300	-0.13479000
C	-0.72852800	-0.36513600	-0.29156500
C	0.70527200	-0.23062200	0.11753200
H	-3.83489200	1.53690700	1.15294900
H	-2.93738600	-2.70313000	0.43538900
H	-5.24163000	-0.12433200	-0.18900400
H	-1.51829600	2.75515200	-0.20128800
H	1.76533900	0.08047600	1.68069500
H	-1.57706700	0.87227100	1.23029900
H	-2.99047800	0.90205600	-1.45771800
H	-0.78613600	-0.47785300	-1.37995700
O	-3.86518600	1.62621600	0.19097400
O	-4.77763100	-0.96485100	-0.30347000
O	-0.94295700	2.00324500	-0.38681600
O	0.83145200	-0.01289700	1.44673000
O	-1.24981700	-1.54107400	0.32612100
C	5.34466800	0.01698700	-0.42549700
C	4.21640400	-0.20006600	-1.27915000
C	3.11416100	-0.16066400	-0.48346600
C	4.85423100	0.17230600	0.82353400
H	6.38354400	0.05189300	-0.70816700
O	3.49717900	0.06668300	0.80983000
H	5.30548600	0.35200700	1.78385100
H	4.21755700	-0.36339700	-2.34403400
C	1.70649700	-0.30762700	-0.76888800
H	1.45375900	-0.48993700	-1.80401900

(**23**)

E = -877.314947

H = -877.312499

G = -877.574780

C	2.91786400	-1.55717600	0.19703600
C	1.39663300	0.66537900	-0.36788200
C	2.80652100	0.92003900	0.13721900
C	3.53967500	-0.38529900	0.25377700
C	0.81679600	-0.53143000	0.38706100
C	-0.62791400	-0.75795200	-0.05314300
H	3.53666500	1.48131600	-1.59440300
H	3.43571000	-2.50476800	0.24818500
H	5.18997100	0.54355000	0.10493400
H	0.96129100	2.54612400	-0.57832800
H	-1.67009900	-0.71082000	1.76326000
H	1.43863200	0.39078500	-1.43131200
H	2.75189700	1.41554600	1.11123100
H	0.85663100	-0.33454000	1.46619500
O	3.51092100	1.83178300	-0.69403000
O	4.89293700	-0.31308000	0.44075100
O	0.55344600	1.77482400	-0.16626500
O	-0.86834300	-1.39636200	-1.04430400
O	1.55620900	-1.69605700	0.08617100
C	-5.01834300	-0.02301100	-0.77121300
C	-3.65306700	-0.45728500	-0.86875400
C	-3.04154300	-0.04508300	0.26815700
C	-5.12683900	0.61405200	0.41400300
H	-5.80479800	-0.17057600	-1.49250500
O	-3.93311600	0.61037900	1.06133700
H	-5.93989900	1.10366600	0.92202400
H	-3.19105700	-1.00303800	-1.67147200
C	-1.66830700	-0.12827100	0.83203500

H	-1.31022600	0.86707600	1.11312000

(24)

E = -877.325728
H = -877.323280
G = -877.584361

C	2.17145100	-1.57993400	-0.67861700
C	1.78382600	1.06308100	-0.00161700
C	3.15198700	0.47474300	0.30243800
C	3.24098500	-0.91479300	-0.25662700
C	0.72163800	0.01013300	0.28639700
C	-0.68051000	0.53011100	0.08038100
H	4.09140900	1.41624800	-1.13947700
H	2.22755700	-2.57098300	-1.10817100
H	5.13411900	-0.76617800	-0.29293800
H	2.26545600	2.80726400	0.69869400
H	1.73742500	1.31580800	-1.07110100
H	3.29732000	0.45779300	1.38698600
H	0.84532800	-0.35202400	1.31426700
H	-0.85212500	0.74884300	-0.97603900
O	4.20769800	1.29311800	-0.18793100
O	4.48661000	-1.48401100	-0.28792100
O	1.52298100	2.19850300	0.79261000
O	0.89423500	-1.09185500	-0.60298100
C	-5.30306100	-0.16140200	-0.24947800
C	-4.27473200	-0.83576000	0.46534400
C	-3.11300400	-0.19839800	0.15270800
C	-4.68656200	0.83275700	-0.94052700
H	-6.35713600	-0.38164200	-0.25408000
O	-3.36101500	0.82621400	-0.70936200
H	-5.04857700	1.59206600	-1.61313400
H	-4.36789200	-1.67975300	1.12841700
C	-1.73372600	-0.43028700	0.58774200
O	-1.47983100	-1.34214900	1.34762300
H	-0.80804900	1.47248900	0.62140200

Transition states

AG-ts1

E = -686.836285
H = -686.833836
G = -687.049264

C	-0.80948600	-1.56168100	-0.43787000
C	1.26272000	0.18062700	-0.71463400
C	-1.51573800	-0.41640500	0.28247500
C	-1.06677100	0.94247100	-0.21551100
C	0.40439600	1.13837400	0.10082000
C	2.65877200	0.01470600	-0.15893400
O	-0.42838200	-2.59754100	0.29583000
O	0.67778800	-1.13352900	-0.78088400
O	-2.91167100	-0.49920600	0.05781300
O	-1.76752200	1.97380300	0.44901900
O	0.83692600	2.43545100	-0.25139700
O	2.53457400	-0.59823500	1.11236400
H	0.74914600	-1.95227500	0.01515700
H	1.31815800	0.56193500	-1.73621400
H	-1.28935300	-0.49765500	1.35081500
H	-3.28783300	-1.17752300	0.62870100
H	-1.26633300	-1.76141100	-1.41416400
H	-1.22482100	1.01476500	-1.30128400
H	-2.70905600	1.76664200	0.39835800
H	0.55809600	0.96259500	1.17228800
H	0.23729900	3.06367300	0.16959600
H	3.24780700	-0.60649800	-0.83825000
H	3.11820200	1.00443900	-0.08852600
H	3.41162300	-0.81318700	1.44348300

AG-ts2

E = -686.809325
H = -686.806876
G = -687.023481

C	1.24796100	-1.44646600	0.26123700
C	-0.32336300	0.42742100	0.80988400
C	1.07295900	0.96033000	0.47692000
C	1.71522900	-0.12938000	-0.36781500
C	-1.37377200	0.68024200	-0.27635400
H	1.93133100	-1.79913600	1.04334900
O	0.64173600	-2.34886600	-0.49288700
H	-0.39231200	-1.72716800	0.19495600
C	-2.64843000	-0.11363900	-0.04095000
H	-3.44083900	0.34377000	-0.63903200
H	-2.93130100	-0.05914600	1.01536800
O	-2.41521200	-1.45447600	-0.44379500
H	-3.15148200	-2.00160400	-0.15337000
O	3.11267600	0.05201600	-0.33161400
H	3.51892500	-0.46104200	-1.03802400
H	1.33288600	-0.08200300	-1.39200900
O	0.98485800	2.20646000	-0.17482400
H	1.87502600	2.53463100	-0.34582400
H	1.64988900	1.04942200	1.40443100
O	-1.74457300	2.04241800	-0.24215100
H	-0.94396700	2.56588000	-0.38285800
H	-0.97600200	0.40267700	-1.26104500
O	-0.06867600	-0.98154900	1.01381300
H	-0.70213400	0.83464200	1.74818900

AG-ts3

E = -686.825874
H = -686.823426
G = -687.037813

C	-1.07453600	0.53455600	0.96390900
C	0.64832400	-0.90893700	0.66180800
C	-0.55127200	-1.49231500	-0.10982900
C	-1.62028600	-0.38434100	-0.08865200
C	1.84266100	-0.36393300	-0.11876300
H	-1.61072000	1.33900700	1.44994700
O	-1.09485700	2.83450100	-0.24007000
H	-0.58936000	3.57549400	0.10462200
C	1.58326600	1.05881700	-0.62080100
H	2.42928500	1.32729100	-1.27348900

H	1.66634500	1.72028900	0.26427500
O	0.35816700	1.14273100	-1.23727200
H	-0.40421700	2.17361400	-0.72787700
O	-2.85584000	-0.89695700	0.35377600
H	-3.57277900	-0.36240900	-0.00490200
H	-1.67444200	0.12473300	-1.04804200
O	-0.17266800	-1.92648400	-1.38540900
H	-0.76585300	-2.63317100	-1.65965800
H	-0.95536200	-2.32427100	0.47407300
O	2.99461100	-0.33039500	0.70930100
H	3.39871900	-1.20348200	0.73375100
H	1.98887900	-1.03470700	-0.96874800
O	0.03544100	0.20458700	1.43681900
H	1.00172200	-1.58933000	1.43285400

AD-ts1

E =-686.812742
H =-686.810294
G = -687.028000

C	-0.61237000	-1.38219100	-0.97820300
C	1.12723100	0.29320500	-0.90792900
C	-1.48489400	-0.63704900	-0.11036900
C	-1.22788200	0.85670200	-0.15505500
C	0.25522300	1.09025000	0.06440200
C	2.52322200	0.00444700	-0.38278700
O	0.44184600	-1.65967500	1.55207100
O	0.55267700	-1.02895600	-1.27707600
O	-2.81674800	-1.02356100	-0.27195200
O	-1.98939300	1.43496500	0.87822900
O	0.50633700	2.46757000	-0.13996300
O	2.55235000	-0.51328000	0.90781900
H	-0.96460500	-1.05189700	0.84995400
H	1.18247600	0.81096300	-1.86586800
H	0.46544800	-1.82692600	2.49825200
H	-3.28781700	-0.81068000	0.54121700
H	-0.90354900	-2.36460100	-1.34646500
H	-1.53289000	1.26183600	-1.12826100
H	-1.82949600	2.38642800	0.86641600
H	0.49200600	0.79517300	1.08730100
H	1.18045100	2.76520800	0.47908800
H	3.01051600	-0.65715300	-1.11160500
H	3.06043700	0.96034100	-0.41385200
H	1.66728800	-1.03738500	1.17044800

AD-ts2

E =-610.371841
H =-610.369393
G = -610.568780

C	-0.75934500	-1.70884100	-0.16885700
C	1.07194500	-0.30918500	-0.55911500
C	-1.59754000	-0.67110800	-0.10628500
C	-1.13448600	0.70841500	0.07739600
C	0.31748500	0.84280600	0.08323700
C	2.56425900	-0.24227000	-0.31620600
O	0.60990300	-1.52694500	0.00079100
O	-2.95667000	-0.79718200	-0.22788300
O	-1.75550700	1.36989300	1.18200400
O	0.45517400	2.03881200	-1.01073600
O	2.86919300	-0.26033100	1.06557500
H	0.87116900	-0.30944500	-1.63747800
H	-3.20001900	-1.72907300	-0.18123400
H	-1.04472500	-2.73421600	-0.36327200
H	-0.62009100	1.81931100	-1.06711300
H	-2.44702500	1.93850800	0.83747400
H	0.78975600	1.25505800	0.97337600
H	0.60547900	2.89828600	-0.58010000
H	3.04656800	-1.07540200	-0.83541200
H	2.95400400	0.69260300	-0.72058500
H	2.49423200	-1.06850200	1.43531400

AD-ts3

E =-533.994643
H =-533.992195
G = -534.170628

C	-0.62700600	-1.48991400	0.08616200
C	1.07552000	0.01114600	-0.67875500
C	-1.58565800	-0.52737800	0.04363100
C	-1.10670300	0.80367500	0.01096400
C	0.28927500	1.11919600	-0.05468000
C	2.57223800	0.08209700	-0.48119300
O	0.66940700	-1.28854800	-0.09431700
O	-2.91217900	-0.85974000	0.09247300
O	-1.79975400	1.88316700	0.04141100
O	2.93259400	0.19593000	0.88129100
H	0.85426600	-0.09369900	-1.74631100
H	-3.40848000	-0.10809800	0.43853000
H	-0.88121900	-2.52719800	0.27724500
H	-0.64584200	2.30028800	-0.24440100
H	0.64620000	1.40860400	0.93779300
H	3.03792700	-0.79658500	-0.93730500
H	2.94425600	0.97380200	-0.98590100
H	2.62634700	-0.59651500	1.33671000

LG-ts

E = -686.833462
H = -686.831014
G = -687.044117

C	-1.09110300	-1.76605900	-0.02480600
C	1.38845200	-0.97831600	-0.12993700
C	0.10308200	-1.27952500	-0.87383100
C	-0.42356700	0.99218100	-0.77430200
C	1.19893200	0.06040800	0.98398800
C	0.41000600	1.27074100	0.44733900
H	3.12600200	-0.27957600	-0.70234100
H	-3.83873200	1.20621300	0.33251600
H	-0.36101600	-0.65879800	1.81057600
H	0.91873700	3.15691200	0.22508700
H	-2.61940300	0.22248000	0.22055700
H	-1.87320500	-2.08441300	-0.72775100
H	-0.73473000	-2.66763900	0.49770300

H	1.73621600	-1.91313800	0.32015300
H	0.30115200	-1.92657200	-1.72525100
H	-0.97746600	1.81619000	-1.21761500
H	2.18502900	0.43733500	1.26590400
H	-0.26386500	1.61959200	1.23190400
O	2.28492000	-0.49961400	-1.11768600
O	0.59496100	-0.49033800	2.11655800
O	1.28962700	2.29411200	0.00847900
O	-1.51725000	-0.77466000	0.82532500
O	-0.39564600	-0.04036700	-1.47693800
O	-3.14580400	0.92022100	-0.26850700

LO-ts1

E = -610.379134
H = -610.376686
G = -610.567326

C	-1.19926100	-0.46568600	-0.20887900
C	-0.02583300	-1.34126200	-0.57796700
C	-0.85183000	0.87935100	0.17896900
O	1.00809600	-0.60537600	-1.22560300
O	0.63360300	-1.87283200	0.56902200
C	0.60610400	1.33794900	0.13660700
C	1.53160400	0.15731800	-0.14775400
C	1.55226700	-0.86910100	0.99931700
H	-1.47431500	-0.28817800	1.32572800
H	-0.33299300	-2.16094600	-1.22459300
H	-1.55465900	1.65854900	-0.10275500
H	0.89662500	1.81203700	1.07644500
H	2.51726600	0.52651200	-0.42187400
H	2.53553400	-1.32188000	1.11846700
H	1.23093500	-0.43503300	1.94887700
O	-2.30294200	-0.57211900	-1.09508000
H	-2.97257500	-1.12330300	-0.68345000
O	-1.19937700	0.67823500	1.86328900
H	-1.98216600	1.18439400	2.13727300
O	0.75137700	2.23281100	-0.95245800
H	0.33199000	3.07067500	-0.72924400

LO-ts2

E =-533.996176
H =-533.993728
G =-534.161344

C	-0.80475500	1.06527700	0.07326300
C	-1.24996200	-0.20407300	-0.61912100
C	0.42009800	1.12842500	0.76619000
O	-0.09037500	-0.66639900	-1.26756100
O	-1.57475500	-1.17291700	0.33843400
C	1.44523100	0.04783700	0.46950900
C	0.71835500	-1.13789500	-0.17445200
C	-0.33279800	-1.76709800	0.75473600
H	-2.06287700	-0.06634500	-1.32795100
H	-0.14588500	2.44929000	0.38214200
H	1.92466700	-0.30227500	1.38466100
H	1.42955300	-1.85505300	-0.57702900
H	-0.41212900	-2.84334600	0.61599900
H	-0.14467100	-1.53873300	1.80425200
O	-1.36120300	2.20431000	-0.03180900
H	0.31587300	1.46328700	1.79672400
O	2.50216700	0.49952800	-0.36379300
H	2.11179100	0.98217700	-1.10170900

LO-ts3

E = -534.022570
H =-534.020121
G =-534.186064

C	0.80564100	1.17424200	-0.02541200
C	1.14394300	-0.14049600	0.69349700
C	-0.49601900	1.23321700	-0.60835600
O	-0.00548400	-0.73484900	1.24226100
O	1.60796200	-1.06160800	-0.27923900
C	-1.34948100	0.01116700	-0.57750500
C	-0.69536700	-1.18398900	0.08040300
C	0.45025900	-1.72870800	-0.79049900
H	1.90171200	0.00222100	1.46095700
H	-1.65487200	1.40768500	0.40512000
H	-1.88371900	-0.24703600	-1.48860800
H	-1.42360400	-1.93630000	0.37173200
H	0.57654000	-2.80171800	-0.65601000
H	0.31617500	-1.49982700	-1.84871600
O	1.66966800	2.04762300	-0.07893200
H	-0.66300800	1.95346600	-1.40024600
O	-2.40638600	0.52282400	0.43166400
H	-3.24915700	0.73699400	-0.00302300

HM-ts1

E = -686.829556
H = -686.827108
G = -687.051084

C	2.25290300	-1.19156500	0.34651000
C	1.96416700	0.15477700	-0.04926800
C	0.60224300	0.80940900	0.15590400
C	-0.58286500	-0.11887700	-0.03724600
C	-1.90869800	0.64260200	0.13739900
H	1.55423100	-2.01774200	0.40701500
H	0.57768400	1.16599200	1.19257800
H	-0.54422600	-0.87701900	0.75486600
H	-1.85179900	1.60561300	-0.37125300
H	1.83370200	-0.52510300	-1.05482300
O	-2.09889900	0.92478600	1.51501200
O	3.50772400	-1.42693400	0.49326800
H	-2.31855700	0.09374400	1.95492300
O	3.01284800	0.93435900	-0.07712000
H	3.89600800	-0.49529800	0.39494200
O	0.51863900	1.90041600	-0.73630100
H	1.41313000	2.26912400	-0.78115000
O	-0.47796500	-0.73974000	-1.30615800
H	-1.10695600	-1.47204600	-1.32084300
C	-3.07232000	-0.13931900	-0.43389500
H	-3.01794600	-0.15348400	-1.52530500

O	-2.98374200	-1.46032900	0.09561900
H	-3.79206800	-1.93951900	-0.11028300
H	-4.00462100	0.34310600	-0.13164000

HM-ts2

E = -687.051084
H = -686.842986
G = -687.052410

C	-0.91356700	-0.39290000	-0.21963300
C	1.28745600	0.64386000	-0.75789100
C	0.71211900	1.27441100	0.51710100
C	-0.33044200	0.28328000	1.04008400
H	1.49101300	1.44609900	1.26500300
H	-1.11732400	0.80330100	1.59246100
C	2.56410400	-0.16621600	-0.61558800
H	2.90690500	-0.45616500	-1.60894700
H	3.32455700	0.48396400	-0.17091700
O	2.39151700	-1.36097300	0.11116600
H	1.98865900	-1.15416800	0.96843500
C	-2.19040700	0.20497400	-0.76797600
H	-2.31489900	-0.13360400	-1.80061200
H	-2.15302700	1.29413500	-0.74231900
O	-3.26210500	-0.20941100	0.05373800
H	-3.23829100	-1.17449800	0.08247900
O	0.10090000	2.48588400	0.11756500
H	-0.23107600	2.94224500	0.89890600
O	0.28598500	-0.69207100	1.84759600
H	-0.06671900	-1.54122600	1.51574300
O	0.21870100	-0.20289600	-1.26034700
O	-0.86148800	-1.73340900	-0.20612700
H	1.44540000	1.43171900	-1.49417400
H	0.20114100	-1.32324600	-0.99137300

HM-ts3

E = -686.796419
H = -686.793970
G = -687.022196

C	-0.84281500	-0.41965500	0.27917900
C	1.27627100	-0.46913200	-0.45064800
C	0.96512400	1.00850300	-0.21613900
C	-0.55517300	1.02602000	-0.04228200
H	-1.04904200	1.26688300	-0.98533900
C	2.59206300	-0.96973800	0.06765400
H	2.65243800	-2.05053400	-0.08538100
H	3.37668900	-0.48905800	-0.52561800
O	2.69096400	-0.63470800	1.43724600
H	3.52282600	-0.97472000	1.78093900
C	-2.15181600	-0.98396500	0.46834900
H	-2.17366300	-1.90987600	1.04069700
H	-2.21511300	-1.22248900	-0.68270600
O	-3.14416800	-0.04310900	0.78901000
H	-3.27695300	-0.03836800	1.74338100
O	-0.93132000	1.87201300	1.01601500
H	-1.89482800	1.93900100	1.01622200
O	0.18720000	-1.16474400	0.23969600
H	1.13556900	-0.71052100	-1.50773100
O	-1.39689000	-1.02130900	-2.05592200
H	-1.57794500	-0.93588600	-2.99599700
O	1.44808300	1.73877800	-1.31333700
H	1.54511200	2.66203400	-1.05872900
H	1.42202900	1.33596100	0.72192000

HM-ts4

E = -610.380644
H = -610.378196
G = -610.577780

C	-2.14284300	-0.69505700	-0.80640100
C	-0.97907100	-0.67077800	0.02222400
C	-0.78514700	0.60231600	0.83071100
C	0.26536700	1.31916700	-0.01652700
H	-2.25194900	-0.53347200	-1.87817500
H	0.83799000	2.03391000	0.57912100
O	-0.44799600	1.95809800	-1.05840400
O	-3.14259500	-1.00229400	-0.08743100
H	0.17931700	2.36363000	-1.66634500
H	-2.20598600	-1.21858800	0.73197800
C	1.12118900	0.16403900	-0.54262600
O	0.25323800	-0.98721200	-0.55672000
H	1.42302000	0.36142900	-1.57587100
C	2.35876700	-0.12038500	0.27776900
H	2.94590200	0.80095800	0.35824200
H	2.06779400	-0.44531000	1.27893500
O	3.09909000	-1.12751000	-0.39620000
H	3.82178800	-1.40924900	0.17234900
O	-0.19663800	0.36215000	2.09615900
H	-0.66856300	-0.36773700	2.51200700
H	-1.69966900	1.19276100	0.91763000

HM-ts5

E = -686.767643
H = -686.765194
G = -686.985856

C	-1.28091800	0.23869700	-0.33374200
C	1.31780700	-0.04567100	-0.81817500
C	0.92043600	-0.78100200	0.46210200
C	-0.60902700	-0.77926900	0.55097200
H	1.26274900	-1.82164100	0.44513200
H	-0.90316700	-0.61731100	1.58685800
C	2.81609700	0.14773000	-0.93643500
H	3.13058100	0.77308700	-1.78918100
O	3.62554000	-0.28885600	-0.15390100
O	1.39847500	-0.12088100	1.61762600
H	2.36279200	-0.14116800	1.57055600
O	-1.21620500	-2.00479600	0.14948700
H	-0.82957800	-2.30650800	-0.68331000
C	-2.70631600	0.61044400	-0.03537100
H	-2.89454000	0.60911000	1.03895900
H	-2.94386000	1.58894100	-0.44756700
O	-3.50114300	-0.33451700	-0.72661600

H	-3.31500500	-1.20996700	-0.36236800
O	-0.70465200	1.91530100	0.93471100
H	-1.14281100	2.72204900	0.63764400
H	-1.08721700	0.15229200	-1.39707900
O	0.70802400	1.18706300	-0.89166600
H	0.09655400	1.77178400	0.30329100
H	1.03472600	-0.69274700	-1.67615400

HM-ts6

E = -610.394229
H = -610.391781
G = -610.589057

C	-2.03619000	-1.18878400	-0.58188800
C	0.51655400	1.42355400	0.01964300
C	-0.84629700	0.84192800	0.40803200
C	-0.85113900	-0.52200800	-0.18135900
C	1.29409800	0.19921900	-0.47906600
C	2.13868100	-0.47503900	0.59042100
H	-1.87497600	-2.07352000	-1.22501800
H	-0.08949800	3.10274700	-0.77216000
H	1.01913300	1.91756900	0.85742400
H	-0.79901200	-0.59700800	1.44987600
H	1.92982300	0.47518800	-1.32109700
H	2.95618100	0.18455100	0.88372100
H	1.54338100	-0.69716700	1.48443400
O	0.35428100	2.30119200	-1.07153400
O	2.71043700	-1.66174900	0.08014700
O	-3.17456900	-0.88675100	-0.21476100
O	0.31327000	-0.70922000	-0.96783400
H	1.99348600	-2.16423700	-0.32730000
O	-0.95399500	0.44018000	1.87484000
H	-0.27656600	0.80735700	2.47157300
H	-1.69159000	1.50207000	0.23698600

HM-ts7

E = -610.367273
H = -610.364825
G = -610.565505

C	0.94900700	-1.84149900	0.11249600
C	0.13327900	1.05151100	-0.44584800
C	1.37177800	0.66857300	0.36524400
C	0.88613200	-0.63033100	1.02586100
C	-1.00874500	0.38146000	0.15985100
C	-1.92520900	-0.44133600	-0.68564800
H	0.51975600	-2.76454600	0.53800800
H	-0.48452700	3.12267800	-0.83222300
H	0.26165500	1.10434700	-1.52419500
H	1.39638300	-0.85283200	1.96525500
H	-1.10984300	2.07306700	0.34766800
H	-2.06215700	0.04557700	-1.65314000
H	-1.51845100	-1.44833300	-0.86516300
O	-0.24457600	2.59285900	-0.05191000
O	-3.23381400	-0.58728500	-0.12631600
O	1.35054300	-1.81197000	-1.02611500
O	-0.48864900	-0.38727400	1.28612700
H	-3.12035100	-0.86818900	0.78795000
O	2.57570100	0.59077700	-0.34696400
H	2.49138000	-0.13200300	-0.98351000
H	1.51506700	1.41311200	1.14903400

HM-ts8

E = -533.985653
H = -533.983205
G = -534.172620

C	-2.49526400	-0.79220200	-0.44512600
C	0.35513800	1.06918400	0.91532400
C	-1.01273000	0.90266200	0.84906800
C	-1.20729500	-0.18165600	0.01085100
C	0.98861400	0.05895000	0.07681900
C	2.06896500	-0.84585200	0.64639600
H	-2.40837800	-1.62605900	-1.15605100
H	1.39170800	3.21545400	-1.36427500
H	0.90350900	1.77965600	1.51084400
H	1.37502600	0.70774100	-0.77414800
H	2.84941800	-0.20279600	1.05234100
H	1.65673900	-1.45258000	1.45657500
O	1.22109200	2.38832700	-0.90034100
O	2.65130700	-1.64468600	-0.35412000
O	-3.54093100	-0.37425100	-0.03614000
O	-0.10716400	-0.72103000	-0.43195400
H	2.04414000	-2.35706700	-0.58028300
H	-1.79116500	1.48224700	1.31543500

HM-ts9

E = -533.999971
H = - 533.997523
G = -534.179710

C	0.44944800	-1.25277800	0.73878300
C	-0.96678200	-0.92501900	0.53839500
C	-0.92288300	0.31042400	-0.28875800
C	1.17583300	-0.34836500	0.05653500
C	2.65174500	-0.23587400	-0.13490300
H	0.84073300	-2.05328500	1.34440500
H	3.15077400	-0.95168100	0.51547700
H	2.89341300	-0.48551600	-1.17365600
O	3.13375300	1.05106900	0.20217900
O	0.44852600	0.60045200	-0.55899000
H	2.70741300	1.69531900	-0.37383800
O	-1.66454000	-1.84051900	-0.58433000
H	-1.03574300	-2.51020600	-0.90487600
H	-1.67660100	-1.00241200	1.35425800
C	-1.77016800	1.45021200	-0.08304000
O	-2.88037200	1.40201800	0.42575800
H	-1.37219600	2.40201700	-0.47888000
H	-1.50988100	-0.79000200	-1.12189900

FU-ts

E = -457.573813
H = -457.571365
G = -457.731945

C	0.58338600	1.31827800	0.10024100
C	-0.79817700	1.28441000	0.06435200
C	-1.11816200	-0.06327100	0.01059000
C	1.06846900	-0.01661300	0.01155600
C	2.42785900	-0.54238100	0.49268700
H	1.22598100	2.18620300	0.12131500
H	2.69115200	-0.13935400	1.48204600
H	2.30373600	-1.63264500	0.59599200
O	3.25114700	-0.13126100	-0.54144200
O	-0.06794900	-0.84219500	0.01530200
H	1.67096600	-0.00347300	-1.03397300
H	-1.50065000	2.10047500	0.06453300
C	-2.45603000	-0.71924500	-0.07689400
O	-3.45628100	-0.05933500	-0.06100300
H	-2.45059400	-1.81594800	-0.14795500

Ch-tsF

E = -610.397287
H = -610.394839
G = -610.591415

C	0.20546000	1.21946400	-1.17130000
C	-0.46355400	-1.22200500	0.11135300
C	0.99335000	-0.77154600	-0.02182400
C	1.06553800	0.75016100	-0.11668000
C	-1.49777300	-0.16444500	-0.29870700
C	-2.00234200	0.71158300	0.85295400
H	-1.39200500	-2.87419100	-0.37925800
H	-0.64125000	-1.41611400	1.17307600
H	0.42440800	1.14678700	0.78104300
H	-2.32359500	-0.63788200	-0.82715200
H	-2.81764000	1.33114800	0.43118700
H	-2.50232100	-0.01812100	1.52288900
O	-0.58675800	-2.41560300	-0.64225900
O	-1.02595700	1.45910200	1.44781300
O	-0.95974200	0.77952200	-1.32615300
O	2.36127900	1.25110500	-0.26358000
H	2.85973200	0.97665600	0.51523300
O	1.78178200	-1.12558700	1.09329900
H	2.10723100	-2.02438200	0.97729800
H	1.41002100	-1.21168300	-0.93314500
H	0.50651900	2.00019700	-1.86891100

Ch-tsR

E = -610.398378
H = -610.395930
G = -610.589643

C	-0.13991300	-1.26320100	-1.11865100
C	0.40109000	1.23835100	0.11747600
C	-1.03075900	0.72932600	-0.05836500
C	-1.02948500	-0.79768500	-0.08421800
C	1.48610200	0.23731100	-0.31124200
C	2.03975100	-0.62016200	0.83975000
H	-2.17850000	2.00943200	0.85785000
H	-0.38963000	-2.09954700	-1.77236600
H	-2.78563000	-1.17898800	0.58636900
H	1.24734200	2.95948600	-0.27564400
H	-0.35231000	-1.14272200	0.82230200
H	0.54719600	1.40025800	1.19206900
H	-1.42480800	1.11309800	-1.00813000
H	2.28011600	0.75399900	-0.85180700
H	2.90825800	-1.17424000	0.42478700
H	2.47357100	0.13634600	1.53150000
O	-1.87422700	1.10780000	1.00505300
O	-2.29485200	-1.37243400	-0.22015000
O	0.48316600	2.46343500	-0.58789300
O	1.11138400	-1.44526600	1.39497600
O	0.98874000	-0.74363100	-1.31891500

Ch-ts1

E = -953.577104
H = -953.574655
G = -953.850561

C	0.99085200	1.53934500	0.43770100
C	1.84177700	-1.07513900	0.18052900
C	2.74027500	-0.00024700	-0.41020300
C	2.20951500	1.35971400	-0.05742100
C	0.38585000	-0.68573700	-0.06758200
C	-0.59219400	-1.73487900	0.43084700
H	4.12959800	-0.11777700	0.96960000
H	0.59755000	2.50442800	0.72573300
H	3.94534600	2.08152200	-0.32000800
H	3.00780600	-2.53805600	-0.33994300
H	-0.97859800	-0.73651700	2.01423800
H	2.00359600	-1.12362100	1.26664300
H	2.76905900	-0.12346600	-1.49712500
H	0.23920000	-0.53235700	-1.14753200
H	-1.39721900	-2.07061500	-0.67493600
H	-0.19769800	-2.73703500	0.20676400
O	4.09208400	-0.14313500	0.00415400
O	3.04010800	2.42026400	-0.29095800
O	2.06969600	-2.32857000	-0.42045400
O	-0.86165000	-1.67077200	1.78452900
O	0.09230400	0.51816400	0.62361700
C	-2.86777800	2.15507300	0.53604800
C	-3.07691900	0.78965900	0.88549800
C	-2.58948100	0.05733600	-0.15353400
C	-2.27498300	2.13753300	-0.68502500
H	-3.12933500	3.03073600	1.10594900
O	-2.10783300	0.87392200	-1.12267200
H	-1.94269500	2.91759900	-1.34941300
H	-3.53013400	0.39391600	1.78045900
C	-2.44383500	-1.38018300	-0.32606300
O	-2.38907000	-1.91827800	-1.55842200
H	-2.94006200	-1.93638200	0.47644100

Ch-ts2G

E = -953.604171
H = -953.601723
G = -953.880628

C	2.45182700	1.57780700	0.42299200
C	1.75141900	-1.05221400	-0.00482700
C	3.08274500	-0.59988400	-0.58068600
C	3.37672300	0.80138500	-0.12881400
C	0.73843500	0.07371900	-0.17635400
C	-0.65389200	-0.31142700	0.24059300
H	4.19559800	-1.54950300	0.72691300
H	2.65384400	2.57818200	0.77945100
H	5.22735300	0.48517000	-0.41331700
H	1.95246400	-2.86692700	-0.66251500
H	-1.02847100	-1.39672800	2.06920500
H	1.87294100	-1.24022500	1.07113400
H	3.03116700	-0.64345700	-1.67284600
H	0.68645500	0.35498900	-1.23797800
H	-0.93379400	-1.29256100	-0.13862000
O	4.14125300	-1.48317300	-0.23580400
O	4.65025200	1.25676000	-0.33249600
O	1.25985900	-2.19535700	-0.66524200
O	-0.57449200	-0.56789400	1.83277700
O	1.14056900	1.20343500	0.58711300
C	-5.16741000	0.02189800	-0.65703800
C	-4.08524700	0.96718200	-0.67257200
C	-3.02201900	0.33798700	-0.09259300
C	-4.69246400	-1.10245800	-0.08216200
H	-6.16716800	0.16454200	-1.03436000
O	-3.37903700	-0.92816200	0.26860500
H	-5.11694000	-2.06664000	0.13638000
H	-4.08867400	1.97134400	-1.05938500
C	-1.67468000	0.75263600	0.24354800
O	-1.34891100	1.96248900	-0.40982600
H	-0.75695800	2.45710700	0.16393700
H	-1.27638800	0.26010500	1.83847100

Ch-ts2F

E = -953.606367
H = -953.603918
G = -953.883988

C	-1.98860900	-1.85107500	-0.04214300
C	-2.00766500	0.88713000	0.29368600
C	-3.28323100	0.26415100	-0.23896800
C	-3.14757300	-1.23212800	-0.23593200
C	-0.79579500	0.18253500	-0.32128300
C	0.49208800	0.80712500	0.10607100
H	-4.28174000	0.49605800	1.43021500
H	-1.90130800	-2.92893300	-0.00094100
H	-5.03553600	-1.38401800	-0.16424700
H	-1.11067100	2.57746800	0.10014800
H	0.57165000	-0.14971100	1.80377300
H	-1.96796700	0.73680500	1.38187100
H	-3.46077600	0.62942600	-1.25492400
H	-0.88866100	0.20727700	-1.41501000
H	1.07484000	2.10832500	-0.55220400
O	-4.44346700	0.64839100	0.49033000
O	-4.29987900	-1.94350900	-0.44964000
O	-2.01601000	2.25986700	-0.02234200
O	0.67064400	0.76734400	1.50925300
O	-0.79224500	-1.20065400	0.09637400
C	4.66986100	-0.86087900	0.97996200
C	3.43412800	-0.16012400	1.11161700
C	2.88288900	-0.11810800	-0.13357600
C	4.77626800	-1.19017500	-0.33019500
H	5.37923200	-1.09029500	1.75698300
O	3.70811000	-0.74535300	-1.02194200
H	5.51995700	-1.72512800	-0.89617400
H	3.01066900	0.26922300	2.00212800
C	1.66438300	0.44599800	-0.69979200
O	2.00898900	2.05800600	-1.19393300
H	2.77505400	2.40655200	-0.70761700
H	1.44565200	0.04751700	-1.68549400

Ch-ts3G

E = -877.210869
H = -877.208421
G = -877.468024

C	-3.01570200	-1.36360400	0.27368400
C	-1.08561400	0.60879300	0.07399600
C	-2.49720200	0.97541600	-0.35892000
C	-3.44154200	-0.14880600	-0.04908500
C	-0.81364600	-0.83999300	-0.35658300
C	0.59381800	-1.23833700	-0.05460800
H	-2.90059900	2.09815300	1.19965300
H	-3.67905800	-2.17882700	0.52530600
H	-4.88544400	1.08608100	-0.04032900
H	-0.36872900	2.35991300	-0.33092100
H	1.91817300	-2.02420400	0.23146100
H	-1.02537400	0.64706600	1.17077600
H	-2.49136900	1.18053300	-1.43368000
H	-0.95278100	-0.91251400	-1.44481900
O	-2.92773600	2.18971000	0.23765100
O	-4.77641200	0.13046900	-0.14013900
O	-0.12735800	1.44458100	-0.52080300
O	0.87408700	-1.94771600	0.96332000
O	-1.68955800	-1.72228600	0.31050700
C	4.17192900	1.26987200	0.79696300
C	2.80568000	0.85567500	0.65725800
C	2.79683700	-0.13356000	-0.27421800
C	4.88416100	0.51816600	-0.07022100
H	4.56235200	2.03825300	1.44357000
O	4.06624800	-0.35124800	-0.72320300
H	5.92496300	0.48615200	-0.34296500
H	1.93836800	1.25551100	1.15495400
C	1.75992900	-1.00744800	-0.84299600
H	1.65343400	-0.96125700	-1.92329000

Ch-ts3F

E = -877.223133
H = -877.220685
G = -877.477781

C	1.65207900	-1.76460900	0.20195000
C	1.91677300	0.87691700	-0.54869300
C	3.09551500	0.24412000	0.17506700
C	2.84814100	-1.21770500	0.38624700

C	0.61362200	0.37255200	0.06599400
C	-0.59698500	1.01544800	-0.54863500
H	4.24679700	0.09556400	-1.40674800
H	1.46815800	-2.82357100	0.32873600
H	4.71991400	-1.51285100	0.52932700
H	2.86211300	2.55852100	-0.69086200
H	1.93501900	0.55928700	-1.60175300
H	3.23071100	0.74860500	1.13695900
H	0.64529300	0.54096900	1.15034700
H	-0.68847700	0.80514400	-1.61170100
O	4.32191700	0.46299900	-0.51590100
O	3.91478500	-1.96688300	0.81218500
O	1.96943500	2.28173600	-0.44948800
O	0.53515000	-1.05499700	-0.14521700
C	-4.98314000	-0.75909800	0.13852600
C	-4.19272700	0.26266900	0.71482200
C	-2.97618600	0.20555900	0.09046700
C	-4.19295400	-1.35395600	-0.80059600
H	-6.00059600	-1.02072500	0.37457600
O	-2.98131800	-0.78817800	-0.84353700
H	-4.36427900	-2.16449700	-1.48939700
H	-4.46953900	0.96489300	1.48408800
C	-1.78140700	0.96492700	0.25432800
O	-1.67049200	1.82084500	1.21159300
H	-0.71731400	2.12353300	0.46248200

