Electronic Supplementary Information

Density functional theory studies on solvent effect in $Al(H_2O)_6^{3+}$ water-exchange reactions: The number and arrangement of outer-sphere water molecules

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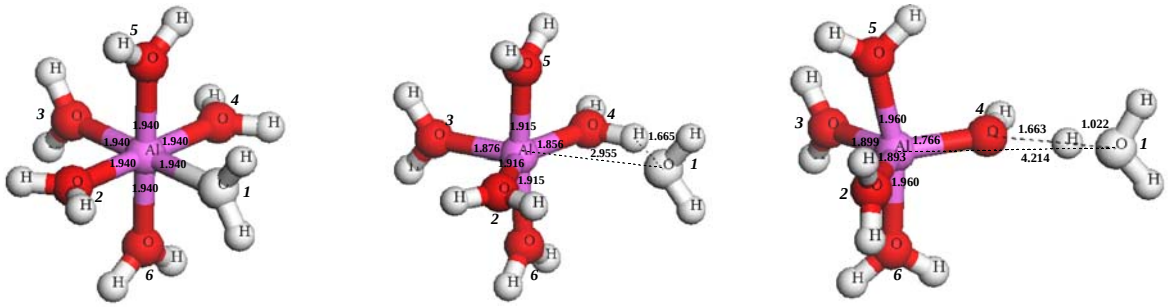


R TS (-144.89 cm^{-1}) P

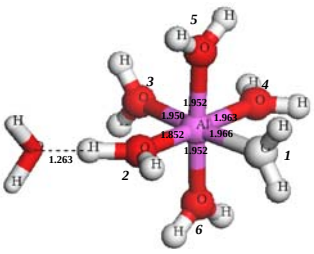
Fig. S1 The optimized R,TS and P structures for the pathway with N_m' = 0 for water-exchange reactions in $Al(H_2O)_6^{3+}$ (the leaving H_2O are colored white to differ from others)

Table S1 Selected structural and energetic parameters for the pathway with N_m' = 0 for water-exchange reactions in $Al(H_2O)_6^{3+}$

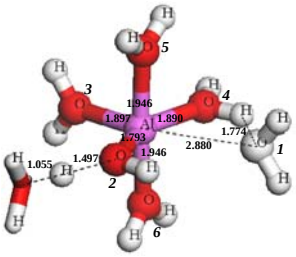
Species	Bond length (Å)					Bond angle (°)			Dihedral angle (°)		$\Delta E_{elec}^{\neq}$ (kJ/mol)	$\Delta G^{\neq}$ (kJ/mol)
	r(Al-O_l)[a]	$\bar{r}$ (Al-O_l)[b]	r(Al-O_L)[c]	$\sum$r(Al-O)[d]	$\Delta\sum$r(Al-O)[e]	θ_x (O_3-Al-O_1)	θ_y (O_2-Al-O_4)	θ_z (O_5-Al-O_6)	horizontal plane D(O_2-$O_3$$O_4$-$O_1$)	axial plane D(O_5-$O_3$$O_6$-$O_1$)		
R	1.940, 1.940, 1.940, 1.940, 1.940, 1.940*	1.940	1.940	11.640		180.0	180.0	180.0	0.0	0.0	0.0	0.0
TS	1.915, 1.878, 1.876, 1.915, 1.916	1.900	2.955	12.455	0.815	167.9	144.2	172.8	-0.1	-12.1	122.0	111.3
P	1.960, 1.900, 1.960, 1.893, 1.766	1.896	4.214	13.693		141.9	116.5	165.7	0.1	-41.8	147.8	129.6

[a] The distance between Al and O of coordinated H_2O. [b] The average bond length between Al and O of coordinated H_2O. [c] The distance between Al and O of leaving H_2O; [d] $\sum$r(Al-O) = $\sum$r(Al-O_l) + r(Al-O_L); [e] $\Delta\sum$r(Al-O) = $\sum$r(Al-$O)_{TS}$ - $\sum$r(Al-$O)_R$; *Parameters of leaving H_2O.

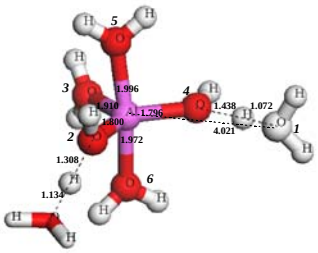
§S2 The optimized R, TS and P structures as well as structural and energetic parameters for seventeen possible pathways with N_m'=1



R

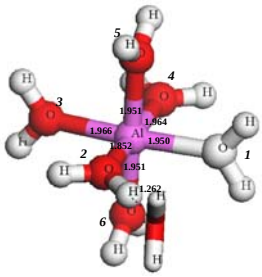


TS (-132.73 cm^{-1})



P

(1) *cis*-2(a)



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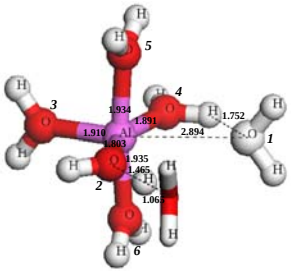
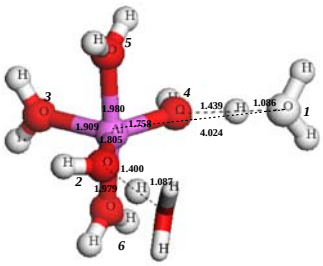


TS (-144.33 cm^{-1})



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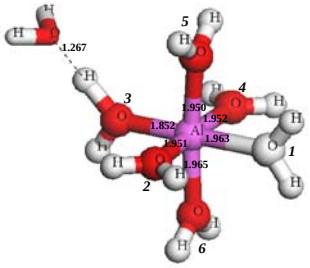
(2) *cis*-2(b)



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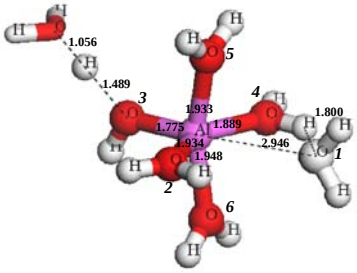
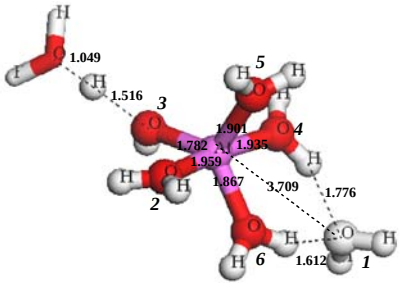


TS (-117.00 cm^{-1})



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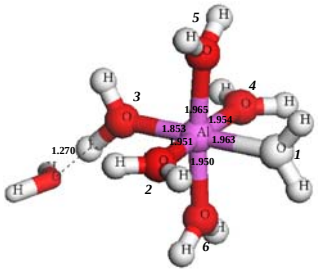
(3) *trans*-3(a)



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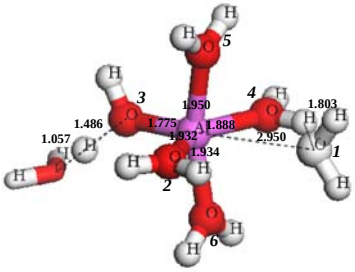
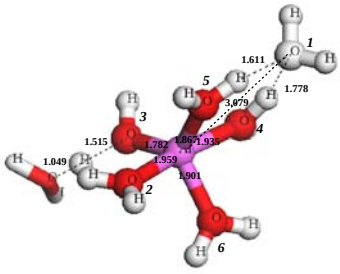


TS (-116.73 cm^{-1})



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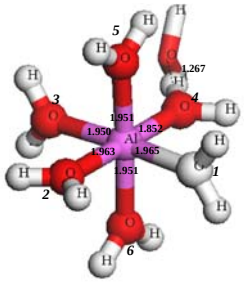
(4) *trans*-3(b)



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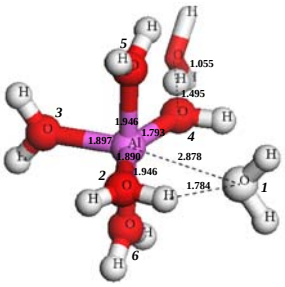
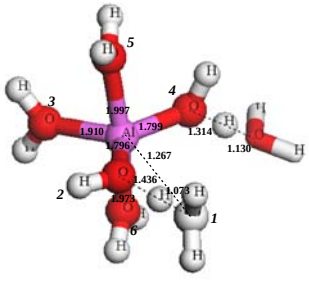


TS (-132.02 cm^{-1})



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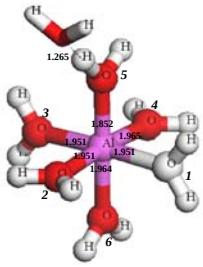
(5) *cis*-4



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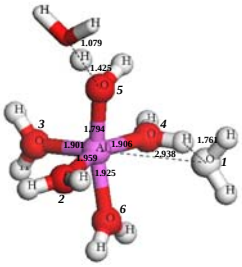
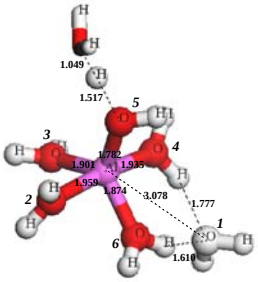


TS (-127.39 cm^{-1})

(6) *cis*-5(a)



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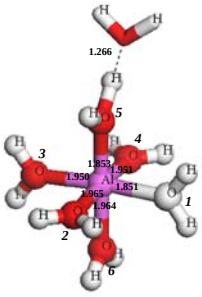