Metal-glucose complexes

Na(I)/site1

E = -849.114936
H = -849.112488
G = -849.348023

C	-0.83978400	-0.82113800	-0.54927000
C	1.50932800	-0.55453400	-0.60267700
C	-1.03827200	0.49734800	0.17147600
C	0.07614700	1.44580300	-0.21078300
C	1.41889800	0.80700200	0.09146200
C	2.76188700	-1.32375400	-0.23694400
O	-1.84252800	-1.69067600	-0.12639000
O	0.40883800	-1.36830600	-0.19766000
O	-2.31070600	1.00403700	-0.19049500
O	-0.12751100	2.63730000	0.51953800
O	2.41312300	1.69441200	-0.38711600
O	2.85200300	-1.55270600	1.15656300
H	-1.81714200	-2.49255000	-0.66288900
H	1.48770400	-0.40310900	-1.69034700
H	-0.99649100	0.30396900	1.25069000
H	-2.35823300	1.92326400	0.10305700
H	-0.88434500	-0.67411200	-1.63700800
H	0.01835200	1.65040300	-1.28904700
H	0.57285600	3.25573400	0.27966100
H	1.50977800	0.66599900	1.17293300
H	3.20241200	1.61672000	0.15781400
H	2.77058300	-2.26665400	-0.79122200
H	3.64118600	-0.74823900	-0.52634200
H	2.06397200	-2.03964500	1.42521600
Na	-3.97141900	-0.62623900	0.36658000

Na(I)/site2

E = -849.115831
H = -849.113383
G = -849.347442

C	1.82547800	-0.76361700	-0.38182700
C	0.56461300	1.22489600	-0.61283600
C	0.67245800	-1.48721000	0.29496700
C	-0.64189700	-0.89863500	-0.17246800
C	-0.65418200	0.59470900	0.06717300
C	0.69475700	2.71050500	-0.34233100
O	3.00002200	-1.26358500	0.15498700
O	1.74639400	0.62146200	-0.10163900
O	0.64694200	-2.85805700	-0.03506400
O	-1.73756600	-1.47536400	0.52115400
O	-1.87173300	1.09425900	-0.47021700
O	0.75873800	2.99076900	1.04260700
H	3.74230800	-1.02151000	-0.41001100
H	0.49149800	1.06622300	-1.69771100
H	0.77392200	-1.34295600	1.37780400
H	1.43606100	-3.27478500	0.32991100
H	1.78439700	-0.91586300	-1.46916700
H	-0.75001400	-1.08624500	-1.24961500
H	-1.63816700	-2.43553800	0.48323000
H	-0.60537300	0.78770400	1.14321700
H	-2.02360500	1.98665700	-0.13889300
H	1.58340000	3.08028000	-0.86165800
H	-0.17139700	3.24102300	-0.73915700
H	1.52456700	2.52603900	1.40001000
Na	-3.75066700	-0.34279900	-0.01624100

Na(I)/site3

E = -849.112893
H = -849.110445
G = -849.347250

C	-1.84184600	-1.00977600	-0.33318500
C	0.51598500	-0.87232300	-0.15441700
C	-2.04421400	0.40313900	0.18784900
C	-0.82152500	1.22934300	-0.14719000
C	0.43306100	0.55687700	0.37730500
C	1.65692200	-1.69067000	0.42350000
O	-2.92614300	-1.76689600	0.07816100
O	-0.66470800	-1.56090500	0.22928300
O	-3.15305000	1.02742700	-0.42020600
O	-0.86679700	2.51816700	0.43315900
O	1.57236600	1.29969700	-0.02833700
O	2.88340200	-1.28144800	-0.17163300
H	-2.95834600	-2.58719700	-0.42667300
H	0.61391300	-0.84994500	-1.24872000
H	-2.16701000	0.34893500	1.27657800
H	-3.94922100	0.54571400	-0.16761600
H	-1.75002600	-1.00225400	-1.42818700
H	-0.74332300	1.31326500	-1.24002800
H	-1.62978400	2.98601200	0.07440400
H	0.38268200	0.51788900	1.47265300
H	1.36366100	2.23204500	0.12204200
H	1.69259800	-1.56686600	1.50992500

H	1.45766700	-2.73867700	0.19458000
H	3.53442400	-1.97644100	-0.03008800
Na	3.81835400	0.83542300	-0.29049700

Na(I)/site4

E = -849.115871
H = -849.113423
G = -849.346789

C	0.72902100	-1.28371900	0.69939300
C	-0.85546800	0.48050600	0.86945600
C	1.61028100	-0.47888200	-0.24335200
C	1.41635700	1.00289900	0.01093200
C	-0.05385600	1.36053300	-0.08233400
C	-2.34938800	0.71175600	0.78039700
O	0.83468800	-2.61681600	0.33898000
O	-0.62751900	-0.88888200	0.54380400
O	2.97472200	-0.76811800	-0.03777600
O	2.10161700	1.79458000	-0.93840100
O	-0.28050800	2.70606200	0.27560800
O	-2.85159100	0.35069800	-0.50309500
H	0.55661400	-3.17596800	1.07321600
H	-0.53339400	0.68052400	1.89980600
H	1.30786400	-0.71492100	-1.27177400
H	3.13227200	-1.68771800	-0.28089900
H	1.03072900	-1.12050400	1.74175500
H	1.77166000	1.23712500	1.02379900
H	3.04423100	1.60409300	-0.86682800
H	-0.38971700	1.17173000	-1.11108600
H	0.34886200	3.24852200	-0.21556200
H	-2.84994900	0.07093800	1.50621800
H	-2.57301600	1.75279400	1.01376700
H	-2.83592300	1.11780700	-1.08416100
Na	-2.01847100	-1.77847100	-1.18801500

K(I)/site2

E = -1286.775542
H = -1286.773093
G = -1287.010152

C	2.10496400	-0.86159800	-0.37950800
C	0.96457700	1.19499500	-0.61013300
C	0.90722600	-1.51521500	0.28882600
C	-0.37257300	-0.85067600	-0.17698900
C	-0.29644500	0.64141200	0.06140800
C	1.18278900	2.67076100	-0.34085500
O	3.24485300	-1.43336400	0.16131700
O	2.10662300	0.52376300	-0.09289400
O	0.80245800	-2.88239500	-0.04338600
O	-1.49246700	-1.37275900	0.51921600
O	-1.47285200	1.22006900	-0.48561300
O	1.25731000	2.94889700	1.04410600
H	4.00356000	-1.23332100	-0.39830600
H	0.88911000	1.03948200	-1.69532100
H	1.01389100	-1.38035600	1.37250200
H	1.56683100	-3.34368100	0.32063100
H	2.06112200	-1.00601400	-1.46786200
H	-0.49231400	-1.03071600	-1.25439400
H	-1.42388600	-2.33634000	0.49726700
H	-0.24218700	0.83123800	1.13799800
H	-1.55243000	2.12752000	-0.17055000
H	2.09451000	2.98559400	-0.85641000
H	0.35278100	3.25345200	-0.74215300
H	1.98809200	2.43445500	1.40681100
K	-3.82998400	-0.10805600	-0.00151000

K(I)/site4

E =-1286.776466
H = -1286.774018
G =-1287.009882

C	0.39530600	-1.30383900	0.88286300
C	-0.24373000	0.99461500	0.94528600
C	1.42528300	-1.04181400	-0.20431900
C	1.92172400	0.38615400	-0.10946100
C	0.74859600	1.34504500	-0.15756300
C	-1.50033200	1.84048600	0.91097500
O	-0.15038900	-2.55938500	0.65093500
O	-0.65820900	-0.35906200	0.79428200
O	2.54311100	-1.88968100	-0.06348300
O	2.77865100	0.71659100	-1.18397000
O	1.16379400	2.67857100	0.04139300
O	-2.23687700	1.63169500	-0.28922500
H	-0.53352500	-2.90313000	1.46580100
H	0.24247200	1.13327400	1.92012300
H	0.93818100	-1.19147000	-1.17647900
H	2.25876700	-2.79870300	-0.21308100
H	0.86042000	-1.24033100	1.87467800
H	2.44703200	0.51776300	0.84645100
H	3.54604200	0.13349600	-1.14922300
H	0.25348700	1.23362000	-1.13185200
H	1.90055000	2.84782900	-0.55861300
H	-2.14586900	1.53901200	1.73622900
H	-1.23605500	2.89078600	1.03689400
H	-1.97548100	2.28613200	-0.94431100
K	-2.66093400	-1.02747300	-0.89014500

Ca(II)/site2

E = -1364.360892
H = -1364.358443
G = -1364.596901

C	2.12120300	-0.82653800	-0.36191800
C	0.93191400	1.20715000	-0.62058800
C	0.93215900	-1.51628300	0.29765700
C	-0.34026000	-0.86462000	-0.19274900
C	-0.29139700	0.61684900	0.08144900
C	1.10025400	2.69302200	-0.37292200
O	3.26634700	-1.36020600	0.19877500
O	2.08173200	0.56420600	-0.08917200
O	0.85117200	-2.87873400	-0.04659100
O	-1.49446300	-1.38804600	0.46437900
O	-1.52420900	1.15507400	-0.40038900

O	1.08938800	3.00657900	1.00499600
H	4.02652600	-1.15464000	-0.35722200
H	0.85608500	1.03242500	-1.70247400
H	1.02333700	-1.38334700	1.38240400
H	1.61209700	-3.33681600	0.32928300
H	2.09285000	-0.98175500	-1.44907900
H	-0.43931600	-1.03549400	-1.27179900
H	-1.44332200	-2.35464200	0.45417600
H	-0.20808600	0.79339500	1.15684400
H	-1.58819500	2.08835400	-0.15906200
H	2.02777000	3.01913900	-0.85079800
H	0.27824700	3.24246600	-0.83431100
H	1.85632100	2.58846800	1.41346700
Ca	-3.54886500	-0.15830100	-0.00764900

Ca(II)/site4

E = -1364.361914
H = -1364.359466
G = -1364.590077

C	0.41658600	-1.31316500	0.83601100
C	-0.29624400	0.97862500	0.90594800
C	1.46901600	-1.00192600	-0.21449400
C	1.92477400	0.43845900	-0.07771800
C	0.73895600	1.38401600	-0.13736900
C	-1.57050800	1.78332300	0.83139500
O	-0.09036200	-2.57413800	0.58579900
O	-0.67127800	-0.38904900	0.68963700
O	2.60170500	-1.82001100	-0.05078300
O	2.80052400	0.81019500	-1.12009900
O	1.12602000	2.70733600	0.15148400
O	-2.23699300	1.39018100	-0.37636500
H	-0.43250000	-2.96395000	1.39896100
H	0.13407900	1.08478900	1.90727200
H	1.00947100	-1.14895800	-1.20059000
H	2.36410600	-2.72883600	-0.26827900
H	0.82111800	-1.21990100	1.84871100
H	2.42012200	0.55933800	0.89509400
H	3.59796200	0.27166500	-1.05510400
H	0.28661000	1.32125400	-1.13534600
H	1.87445500	2.92555900	-0.41778000
H	-2.20560000	1.56498300	1.69078900
H	-1.32852700	2.84481900	0.80583000
H	-2.90483900	2.04421800	-0.61093500
Ca	-2.49844300	-0.95835400	-0.78793300

Mg(II)/site2

E = -886.757628
H = -886.755179
G = -886.983107

C	1.81388200	-0.79239400	-0.38287000
C	0.58560200	1.23526700	-0.63562000
C	0.65639200	-1.50297500	0.31266800
C	-0.62099700	-0.87626800	-0.18041000
C	-0.62131500	0.60954100	0.06129700
C	0.74304300	2.71372000	-0.33326300
O	2.98163700	-1.29376000	0.15494000
O	1.74422600	0.59928000	-0.11527000
O	0.58611200	-2.86738000	-0.01736400
O	-1.78080500	-1.38895100	0.49669100
O	-1.88989500	1.05476100	-0.45781600
O	0.80869900	2.95671700	1.05596000
H	3.72302900	-1.08968900	-0.42640500
H	0.50854700	1.08682700	-1.72052300
H	0.76285100	-1.35211700	1.39311500
H	1.35852200	-3.31523600	0.34734400
H	1.76245000	-0.95538600	-1.46771700
H	-0.72818300	-1.07818900	-1.25260700
H	-1.75902900	-2.35793500	0.49392100
H	-0.57333000	0.82143800	1.13163400
H	-2.03642400	1.99139800	-0.26550100
H	1.63841700	3.07440600	-0.84600500
H	-0.11109900	3.27142600	-0.71957900
H	1.59630100	2.51702300	1.39761300
Mg	-3.42345700	-0.28505400	-0.00443600

Mg(II)/site4

E = -886.759632
H = -886.757183
G = -886.985569

C	-0.65418000	-1.33391900	-0.65376500
C	0.83078700	0.56534100	-0.81357800
C	-1.60651100	-0.55489400	0.24164300
C	-1.49429700	0.93275800	-0.04093400
C	-0.05511100	1.39353400	0.10866700
C	2.30333000	0.88615500	-0.71742700
O	-0.66063200	-2.65217800	-0.27404600
O	0.69239900	-0.82349800	-0.45114900
O	-2.93653800	-0.93054600	-0.01499400
O	-2.26216400	1.69370000	0.86325900
O	0.09851400	2.73889100	-0.26789800
O	2.75675700	0.32067200	0.52887900
H	-0.41995900	-3.22032600	-1.01566900
H	0.50879300	0.69667500	-1.85030700
H	-1.33166800	-0.74578100	1.28771300
H	-3.07954200	-1.82749200	0.30849600
H	-0.89336100	-1.19789000	-1.71175700
H	-1.81998400	1.12327000	-1.07269400
H	-3.19235400	1.47229500	0.73712700
H	0.25231700	1.23626900	1.15255200
H	-0.59118400	3.25088700	0.17329200
H	2.85306200	0.42936000	-1.53910300
H	2.44805700	1.96427900	-0.71129400
H	3.63461300	0.64546700	0.76325600
Mg	2.01503400	-1.49476600	0.97152800

Na(I)/intermediates

Local minima

Na(I)/(2)

E = -849.098286

H = -849.095837
G = -849.341220

C	2.06528200	-0.25913700	-0.72812900
C	0.92859000	-0.35116400	0.29032800
C	-0.28103200	0.49368400	-0.11908000
C	-1.43875100	0.32148100	0.86122100
H	0.60489600	-1.39661100	0.31611900
H	-0.60632900	0.13801100	-1.10636600
H	-1.11266700	0.67454400	1.84395200
O	-1.75730700	-1.07001700	0.90599200
H	-2.14562800	-1.27909300	1.76237500
O	1.46851700	0.04193000	1.54040000
H	0.94304100	-0.33926700	2.25102600
O	-0.00412100	1.87773000	-0.15129200
H	0.90366300	1.99100000	-0.46750800
C	-2.65946000	1.12184700	0.45238300
H	-2.39234700	2.17522100	0.36111700
O	-3.11426800	0.60081700	-0.79525000
H	-3.82047200	1.16023300	-1.13264400
H	-3.43611300	1.00986900	1.21420800
C	3.22506000	-1.08795300	-0.22679000
H	3.01831900	-2.14801900	-0.01186700
O	4.31443000	-0.60556000	-0.06142100
O	2.48295000	1.06531700	-0.96098000
H	3.38201200	1.15310100	-0.60817500
H	1.71864200	-0.70142300	-1.67011900
Na	-3.20152400	-1.74107700	-0.88648300

Na(I)/(3)

E = -849.106424
H = -849.103976
G = -849.342894

C	-2.11422200	0.95685000	0.45594100
C	0.04640600	0.03775100	0.46715400
C	-0.98532600	-1.10530900	0.43951400
C	-2.20215500	-0.43344900	-0.16010800
C	0.98574200	0.03706900	-0.74305600
H	-2.51442800	0.95055500	1.47408800
O	-2.79977900	1.95358900	-0.21719900
H	-2.48708200	1.98397100	-1.13080600
C	1.81099300	1.30057700	-0.81960200
H	1.15035900	2.16641500	-0.86257400
H	2.42848800	1.26829000	-1.72086200
O	2.63695000	1.34917300	0.34416100
H	3.06214600	2.21098700	0.39145100
O	-3.36822400	-1.14578100	0.16349100
H	-4.11195000	-0.77285500	-0.32240100
H	-2.07062300	-0.35166600	-1.24747000
O	-0.50481900	-2.20579800	-0.30634700
H	-1.12037500	-2.94157800	-0.21826300
H	-1.22687800	-1.41492000	1.46087900
O	1.89880900	-1.04958800	-0.64586400
H	1.37438000	-1.86332400	-0.62734600
H	0.39797400	-0.03842500	-1.66473900
O	-0.72129600	1.24319700	0.46565400
H	0.65474100	0.00281100	1.37277100
Na	3.82559000	-0.64723000	0.62046000

Na(I)/(4)

E = -772.691102
H = -772.688654
G = -772.895108

C	-0.67505000	-0.82635400	0.93070800
C	-1.94690700	-0.41721000	0.19728200
C	-1.36807700	0.52233300	-0.87240600
C	0.14568700	0.17607300	-0.87606000
C	1.05045300	1.16407900	-0.15898800
C	0.89753000	0.94652900	1.36445400
O	-2.56215600	-1.50730400	-0.45345100
O	-1.64092600	1.86544500	-0.53472700
O	2.37214300	0.80970300	-0.57300500
O	0.24670500	-1.04085300	-0.11434600
O	-0.31121500	0.29130600	1.72127900
H	-2.63462600	0.12015600	0.85079000
H	-0.73228100	-1.72923300	1.53823000
H	-1.81041800	0.26402000	-1.83500500
H	0.52999600	-0.01847700	-1.87565700
H	0.83363400	2.19117200	-0.44951000
H	1.75829200	0.37050600	1.71727900
H	0.87957600	1.89473300	1.89818700
H	-2.99482400	-2.06137000	0.20504700
H	-1.55338600	2.41138900	-1.32301300
H	3.00575600	1.43290100	-0.20017500
Na	2.66000500	-1.60135200	-0.40019200

Na(I)/(5)

E = -772.690823
H = -772.688374
G = -772.907900

C	-0.21675600	-2.24204900	-0.18270200
C	-1.36351800	-0.33793800	0.57390300
C	0.95593800	-1.65834500	0.04297200
C	1.08596200	-0.19316800	0.34191100
C	-0.21774500	0.47921700	-0.01156800
C	-2.70498200	0.34624900	0.42158800
O	-1.41922200	-1.58206200	-0.12354700
O	2.17276900	-2.28375800	0.02867200
O	2.10851000	0.41505400	-0.43785200
O	-0.17576800	1.80800000	0.47951200
O	-2.86404900	0.94907200	-0.85126700
H	-1.17748800	-0.54056900	1.63667300
H	2.08510500	-3.19770500	-0.26619800
H	-0.32266700	-3.29188300	-0.42438200
H	1.30447000	-0.03925800	1.40615100
H	2.90815100	-0.12118200	-0.36679000
H	-0.31610400	0.48151200	-1.10145800
H	-0.91654600	2.29293000	0.09301100
H	-3.49734600	-0.37884100	0.62452900
H	-2.78193500	1.14811000	1.15573900
H	-2.89320400	0.25490200	-1.51931200
Na	1.98147700	2.77979400	-0.10170300

Na(I)/(6)

E = -696.281117

H = -696.278669

G = -696.478598

C	-0.72944300	1.30660500	0.67562800
C	0.70611900	-0.52965100	0.96203700
C	-1.70687200	0.50311800	0.25421100
C	-1.36413800	-0.83083200	-0.25032900
C	-0.15867200	-1.32764000	0.02570300
C	2.17297400	-0.86561700	0.86657400
O	0.57774700	0.87806200	0.68588100
O	-3.03053700	0.81760700	0.15914900
O	-2.27940200	-1.46419400	-1.02040700
O	2.60699700	-0.60264600	-0.46387400
H	0.39242900	-0.67938200	2.00562200
H	-3.16935000	1.76461800	0.27826600
H	-0.86220800	2.34276100	0.95669300
H	-3.06990800	-0.91074400	-1.08512900
H	0.17733700	-2.28008600	-0.36129200
H	2.73394200	-0.25680300	1.57950000
H	2.30354900	-1.92123500	1.11593800
H	3.51849300	-0.89647500	-0.56183200
Na	1.95067900	1.47916600	-1.27424600

Na(I)/(7)

E = -696.307174

H = -696.304725

G = -696.502985

C	-0.52001900	1.31911800	-0.09878900
C	0.53151400	-0.76288700	0.25907800
C	-1.73444000	0.77706200	0.06264900
C	-1.92479700	-0.67004400	-0.05024200
C	-0.67699500	-1.46697900	-0.32774600
C	1.82784000	-1.44000300	-0.10384300
O	0.61770700	0.59232100	-0.22171800
O	-2.84384700	1.54268500	0.23009200
O	-3.04161400	-1.14605500	0.01244400
O	2.88589500	-0.67433100	0.46016000
H	0.43723400	-0.69814200	1.34923500
H	-3.59863500	0.93378800	0.24020300
H	-0.35739200	2.38828200	-0.14962300
H	-0.78366100	-2.46823100	0.08887000
H	-0.57654100	-1.55726000	-1.41533300
H	1.81836500	-2.45301800	0.30346300
H	1.92693200	-1.49169900	-1.19217500
H	3.70959200	-1.16560600	0.37550500
Na	2.86003300	1.58702900	-0.17223700

Na(I)/(8)

E = -772.70964

H = -772.707192

G = -772.908843

C	-0.02379100	0.92286200	-1.07309400
C	-0.42506500	-0.53368000	-1.28628500
C	-0.39230100	1.35419200	0.35740100
C	-0.09132900	0.24123200	1.38698800
C	-0.43499600	-1.14209300	0.85015800
C	-1.86500100	-1.27364300	0.35371900
O	0.29068500	-1.33733900	-0.37384800
O	-1.79679900	-0.69539200	-0.96275200
O	1.37551800	0.96650100	-1.29937800
O	-1.74292400	1.76843200	0.43188500
O	1.30144400	0.18704200	1.67564800
H	-0.55596800	1.55857200	-1.78534000
H	-0.22227300	-0.88119400	-2.29801700
H	0.21490300	2.22383500	0.62169400
H	-0.67017000	0.44151500	2.29238100
H	-0.13751900	-1.91743900	1.55233600
H	-2.15892200	-2.31927900	0.27326200
H	-2.58898200	-0.72533000	0.95445900
H	1.65474500	1.87906300	-1.42960600
H	-2.26927700	1.21431600	-0.15821500
H	1.56083800	0.98025300	2.15752800
Na	2.64946500	-0.63468200	-0.13511300

Na(I)/(9)

E = -696.292975

H = -696.290526

G = -696.479502

C	0.92791900	-1.07436500	0.25481400
C	1.03601800	-0.08233800	-0.89226600
C	0.07510300	-0.84192900	1.24854200
O	-0.21117700	0.54403900	-1.08700100
O	1.90710500	0.96134100	-0.53851000
C	-0.78336500	0.39554400	1.21817900
C	-0.31635300	1.32831300	0.11246000
C	1.13034900	1.82440400	0.30590300
H	1.36718400	-0.53875500	-1.82523900
H	0.00062700	-1.52173100	2.08863900
H	-0.73312600	0.92277800	2.17489500
H	-1.03529400	2.12507800	-0.05972100
H	1.26439500	2.84480100	-0.04463000
H	1.45593400	1.73761400	1.34312600
O	1.77877100	-2.12526900	0.26153100
H	2.27418800	-2.17818300	-0.56409300
O	-2.15329800	0.09066500	0.91719200
H	-2.51526800	-0.45791600	1.62221800
Na	-2.27889800	-0.72706100	-1.33151600

Na(I)/(10)

E = -696.310159

H = -696.307711

G = -696.495909

C	-0.54652100	1.39513400	0.15568600
C	-0.92882400	0.43870400	-0.97827100
C	-0.32740000	0.69478900	1.47777400
O	0.11036700	-0.51460200	-1.08485000
O	-2.07926700	-0.28034800	-0.61324200
C	0.39186200	-0.64941700	1.28515600
C	-0.13165700	-1.36648300	0.04814000
C	-1.65144300	-1.49759900	0.01708800
H	-1.06998800	0.95495900	-1.92553500
H	0.22131200	1.34551400	2.15785900
H	0.25077600	-1.28418100	2.16261100
H	0.39601000	-2.30296400	-0.11579100
H	-1.96770500	-2.34002600	-0.59518400
H	-2.09184400	-1.57494800	1.01127700
O	-0.43196000	2.57983200	-0.02006400
H	-1.31669000	0.51572300	1.91081100
O	1.78042500	-0.45299500	1.03834900
H	2.21069900	-0.13484500	1.83954200
Na	2.49952800	0.00681000	-1.18550800

Na(I)/(11)

E = -619.892225
H = -619.889777
G = -620.065281

C	-0.19019200	1.37490100	0.15177300
C	0.02342500	0.13307800	1.02369700
C	-1.19078300	1.18748300	-0.91389500
C	-1.79055500	-0.00019500	-1.01571000
C	-1.47925900	-1.08371400	-0.02032100
C	-0.11968400	-1.73081700	-0.32965300
O	-1.19257100	-0.50182200	1.25564100
O	0.79843800	-0.78663600	0.24539400
O	0.47148100	2.37543400	0.30690600
H	0.52996900	0.36598800	1.95790900
H	-2.28666700	-1.80008900	0.09458100
H	-0.02092700	-2.68665000	0.18315200
H	0.08496000	-1.83542400	-1.39263600
Na	3.03733700	-0.34597100	-0.47849400
H	-2.47847500	-0.22534000	-1.82211200
H	-1.37606200	2.00697700	-1.59632900

Na(I)/(12)

E = -849.101805
H = -849.099357
G = -849.345705

C	2.18744000	0.44886000	-0.58686800
C	3.52323800	-0.21449100	-0.32498200
C	0.94114900	-0.18540500	0.02257300
C	-0.24350700	0.77765600	0.01149600
C	-1.38203500	0.24008800	0.88225900
H	0.69222300	-1.03766900	-0.62538800
H	-0.58680600	0.87678700	-1.02298900
H	-1.11693600	0.43148000	1.92507600
H	3.99923700	0.33625600	0.49425500
O	-1.58575200	-1.15285200	0.67437000
O	2.13111200	1.45088800	-1.25943700
H	-0.85937800	-1.62269000	1.10363000
O	3.32343600	-1.57699600	0.01045400
H	4.16620600	-1.96439600	0.26867800
O	1.16920600	-0.62496100	1.34946500
H	1.88573900	-1.27544000	1.31756700
O	0.07651600	2.04323600	0.55538700
H	0.66427900	2.48591500	-0.06840500
C	-2.69156100	0.93499400	0.59325700
H	-2.54575500	2.01431000	0.66184800
O	-3.10237400	0.55888100	-0.72086800
H	-3.87375200	1.07724300	-0.97067200
H	-3.43854200	0.62017500	1.32597100
H	4.13475200	-0.10056100	-1.22203800
Na	-3.02061500	-1.76701700	-1.05899200

Na(I)/(13)

E = -849.113657
H = -849.111208
G = -849.342423

C	-0.42183700	0.19779200	-0.37986500
C	1.87922200	0.06038200	-0.76025100
C	1.73105400	0.85878400	0.53170300
C	0.28483500	0.58992400	0.95756200
H	2.43140600	0.54205700	1.30951200
H	-0.17089300	1.49345800	1.36929100
C	2.33483900	-1.38271800	-0.60680500
H	2.41448200	-1.82591400	-1.59891400
H	3.32433300	-1.40065200	-0.14052000
O	1.41872500	-2.19600700	0.11454900
H	1.34852800	-1.86453600	1.02252500
C	-1.42142600	1.23807100	-0.83815200
H	-1.71871300	1.00876900	-1.86476500
H	-0.94078900	2.21816700	-0.80769300
O	-2.53255800	1.17606700	0.04637500
H	-3.08704900	1.95141400	-0.08664900
O	1.91581100	2.21872200	0.18803300
H	1.81585200	2.75703300	0.98096100
O	0.28268300	-0.44027100	1.92350400
H	-0.62376600	-0.74869900	2.04541900
O	0.58292900	0.12615800	-1.36137600
O	-1.10935300	-1.02378400	-0.27458300
H	2.57641700	0.57232800	-1.42571500
H	-0.42899000	-1.71946000	-0.20393300
Na	-3.42971200	-1.02222400	0.08030100

Na(I)/(14)

E = -772.682084
H = -772.679636
G = -772.903613

C	-0.92382900	-0.68378600	-0.07818200
C	0.89674300	0.68168500	-0.28287300
C	-0.26587300	1.56575700	0.14416000
C	-1.47410800	0.71112300	-0.23028800
H	-1.72930800	0.91232600	-1.27830600
C	2.17903200	0.93398700	0.45646700

H	2.50555600	1.95762700	0.25876900
H	2.01645900	0.80459400	1.53048000
O	3.13169800	-0.01054400	-0.02213100
H	3.99065700	0.17902600	0.36931200
C	-1.62242500	-1.80467400	-0.01497600
H	-1.17432700	-2.78152400	0.11660900
O	-2.98928600	-1.73303000	-0.16828900
H	-3.40490800	-2.48637200	0.26340800
O	-2.56603100	1.00187800	0.61253300
H	-3.23683600	0.32211800	0.46572600
O	0.45649800	-0.65680500	0.00150200
H	1.05715000	0.78316800	-1.36232900
O	-0.17699900	2.80422100	-0.51246500
H	-0.82137000	3.40770800	-0.12726900
H	-0.26023100	1.68848000	1.23390400
Na	2.31571500	-2.22340600	-0.06594200

Na(I)/(15)

E = -772.692179
H = -772.689731
G = -772.905258

C	-0.04998200	-1.98961000	0.47967700
C	-1.34089400	0.88919100	0.24214900
C	-1.81556100	-0.37301400	-0.47224000
C	-0.49418000	-1.13405500	-0.68636300
C	0.05419100	1.11539200	-0.33902500
C	1.05781100	1.51966700	0.71413300
H	-0.75347700	-2.76252300	0.82660500
H	-2.96294200	1.93422900	0.49630500
H	-1.27000700	0.68383100	1.32047800
H	-0.56839400	-1.80244400	-1.55047800
H	0.00914300	1.86946900	-1.12741400
H	0.78726400	2.50822900	1.09448300
H	1.04214800	0.80266800	1.54121800
O	-2.13438700	2.02615300	0.01298100
O	2.34166600	1.53348600	0.10174400
O	1.03796100	-1.86444800	0.98612900
O	0.45671200	-0.12583800	-0.95617200
H	2.96607900	1.97671700	0.68538000
O	-2.84048200	-1.08715500	0.16488400
H	-2.69501300	-1.10719900	1.11795400
H	-2.19730400	-0.08461300	-1.45325600
Na	2.75294900	-0.73103500	-0.45979900

Na(I)/(16)

E = -696.290164
H = -696.287716
G = -696.487350

C	1.14134600	-2.12979700	0.30564600
C	-2.01510000	-0.10732000	0.21815800
C	-1.24357600	-1.34388900	0.61755300
C	-0.00634200	-1.22903100	0.14522800
C	-0.88881500	0.79646100	-0.30380600
C	-0.46038600	1.84271300	0.69842900
H	0.93530500	-3.11325200	0.74884800
H	-3.67674900	-0.85684800	-0.49059000
H	-2.52963400	0.35679200	1.06391800
H	-1.14776800	1.24469800	-1.26198500
H	-1.25501500	2.58443500	0.80690200
H	-0.27813600	1.37043900	1.67008300
O	-2.92824700	-0.35812000	-0.83676300
O	0.73349700	2.43195600	0.19813100
O	2.25612500	-1.78688500	-0.01536400
O	0.25003100	-0.06869100	-0.52175600
H	0.97012100	3.18232600	0.75304000
H	-1.64011600	-2.18696000	1.16203200
Na	2.45163400	0.79067900	-0.46668000

Na(I)/(17)

E = -696.288046
H = -696.285598
G = -696.485545

C	-0.74957000	1.98248600	-0.26487200
C	-1.00768200	-1.28245500	-0.73851100
C	-1.98649000	-0.21251900	-0.34014800
C	-1.07030300	0.71406800	0.48559500
C	0.11588100	-1.12093100	-0.05429200
C	1.34646000	-1.95005300	0.01643800
H	-1.61833100	2.60747300	-0.52461200
H	-1.21498600	-2.08339800	-1.43012500
H	1.41959200	-2.39979500	1.01101300
H	1.28546000	-2.74142600	-0.73158200
O	2.46197800	-1.09570400	-0.22130900
O	0.36777500	2.30724800	-0.57274000
O	0.13205400	-0.00546900	0.75405800
H	3.27337200	-1.59714800	-0.09002600
Na	2.28214200	1.19157500	0.29063000
H	-1.55817500	0.97738700	1.42728400
O	-3.02644700	-0.67713100	0.50657300
H	-3.64479500	-1.19677900	-0.01945900
H	-2.41834300	0.31122300	-1.19734100

Na(I)/(18)

E = -619.907063
H = -619.904614
G = -620.078351

C	-2.38274800	0.06759800	0.00300200
C	0.61779700	2.17450600	-0.01197800
C	-0.80300500	2.12884100	-0.01048400
C	-1.14596300	0.80965700	0.00543400
C	1.03764000	0.87784900	0.00474900
C	2.37477500	0.21215600	0.01740000
H	-3.30836200	0.65827600	-0.00121900
H	1.24670500	3.04869800	-0.02399600
H	2.95201200	0.54231000	-0.85004700
H	2.91654600	0.50254400	0.92149300

O	2.15244800	-1.18831600	-0.01719100
O	-2.39924200	-1.15084900	0.00451600
O	-0.01674600	0.04777200	0.01591400
H	3.00556600	-1.63364800	-0.00517900
H	-1.48748000	2.96169400	-0.02201500
Na	-0.12796700	-2.30658000	-0.00851600

Na(I)/(19)

E = -505.420797
H = -505.418349
G = -505.568315

C	2.45835100	-0.36532300	-0.00012700
C	1.80430400	0.89570100	0.00006500
C	0.46700000	0.63043800	0.00001000
C	1.46938200	-1.29780400	0.00002500
H	3.51718700	-0.55937200	-0.00030700
O	0.25560900	-0.71450100	0.00011400
H	1.47904400	-2.37481200	-0.00022000
H	2.25260100	1.87622000	0.00008200
C	-0.68470600	1.49663700	0.00015400
O	-1.83240600	1.08792500	-0.00030400
H	-0.46316100	2.57234900	0.00053500
Na	-2.47793500	-1.15087900	0.00006100

Na(I)/adduct (5)+(19)

E = -1115.908298
H = -1115.905850
G = -1116.215432

C	2.32091400	-2.49337800	-0.04538400
C	1.88118500	0.11663800	0.62333300
C	0.65256900	-0.68134400	0.22932600
C	1.04718700	-2.12626100	0.05498800
C	3.06070700	-0.26385700	-0.25419900
C	4.33010300	0.51645400	0.03616200
H	-1.17920600	-0.65372300	0.88878500
H	2.62430800	-3.52516400	-0.15720900
H	-0.77579400	-2.67664500	-0.24281400
H	0.79929100	1.66859500	1.00835800
H	5.14595300	2.15740700	-0.64323100
H	2.13317500	-0.13879000	1.66008800
H	0.25849500	-0.28419400	-0.71542900
H	2.79469400	-0.14028900	-1.31280100
H	4.45188900	0.65502900	1.11454100
H	5.17045400	-0.06799800	-0.34299800
O	-0.30001500	-0.47984400	1.25773900
O	0.06388700	-3.07550700	0.03301600
O	1.61819200	1.50559500	0.52127800
O	4.26382700	1.77256100	-0.63000900
O	3.38501500	-1.62511400	-0.00580000
C	-5.47135800	1.61202700	0.03153000
C	-5.30945600	0.41929800	-0.71794800
C	-4.07470500	-0.06773100	-0.39478500
C	-4.32416300	1.75586200	0.75031700
H	-6.31918600	2.27525600	0.04189400
O	-3.46782800	0.75093900	0.50547600
H	-3.99165900	2.50151700	1.45339200
H	-6.00500700	-0.03091600	-1.40805400
C	-3.37461100	-1.24116400	-0.83578500
O	-2.25727000	-1.54199100	-0.44633300
H	-3.91194100	-1.86787400	-1.55943400
Na	2.53889400	3.30867500	-0.59394100

Na(I)/(20)

E = -1115.917778
H = -1115.915329
G = -1116.218014

C	1.86303000	-1.70813700	-0.27262300
C	1.37555100	0.97904600	-0.03473000
C	2.74305900	0.50375400	0.41476600
C	2.89430600	-0.94283300	0.06493900
C	0.33108000	-0.04718200	0.39377700
C	-1.08544500	0.38541700	0.05662700
H	3.64863100	2.16719400	-0.02742100
H	1.96070500	-2.75288900	-0.53892000
H	4.25332900	-2.31943500	-0.06479700
H	0.55571900	2.75289900	0.00795100
H	-0.93738100	-0.07805600	-1.82549600
H	1.37791600	1.04966300	-1.12672600
H	2.83259300	0.64262700	1.49947700
H	0.41154100	-0.23198700	1.47091700
H	-1.30549100	1.30109400	0.61036700
O	3.77871700	1.23309300	-0.23396600
O	4.19557500	-1.37837900	0.14036700
O	1.16491300	2.24543400	0.55484500
O	-1.21475100	0.69368000	-1.31444500
O	0.56716300	-1.26897100	-0.30718400
C	-5.55611100	0.62908500	-0.02917100
C	-4.39245200	0.56012000	0.80619100
C	-3.50545600	-0.22607700	0.14957100
C	-5.27860700	-0.11921600	-1.12026100
H	-6.47280800	1.16092700	0.16337300
O	-4.03390300	-0.65169100	-1.02453200
H	-5.83417200	-0.36857000	-2.00790000
H	-4.23708000	1.02853400	1.76431200
C	-2.11747500	-0.66865700	0.47878500
O	-1.95082400	-0.84173400	1.87306700
H	-2.62617400	-1.45163300	2.19013300
H	-1.90981000	-1.59750200	-0.06596300
Na	5.87259000	0.21579600	-0.45470500

Na(I)/(21)

E = -1039.516702
H = -1039.514253
G = -1039.794486

C	1.98827000	1.85533900	0.28348300
C	1.11101600	-0.76001300	0.12924000
C	2.53414400	-0.48411300	-0.33443700
C	2.88955800	0.94568600	-0.06707500

C	0.21381900	0.40870500	-0.26883300
C	-1.21451600	0.18332800	0.11830000
H	3.35189400	-1.32280500	1.24103900
H	2.23495400	2.88661700	0.50269500
H	4.43371300	2.12279000	-0.06724300
H	1.16132200	-2.66872300	-0.22127100
H	-2.26912400	-0.25070800	1.65614800
H	1.10167800	-0.83244900	1.22468500
H	2.60997900	-0.70009200	-1.40407300
H	0.27883500	0.56415400	-1.35124400
O	3.46180100	-1.37641300	0.28184800
O	4.23125900	1.19367600	-0.22981700
O	0.59097300	-1.92803600	-0.45868300
O	-1.33769400	-0.11717500	1.43147400
O	0.65107000	1.59438300	0.39740300
C	-5.84911800	-0.07986700	-0.44606000
C	-4.72232900	0.19418600	-1.28505800
C	-3.61937800	0.10669800	-0.49432600
C	-5.35682700	-0.31399500	0.78994900
H	-6.88832200	-0.09830800	-0.72912500
O	-4.00005900	-0.20471400	0.78184500
H	-5.80650600	-0.55707400	1.73686700
H	-4.72498300	0.42721100	-2.33701800
C	-2.21356100	0.28988200	-0.76702300
H	-1.96132900	0.54218400	-1.78762300
Na	5.73932900	-0.68014300	-0.18594200

Na(I)/(22)

E = -1039.513204
H = -1039.510755
G = -1039.789757

C	1.80402500	-1.73327000	-0.25704600
C	1.20997500	0.97242900	-0.13205900
C	2.63112200	0.55789700	0.21902500
C	2.81753200	-0.91016500	-0.01978800
C	0.23846400	-0.07919800	0.39090800
C	-1.19022200	0.30756300	0.17750300
H	3.43709100	1.21947500	-1.44463600
H	1.92044500	-2.79230600	-0.44689200
H	4.23610200	-2.23143300	-0.12086900
H	1.51620600	2.86936300	0.14530100
H	1.10629600	1.01190800	-1.22591200
H	2.81615100	0.79081800	1.27182200
H	0.44883200	-0.24486900	1.45828200
H	-1.40657500	1.35843500	0.05333400
O	3.59193500	1.32906000	-0.49668600
O	4.13542400	-1.28629300	0.04474900
O	0.88100700	2.21062500	0.45024400
O	0.49624300	-1.31981000	-0.28922300
C	-5.80529800	0.06199800	-0.21679000
C	-4.74141800	-0.88518100	-0.08036200
C	-3.59967600	-0.15603200	0.01585300
C	-5.22394000	1.28366900	-0.19266900
H	-6.85798400	-0.14122000	-0.31910800
O	-3.88064200	1.16935800	-0.04980000
H	-5.60818000	2.28688100	-0.26147600
H	-4.80780900	-1.95965500	-0.05797200
C	-2.20932500	-0.55801200	0.17474700
O	-2.09928100	-1.90366800	0.32196800
H	-1.16845800	-2.15043300	0.21445400
Na	5.79845000	0.47442400	0.03706500

Na(I)/(23)

E = -1039.518855
H = -1039.516406
G = -1039.799467

C	2.28291500	1.88950500	-0.19232300
C	0.98170500	-0.48600500	0.33472200
C	2.41683500	-0.58869000	-0.15877900
C	3.01106800	0.78232200	-0.27334600
C	0.28806700	0.67751700	-0.37248300
C	-1.16436500	0.75894500	0.09794100
H	3.14881200	-1.08338200	1.59476000
H	2.70109700	2.88630600	-0.24774900
H	4.73017100	1.64098400	-0.54211300
H	0.68710300	-2.40061300	0.50911300
H	-2.19757500	0.71212700	-1.72419900
H	0.98944400	-0.25372300	1.40898400
H	2.42596500	-1.09049100	-1.13059400
H	0.33144000	0.52718900	-1.45835300
O	3.19506600	-1.42604300	0.69169000
O	4.37005300	0.74915700	-0.46614900
O	0.24824200	-1.65838300	0.07643000
O	-1.43220300	1.31349300	1.13107700
O	0.92248500	1.89411900	-0.03437400
C	-5.51020400	-0.23941400	0.77002800
C	-4.16435900	0.24414200	0.89938000
C	-3.53426900	-0.07404900	-0.25746400
C	-5.58978900	-0.80868900	-0.45128300
H	-6.30419200	-0.16539400	1.49431700
O	-4.39594300	-0.71782700	-1.09200400
H	-6.38133400	-1.29954500	-0.99103500
H	-3.72767400	0.76005400	1.73517800
C	-2.16584100	0.10302300	-0.81094400
H	-1.74836300	-0.86074800	-1.12164900
Na	5.54299300	-1.28732300	0.04611700

Na(I)/(24)

E = -1039.530054
H = -1039.527606
G = -1039.808372

C	1.60292900	-1.59618400	-0.62929500
C	1.29677200	1.07311000	0.00785400
C	2.65881500	0.45352900	0.28623100
C	2.69514500	-0.94865500	-0.24036900
C	0.21344100	0.04991200	0.32152300
C	-1.18103700	0.59481700	0.12913500
H	3.55964400	1.36534600	-1.20157800
H	1.61639600	-2.60209100	-1.02976700
H	3.96085200	-2.37706400	-0.59340800

H	1.79730700	2.83865000	0.64384500
H	1.23476700	1.32265000	-1.06144200
H	2.83589800	0.45781800	1.36573100
H	0.34321100	-0.30862200	1.34943200
H	-1.35779600	0.82117400	-0.92428500
O	3.71597200	1.24359100	-0.25515200
O	3.96634700	-1.47080700	-0.26331300
O	1.07921100	2.21477100	0.80352800
O	0.34692000	-1.06371000	-0.56252500
C	-5.78242600	-0.21008200	-0.31039800
C	-4.76186800	-0.82808800	0.46288500
C	-3.60640100	-0.17355600	0.16130300
C	-5.16866500	0.77185800	-1.02154200
H	-6.83003900	-0.45790100	-0.33898500
O	-3.85162600	0.80900700	-0.74915900
H	-5.52824100	1.49452900	-1.73469300
H	-4.85619300	-1.64754600	1.15587800
C	-2.23755200	-0.35949900	0.64485000
O	-1.98945700	-1.23438900	1.44917000
H	-1.28912600	1.53419200	0.67928000
Na	5.81813300	0.05529000	-0.05122400

Na(I)/Transition states

Na(I)/AG-ts1

E = -849.047531
H = -849.042417
G = -849.280270

C	-1.11057700	0.36618900	-0.86456300
C	-0.42794900	1.37177400	0.05807600
C	1.07844400	1.37037300	-0.11074700
C	1.62473900	0.01060300	0.27979600
C	1.16106400	-1.05323600	-0.70509100
H	-1.25584400	0.78069100	-1.86648900
H	1.27347300	-0.23122200	1.29029100
H	1.73981300	-0.94500300	-1.62405200
O	-0.23033600	-0.88748100	-1.05889900
O	-2.13206100	-0.33068800	-0.34171700
H	-1.13229600	-1.25600300	-0.45572000
O	3.03411600	-0.01371000	0.22904400
H	3.35541600	0.73227900	0.75069900
C	1.30265500	-2.46128600	-0.17446400
H	2.34407600	-2.60795100	0.12411200
O	0.41582900	-2.58432400	0.92360500
H	0.43644000	-3.49126200	1.24374300
H	1.05213700	-3.17415800	-0.96406600
Na	-4.07862800	-0.50340800	0.70581800
O	-0.88089600	2.67832700	-0.24065700
H	-1.71727400	2.84166900	0.20727100
H	-0.66850000	1.10251900	1.09166900
O	1.67831600	2.31360400	0.75070600
H	1.24896000	3.16496600	0.60013100
H	1.33851000	1.58863500	-1.15628500

Na(I)/AG-ts2

E = -849.040641
H = -849.038193
G = -849.275937

C	-1.29331100	-0.63707600	0.53622700
C	1.09696900	-0.02415000	0.78449300
C	0.95845700	-1.49845500	0.39611300
C	-0.40880300	-1.59360400	-0.26838600
C	1.63419300	0.87682500	-0.33195800
H	-1.80752000	-1.13883700	1.36189800
O	-1.96881900	0.31829000	-0.11926100
H	-0.89212300	0.98623700	0.44680500
C	1.44099000	2.35236400	-0.02284600
H	2.09851300	2.92172500	-0.68420500
H	1.72288300	2.55768300	1.01489100
O	0.07757900	2.67441000	-0.25905400
H	-0.09388100	3.56640500	0.05883100
O	-0.83334800	-2.93500700	-0.22477000
H	-1.53777300	-3.07123400	-0.86701500
H	-0.34762900	-1.22421600	-1.29656600
O	2.02399000	-1.88245100	-0.44012000
H	1.97615900	-2.83190900	-0.59866400
H	0.93710700	-2.11049800	1.30391300
O	3.02528700	0.67296300	-0.44671300
H	3.16724000	-0.25955400	-0.65804200
H	1.12173400	0.65696100	-1.27736700
O	-0.26160500	0.32329100	1.16030200
H	1.72268800	0.11372200	1.66647900
Na	-4.10391200	0.87328400	-0.39962600

Na(I)/AG-ts3

E = -849.034098
H = -849.031649
G = -849.264942

C	-0.92297900	-0.88794900	-1.06050700
C	-1.32765800	-1.34713300	0.30434900
C	-1.42972000	-0.02729600	1.09299800
C	-1.26676700	1.07292400	0.01157800
C	-0.01806800	1.94048900	0.12431000
C	1.23513100	1.14767000	-0.30095600
O	1.68692800	-1.78718700	-1.84385300
O	-2.60777800	-1.91611800	0.11997300
O	-0.48927600	0.05219000	2.12044900
O	-0.14568700	3.13181200	-0.62311800
O	-1.11018600	0.32744200	-1.27415400
O	1.23257600	-0.15832600	0.18487700
H	-0.61177900	-2.03250500	0.75299900
H	-0.65280900	-1.51476700	-1.90531100
H	-2.42316100	0.03527900	1.53404800
H	1.61692000	-1.15932600	-1.07647800
H	-2.15378700	1.68361900	-0.13376700
H	0.05280700	2.24348700	1.16957900
H	1.24972500	1.16057500	-1.40574600
H	2.11389700	1.72233000	0.02052700
H	-2.52227200	-2.85584800	-0.08158500
H	0.37375900	-0.06854800	1.64928300
H	2.26391000	-1.36473200	-2.48620000
H	-0.01849300	2.93161900	-1.55833800

Na	3.14173100	-0.85199300	1.18336000

Na(I)/AD-ts1

E = -849.02484
H = -849.022392
G = -849.259408

C	-0.18614300	-1.10994800	-1.32712200
C	0.21140900	1.23303700	-0.89664000
C	-1.16293900	-1.22422100	-0.28031000
C	-1.86105600	0.08843200	0.02667200
C	-0.80908000	1.16136400	0.24825200
C	1.56393000	1.77929800	-0.48620100
O	1.12376800	-1.03839200	1.32321700
O	0.49073900	-0.07560200	-1.54402600
O	-2.00298100	-2.31797000	-0.48041100
O	-2.62313900	-0.12500000	1.18969700
O	-1.47350600	2.40652400	0.31407000
O	2.24519300	0.96876200	0.42790300
H	-0.35967200	-1.37362200	0.55422100
H	-0.20738900	1.82971200	-1.70750100
H	1.01762100	-1.07843100	2.27806500
H	-2.43534800	-2.51432800	0.35895200
H	0.09856200	-1.97631500	-1.92203700
H	-2.50833200	0.37004400	-0.81242400
H	-3.14737400	0.66710700	1.35752100
H	-0.30354800	0.93850100	1.18850300
H	-1.07180300	2.95342200	0.99631200
H	2.17061400	1.90980300	-1.38684800
H	1.37127700	2.77929600	-0.07595100
H	1.65512900	0.23003500	0.87899400
Na	3.19117700	-1.34996100	0.43097100

Na(I)/AD-ts2

E = -772.574434
H = -772.571986
G = -772.793373

C	1.70048600	1.48918000	-0.54599100
C	-0.50230200	0.92236700	-0.02517000
C	2.10618000	0.23171200	-0.38555100
C	1.28834800	-0.72618700	0.38304300
C	-0.00942100	-0.29546500	0.72641900
C	-1.74288400	1.53778300	0.58677600
O	0.50448700	1.91808100	0.00139100
O	3.26582000	-0.30271300	-0.86269100
O	1.95863200	-1.50815400	1.33244500
O	-0.89331000	-1.68263100	-0.27741100
O	-2.78316600	0.57446300	0.49662800
H	-0.69056400	0.63973800	-1.06826400
H	3.83693600	0.39292500	-1.20949700
H	2.24841700	2.26014700	-1.07056600
H	0.40468500	-1.49776000	-0.34875000
H	2.59642800	-2.06284400	0.87035000
H	-0.45291100	-0.54625800	1.68393800
H	-1.01819000	-2.43203900	0.32392000
H	-1.54465200	1.79930600	1.62948600
H	-1.99442500	2.44390800	0.03256400
H	-3.56661100	0.92096400	0.93582400
Na	-3.02556800	-1.16970900	-1.06718700

Na(I)/AD-ts3

E = -696.198296
H = -696.195848
G = -696.393720

C	-0.16019600	1.65823000	0.12674700
C	-1.64703000	-0.04703700	-0.67457500
C	0.93109800	0.85985700	-0.04068700
C	0.66330600	-0.52108400	-0.13680000
C	-0.65806000	-1.05171600	-0.17802000
C	-3.09645800	-0.36859100	-0.39269000
O	-1.40723500	1.26898500	-0.02065500
O	2.23102100	1.30615500	0.07434800
O	1.52699700	-1.47795000	-0.20062700
O	-3.33093100	-0.65038100	0.97181100
H	-1.51869100	0.16404700	-1.74067800
H	2.43904200	1.92225000	-0.63838300
H	-0.06056800	2.70346500	0.40325800
H	0.44185100	-2.05202200	-0.49461400
H	-0.91357600	-1.49925000	0.78599200
H	-3.72297100	0.45895600	-0.73725200
H	-3.36336600	-1.26315700	-0.95544800
H	-3.16549900	0.15319700	1.47759600
Na	3.77354600	-0.66726500	0.27969600

Na(I)/LG-ts

E = -849.040899
H = -849.038450
G = -849.275769

C	0.61799300	-1.18057000	1.59533300
C	-0.64265500	1.02973300	1.06016600
C	0.62267800	0.36324500	1.56447800
C	1.52304300	0.52852500	-0.57792600
C	-1.02863800	0.56128700	-0.35083800
C	0.19544600	0.61825700	-1.27973700
H	-1.13392400	2.89783200	0.74459400
H	3.04674900	-2.72533300	-1.31481300
H	-0.75735400	-1.33029600	-0.10410800
H	0.59383700	1.75098800	-2.83659800
H	2.02473100	-1.97330700	-0.40213200
H	1.52719400	-1.49710700	2.12075300
H	-0.24244800	-1.46706700	2.21780300
H	-1.45147300	0.76574700	1.74872700
H	0.93239000	0.80044200	2.51058300
H	2.42707600	0.54156200	-1.18182500
H	-1.76124400	1.26204500	-0.75724000
H	0.13469500	-0.21063300	-1.98676500
O	-0.36594800	2.41730000	1.07304600
O	-1.58477400	-0.72406300	-0.33285400
O	0.27279500	1.87316900	-1.93567700
O	0.55360100	-1.68578000	0.31494600

O	1.72387900	0.66657000	0.64853600
O	2.91109500	-1.90082000	-0.84045800
Na	-3.74114700	-1.40988600	-0.38619600

Na(I)/LO-ts1

E = -772.589400
H = -772.586952
G = -772.789756

C	-0.04341600	-1.10943200	-0.85498300
C	0.34454500	0.24431400	-1.36763200
C	0.19156900	-1.17193200	0.62024000
O	-0.27509700	1.30965800	-0.60846100
O	1.74149900	0.46391100	-1.18881600
C	0.16033300	0.13053100	1.43329600
C	0.52606800	1.33656200	0.57152700
C	1.92815800	1.25385200	-0.01509500
H	1.57970800	-2.01402700	-0.33515000
H	0.06754800	0.39813200	-2.40991200
H	-0.43832200	-1.92388600	1.09025500
H	0.79290600	0.09361100	2.32335900
H	0.32679600	2.25765600	1.11498900
H	2.29245700	2.24363600	-0.29219700
H	2.64503200	0.76793300	0.64769300
O	-1.45083600	-1.29332800	-1.12193300
H	-1.56240300	-2.05342000	-1.69585100
O	1.63713100	-1.72716500	0.64422800
H	1.75840100	-2.49156100	1.23638700
O	-1.20700900	0.32933300	1.78345200
H	-1.45112100	-0.27146300	2.49646200
Na	-2.56545900	0.56643200	-0.23344700

Na(I)/LO-ts2

E = -696.195753
H = -696.193305
G = -696.383925

C	0.36515000	0.97408500	0.44770600
C	0.43374000	-0.40793200	1.05917900
C	-0.73352300	1.37733400	-0.30055000
O	-0.84827200	-0.91965700	1.19777400
O	1.06268000	-1.20617300	0.06726000
C	-1.76413400	0.32694900	-0.66083300
C	-1.27612000	-1.03772200	-0.16572100
C	0.00920300	-1.52653400	-0.86817800
H	0.99072500	-0.44458300	1.99362100
H	-1.03154400	2.42284200	-0.23397100
H	-1.89010800	0.27257800	-1.74752600
H	-2.08818500	-1.75840200	-0.20472100
H	0.01172400	-2.60314100	-1.01515000
H	0.18513700	-1.01707100	-1.81624000
O	1.43079200	1.68442700	0.26857800
H	0.54690400	1.92236200	-0.71752300
O	-3.01928600	0.54858500	-0.03995500
H	-3.35476000	1.41056500	-0.30824300
Na	3.21971800	0.06366500	-0.45173800

Na(I)/LO-ts3

E = -696.230956
H = -696.228507
G = -696.417309

C	-0.34829800	0.77037100	0.60727000
C	-0.71696900	-0.50221500	-0.16613800
C	0.37460900	-1.25065500	-0.67388200
C	1.75795900	-0.70447200	-0.50933700
C	1.80632900	0.64381400	0.17612000
H	-1.12497900	1.05387100	1.31519200
H	0.18819400	-1.94227600	-1.48642600
H	2.41371800	-0.76150500	-1.37415900
H	2.79812200	0.86864000	0.55917200
O	-1.91474100	-0.76609900	-0.32352300
H	1.12922200	-2.04459900	0.38810900
O	2.25685900	-1.72960700	0.51683700
H	2.87401400	-2.36765300	0.12000400
C	1.22257000	1.73957500	-0.73245300
O	-0.15274400	1.80559200	-0.33869900
O	0.88378200	0.62636600	1.26193800
H	1.30164400	1.49131700	-1.79167300
H	1.68731200	2.70511100	-0.54165400
Na	-4.03906300	-0.24285700	0.15177600

Na(I)/Ch-tsF

E = -772.613969
H = -772.611521
G = -772.826476

C	-0.62018200	0.27063900	1.61665200
C	-1.32703900	-0.80692100	-0.78614700
C	-1.14529200	0.71448200	-0.79305500
C	-0.47457000	1.18316100	0.49936600
C	-0.36366200	-1.53665200	0.14378200
C	1.14510300	-1.51361400	-0.17441200
H	-2.86091500	-1.96265000	-0.37687800
H	-1.15676500	-1.18910900	-1.79682000
H	0.62951000	0.94820300	0.30182800
H	-0.69741700	-2.56725000	0.26284100
H	1.57704300	-2.35788500	0.39182900
H	1.18834400	-1.81563000	-1.23906200
O	-2.66276100	-1.01935100	-0.36227500
O	1.76940000	-0.33063300	0.10993100
O	-0.54692700	-0.97534900	1.50472000
O	-0.78070500	2.49152300	0.88169500
H	-0.17818600	3.09328900	0.43283300
O	-0.33723700	1.17976200	-1.85061400
H	-0.87075900	1.22724800	-2.65144800
H	-2.14044000	1.16329700	-0.83665700
H	-0.72234200	0.64204700	2.63516500
Na	3.85560200	0.19856800	-0.22076300

Na(I)/Ch-tsR

E = -772.613966 H = -772.611517
G = -772.826442

C	0.62088300	0.27061000	-1.61661700
C	1.32645800	-0.80743900	0.78637900
C	1.14537100	0.71405500	0.79331100
C	0.47529600	1.18319400	-0.49934000
C	0.36299700	-1.53659400	-0.14388800
C	-1.14584700	-1.51291500	0.17388100
H	0.87065800	1.22719100	2.65155900
H	0.72368300	0.64197200	-2.63508100
H	0.18072600	3.09356800	-0.43224900
H	2.85976900	-1.96391600	0.37715500
H	-0.62896700	0.94904500	-0.30220200
H	1.15569700	-1.18961200	1.79698300
H	2.14070500	1.16241400	0.83725300
H	0.69625800	-2.56735900	-0.26292700
H	-1.57796000	-2.35706400	-0.39242200
H	-1.18943100	-1.81486400	1.23854300
O	0.33723300	1.17964300	1.85066500
O	0.78240800	2.49134300	-0.88161300
O	2.66219700	-1.02049300	0.36288200
O	-1.76964100	-0.32970800	-0.11061700
O	0.54704400	-0.97532800	-1.50472100
Na	-3.85600200	0.19904500	0.22075100

Na(I)/HM-ts1

E = -849.038220
H = -849.035772
G = -849.277205

C	-1.43464900	1.78320400	0.32785800
C	-1.48388600	0.44400600	-0.16798400
C	-0.30125600	-0.51313200	-0.04793800
C	1.05912900	0.16085200	-0.02101100
C	2.19002800	-0.88124600	0.00034200
H	-0.53860300	2.38505600	0.42286800
H	-0.42803300	-1.03969400	0.90518500
H	1.12860300	0.72581800	0.91676400
H	1.98487700	-1.66637200	-0.72785800
H	-1.19553100	1.15043800	-1.11904600
O	2.21299000	-1.50656400	1.27341600
O	-2.56937500	2.35646100	0.52385500
H	2.55908600	-0.86657200	1.90849800
O	-2.68000900	-0.07748200	-0.25640700
H	-3.23631300	1.63058600	0.39788000
O	-0.36889200	-1.42498300	-1.12388300
H	-1.30227700	-1.64701100	-1.24014900
O	1.15563600	1.04236600	-1.12574500
H	1.92801400	1.60353500	-0.98074700
C	3.52414300	-0.24864300	-0.33535200
H	3.55601800	0.02227100	-1.39388400
O	3.65510400	0.90724400	0.48853000
H	4.55365600	1.24452000	0.42303200
H	4.31839900	-0.97023100	-0.13152000
Na	-4.17205300	-1.58353900	0.34957700

Na(I)/HM-ts2

E = -849.051422
H = -849.048974
G = -849.279838

C	-0.46115200	0.74258400	0.51508200
C	0.89228100	-0.89250600	-0.83703300
C	1.31505300	0.54736800	-1.15474100
C	0.84151900	1.40271000	0.02407900
H	2.39742900	0.63039400	-1.28276000
H	0.64949900	2.42693300	-0.30848400
C	1.90839600	-1.77986100	-0.13766200
H	1.51343800	-2.79483000	-0.09439900
H	2.81771600	-1.79568400	-0.74666400
O	2.16164500	-1.39486800	1.19325100
H	2.46600800	-0.47489700	1.20218800
C	-1.74941100	1.28602900	-0.05286500
H	-1.72691300	1.27430900	-1.14214100
H	-1.85693800	2.31954800	0.28994900
O	-2.83348700	0.48749200	0.38053900
H	-2.77492200	0.44361000	1.34569700
O	0.62059300	0.90576300	-2.33338600
H	0.91789700	1.77548400	-2.62394900
O	1.79367600	1.38582600	1.05943000
H	1.28436500	1.22090600	1.87472400
O	-0.28918600	-0.74845300	-0.00325900
O	-0.48607600	0.40424500	1.80551100
H	0.58022300	-1.37080700	-1.76559800
H	-0.17013200	-0.75538300	1.14971800
Na	-2.75591800	-1.73250700	-0.44146600

Na(I)/HM-ts3

E = -849.013370
H = -849.010922
G = -849.259432

C	-0.58885000	-0.56684000	-0.53955200
C	1.15793300	0.72312000	0.05222200
C	1.37073500	-0.61193300	0.76313900
C	0.00057400	-1.28184400	0.64877300
H	-0.61648300	-1.01412900	1.51319000
C	2.34436600	1.29635900	-0.66622400
H	2.04317600	2.20116000	-1.20095500
H	3.07978500	1.57072200	0.09723300
O	2.84260700	0.31390000	-1.54953300
H	3.60809700	0.66889900	-2.01170500
C	-1.90570400	-0.79030000	-1.07504100
H	-2.04357800	-0.46643700	-2.10560100
H	-2.32711600	0.02753500	-0.34784400
O	-2.46588200	-2.03001800	-0.73839800
H	-2.32771300	-2.64827400	-1.46481900
O	0.11795500	-2.66339400	0.45368200
H	-0.76587100	-3.05183600	0.48835600
O	0.10100100	0.42597600	-0.92467300
H	0.71492000	1.44479600	0.74309000

O	-1.99485200	1.12076000	0.87215900
H	-2.47839400	0.94639700	1.68465500
O	1.79513300	-0.35183500	2.07340700
H	2.22572600	-1.13672800	2.42781400
H	2.09802700	-1.21158300	0.20873400
Na	-1.87751000	3.23045300	0.30679900

Na(I)/HM-ts4

E = -772.582047
H = -772.579598
G = -772.802065

C	-1.59531700	-0.45144100	-0.71695600
C	-0.41103800	-0.47939700	0.05761700
C	-0.04836600	0.80347300	0.79842500
C	1.07325300	1.32365500	-0.10153900
H	-1.72980000	-0.42147600	-1.79677500
H	1.73999700	1.99177100	0.44843500
O	0.43356200	1.98561300	-1.17487700
O	-2.60207100	-0.54635300	0.07027000
H	1.09645500	2.24507400	-1.82346200
H	-1.64155400	-0.81315100	0.86473400
C	1.76582800	0.03939400	-0.56160200
O	0.75088500	-0.98492600	-0.51537100
H	2.08437000	0.13627500	-1.60384700
C	2.95877300	-0.36535300	0.27372500
H	3.66639100	0.47027200	0.30048400
H	2.63503300	-0.59057900	1.29228700
O	3.54523700	-1.50075700	-0.34410900
H	4.25659000	-1.82256200	0.21749500
O	0.52745800	0.57071100	2.06765800
H	-0.08195500	0.03854300	2.59064100
H	-0.88059200	1.50781400	0.85062300
Na	-4.98584500	-0.37802500	-0.06065400

Na(I)/HM-ts6

E = -772.609818
H = -772.607370
G = -772.822587

C	0.03623700	-2.24153200	-0.55833000
C	-1.44149600	1.02000500	-0.11843200
C	-1.79426000	-0.48254100	-0.09480900
C	-0.51152000	-1.18014500	0.21482700
C	0.08480600	0.95819400	-0.19690000
C	0.85573600	2.13884500	0.31928600
H	-0.69485800	-2.93448900	-1.00541600
H	-2.84700200	1.97731700	-1.07414600
H	-1.74669300	1.49984600	0.81895100
H	0.35899600	0.76514800	-1.24474800
H	0.59962000	3.03014900	-0.25824500
H	0.61938100	2.30541700	1.37417200
O	-1.93738400	1.70435300	-1.23472500
O	2.22807500	1.79155000	0.15703100
O	1.24563000	-2.44912200	-0.68013800
O	0.41612100	-0.17588100	0.59808000
H	2.78130100	2.50817800	0.48292900
H	-2.38204900	-0.80783000	-0.94710900
Na	2.66390900	-0.67686500	0.14454400
H	-1.57041200	-1.46504500	1.33692600
O	-2.57467300	-0.93236600	1.13294300
H	-2.82045000	-0.21840600	1.74731900

Na(I)/HM-ts7

E = -772.582708
H = -772.580259
G = -772.796973

C	0.58507500	-2.29684500	-0.35799700
C	-1.71976500	0.51397700	0.26063200
C	-1.47648900	-0.99218300	0.30783600
C	-0.31538100	-1.13333100	-0.68472700
C	-0.48444700	1.14601500	-0.21499800
C	0.27588800	2.00089900	0.75276900
H	0.11492600	-3.29249500	-0.36062800
H	-3.01902700	0.16390100	-1.48994600
H	-2.24317800	0.92523200	1.11784500
H	-1.83401500	1.38470100	-1.35018200
H	-0.34248800	2.83835200	1.08684600
H	0.60278000	1.43763500	1.63610100
O	-2.69086000	0.90294200	-0.94391300
O	1.49520700	2.46263800	0.15986900
O	1.75732700	-2.15665400	-0.12192700
O	0.41048900	0.05747800	-0.59826600
H	1.26275000	2.88117500	-0.67863400
H	-2.33745500	-1.60891100	0.04573200
Na	2.63989800	0.25380700	-0.14420000
H	-0.71796300	-1.29017700	-1.69773600
O	-0.97381300	-1.30657300	1.58869400
H	-1.70129100	-1.34112500	2.22005300

Na(I)/HM-ts8

E = -696.190508
H = -696.188060
G = -696.392529

C	2.64691500	-0.35653100	-0.19608500
C	-0.29132600	1.87880600	-0.39441200
C	1.13912500	1.66984400	-0.49720700
C	1.35676900	0.35602600	-0.26470200
C	-0.85810300	0.56503900	-0.11814700
C	-2.01620800	-0.02538400	-0.84854800
H	3.53173600	0.25790000	-0.41863300
H	0.07980400	2.58211100	1.81025800
H	-0.81251600	2.66612600	-0.92031900
H	-1.01804700	1.28492100	1.10834300
H	-2.82072300	0.71209500	-0.89479500
H	-1.74148800	-0.31811700	-1.86785200
O	-0.71210300	2.46851100	1.26037400
O	-2.42340400	-1.18604100	-0.11916400

O	2.72550800	-1.52622600	0.08010100
O	0.24163200	-0.35410300	-0.07072900
H	-3.10631900	-1.64310800	-0.62190400
H	1.89101800	2.41160900	-0.71194700
Na	-0.59268700	-2.51795100	0.65698200

Na(I)/HM-ts9

E = -696.212304
H = -696.209856
G = -696.409163

C	1.08567100	1.89519300	0.24046100
C	0.78849000	-1.62749200	0.66941400
C	1.81399700	-0.57616800	0.53820500
C	1.08687500	0.52509200	-0.16718300
C	-0.31421000	-1.20327400	0.03944700
C	-1.64102500	-1.84167600	-0.17359800
H	2.04024200	2.26976400	0.64224300
H	0.90408700	-2.56357100	1.18952500
H	-1.72352100	-2.15961500	-1.21719700
H	-1.73017700	-2.71521700	0.47360900
O	-2.62757000	-0.85985800	0.12800900
O	0.12371000	2.64715100	0.11301900
O	-0.20800400	0.03667100	-0.49414700
H	-3.49478500	-1.21005400	-0.10044200
Na	-2.00787000	1.54455300	-0.06166100
H	2.21236300	0.04374800	-1.04829600
O	2.80931500	-0.90274900	-0.63823800
H	3.73220900	-0.70718700	-0.40038300
H	2.44775500	-0.34772000	1.38960200

Na(I)/FU-ts

E = -619.788381
H = -619.785933
G = -619.969188

C	-0.20736700	1.58924200	0.05566600
C	-1.57589200	1.58395200	-0.16245600
C	-1.94988100	0.25494800	-0.05970700
C	0.21359100	0.24421300	0.22627800
C	1.48474100	-0.26883000	0.90158400
H	0.46665100	2.43297500	0.03375000
H	1.70299300	0.28299900	1.82442300
H	1.29463300	-1.31885400	1.16532100
O	2.41652400	-0.07892000	-0.11536400
O	-0.94358100	-0.54088500	0.19796700
H	0.92180700	0.11731200	-0.75483500
H	-2.22828600	2.41328500	-0.38025500
C	-3.30066600	-0.36012100	-0.23749200
O	-3.45908500	-1.54572600	-0.17755700
H	-4.11731300	0.35118700	-0.42100800
Na	4.53286300	-0.47409900	-0.45918200

Na(I)/Ch-ts1

E = -1115.786763
H = -1115.784315
G = -1116.080992

C	-1.30741100	1.59760500	-0.32305200
C	-2.02538200	-1.07319800	-0.27156000
C	-2.87711800	-0.11511200	0.54671600
C	-2.44371100	1.30130800	0.29576200
C	-0.56416300	-0.63758300	-0.17276800
C	0.35984500	-1.57693400	-0.92792400
H	-4.42800700	-0.14441200	-0.65452500
H	-0.98531300	2.60692400	-0.53787300
H	-4.15477900	1.90492400	0.85395200
H	-3.04673300	-2.65510500	0.20583500
H	0.42973000	-0.39740100	-2.42806700
H	-2.32835200	-1.01486100	-1.32631800
H	-2.76173700	-0.36004500	1.60710700
H	-0.27448900	-0.60785700	0.88851000
H	1.31542700	-1.98770000	0.00780800
H	0.04399300	-2.61746700	-0.75813700
O	-4.26401900	-0.27834400	0.28856100
O	-3.27012800	2.28452400	0.76072100
O	-2.11826700	-2.39290100	0.21038700
O	0.42301900	-1.35645200	-2.28441000
O	-0.40691700	0.64842300	-0.74476900
C	2.49256600	2.40431900	-0.84157000
C	2.66207600	1.11280100	-1.42353000
C	2.36102100	0.21934000	-0.44595400
C	2.10999800	2.19071600	0.44098000
H	2.64338800	3.36246100	-1.30958900
O	2.03359700	0.86660700	0.70481000
H	1.88195200	2.85138000	1.26029100
H	2.96682400	0.87209400	-2.42951100
C	2.26531500	-1.23128100	-0.43063400
O	2.43077900	-1.88065600	0.75468800
H	2.66793500	-1.69323700	-1.33504100
Na	2.65522100	-0.76374500	2.70516800

Na(I)/Ch-ts2G

E = -1115.811593
H = -1115.809144
G = -1116.107912

C	-1.57640500	-1.76082000	-0.01619400
C	-1.50322100	0.98313700	0.29172000
C	-2.80784200	0.39141400	-0.20723300
C	-2.71582800	-1.10506700	-0.20635200
C	-0.31918400	0.22684700	-0.31334400
C	0.98747200	0.82160000	0.09332400
H	-3.73000500	0.70302600	1.49608100
H	-1.51314500	-2.84216700	0.01237600
H	-3.84799500	-2.66468000	-0.44326600
H	-0.56167600	2.64064900	0.04753300
H	1.06660900	-0.10046200	1.81167800
H	-1.45483900	0.85754500	1.38293600

H	-3.00282600	0.75860200	-1.21895800
H	-0.41682600	0.22375500	-1.40653700
H	1.60547300	2.09641400	-0.60743600
O	-3.92845500	0.82963100	0.55930500
O	-3.93683800	-1.70473000	-0.41691600
O	-1.47703600	2.34581100	-0.05808900
O	1.17232200	0.80875900	1.49609700
O	-0.36720900	-1.14664500	0.14199800
C	5.13428000	-0.91655400	0.98473900
C	3.91595400	-0.18369000	1.10501500
C	3.35395800	-0.16869500	-0.13580300
C	5.22039400	-1.28991700	-0.31486800
H	5.84612000	-1.13653700	1.76223700
O	4.15563300	-0.84297800	-1.01086200
H	5.94607500	-1.85925900	-0.87053400
H	3.51178700	0.28423700	1.98499200
C	2.14684600	0.41233300	-0.71225600
O	2.52735200	1.98744600	-1.25068700
H	3.31086500	2.32786600	-0.78636000
H	1.91038100	-0.01439400	-1.68209000
Na	-5.89588000	-0.35968000	-0.05290100

Na(I)/Ch-ts2F

E = -1115.808069
H = -1115.805620
G = -1116.104289

C	1.92772500	1.67183700	0.52465500
C	1.29962900	-0.98838200	0.14545100
C	2.64950500	-0.52234600	-0.37747600
C	2.89070200	0.89578900	0.04263700
C	0.27396800	0.11403600	-0.09077000
C	-1.12628100	-0.28719100	0.28301800
H	3.71975200	-1.40538900	1.01381600
H	2.08610800	2.69253900	0.84847200
H	4.32730800	2.19625800	0.14446300
H	1.53844800	-2.82945000	-0.42434700
H	-1.56514000	-1.30593000	2.13164400
H	1.37537300	-1.15688600	1.22846900
H	2.65258600	-0.60043200	-1.46860400
H	0.25692500	0.37290000	-1.15862700
H	-1.36865900	-1.28733700	-0.07160600
O	3.70256500	-1.38204600	0.04731100
O	4.19599000	1.28243300	-0.13474900
O	0.86062900	-2.14923700	-0.51786100
O	-1.11031100	-0.48093500	1.88298300
O	0.62639500	1.26795100	0.66274400
C	-5.59813600	-0.10397300	-0.81640400
C	-4.53431900	0.86197300	-0.84224400
C	-3.48874300	0.29465600	-0.17408000
C	-5.13012000	-1.17871100	-0.14868100
H	-6.58158700	-0.00635600	-1.24735000
O	-3.83892800	-0.95354000	0.25155000
H	-5.54667300	-2.13534800	0.11370700
H	-4.53833800	1.83892700	-1.29331900
C	-2.16533100	0.75578400	0.19869500
O	-1.82987700	1.93754100	-0.49930300
H	-1.33858600	2.50665100	0.09932500
H	-1.82152900	0.33633600	1.83007200
Na	5.81461000	-0.40678500	-0.70512000

Na(I)/Ch-ts3G

E = -1039.415819
H = -1039.413370
G = -1039.691811

C	-2.97424100	1.02801600	0.23701700
C	-1.01840500	-0.90202200	-0.14653700
C	-2.42467500	-1.39106400	0.16664900
C	-3.38241900	-0.23342100	0.19394200
C	-0.76295800	0.35601000	0.69754200
C	0.63882100	0.83696600	0.54493700
H	-2.83461300	-2.03571000	-1.64096900
H	-3.64243200	1.87671300	0.24328600
H	-4.80977800	-1.44390900	-0.12605300
H	-0.30127700	-2.69678800	-0.24565500
H	1.93445600	1.70512000	0.56202600
H	-0.96481200	-0.61122800	-1.20535800
H	-2.41173900	-1.88622600	1.14246300
H	-0.92391200	0.11037300	1.75612000
O	-2.84910700	-2.39163600	-0.74239100
O	-4.70993000	-0.54012300	0.20343100
O	-0.04831600	-1.86327600	0.17114900
O	0.90043800	1.85729100	-0.18847800
O	-1.64088900	1.39045800	0.29476900
C	4.29388300	-1.09337300	-1.09549600
C	2.91084400	-0.86273400	-0.79663800
C	2.88130000	-0.17710300	0.37515200
C	4.99400000	-0.54676700	-0.07681700
H	4.70568700	-1.61297100	-1.94464600
O	4.15287300	0.02720900	0.82214900
H	6.04390500	-0.49355300	0.15466200
H	2.04610400	-1.18647100	-1.35164900
C	1.79831600	0.37316600	1.20746600
H	1.69204300	-0.05731400	2.19875200
Na	-0.79099700	3.28786600	-1.07921100

Na(I)/Ch-ts3F

E = -1039.427764
H = -1039.425316
G = -1039.702340

C	1.22227400	-1.61218100	0.16489800
C	1.37454800	1.05340500	-0.55620700
C	2.60052100	0.44302700	0.11042500
C	2.40025700	-1.02167100	0.32840400
C	0.10314000	0.48146000	0.06474200
C	-1.13873000	1.08722800	-0.51984400
H	3.63646500	0.39827200	-1.55656900
H	1.06920400	-2.67594400	0.30380200
H	3.38504200	-2.59521100	0.89279300
H	2.23864800	2.78142400	-0.69350100

H	1.37772500	0.77139600	-1.61962500
H	2.77280200	0.94621700	1.06643600
H	0.14283700	0.61905500	1.15282100
H	-1.22730800	0.90888700	-1.58906300
O	3.78114300	0.70425300	-0.65090300
O	3.55383400	-1.66108200	0.72153100
O	1.37625300	2.45368700	-0.41007100
O	0.08477800	-0.94467000	-0.18550500
C	-5.40832000	-0.96554000	0.13798400
C	-4.67586800	0.08455800	0.73819300
C	-3.46117500	0.11532100	0.10750300
C	-4.58983800	-1.48816500	-0.82003700
H	-6.40732000	-1.29255700	0.37048200
O	-3.41357700	-0.85210400	-0.85299100
H	-4.71807400	-2.28862100	-1.52981900
H	-4.98910100	0.74900000	1.52675800
C	-2.31458400	0.94083700	0.28728700
O	-2.24712300	1.77293300	1.26833400
H	-1.31769400	2.15326100	0.52958400
Na	5.66190700	-0.63354500	0.16024200

K(I)/intermediates

Local minima

K(I)/(2)