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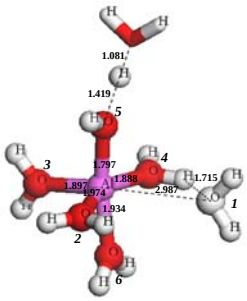
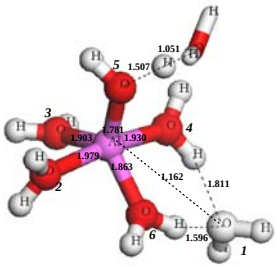


TS (-120.76 cm^{-1})

(7) *cis*-5(b)



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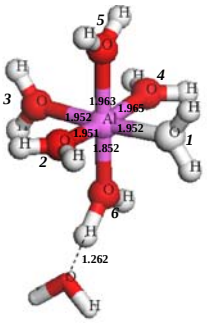

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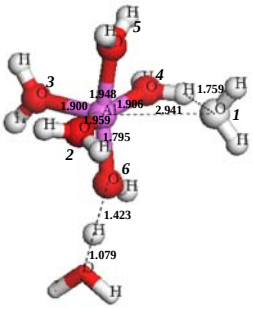
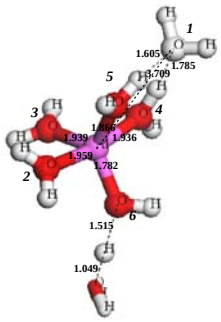


TS (-126.73 cm^{-1})

(8) *cis*-6(a)



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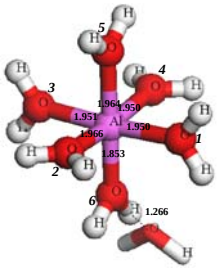

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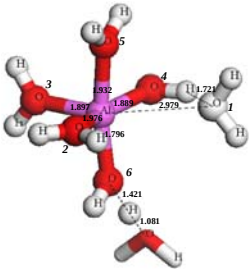
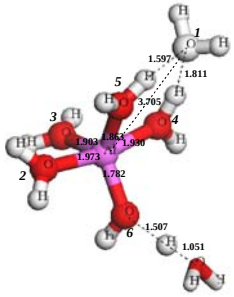


TS (-121.85 cm^{-1})

(9) *cis*-6(b)



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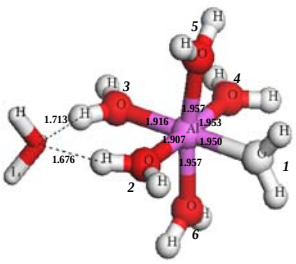

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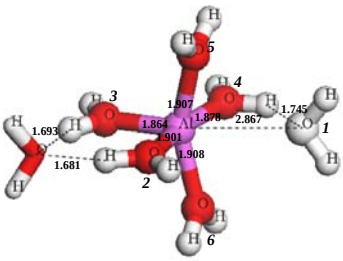
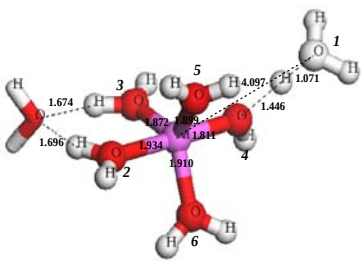


TS (-136.66 cm^{-1})

(10) *cis*-2//*trans*-3



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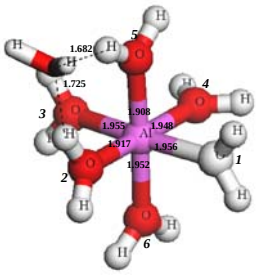

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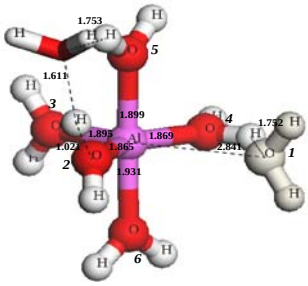
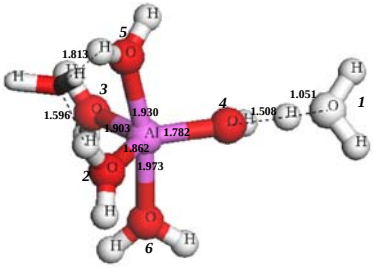


TS (-154.88 cm^{-1})



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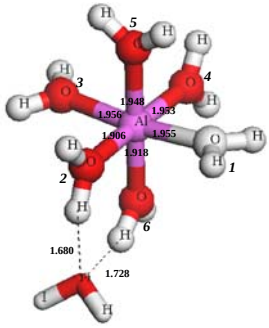
(11) *cis*-2//*cis*-5



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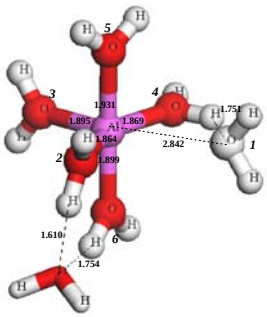
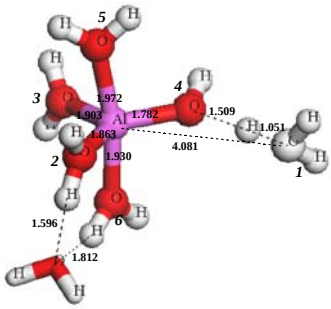


TS (-151.68 cm^{-1})



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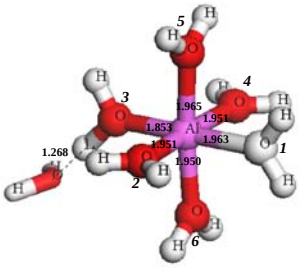
(12) *cis*-2//*cis*-6



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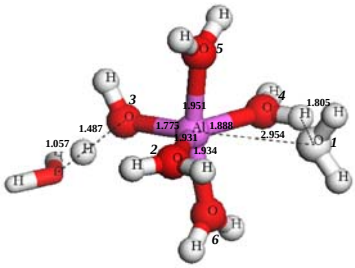
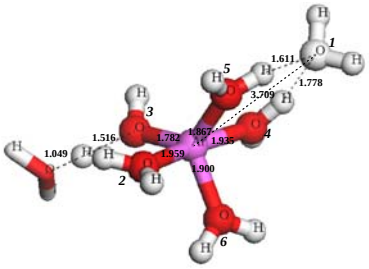


TS (-114.40 cm^{-1})



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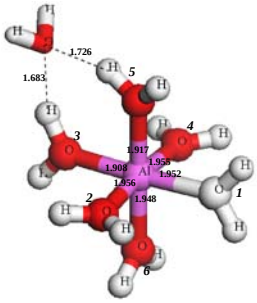
(13) *trans*-3//*cis*-4



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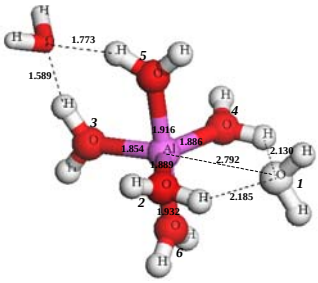
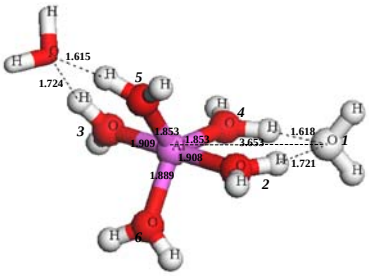


TS (-141.97 cm^{-1})



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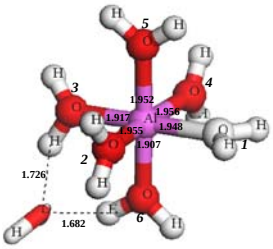
(14) *trans*-3//*cis*-5



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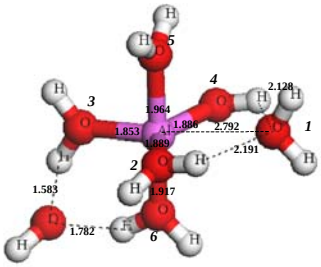
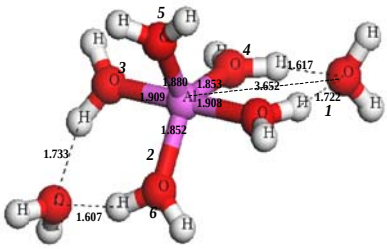


TS (-140.55 cm^{-1})



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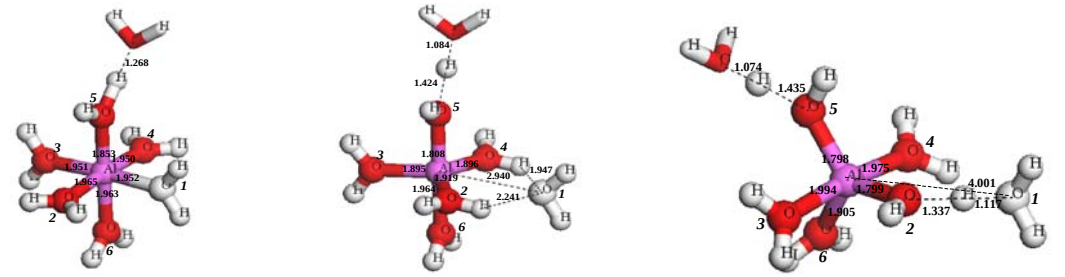
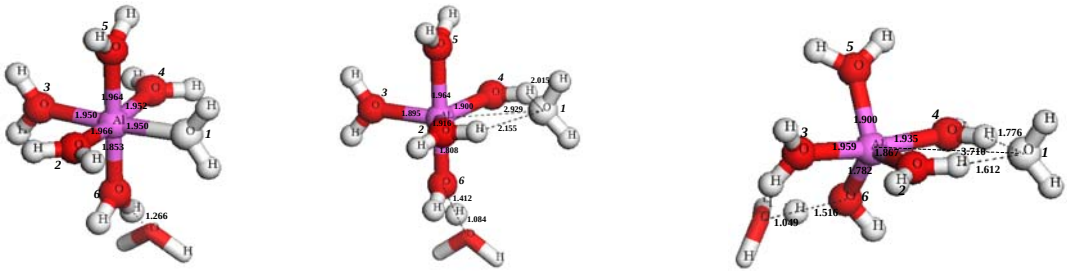
(15) *trans*-3/ *cis*-6