E = -1286.758116
H = -1286.755668
G = -1287.004156

C	2.18427400	-0.62596300	-0.54509600
C	1.17372500	-0.12480000	0.48709800
C	-0.01023300	0.58483600	-0.17943700
C	-1.10671000	0.91812100	0.82869700
H	0.78225700	-1.00352500	1.01017900
H	-0.43146900	-0.11143600	-0.91780500
H	-0.68179300	1.54646800	1.61831000
O	-1.56217500	-0.32340500	1.36315800
H	-1.98419300	-0.16385300	2.21438500
O	1.88619700	0.72005500	1.37399000
H	1.41844700	0.77937700	2.21293900
O	0.35792200	1.80086600	-0.79161100
H	1.22407600	1.66865000	-1.20349900
C	-2.25246200	1.68280000	0.19740900
H	-1.87659900	2.62262800	-0.20875000
O	-2.81094400	0.87007700	-0.83100100
H	-3.43448100	1.39590100	-1.34104900
H	-3.00474900	1.89648700	0.96275700
C	3.34614900	-1.25765600	0.18473800
H	3.10497600	-2.07533300	0.88189700
O	4.47420900	-0.87551300	0.01682200
O	2.64460700	0.39851900	-1.39459400
H	3.58551400	0.53270400	-1.20204100
H	1.70145800	-1.40702300	-1.14509100
K	-3.17528600	-1.76157200	-0.34825300

K(I)/(3)

E = -1286.765714
H = -1286.763265
G = -1287.002811

C	2.45601600	0.87349600	-0.53080100
C	0.25790600	0.04762800	-0.43108200
C	1.24143600	-1.13562900	-0.41697500
C	2.50451500	-0.50077200	0.12427600
C	-0.61250200	0.12320500	0.82709400
H	2.83116100	0.82169200	-1.55712100
O	3.19902600	1.86070600	0.09585800
H	2.90458900	1.93601400	1.01291800
C	-1.34442700	1.44060500	0.92966200
H	-0.61843300	2.25242100	0.98004000
H	-1.94793000	1.43786300	1.84159000
O	-2.18017900	1.57686300	-0.21771100
H	-2.48253100	2.48841500	-0.27582000
O	3.62829300	-1.27294800	-0.21195900
H	4.40193900	-0.91851300	0.23981100
H	2.41160300	-0.38194700	1.21216800
O	0.74543600	-2.20065600	0.36861300
H	1.34368200	-2.95204300	0.29338300
H	1.43320300	-1.47509800	-1.43967500
O	-1.59181500	-0.90683500	0.79671600
H	-1.11743500	-1.75003000	0.77849900
H	0.01889200	0.02290500	1.71785800
O	1.07659400	1.21689200	-0.51750300
H	-0.40190800	0.01041800	-1.29950000
K	-3.93754300	-0.46186600	-0.47522600

K(I)/(4)

E = -1210.352721
H = -1210.350273
G = -1210.560801

C	-0.80699800	-0.81962900	0.97897200
C	-2.09666600	-0.70717900	0.17563500
C	-1.66249000	0.25896600	-0.93729000
C	-0.11069600	0.26458800	-0.83225400
C	0.49619700	1.46490400	-0.11869300
C	0.38655100	1.21358100	1.39980000
O	-2.46404300	-1.93499700	-0.41540400
O	-2.25711600	1.52297400	-0.74091700
O	1.86969800	1.49462600	-0.50731200
O	0.19388600	-0.87682200	-0.01036100
O	-0.71207100	0.37831600	1.73269300
H	-2.90245000	-0.27527900	0.76988600
H	-0.71383300	-1.69396600	1.62335000
H	-1.96246700	-0.16716200	-1.89539600
H	0.37106900	0.12468600	-1.79867800
H	0.00256900	2.38895900	-0.41677800
H	1.32481200	0.76430800	1.73878400
H	0.23050000	2.13994200	1.94880400
H	-2.79281000	-2.52497300	0.27163100
H	-2.21883200	2.01933100	-1.56512100
H	2.27805900	2.30541100	-0.18381200
K	2.95290300	-1.04239100	-0.26101500

K(I)/(5)

E = -1210.351101
H = -1210.348653
G = -1210.568651

C	1.99419400	1.57023100	-0.18141200
C	1.54935700	-0.60658300	0.56921700
C	0.73617900	1.93174700	0.04871600
C	-0.35652000	0.94262800	0.33882500
C	0.14867000	-0.43795800	-0.01008000
C	2.07967300	-2.01611600	0.42011400
O	2.43179900	0.27076600	-0.12919200
O	0.26356800	3.21661300	0.03791700
O	-1.51237000	1.20531700	-0.44601500
O	-0.76570100	-1.39471900	0.49580600
O	1.81326400	-2.56316600	-0.86007700
H	1.55095300	-0.33105900	1.63192200
H	0.94290800	3.83120400	-0.26365500
H	2.78280500	2.27202600	-0.42035000
H	-0.62559900	0.97762000	1.40253000
H	-1.68066700	2.15603500	-0.42387700
H	0.21205400	-0.51123700	-1.10023500
H	-0.54683600	-2.24925800	0.10255900
H	3.15003900	-2.01678800	0.64178700
H	1.58324500	-2.66297100	1.14334400
H	2.30867500	-2.06126700	-1.51721400
K	-3.39112500	-0.71507800	-0.05771600

K(I)/(6)

E = -1133.944371
H = -1133.941922
G = -1134.137265

C	0.88605300	-0.09423800	1.52051300
C	-0.60577600	1.33180700	0.39944300
C	1.78149800	0.02780800	0.53801300
C	1.32711600	0.47725100	-0.78290600
C	0.12791400	1.05386200	-0.88539400
C	-2.08927300	1.52530500	0.21252300
O	-0.43178400	0.23430300	1.31440100
O	3.10273000	-0.30147900	0.59336400
O	2.13374600	0.23249500	-1.83982700
O	-2.61404900	0.37730600	-0.44123300
H	-0.20454600	2.22953600	0.89229600
H	3.30746800	-0.77710900	1.40723700
H	1.09205600	-0.52484600	2.49149500
H	2.94148100	-0.19628300	-1.52465600
H	-0.28235300	1.36634900	-1.83622500
H	-2.56018800	1.66407300	1.18839500
H	-2.24512100	2.42319900	-0.39154200
H	-3.55759000	0.50034500	-0.58550300
K	-1.29376500	-1.94510700	-0.24569900

K(I)/(7)

E = -1133.967267
H = -1133.941922
G = -1134.137265

C	0.60253100	-1.23651800	-0.19388400
C	-0.09437700	0.97757900	0.22803600
C	1.88538200	-0.92164300	0.03241000
C	2.32535300	0.47202200	-0.00113300
C	1.24410900	1.48248400	-0.27927000
C	-1.22745100	1.89109600	-0.16119600
O	-0.39423300	-0.32704000	-0.30654200
O	2.83813400	-1.87798600	0.18771500
O	3.50442500	0.74553800	0.11696700
O	-2.42819400	1.36819700	0.38916000
H	-0.06305200	0.86537500	1.31813200
H	3.68761200	-1.41325800	0.23854900
H	0.27130000	-2.26089700	-0.31166200
H	1.50059000	2.42990300	0.19407200
H	1.21012400	1.64064100	-1.36309300
H	-1.01801300	2.88688300	0.23611400
H	-1.29310600	1.94837700	-1.25185700
H	-3.13062700	2.01762000	0.27932600
K	-3.03890300	-1.23023300	-0.00988300

K(I)/(8)

E = -1210.37000
H = -1210.367552
G = -1210.571419

C	-0.42488300	0.91374800	-1.10399900
C	-0.57855300	-0.59445400	-1.26993100
C	-0.88230500	1.32497100	0.30750200
C	-0.43740800	0.30730300	1.38197400
C	-0.53758900	-1.12893500	0.88449300
C	-1.91808600	-1.5055300	0.36908700
O	0.23226600	-1.24803000	-0.32110100
O	-1.91664100	-0.95804500	-0.96111600
O	0.94543400	1.19220600	-1.32839500
O	-2.28295200	1.52762800	0.34702700
O	0.93004100	0.49631300	1.72215300
H	-1.05419600	1.42388900	-1.83867200
H	-0.30420400	-0.93724900	-2.26639300
H	-0.42114200	2.28603700	0.54914100
H	-1.07871900	0.43344700	2.25891000
H	-0.13545000	-1.82417000	1.61772900
H	-2.03475600	-2.58726200	0.31452800
H	-2.73499200	-1.06841800	0.94117000
H	1.05563400	2.13491100	-1.49290000
H	-2.70404000	0.87163400	-0.22266000
H	1.02558000	1.32579000	2.20295000
K	2.83126500	-0.31798900	-0.06037400

K(I)/(9)

E = -1133.953392
H = -1133.950943
G = -1134.144433

C	-1.02147900	1.11057700	0.45663100
C	-1.06176000	0.47771300	-0.92474500
C	-0.47472300	0.44600300	1.47030900

O	0.05817600	-0.35983900	-1.08124800
O	-2.16971100	-0.38194200	-1.02938800
C	0.10023900	-0.92756700	1.24221300
C	-0.25165700	-1.41324200	-0.15557500
C	-1.77085800	-1.58653900	-0.35904000
H	-1.09002400	1.21047400	-1.73171600
H	-0.45543700	0.87020500	2.46705000
H	-0.30545500	-1.63676700	1.96970600
H	0.33044700	-2.29063900	-0.42543700
H	-2.00596300	-2.42667500	-1.00806300
H	-2.29942300	-1.68663500	0.58967400
O	-1.62356800	2.31111500	0.62036100
H	-1.88902900	2.68487500	-0.22775300
O	1.53042700	-0.93452400	1.32913100
H	1.78939300	-0.71031100	2.23025100
K	2.65496500	0.54028100	-0.68175300

K(I)/(10)

E = -1133.970848
H = -1133.968399
G = -1134.158896

C	-0.98997400	1.36284400	-0.08544500
C	-0.98959200	0.26910300	-1.15756900
C	-1.07440800	0.81621800	1.32101200
O	0.11659200	-0.56725200	-0.89474600
O	-2.13215700	-0.53663000	-1.00313000
C	-0.22182100	-0.45318300	1.47661900
C	-0.33322500	-1.33039900	0.23675000
C	-1.77489400	-1.63993300	-0.15643000
H	-0.92813500	0.67863500	-2.16388300
H	-0.78188100	1.58234400	2.03813200
H	-0.54854100	-1.02238100	2.35028700
H	0.29926000	-2.21103100	0.32260000
H	-1.84252400	-2.56195900	-0.73139900
H	-2.45031600	-1.68469000	0.69791900
O	-0.92269200	2.53137100	-0.36506800
H	-2.12517900	0.56897000	1.50294100
O	1.15798700	-0.12764600	1.58841300
H	1.31277100	0.32642500	2.42407800
K	2.82158900	-0.01173500	-0.57126600

K(I)/(11)

E = -1057.55218
H = -1057.549731
G = -1057.726023

C	-0.96791900	1.34520600	0.08273400
C	-0.34503400	0.23996500	0.94167200
C	-1.98218900	0.85833600	-0.86917700
C	-2.25539000	-0.44737000	-0.88847800
C	-1.57002000	-1.36910700	0.08300200
C	-0.12602300	-1.64706200	-0.36396800
O	-1.32275800	-0.68022500	1.31295000
O	0.56405000	-0.47651100	0.10117200
O	-0.59143300	2.49196500	0.16025200
H	0.16984300	0.63790700	1.81396200
H	-2.14308600	-2.26677900	0.29326400
H	0.27238700	-2.52624300	0.14114400
H	-0.01030800	-1.73142000	-1.44225400
H	-2.93858300	-0.87740400	-1.61137800
H	-2.44359900	1.57296000	-1.53865900
K	3.23020700	0.03312300	-0.21925200

K(I)/(12)

E = -1286.761183
H = -1286.758734
G = -1287.007282

C	2.39054500	0.15463000	-0.71872400
C	3.65979100	-0.58946000	-0.35987000
C	1.14155900	-0.12423200	0.11151000
C	0.07384100	0.94522500	-0.09923900
C	-1.04359800	0.80326900	0.93871800
H	0.74293000	-1.07886600	-0.25964500
H	-0.33988400	0.81377900	-1.10397100
H	-0.67725500	1.23586300	1.87373100
H	4.26464500	0.08605000	0.25566200
O	-1.40187600	-0.55910600	1.13592400
O	2.38756500	0.94025700	-1.63624300
H	-0.69297200	-0.96958100	1.64795000
O	3.33397800	-1.77861000	0.33936600
H	4.14610000	-2.19559000	0.64542800
O	1.43979700	-0.21823900	1.49295700
H	2.06898500	-0.94628100	1.60159700
O	0.57583000	2.25743000	0.06568500
H	1.14998500	2.44418000	-0.68642800
C	-2.28908500	1.55551900	0.53443300
H	-2.02389600	2.59621400	0.33820900
O	-2.82435200	0.93936400	-0.63472000
H	-3.53364800	1.49059700	-0.97929400
H	-3.01498600	1.51358000	1.35040300
H	4.20072000	-0.79513700	-1.28536000
K	-3.05139900	-1.75333100	-0.62857900

K(I)/(13)

E = -1286.773451
H = -1286.771003
G = -1287.005625

C	-0.07947200	0.31628200	-0.41063300
C	2.19255700	-0.12557700	-0.73410400
C	2.12003300	0.66120900	0.57226100
C	0.63672700	0.60406600	0.94815800
H	2.73734800	0.22640400	1.36350000
H	0.30202000	1.56405000	1.34835100
C	2.44528700	-1.61884200	-0.59821600
H	2.46863800	-2.05639900	-1.59583700
H	3.41990500	-1.77880500	-0.12804800
O	1.42145000	-2.30808400	0.10812700
H	1.39643000	-1.99103000	1.02303000
C	-0.92656300	1.47869300	-0.88132800
H	-1.26140800	1.27557200	-1.90238700
H	-0.30931900	2.37952200	-0.87454000

O	-2.02828500	1.59713800	0.00798100
H	-2.43359300	2.46249800	-0.10813800
O	2.52138300	1.98363500	0.26902500
H	2.46828700	2.51697000	1.06992300
O	0.44842500	-0.41520800	1.90725000
H	-0.49303900	-0.62647800	1.94333600
O	0.93587800	0.12710400	-1.36723000
O	-0.91439000	-0.81030100	-0.33436200
H	2.97184600	0.29775500	-1.37003700
H	-0.32411800	-1.58302700	-0.25034200
K	-3.59737400	-0.63033100	0.07252800

K(I)/(14)

E = -1210.342658
H = -1210.340209
G = -1210.567526

C	-0.91076300	-0.80427600	-0.01080700
C	0.38772600	1.06621900	-0.22361000
C	-1.02430900	1.54258300	0.08904100
C	-1.86743800	0.32714100	-0.28621600
H	-2.09827100	0.38263200	-1.35769600
C	1.45952300	1.75498600	0.57208200
H	1.40836500	2.82743200	0.36662100
H	1.28917100	1.58228300	1.63885800
O	2.71300000	1.21553000	0.16972700
H	3.42037200	1.71101300	0.59528200
C	-1.21801700	-2.08397100	0.12107700
H	-0.48933600	-2.85347800	0.34335100
O	-2.52536200	-2.47050600	-0.08311000
H	-2.71048900	-3.26821000	0.42332500
O	-3.05175300	0.28844700	0.47661500
H	-3.44378300	-0.58739800	0.36131400
O	0.38268900	-0.33306700	0.10427400
H	0.58212800	1.18225100	-1.29630000
O	-1.29297800	2.71175100	-0.64196500
H	-2.11971700	3.09353900	-0.32810200
H	-1.13137700	1.71092500	1.16757600
K	2.86988600	-1.46812200	-0.19410300

K(I)/(15)

E = -1210.353070
H = -1210.350622
G = -1210.569054

C	-0.20536600	-2.01406200	0.46386600
C	-1.66747400	0.78584500	0.23491400
C	-2.01982700	-0.49105900	-0.51994800
C	-0.63361800	-1.14160700	-0.69549800
C	-0.30509700	1.15467000	-0.34129900
C	0.62011400	1.74565500	0.69254800
H	-0.85721300	-2.87177700	0.69541800
H	-3.38971000	1.65180600	0.49453600
H	-1.57204600	0.55263100	1.30646000
H	-0.61671600	-1.77888100	-1.58573800
H	-0.43614200	1.85542000	-1.16983800
H	0.17389000	2.66943400	1.07079500
H	0.73671400	1.04216800	1.52497600
O	-2.56307100	1.85026200	0.04058400
O	1.87564200	1.99482300	0.07307800
O	0.80749100	-1.81550400	1.08661400
O	0.25801700	-0.06053100	-0.87324300
H	2.37986800	2.60609000	0.61970800
O	-3.00740500	-1.29317900	0.07137900
H	-2.89251800	-1.31539300	1.02867400
H	-2.39243000	-0.21334800	-1.50750300
K	2.90360700	-0.51798800	-0.24591000

K(I)/(16)

E = -1133.951798
H = -1133.949350G
G = -1134.152298

C	-0.49479400	2.35298000	0.33822900
C	2.29247500	-0.14690100	0.16905800
C	1.73770700	1.19884400	0.56860900
C	0.47207900	1.26202300	0.16475000
C	1.02143700	-0.87698200	-0.29284000
C	0.51801400	-1.87505000	0.72190100
H	-0.09828100	3.28889300	0.75536700
H	4.02290200	0.32125100	-0.61395300
H	2.76359100	-0.66971200	1.00601900
H	1.16592900	-1.34270800	-1.26686500
H	1.24103800	-2.69029200	0.80428800
H	0.41844200	-1.38825000	1.69863300
O	3.19320900	-0.05985300	-0.92280700
O	-0.74285000	-2.34656800	0.26670300
O	-1.66276500	2.21883000	0.05349400
O	0.00229200	0.13966000	-0.44520600
H	-1.01071200	-3.09496300	0.81004900
H	2.28592400	1.98519100	1.06445100
K	-2.65207600	-0.39555000	-0.31019500

K(I)/(17)

E = -1133.948460
H = -1133.946011
G = -1134.150496

C	-1.59134000	-1.13887300	0.66221100
C	-2.28436600	0.13313200	0.26130500
C	-1.12731600	0.87253400	-0.44044900
C	-0.40768100	-1.19668900	0.06662100
C	0.59607900	-2.29069400	0.01732100
H	-2.02110300	-1.90748500	1.28460500
H	0.27914800	-3.08610900	0.69335900
H	0.64082900	-2.68618700	-1.00234900
O	1.86073100	-1.75916200	0.39700700
O	-0.08893800	-0.07787900	-0.66894800
H	2.51261000	-2.46739900	0.36342100
H	-2.66390800	0.70268900	1.11420400
O	-3.32739500	-0.05955500	-0.68263800
H	-4.08282100	-0.45400700	-0.23247600
K	2.58714400	0.73883400	-0.33403200

C	-0.61772400	2.00966700	0.41089400
O	0.50638400	2.07881200	0.83240100
H	-1.36297100	2.79132000	0.63191800
H	-1.46969600	1.27714900	-1.39607800

K(I)/(18)

E = -1057.567954
H = -1057.565510
G = -1057.749775

C	-2.49822600	0.08125600	-0.18317300
C	-2.14783900	-1.29777800	-0.21208200
C	-0.80897600	-1.35685300	0.03385500
C	-1.34895900	0.75715100	0.09047500
C	-1.01809100	2.19221300	0.30025400
H	-3.46867600	0.51867500	-0.34778200
H	-1.77067200	2.80504000	-0.19930500
H	-1.03780000	2.41955300	1.37082700
O	0.28235200	2.41292500	-0.22935200
O	-0.32023800	-0.10082700	0.22798800
H	0.52647600	3.33016700	-0.06604700
H	-2.79285700	-2.13870200	-0.41034300
K	2.32732500	0.42686700	-0.10817700
C	0.16130100	-2.42771000	0.04494700
O	1.35444400	-2.22369800	0.16867700
H	-0.24336400	-3.44207400	-0.07614200

K(I)/(19)

E = -943.081178
H = -943.078729
G = -943.233141

C	-2.63410400	-0.81420200	0.00011000
C	-2.31371300	0.57089800	-0.00019100
C	-0.95349200	0.64787200	-0.00027100
C	-1.44542900	-1.47109000	0.00019800
H	-3.61164700	-1.26486100	0.00025700
O	-0.41309900	-0.60339200	-0.00003200
H	-1.18681700	-2.51683800	0.00038000
H	-2.99166700	1.40916400	-0.00044200
C	-0.05735200	1.77993200	-0.00001200
O	1.15463000	1.67733200	0.00038700
H	-0.55024000	2.76251800	-0.00021500
K	2.46487700	-0.69799800	-0.00009600

K(I)/adduct (5)+(19)

E = -1553.567612
H = -1553.565164
G = -1553.879018

C	2.07946000	-2.77494000	-0.25200400
C	1.82034300	-0.25456600	0.76983400
C	0.53950400	-0.90838400	0.28508400
C	0.83400700	-2.33901500	-0.09033000
C	2.97095300	-0.59365600	-0.16251700
C	4.29055400	0.05553600	0.21488200
H	-1.28590400	-0.85186400	0.96281000
H	2.31007400	-3.80020100	-0.50755900
H	-1.02123400	-2.71637500	-0.44976100
H	0.86902600	1.30248400	1.39301000
H	5.20431700	1.73532800	-0.16899800
H	2.05605100	-0.66551000	1.75990600
H	0.17113500	-0.35936700	-0.59165800
H	2.71252000	-0.31479100	-1.19371500
H	4.40894600	0.06463800	1.30248900
H	5.09061100	-0.54536200	-0.22302900
O	-0.39660600	-0.78945400	1.34181700
O	-0.21196200	-3.20692400	-0.23506100
O	1.65771100	1.14931500	0.85566100
O	4.32139700	1.37727700	-0.30816500
O	3.20100400	-1.99572700	-0.10250100
C	-5.67069600	1.62162300	0.09238300
C	-5.41688500	0.54706300	-0.79669800
C	-4.22237300	0.00796300	-0.41023500
C	-4.61253800	1.65039600	0.94875400
H	-6.51941100	2.28370200	0.10298700
O	-3.72639200	0.68381900	0.66013200
H	-4.36791100	2.28328700	1.78567300
H	-6.02709300	0.20591400	-1.61759700
C	-3.47618500	-1.09840100	-0.93882000
O	-2.40419800	-1.46820000	-0.48592200
H	-3.93565500	-1.60816300	-1.79566000
K	2.42052800	3.23703800	-0.65939900

K(I)/(20)

E = -1553.577832
H = -1553.575383
G = -1553.883230

C	1.50232900	-1.71085700	-0.29668900
C	1.02934400	0.96104600	0.07833700
C	2.38805200	0.45376900	0.52223200
C	2.53278400	-0.97689900	0.10899900
C	-0.02845100	-0.07936500	0.43096100
C	-1.43733100	0.38580000	0.10510800
H	3.29249300	2.13246600	0.16531600
H	1.59606200	-2.74219600	-0.61256600
H	3.85241700	-2.38730300	0.02414300
H	0.21063300	2.73068300	0.20503200
H	-1.26503400	0.07947700	-1.80745300
H	1.05010300	1.08941900	-1.00824600
H	2.46156000	0.53853600	1.61402100
H	0.03664900	-0.33308700	1.49501300
H	-1.66549400	1.25300800	0.72899200
O	3.43465600	1.20808600	-0.07522500
O	3.82184200	-1.44048400	0.20801100
O	0.81757000	2.19702400	0.72928300
O	-1.54076300	0.80904400	-1.23737700
O	0.21151500	-1.25497700	-0.34287100
C	-5.91547000	0.62141300	-0.05141400
C	-4.78133100	0.46065100	0.81185500
C	-3.86073900	-0.22989900	0.09670500
C	-5.58888100	0.01595300	-1.21520000

H	-6.84510200	1.11823600	0.17036100
O	-4.34115800	-0.51278800	-1.13939200
H	-6.10749200	-0.12590800	-2.14772100
H	-4.66662700	0.80980100	1.82475200
C	-2.47890700	-0.69697400	0.41843200
O	-2.34332900	-0.98170800	1.79716700
H	-3.00823000	-1.63399900	2.04406500
H	-2.25676600	-1.57851300	-0.19486300
K	5.92967200	0.19094600	-0.42492500

K(I)/(21)

E = -1477.177202
H = -1477.174753
G = -1477.459261

C	1.58995700	2.00491100	0.14879000
C	0.76318700	-0.61888400	0.30085300
C	2.19035100	-0.37905700	-0.16931100
C	2.51907800	1.07873000	-0.05940100
C	-0.14551800	0.46710500	-0.26730100
C	-1.57846000	0.25667100	0.11088600
H	3.04657400	-0.96996000	1.49334400
H	1.81375300	3.05966600	0.24783900
H	4.03098700	2.28643600	-0.15256500
H	0.87551300	-2.55184300	0.19453400
H	-2.66668700	0.01720300	1.66768300
H	0.73362100	-0.54356900	1.39569300
H	2.28323200	-0.71269000	-1.20744300
H	-0.05442000	0.48333000	-1.35880100
O	3.11009200	-1.19141600	0.55448800
O	3.86027400	1.33832600	-0.20522300
O	0.27978100	-1.86727900	-0.13269400
O	-1.73327200	0.14894600	1.45046000
O	0.25258100	1.73686100	0.25146800
C	-6.17310000	-0.33221200	-0.53016000
C	-5.03212800	-0.13304000	-1.37106900
C	-3.95632000	-0.02375700	-0.54620800
C	-5.71561600	-0.33032100	0.74094600
H	-7.19803400	-0.45932400	-0.83560200
O	-4.36747400	-0.14336900	0.75278400
H	-6.18604800	-0.44250800	1.70231100
H	-5.00788100	-0.07803000	-2.44674500
C	-2.55183600	0.18630900	-0.80634700
H	-2.27723600	0.29178500	-1.84649200
K	5.68069600	-0.71662000	-0.29126700

K(I)/(22)

E = -1477.173525
H = -1477.171077
G = -1477.456385

C	-1.39368300	1.80060300	-0.29693200
C	-0.86414400	-0.91457700	-0.16332100
C	-2.27957200	-0.46867500	0.17504200
C	-2.43034300	1.00303000	-0.06924600
C	0.12837900	0.11199900	0.36712900
C	1.54966600	-0.30650100	0.16265200
H	-3.09869100	-1.10121900	-1.49082400
H	-1.48298900	2.86217300	-0.48793800
H	-3.80092100	2.36802800	-0.16255700
H	-1.23103100	-2.79823000	0.11825800
H	-0.75380900	-0.95498800	-1.25652500
H	-2.47646300	-0.69283800	1.22795100
H	-0.08485500	0.28382400	1.43298900
H	1.74446200	-1.35880500	0.01659500
O	-3.24522700	-1.22771000	-0.54379000
O	-3.73678500	1.41620000	-0.01719800
O	-0.57065700	-2.16216900	0.41821800
O	-0.09468900	1.35778400	-0.31612400
C	6.17401700	-0.13731000	-0.18022700
C	5.12559700	0.82513600	-0.03186900
C	3.97033200	0.11428500	0.03586700
C	5.57105500	-1.34868900	-0.19070800
H	7.23107300	0.04972600	-0.26717400
O	4.22855400	-1.21395500	-0.05837800
H	5.93857200	-2.35656200	-0.27942900
H	5.21070500	1.89748700	0.01658700
C	2.58600500	0.53783500	0.18951900
O	2.49834400	1.88195000	0.36511900
H	1.57496200	2.14883400	0.24255400
K	-5.80164200	-0.42458200	0.11154200

K(I)/(23)

E = -1477.179316
H = -1477.176867
G = -1477.463427

C	1.84674800	2.10701500	-0.24631000
C	0.65150700	-0.27990900	0.42798000
C	2.09443900	-0.35265400	-0.04791600
C	2.62999800	1.03427100	-0.24255100
C	-0.08377600	0.78981200	-0.37805000
C	-1.55180500	0.82840400	0.04414600
H	2.89193800	-0.67362700	1.71567400
H	2.21888800	3.11689300	-0.36010600
H	4.29741100	1.95900900	-0.57655600
H	0.46443700	-2.18402100	0.75538200
H	-2.52393300	0.54772500	-1.79005300
H	0.63787000	0.03935000	1.47944100
H	2.12864200	-0.90995700	-0.98918100
H	-0.00262400	0.56514600	-1.44905200
O	2.89254100	-1.11032700	0.85332300
O	3.99131200	1.05871900	-0.41300100
O	-0.01640600	-1.50710600	0.26381100
O	-1.88810800	1.46299700	1.00923100
O	0.48359800	2.05673500	-0.11358700
C	-5.85912200	-0.35534900	0.67529500
C	-4.57916700	0.29163000	0.74652900
C	-3.85057700	-0.19413900	-0.28790400
C	-5.80586500	-1.17797400	-0.39364000
H	-6.69797400	-0.22052200	1.33740200
O	-4.59060600	-1.09324100	-0.99321800

H	-6.50814400	-1.86078700	-0.84022400
H	-4.24672800	1.01757400	1.46637100
C	-2.48167400	0.02643700	-0.82411100
H	-1.99640700	-0.93218300	-1.03319200
K	5.48914500	-1.24800400	-0.07416800

K(I)/(24)

E = -1477.189568
H = -1477.18712
G = -1477.472486

C	0.73601700	-1.46658900	0.26433200
C	0.95025600	1.16869200	-0.52005800
C	2.21994400	0.50241000	-0.00848900
C	1.96111200	-0.95268800	0.24235300
C	-0.23347800	0.67871800	0.29890500
C	-1.53817600	1.34244100	-0.09855000
H	3.08226000	0.32568800	-1.76202600
H	0.53447600	-2.51777800	0.42808700
H	2.90312600	-2.58955400	0.66849400
H	1.82594600	2.86610800	-0.85869400
H	0.78894100	0.86532400	-1.56504800
H	2.52771200	0.99575500	0.91881200
H	-0.03552800	0.85178300	1.36439300
H	-1.73689500	1.16370300	-1.15467400
O	3.30855200	0.70747600	-0.90345100
O	3.11187000	-1.67204500	0.45480900
O	1.02518300	2.57008500	-0.40942200
O	-0.40030700	-0.72409800	0.09173300
C	-5.48174400	-1.24296200	-0.31434600
C	-4.81084900	-0.57276700	0.74380000
C	-3.71548600	0.01844500	0.18833200
C	-4.74272000	-1.00829000	-1.43130100
H	-6.38836100	-1.82156000	-0.26066200
O	-3.67213600	-0.24741700	-1.14690900
H	-4.85353400	-1.30821400	-2.45980900
H	-5.08852300	-0.52626800	1.78384800
C	-2.65402500	0.82468100	0.78625800
O	-2.66135500	1.05729100	1.97936800
H	-1.44843300	2.41555600	0.07334900
K	5.58153800	-0.52649600	0.07302600

K(I)/Transition states

K(I)/AG-ts1

E = -1286.703826
H = -1286.701378
G = -1286.944157

C	-0.72961900	-0.43334800	0.85237600
C	0.00869300	-1.40318800	-0.06552200
C	1.51201400	-1.32728700	0.11007100
C	1.99123400	0.05786600	-0.28145700
C	1.46806800	1.10003600	0.69681700
H	-0.84564000	-0.84657100	1.85901400
H	1.77975500	-1.53067900	1.15669200
H	1.63294000	0.27867300	-1.29422400
H	2.03702300	1.01664600	1.62456500
H	-0.23967400	-1.14519900	-1.10015300
O	0.08092300	0.87154800	1.02967600
O	-1.78963400	0.19616400	0.32443200
H	-0.83653600	1.17878700	0.41754400
O	-0.38270000	-2.73067300	0.22910300
H	-1.21433200	-2.92735500	-0.21448900
O	2.16222900	-2.24066200	-0.74769200
H	1.77096800	-3.11110400	-0.60221500
O	3.39743700	0.15296700	-0.22352100
H	3.75796000	-0.57899100	-0.73921900
C	1.55667500	2.51374400	0.17046500
H	2.59702700	2.70985100	-0.10213800
O	0.69179300	2.59879000	-0.94832000
H	0.68128000	3.50585800	-1.26859800
H	1.25405600	3.21169800	0.95520300
K	-4.23671600	0.23191500	-0.36304800

K(I)/AG-ts2

E = -1286.702294
H = -1286.699846
G = -1286.934720

C	-0.33614100	1.53274500	0.90336400
C	-1.04989000	-0.83640200	0.74703400
C	-2.09744100	0.07494700	0.10543000
C	-1.34281600	1.35478500	-0.23727000
C	-0.19078400	-1.61182100	-0.25943000
H	-0.70688400	2.19621200	1.69097600
O	0.96813200	1.59445500	0.61518800
H	0.79393400	0.34263800	1.16300500
C	1.03353700	-2.24544700	0.38080800
H	1.39781200	-3.02446400	-0.29189000
H	0.76478600	-2.70077800	1.33798600
O	2.02353600	-1.23582800	0.56248600
H	2.70070000	-1.57076300	1.16034900
O	-2.27816000	2.40229500	-0.33727000
H	-1.87900400	3.14898000	-0.79625000
H	-0.78925400	1.22184000	-1.17175600
O	-2.67867900	-0.55858800	-1.00907600
H	-3.42076200	-0.03093900	-1.32485900
H	-2.85751600	0.32484900	0.85333400
O	-0.95391400	-2.67893500	-0.77640100
H	-1.74709400	-2.30305000	-1.18155900
H	0.14973600	-0.94588600	-1.06385100
O	-0.27454900	0.10418200	1.53249200
H	-1.49285500	-1.55218500	1.43956100
K	2.97561500	0.96105500	-0.86073700

K(I)/AG-ts3

E = -1286.694477
H = -1286.692029
G = -1286.928520

C	0.72354000	-1.15072900	1.15344000

C	0.53394100	-1.79533200	-0.18301000
C	1.27059600	-0.83435200	-1.13941800
C	1.95894200	0.18798600	-0.19560600
C	1.47438100	1.63032300	-0.29810900
C	0.06933800	1.78249400	0.31912600
O	-2.02716800	-0.54506900	1.77900300
O	1.21664400	-3.02775400	-0.08906500
O	0.41596900	-0.24705800	-2.07105400
O	2.39470400	2.52876500	0.28413800
O	1.59640500	-0.26251600	1.18631600
O	-0.76622400	0.72368700	-0.01712700
H	-0.51603500	-1.90419800	-0.44798200
H	0.30120700	-1.48559000	2.09652600
H	2.02807200	-1.40252400	-1.67733400
H	-1.48760100	0.06329200	1.17831200
H	3.04440800	0.14153200	-0.21387400
H	1.45120800	1.86535900	-1.36316500
H	0.21251200	1.84882400	1.41251300
H	-0.32838800	2.75526900	0.00260000
H	0.61108000	-3.71610700	0.21157200
H	-0.25500500	0.21647500	-1.49684800
H	-2.18111300	-0.07242600	2.60217300
H	2.30015300	2.49908700	1.24368900
K	-3.36882000	0.36359000	-0.52970600

K(I)/AD-ts1

E = -1286.684779
H = -1286.682331
G = -1286.921771

C	0.32862700	-1.06075900	1.35175700
C	0.34958600	1.31110800	0.89475400
C	1.23739800	-1.36158900	0.27862500
C	2.15140300	-0.19960200	-0.06446700
C	1.30218100	1.04167000	-0.27638500
C	-0.89582600	2.08712400	0.51493000
O	-1.03879600	-0.77472700	-1.25408500
O	-0.13949900	0.08123000	1.57379900
O	1.87379100	-2.58533900	0.48042200
O	2.83181800	-0.55896200	-1.24180300
O	2.17690200	2.14654000	-0.38518100
O	-1.73845600	1.40665700	-0.36564900
H	0.40012700	-1.37496600	-0.53119500
H	0.89393300	1.83080300	1.68331200
H	-0.95484800	-0.79964700	-2.21213700
H	2.25081000	-2.86309100	-0.36255100
H	-0.08987700	-1.85525600	1.96811100
H	2.86058100	-0.02959700	0.75439500
H	3.48237800	0.12635200	-1.43573200
H	0.73477300	0.90038100	-1.19683100
H	1.87105900	2.73467600	-1.08245500
H	-1.43632600	2.33502300	1.43383100
H	-0.53700700	3.03328600	0.08710000
H	-1.32767700	0.52690500	-0.80205700
K	-3.51127500	-0.69451500	-0.26100600

K(I)/AD-ts2

E = -1210.234019
H = -1210.231571
G = -1210.455741

C	2.03465900	1.25315700	-0.86805300
C	-0.12179000	1.03975600	-0.00850200
C	2.34077500	-0.00379500	-0.54796800
C	1.54876400	-0.75034300	0.44300500
C	0.33869800	-0.11645100	0.85782000
C	-1.20251400	1.88151700	0.63766600
O	0.97588900	1.89913000	-0.24653100
O	3.37544200	-0.71547800	-1.08419300
O	2.28776500	-1.37068400	1.47484400
O	-0.74307400	-1.44882400	0.30593900
O	-2.34881600	1.05738800	0.79533100
H	-0.47269800	0.64136800	-0.96878400
H	3.94521000	-0.13179400	-1.59894100
H	2.55919400	1.86104400	-1.59290000
H	0.41338500	-1.59862800	0.00099400
H	2.59260300	-2.22588500	1.15840400
H	0.06896600	-0.09843000	1.90986200
H	-0.92619600	-2.02207100	1.06780000
H	-0.84742000	2.24804200	1.60461000
H	-1.41608000	2.73571600	-0.00850900
H	-3.00931600	1.54210600	1.30078300
K	-3.20614900	-0.95509300	-0.83790800

K(I)/AD-ts3

E = -1133.859128
H = -1133.856680
G = -1134.057274

C	-0.61974600	1.68870600	0.16102000
C	-2.05565400	-0.05234900	-0.64978200
C	0.50359900	0.96400000	-0.10516100
C	0.30640900	-0.42478100	-0.26070100
C	-0.98915000	-1.02305400	-0.25904200
C	-3.46949500	-0.46900900	-0.31595000
O	-1.85103300	1.23912000	0.06170700
O	1.77569100	1.49327700	-0.03834800
O	1.20765200	-1.33322900	-0.41807700
O	-3.61992700	-0.83833600	1.03970900
H	-1.99619300	0.22039100	-1.70803300
H	1.92089200	2.10284700	-0.77198800
H	-0.55933100	2.72309500	0.48538800
H	0.13557000	-1.94659200	-0.68144900
H	-1.16581200	-1.52320200	0.69674200
H	-4.15585600	0.33973600	-0.58215700
H	-3.71747100	-1.34486500	-0.91565500
H	-3.48234000	-0.05433600	1.58293200
K	3.72977400	-0.47920000	0.27957800

K(I)/LG-ts

E = -1286.699677

H = -1286.697228
G = -1286.935884

C	-1.03487000	-0.99050500	-1.74705900
C	-0.28067200	1.38926200	-1.01985300
C	-1.42153100	0.45866300	-1.38074300
C	-1.74634700	0.03674900	0.88907900
C	0.56683700	0.85499900	0.14439000
C	-0.34601900	0.40570800	1.29879800
H	-0.21668600	3.25649500	-0.43109600
H	-2.11014300	-3.57361400	1.23090600
H	0.74863100	-0.96357100	-0.44819000
H	-0.59435200	1.11831800	3.11493600
H	-1.60816200	-2.43584300	0.28167600
H	-1.94075300	-1.48057300	-2.12528800
H	-0.32712300	-0.90893700	-2.58546200
H	0.35855200	1.48465300	-1.90310700
H	-2.06855600	0.91964300	-2.12293200
H	-2.43716700	-0.29964900	1.65850800
H	1.17306100	1.67783000	0.52999600
H	0.10227600	-0.46744400	1.77608300
O	-0.89517600	2.61620900	-0.67245600
O	1.41509800	-0.18139000	-0.26476200
O	-0.55553100	1.46641300	2.21668500
O	-0.50807700	-1.63873000	-0.65226200
O	-2.28547100	0.28090000	-0.21177700
O	-2.33480700	-2.69736000	0.90700800
K	3.98988100	-0.52762600	0.07035800