R TS (-115.12 cm^{-1}) P

(16) *cis*-4//*cis*-5



R TS (-116.43cm^{-1}) P

(17) *cis*-4//*cis*-6

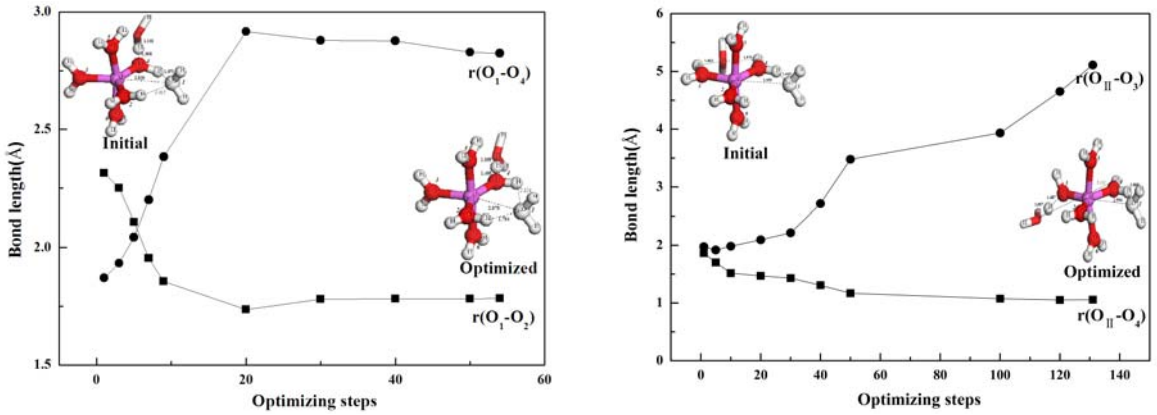
Fig. S2 The optimized R,TS and P structures for the seventeen possible pathways with N_m' = 1 for water-exchange reactions in $Al(H_2O)_6^{3+}$ (the leaving H_2O are colored white to differ from others and the explicit H_2O are showed by stick model)

Table S2 Selected structural and energetic parameters for the seventeen possible pathways with N_m' = 1 for water-exchange reactions in $Al(H_2O)_6^{3+}$

No.	Species	Bond length (Å)					Bond angle (°)			二面角 (°)		$\Delta E_{elec}^{\neq}$ (kJ/mol)	$\Delta G^{\neq}$ (kJ/mol)
		r(Al-O$_l$)[a]	r (Al-O$_l$)[b]	r(Al-O$_L$)[c]	$\sum$r(Al-O)[d]	$\Delta\sum$r(Al-O)[e]	θ_x (O$_3$-Al-O$_1$)	θ_y (O$_2$-Al-O$_4$)	θ_z (O$_5$-Al-O$_6$)	horizontal plane D(O$_2$-O$_5$O$_4$-O$_1$)	axial plane D(O$_5$-O$_3$O$_6$-O$_1$)		
1	R	1.852, 1.950, 1.952, 1.963, 1.952, 1.966*	1.939	1.966	11.635		173.5	179.8	175.8	0.0	-1.7	0.0	0.0
	TS	1.793, 1.897, 1.946, 1.890, 1.946	1.894	2.880	12.352	0.717	163.2	147.2	174.8	0.0	-10.6	110.8	106.5
	P	1.800, 1.910, 1.996, 1.796, 1.972	1.895	4.021	13.495		138.5	125.1	170.2	14.6	-38.0	133.3	117.1
2	R	1.852, 1.966, 1.951, 1.964, 1.951, 1.950*	1.939	1.950	11.634		173.4	180.0	175.8	0.0	-1.7	0.0	0.0
	TS	1.803, 1.910, 1.934, 1.891, 1.935	1.895	2.894	12.367	0.733	158.8	153.5	172.8	0.2	-14.8	114.3	110.1
	P	1.805, 1.909, 1.980, 1.805, 1.979	1.896	4.024	13.502		137.5	132.9	172.7	-33.0	-35.9	145.4	125.9
3	R	1.951, 1.853, 1.950, 1.952, 1.965, 1.963*	1.939	1.963	11.634		179.8	175.8	173.6	-0.4	0.0	0.0	0.0
	TS	1.934, 1.775, 1.933, 1.889, 1.948	1.895	2.946	12.425	0.791	172.1	140.1	160.9	0.3	-8.6	117.1	113.2
	P	1.959, 1.782, 1.901, 1.935, 1.867	1.889	3.709	13.153		121.3	169.6	117.1	69.9	-93.6	99.5	97.2
4	R	1.951, 1.853, 1.965, 1.951, 1.950, 1.963*	1.939	1.963	11.633		179.9	175.8	173.6	0.4	0.1	0.0	0.0
	TS	1.932, 1.775, 1.950, 1.888, 1.934	1.896	2.950	12.429	0.796	172.8	138.5	161.5	-0.3	-7.7	118.2	113.2
	P	1.959, 1.782, 1.867, 1.935, 1.901	1.889	3.709	13.153		121.2	169.5	117.2	-70.1	-32.3	99.8	97.0
5	R	1.951, 1.950, 1.951, 1.963, 1.853, 1.965*	1.939	1.965	11.633		173.5	179.8	175.8	0.0	1.7	0.0	0.0
	TS	1.946, 1.897, 1.946, 1.890, 1.793	1.894	2.878	12.350	0.717	163.9	146.4	174.8	0.1	10.0	112.6	109.4
	P	1.973, 1.910, 1.997, 1.796, 1.799	1.895	4.019	13.494		138.5	125.1	170.2	1.0	37.9	133.9	117.8
6	R	1.951, 1.951, 1.852, 1.965, 1.964, 1.951*	1.939	1.951	11.634		175.8	173.5	179.9	-1.6	-0.4	0.0	0.0
	TS	1.959, 1.901, 1.794, 1.906, 1.925	1.897	2.938	12.423	0.789	158.7	159.1	163.5	0.5	-21.2	119.1	114.8
	P	1.959, 1.901, 1.782, 1.934, 1.867	1.889	3.708	13.151		106.1	169.7	125.5	76.5	-108.2	99.1	96.4
7	R	1.965, 1.950, 1.853, 1.951, 1.964, 1.951*	1.939	1.951	11.634		175.8	173.4	179.8	-1.7	0.5	0.0	0.0
	TS	1.974, 1.897, 1.797, 1.888, 1.934	1.898	2.988	12.478	0.844	161.6	151.2	168.8	2.4	-16.9	124.9	120.2
	P	1.973, 1.903, 1.781, 1.930, 1.863	1.890	3.706	13.156		105.1	168.3	125.0	76.3	-110.8	100.1	95.2
8	R	1.951, 1.952, 1.963, 1.965, 1.852, 1.952*	1.939	1.952	11.635		175.8	173.5	179.8	1.6	-0.3	0.0	0.0
	TS	1.959, 1.900, 1.926, 1.906, 1.795	1.897	2.941	12.427	0.792	158.9	158.4	164.0	-0.4	-19.4	119.0	114.7
	P	1.959, 1.900, 1.866, 1.936, 1.782	1.889	3.709	13.152		106.1	169.6	125.3	-76.2	-32.1	98.9	96.7
9	R	1.966, 1.952, 1.964, 1.950, 1.853, 1.950*	1.939	1.950	11.635		175.8	173.6	179.9	1.6	0.4	0.0	0.0
	TS	1.976, 1.897, 1.932, 1.889, 1.796	1.898	2.979	12.469	0.834	160.9	153.3	167.5	-2.3	-16.0	123.8	119.1
	P	1.973, 1.903, 1.863, 1.930, 1.782	1.890	3.705	13.156		105.1	168.4	125.2	-76.3	-31.8	100.0	95.2
10	R	1.907, 1.917, 1.957, 1.952, 1.957, 1.949*	1.940	1.949	11.639		179.0	178.0	172.1	0.5	2.1	0.0	0.0
	TS	1.901, 1.864, 1.907, 1.878, 1.908	1.892	2.867	12.325	0.686	162.1	167.8	153.2	0.0	-18.9	99.1	99.9
	P	1.934, 1.872, 1.899, 1.811, 1.910	1.885	4.097	13.523		101.9	179.8	116.1	-124.3	-57.0	122.2	114.5
11	R	1.917, 1.955, 1.908, 1.948, 1.952, 1.956*	1.939	1.956	11.636		172.5	179.3	177.7	1.8	-6.7	0.0	0.0
	TS	1.865, 1.895, 1.899, 1.869, 1.931	1.892	2.840	12.299	0.663	162.9	148.6	175.1	1.4	-16.8	89.1	85.7
	P	1.862, 1.903, 1.930, 1.782, 1.973	1.890	4.080	13.530		137.8	125.1	168.4	-72.8	-39.6	114.5	102.2
12	R	1.918, 1.955, 1.953, 1.949, 1.906, 1.956*	1.940	1.956	11.637		172.4	179.7	165.2	-1.5	-6.6	0.0	0.0
	TS	1.864, 1.895, 1.931, 1.869, 1.899	1.892	2.842	12.300	0.663	162.9	148.5	175.1	-1.4	-16.3	87.6	84.9
	P	1.863, 1.903, 1.972, 1.782, 1.930	1.890	4.081	13.531		138.0	125.1	168.4	71.2	-46.3	113.3	101.6
13	R	1.951, 1.853, 1.965, 1.951, 1.950, 1.963*	1.939	1.963	11.633		179.8	175.8	173.6	0.4	0.0	0.0	0.0
	TS	1.931, 1.775, 1.951, 1.889, 1.934	1.896	2.954	12.434	0.801	172.8	138.0	161.7	0.0	-7.8	118.4	113.3
	P	1.959, 1.782, 1.867, 1.935, 1.900	1.889	3.709	13.152		121.3	169.6	117.1	-69.9	-32.2	98.8	96.4
14	R	1.956, 1.908, 1.917, 1.955, 1.948, 1.952*	1.939	1.952	11.636		177.7	172.6	179.2	-6.4	-1.0	0.0	0.0
	TS	1.889, 1.854, 1.916, 1.886, 1.932	1.895	2.792	12.269	0.633	173.4	135.6	177.9	5.0	-0.9	102.2	97.7
	P	1.908, 1.909, 1.853, 1.853, 1.889	1.882	3.653	13.065		135.2	86.7	118.6	0.3	-69.7	79.9	78.6
15	R	1.956, 1.907, 1.948, 1.955, 1.917, 1.952*	1.939	1.952	11.635		177.7	172.5	179.2	6.5	-1.0	0.0	0.0
	TS	1.889, 1.854, 1.932, 1.886, 1.917	1.896	2.792	12.270	0.635	173.3	135.6	178.0	-5.2	-0.7	102.1	97.3
	P	1.908, 1.909, 1.890, 1.853, 1.852	1.882	3.652	13.064		135.3	86.8	118.7	-0.8	-66.8	80.2	78.4
16	R	1.965, 1.951, 1.853, 1.950, 1.963, 1.952*	1.939	1.952	11.634		175.8	173.6	179.8	-1.7	0.5	0.0	0.0
	TS	1.919, 1.895, 1.808, 1.896, 1.964	1.896	2.941	12.423	0.789	167.6	130.4	179.6	4.7	-0.6	131.6	126.0
	P	1.799, 1.994, 1.798, 1.975, 1.905	1.894	4.001	13.472		115.1	90.7	112.7	3.8	79.4	134.8	118.8
17	R	1.966, 1.950, 1.964, 1.952, 1.853, 1.950*	1.939	1.950	11.635		175.8	173.5	179.8	1.7	0.5	0.0	0.0
	TS	1.916, 1.895, 1.964, 1.900, 1.808	1.897	2.929	12.412	0.777	167.7	130.4	179.5	-4.4	0.2	131.7	125.5
	P	1.867, 1.959, 1.900, 1.935, 1.782	1.889	3.710	13.153		128.9	85.1	117.6	-7.2	67.2	99.2	95.7

[a] The distance between Al and O of coordinated H_2O. [b] The average bond length between Al and O of coordinated H_2O. [c] The distance between Al and O of leaving H_2O; [d] $\sum r(Al\text{-}O) = \sum r(Al\text{-}O_l) + r(Al\text{-}O_L)$; [e] $\Delta\sum r(Al\text{-}O) = \sum r(Al\text{-}O)_{TS} - \sum r(Al\text{-}O)_R$; *Parameters of leaving H_2O; using the labeling in Fig.S2.

All the TS structures related to H-bond donated by the *cis*-4 inner-sphere H_2O (using the label in Fig. 1) are changed after optimizations: *cis*-4(No.5) → *cis*-2(a)(No.1), *trans*-3//*cis*-4(No.13) → *trans*-3(b)(No.4), *cis*-4//*cis*-5(No.16) → *cis*-5(b)(No.7) and *cis*-4//*cis*-6(No.17) → *cis*-6(b)(No.9). This demonstrates that *cis*-4 is not a good H-bond donor. The possible reason is that the rotation ability of *cis*-4 is limited by the H-bond between the leaving H_2O and *cis*-4. In this situation, it is difficult for *cis*-4 to donate the double H-bonds sites through the rotation of the coordination bond. It is also difficult for *cis*-4 to donate a single H-bond site, because there will be proton migration if the explicit H_2O forms a single H-bond with the inner-sphere H_2O, making the leaving H_2O transfer to the *cis*-2. There are two kinds of ways to change the TS structures during the optimization, one is changing the H-bonding site of leaving H_2O, including *cis*-4(No.5) → *cis*-2(a)(No.1). Another is changing the H-bonding site of explicit H_2O, including *trans*-3//*cis*-4(No.13) → *trans*-3(b)(No.4), *cis*-4//*cis*-5(No.16) → *cis*-5(b)(No.7) and *cis*-4//*cis*-6(No.17) → *cis*-6(b)(No.9). The detailed processes described by the related bond lengths are showing in Fig. S3, taking *cis*-4(No.5) → *cis*-2(a)(No.1) and *trans*-3//*cis*-4(No.13) → *trans*-3(b)(No.4) as examples. In Fig. S3 (A), the leaving H_2O forms a single H-bond with *cis*-4 with a length of 1.871 Å, while the distance between leaving H_2O and *cis*-2 is 2.315 Å in the initial structure of TS. During the optimization, the leaving H_2O is gradually away from the *cis*-4 and close to the *cis*-2, until forms a single H-bond with *cis*-2 with a bond length of 1.784 Å. Finally, the previous H-bond between the leaving H_2O and *cis*-4 is broken with a distance of 2.824 Å and the H-bond between the leaving H_2O and *cis*-2 is made. In Fig. S3 (B), the explicit H_2O forms double H-bond with *trans*-3 and *cis*-4 with the bond lengths of 1.863 Å and 1.975 Å in the initial structure of TS, respectively. During the optimization, the distance between the explicit H_2O and *cis*-4 continues to increase until reaches 5.111 Å in the optimized structure.



(A) changing the H-bonding site of leaving H_2O (*cis*-4(No.5) → *cis*-2(a)(No.1))

(B) changing the H-bonding site of explicit H_2O (*trans*-3//*cis*-4(No.13) → *trans*-3(b)(No.4))

Fig. S3 Description of the changing of the TS configuration during the optimization process

§S3 The results of N_m' = 2 ~ 7 as well as the structural and energetic parameters for the optimal pathways with N_m' = 0 ~ 7