K(I)/LO-ts1

E = -1210.251364
H = -1210.248916
G = -1210.456463

C	-0.27747700	1.23148900	-0.63732100
C	-0.49491100	-0.04476300	-1.39219200
C	-0.53089700	1.03405800	0.80817100
O	0.16128300	-1.17233500	-0.77203700
O	-1.87463000	-0.40939300	-1.37372600
C	-0.48464300	-0.38105000	1.40277000
C	-0.70079100	-1.44537900	0.32883000
C	-2.07255500	-1.36296300	-0.33155500
H	-1.90766800	1.91244100	-0.08008900
H	-0.13586700	0.01090500	-2.41903700
H	0.03177900	1.72917900	1.42682800
H	-1.20285500	-0.51553700	2.21475100
H	-0.46297200	-2.42769500	0.73141700
H	-2.35619000	-2.32357500	-0.76305000
H	-2.85423900	-1.01746900	0.34630500
O	1.04607000	1.73394700	-0.88412500
H	0.97370000	2.57006100	-1.34891300
O	-2.03741800	1.51782300	0.87006100
H	-2.20455300	2.20944800	1.53565800
O	0.84946800	-0.57468500	1.86235300
H	0.96868100	-0.11965600	2.70359500
K	2.70313900	-0.26206900	-0.15999400

K(I)/LO-ts2

E = -1133.857524
H = -1133.855076
G = -1134.047662

C	0.01600800	0.97244800	0.53170200
C	0.03782100	-0.41160700	1.14294800
C	-1.02417300	1.37633000	-0.29804600
O	-1.25776200	-0.90989000	1.19549200
O	0.72240000	-1.21979500	0.19699800
C	-2.02810600	0.32896200	-0.73754900
C	-1.59277000	-1.03484500	-0.19275500
C	-0.26968400	-1.54565200	-0.79987800
H	0.52837500	-0.45412000	2.11369300
H	-1.34178600	2.41549200	-0.22058100
H	-2.06478400	0.26397900	-1.83012600
H	-2.40909100	-1.74620700	-0.28110400
H	-0.26831000	-2.62445200	-0.93097000
H	-0.02670200	-1.05158100	-1.74152000
O	1.07928800	1.70020300	0.44798700
H	0.27599000	1.95368700	-0.59973200
O	-3.32885200	0.56640800	-0.22549200
H	-3.65939700	1.39661500	-0.58499900
K	3.17950200	0.03354500	-0.35384600

K(I)/LO-ts3

E = -1133.889638
H = -1133.887190
G = -1134.077633

C	-0.11494000	-1.03647600	0.29615000
C	-0.09345700	0.31381300	1.02277600
C	1.00222300	-1.31138900	-0.53496000
O	1.19893400	0.79786100	1.22770300
O	-0.70464700	1.23751000	0.12500000
C	1.98038100	-0.20561400	-0.78153200
C	1.62210500	1.09816500	-0.09945200
C	0.35612800	1.72747400	-0.71279800
H	-0.64659300	0.28491400	1.95957900
H	2.31080900	-1.58556400	0.20810800
H	2.30929300	-0.06810700	-1.80852400
H	2.46908700	1.77713600	-0.05349100
H	0.37750400	2.81256900	-0.64114100
H	0.19323100	1.42165800	-1.74678200
O	-1.13394400	-1.72424700	0.42492800
H	0.88841300	-2.07180400	-1.29819200
O	3.15583400	-0.79236100	0.00812500
H	3.86116500	-1.12100800	-0.57467200
K	-3.17931400	-0.05872300	-0.28800100

K(I)/Ch-tsF

E = -1210.271094
H = -1210.268646
G = -1210.486027

C	0.77097800	0.28543600	-1.60324600
C	1.85506000	-0.64065700	0.70992000
C	1.41434200	0.82409500	0.76255800
C	0.58358300	1.17644300	-0.47381700
C	0.93009600	-1.52148500	-0.12228300
C	-0.53285100	-1.71608000	0.34304100
H	3.49725300	-1.51264200	0.07661400
H	1.86866500	-1.04631700	1.72576500
H	-0.45357500	0.78143700	-0.19427800
H	1.40122800	-2.49283800	-0.27200100
H	-0.86886700	-2.65326600	-0.13533300
H	-0.42757100	-1.95144600	1.42020200
O	3.15055700	-0.61522900	0.13595700
O	-1.36978600	-0.67347700	0.06918200
O	0.90085600	-0.95592300	-1.49116400
O	0.65744600	2.51228400	-0.87706700
H	0.01451100	3.02307400	-0.37464400
O	0.61293900	1.12742200	1.88214300
H	1.18276500	1.23595600	2.65133500
H	2.31562800	1.44126400	0.74670300
H	0.72571600	0.65962900	-2.62483200
K	-3.73679400	0.04779100	0.08058000

K(I)/Ch-tsR

E = -1210.271093
H = -1210.26865
G = -1210.485995

C	0.77087300	0.28549000	-1.60318200
C	1.85516700	-0.64068900	0.70982000
C	1.41436000	0.82402300	0.76263400
C	0.58358300	1.17646300	-0.47370700
C	0.93009800	-1.52147000	-0.12231400
C	-0.53282400	-1.71597800	0.34319700
H	1.18272000	1.23542100	2.65150500
H	0.72553100	0.65972300	-2.62474900
H	0.01462300	3.02312300	-0.37443300
H	3.49725600	-1.51253100	0.07604600
H	-0.45358800	0.78150000	-0.19417600
H	1.86895100	-1.04643700	1.72562900
H	2.31560500	1.44125600	0.74684400
H	1.40117200	-2.49284000	-0.27209400
H	-0.86887200	-2.65331900	-0.13484300
H	-0.42744100	-1.95098900	1.42042600
O	0.61292600	1.12714900	1.88225100
O	0.65748900	2.51231400	-0.87691700
O	3.15056900	-0.61513200	0.13565700
O	-1.36979700	-0.67347000	0.06908900
O	0.90075300	-0.95587500	-1.49115900
K	-3.73679100	0.04779800	0.08051500

K(I)/HM-ts1

E = -1286.697301
H = -1286.694853
G = -1286.942384

C	0.88973200	1.96944800	-0.30108400
C	1.04427300	0.58806000	0.03100200
C	-0.08306500	-0.42400800	-0.16035400
C	-1.48027200	0.13940100	0.03134300
C	-2.53948300	-0.96923800	-0.08329600
H	-0.04109000	2.52387200	-0.28241800
H	-0.00728800	-0.78095200	-1.19397200
H	-1.66857200	0.84709700	-0.78510000
H	-2.22255000	-1.84365800	0.48570600
H	0.76746800	1.15133100	1.07381200
O	-2.62943800	-1.37875000	-1.43863200
O	1.97832400	2.62968800	-0.48403600
H	-3.07654400	-0.67623300	-1.92788700
O	2.27125200	0.13547700	-0.00736100
H	2.68725100	1.93187000	-0.48050700
O	0.13727200	-1.48805200	0.74076900
H	1.09211800	-1.64080700	0.75071000
O	-1.53278400	0.81273900	1.27714300
H	-2.34218900	1.33899400	1.29095000
C	-3.87965000	-0.50691000	0.44748300
H	-3.83985500	-0.40619900	1.53507000
O	-4.16057700	0.74693200	-0.16927200
H	-5.07099000	0.99607600	0.01687800
H	-4.63687500	-1.25093700	0.18949200
K	4.53355300	-0.98080200	0.00988500

K(I)/HM-ts2

E = -1286.712151
H = -1286.709703
G = -1286.944920

C	0.04332000	-1.00419700	-0.42033500
C	0.83766200	1.10480300	0.69410500
C	1.58954800	-0.11120100	1.25026100
C	1.43440800	-1.22092700	0.20762000
H	2.64497600	0.11306600	1.42450100
H	1.49018200	-2.20114700	0.68925100
C	1.64127300	2.11966300	-0.10220300
H	1.00656000	2.98092900	-0.31118200
H	2.47405100	2.45614000	0.52346100
O	2.07300700	1.63223100	-1.35100700
H	2.59389500	0.82719000	-1.21111100
C	-1.09946100	-1.78546200	0.18292200
H	-1.18324700	-1.58554900	1.25114500
H	-0.88555600	-2.84940200	0.03821600
O	-2.31272200	-1.41745800	-0.44009300
H	-2.15178300	-1.46064200	-1.39396700
O	0.92722200	-0.46631400	2.44853700
H	1.42058400	-1.17004900	2.88544600
O	2.42013000	-1.09973500	-0.78935200
H	1.94462400	-1.20303300	-1.63469200
O	-0.20205200	0.53530700	-0.14573900
O	0.02571300	-0.88043600	-1.75006800
H	0.34601400	1.61276000	1.52407000
H	-0.01044000	0.40602400	-1.28070400

K	-3.14846000	1.10678400	0.14963800

K(I)/HM-ts3

E = -1286.669875
H = -1286.667426
G = -1286.921485

C	-0.13677300	0.85337800	-0.49933500
C	-0.70131900	-1.22209200	0.16139500
C	-1.83199400	-0.31267200	0.63727700
C	-1.20928200	1.07970300	0.53418800
H	-0.69192900	1.32384000	1.46911500
C	-1.10439600	-2.49095000	-0.53039900
H	-0.21076000	-3.00764200	-0.89142600
H	-1.59226500	-3.12224400	0.21944600
O	-1.97687000	-2.16071700	-1.59020500
H	-2.25531700	-2.97055100	-2.02865100
C	0.77980100	1.85489400	-0.98391900
H	1.23625400	1.62641400	-1.94632000
H	1.52503200	1.58413100	-0.12418200
O	0.34190300	3.17496300	-0.81127300
H	-0.07503900	3.47947000	-1.62520000
O	-2.15343800	2.03907100	0.15070700
H	-1.73413900	2.90863700	0.18384400
O	0.03958100	-0.37097800	-0.78247200
H	-0.00405400	-1.41071200	0.98208900
O	1.82160800	0.57260100	1.18931200
H	1.98822000	1.00854100	2.02964800
O	-2.20087600	-0.70239500	1.93146500
H	-3.07977200	-0.36039200	2.12633200
H	-2.67049600	-0.37151400	-0.06277700
K	3.46383000	-1.03589000	0.16066200

K(I)/HM-ts4

E = -1210.242061
H = -1210.239612
G = -1210.467020

C	-1.15197300	-0.53869300	-0.66033000
C	0.03965800	-0.53215800	0.10804500
C	0.37599100	0.77626300	0.81356400
C	1.45625200	1.31770700	-0.12319300
H	-1.29421700	-0.51394200	-1.73953300
H	2.11191600	2.02099900	0.39539800
O	0.76668000	1.93402800	-1.19328900
O	-2.14966600	-0.65201600	0.13227400
H	1.40255800	2.19768000	-1.86670400
H	-1.18183600	-0.88520900	0.92618700
C	2.18316300	0.04875500	-0.57419900
O	1.21056100	-1.01250200	-0.47211500
H	2.46569000	0.13300100	-1.62793100
C	3.41606900	-0.29051400	0.23163000
H	4.08726100	0.57494000	0.22689000
H	3.13102800	-0.51431000	1.26198500
O	4.03492100	-1.40867600	-0.38672700
H	4.75995600	-1.70583800	0.17100900
O	0.98986000	0.58647400	2.07242500
H	0.43488000	0.00220800	2.60046500
H	-0.47828800	1.45322100	0.87438500
K	-4.85119800	-0.15944100	-0.06398900

K(I)/HM-ts6

E = -1210.271154
H = -1210.268705
G = -1210.487686

C	0.03447300	-2.25041500	-0.52071600
C	-1.83320400	0.83245500	-0.12079900
C	-1.97319700	-0.70069400	-0.09080700
C	-0.60493200	-1.21124600	0.20850100
C	-0.31332000	0.99404400	-0.20825900
C	0.23991900	2.28095600	0.33436800
H	-0.64485700	-3.02152400	-0.92366200
H	-3.37110600	1.56168900	-1.07250500
H	-2.19541800	1.26638400	0.81884600
H	-0.02173900	0.87491400	-1.26232900
H	-0.20283400	3.12081000	-0.20748300
H	-0.00443400	2.36557300	1.39757200
O	-2.42886800	1.44147200	-1.23242400
O	1.64871200	2.22715000	0.14307100
O	1.25430200	-2.36893300	-0.65071200
O	0.19555200	-0.09312200	0.55622600
H	2.04039600	3.05497200	0.43912100
H	-2.51971400	-1.11103100	-0.93402000
H	-1.60429300	-1.62133200	1.35134100
O	-2.67733400	-1.24368500	1.14820300
H	-3.02218000	-0.56356500	1.75353100
K	2.85835900	-0.27897600	0.06899700

K(I)/HM-ts7

E = -1210.244635
H = -1210.242187
G = -1210.462056

C	-0.08212100	2.37396900	-0.37538400
C	1.92566000	-0.65595000	0.26102500
C	1.83274900	0.86611700	0.29184000
C	0.66980400	1.10510200	-0.68019800
C	0.62766400	-1.16311400	-0.19154600
C	-0.18179800	-1.99229000	0.75244200
H	0.51025400	3.30231700	-0.40431400
H	3.22104900	-0.44868400	-1.52541300
H	2.43021000	-1.11253100	1.10605300
H	1.91086500	-1.53358200	-1.34472700
H	0.41558500	-2.83232100	1.11837300
H	-0.52869700	-1.41307500	1.61827000
O	2.83423900	-1.14957100	-0.96761700
O	-1.38528900	-2.45276300	0.12803300
O	-1.26053500	2.38975200	-0.13078100
O	-0.17407100	0.00108200	-0.54361200
H	-1.13082800	-2.84715700	-0.71559100
H	2.74383100	1.39340900	0.00497300
H	1.06768500	1.18956100	-1.70433700

O	1.38883800	1.24611200	1.57716500
H	2.12638400	1.20799300	2.19651100
K	-2.77597600	-0.02030700	-0.06338900

K(I)/HM-ts8

E = -1133.852501
H = -1133.850052
G = -1134.059867

C	0.48316000	2.54384200	-0.23006500
C	-2.21959400	0.02660800	-0.35351000
C	-1.81046800	1.40728200	-0.44741700
C	-0.46592700	1.41815300	-0.29347900
C	-0.99928300	-0.73356800	-0.15270700
C	-0.61421600	-1.99402700	-0.85486200
H	0.06102200	3.54655600	-0.38151100
H	-3.45205400	-0.83666100	1.57076500
H	-3.13048700	-0.36367300	-0.78445600
H	-1.60337700	-0.81987400	1.08134900
H	-1.44264400	-2.70413600	-0.79559600
H	-0.38224100	-1.80479900	-1.90826100
O	-2.69249700	-0.24802700	1.43811300
O	0.54734500	-2.49020100	-0.19103600
O	1.65810400	2.35893100	-0.02334500
O	0.07052200	0.20339200	-0.16094000
H	0.85755300	-3.27134300	-0.66151100
H	-2.44549400	2.26494300	-0.59539400
K	2.55936200	-0.55860600	0.41918500

K(I)/HM-ts9

E = -1133.873689
H = -1133.871240
G = -1134.072559

C	1.55555900	1.39747800	0.63402700
C	2.18254600	0.07022500	0.52035900
C	1.11723700	-0.75411400	-0.12782600
C	0.35253700	1.33300700	0.04770500
C	-0.67276100	2.38621900	-0.18123500
H	1.98801100	2.26439800	1.10462200
H	-0.41895100	3.26414000	0.41475700
H	-0.66775400	2.66308800	-1.24007900
O	-1.93691800	1.84797900	0.18670400
O	0.02793200	0.10785900	-0.42742000
H	-2.61570200	2.50263500	-0.00856400
H	2.74444300	-0.32730800	1.36017200
O	3.19106000	0.03133300	-0.69554200
H	4.00665700	-0.45221400	-0.47763100
K	-2.51558600	-0.85533700	-0.08256400
C	0.74362600	-2.07087500	0.27947900
O	-0.38006200	-2.54679500	0.15667400
H	1.57175600	-2.68267100	0.67520300
H	2.29911700	-0.67531900	-1.05813800

K(I)/FU-ts

E = -1057.446217
H = -1057.443768
G = -1057.629258

C	-0.63630600	1.55437900	0.14056100
C	-1.97504100	1.58632900	-0.21547300
C	-2.40114100	0.27191000	-0.12489400
C	-0.27893300	0.20148100	0.38148300
C	0.89418500	-0.33367700	1.20243500
H	0.06355000	2.37664800	0.17231600
H	1.02839300	0.23346700	2.13238300
H	0.63904300	-1.37001900	1.46608400
O	1.94012900	-0.20376200	0.29485600
O	-1.45288200	-0.54812200	0.24938500
H	0.52603600	0.02272900	-0.51243900
H	-2.57499600	2.43099400	-0.51114000
C	-3.74764700	-0.30489800	-0.42183900
O	-3.94718500	-1.48450500	-0.36643800
H	-4.52206700	0.42825300	-0.68620300
K	4.28362300	-0.21495300	-0.48721400

K(I)/Ch-ts1

E = -1553.446485
H = -1553.444037
G = -1553.744049

C	1.51694100	1.62878200	-0.12222900
C	2.17073400	-0.97967200	0.52069500
C	2.92984400	-0.34520100	-0.63401100
C	2.56036100	1.10573100	-0.75476900
C	0.71767200	-0.51228000	0.46162200
C	-0.13716700	-1.15016500	1.54277300
H	4.62095200	-0.11456500	0.33158300
H	1.24638600	2.67421600	-0.17170400
H	4.19874400	1.42835300	-1.65751100
H	3.09702700	-2.68131000	0.38544100
H	-0.04924600	0.42127700	2.62452000
H	2.60296000	-0.63516400	1.47053400
H	2.67366600	-0.87540600	-1.55644300
H	0.30801800	-0.76561500	-0.52825200
H	-1.18475800	-1.77119000	0.84726700
H	0.14701800	-2.20599000	1.66324700
O	4.33476800	-0.50567900	-0.50466500
O	3.34190400	1.86915800	-1.57461300
O	2.18034000	-2.38525600	0.43873700
O	-0.06719200	-0.53689500	2.77285500
O	0.65683300	0.88953600	0.65474500
C	-2.19709700	2.73386600	0.56766600
C	-2.33199000	1.65022800	1.48514000
C	-2.15078500	0.51733200	0.75771600
C	-1.95077200	2.17285100	-0.64118200
H	-2.28090400	3.78708500	0.77562700
O	-1.92769300	0.82345100	-0.54913000
H	-1.79536900	2.58434200	-1.62433100
H	-2.53892000	1.69678100	2.54235000

C	-2.08123500	-0.88703400	1.13053700
O	-2.35952200	-1.82796300	0.19122500
H	-2.40179700	-1.06556800	2.16023800
K	-2.74728000	-1.29972100	-2.34629200

K(I)/Ch-ts2G

E = -1553.471759
H = -1553.469311
G = -1553.772093

C	-1.22601800	-1.73944200	0.08857900
C	-1.14635200	1.00636300	0.35238100
C	-2.46144400	0.40957200	-0.11637800
C	-2.37002100	-1.08792400	-0.09195400
C	0.02615600	0.24122200	-0.26288700
C	1.34289900	0.83803400	0.10755200
H	-3.39400900	0.68415400	1.58494800
H	-1.16240600	-2.82036700	0.13230300
H	-3.48683700	-2.65669800	-0.30182200
H	-0.20573400	2.65725100	0.06350200
H	1.45325500	-0.07278300	1.82958800
H	-1.08049500	0.89738800	1.44440400
H	-2.66584100	0.75901100	-1.13299700
H	-0.09282800	0.22192000	-1.35383900
H	1.95800700	2.10681000	-0.61179000
O	-3.56784900	0.87031600	0.65329900
O	-3.58960600	-1.69798800	-0.27386900
O	-1.12402000	2.36390000	-0.01865700
O	1.56208500	0.83310700	1.50547300
O	-0.01318400	-1.12453500	0.21443000
C	5.48833400	-0.95208500	0.90656900
C	4.28515700	-0.19912700	1.05348100
C	3.69367600	-0.17928100	-0.17348200
C	5.53686200	-1.33148000	-0.39310800
H	6.21503400	-1.18093300	1.66759400
O	4.46294700	-0.86961500	-1.06494900
H	6.23873000	-1.91533800	-0.96413100
H	3.91025300	0.27808200	1.94146500
C	2.48080400	0.41656600	-0.72229200
O	2.86687900	1.98624000	-1.26938900
H	3.66141700	2.31954400	-0.81881600
H	2.21684200	-0.00806000	-1.68603100
K	-5.90756300	-0.24715200	-0.22399200

K(I)/Ch-ts2F

E = -1553.468538
H = -1553.466089
G = -1553.769531

C	1.53635900	1.75057300	0.54815800
C	0.96990200	-0.92735700	0.21170600
C	2.33074800	-0.44976100	-0.27298100
C	2.52866500	0.98702300	0.10521800
C	-0.07033900	0.14859200	-0.07137000
C	-1.47028000	-0.27931400	0.27272400
H	3.35149700	-1.25882400	1.19454100
H	1.66219700	2.78451900	0.84342800
H	3.91124500	2.34150900	0.16311600
H	1.26833300	-2.77162100	-0.31240600
H	-1.92049300	-1.32368100	2.10633700
H	1.01497800	-1.07284200	1.29971300
H	2.38138100	-0.56399600	-1.35993000
H	-0.06428300	0.39352500	-1.14269000
H	-1.68599300	-1.28147200	-0.09344800
O	3.37238200	-1.28049100	0.22821500
O	3.82303300	1.40888500	-0.06769200
O	0.57639800	-2.11132800	-0.43963400
O	-1.47851200	-0.48738600	1.87293900
O	0.24253100	1.31720900	0.67629600
C	-5.93460500	-0.18193200	-0.86974000
C	-4.89347700	0.80873500	-0.87381500
C	-3.83894800	0.25541400	-0.20784000
C	-5.44593700	-1.25575800	-0.21550000
H	-6.91752100	-0.10018300	-1.30509300
O	-4.16268900	-1.00712600	0.19632400
H	-5.84147400	-2.22600400	0.02886000
H	-4.91828100	1.79276000	-1.30861300
C	-2.52947400	0.74181600	0.18118000
O	-2.21316700	1.93666700	-0.50275900
H	-1.72937600	2.50558900	0.10220400
H	-2.20517600	0.31620300	1.81222900
K	5.85881400	-0.38605800	-0.55706300

K(I)/Ch-ts3G

E = -1477.07645
H = -1477.074002
G = -1477.358360

C	2.94950600	0.60484800	-0.45774100
C	0.89829800	-1.14791600	0.19866200
C	2.27472200	-1.74757400	-0.05136700
C	3.29136700	-0.65960900	-0.24799600
C	0.69807600	0.00554100	-0.79692500
C	-0.67537200	0.57684400	-0.70132600
H	2.67352400	-2.15447100	1.82697800
H	3.66514200	1.40316800	-0.59149900
H	4.65944500	-1.88967200	0.21948900
H	0.08905100	-2.87504000	0.52904600
H	-1.93162300	1.49580200	-0.82600100
H	0.86757900	-0.72435400	1.21236400
H	2.22392300	-2.37330400	-0.94786800
H	0.82882500	-0.38421300	-1.81577000
O	2.65956400	-2.63243500	0.98672700
O	4.60027700	-1.03877900	-0.23635000
O	-0.12207400	-2.09054900	0.00695300
O	-0.88003800	1.69809300	-0.11538200
O	1.63763600	1.03201800	-0.54059400
C	-4.39373500	-0.93970000	1.21229400
C	-3.00541900	-0.80192900	0.88172000
C	-2.95920100	-0.30215300	-0.38028100
C	-5.08125400	-0.53059200	0.12331100
H	-4.81647000	-1.31355200	2.13020300

O	-4.22597100	-0.12647100	-0.85229200
H	-6.12996300	-0.47972000	-0.11394200
H	-2.15035800	-1.06603700	1.48147200
C	-1.86696600	0.08558800	-1.28828300
H	-1.79721600	-0.47756800	-2.21403800
K	1.03594100	3.43388700	0.74550900

K(I)/Ch-ts3F

E = -1477.088237
H = -1477.085788
G = -1477.366836

C	0.88699100	-1.62924700	-0.03993600
C	1.00194900	1.05464500	-0.66627500
C	2.24305100	0.43946300	-0.03273100
C	2.06615000	-1.03802400	0.11780200
C	-0.24964900	0.45814300	-0.02955400
C	-1.51402900	1.07441100	-0.55111400
H	3.32304600	0.41727700	-1.67208700
H	0.74624300	-2.69963700	0.05479900
H	3.06393300	-2.62806200	0.59328500
H	1.86148100	2.78421900	-0.76954900
H	0.98858100	0.79606000	-1.73537500
H	2.40246600	0.90150400	0.94674700
H	-0.17785900	0.56113900	1.06086700
H	-1.65314400	0.90796400	-1.61678800
O	3.41421100	0.77020500	-0.77667500
O	3.23151200	-1.68878200	0.45123700
O	1.00016500	2.45125200	-0.48830800
O	-0.26716300	-0.95886700	-0.32690400
C	-5.76211300	-0.95279000	0.30134300
C	-4.99479700	0.08958600	0.87071700
C	-3.81217300	0.11681100	0.18169600
C	-4.99439800	-1.47501700	-0.69809800
H	-6.75034700	-1.27515300	0.58133200
O	-3.81728300	-0.84545000	-0.78493900
H	-5.16120000	-2.27127300	-1.40449700
H	-5.26497000	0.75082700	1.67768600
C	-2.65101700	0.93154400	0.31038500
O	-2.52844100	1.75421500	1.29421300
H	-1.63193700	2.13273400	0.51417000
K	5.61420500	-0.35028100	0.43342100

Ca(II)/intermediates

Local minima

Ca(II)/(2)

E = -1364.344778
H = -1364.342329
G = -1364.589269

C	2.31056600	-0.44610900	-0.69967300
C	1.20759700	-0.25550900	0.35560100
C	0.07868000	0.63127900	-0.17298900
C	-1.06054900	0.72161300	0.84063000
H	0.77953600	-1.24092800	0.56682200
H	-0.30220800	0.17239900	-1.09627300
H	-0.66392400	1.12332300	1.77281300
O	-1.59650400	-0.59559800	1.05457700
H	-1.45055800	-0.88511300	1.96142400
O	1.72889500	0.34452200	1.52640500
H	2.02435200	-0.33463200	2.14112700
O	0.49064900	1.96005000	-0.40497400
H	1.39542600	1.93514600	-0.74978300
C	-2.19978300	1.59370800	0.36322200
H	-1.81752300	2.54533300	-0.00042400
O	-2.84535600	0.87603300	-0.70206900
H	-3.37925200	1.47819800	-1.23150500
H	-2.91262300	1.75872600	1.17208000
C	3.39209500	-1.33257700	-0.13269500
H	3.09272800	-2.34820400	0.17230900
O	4.52008300	-0.93686800	0.00076600
O	2.85680400	0.77848200	-1.12297700
H	3.75549900	0.83734700	-0.76395100
H	1.87335400	-0.96703500	-1.56087300
Ca	-3.30015100	-1.44809800	-0.42610800

Ca(II)/(3)

E = -1364.355065
H = -1364.352617
G = -1364.58653

C	2.45601600	0.87349600	-0.53080100
C	0.25790600	0.04762800	-0.43108200
C	1.24143600	-1.13562900	-0.41697500
C	2.50451500	-0.50077200	0.12427600
C	-0.61250200	0.12320500	0.82709400
H	2.83116100	0.82169200	-1.55712100
O	3.19902600	1.86070600	0.09585800
H	2.90458900	1.93601400	1.01291800
C	-1.34442700	1.44060500	0.92966200
H	-0.61843300	2.25242100	0.98004000
H	-1.94793000	1.43786300	1.84159000
O	-2.18017900	1.57686300	-0.21771100
H	-2.48253100	2.48841500	-0.27582000
O	3.62829300	-1.27294800	-0.21195900
H	4.40193900	-0.91851300	0.23981100
H	2.41160300	-0.38194700	1.21216800
O	0.74543600	-2.20065600	0.36861300
H	1.34368200	-2.95204300	0.29338300
H	1.43320300	-1.47509800	-1.43967500
O	-1.59181500	-0.90683500	0.79671600
H	-1.11743500	-1.75003000	0.77849900
H	0.01889200	0.02290500	1.71785800
O	1.07659400	1.21689200	-0.51750300
H	-0.40190800	0.01041800	-1.29950000
K	-3.93754300	-0.46186600	-0.47522600

Ca(II)/(4)

E = -1287.948697
H = -1287.946248

G = -1288.149846

C	-0.44099400	-1.03440800	0.70053800
C	-1.88658100	-0.71778200	0.29296800
C	-1.72938500	0.29807400	-0.85238800
C	-0.20590400	0.47502900	-0.96218500
C	0.34802100	1.51147700	0.00485900
C	-0.09313000	1.18424900	1.42533900
O	-2.53322700	-1.86175700	-0.21613100
O	-2.41466400	1.49414200	-0.56607200
O	1.77230200	1.38721000	-0.12537100
O	0.30261100	-0.80126400	-0.51001200
O	0.06467300	-0.21137100	1.70507600
H	-2.44130400	-0.27828000	1.12430500
H	-0.28696700	-2.06709800	1.00250900
H	-2.10628400	-0.17082100	-1.76221900
H	0.15659100	0.64306800	-1.97443700
H	0.03084000	2.51639500	-0.27122200
H	0.52488900	1.71148000	2.14950300
H	-1.13306100	1.48769500	1.56220200
H	-2.80580500	-2.42489600	0.51698100
H	-2.60200400	1.95994100	-1.38774600
H	2.21390500	2.15205100	0.26209800
Ca	2.74817300	-0.79425300	-0.35883400

Ca(II)/(5)

E = -1287.935399
H = -1287.932951
G = -1288.147834

C	1.95454000	1.61371500	-0.22450900
C	1.57098100	-0.56919800	0.56601400
C	0.69400700	1.96137100	0.02155200
C	-0.34454600	0.94579400	0.38801500
C	0.17612500	-0.40409500	-0.01892700
C	2.09528700	-1.98334300	0.42265800
O	2.42166200	0.32395300	-0.15308700
O	0.17763400	3.22570500	-0.00674900
O	-1.57525500	1.13711300	-0.31385100
O	-0.76734600	-1.37973200	0.41198100
O	1.67339800	-2.59821600	-0.78404700
H	1.58265300	-0.28250400	1.62449900
H	0.82429800	3.85973000	-0.33953400
H	2.72428700	2.32275400	-0.49958600
H	-0.55209600	0.97133800	1.46375500
H	-1.81184100	2.07519900	-0.30117600
H	0.25595600	-0.43249400	-1.10892500
H	-0.48820100	-2.23670200	0.05476000
H	3.18347900	-1.97374100	0.51503200
H	1.69053400	-2.59107000	1.23195400
H	2.15492200	-2.20904700	-1.52257000
Ca	-3.09415500	-0.72797500	-0.06405100

Ca(II)/(6)

E = -1211.525137
H = -1211.522689
G = -1211.722666

C	0.86348300	-0.90801200	1.16218700
C	-0.37862100	1.05868300	0.84323400
C	1.85498100	-0.41421200	0.41958000
C	1.56466100	0.66837400	-0.53202900
C	0.44142800	1.37144400	-0.37550400
C	-1.80817900	1.52260500	0.76597900
O	-0.41697800	-0.37769700	1.02613700
O	3.14391400	-0.83440100	0.39827600
O	2.43775400	0.86827100	-1.54040400
O	-2.42362400	0.82606200	-0.32278100
H	0.07339100	1.48127900	1.74979300
H	3.26167900	-1.64373900	0.91016000
H	0.93235900	-1.75093000	1.83478600
H	3.18410400	0.26086400	-1.44156700
H	0.15459400	2.16415800	-1.05293500
H	-2.32918700	1.29535800	1.69659700
H	-1.82666500	2.59770800	0.58469900
H	-3.31095800	1.17059500	-0.47775900
Ca	-1.86471800	-1.46132300	-0.69971400

Ca(II)/(7)

E = -1211.550765
H = -1211.548317
G = -1211.747593

C	-0.43446500	1.83317400	0.08789100
C	-2.02737400	0.14482600	-0.26234800
C	0.57352900	0.94509100	-0.02258600
C	0.33289600	-0.46216800	0.14809200
C	-1.09208300	-0.85351500	0.39237800
C	-3.48064600	-0.07635100	0.09889500
O	-1.71702600	1.49501800	0.13248000
O	1.90939500	1.27403500	-0.11071400
O	1.27120600	-1.25943200	0.17708600
O	-3.81377400	-1.36572300	-0.37524900
H	-1.90382700	0.10193900	-1.35050400
H	2.04168300	2.17529000	-0.42996500
H	-0.26861200	2.90330800	0.15030000
H	-1.27782000	-1.85344200	0.00353800
H	-1.24388200	-0.87815900	1.47819200
H	-3.59864600	-0.00320600	1.18481200
H	-4.08720600	0.69907700	-0.37631900
H	-4.73489800	-1.54568300	-0.16381800
Ca	3.53218300	-0.59683300	-0.08695000

Ca(II)/(8)

E = -1287.958934
H = -1287.956486
G = -1288.157048

C	-0.36126300	0.87961400	-1.12265800
C	-0.57479700	-0.62491200	-1.24876000
C	-0.83230700	1.36129600	0.26001400
C	-0.41478700	0.37013100	1.36871900
C	-0.58141300	-1.08013800	0.94279500
C	-1.95604800	-1.43521700	0.40726500

O	0.22281900	-1.25236500	-0.24672500
O	-1.90909700	-0.94817600	-0.94645000
O	1.04515700	1.05863200	-1.28159500
O	-2.22244900	1.59474900	0.27897300
O	0.98989700	0.49899500	1.62782500
H	-0.90417000	1.40879900	-1.90659000
H	-0.28173700	-1.01545400	-2.22153200
H	-0.34661300	2.31668800	0.47235000
H	-0.99126300	0.57560500	2.27170400
H	-0.21351400	-1.76265500	1.70451400
H	-2.10493500	-2.51335700	0.39374800
H	-2.76960500	-0.94826600	0.94115200
H	1.24566200	1.95524400	-1.57543200
H	-2.66301500	0.96089700	-0.30049800
H	1.16096200	1.27744400	2.17155900
Ca	2.55906500	-0.33471300	-0.05257200

Ca(II)/(9)

E = -1211.536233
H = -1211.533784
G = -1211.720023

C	1.21443300	-1.08459900	0.20233000
C	1.05251500	-0.17613700	-1.00561900
C	0.64438300	-0.75585200	1.35910300
O	-0.19083100	0.51117600	-0.90575100
O	2.00592900	0.84256100	-0.97285700
C	-0.17056700	0.50183900	1.44780700
C	0.06364700	1.37165100	0.22689500
C	1.53261900	1.77655600	0.00983000
H	1.10069800	-0.70481000	-1.95671100
H	0.77269500	-1.37231500	2.23967800
H	0.05023800	1.06145400	2.35785400
H	-0.63193200	2.20580100	0.18575800
H	1.62446500	2.77475200	-0.40903000
H	2.11278500	1.69622900	0.92925700
O	2.01574000	-2.16049700	0.07178600
H	2.32444100	-2.26342300	-0.83625200
O	-1.58810400	0.21208600	1.41102400
H	-1.85672400	-0.23296300	2.22413100
Ca	-2.47303600	-0.41040400	-0.75051900

Ca(II)/(10)

E = -1211.551731
H = -1211.549283
G = -1211.736050

C	-0.99939000	1.34345900	-0.08542700
C	-0.95712500	0.22843500	-1.13868300
C	-1.02594200	0.83316200	1.33913300
O	0.16596700	-0.60151500	-0.83925800
O	-2.07560700	-0.59438100	-0.99080100
C	-0.14181200	-0.40810800	1.50146500
C	-0.29688700	-1.34336900	0.31255800
C	-1.73816100	-1.64983300	-0.07744300
H	-0.87561700	0.61629400	-2.15140200
H	-0.73497800	1.62778300	2.02425900
H	-0.37054400	-0.93213900	2.42970700
H	0.32444000	-2.22986300	0.41684600
H	-1.81239400	-2.59955500	-0.60287400
H	-2.41819800	-1.64150900	0.77354300
O	-1.01376100	2.50360000	-0.39679500
H	-2.06308000	0.56383200	1.56363200
O	1.24838100	-0.04572600	1.47911000
H	1.50416400	0.36166100	2.31533600
Ca	2.54011400	0.00576000	-0.59483600

Ca(II)/(11)

E = -1135.130437
H = -1135.127988
G = -1135.300649

C	-0.97968900	1.33923600	0.07781800
C	-0.31116100	0.26046700	0.93702700
C	-2.00753300	0.81923000	-0.83917300
C	-2.23682100	-0.49476300	-0.84843600
C	-1.49765600	-1.39250500	0.10668400
C	-0.06200200	-1.64346700	-0.37711400
O	-1.23443800	-0.69408700	1.32853900
O	0.61116900	-0.44346500	0.07090900
O	-0.62128800	2.49147600	0.13663600
H	0.21585300	0.67866700	1.79175300
H	-2.03964600	-2.30425600	0.33638500
H	0.37563600	-2.50315800	0.12610000
H	0.03266300	-1.72331000	-1.45687800
H	-2.92538300	-0.95004300	-1.55015000
H	-2.51181600	1.51668500	-1.49524800
Ca	2.96891600	0.05624200	-0.21907300

Ca(II)/(12)

E = -1364.349746
H = -1364.347297
G = -1364.589690

C	2.47321300	0.24865500	-0.65935800
C	3.73901200	-0.49252600	-0.28652800
C	1.17157200	-0.16715500	0.01995300
C	0.11698200	0.93832400	-0.07149200
C	-1.01501600	0.67774000	0.92343300
H	0.80930400	-1.03694400	-0.54720700
H	-0.27741000	0.95067100	-1.09287000
H	-0.65571200	0.95243300	1.91635300
H	4.23946300	0.10069400	0.48745600
O	-1.40581200	-0.69909100	0.91891400
O	2.50374900	1.13989500	-1.47321200
H	-0.70618100	-1.20762800	1.35566500
O	3.40819900	-1.78805200	0.18420100
H	4.20271600	-2.21226700	0.52517400
O	1.35681500	-0.51144100	1.38085100
H	2.01290500	-1.22452800	1.41204900
O	0.61674600	2.20884600	0.28694700
H	1.20468200	2.50285800	-0.41921300
C	-2.25316300	1.48171400	0.61303800

H	-1.97600700	2.51507100	0.40731900
O	-2.85605600	0.88633900	-0.54677700
H	-3.52016800	1.48005000	-0.91483700
H	-2.95254600	1.44182200	1.44868500
H	4.38047500	-0.52841900	-1.16852300
Ca	-3.05731200	-1.48731400	-0.63258500

Ca(II)/(13)