§S3.1 The PES profiles of all the tested pathways with N_m' = 2 ~ 7

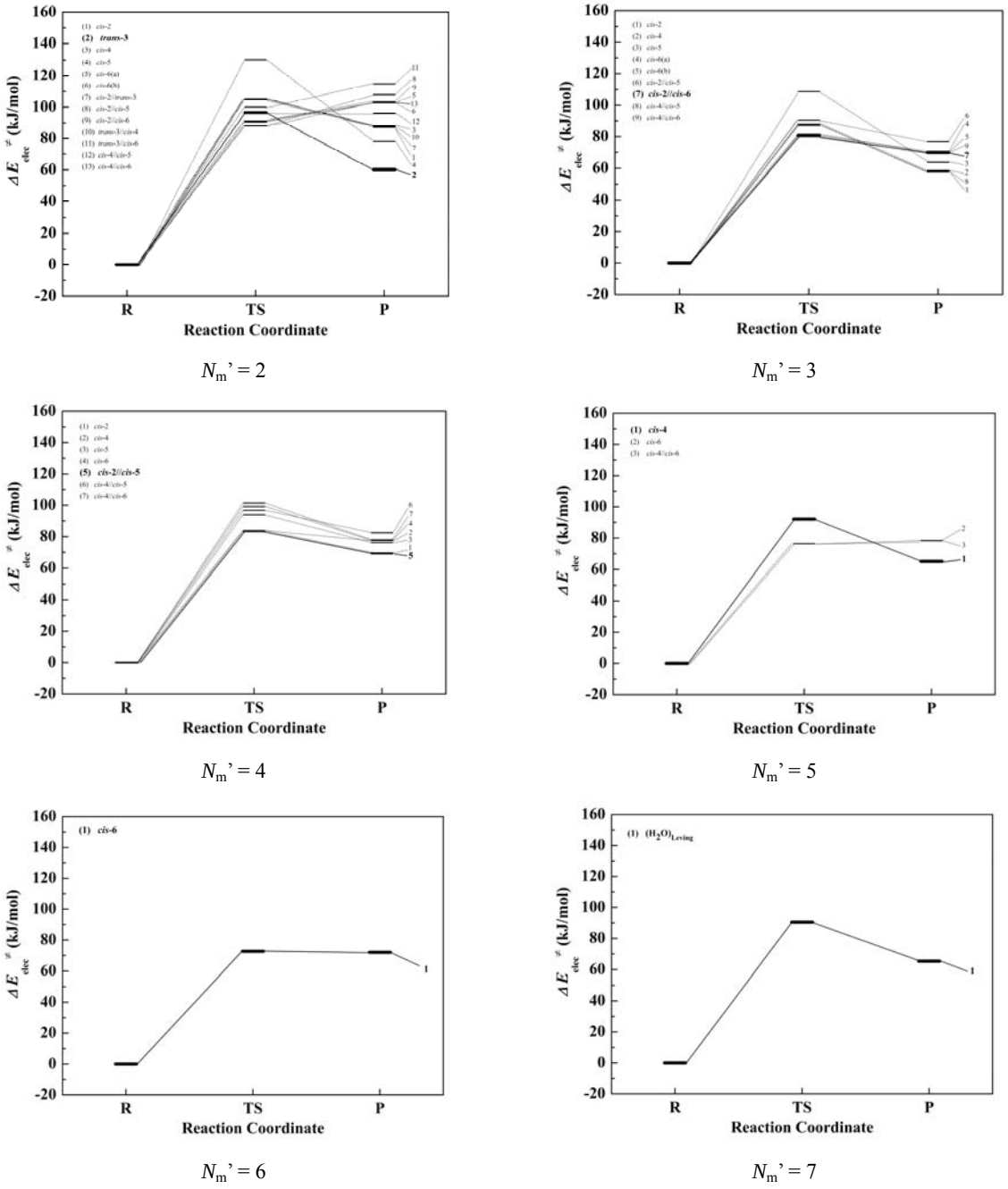
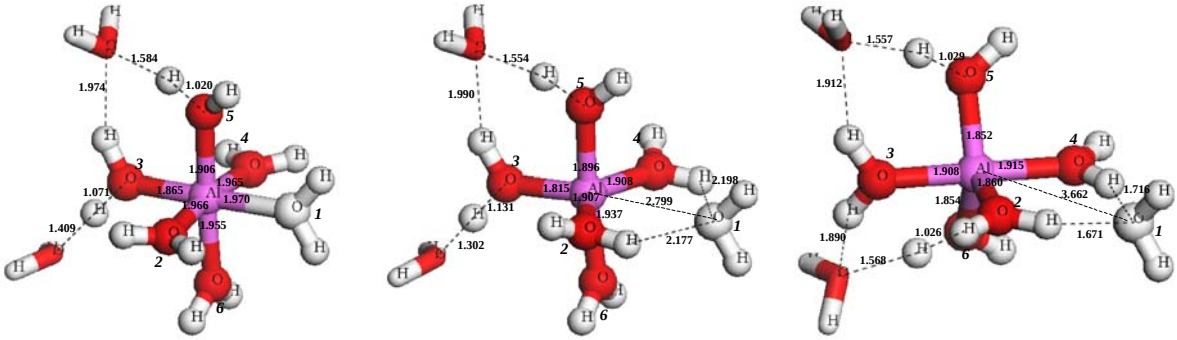


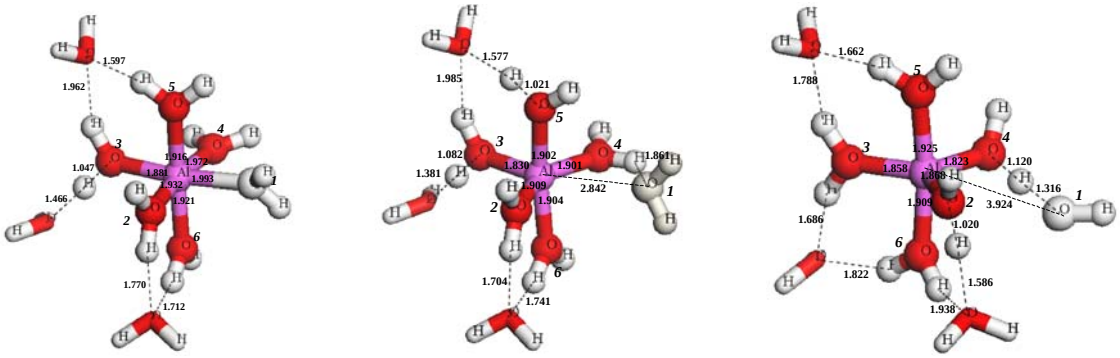
Fig. S4 The PES profiles of all the tested pathways with N_m' = 2 ~ 7 for water-exchange reactions in $Al(H_2O)_6^{3+}$ (the optimal pathway is shown by solid line)

§S3.2 The optimized R, TS and P structures for the optimal pathways with N_m' = 2 ~ 7