E = -1364.360516
H = -1364.358068
G = -1364.587132

C	-0.08238200	0.37285100	-0.37185000
C	2.14075800	-0.17852900	-0.78012800
C	2.16633500	0.62852400	0.51482600
C	0.69660700	0.65309800	0.95653500
H	2.79113000	0.17234000	1.28712700
H	0.42864700	1.63854900	1.34427800
C	2.29747900	-1.68406800	-0.63935000
H	2.23814400	-2.13156900	-1.63068900
H	3.27848100	-1.90975100	-0.21388800
O	1.26392200	-2.29417900	0.12895000
H	1.34746200	-2.02025100	1.05368300
C	-0.95473000	1.52061100	-0.83137100
H	-1.22507000	1.36643000	-1.87771900
H	-0.41299100	2.46007700	-0.72424400
O	-2.11934700	1.50704200	-0.00097800
H	-2.57581800	2.35424800	-0.05970400
O	2.62056300	1.92184900	0.17201700
H	2.69778400	2.45104900	0.97362100
O	0.51189300	-0.33390800	1.94491500
H	-0.41975000	-0.37199000	2.19005000
O	0.87442300	0.15154200	-1.36393900
O	-0.93842100	-0.75066700	-0.24399100
H	2.91415100	0.18799100	-1.45589400
H	-0.35354900	-1.53357300	-0.13069700
Ca	-3.29986400	-0.60759600	0.05281600

Ca(II)/(14)

E = -1287.926181
H = -1287.923733
G = -1288.142847

C	-0.90262300	-0.78295100	-0.07013000
C	0.39654600	1.10482400	-0.28581400
C	-0.99359900	1.56801100	0.12191800
C	-1.86301000	0.36451800	-0.23917700
H	-2.17066600	0.45804200	-1.28794900
C	1.52795100	1.72778900	0.47949100
H	1.62174400	2.77873800	0.20528600
H	1.36057100	1.63507800	1.55453600
O	2.70744200	1.00440800	0.10694900
H	3.49386500	1.47297400	0.40937700
C	-1.21025500	-2.06513800	0.01919200
H	-0.48159100	-2.85137200	0.17132300
O	-2.52458500	-2.42825100	-0.12828200
H	-2.67843100	-3.28331200	0.28733900
O	-2.98561600	0.30649500	0.60858800
H	-3.42721200	-0.53946800	0.45769900
O	0.40867400	-0.31183900	-0.00232200
H	0.53401900	1.24725000	-1.36231400
O	-1.29524100	2.75541300	-0.56123800
H	-2.09531000	3.13925300	-0.18627300
H	-1.04097900	1.70401700	1.20852900
Ca	2.63342700	-1.39366600	-0.08999900

Ca(II)/(15)

E = -1287.940808
H = -1287.938359
G = -1288.150513

C	-0.05092900	-2.08511100	0.39254100
C	-1.72243100	0.77838900	0.22548700
C	-1.98954200	-0.56519800	-0.45358900
C	-0.57370500	-1.13989400	-0.65881700
C	-0.37248300	1.20138700	-0.33952000
C	0.50155100	1.91164600	0.66771400
H	-0.68711600	-2.92477600	0.69911000
H	-3.48300000	1.58362200	0.42025300
H	-1.64204300	0.61998500	1.30975200
H	-0.52876400	-1.69917400	-1.60081500
H	-0.51441400	1.80900200	-1.23513200
H	0.15472100	2.93702500	0.79684300
H	0.47328700	1.39388500	1.63039400
O	-2.67057700	1.76979400	-0.06375800
O	1.83697300	1.88507100	0.15191000
O	1.06882700	-1.95777500	0.83685200
O	0.29808500	-0.01956100	-0.73738600
H	2.37031700	2.56329000	0.58196500
O	-2.88399800	-1.41256300	0.21213600
H	-2.74657200	-1.36828800	1.16608100
H	-2.42112800	-0.36662700	-1.43549900
Ca	2.65377300	-0.36374900	-0.22669400

Ca(II)/(16)

E = -1211.538335
H = -1211.535887
G = -1211.732425

C	0.60757300	-2.26170200	0.37011500
C	-2.29321300	0.10572300	0.16447300
C	-1.70648500	-1.22443600	0.56829300
C	-0.44086400	-1.26528800	0.17378600
C	-1.03384400	0.87981200	-0.28124500
C	-0.50473500	1.83748400	0.75992400
H	0.32814300	-3.24379300	0.76437200
H	-3.82903600	0.62426400	-0.92301100
H	-2.77564400	0.60565300	1.00829700
H	-1.17520700	1.36426500	-1.24526000
H	-1.13045800	2.72942500	0.79338600

H	-0.49007100	1.36324400	1.74546400
O	-3.21262000	-0.11527600	-0.88147300
O	0.82815100	2.16760800	0.35765100
O	1.76219300	-1.97542400	0.11239500
O	0.00042100	-0.12644800	-0.45592400
H	1.13438900	2.94391600	0.83998700
H	-2.24422900	-2.01500700	1.06789100
Ca	2.36931800	0.37974000	-0.38222000

Ca(II)/(17)

E = -1211.536657
H = -1211.534208
G = -1211.732199

C	1.31328000	1.72902000	-0.33322600
C	1.22481200	-1.80791300	0.09363100
C	2.16430900	-0.64672800	-0.10974200
C	1.25361200	0.33339900	-0.88130900
C	0.00044300	-1.44602500	-0.24224000
C	-1.32158400	-2.11549000	-0.17176300
H	2.27933800	2.24388100	-0.38129000
H	1.50703400	-2.75429700	0.52677600
H	-1.66505400	-2.38494100	-1.17293200
H	-1.25740700	-3.00585400	0.45091500
O	-2.21667400	-1.15292600	0.40326600
O	0.33518100	2.27132200	0.12724000
O	-0.08719600	-0.15385100	-0.74574600
H	-3.09120100	-1.54638300	0.50805100
H	3.05175300	-0.89346600	-0.69068300
H	1.50859200	0.35178900	-1.94395900
O	2.52764900	-0.03156000	1.11754900
H	3.27761500	-0.49929400	1.50089800
Ca	-1.89457900	1.23735500	0.19258200

Ca(II)/(18)

E = -1135.15734
H = -1135.14904
G = -1135.33074

C	0.46505	1.57871	-0.08258
C	-0.93082	1.34003	-0.18579
C	-1.10423	0.00694	0.0367
C	1.03967	0.37591	0.20016
C	2.44986	-0.05118	0.41524
H	0.98561	2.51418	-0.20376
H	3.08446	0.83264	0.39159
H	2.54819	-0.51995	1.39879
O	2.91163	-0.92263	-0.60503
O	0.09889	-0.58652	0.27764
H	2.44992	-1.7639	-0.52313
H	-1.71393	2.04934	-0.39799
C	-2.27716	-0.84845	0.06428
O	-2.29935	-1.93108	0.60687
H	-3.16336	-0.44226	-0.45116
Ca	-0.09401	-2.81418	0.26537

Ca(II)/(19)

E = -1020.660773
H = -1020.658324
G = -1020.80971

C	-2.64574600	-0.71918800	-0.03843900
C	-2.27997500	0.65333800	-0.05656600
C	-0.92009500	0.68777300	0.01509100
C	-1.48628000	-1.41971000	0.04544100
H	-3.63715700	-1.13593500	-0.08333400
O	-0.42326300	-0.58553400	0.07852500
H	-1.26598500	-2.47303400	0.08954000
H	-2.93025600	1.51116800	-0.11745900
C	0.05069600	1.73915700	0.01381600
O	1.25492000	1.50576500	0.03925100
H	-0.32327900	2.76762600	-0.01385300
Ca	2.25959100	-0.68399500	-0.03465800

Ca(II)/adduct (5) and (19)

E = -1631.154999
H = -1631.152551
G = -1631.458576

C	1.92647100	-2.88408500	-0.03717700
C	1.74695000	-0.24155300	0.59138200
C	0.44875500	-0.91025600	0.19009500
C	0.69544600	-2.39064200	0.05122300
C	2.89681300	-0.74342200	-0.26004600
C	4.22985200	-0.10389800	0.07856200
H	-1.37557800	-0.67005800	0.82623300
H	2.12783000	-3.94180200	-0.13268500
H	-1.17196600	-2.75736800	-0.25506100
H	0.76663700	1.39422700	0.91227500
H	5.16337700	1.41961100	-0.75459600
H	1.95510700	-0.49022100	1.63743700
H	0.11324100	-0.49725900	-0.77034500
H	2.67279600	-0.59203000	-1.32426100
H	4.38033100	-0.07695200	1.15941400
H	5.01766600	-0.70024900	-0.37935200
O	-0.48487500	-0.57587100	1.19898100
O	-0.37850900	-3.23235700	0.03918600
O	1.60162200	1.17391000	0.47056000
O	4.26942500	1.22771500	-0.44972700
O	3.07374200	-2.12508300	0.00164800
C	-5.64015900	1.77114200	0.06209800
C	-5.52978500	0.56173900	-0.66944200
C	-4.29612500	0.05221900	-0.37739500
C	-4.46708600	1.90117900	0.74072300
H	-6.47204600	2.45378000	0.08813200
O	-3.64149200	0.87292800	0.48727500
H	-4.09671300	2.65052000	1.42057300
H	-6.25744300	0.11468600	-1.32775100
C	-3.64238200	-1.14552900	-0.82124500
O	-2.51824200	-1.46965700	-0.46946400
H	-4.22222700	-1.77111900	-1.51180600

Ca	2.79065600	3.06451000	-0.35542700

Ca(II)/(20)

E = -1631.158839
H = -1631.156391
G = -1631.455759

C	1.48872200	-1.75494100	-0.30368600
C	1.00668800	0.97182700	-0.07866500
C	2.39244700	0.47462800	0.30235400
C	2.51926700	-0.98425100	0.01452900
C	-0.02433000	-0.06636600	0.35007600
C	-1.44112700	0.36463500	0.00371700
H	3.19602300	1.26234700	-1.32882200
H	1.57388300	-2.80527200	-0.55207300
H	3.91135200	-2.36551900	-0.01590000
H	1.26364800	2.87966000	0.22617700
H	-1.35095700	-0.21069600	-1.85033700
H	0.94917500	1.07785000	-1.17001800
H	2.57491700	0.68152400	1.36002400
H	0.05696800	-0.24242000	1.42819700
H	-1.63889900	1.31074900	0.50961300
O	3.42913200	1.19332600	-0.39169200
O	3.83302100	-1.40991200	0.10148700
O	0.69297800	2.18159200	0.56636800
O	-1.57774500	0.60162400	-1.37938300
O	0.20611500	-1.29738300	-0.33751000
C	-5.90916000	0.67898000	0.04548400
C	-4.73137600	0.59014700	0.85883700
C	-3.86632400	-0.20190500	0.18055400
C	-5.66072100	-0.06468000	-1.05571300
H	-6.81526400	1.22096200	0.25887400
O	-4.42080800	-0.61312800	-0.98637500
H	-6.23480200	-0.30056500	-1.93524000
H	-4.55324000	1.05037200	1.81689700
C	-2.47731400	-0.66076400	0.48336500
O	-2.27822700	-0.80037800	1.87675200
H	-2.96165700	-1.38156100	2.22865200
H	-2.30014300	-1.60789400	-0.04116100
Ca	5.67363200	0.22503300	-0.06685800

Ca(II)/(21)

E = -1554.7595
H = -1554.757052
G = -1555.035125

C	1.60939100	1.95531500	0.23552700
C	0.73889300	-0.67614800	0.09403400
C	2.16281400	-0.38778100	-0.35400600
C	2.50765600	1.03990600	-0.09959100
C	-0.16021400	0.49165900	-0.31368500
C	-1.57973900	0.25493600	0.09769300
H	2.89214800	-1.27290600	1.26155400
H	1.85531700	2.98540800	0.46050200
H	4.08588600	2.20442300	-0.17233200
H	0.70492800	-2.60452300	-0.17611500
H	-2.60030000	-0.16559000	1.66263400
H	0.71379700	-0.75027900	1.18881200
H	2.27238100	-0.63688500	-1.41281500
H	-0.10821400	0.62810300	-1.39873900
O	3.11103800	-1.23548500	0.31911900
O	3.86796300	1.26493500	-0.22621800
O	0.22597500	-1.83704700	-0.50844900
O	-1.67637600	-0.01037400	1.42079700
O	0.27601400	1.69533200	0.32475500
C	-6.19933500	-0.24367200	-0.40044600
C	-5.09783400	0.06174200	-1.26168300
C	-3.98418700	0.06340700	-0.48150000
C	-5.68289100	-0.40572200	0.83715800
H	-7.23837000	-0.33003500	-0.67045600
O	-4.33458500	-0.22242200	0.80940100
H	-6.10913200	-0.63901600	1.79733100
H	-5.12380600	0.25479300	-2.32126700
C	-2.59118900	0.30038700	-0.77812200
H	-2.36041100	0.52795000	-1.80955900
Ca	5.44576800	-0.60825600	-0.04885300

Ca(II)/(22)

E = -1554.755334
H = -1554.752886
G = -1555.029650

C	-1.40520000	1.75126200	-0.27242500
C	-0.85701700	-0.97574100	-0.08626000
C	-2.26000800	-0.51360700	0.28375300
C	-2.41650500	0.94933400	0.02471600
C	0.14062800	0.08175100	0.38155400
C	1.55995200	-0.32289300	0.14594900
H	-3.04734200	-1.27533500	-1.36703400
H	-1.51191400	2.80481500	-0.49600100
H	-3.83420800	2.30282900	0.02348600
H	-1.06603700	-2.89645300	0.16429200
H	-0.77452800	-1.05796900	-1.17897900
H	-2.44455200	-0.74103100	1.33688500
H	-0.04436100	0.28223300	1.44749600
H	1.76482600	-1.37015400	-0.01960900
O	-3.27817600	-1.23936500	-0.42730000
O	-3.73697400	1.34583400	0.11413500
O	-0.53172600	-2.18922900	0.54254400
O	-0.11347700	1.31238000	-0.32394500
C	6.17808100	-0.06814900	-0.24322700
C	5.11254100	0.87338900	-0.08732000
C	3.97354000	0.13914200	0.00319400
C	5.60020400	-1.29190000	-0.23525700
H	7.22963300	0.13994600	-0.34716500
O	4.25736000	-1.18420600	-0.08440200
H	5.98768800	-2.29258800	-0.32028000
H	5.17562900	1.94768700	-0.04935500
C	2.58436400	0.53675900	0.17518800
O	2.47798900	1.87593200	0.37136400

H	1.55423000	2.13803200	0.24697400
Ca	-5.54262600	-0.31544300	-0.07595300

Ca(II)/(23)

E = -1554.760497
H = -1554.758049
G = -1555.038636

C	1.76898300	1.98476800	-0.19531700
C	0.70408300	-0.54085500	0.24280300
C	2.13284000	-0.47385000	-0.27900800
C	2.58127200	0.94920300	-0.34679100
C	-0.10803600	0.59575100	-0.37727200
C	-1.53773300	0.54303500	0.17482100
H	2.81917800	-1.09614200	1.47500100
H	2.09974600	3.01537000	-0.20383800
H	4.21790700	1.95628300	-0.73101000
H	0.42169900	-2.46725800	0.41676500
H	-2.56574300	0.65581400	-1.65346000
H	0.70670700	-0.38410600	1.32999500
H	2.18665100	-0.94862900	-1.26180500
H	-0.10414700	0.49488800	-1.46890100
O	3.04549600	-1.22445000	0.54248400
O	3.94439400	1.04686300	-0.55445200
O	0.05884100	-1.74088500	-0.10226600
O	-1.74633100	0.91034600	1.30016900
O	0.42439700	1.85808800	-0.01885600
C	-5.95639200	-0.11869400	0.77015500
C	-4.58641800	0.28620000	0.91267400
C	-3.95607000	-0.10322800	-0.22216900
C	-6.04798300	-0.71895500	-0.43542400
H	-6.75635000	0.02194700	1.47772900
O	-4.83951200	-0.71870200	-1.05486500
H	-6.85713700	-1.17987500	-0.97537000
H	-4.13419700	0.79512400	1.74453900
C	-2.57737900	0.00939200	-0.76675600
H	-2.21703400	-0.96459900	-1.11984000
Ca	5.42907200	-0.77127500	0.16031000

Ca(II)/(24)

E = -1554.77311
H = -1554.770661
G = -1555.050376

C	1.31306600	-1.63034800	-0.63643100
C	0.90676900	1.02555600	0.05818200
C	2.27269000	0.42723500	0.35970500
C	2.36349000	-0.95695100	-0.18788800
C	-0.15838200	-0.04093600	0.29759000
C	-1.55207900	0.47973200	0.04585200
H	3.11552100	1.49376700	-1.08141800
H	1.37430800	-2.62122500	-1.06871200
H	3.71557800	-2.36459300	-0.39450600
H	1.21876000	2.84862900	0.67697700
H	0.87019800	1.31534500	-1.00165600
H	2.43967700	0.43416000	1.43992700
H	-0.06986100	-0.41397800	1.32453700
H	-1.69417800	0.68234900	-1.01845800
O	3.33968700	1.22971600	-0.17712300
O	3.66834100	-1.42208900	-0.18969600
O	0.62572200	2.12068400	0.89439700
O	0.04558000	-1.13965900	-0.59414100
C	-6.18739200	-0.06709500	-0.25683700
C	-5.17592200	-0.79726000	0.42623000
C	-3.99662200	-0.18853100	0.12226300
C	-5.54462000	0.92810200	-0.92200600
H	-7.24807100	-0.25234000	-0.25742900
O	-4.21803500	0.87104500	-0.70420600
H	-5.88697300	1.72069200	-1.56585300
H	-5.29215500	-1.65792700	1.06378300
C	-2.62205200	-0.47139200	0.53658200
O	-2.37920600	-1.41174800	1.26444000
H	-1.68944000	1.43100000	0.56741000
Ca	5.53881200	0.15759300	-0.08467000

Ca(II)/Transition states

Ca(II)/AG-ts1

E = -1364.293576
H = -1364.291127
G = -1364.528877

C	0.74446400	0.36646000	0.82687100
C	0.04840000	1.37551200	-0.07040800
C	-1.45645800	1.35986500	0.12814900
C	-1.98729500	-0.01095400	-0.26300400
C	-1.47009900	-1.07085100	0.69794300
H	0.93006500	0.77335400	1.82236300
H	-1.70434500	1.57230600	1.17488000
H	-1.65950900	-0.22605400	-1.28757300
H	-2.00941900	-0.97259200	1.64228100
H	0.26320300	1.10177300	-1.11102000
O	-0.06411300	-0.88592300	0.99704800
O	1.79359800	-0.29986000	0.25790100
H	0.84676300	-1.24044000	0.36269500
O	0.60639900	2.63014400	0.23941100
H	0.08253900	3.29531200	-0.22594200
O	-1.98293800	2.36143800	-0.72140900
H	-2.76404800	2.75162800	-0.31662800
O	-3.39195300	-0.07811400	-0.16739600
H	-3.77226200	0.40914200	-0.90674800
C	-1.58879600	-2.49300000	0.17984900
H	-2.63157700	-2.68170800	-0.08003600
O	-0.71278900	-2.70764700	-0.91071800
H	-1.17116500	-2.53053300	-1.73785000
H	-1.29498700	-3.18363900	0.97043700
Ca	3.95789100	-0.21955200	-0.34309700

Ca(II)/AG-ts2

E = -1364.290118
H = -1364.287670
G = -1364.525356

C	0.81314400	0.83271800	0.65756600
C	-1.46161400	-0.07206900	0.76889000
C	-1.50106300	1.40106300	0.35486900
C	-0.11467800	1.66780700	-0.22383700
C	-1.80808600	-1.05306600	-0.35528200
H	1.23971600	1.40038200	1.48655000
O	1.65737500	-0.04565600	0.03894500
H	0.68063100	-0.83940400	0.54396800
C	-1.41772800	-2.48104900	-0.01147600
H	-1.94101600	-3.14677500	-0.70134300
H	-1.72630000	-2.71882500	1.01130500
O	-0.00820200	-2.59665200	-0.16332700
H	0.27174500	-3.45770700	0.16343300
O	0.14314300	3.04779400	-0.17346700
H	0.81967200	3.27503200	-0.81958300
H	-0.06374400	1.28315400	-1.24663000
O	-2.54551600	1.61611300	-0.56181600
H	-2.65481700	2.56269100	-0.70651900
H	-1.62486000	2.02739700	1.24447300
O	-3.20565900	-1.05283400	-0.53660200
H	-3.47028500	-0.15528100	-0.77982200
H	-1.28750900	-0.77084700	-1.27943400
O	-0.08511300	-0.23107200	1.21820700
H	-2.10166500	-0.28463800	1.62429500
Ca	3.85751800	-0.34245700	-0.31302900

Ca(II)/AG-ts3

E = -1364.264666
H = -1364.262217
G = -1364.494696

C	-1.26174100	0.58901900	1.15225500
C	-2.37779300	-0.24359300	0.60673900
C	-1.63814800	-1.37424300	-0.14952300
C	-0.14057600	-1.13828000	0.20411700
C	0.75206000	-0.76923000	-0.96909800
C	0.48619100	0.67298200	-1.43993800
O	-1.35567100	3.04705800	-0.10097500
O	-3.17260200	-0.63096400	1.70328500
O	-1.89395100	-1.35242100	-1.51567500
O	2.13841100	-0.90282500	-0.61370800
O	-0.13589400	0.04941000	1.11049900
O	-0.87096900	0.93292600	-1.47191200
H	-3.00365800	0.33223800	-0.07084300
H	-1.36082400	1.51894800	1.70215200
H	-1.95761700	-2.33775500	0.24890600
H	-1.20185000	2.29255400	-0.75031100
H	0.29835700	-1.93165800	0.80378900
H	0.52761500	-1.47440600	-1.76948700
H	1.00916800	1.34692400	-0.74004400
H	0.97704200	0.79730800	-2.41486100
H	-2.72016200	-1.29864500	2.23357200
H	-1.59584300	-0.41679800	-1.77249000
H	-2.11861500	3.53124400	-0.42845800
H	2.44642600	-1.77583800	-0.88743200
Ca	3.80527100	0.19252300	0.72630400

Ca(II)/AD-ts1

E = -1364.246732
H = -1364.244283
G = -1364.481905

C	2.24708300	-0.74777500	-0.20650400
C	0.94171300	1.22852700	-0.62574600
C	1.08152700	-1.63783700	-0.05864400
C	-0.21178300	-0.96810600	-0.36682600
C	-0.15412000	0.46730900	0.11096700
C	1.23013200	2.57774500	0.00882600
O	2.52181100	-0.64782200	1.51317600
O	2.18921000	0.51974700	-0.62883600
O	1.24875000	-2.91152400	-0.64468200
O	-1.33268600	-1.61387200	0.27183400
O	-1.43084700	1.04263900	-0.15444400
O	0.00628300	3.30216300	0.00213600
H	3.36256200	-1.04941500	1.78299800
H	0.63518800	1.35916100	-1.66769900
H	1.70082200	-1.40196800	1.36971600
H	1.19766500	-2.84235500	-1.60768000
H	3.16948600	-1.21945900	-0.52950900
H	-0.46841500	-0.97736000	-1.43536900
H	-1.00135100	-2.05542600	1.06697300
H	0.03715700	0.48670000	1.19053600
H	-1.36292100	2.00222800	-0.00241000
H	1.59124300	2.41903900	1.02902700
H	1.99911000	3.09658500	-0.56696800
H	0.11493300	4.12340100	0.49192300
Ca	-3.37014800	-0.34954700	0.14162700

Ca(II)/AD-ts2

E = -1287.828611
H = -1287.826162
G = -1288.045418

C	2.18424800	1.30039600	-0.70123500
C	-0.03833600	1.03405500	-0.02888100
C	2.45571800	0.02157800	-0.45800900
C	1.58459600	-0.73126100	0.47760500
C	0.36281100	-0.14527800	0.82195700
C	-1.14323300	1.86876700	0.58856100
O	1.07416300	1.90194100	-0.16523800
O	3.50246100	-0.71612100	-0.90778100
O	2.17290800	-1.61358800	1.33893800
O	-1.10031900	-1.50508900	-0.11815200
O	-2.31816600	1.06710500	0.67943900
H	-0.32587700	0.66542400	-1.02016400
H	4.17997300	-0.15507200	-1.30507700
H	2.81083600	1.96439400	-1.28088800
H	0.69183700	-1.27796700	-0.15430600
H	2.94119300	-2.00483800	0.89983400
H	-0.15310300	-0.39660000	1.73894300
H	-1.09263200	-2.29173000	0.44136500

H	-0.83924500	2.20260600	1.58197000
H	-1.31501800	2.73716300	-0.04781500
H	-2.97621500	1.54664600	1.19664300
Ca	-3.15024700	-0.80767800	-0.64340700

Ca(II)/AD-ts3

E = -1211.440109
H = -1211.437661
G = -1211.633943

C	-0.61311500	1.71455400	0.15206600
C	-2.03164900	-0.04665600	-0.67902400
C	0.50404000	0.96900100	-0.07888200
C	0.29898500	-0.41213400	-0.19689800
C	-0.96720500	-1.01425600	-0.26429300
C	-3.44397600	-0.46623600	-0.34160300
O	-1.83372600	1.25567200	0.01807600
O	1.80855100	1.42189000	0.02157200
O	1.25092500	-1.30534100	-0.28549900
O	-3.58754100	-0.82802500	1.01538000
H	-1.96562900	0.21239800	-1.73940400
H	1.97761000	2.14937400	-0.59184300
H	-0.56436500	2.75004900	0.47391500
H	0.20012500	-1.91827100	-0.66217400
H	-1.18057100	-1.62740900	0.61311700
H	-4.13241400	0.33805400	-0.61391200
H	-3.68736300	-1.34670800	-0.93648100
H	-3.48299200	-0.03627900	1.55476700
Ca	3.46237200	-0.46702100	0.20988000

Ca(II)/LG-ts

E = -1364.279029
H = -1364.276581
G = -1364.505349

C	-2.31681100	-1.28121100	-0.61635200
C	0.19523600	-1.49379400	0.04100300
C	-0.83142500	-1.18795600	-1.03772200
C	-0.52173400	1.09606500	-0.59655200
C	0.05925000	-0.59122200	1.27124800
C	0.00298600	0.87363700	0.79986400
H	1.71014300	-1.93617700	-1.15578400
H	-3.38428400	2.66840600	0.21769300
H	-1.84631500	-0.69572000	1.47337900
H	1.36940900	2.30709200	1.03347700
H	-2.96876700	1.19842300	-0.13993600
H	-2.91036200	-1.18535800	-1.53409700
H	-2.45407800	-2.30674100	-0.24124900
H	0.08543300	-2.53451900	0.34762400
H	-0.63020100	-1.75647700	-1.94378000
H	-0.57575500	2.11185300	-0.97528500
H	0.97077900	-0.69047400	1.86428500
H	-0.59601000	1.45888800	1.49677800
O	1.51183500	-1.26599400	-0.48807200
O	-1.02498300	-0.93595800	2.06073100
O	1.33479000	1.40121700	0.69909800
O	-2.61674500	-0.31555300	0.31141400
O	-0.68057800	0.20803200	-1.45890100
O	-2.92446600	2.14688300	-0.44634500
Ca	3.34530800	0.34793300	-0.25177200

Ca(II)/LO-ts1

E = -1287.843991
H = -1287.841543
G = -1288.040708

C	-0.34856700	1.01078200	-0.99779900
C	-0.51654600	-0.44778300	-1.30311300
C	-0.69888200	1.26938000	0.44932400
O	0.25665500	-1.25458200	-0.35788300
O	-1.84525700	-0.87587100	-1.11093800
C	-0.44275000	0.13661900	1.44820800
C	-0.59199800	-1.23655400	0.80169600
C	-1.95674800	-1.48210200	0.17842100
H	-2.00483000	1.67804400	-0.76455300
H	-0.16428000	-0.71569400	-2.29832600
H	-0.24055200	2.18954200	0.80373800
H	-1.03418500	0.21026000	2.36171300
H	-0.26912000	-2.01718500	1.48626000
H	-2.14366700	-2.54908200	0.06205500
H	-2.77179900	-1.01932300	0.73432600
O	1.06739400	1.27661800	-1.17419100
H	1.19841500	1.99707500	-1.79617100
O	-2.17224200	1.52586800	0.26677700
H	-2.49708900	2.32279700	0.72382600
O	0.95905000	0.23422500	1.73965300
H	1.12263600	0.89037400	2.42831400
Ca	2.50063100	-0.28694600	-0.10544700

Ca(II)/LO-ts2

E = -1211.435046
H = -1211.432598
G = -1211.619599

C	0.01972800	0.97447900	0.53577900
C	0.03013000	-0.41135100	1.13538100
C	-1.01595000	1.39646500	-0.26412400
O	-1.23612500	-0.94855600	1.16850200
O	0.75518900	-1.17175200	0.15960500
C	-2.03254900	0.35467300	-0.69633200
C	-1.57245500	-1.02704400	-0.22287400
C	-0.24453900	-1.50886200	-0.84601600
H	0.52210400	-0.45890400	2.10528400
H	-1.21549700	2.46053100	-0.38867900
H	-2.09073400	0.34313300	-1.78988400
H	-2.37833000	-1.74587500	-0.33735400
H	-0.22273600	-2.58637900	-0.97619200

H	-0.00513900	-1.00569200	-1.78210100
O	1.16635400	1.60629300	0.38980500
H	0.31913500	1.78309600	-0.65934000
O	-3.31051000	0.56314500	-0.13387800
H	-3.68232000	1.38056900	-0.48275600
Ca	2.93240300	0.03831600	-0.31060600

Ca(II)/LO-ts3

E = -1211.47216
H = -1211.469711
G = -1211.655465

C	-0.11860600	-0.97909200	0.33610200
C	-0.03711100	0.36413900	1.06069300
C	0.98422400	-1.35679700	-0.44829900
O	1.24483200	0.86959800	1.17219900
O	-0.71614100	1.23800900	0.14742200
C	1.97984800	-0.27291900	-0.76821900
C	1.60963800	1.07937600	-0.19017300
C	0.30458700	1.64085300	-0.80064600
H	-0.54177300	0.35937900	2.02391000
H	2.24663600	-1.59039000	0.30461900
H	2.28661400	-0.21938400	-1.80943800
H	2.44109700	1.77728200	-0.22829600
H	0.31345100	2.72611500	-0.83996700
H	0.08948000	1.22441200	-1.78432100
O	-1.23653600	-1.53627700	0.38667400
H	0.84056000	-2.15045300	-1.17101100
O	3.13078800	-0.80315600	0.05691800
H	3.84626300	-1.16285900	-0.49397800
Ca	-2.96206800	-0.09814300	-0.26219900

Ca(II)/Ch-tsF

E = -1287.843988
H = -1287.841539
G = -1288.048748

C	-2.07503000	0.75355400	-0.89689000
C	0.14680600	-0.79562100	-0.03059400
C	0.23131200	0.67615400	-0.33164000
C	-1.11559000	1.29372400	0.03705600
C	-1.20483900	-1.40214500	-0.43052600
C	-2.04255500	-1.69136400	0.82015900
H	1.32756400	-2.33030300	-0.46046600
H	0.21948700	-0.90617100	1.05468200
H	-1.54488600	0.66915800	0.98453000
H	-1.09138700	-2.25631700	-1.09430800
H	-2.97578600	-2.17697700	0.48844700
H	-1.46464400	-2.46709400	1.35785900
O	1.29924100	-1.38068800	-0.63967800
O	-2.27607100	-0.54712100	1.54056000
O	-2.05147900	-0.46260300	-1.22679500
O	-1.07156800	2.68725500	0.06861700
H	-1.33926800	2.99531100	0.94069000
O	1.30515900	1.18694300	0.44107200
H	1.29795200	2.15422300	0.39210600
H	0.45297100	0.83424300	-1.39286900
H	-2.86143000	1.35055400	-1.35671700
Ca	3.33482700	-0.13713700	0.13052200

Ca(II)/Ch-tsR

E = -1287.882061
H = -1287.879613
G = -1288.079225

C	1.79348700	0.44523500	-1.18507500
C	0.91317800	-0.61718300	1.17423100
C	0.45307300	0.81937000	0.88509000
C	0.73902400	1.18379100	-0.56986700
C	1.01308200	-1.47994400	-0.08237200
C	-0.28693000	-1.80233800	-0.80010500
H	-1.03869000	1.59951500	1.90616100
H	2.46219300	0.89826900	-1.91448700
H	1.29439300	3.03853700	-0.36169000
H	2.52273600	-1.34698000	2.02392700
H	-0.15526100	0.53000900	-1.07501700
H	0.18921400	-1.08695900	1.84668700
H	1.02995700	1.47649600	1.53711400
H	1.54278800	-2.40459200	0.14340700
H	-0.02135500	-2.33985300	-1.71920500
H	-0.80741500	-2.52542100	-0.15478700
O	-0.93404900	1.01718100	1.14575500
O	0.67646600	2.52986400	-0.90196900
O	2.18411500	-0.47942100	1.77425700
O	-1.07138600	-0.67649200	-1.07597000
O	1.93207600	-0.80388000	-1.03493800
Ca	-2.85329200	-0.09153100	0.09896900

Ca(II)/HM-ts1

E = -1364.298204
H = -1364.295756
G = -1364.533806

C	-1.04681500	2.29810200	0.12242500
C	-1.26467200	0.89679800	0.02858000
C	-0.18749300	-0.13011600	0.38239100
C	1.20669200	0.18159800	-0.13201500
C	2.24615800	-0.74623100	0.52067000
H	-0.07629100	2.77882200	0.09561400
H	-0.16653500	-0.22383600	1.46932100
H	1.47856900	1.20762300	0.13332100
H	1.85295300	-1.76307200	0.58242100
H	-0.93218800	1.34630700	-1.08636700
O	2.45418800	-0.31510800	1.85260200
O	-2.08141400	3.06909900	0.13370000
H	2.97102000	0.50056400	1.82532300
O	-2.50993900	0.50683500	0.07694100
H	-2.86954900	2.48462200	0.21964600
O	-0.62575400	-1.38490700	-0.13552600
H	-0.25532300	-1.47789400	-1.02858200

O	1.13454700	0.02914400	-1.53717000
H	1.95188700	0.37121000	-1.92220800
C	3.53013800	-0.77070000	-0.28200700
H	3.38215400	-1.33047100	-1.20940100
O	3.86618200	0.58602100	-0.55524400
H	4.75292100	0.62726100	-0.92648700
H	4.30749900	-1.26238800	0.30670900
Ca	-3.06018300	-1.67820600	-0.04910000

Ca(II)/HM-ts2

E = -1364.291182
H = -1364.288734
G = -1364.519495

C	0.01000800	-1.07643700	-0.50379900
C	0.79695000	1.06015100	0.74369400
C	1.49017600	-0.20738700	1.26344600
C	1.37450500	-1.27374400	0.16592900
H	2.54113600	-0.02026800	1.49644000
H	1.41889800	-2.26991100	0.61754000
C	1.64414400	2.06548500	-0.02289600
H	1.05560300	2.97120000	-0.16901300
H	2.51280800	2.32221900	0.59065400
O	2.00761700	1.61742900	-1.30711100
H	2.54461300	0.81693700	-1.21412500
C	-1.16986700	-1.81199000	0.07514400
H	-1.16622400	-1.75499300	1.16210400
H	-1.10525700	-2.85944100	-0.22929900
O	-2.37256500	-1.21892000	-0.39517300
H	-2.46986400	-1.42615400	-1.33460000
O	0.76110700	-0.60515900	2.40624000
H	1.25301700	-1.28542000	2.88042100
O	2.40670300	-1.10296200	-0.77234100
H	2.02551300	-1.27337700	-1.64916000
O	-0.26848100	0.57208200	-0.10823700
O	0.00468000	-0.81797700	-1.78688300
H	0.34763300	1.56180000	1.60197400
H	-0.01237200	0.39256600	-1.26394300
Ca	-2.70667400	1.13662100	0.14449700

Ca(II)/HM-ts3

E = -1364.284239
H = -1364.281791
G = -1364.527136

C	-0.19830100	-0.49131500	0.94695700
C	-2.39534600	-0.03671100	0.53078700
C	-1.56753100	1.05364700	-0.15995700
C	-0.23945400	0.96066400	0.59138300
H	-1.39953300	0.78636400	-1.20630300
H	-0.35035000	1.48497100	1.55548100
C	-3.37753800	-0.78350800	-0.32509800
H	-3.80480700	-1.60815200	0.25128500
H	-4.18112700	-0.08426300	-0.58029700
O	-2.68785700	-1.24158100	-1.46674000
H	-3.29053000	-1.75490800	-2.01387000
C	0.96528600	-1.32563800	1.15030600
H	1.12935200	-1.69189300	0.06912900
H	0.79023000	-2.15968400	1.82814900
O	2.14207600	-0.59269500	1.39913100
H	2.19918400	-0.32137600	2.32318500
O	-2.10728600	2.33281400	-0.01352800
H	-2.60550900	2.56973700	-0.80296100
O	0.88456500	1.41771000	-0.10669900
H	0.80920400	2.37702600	-0.20535800
O	-1.35399400	-1.00155400	0.97290000
O	1.87903600	-1.21681400	-1.33851100
H	-2.86528200	0.34318100	1.43783100
H	1.89695600	-1.80289400	-2.09693200
Ca	3.12486000	0.40080100	-0.62690200

Ca(II)/HM-ts4

E = -1287.820934
H = -1287.818486
G = -1288.041074

C	-1.16635900	-0.46290100	-0.77772300
C	0.00875600	-0.44158900	-0.02460100
C	0.36375100	0.81086000	0.78219400
C	1.52159900	1.32903900	-0.07390300
H	-1.30024000	-0.56409400	-1.85246700
H	2.17963500	1.96802600	0.51887700
O	0.93028700	2.02974100	-1.14767500
O	-2.19084900	-0.47672300	0.02773700
H	1.62132500	2.32134300	-1.75206000
H	-1.18521200	-0.75960200	0.80181400
C	2.20742000	0.04387900	-0.54336100
O	1.16932300	-0.96303400	-0.55584100
H	2.55729000	0.15747900	-1.57298100
C	3.36297800	-0.40766300	0.31901700
H	4.08559600	0.41242300	0.38862700
H	3.00235100	-0.65001200	1.32111000
O	3.94315900	-1.53940700	-0.30909800
H	4.64009200	-1.88193300	0.25849800
O	0.90397700	0.52916500	2.05174100
H	0.24536700	0.07646700	2.58898900
H	-0.46002600	1.52445000	0.82640100
Ca	-4.56111200	-0.22361200	-0.00757300

Ca(II)/HM-ts6

E = -1287.823347
H = -1287.820899
G = -1288.030459

C	0.10561700	-1.63814700	0.80215200
C	-1.87382000	0.79268600	0.20312100
C	-1.92898700	-0.58315300	-0.43093500
C	-0.52912400	-1.06465800	-0.32858500

C	-0.42972600	1.19030600	-0.27233000
C	0.42605800	1.62924000	0.89281500
H	-0.46545900	-2.30421800	1.46149700
H	-3.61503900	1.66029300	0.17681600
H	-1.90788600	0.73329800	1.29578600
H	-1.51270900	-2.23131200	-0.44678100
H	-0.48396700	1.95529100	-1.04487800
H	0.08555100	2.60670100	1.23833300
H	0.36013000	0.91420200	1.71642400
O	-2.77918300	1.73307900	-0.29691000
O	1.77312600	1.69558600	0.42461800
O	1.33114100	-1.50447400	0.99162700
O	0.19256300	0.00777800	-0.89620700
H	2.30555400	2.22215900	1.03222100
O	-2.64572600	-1.78986500	-0.02379200
H	-2.75315400	-1.87223300	0.93855300
H	-2.19618900	-0.46087100	-1.48080300
Ca	2.62938500	-0.31588900	-0.58396400