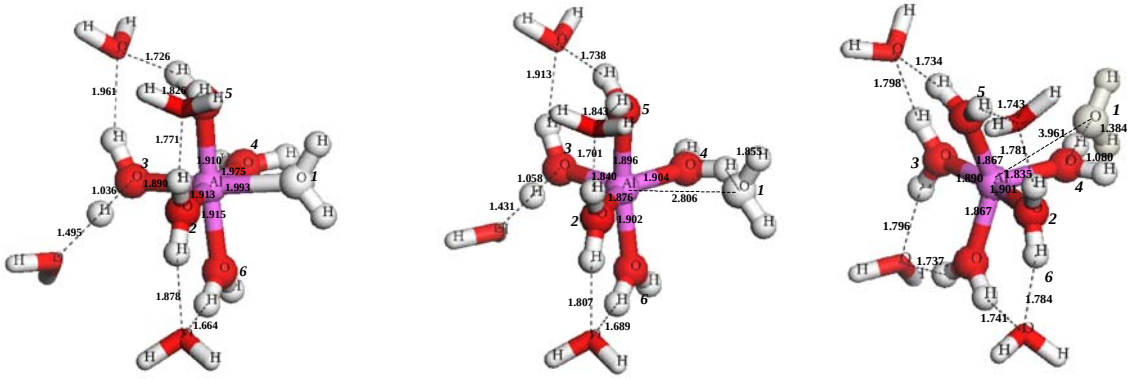
R TS (-134.43 cm^{-1}) P

(1) N_m' = 2



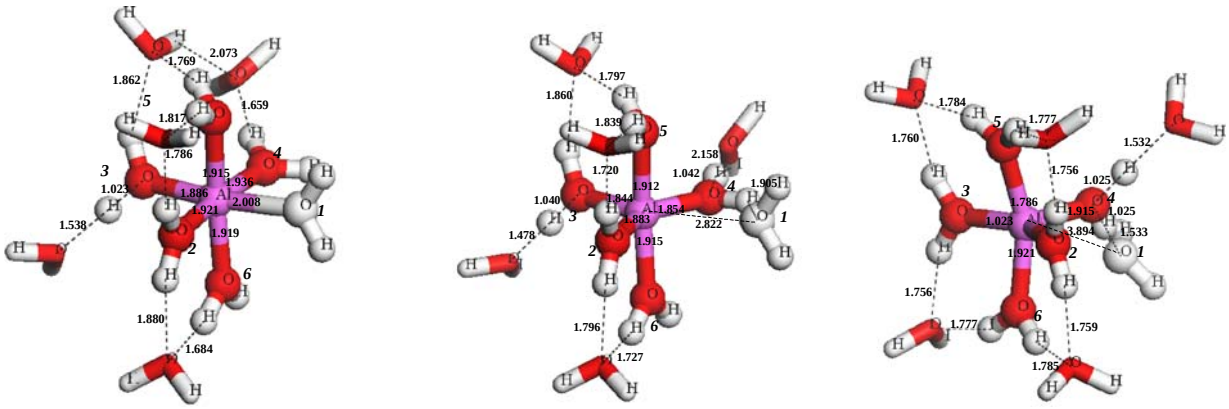
R TS (-133.28 cm^{-1}) P

(2) N_m' = 3



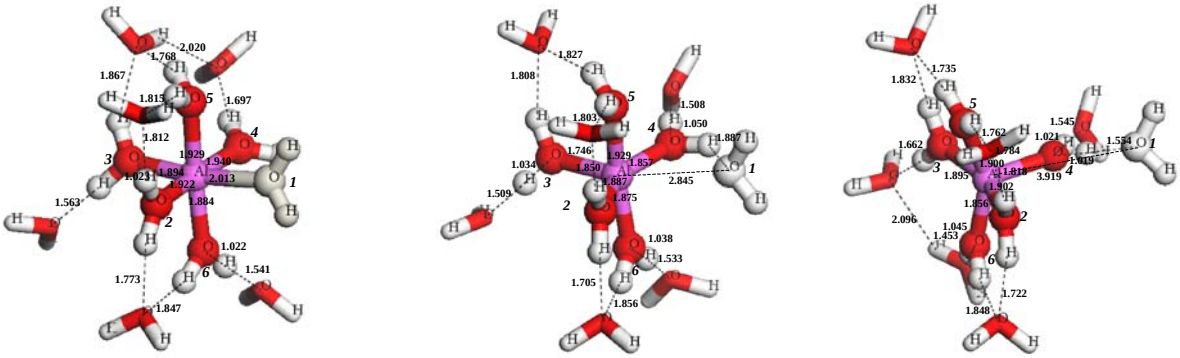
R TS (-134.58 cm^{-1}) P

(3) N_m' = 4



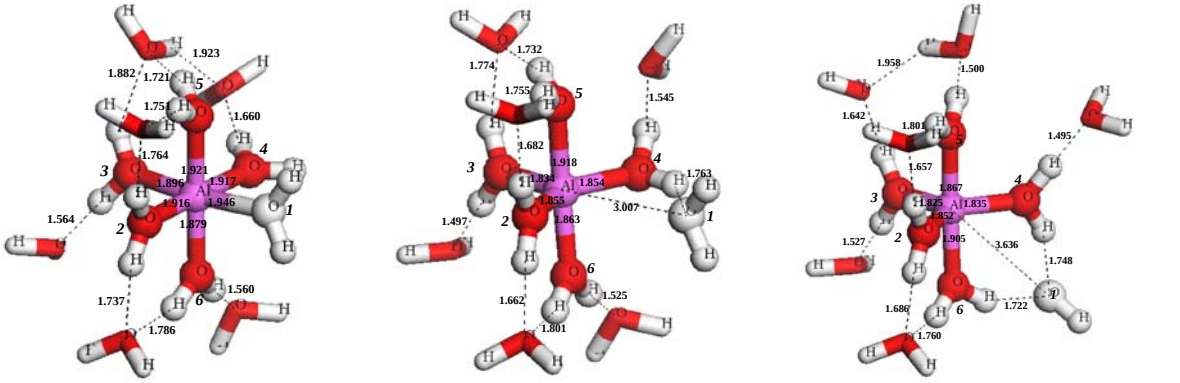
R TS (-102.54 cm^{-1}) P

(4) N_m' = 5



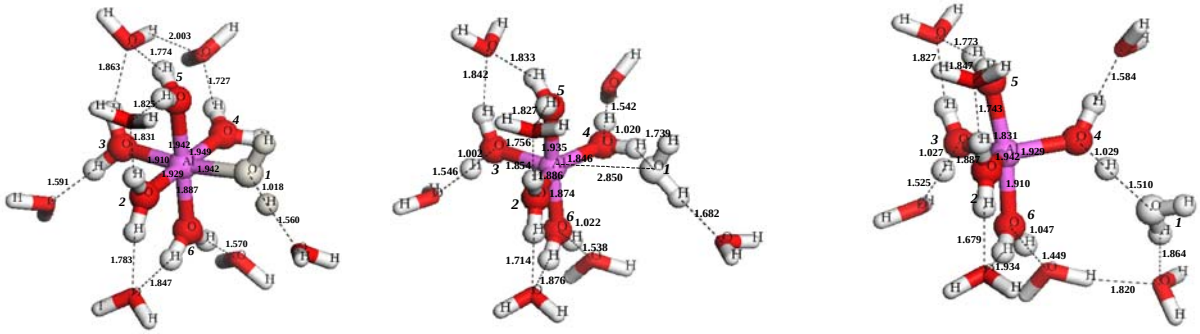
R TS (-97.42 cm^{-1}) P

(5) N_m' = 6 (without PCM)



R TS (-87.39 cm^{-1}) P

(6) N_m' = 6 (with PCM)



R TS (-102.79 cm^{-1}) P

(7) N_m' = 7

Fig. S5 The optimized R,TS and P structures for the optimal pathways with N_m' = 2 ~ 7 for water-exchange reactions in $Al(H_2O)_6^{3+}$ (the leaving H_2O are colored white to differ from others and the explicit H_2O are showed by stick model)

§S3.3 The structural and energetic parameters for the optimal pathways with N_m' = 0 ~ 7

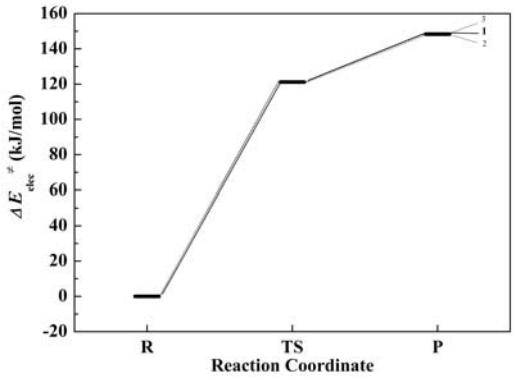
Table S3 Selected structural and energetic parameters for the optimal pathways with N_m' = 0 ~ 7 for water-exchange reactions in $Al(H_2O)_6^{3+}$

N_m'	Species	Bond length (Å)					Bond angle (°)			Dihedral angle (°)		$\Delta E_{elec}^{\neq}$ (kJ/mol)	$\Delta G^{\neq}$ (kJ/mol)
		r(Al-O_I)[a]	r (Al-O_I)[b]	r(Al-O_L)[c]	$\sum$r(Al-O)[d]	$\Delta\sum$r(Al-O)[e]	θ_x (O_3-Al-O_1)	θ_y (O_2-Al-O_4)	θ_z (O_5-Al-O_6)	horizontal plane D(O_2-$O_3$$O_4$-$O_1$)	axial plane D(O_5-$O_3$$O_6$-$O_1$)		
0	R	1.940, 1.940, 1.940, 1.940, 1.940, 1.940*	1.940	1.940	11.640		180.0	180.0	179.9	0.0	0.0	0.0	0.0
	TS	1.915, 1.878, 1.876, 1.915, 1.916	1.900	2.955	12.455	0.815	167.9	144.2	172.8	0.2	-12.1	122	111
	P	1.960, 1.900, 1.960, 1.893, 1.766	1.896	4.214	13.693		141.9	116.5	165.7	-2.0	-41.8	148	130
1	R	1.956, 1.908, 1.917, 1.955, 1.948, 1.952*	1.939	1.952	11.636		177.7	172.6	179.2	-6.4	-1.0	0.0	0.0
	TS	1.889, 1.854, 1.916, 1.886, 1.932	1.895	2.792	12.269	0.633	173.4	135.6	177.9	5.0	-0.9	102	97.7
	P	1.908, 1.909, 1.853, 1.853, 1.889	1.882	3.653	13.065		135.2	86.7	118.6	0.3	-69.7	79.9	78.6
2	R	1.966, 1.865, 1.906, 1.965, 1.955, 1.970*	1.938	1.970	11.627		179.0	171.2	176.6	-5.7	-1.0	0.0	0.0
	TS	1.907, 1.815, 1.896, 1.907, 1.938	1.893	2.799	12.262	0.635	173.7	136.3	175.3	2.5	0.3	96.5	89.2
	P	1.860, 1.908, 1.852, 1.915, 1.854	1.878	3.662	13.051		136.0	87.4	127.9	0.1	64.3	60.3	67.2
3	R	1.932, 1.881, 1.916, 1.972, 1.921, 1.992*	1.936	1.992	11.614		171.9	171.9	175.4	-6.5	-7.9	0.0	0.0
	TS	1.889, 1.830, 1.902, 1.902, 1.904	1.885	2.842	12.269	0.655	162.9	147.8	168.6	-8.5	-17.1	80.2	76.6
	P	1.868, 1.858, 1.925, 1.823, 1.909	1.877	3.924	13.307		121.0	115.1	171.0	105.7	-64.2	69.6	65.6
4	R	1.913, 1.890, 1.910, 1.975, 1.915, 1.993*	1.933	1.993	11.596		167.7	173.9	172.7	-5.5	-11.4	0.0	0.0
	TS	1.876, 1.840, 1.896, 1.904, 1.902	1.884	2.806	12.224	0.628	158.7	148.7	168.2	-9.0	-19.3	83.4	78.8
	P	1.890, 1.901, 1.867, 1.835, 1.867	1.872	3.961	13.321		122.1	97.8	138.8	27.0	-69.1	69.3	65.2
5	R	1.921, 1.886, 1.915, 1.936, 1.919, 2.008*	1.931	2.008	11.585		171.9	173.9	172.6	-3.9	-8.6	0.0	0.0
	TS	1.883, 1.844, 1.912, 1.854, 1.915	1.882	2.822	12.230	0.645	164.4	147.7	168.8	-8.0	-16.4	92.2	78.1
	P	1.883, 1.883, 1.894, 1.810, 1.894	1.873	3.896	13.260		86.7	106.8	156.4	138.1	-97.9	65.2	53.0
6	R	1.922, 1.894, 1.929, 1.940, 1.884, 2.013*	1.930	2.013	11.582		171.2	174.8	172.7	-3.6	-7.8	0.0	0.0
	TS	1.887, 1.850, 1.929, 1.857, 1.875	1.880	2.851	12.249	0.667	162.6	148.3	168.5	-7.8	-16.5	72.7	58.4
	P	1.902, 1.895, 1.900, 1.818, 1.856	1.874	3.919	13.290		129.9	102.0	148.5	-59.4	-52.1	72.1	57.1
6**	R	1.916, 1.896, 1.921, 1.917, 1.879 ,1.946*	1.912	1.946	11.474		177.6	173.0	175.1	-2.6	-6.6	0.0	0.0
	TS	1.855, 1.834, 1.918, 1.854, 1.863	1.865	3.007	12.330	0.856	139.9	162.1	172.9	5.7	-18.9	74.9	67.6
	P	1.852, 1.825, 1.835, 1.867, 1.905	1.857	3.636	13.270		117.8	106.4	174.5	118.3	-80.7	60.8	57.5
7	R	1.929, 1.910, 1.942, 1.949, 1.887, 1.942*	1.926	1.942	11.559		170.9	177.8	175.7	-4.0	-7.7	0.0	0.0
	TS	1.886, 1.854, 1.935, 1.846, 1.874	1.879	2.850	12.245	0.686	161.7	146.4	170.1	-8.3	-17.7	90.6	75.7
	P	1.875, 1.855, 1.933, 1.816, 1.869	1.870	3.879	13.227		122.6	116.7	171.2	97.2	-67.1	65.4	61.6

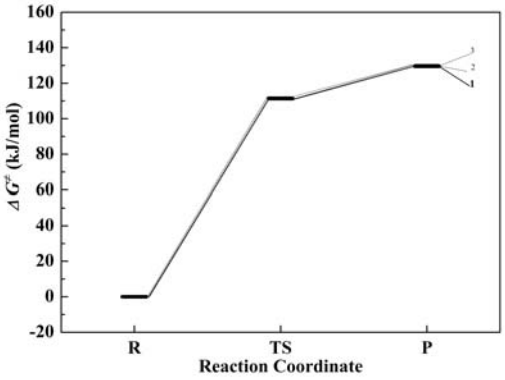
[a] The distance between Al and O of coordinated H_2O. [b] The average bond length between Al and O of coordinated H_2O. [c] The distance between Al and O of leaving H_2O; [d] $\sum$r(Al-O) = $\sum$r(Al-O_I) + r(Al-O_L); [e] $\Delta\sum$r(Al-O) = $\sum$r(Al-O)$_{TS}$ - $\sum$r(Al-O)$_R$; *Parameters of leaving H_2O; ** The results obtained under PCM model with N'_m = 6.