Ca(II)/HM-ts7

E = -1287.837778
H = -1287.835330
G = -1288.046771

C	-0.27879400	2.30152400	-0.29736200
C	1.98397100	-0.57205800	0.20419400
C	1.76646400	0.93798300	0.29908800
C	0.59220100	1.13476100	-0.66399500
C	0.70824700	-1.17895500	-0.23764900
C	-0.05734100	-1.96385800	0.78462300
H	0.18502300	3.29543500	-0.26624000
H	3.25743800	-0.23403300	-1.53272800
H	2.50443500	-1.00157500	1.05473100
H	2.01768200	-1.41786400	-1.42653200
H	0.47004000	-2.87696000	1.06251300
H	-0.26502200	-1.38652800	1.69429400
O	2.87972500	-0.96371300	-1.00607700
O	-1.36563000	-2.27189300	0.26146300
O	-1.45553700	2.15378000	-0.06168400
O	-0.17317900	-0.03793900	-0.56201600
H	-1.25017000	-2.82799400	-0.52108200
H	2.63304500	1.54762800	0.03972900
H	0.96166600	1.28399100	-1.68856200
O	1.28130900	1.22084000	1.59153200
H	2.01640300	1.25975200	2.21416700
Ca	-2.50762700	-0.12034100	-0.14747100

Ca(II)/HM-ts8

E = -1211.437760
H = -1211.435312
G = -1211.632106

C	0.63917300	2.40158100	-0.18193400
C	-2.21093300	0.01395500	-0.38259500
C	-1.70395300	1.39229500	-0.53103100
C	-0.40629700	1.37482500	-0.19190800
C	-1.04790400	-0.78473000	0.06859300
C	-0.52561000	-1.95785100	-0.70425800
H	0.36097500	3.43799900	-0.39966300
H	-3.86042400	-0.58477400	0.94047300
H	-2.92267100	-0.36745700	-1.10871500
H	-2.13797400	-0.72514800	1.25172000
H	-1.22245500	-2.79391500	-0.65619900
H	-0.31911400	-1.71445500	-1.75310200
O	-3.02850400	-0.08288000	1.01787100
O	0.72375300	-2.30501900	-0.07077000
O	1.78783700	2.07705600	0.04569900
O	0.05270700	0.15616000	0.15120600
H	1.03625400	-3.14604200	-0.42395100
H	-2.26302100	2.24766600	-0.87411800
Ca	2.32876200	-0.48784300	0.27051500

Ca(II)/HM-ts9

E = -1211.466046
H = -1211.463598
G = -1211.656262

C	-0.61662600	-2.05602600	0.34058600
C	-1.60781400	1.34938200	0.63296400
C	-2.21161500	0.00337900	0.48802900
C	-1.10274000	-0.80395900	-0.11981500
C	-0.39162300	1.32128700	0.08515200
C	0.67006600	2.34861200	-0.07846000
H	-1.35425000	-2.77681900	0.71203100
H	-2.06597000	2.19340700	1.12150500
H	0.65360900	2.74406500	-1.09671600
H	0.51320800	3.15867300	0.63194000
O	1.91302900	1.68154300	0.16833200
O	0.57902700	-2.36607200	0.27820800
O	-0.03424800	0.10062700	-0.41025200
H	2.63380200	2.31965300	0.11162800
H	-2.76467900	-0.40411300	1.32705100
H	-2.23045400	-0.74136000	-1.09287600
O	-3.18565800	-0.11895000	-0.70324700
H	-3.32719000	0.73702800	-1.14524600
Ca	2.26634200	-0.72918800	-0.16621900

Ca(II)/FU-ts

E = -1135.046967
H = -1135.044519
G = -1135.227634

C	-0.83113900	1.72173800	-0.06381200
C	-2.16886400	1.51938200	-0.37613900
C	-2.39993000	0.18112500	-0.11860000
C	-0.28470900	0.47165500	0.31330300
C	0.98412300	0.15366500	1.08489200
H	-0.25851400	2.63390300	-0.14831000
H	1.19698000	0.91307600	1.84112300
H	0.85207300	-0.81636400	1.57353200
O	1.92338300	0.13716800	0.03318100
O	-1.33098600	-0.44635100	0.31081300
H	0.51344200	0.29892700	-0.62622100

H	-2.88658200	2.23148200	-0.74867700
C	-3.65221300	-0.61564000	-0.28688000
O	-3.67222300	-1.79522500	-0.08068100
H	-4.53331100	-0.04142700	-0.60270200
Ca	3.99354500	-0.44879400	-0.33559200

Ca(II)/Ch-ts1

E = -1631.034891
H = -1631.032443
G = -1631.328227

C	-1.91922900	1.46410200	0.26845400
C	-2.08284700	-1.18301600	-0.52208000
C	-2.96548200	-0.75497300	0.64005400
C	-2.86230600	0.72972900	0.84523900
C	-0.74004500	-0.46390200	-0.40591400
C	0.20853100	-0.87875000	-1.51779200
H	-4.65140900	-0.77010100	-0.36253000
H	-1.83898800	2.53630600	0.37892100
H	-4.54705200	0.70749500	1.72097200
H	-2.67688800	-3.03302000	-0.52742800
H	-0.20981600	0.67929300	-2.53573700
H	-2.55569000	-0.87806600	-1.46558900
H	-2.63847200	-1.28135300	1.54193000
H	-0.29491000	-0.69930900	0.57159400
H	1.35065900	-1.39111700	-0.93750500
H	0.11735700	-1.96773200	-1.67644700
O	-4.31583400	-1.15281300	0.45938000
O	-3.78007900	1.29553100	1.68250300
O	-1.83183400	-2.56829100	-0.50470000
O	0.00784500	-0.24855500	-2.71899500
O	-0.92774400	0.93263000	-0.52447500
C	1.56322200	3.20115700	-0.12888100
C	1.88462500	2.26554300	-1.15392300
C	1.87530700	1.04310300	-0.55870100
C	1.38958600	2.47111800	1.00152100
H	1.48015900	4.27123800	-0.21650900
O	1.58447600	1.15718500	0.76173500
H	1.15159700	2.73739500	2.01775500
H	2.09476100	2.46349400	-2.19290200
C	2.02590800	-0.29099200	-1.11006200
O	2.53546500	-1.29169000	-0.30976600
H	2.36766600	-0.28271200	-2.14527500
Ca	3.72045300	-1.68512500	1.54579100

Ca(II)/Ch-ts2G

E = -1631.059221
H = -1631.056772
G = -1631.355054

C	-1.26992900	-1.69851200	-0.17346400
C	-1.14156400	1.01046700	0.22925900
C	-2.42005000	0.48225300	-0.38116500
C	-2.38535400	-1.00573900	-0.36382800
C	0.05053500	0.27473100	-0.38180100
C	1.34791800	0.81614700	0.10922400
H	-3.56123000	1.85740400	0.44582000
H	-1.24708600	-2.78115900	-0.14145700
H	-3.58792200	-2.52274600	-0.67630700
H	-0.21770400	2.70393200	0.19263700
H	1.37488600	-0.20616900	1.77430600
H	-1.15893200	0.80928400	1.30699900
H	-2.52784700	0.86764300	-1.40059800
H	-0.00416600	0.33938100	-1.47535300
H	2.00492500	2.12686200	-0.49628600
O	-3.56948300	0.89273200	0.37749900
O	-3.64102700	-1.56678200	-0.54771000
O	-1.10640000	2.39300700	-0.02887600
O	1.47895400	0.72054800	1.51399500
O	-0.04551100	-1.13042500	-0.01816600
C	5.43451200	-1.03543300	1.04334800
C	4.22647600	-0.28512300	1.16213300
C	3.70990800	-0.19023600	-0.09445900
C	5.56001400	-1.33819200	-0.27135300
H	6.11290000	-1.31430800	1.83166800
O	4.52934600	-0.83127200	-0.97768500
H	6.29454200	-1.89045600	-0.83261200
H	3.80068000	0.14159900	2.05291800
C	2.53264600	0.44331100	-0.67933700
O	2.94472800	2.03213400	-1.11013500
H	3.71959000	2.33764700	-0.60781400
H	2.32484500	0.07091700	-1.67768900
Ca	-5.59615000	-0.37307100	0.24205200

Ca(II)/Ch-ts2F

E = -1631.049843
H = -1631.047394
G = -1631.343432

C	1.54617400	1.71306300	0.53851700
C	0.95813000	-0.97640200	0.12494900
C	2.30329100	-0.47211100	-0.36576600
C	2.50603900	0.95254300	0.03274900
C	-0.07749100	0.13326100	-0.08587900
C	-1.47519200	-0.28255500	0.27752300
H	3.26766500	-1.45920400	1.05593500
H	1.69243500	2.73365700	0.86792500
H	3.92630200	2.30235100	-0.03219100
H	0.20840300	-2.77821600	-0.05030700
H	-1.92454300	-1.31933900	2.12024200
H	1.01907400	-1.19210000	1.19798200
H	2.34382600	-0.57864700	-1.45316300
H	-0.09265700	0.41027100	-1.14895200
H	-1.71698400	-1.27821400	-0.09110000
O	3.39781000	-1.26245200	0.11754500
O	3.81471800	1.35246300	-0.16761500
O	0.62788700	-2.12495300	-0.61868800
O	-1.46069800	-0.49649400	1.88051300
O	0.26101500	1.28153500	0.68626800
C	-5.94563400	-0.14075100	-0.81798000
C	-4.89774600	0.84280700	-0.82427400
C	-3.84207000	0.27776400	-0.17157300
C	-5.45889100	-1.22196300	-0.17467700
H	-6.93133100	-0.04961800	-1.24500500

O	-4.17076000	-0.98465900	0.22808500
H	-5.85923000	-2.19089200	0.06709800
H	-4.91922500	1.82951100	-1.25310700
C	-2.52239300	0.75024900	0.20481000
O	-2.19849200	1.94388300	-0.47535600
H	-1.75095000	2.52846000	0.14208000
H	-2.17321200	0.32315100	1.82724000
Ca	5.60866500	-0.32055900	-0.38205400

Ca(II)/Ch-ts3G

E = -1554.659397
H = -1554.656949
G = -1554.932745

C	-1.90151100	2.11278400	-0.33464200
C	-0.26215700	-0.12998200	0.02395800
C	-1.73519200	-0.26312900	0.37562300
C	-2.48681700	0.97348900	0.00078700
C	0.17074400	1.31187800	0.40646400
C	1.62610300	1.51791300	0.17426400
H	-2.05205500	-1.47258100	-1.16232900
H	-2.43416900	3.00538700	-0.63444800
H	-4.34756700	1.58635200	-0.08141600
H	1.28978400	-1.27920100	0.33985800
H	3.09887900	2.04734400	-0.08865800
H	-0.13654600	-0.24606800	-1.06019200
H	-1.81782800	-0.45411600	1.44916100
H	-0.00833000	1.44027400	1.48432400
O	-2.34537900	-1.40162100	-0.24269000
O	-3.85193200	0.76537800	0.03423700
O	0.42542200	-1.11040500	0.74365900
O	2.05851400	2.27866200	-0.73925000
O	-0.54624300	2.27801500	-0.33086500
C	4.28943700	-1.77218000	-1.06773700
C	3.23108200	-0.80439200	-0.97562400
C	3.41563900	-0.14931500	0.20678900
C	5.01775100	-1.64333800	0.05944100
H	4.46854200	-2.47030400	-1.86827900
O	4.49733100	-0.65634700	0.84678400
H	5.88256000	-2.15102200	0.44919900
H	2.47070700	-0.59788200	-1.71290800
C	2.72929500	0.95131700	0.89613100
H	2.61779300	0.79373600	1.96515100
Ca	-4.77498500	-1.50308200	-0.00835900

Ca(II)/Ch-ts3F

E = -1554.671305
H = -1554.668856
G = -1554.944868

C	0.89411700	-1.58166600	0.11495600
C	0.99793500	1.10621200	-0.57541400
C	2.22293700	0.50565100	0.09935700
C	2.05258600	-0.96110300	0.28887100
C	-0.26385400	0.49757400	0.03931900
C	-1.51526700	1.07830100	-0.54354700
H	3.25992300	0.57719100	-1.58886900
H	0.76998000	-2.65244800	0.22429800
H	3.11125100	-2.50131800	0.88504800
H	1.76502500	2.88093900	-0.77573500
H	1.01072100	0.83924700	-1.64213000
H	2.38870800	1.00827400	1.05599300
H	-0.22859400	0.63249700	1.12755400
H	-1.60975300	0.88870100	-1.61010400
O	3.42584400	0.76246100	-0.65264900
O	3.24263300	-1.57545900	0.64470100
O	0.96240900	2.50005300	-0.40024600
O	-0.25382100	-0.93234800	-0.21011200
C	-5.75531700	-1.01394300	0.18070600
C	-5.03129100	0.05382500	0.75820300
C	-3.82043900	0.08702900	0.11949700
C	-4.93662700	-1.54409800	-0.77337300
H	-6.74936900	-1.34748800	0.42470500
O	-3.76781700	-0.89614000	-0.82477200
H	-5.06043400	-2.35817500	-1.46830500
H	-5.34756600	0.72861800	1.53677200
C	-2.68421100	0.92937500	0.27641900
O	-2.61831300	1.77892000	1.24162000
H	-1.69992000	2.15829100	0.48956800
Ca	5.37495700	-0.44485800	0.15214500

Mg(II)/intermediates

Local minima

Mg(II)/(2)

E = -886.743954
H = -886.741505
G = -886.979906

C	2.12943000	-0.26847500	-0.72962500
C	0.99852400	-0.37973300	0.30561800
C	-0.21564500	0.45197600	-0.11555600
C	-1.39129800	0.20494400	0.82865400
H	0.68754200	-1.42912100	0.34275100
H	-0.50244800	0.13848000	-1.12843800
H	-1.06260700	0.33357900	1.85893200
O	-1.85589300	-1.15290600	0.62931100
H	-1.71361000	-1.70497500	1.40692600
O	1.42582800	0.08147100	1.57249800
H	1.74550700	-0.65614600	2.10161800
O	0.03236000	1.83630500	-0.06507600
H	0.93362700	1.98610700	-0.38835700
C	-2.57589200	1.10367500	0.55281800
H	-2.25356200	2.13234800	0.41802600
O	-3.15694300	0.60700100	-0.67402600
H	-3.79585000	1.23072900	-1.03874100
H	-3.31197800	1.02829600	1.35220200
C	3.32303000	-1.06440300	-0.25928300
H	3.16622700	-2.14095000	-0.08431100
O	4.38785600	-0.53874800	-0.06900400

O	2.49735300	1.06844900	-0.96274100
H	3.39653700	1.18915700	-0.61999400
H	1.77938700	-0.72112300	-1.66623700
Mg	-3.27684600	-1.40723900	-0.79148600

Mg(II)/(3)

E = -886.754754
H = -886.752305
G = -886.979372

C	2.45601600	0.87349600	-0.53080100
C	0.25790600	0.04762800	-0.43108200
C	1.24143600	-1.13562900	-0.41697500
C	2.50451500	-0.50077200	0.12427600
C	-0.61250200	0.12320500	0.82709400
H	2.83116100	0.82169200	-1.55712100
O	3.19902600	1.86070600	0.09585800
H	2.90458900	1.93601400	1.01291800
C	-1.34442700	1.44060500	0.92966200
H	-0.61843300	2.25242100	0.98004000
H	-1.94793000	1.43786300	1.84159000
O	-2.18017900	1.57686300	-0.21771100
H	-2.48253100	2.48841500	-0.27582000
O	3.62829300	-1.27294800	-0.21195900
H	4.40193900	-0.91851300	0.23981100
H	2.41160300	-0.38194700	1.21216800
O	0.74543600	-2.20065600	0.36861300
H	1.34368200	-2.95204300	0.29338300
H	1.43320300	-1.47509800	-1.43967500
O	-1.59181500	-0.90683500	0.79671600
H	-1.11743500	-1.75003000	0.77849900
H	0.01889200	0.02290500	1.71785800
O	1.07659400	1.21689200	-0.51750300
H	-0.40190800	0.01041800	-1.29950000
K	-3.93754300	-0.46186600	-0.47522600

Mg(II)/(4)

E = -810.345009
H = -810.342561
G = -810.541411

C	-0.36650100	-1.07586300	0.66900200
C	-1.73607900	-0.48721300	0.31129100
C	-1.42815000	0.54259000	-0.79082500
C	0.09252700	0.43501200	-0.96823100
C	0.89541100	1.27772000	0.01483800
C	0.42732500	1.00977400	1.43658400
O	-2.57727600	-1.47395500	-0.23684000
O	-1.84844300	1.83202400	-0.42079800
O	2.24263600	0.78713000	-0.16704500
O	0.37255200	-0.93867000	-0.58060600
O	0.31620900	-0.39915000	1.66835000
H	-2.18803800	-0.00114200	1.17825400
H	-0.39068900	-2.13100200	0.92457500
H	-1.92183700	0.20298300	-1.70190100
H	0.43470500	0.57591300	-1.99140000
H	0.85207600	2.33797000	-0.22545300
H	1.14842600	1.38276500	2.16074300
H	-0.53023700	1.50733300	1.60134400
H	-2.93631200	-2.01827600	0.47275900
H	-1.98753100	2.36341100	-1.21207500
H	2.90070000	1.37262300	0.22705300
Mg	2.43884300	-1.18864400	-0.63119500

Mg(II)/(5)

E = -810.330938
H = -810.328489
G = -810.538136

C	-0.23946600	2.25559400	-0.21976400
C	1.28345100	0.63820100	0.57779500
C	-1.28057400	1.45903900	0.01181500
C	-1.08208700	0.02727400	0.38777000
C	0.30779300	-0.36020100	-0.02064200
C	2.72448400	0.19423200	0.41526900
O	1.07242400	1.85532300	-0.13934200
O	-2.59926000	1.80346600	-0.01859800
O	-1.94204300	-0.88073000	-0.32947300
O	0.49156200	-1.72529000	0.37631900
O	2.92175900	-0.56300200	-0.76800600
H	1.06694000	0.81602300	1.63720500
H	-2.71324500	2.71711300	-0.30710600
H	-0.34380700	3.29751900	-0.49149100
H	-1.24423400	-0.12912000	1.45862400
H	-2.86850400	-0.60978200	-0.25448900
H	0.38410900	-0.30010300	-1.10876300
H	1.34013400	-2.03316500	0.01628600
H	3.37647600	1.06897600	0.45435400
H	2.98437200	-0.46291500	1.24509900
H	2.93376600	0.02821200	-1.52924400
Mg	-1.22942900	-2.79964400	-0.08342800

Mg(II)/(6)

E = -733.922683
H = -733.920235
G = -734.111619

C	0.69561000	1.35528700	-0.54282000
C	-0.68082100	-0.53590300	-0.92276000
C	1.70534300	0.55288800	-0.21155000
C	1.42541700	-0.82709300	0.21720600
C	0.23652500	-1.35966400	-0.06998900
C	-2.13937300	-0.91625800	-0.85108400
O	-0.61140300	0.85280100	-0.48718900
O	3.01730900	0.87996600	-0.18184100
O	2.38325800	-1.47431000	0.90730900
O	-2.59675300	-0.53409500	0.46083200
H	-0.36929800	-0.53978500	-1.97347000
H	3.15432200	1.82429700	-0.32867600
H	0.76001600	2.40123800	-0.80206500
H	3.16825000	-0.91263300	0.97407200
H	-0.03787400	-2.36101900	0.23178800
H	-2.71555400	-0.38085300	-1.60452800

H	-2.25090300	-1.99076400	-0.98387700
H	-3.49063100	-0.85877900	0.62768200
Mg	-1.93448500	1.28398800	1.04601300

Mg(II)/(7)

E = -733.922683
H = -733.920235
G = -734.111619

C	0.07458400	1.76903700	0.07564400
C	-1.64733800	0.20394500	-0.26746900
C	1.00954900	0.80075100	-0.03951200
C	0.65979400	-0.57324200	0.12024900
C	-0.78168000	-0.87693300	0.35122200
C	-3.10384600	0.09145900	0.12853400
O	-1.22029700	1.52387200	0.13609100
O	2.37496100	0.99614100	-0.15565700
O	1.54944600	-1.43890400	0.14597600
O	-3.53937200	-1.16637000	-0.34574600
H	-1.55193100	0.17172600	-1.35808100
H	2.65369500	1.91678300	-0.06349800
H	0.31963400	2.82365600	0.14207100
H	-1.03327500	-1.84723500	-0.07444900
H	-0.93202300	-0.93584000	1.43610200
H	-3.18842400	0.16360700	1.21737100
H	-3.66245100	0.91301200	-0.32701600
H	-4.45702500	-1.29581300	-0.08757100
Mg	3.43896000	-0.80982600	-0.11185500

Mg(II)/(8)

E = -810.359976
H = -810.357527
G = -810.552785

C	0.00014300	0.89918200	-1.09677700
C	-0.44647900	-0.54970400	-1.27312500
C	-0.38056100	1.39487300	0.31039800
C	-0.07320500	0.31596400	1.37281800
C	-0.45874600	-1.08372400	0.91683200
C	-1.87309100	-1.23999200	0.40242200
O	0.29857200	-1.31074800	-0.30490200
O	-1.79344400	-0.70068400	-0.93160500
O	1.42552400	0.82951000	-1.24660300
O	-1.72409000	1.80431100	0.36980000
O	1.35473100	0.21527700	1.54349700
H	-0.43060800	1.54567100	-1.86018600
H	-0.23398900	-0.95047800	-2.26182300
H	0.22899600	2.26956300	0.54590900
H	-0.54970800	0.57343900	2.31778900
H	-0.16331200	-1.83743800	1.64201900
H	-2.15351300	-2.28988500	0.34613700
H	-2.60853100	-0.68149300	0.97771600
H	1.80692100	1.67094800	-1.52699300
H	-2.26255200	1.24539700	-0.20471700
H	1.70479000	0.93968600	2.07771200
Mg	2.29690000	-0.63386200	-0.10753800

Mg(II)/(9)

E = -733.931758
H = -733.929310
G = -734.111168

C	1.09311800	-1.01188800	0.04420300
C	0.98007200	0.16441800	-0.91530000
C	0.29448200	-1.08128000	1.10748500
O	-0.37003400	0.65939700	-0.89625800
O	1.72200000	1.23944700	-0.44143900
C	-0.74855100	-0.02220600	1.30215700
C	-0.44336400	1.19792700	0.45291300
C	0.95907300	1.79636700	0.64028500
H	1.26001500	-0.06930300	-1.94108800
H	0.38812700	-1.88267700	1.82819200
H	-0.88101800	0.24774300	2.34868500
H	-1.24405800	1.93183000	0.48634400
H	0.95863500	2.87587300	0.52116700
H	1.39035300	1.51796200	1.60136000
O	2.08522900	-1.89390100	-0.16630100
H	2.55687700	-1.71868300	-0.98935800
O	-2.04066300	-0.46024600	0.77482500
H	-2.42399000	-1.16030800	1.31870900
Mg	-2.16551500	-0.36333700	-1.26092300

Mg(II)/(10)

E = -733.944763
H = -733.942315
G = -734.124006

C	-0.89878800	1.26866000	-0.04160700
C	-0.97996400	0.07583700	-1.00425300
C	-0.45259300	0.90338900	1.36141900
O	0.27459600	-0.63159900	-0.94481900
O	-1.92053400	-0.83227900	-0.53180600
C	0.56278900	-0.23785200	1.35602300
C	0.18717900	-1.30585200	0.34042400
C	-1.26815000	-1.75077200	0.35971600
H	-1.18803400	0.37468100	-2.02841700
H	-0.06316700	1.78566900	1.86696600
H	0.69610200	-0.66707500	2.34711300
H	0.90094500	-2.12593800	0.33542900
H	-1.37926100	-2.75487700	-0.04211700
H	-1.71197300	-1.69431200	1.35298300
O	-1.20283800	2.37492000	-0.39042100
H	-1.34420200	0.57902700	1.90754300
O	1.84113000	0.23276500	0.86773000
H	2.34245900	0.70275700	1.54581200
Mg	2.24212100	0.07743000	-1.12676000

Mg(II)/(11)

E = -657.518416
H = -657.515968
G = -657.680859

C	-0.41235100	1.38217400	0.12513200
C	0.01407100	0.21634600	1.02136200
C	-1.36928800	0.99981500	-0.92582600
C	-1.75665800	-0.27471400	-0.99218700
C	-1.27725400	-1.26695400	0.03258400
C	0.14717300	-1.73836100	-0.27616300
O	-1.04826900	-0.61572200	1.28755100
O	0.92605300	-0.60578300	0.20906600
O	0.07560500	2.47791600	0.26140600
H	0.51802500	0.53399800	1.93031000
H	-1.97424400	-2.08415100	0.18796000
H	0.40897500	-2.61323900	0.31303000
H	0.34993400	-1.88372500	-1.33308300
H	-2.39490400	-0.63719500	-1.78896300
H	-1.68911600	1.75705300	-1.62969400
Mg	2.75667200	-0.08615500	-0.47109700

Mg(II)/(12)

E = -886.749052
H = -886.746603
G = -886.981798

C	2.26041100	0.47438600	-0.51586500
C	3.55090600	-0.24879800	-0.19904000
C	0.95023600	-0.17170400	-0.07347400
C	-0.18591400	0.85272900	-0.01602000
C	-1.35182900	0.31229100	0.81328900
H	0.70716500	-0.91034200	-0.85052700
H	-0.51187700	1.05743800	-1.04114700
H	-1.10461500	0.44204400	1.86647100
H	3.93832100	0.17976500	0.73258300
O	-1.57696600	-1.08428100	0.55693800
O	2.27413600	1.52753900	-1.10500200
H	-0.83110300	-1.58572900	0.92688900
O	3.29180000	-1.63609300	-0.06476200
H	4.09953200	-2.08181100	0.21172900
O	1.05469800	-0.80686600	1.18925300
H	1.77015300	-1.45910700	1.12840400
O	0.16863800	2.04633300	0.64466100
H	0.77577600	2.53106900	0.07237900
C	-2.65906500	1.00666600	0.51003000
H	-2.49499700	2.07428600	0.37699700
O	-3.13327400	0.42308100	-0.72270600
H	-3.87527400	0.92557700	-1.07977000
H	-3.39264300	0.82813100	1.29495500
H	4.26041000	-0.04003300	-1.00130100
Mg	-2.94679800	-1.58936700	-0.81152000

Mg(II)/(13)

E = -886.759512
H = -886.757064
G = -886.980095

C	-0.40056800	0.29491500	-0.32587000
C	1.85342900	-0.00317400	-0.80630600
C	1.82773200	0.79572900	0.49398700
C	0.38233000	0.64176500	0.98653800
H	2.52692300	0.41484500	1.24211800
H	0.01503000	1.58039600	1.40568500
C	2.16945900	-1.48570400	-0.69882000
H	2.13620700	-1.91624700	-1.69862500
H	3.17446400	-1.62147800	-0.29380400
O	1.21412500	-2.21158900	0.07424500
H	1.33223400	-1.99951000	1.01087200
C	-1.42172500	1.32086700	-0.78215600
H	-1.59365300	1.19802700	-1.85135700
H	-1.06481700	2.32711200	-0.56974500
O	-2.63305700	1.05983900	-0.05577300
H	-3.27365500	1.77093700	-0.18147100
O	2.10716000	2.13511100	0.14529700
H	2.16092700	2.66497000	0.94873500
O	0.35340400	-0.38117800	1.95202100
H	-0.53159000	-0.45690900	2.32463600
O	0.53644900	0.18706300	-1.34395900
O	-1.11591800	-0.93500200	-0.16942600
H	2.55518100	0.45371100	-1.50432700
H	-0.43401300	-1.64653700	-0.07740900
Mg	-3.09704100	-0.91580600	0.10176900

Mg(II)/(14)

E = -810.322529
H = -810.320081
G = -810.534576

C	-0.91320000	-0.65897100	-0.08543200
C	0.93865900	0.73838300	-0.27163800
C	-0.24565200	1.59820400	0.13637500
C	-1.44140200	0.73544400	-0.27584700
H	-1.65487500	0.92610000	-1.33486700
C	2.19722300	0.88821300	0.53753000
H	2.71244300	1.81176500	0.28014500
H	1.98322100	0.85086800	1.60600100
O	3.00842500	-0.24722600	0.17038900
H	3.89964400	-0.17844900	0.53411700
C	-1.59082100	-1.78112000	0.07023400
H	-1.11701500	-2.73848600	0.25032500
O	-2.95113900	-1.74281000	-0.04409400
H	-3.34083900	-2.51878100	0.37221300
O	-2.55104800	1.04729800	0.52747300
H	-3.24593800	0.39988300	0.35073200
O	0.48984200	-0.62826700	-0.05873100
H	1.14014500	0.86750600	-1.33835400
O	-0.14775300	2.83135700	-0.52074800
H	-0.81432600	3.42954700	-0.16497100
H	-0.27418300	1.71819200	1.22506300
Mg	2.02135500	-1.98099000	-0.25350500

Mg(II)/(15)

E = -810.342430
H = -810.339981
G = -810.545641

C	0.18970800	-1.97781000	0.42993500
C	-1.45134500	0.84565900	0.22948400
C	-1.79919700	-0.51026100	-0.39393400

C	-0.42242100	-1.14558000	-0.66403200
C	-0.06916400	1.17565300	-0.33364000
C	0.89991000	1.63489000	0.73472600
H	-0.39312900	-2.77778200	0.89653500
H	-3.14523700	1.78502300	0.41015100
H	-1.39347200	0.73212600	1.31983300
H	-0.46390900	-1.78940900	-1.54903600
H	-0.14454700	1.90143100	-1.14169400
H	0.72799700	2.68338600	0.97138600
H	0.80780900	1.03401400	1.64199500
O	-2.33857200	1.87574500	-0.10980800
O	2.21695100	1.45571300	0.18713600
O	1.34913700	-1.78965900	0.75096500
O	0.45422000	-0.05343900	-0.92572000
H	2.87408200	1.95377500	0.68970300
O	-2.67737200	-1.31408800	0.33751400
H	-2.52994400	-1.21166100	1.28547300
H	-2.26825800	-0.32145500	-1.36025200
Mg	2.48406300	-0.45991000	-0.42500200

Mg(II)/(16)

E = -733.937564

H = -733.935116

G = -734.125226

C	1.11870600	-2.05135100	0.26393700
C	-2.03412200	-0.02403800	0.26694000
C	-1.29508900	-1.30151200	0.62415100
C	-0.08293600	-1.24783600	0.09162800
C	-0.90455100	0.84461400	-0.30734200
C	-0.31779300	1.83325200	0.68050700
H	1.04612300	-3.07011600	0.64930700
H	-3.79825200	-0.60365400	-0.33589400
H	-2.47837300	0.44550500	1.14814000
H	-1.19200800	1.31646500	-1.24374200
H	-0.92052600	2.73841800	0.71600700
H	-0.23715500	1.39738100	1.67841600
O	-2.99907700	-0.24135500	-0.73563900
O	1.00231100	2.13518800	0.18874700
O	2.20029600	-1.53852900	0.00647600
O	0.17517400	-0.08321800	-0.60925000
H	1.34985600	2.93264700	0.60594000
H	-1.69833300	-2.11547100	1.20692500
Mg	2.16614600	0.53861400	-0.41222500

Mg(II)/(17)

E = -733.936757

H = -733.934309

G = -734.123975

C	-0.73200700	1.97572200	-0.22921600
C	-1.01535100	-1.37369000	-0.69012300
C	-1.97295400	-0.25728400	-0.35480200
C	-1.05817800	0.68707100	0.46223600
C	0.12859300	-1.19079300	-0.06324600
C	1.41541400	-1.92726800	0.01043500
H	-1.55742800	2.63962800	-0.50551200
H	-1.25532900	-2.20622000	-1.33228100
H	1.51506400	-2.43939300	0.96833900
H	1.49748400	-2.63563300	-0.81050900
O	2.43903100	-0.91494100	-0.09154900
O	0.41722500	2.28597100	-0.47258700
O	0.17920200	-0.00379500	0.67919000
H	3.32080500	-1.30659600	-0.07997700
H	-1.52667700	0.90551600	1.42509700
Mg	1.96093800	1.05158100	0.17334600
O	-3.03818700	-0.65023500	0.47969900
H	-3.74116000	-1.02716100	-0.06133300
H	-2.35529800	0.23233900	-1.25370500

Mg(II)/(18)

E = -657.545312

H = -657.542864

G = -657.715215

C	-2.31154500	-0.11065500	-0.04407000
C	0.53215900	2.21447200	0.07565400
C	-0.89218600	2.12180800	0.04955600
C	-1.20125400	0.79837300	-0.05224800
C	1.00554400	0.94250000	-0.01475900
C	2.31218800	0.21694000	-0.04022700
H	-3.33448300	0.26783800	-0.04647400
H	1.12026600	3.11234500	0.15878400
H	2.86947800	0.46251300	-0.94476900
H	2.90633500	0.47285700	0.83688500
O	1.98281200	-1.18319900	-0.03072500
O	-2.07964300	-1.32301500	-0.02925400
O	-0.03228200	0.09184300	-0.10032700
H	2.78882200	-1.71229400	-0.06075700
H	-1.59655200	2.93528900	0.11394900
Mg	-0.03253400	-1.94368300	0.11511700

Mg(II)/(19)

E = -543.052819

H = -543.05037

G = -543.195401

C	2.39894200	-0.27408500	0.01670400
C	1.73259200	0.97998900	0.04145200
C	0.39931200	0.70861700	-0.00005700
C	1.43464300	-1.22577400	-0.03672700
H	3.46034700	-0.45194400	0.03379900
O	0.20506200	-0.65192900	-0.04577000
H	1.45761600	-2.30160400	-0.07691700
H	2.17419000	1.96262700	0.08623800
C	-0.80614700	1.46284400	-0.01014100
O	-1.89948900	0.88554000	-0.04441800
H	-0.75295500	2.55236700	0.01011400
Mg	-1.97831900	-1.12832300	0.05007300

Mg(II)/adduct (5)+(19)

E = -1153.555715

H = -1153.553267

G = -1153.853228

C	2.17824100	-2.52880600	0.17098200
C	1.92943600	0.14917000	0.55039800
C	0.66858800	-0.56220000	0.11290600
C	0.94029000	-2.04705900	0.12407600
C	3.13573200	-0.40850000	-0.18135500
C	4.43473500	0.29264900	0.16120500
H	-1.19957000	-0.30372400	0.59197700
H	2.39712800	-3.58694000	0.18304700
H	-0.88744000	-2.47351100	-0.30961600
H	0.91478700	1.82116200	0.65099200
H	5.35127500	1.86764900	-0.64263500
H	2.06642600	0.00453800	1.62580200
H	0.40764900	-0.24128600	-0.90415800
H	2.96873200	-0.36961400	-1.26612000
H	4.54141500	0.42377300	1.23839500
H	5.26275700	-0.29893200	-0.22397100
O	-0.33847800	-0.15050200	1.01349600
O	-0.12207000	-2.90072500	0.10747900
O	1.78161700	1.55752500	0.30259900
O	4.44337200	1.58186300	-0.48415400
O	3.31316300	-1.74931300	0.22795800
C	-5.79065900	1.38782900	0.25256300
C	-5.54769800	0.24037100	-0.54358000
C	-4.21954900	-0.04736100	-0.40003300
C	-4.59329400	1.70685700	0.81694300
H	-6.72228400	1.90813600	0.39424400
O	-3.63153000	0.85157900	0.43409300
H	-4.29052300	2.49147000	1.49034700
H	-6.25117300	-0.31201400	-1.14578100
C	-3.41599000	-1.09874900	-0.95267200
O	-2.22243500	-1.22657700	-0.72052800
H	-3.94298900	-1.80148100	-1.61046200
Mg	2.93964200	2.88789800	-0.64901800

Mg(II)/(20)

E = -1153.558794
H = -1153.556346
G = -1153.851706

C	1.85017300	-1.72461500	-0.06682300
C	1.35540300	0.97881600	-0.00243900
C	2.71838700	0.52923700	0.47184000
C	2.87176000	-0.92212600	0.19005700
C	0.31216900	-0.01364200	0.51185800
C	-1.09271500	0.37800200	0.08100700
H	3.70485700	2.14845700	-0.13696400
H	1.96016500	-2.77295200	-0.31230200
H	4.33576800	-2.25353100	0.09385800
H	0.58387500	2.77336600	-0.09461700
H	-0.94391000	-0.34768200	-1.71731800
H	1.34874000	0.96986900	-1.09623700
H	2.85513500	0.76257200	1.53155200
H	0.36322900	-0.07869900	1.60359700
H	-1.31588100	1.36096300	0.50215000
O	3.76237000	1.19167500	-0.26877800
O	4.21490300	-1.29565800	0.15363500
O	1.15227100	2.27739500	0.50437000
O	-1.17433800	0.50231100	-1.32034700
O	0.55780100	-1.31491500	-0.03966200
C	-5.53898900	0.61261200	-0.29119800
C	-4.44033200	0.65306200	0.63030700
C	-3.51460300	-0.20943300	0.14692900
C	-5.18819300	-0.26933600	-1.25392400
H	-6.46222500	1.16498000	-0.23750200
O	-3.95810300	-0.78350900	-0.99834800
H	-5.67782400	-0.63012100	-2.14202000
H	-4.35248500	1.24195900	1.52847300
C	-2.14999900	-0.59742600	0.61463100
O	-2.04754200	-0.54395500	2.02320300
H	-2.72659400	-1.11122700	2.40495000
H	-1.92575700	-1.60151000	0.23432100
Mg	5.42463700	0.13465900	-0.73233300

Mg(II)/(21)

E = -1077.156134
H = -1077.153686
G = -1077.420758

C	2.05799500	1.88712700	-0.00496200
C	1.03349100	-0.68033100	0.14526700
C	2.45862400	-0.53194300	-0.35231000
C	2.89933700	0.88140500	-0.18881300
C	0.20187900	0.47167700	-0.43392400
C	-1.21905700	0.37144800	0.02412100
H	3.13100500	-1.44752000	1.30059900
H	2.37256700	2.91098800	0.15043000
H	4.60978600	1.86374800	-0.43132200
H	0.74573100	-2.60678300	0.26721800
H	-2.22859000	0.32953400	1.65036500
H	1.01478100	-0.59311900	1.23855000
H	2.52877700	-0.87122600	-1.38802900
H	0.24199400	0.42821300	-1.52656700
O	3.38277300	-1.38587300	0.36645700
O	4.28936500	0.98929400	-0.17455000
O	0.45118500	-1.87959800	-0.29134500
O	-1.30613700	0.42161900	1.37325700
O	0.71086800	1.73980500	-0.00354600
C	-5.81981900	-0.36389300	-0.30748500
C	-4.72643100	-0.25301800	-1.22413900
C	-3.61950700	0.00640200	-0.47810100
C	-5.30615900	-0.16362300	0.92565300
H	-6.85198300	-0.56702400	-0.53924000
O	-3.96676100	0.06345700	0.84366400
H	-5.72872100	-0.14679100	1.91512700
H	-4.75250800	-0.35792400	-2.29612000
C	-2.23310400	0.19900200	-0.83218700
H	-2.00757000	0.17081700	-1.88910200
Mg	5.33924100	-0.80400500	0.08315600

Mg(II)/(22)