§S4 The results of "Independent-minimum" method (Method-II)

§S4.1 The PES and GES profiles of all the tested pathways with N_m' = 0 ~ 12

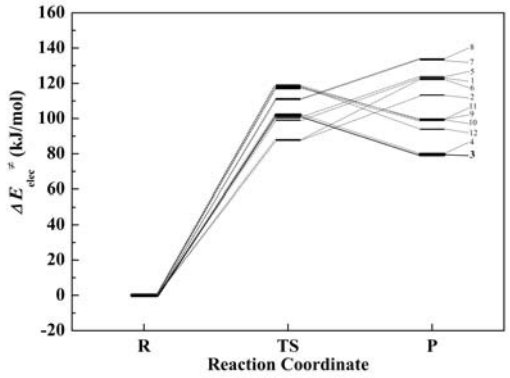


PES profiles

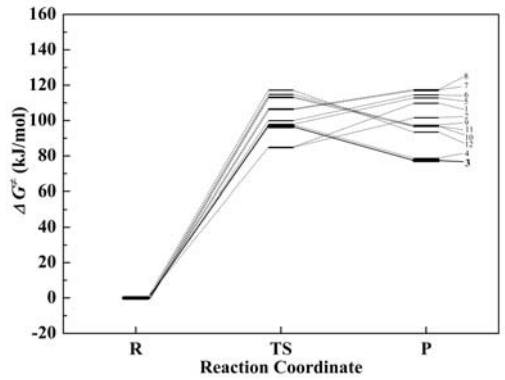


GES profiles

(1) N_m' = 0

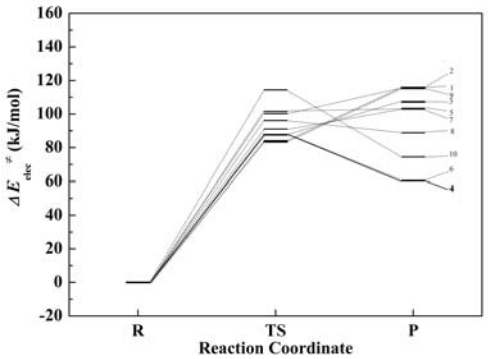


PES profiles

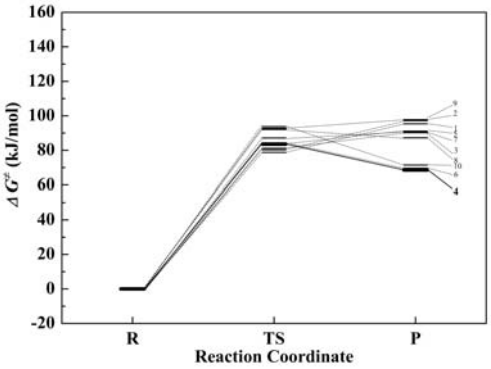


GES profiles

(2) N_m' = 1

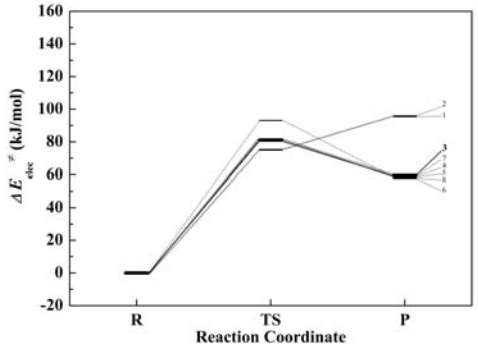


PES profiles

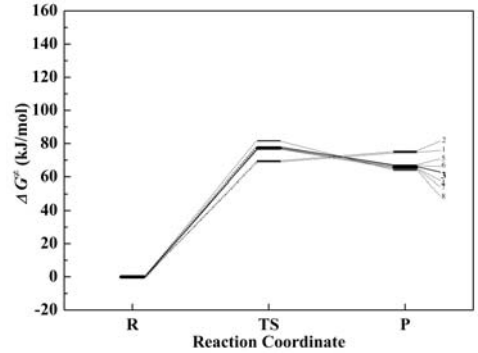


GES profiles

(3) N_m' = 2

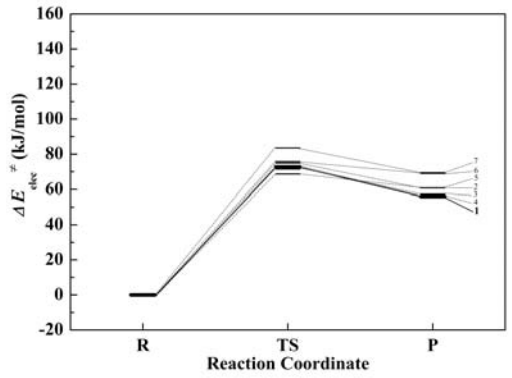


PES profiles

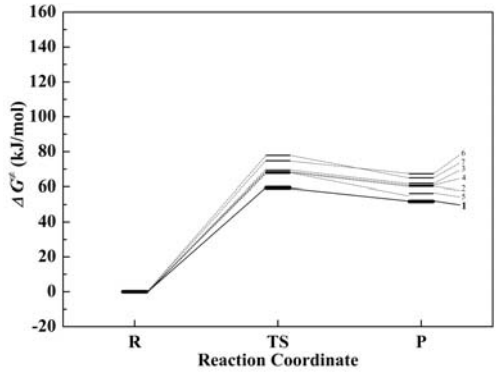


GES profiles

(4) N_m' = 3

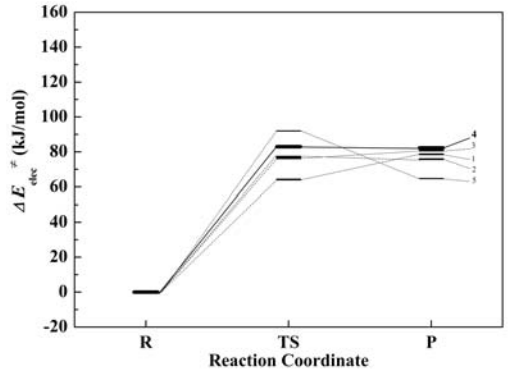


PES profiles

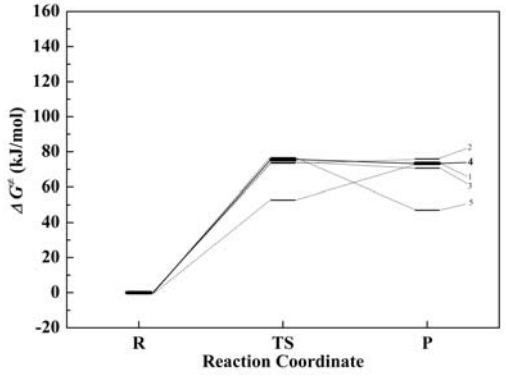


GES profiles

(5) N_m' = 4

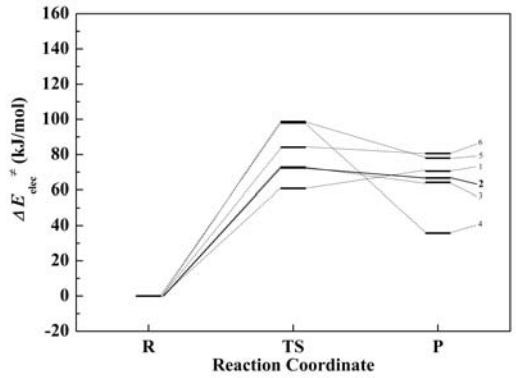


PES profiles

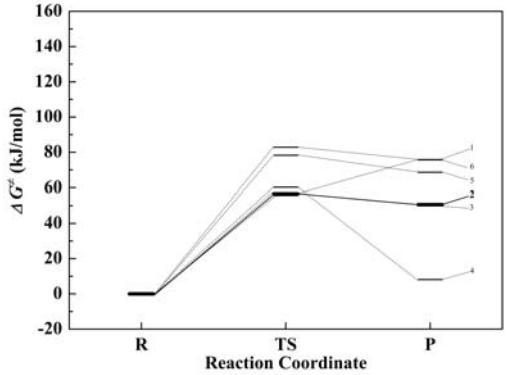


GES profiles

(6) N_m' = 5

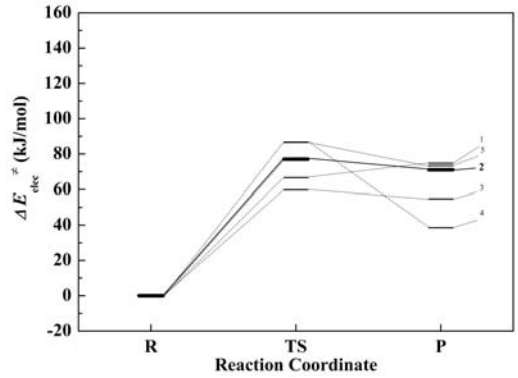


PES profiles

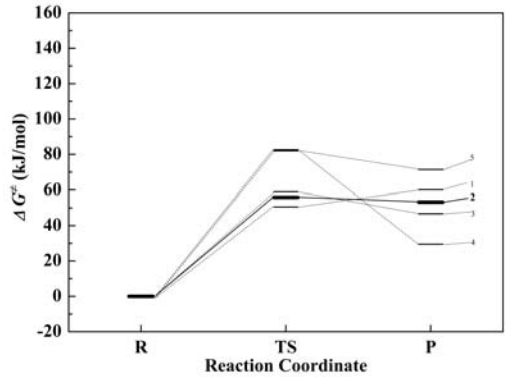


GES profiles

(7) N_m' = 6

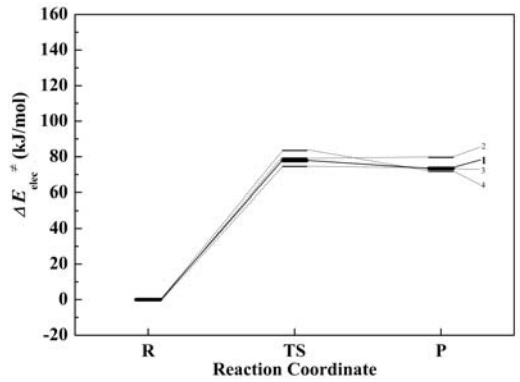


PES profiles