E = -1077.154504

H = -1077.152055
G = -1077.423857

C	-1.80841600	1.71741900	-0.25028400
C	-1.20736000	-0.97367300	-0.04980000
C	-2.58338600	-0.54036400	0.40156700
C	-2.79536100	0.89044200	0.05563600
C	-0.21216500	0.08880200	0.42427600
C	1.20631600	-0.29076800	0.15593900
H	-3.49209300	-2.22559300	-0.12513100
H	-1.95317600	2.75278700	-0.52937700
H	-4.31536300	2.15175200	-0.11174300
H	-0.42792000	-2.77180000	-0.04809300
H	-1.18551100	-1.02184700	-1.14319200
H	-2.69534200	-0.71947600	1.47528800
H	-0.37893400	0.26502400	1.49696400
H	1.43203000	-1.33214200	-0.02113100
O	-3.61585400	-1.27803300	-0.28268000
O	-4.14802000	1.21346100	0.05226400
O	-0.97532100	-2.23375100	0.53307100
O	-0.50193700	1.33519600	-0.24884700
C	5.81450900	-0.05815700	-0.27835200
C	4.76084500	0.89132600	-0.09217400
C	3.61402400	0.16812700	-0.01496900
C	5.22261000	-1.27498900	-0.29939600
H	6.86796000	0.14011900	-0.38185300
O	3.88221600	-1.15588200	-0.13883900
H	5.59790300	-2.27754500	-0.41290200
H	4.83757100	1.96336300	-0.02506800
C	2.22927100	0.57091700	0.17952300
O	2.12638800	1.90600700	0.39179800
H	1.19994600	2.17178000	0.30330300
Mg	-5.42268100	-0.37724200	-0.36024900

Mg(II)/(23)

E = -1077.155428
H = -1077.152979
G = -1077.427469

C	2.23916900	1.84547300	-0.16895000
C	0.98741700	-0.59778100	0.22302500
C	2.41659900	-0.63101700	-0.29417400
C	2.96894700	0.75236300	-0.33118600
C	0.27042400	0.59441600	-0.41738800
C	-1.16404300	0.64263000	0.12478900
H	2.98967900	-1.42272500	1.46270200
H	2.65862500	2.84132500	-0.11548700
H	4.68478200	1.35038400	-1.12692400
H	0.46947700	-2.46828900	0.48061800
H	-2.23609900	0.81094100	-1.66792200
H	0.99197200	-0.42928600	1.30810800
H	2.44781900	-1.11670400	-1.27147000
H	0.27455500	0.48438800	-1.50762500
O	3.29033400	-1.43597900	0.54156900
O	4.36502000	0.77152300	-0.42222500
O	0.26202300	-1.74796900	-0.12456400
O	-1.35769300	1.06417100	1.23315500
O	0.89076000	1.82262000	-0.07021400
C	-5.55419500	-0.10460900	0.81869000
C	-4.19334600	0.33987100	0.92768300
C	-3.58502300	-0.01608000	-0.22984900
C	-5.66276000	-0.69139000	-0.39207800
H	-6.33764900	0.00333900	1.55016100
O	-4.47328300	-0.64683000	-1.04552800
H	-6.47313700	-1.16912900	-0.91538900
H	-3.73299700	0.85268500	1.75279600
C	-2.22262900	0.12971300	-0.80656600
H	-1.86924600	-0.82808000	-1.20454000
Mg	5.27596300	-0.92588900	0.30278800

Mg(II)/(24)

E = -1077.168081
H = -1077.165633
G = -1077.440113

C	1.59984900	-1.58374000	-0.61734400
C	1.28490600	1.10151400	0.04284100
C	2.62652400	0.45678500	0.35813700
C	2.66444300	-0.93258700	-0.17504700
C	0.19741700	0.06209600	0.32043000
C	-1.19577300	0.59376500	0.09075900
H	3.51645400	1.56898200	-1.05958800
H	1.63792700	-2.57260300	-1.05611100
H	4.02418600	-2.38446800	-0.20230400
H	1.55319500	2.96683300	0.56323700
H	1.24909500	1.37028800	-1.02161700
H	2.79945100	0.48368300	1.43626500
H	0.30141800	-0.29189700	1.35228800
H	-1.36011300	0.78672500	-0.97128100
O	3.75292400	1.18660700	-0.20082700
O	3.96817600	-1.42026800	-0.21642700
O	1.03709000	2.21200100	0.86616600
O	0.35180600	-1.06618900	-0.54787100
C	-5.79687400	-0.22370500	-0.31179500
C	-4.77181900	-0.83054700	0.46372500
C	-3.61842400	-0.18021200	0.14517000
C	-5.18764500	0.74810800	-1.04086200
H	-6.84463000	-0.47186800	-0.32993300
O	-3.86896700	0.78953200	-0.77742300
H	-5.55201200	1.46022500	-1.76212600
H	-4.86216600	-1.63975000	1.16928400
C	-2.24821100	-0.35890400	0.62217200
O	-1.98974300	-1.22487600	1.43263400
H	-1.31790200	1.54704700	0.61227900
Mg	5.45987100	0.02057500	-0.21412700

Mg(II)/Transition states

Mg(II)/AG-ts1

E = -886.691207
H = -886.688759
G = -886.914300

C	1.03668200	-0.64103300	-0.44447700
C	0.25329900	-1.37755500	0.62868000

C	-1.16276800	-1.63088400	0.12708300
C	-1.92382900	-0.31499100	-0.06845300
C	-1.16945000	0.64794700	-1.00687600
H	1.38459700	-1.28532700	-1.24748300
H	-1.48269700	0.45174000	-2.03067800
O	0.28063400	0.47615000	-1.02516500
O	2.00507900	0.20892000	0.09544300
H	1.11502900	1.02776400	-0.35331400
C	-1.37670100	2.11293700	-0.67714600
H	-2.44134600	2.27719600	-0.49868500
O	-0.59825700	2.39412600	0.47451100
H	-0.74269000	3.30963800	0.73348000
H	-1.05179100	2.72700900	-1.52036200
O	0.17591000	-0.61021100	1.80673500
H	1.03363200	-0.18521000	1.94188900
O	-1.00598100	-2.30881600	-1.10485800
H	-1.85138200	-2.68471500	-1.37252400
H	0.75574700	-2.33339400	0.80687900
H	-1.70290200	-2.23202000	0.86244100
O	-2.32789300	0.25341500	1.15206800
H	-1.53235800	0.44960800	1.66492900
H	-2.85183400	-0.55470000	-0.59314900
Mg	3.93238800	0.24543500	-0.07801400

Mg(II)/AG-ts2

E = -886.688421
H = -886.685972
G = -886.916785

C	1.26248900	0.50675300	0.72843700
C	-1.14280900	0.14839700	0.76395500
C	-0.84380000	1.58836900	0.34196400
C	0.59262000	1.53844700	-0.17689600
C	-1.64403000	-0.74939000	-0.37305500
H	1.82315500	0.95040300	1.55101600
O	1.87579300	-0.57257600	0.12283300
H	0.76811400	-1.11285000	0.62442700
C	-1.58522700	-2.22349400	-0.00844000
H	-2.18911900	-2.77396100	-0.73291600
H	-2.00251600	-2.37893200	0.99084400
O	-0.22360300	-2.63345300	-0.06798400
H	-0.14305400	-3.51510300	0.31054100
O	1.15428600	2.82113800	-0.08752800
H	1.90115800	2.89510300	-0.69064200
H	0.59315100	1.16271800	-1.20402300
O	-1.77386900	2.00870200	-0.62416500
H	-1.72074500	2.96497600	-0.72949500
H	-0.86494500	2.23956400	1.22096000
O	-2.99935100	-0.45242100	-0.61473800
H	-3.05528100	0.47906100	-0.86799300
H	-1.03693600	-0.59460800	-1.27502300
O	0.14692000	-0.30026500	1.27593200
H	-1.84834600	0.09060600	1.59148500
Mg	3.54154200	-1.01920700	-0.70664700

Mg(II)/AG-ts3

E = -886.656005
H = -886.653557
G = -886.883298

C	1.17312300	0.42283500	-1.15554100
C	2.12229300	-0.39888600	-0.34365300
C	1.19365900	-1.39233300	0.38609700
C	-0.20841800	-1.11112000	-0.22869300
C	-1.22770300	-0.55617100	0.75014800
C	-0.95029900	0.92137100	1.07305700
O	1.55871400	2.88410300	-0.07015600
O	2.92021200	-1.06595100	-1.29877400
O	1.23519400	-1.24792100	1.76823700
O	-2.57327700	-0.71296200	0.23304200
O	0.01865200	-0.04507500	-1.24494800
O	0.39287000	1.08989700	1.34088900
H	2.69696400	0.20214100	0.35860200
H	1.42682100	1.27173100	-1.78146400
H	1.50383300	-2.40387500	0.12791500
H	1.07272400	2.29492700	0.58476600
H	-0.60992000	-1.94490200	-0.79899300
H	-1.15961500	-1.15435400	1.65775500
H	-1.26574300	1.52300100	0.20255300
H	-1.60446300	1.20706700	1.90802400
H	3.72054100	-0.55506100	-1.46957300
H	0.97523000	-0.28116500	1.89533800
H	1.25946500	3.78351300	0.08565500
H	-2.93425100	-1.55379400	0.54478800
Mg	-3.84303600	0.25665500	-1.00251600

Mg(II)/AD-ts1

E = -886.646497
H = -886.644049
G = -886.874496

C	1.76660600	1.15268900	-0.08454500
C	-0.58419200	1.25000900	-0.61096400
C	1.83783800	-0.33085100	-0.09237400
C	0.54065200	-0.96108600	-0.43961900
C	-0.58645400	-0.10201100	0.08136600
C	-1.58627200	2.20798400	0.00777500
O	1.79757300	1.29075000	1.58557700
O	0.70117300	1.87159800	-0.49652000
O	2.95584700	-0.85075000	-0.77965700
O	0.37689100	-2.28076300	0.16466400
O	-1.79190500	-0.83614700	-0.17083500
O	-2.86085800	1.58591500	-0.11680800
H	2.55986400	1.79174300	1.92001000
H	-0.80189100	1.11192500	-1.67404400
H	1.99999800	0.22263000	1.44209000
H	2.84562300	-0.73575200	-1.73334000
H	2.68522100	1.65254800	-0.37395600
H	0.39491000	-1.14510600	-1.51203500
H	1.01598900	-2.35241000	0.89033500
H	-0.47796500	0.03848900	1.16278600

H	-2.55368300	-0.23545800	-0.05020100
H	-1.32593800	2.36972200	1.05752300
H	-1.55907700	3.16176000	-0.52192200
H	-3.52792100	2.11842500	0.32846100
Mg	-1.58449800	-2.79531100	0.36692500

Mg(II)/AD-ts2

E = -810.226471
H = -810.224022
G = -810.434969

C	-0.11842100	-1.80112100	-0.27518500
C	1.64848800	-0.26415300	-0.51634000
C	-1.00947700	-0.82501500	-0.39965500
C	-0.70376900	0.60252100	-0.34379700
C	0.72655000	0.84561400	-0.02047000
C	3.07099200	-0.08789300	-0.02537400
O	1.20713200	-1.52987700	-0.04601200
O	-2.38369700	-1.06723800	-0.52097700
O	-1.63535800	1.17487300	0.64644700
O	0.98313500	2.00453300	-0.99867500
O	3.13128300	-0.06762500	1.38578200
H	1.62725700	-0.26819000	-1.61207200
H	-2.58358200	-2.01321200	-0.54807100
H	-0.34404000	-2.85692100	-0.33773100
H	-0.03184700	1.79488400	-1.34753800
H	-1.69324700	2.12809700	0.51169400
H	0.96861600	1.20531500	0.97849600
H	1.06646500	2.87282600	-0.56432900
H	3.68807400	-0.88965500	-0.43925700
H	3.45897200	0.86689400	-0.38118400
H	2.86178400	-0.93550300	1.70800700
Mg	-3.42704900	0.26320200	0.64869900

Mg(II)/AD-ts3

E = -733.833224
H = -733.830775
G = -734.023516

C	0.11613500	1.70915300	-0.19821100
C	1.61862100	0.05127700	0.66363500
C	-0.93088300	0.85674500	-0.01753100
C	-0.61111700	-0.50426200	0.01403900
C	0.67038800	-1.00136300	0.16975400
C	3.07433900	-0.26954900	0.46472400
O	1.36025900	1.33088300	-0.04647200
O	-2.28747500	1.15500700	-0.10507500
O	-1.54120200	-1.45587500	0.00859900
O	3.26921900	-0.66509100	-0.87725800
H	1.44106900	0.29576600	1.71428200
H	-2.53701700	1.90686700	0.45152800
H	-0.00384300	2.74586300	-0.49555100
H	-0.48498900	-1.93928000	0.56476100
H	1.00389700	-1.72060100	-0.57597300
H	3.66936800	0.61294100	0.71415200
H	3.32889600	-1.07394100	1.16180700
H	4.19125700	-0.91310800	-0.99616700
Mg	-3.38666200	-0.65715900	-0.07963800

Mg(II)/LG-ts

E = -886.682849
H = -886.680121
G = -886.908288

O	3.18836800	-1.05238400	-0.12264900
O	-2.75994100	1.13621900	-0.20824200
O	-1.61102600	-1.26158600	0.47419100
O	0.64121000	-2.45846300	-0.67419500
O	0.78005800	1.03666400	1.34492100
O	0.13357800	1.90803400	-0.86062500
C	-0.34869600	0.69568700	0.87430400
C	-0.48537700	-0.52385600	-0.00212600
C	0.79621200	-1.32065200	0.12882500
C	1.94841800	-0.42408600	-0.31571400
C	1.87448900	0.95623500	0.37918400
C	1.49988900	2.12298900	-0.54503700
H	-3.25778300	1.89870900	-0.50558500
H	-1.40084800	-2.20702600	0.41081200
H	1.39603800	-3.04511000	-0.54308300
H	-0.37948600	2.72577800	-0.83068000
H	-1.22943500	1.10284200	1.36249500
H	-0.64952800	-0.22983000	-1.03709900
H	0.94178300	-1.60231100	1.18074100
H	1.86027100	-0.28093800	-1.39487400
H	2.78306900	1.15862700	0.93857800
H	2.10939700	2.08521400	-1.44746800
H	1.64445700	3.06905600	-0.02801100
Mg	-3.48588000	-0.57822800	-0.13867300
H	3.32504800	-1.24204900	0.81442800

Mg(II)/LO-ts1

E = -810.247423
H = -810.244975
G = -810.439539

C	-0.00579900	1.02813500	-0.95539800
C	-0.42034400	-0.36913300	-1.31781900
C	-0.24254300	1.27355900	0.52230300
O	0.29439200	-1.31875600	-0.44248800
O	-1.77302200	-0.61455300	-1.06106100
C	-0.08923100	0.06314800	1.44882400
C	-0.49301000	-1.23841600	0.76742700
C	-1.90780200	-1.24386900	0.21535700
H	-1.45783100	1.92903300	-0.64047800
H	-0.16119400	-0.63873100	-2.34003000
H	0.37399800	2.09461700	0.88104700
H	-0.55461100	0.17636400	2.42687900
H	-0.25514600	-2.09277800	1.39519400
H	-2.26908300	-2.26170200	0.07774300

H	-2.60532800	-0.68015200	0.83396300
O	1.43706500	1.03187500	-1.16539300
H	1.70974200	1.66995400	-1.83086500
O	-1.64843100	1.75571200	0.40623800
H	-1.83427800	2.56570000	0.91541700
O	1.34204100	-0.07606800	1.58473100
H	1.69757700	0.49304200	2.27930400
Mg	2.25768100	-0.54679800	-0.22154700

Mg(II)/LO-ts2

E = -733.826116
H = -733.823668
G = -734.005027

C	0.35373600	0.97072500	0.48840400
C	0.39236000	-0.41494700	1.08238800
C	-0.71248500	1.41188500	-0.24041600
O	-0.85069000	-0.97512700	1.16389900
O	1.09682700	-1.14372700	0.04738300
C	-1.75251600	0.36785500	-0.62261000
C	-1.25891800	-1.02371000	-0.21004700
C	0.03509900	-1.49674200	-0.90720500
H	0.93660300	-0.46478100	2.02421000
H	-0.86933200	2.47230900	-0.44317900
H	-1.86416200	0.38412600	-1.71210500
H	-2.06799200	-1.74240500	-0.29933600
H	0.06299100	-2.57465900	-1.02527300
H	0.22223500	-0.99529300	-1.85492200
O	1.53617100	1.54984000	0.24839300
H	0.60587300	1.71903500	-0.73881600
O	-2.99079700	0.56051400	0.01577000
H	-3.40296100	1.36456500	-0.31950200
Mg	2.80841700	0.08455900	-0.41481000

Mg(II)/LO-ts3

E = -733.856716
H = -733.854268
G = -734.040955

C	-1.01792200	1.24009400	-0.12661200
C	-0.97137000	-0.02719500	-0.99135600
C	-0.26278400	1.13773000	1.16711200
O	0.28387900	-0.68515700	-0.77493500
O	-1.93300200	-0.91328300	-0.50553600
C	0.22119700	-0.13964100	1.52299800
C	0.12697800	-1.25129600	0.53494600
C	-1.33095300	-1.75262700	0.48341000
H	-1.11178600	0.17549500	-2.04969600
H	0.91422000	1.30779700	0.89755900
H	0.55546800	-0.35351000	2.53233800
H	0.85983200	-2.03408500	0.69390800
H	-1.35358400	-2.78513200	0.14214300
H	-1.85663800	-1.65607700	1.43278400
O	-1.65104300	2.20357400	-0.44913500
H	-0.50556200	1.84821500	1.94931900
O	2.20752200	0.43178600	0.69060000
H	2.98626900	0.57691100	1.23848700
Mg	2.30517100	-0.05144700	-1.17231500

Mg(II)/Ch-tsF

E = -810.237469
H = -810.235021
G = -810.438010

C	-1.66435100	0.80877500	-0.94860700
C	0.41032700	-0.83046500	0.06359300
C	0.58137300	0.62711400	-0.25194200
C	-0.73958100	1.32174800	0.04142700
C	-0.92700500	-1.38385500	-0.43187100
C	-1.86795700	-1.61350300	0.75812700
H	1.63130700	-2.38897000	-0.26573000
H	0.42046300	-0.93916500	1.15070600
H	-1.26831800	0.72282800	0.96220200
H	-0.80477600	-2.24882900	-1.07937300
H	-2.79360900	-2.06392400	0.36365200
H	-1.36659100	-2.39950000	1.35247600
O	1.59773400	-1.44378700	-0.47252900
O	-2.10458300	-0.44298700	1.43279300
O	-1.66298300	-0.40702600	-1.28523700
O	-0.62465700	2.70953700	0.04844300
H	-0.93032200	3.05178100	0.89509500
O	1.68094900	1.05246300	0.55543800
H	1.78162800	2.01549500	0.50079600
H	0.86205700	0.75776900	-1.30273500
H	-2.39649400	1.43567000	-1.45562100
Mg	3.25134600	-0.27230500	0.10524200

Mg(II)/Ch-tsR

E = -810.27833
H = -810.275881
G = -810.483292

C	-0.78359500	-0.28760600	-1.59622900
C	-1.32190900	0.73093400	0.85831200
C	-0.96724800	-0.75666700	0.86742600
C	-0.46517700	-1.15444000	-0.52330800
C	-0.48870000	1.52010700	-0.14006900
C	1.01897500	1.57577800	0.07445000
H	0.15629700	-1.94309900	1.92302200
H	-0.93445800	-0.65559700	-2.60882500
H	-1.33107300	-2.88253800	-0.74580100
H	-3.25219800	0.60182200	1.14392800
H	0.67855000	-0.66813600	-0.45194500
H	-1.13013900	1.14475300	1.85196100
H	-1.88186800	-1.32585300	1.06666100
H	-0.88041400	2.53368800	-0.19016600
H	1.40864900	2.37608100	-0.56183000

H	1.16914200	1.87513000	1.11821200
O	-0.01172700	-0.99490800	1.87104700
O	-0.44160200	-2.51274400	-0.81616500
O	-2.66087600	0.91666700	0.45111900
O	1.67095800	0.36673800	-0.23866200
O	-0.74748800	0.98215900	-1.48988800
Mg	3.46411000	-0.07401500	0.16597300

Mg(II)/HM-ts1

E = -886.702568
H = -886.700120
G = -886.932189

C	-1.69463600	1.91036300	0.05748900
C	-1.63541300	0.49737700	0.04309100
C	-0.39198200	-0.28103000	0.47615000
C	0.92432200	0.18623800	-0.12090200
C	2.11334700	-0.43853900	0.63585900
H	-0.82011700	2.54898900	0.07230200
H	-0.34357600	-0.25837400	1.56559900
H	1.01070600	1.27301500	-0.02390200
H	1.87822700	-1.46547100	0.92441000
H	-1.34756000	0.98961800	-1.08361700
O	2.29714000	0.27919100	1.83993200
O	-2.84387700	2.49677400	-0.02897500
H	2.69723200	1.13145500	1.62394800
O	-2.77488500	-0.14265100	0.04745700
H	-3.54386300	1.81568400	0.05498000
O	-0.62065600	-1.64347100	0.09023000
H	-0.12957800	-1.79872100	-0.73628100
O	0.86411300	-0.19426200	-1.48139800
H	1.63336700	0.18085000	-1.93184100
C	3.35681700	-0.45704600	-0.22915500
H	3.26564100	-1.22909900	-0.99761400
O	3.46458500	0.83530800	-0.81781600
H	4.31589700	0.91619500	-1.25954000
H	4.22140800	-0.68379100	0.39780100
Mg	-2.66365600	-2.08097000	-0.08140800

Mg(II)/HM-ts2

E = -886.710273
H = -886.707824
G = -886.930421

C	-0.55331300	0.28850600	0.22619100
C	1.56092400	0.10444800	-0.99155500
C	1.73352900	1.03570800	0.21127500
C	0.60584000	0.65975900	1.17377700
H	2.71067800	0.91607400	0.68308800
H	0.33766700	1.50563900	1.81019000
C	2.29494700	-1.23255600	-0.98907000
H	2.24973000	-1.65192300	-1.99343100
H	3.34450600	-1.04885500	-0.74278200
O	1.69890500	-2.18361600	-0.13747500
H	1.73749100	-1.85321300	0.77195500
C	-1.54608500	1.39515400	-0.04608700
H	-1.10683200	2.14032000	-0.70740700
H	-1.84370700	1.85741200	0.89545300
O	-2.67994200	0.77333900	-0.66163800
H	-3.31513400	1.43332800	-0.96510700
O	1.52754000	2.34504300	-0.27628700
H	1.75158300	2.98227800	0.41170700
O	1.01373800	-0.44481600	1.93933800
H	0.22583700	-0.90816700	2.25715000
O	0.12573100	-0.16293800	-1.02131600
O	-1.13219400	-0.94219100	0.48244700
H	1.80507100	0.65719700	-1.89740700
H	-0.30555100	-1.17229500	-0.51158400
Mg	-3.04971800	-1.12020800	-0.00996300

Mg(II)/HM-ts3

E = -886.698413
H = -886.695965
G = -886.929863

C	-0.14344500	-0.46404600	-0.87481500
C	2.08838900	-0.07199600	-0.62553500
C	1.34433500	1.01211600	0.16731100
C	-0.03209300	0.98028700	-0.49338900
H	1.24411500	0.70199200	1.21095200
H	0.00896600	1.54975500	-1.43343100
C	3.12878700	-0.85543200	0.12177600
H	3.47838600	-1.67791700	-0.50749800
H	3.97087700	-0.18109400	0.31147500
O	2.53952000	-1.31959200	1.31561000
H	3.17030900	-1.87570100	1.78333600
C	-1.34785000	-1.22624100	-0.95814400
H	-1.49267100	-1.49223700	0.20820900
H	-1.30586800	-2.12989400	-1.55987800
O	-2.50217200	-0.42705100	-1.14926100
H	-2.60913800	-0.14370900	-2.06656900
O	1.90700900	2.28157200	0.03631700
H	2.47624900	2.46680400	0.79112400
O	-1.09852600	1.43244400	0.31271600
H	-0.97642100	2.37454500	0.49904300
O	0.99476700	-1.00644200	-0.99871800
O	-2.15949200	-1.01996700	1.50197900
H	2.48436700	0.32672400	-1.55975400
H	-2.63559300	-1.67253300	2.02002700
Mg	-2.95759700	0.49812000	0.67755000

Mg(II)/HM-ts4

E = -810.231600
H = -810.229152
G = -810.445829

C	-1.49881300	-0.75405200	-0.63506900
C	-0.28000500	-0.15870800	-0.46761300
C	-0.01339700	1.00953400	0.45161100

C	1.44519200	1.34378400	0.10941800
H	-1.66591800	-1.57079900	-1.32507800
H	1.98536400	1.68473500	0.99521000
O	1.39102200	2.32706900	-0.89945800
O	-2.60634500	-0.13398600	0.00333700
H	2.28615400	2.56446600	-1.16615000
H	-1.71067000	-0.94116800	0.56707600
C	1.98806900	0.01733800	-0.41840100
O	0.81626100	-0.63018300	-1.01460600
H	2.69750900	0.14477400	-1.23464700
C	2.55249300	-0.89766500	0.64903700
H	3.43306900	-0.42000800	1.08034000
H	1.81422200	-1.03875200	1.44582500
O	2.97235800	-2.13024800	0.10546200
H	2.19662300	-2.61234800	-0.20140200
O	-0.20792700	0.54771000	1.76956500
H	-0.32255700	1.30578300	2.35426500
H	-0.66741600	1.84857600	0.20661900
Mg	-4.51088000	-0.34746200	-0.04753000

Mg(II)/HM-ts6

E = -810.270762
H = -810.268314
G = -810.473772

C	0.31709200	-2.15558900	-0.60371500
C	-1.56894500	0.92555700	-0.02480700
C	-1.77860400	-0.60957800	-0.15475400
C	-0.42885600	-1.20474900	0.12726100
C	-0.05709500	1.01150900	-0.20377300
C	0.76889900	2.15852800	0.30464000
H	-0.19587800	-2.98497300	-1.09621800
H	-3.10537200	1.85741600	-0.77390900
H	-1.84450500	1.25914200	0.98153600
H	0.16321200	0.85172400	-1.26831100
H	0.61641800	3.05804200	-0.28791600
H	0.58375000	2.35063000	1.36163100
O	-2.19341200	1.67100800	-1.02312500
O	2.11586400	1.66384400	0.12532600
O	1.56618000	-2.10048200	-0.62370000
O	0.40224900	-0.12760300	0.54305700
H	2.76930300	2.35328400	0.29164900
H	-2.29572900	-0.89090900	-1.06645100
H	-1.39863100	-1.66360800	1.18615000
O	-2.50464600	-1.25599700	0.98243600
H	-2.92306400	-0.64547000	1.61474300
Mg	2.41880500	-0.42545900	0.19633600

Mg(II)/HM-ts7

E = -810.241891
H = -810.239442
G = -810.442620

C	0.80536900	-2.11461000	-0.28007500
C	-1.79642200	0.40390200	0.24945100
C	-1.40044500	-1.07236500	0.32187800
C	-0.27202500	-1.15832100	-0.71177400
C	-0.62866400	1.17426500	-0.24466700
C	0.17107800	1.88779400	0.81621900
H	0.56381400	-3.17741000	-0.18496200
H	-3.08216400	-0.03916600	-1.43045500
H	-2.29532600	0.75842600	1.14616700
H	-2.01558600	1.31592300	-1.31686500
H	-0.30924700	2.81070800	1.13593000
H	0.37443600	1.27033500	1.69760700
O	-2.78327900	0.71184500	-0.88469800
O	1.49382700	2.16964600	0.29051300
O	1.92901900	-1.71201800	-0.05163300
O	0.30464700	0.12889600	-0.76598200
H	1.42951400	2.85394500	-0.39082600
H	-2.20562500	-1.77876700	0.11814700
H	-0.65051500	-1.46036700	-1.69479900
O	-0.80182600	-1.28674200	1.57992000
H	-1.47862800	-1.45801300	2.24539400
Mg	2.27140500	0.34061500	-0.29804100

Mg(II)/HM-ts8

E = -733.834830
H = -733.832381
G = -734.019729

C	-1.25006300	-2.07091600	-0.18183500
C	1.95703900	-0.19220800	-0.43596400
C	1.24153600	-1.48733900	-0.59568300
C	-0.00066800	-1.30825200	-0.13139700
C	0.95968400	0.76158700	0.13331300
C	0.43776000	1.93076800	-0.66612300
H	-1.24641100	-3.12915300	-0.44913900
H	2.95280200	-1.05865500	1.28055700
H	2.62170600	0.11520000	-1.23655400
H	2.16468500	0.48536100	1.22537900
H	1.11907900	2.77758100	-0.62924900
H	0.21995300	1.67508200	-1.70880500
O	2.92661200	-0.20072200	0.81734100
O	-0.81923500	2.28551000	-0.02907000
O	-2.28841800	-1.46760100	0.04282700
O	-0.22530600	-0.06637300	0.34419300
H	-1.14293400	3.12225100	-0.38334100
H	1.62584100	-2.37737200	-1.06756400
Mg	-2.09463900	0.68177900	0.40270900

Mg(II)/HM-ts9

E = -733.868308
H = -733.865859
G = -734.051988

C	0.73120200	1.98088100	0.30777700
C	1.04182900	-1.50959700	0.68570100
C	1.93829100	-0.33416900	0.50718700
C	1.05138700	0.67954100	-0.16328100

C	-0.11501600	-1.24880000	0.08418500
C	-1.42149500	-1.94867300	-0.04511700
H	1.53390800	2.61618000	0.69026800
H	1.28268900	-2.39635600	1.24853200
H	-1.50708800	-2.43711900	-1.01673600
H	-1.54796400	-2.67458600	0.75476900
O	-2.41319300	-0.90633400	0.05506600
O	-0.42927100	2.42452400	0.24181300
O	-0.15590200	-0.00913900	-0.50727700
H	-3.30315800	-1.27870100	0.03912200
H	2.16682200	0.36136800	-1.07866100
Mg	-1.91129600	1.09466700	-0.19908100
O	2.93826900	-0.46803600	-0.64031000
H	2.90447500	-1.34440800	-1.06350600
H	2.52945900	-0.02559800	1.36214100

Mg(II)/FU-ts

E = -657.449589
H = -657.447141
G = -657.624138

C	-0.48059800	1.83380400	-0.14842800
C	-1.80806400	1.49450600	-0.36970100
C	-1.89140500	0.14628400	-0.07467700
C	0.20690300	0.65425700	0.21600900
C	1.53176300	0.44497400	0.91768800
H	-0.01099500	2.79740100	-0.28147900
H	1.84117000	1.34317200	1.45328000
H	1.45090600	-0.39119200	1.61435600
O	2.36261500	0.18025400	-0.20988700
O	-0.74239600	-0.36325200	0.29796700
H	0.98209600	0.43479600	-0.75843800
H	-2.61524600	2.12325700	-0.70671500
C	-3.06720700	-0.77170700	-0.15217500
O	-2.95716900	-1.94373500	0.06828500
H	-4.01819200	-0.29084200	-0.41804600
Mg	3.84312600	-0.98461900	-0.37384900

Mg(II)/Ch-ts1

E = -1153.426788
H = -1153.424339
G = -1153.720574

C	0.27455000	1.66658500	0.30525800
C	1.96468600	-0.38032100	0.08093600
C	2.49734800	0.92964500	-0.42328900
C	1.51070000	1.99548700	-0.08152100
C	0.54433800	-0.59531000	-0.41993700
C	0.02268500	-1.97500300	-0.26313100
H	3.74518700	1.40054100	1.07480900
H	-0.45197700	2.43312200	0.55164600
H	2.72425900	3.49777400	0.03185700
H	2.53204200	-2.22719900	0.02980400
H	0.42268800	-2.87628100	1.47649000
H	1.92720700	-0.36154400	1.17460200
H	2.69136000	0.88949100	-1.49870200
H	0.44085600	-0.26231600	-1.45930300
H	-2.07559500	-2.97697900	-0.30484600
H	0.06820100	-2.48355100	-1.22886600
O	3.82286000	1.12604600	0.14788200
O	1.84446700	3.30824700	-0.31441000
O	2.90066300	-1.38860800	-0.32244900
O	0.87332200	-2.74570300	0.64004700
O	-0.21174900	0.40266800	0.37504800
C	-4.37229300	1.76776200	0.40246200
C	-3.39795500	0.93782100	0.97576200
C	-3.38707600	-0.22365200	0.22843000
C	-4.88690500	1.06030400	-0.65379100
H	-4.66916500	2.75480700	0.71219600
O	-4.30771700	-0.13180400	-0.77585700
H	-5.65334000	1.29375500	-1.37527900
H	-2.76668400	1.13751800	1.82731000
C	-2.61690500	-1.37321700	0.37172500
O	-2.87865800	-2.41708000	-0.35550700
H	-1.88762600	-1.42155700	1.16383800
Mg	4.80733700	-0.74069300	-0.03925300

Mg(II)/Ch-ts2G

E = -1153.45573
H = -1153.453281
G = -1153.746262

C	-1.53565200	-1.71677200	-0.13569200
C	-1.50189900	0.99510100	0.22044000
C	-2.74810700	0.42393400	-0.41398100
C	-2.66935100	-1.06043300	-0.34532300
C	-0.27706200	0.30313100	-0.38253100
C	0.99058900	0.87166400	0.14947200
H	-4.01472500	1.75897800	0.36494200
H	-1.50156700	-2.79422800	-0.02938000
H	-4.01111000	-2.26474500	-1.16773000
H	-0.60452400	2.69561400	0.15978200
H	1.05154800	-0.26072200	1.74467100
H	-1.52942800	0.78520600	1.29641600
H	-2.86359900	0.80074200	-1.43413500
H	-0.31212200	0.39073200	-1.47408100
H	1.68189700	2.25808000	-0.32558200
O	-3.93275700	0.79603600	0.32759600
O	-3.91480400	-1.71000100	-0.38130000
O	-1.49854800	2.37646200	-0.03186600
O	1.11674700	0.68509200	1.54628300
O	-0.33124500	-1.12254600	-0.05803200
C	5.02842800	-1.16612800	0.95185300
C	3.85075400	-0.37911900	1.13263000
C	3.35319500	-0.14509000	-0.11274600
C	5.15540600	-1.34938900	-0.38411200
H	5.68711400	-1.54605200	1.71427300
O	4.15405900	-0.73473200	-1.04648900
H	5.87206900	-1.87676100	-0.99056200
H	3.43699700	-0.01677000	2.05729100
C	2.20331300	0.58607000	-0.64579400
O	2.64413100	2.16840700	-0.87402400

H	3.39020900	2.40518500	-0.29544800
H	2.00470400	0.31536200	-1.67867000
Mg	-5.44048500	-0.54151500	0.33296500

Mg(II)/Ch-ts2F

E = -1153.444747
H = -1153.442298
G = -1153.735684

C	1.91671000	1.64084600	0.52417800
C	1.28504000	-1.03777500	0.13657400
C	2.58039600	-0.53858100	-0.47166200
C	2.82482900	0.87206200	-0.05496300
C	0.25182400	0.08561900	-0.04155400
C	-1.14393000	-0.30009800	0.35827700
H	3.63939900	-1.68060600	0.79441800
H	2.10731500	2.64478200	0.88059200
H	4.28707400	2.19315900	-0.29185700
H	0.49195700	-2.82557400	0.06012900
H	-1.54575100	-1.31048500	2.22893500
H	1.42310300	-1.21709700	1.20936600
H	2.52777200	-0.63482700	-1.55866100
H	0.20793700	0.36336600	-1.10365400
H	-1.41198600	-1.29514500	0.00785800
O	3.73902800	-1.31992900	-0.09873900
O	4.14638100	1.23749000	-0.28806400
O	0.90426600	-2.20360400	-0.54815800
O	-1.10663500	-0.48282900	1.96077900
O	0.63539200	1.23362600	0.71354400
C	-5.57832800	-0.04487600	-0.88443800
C	-4.50867100	0.91296700	-0.82781700
C	-3.49251200	0.30797400	-0.14919400
C	-5.14133700	-1.15112700	-0.24778100
H	-6.54454800	0.07908200	-1.34642000
O	-3.86486800	-0.95345800	0.20918800
H	-5.57335000	-2.11523100	-0.04405400
H	-4.48907600	1.90910500	-1.23437300
C	-2.17545200	0.74845100	0.27578000
O	-1.81628300	1.94341000	-0.38621800
H	-1.38963900	2.52408100	0.24914800
H	-1.83249200	0.32522500	1.90339300
Mg	5.50771900	-0.29752000	-0.49648900

Mg(II)/Ch-ts3G

E = -1077.058502
H = -1077.056053
G = -1077.324807

C	-2.38817400	1.80039000	-0.30001800
C	-0.53364700	-0.22713400	0.07859400
C	-1.95853900	-0.49135200	0.51858600
C	-2.84380400	0.61241400	0.06123100
C	-0.22140300	1.24757600	0.44534200
C	1.19451900	1.57422100	0.12821600
H	-1.89829600	-2.44404300	0.16425900
H	-3.01481300	2.60634100	-0.65722300
H	-4.78750400	0.94112600	-0.16194200
H	1.11244900	-1.26431900	0.30702400
H	2.60278700	2.20207000	-0.25098300
H	-0.47220700	-0.33839300	-1.00954100
H	-1.98685200	-0.61585200	1.60518500
H	-0.35294300	1.36998600	1.52936800
O	-2.46230600	-1.69655900	-0.08387900
O	-4.17592700	0.21585100	0.02665900
O	0.25916500	-1.15762000	0.75605800
O	1.51371400	2.31225800	-0.84685900
O	-1.07004000	2.13614700	-0.25704900
C	4.01336800	-1.60608400	-1.06336500
C	2.94477200	-0.64581700	-1.01852800
C	3.09713000	0.03760800	0.15340300
C	4.71700700	-1.44306600	0.07467100
H	4.21532000	-2.32118500	-1.84326100
O	4.16883600	-0.44342000	0.82770200
H	5.57916200	-1.93058800	0.49479300
H	2.20224800	-0.46156800	-1.77963300
C	2.37584300	1.13477600	0.81376200
H	2.33169000	1.02952100	1.89397100
Mg	-4.48175100	-1.80562900	-0.25203600

Mg(II)/Ch-ts3F

E = -1077.075165
H = -1077.072717
G = -1077.341252

C	1.18447900	-1.57146500	0.17920400
C	1.37600400	1.08167500	-0.49885600
C	2.53802700	0.50335100	0.27910400
C	2.33720100	-0.96222700	0.42383400
C	0.06921600	0.52395400	0.07666900
C	-1.12107400	1.14084900	-0.59101600
H	3.97126000	1.59024500	-0.59843500
H	1.07955300	-2.64874600	0.21554900
H	3.51620500	-2.05453800	1.58061400
H	0.66036700	2.85993200	-0.75977700
H	1.46002800	0.75971100	-1.54508600
H	2.64147500	1.01774500	1.23874000
H	0.05274100	0.69359600	1.16026200
H	-1.17067200	0.89416500	-1.65037500
O	3.78642900	0.65425300	-0.43910900
O	3.51392000	-1.67979700	0.68916100
O	1.46291900	2.47769300	-0.37969000
O	0.04760000	-0.91927300	-0.11873500
C	-5.28988800	-1.10254100	0.16272400
C	-4.64669000	0.04454500	0.67463400
C	-3.42463200	0.10876400	0.05588000
C	-4.41775800	-1.64701500	-0.73621400
H	-6.26625300	-1.48077900	0.41265100
O	-3.29130700	-0.93412200	-0.81401400
H	-4.47525900	-2.51638500	-1.37041800
H	-5.01969900	0.74925300	1.40006100

C	-2.34537700	1.02188500	0.17677800
O	-2.35529600	1.95458800	1.05504200
H	-1.39079100	2.28989000	0.36833500
Mg	5.17249000	-0.78595600	-0.13415100