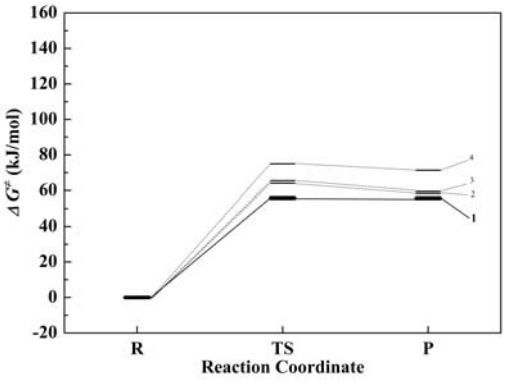


GES profiles

(8) N_m' = 7

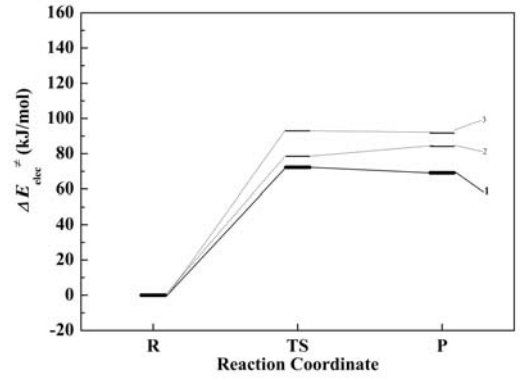


PES profiles

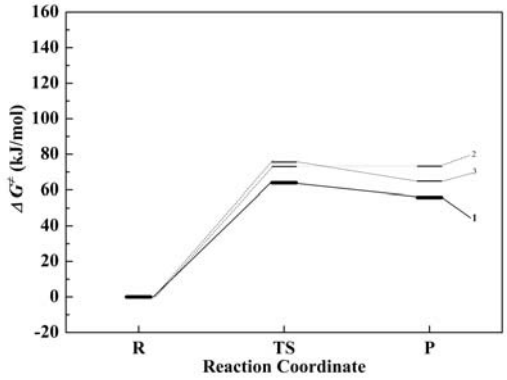


GES profiles

(9) N_m' = 8

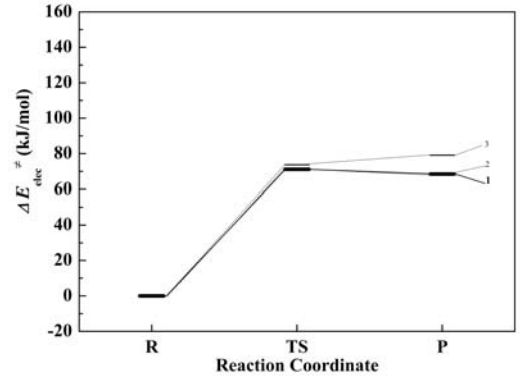


PES profiles

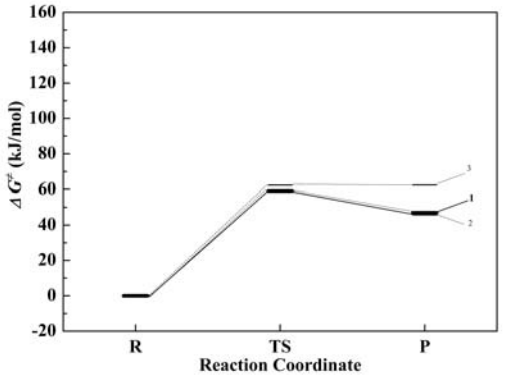


GES profiles

(10) N_m' = 9

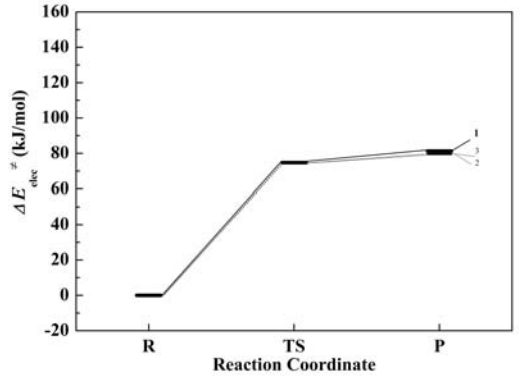


PES profiles

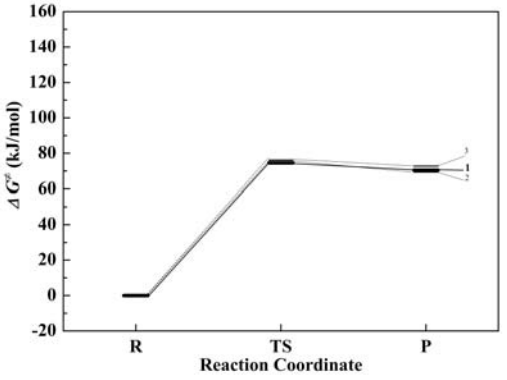


GES profiles

(11) N_m' = 10

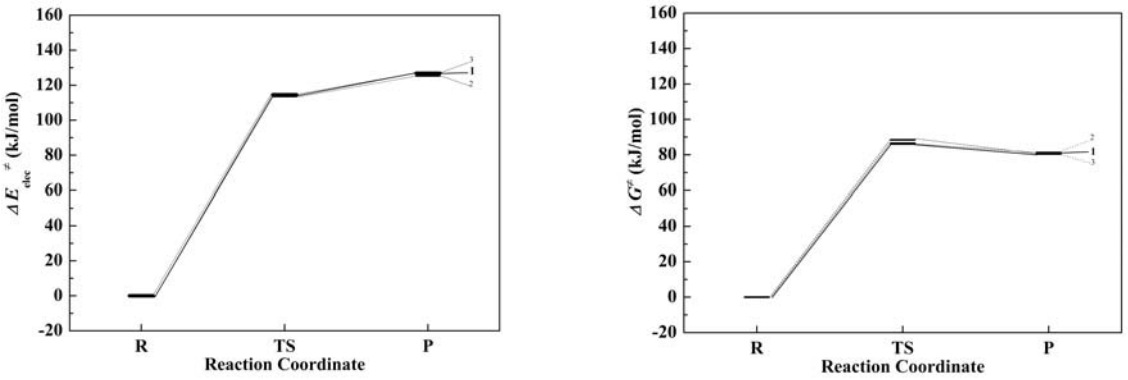


PES profiles



GES profiles

(12) N_m' = 11

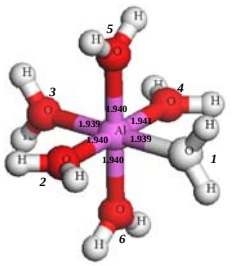


PES profiles GES profiles

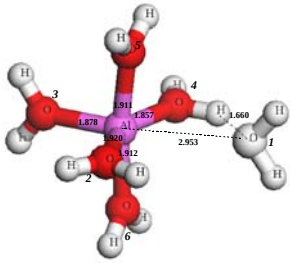
(13) N_m' = 12

Fig. S6 The PES and GES profiles of all the tested pathways with N_m' = 0 ~ 12 obtained by "Independent-minimum" method (Method-II) (different pathways are numbered by $\Delta G_a^{\neq}$ from low to high and the optimal pathway is shown by solid line)

§S4.2 The optimized R, TS and P structures as well as structural and energetic parameters for the optimal pathways with N_m' = 0 ~ 12

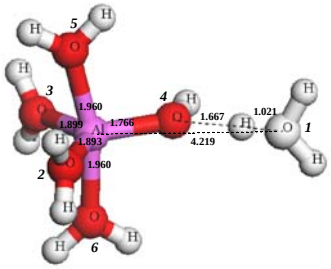


R

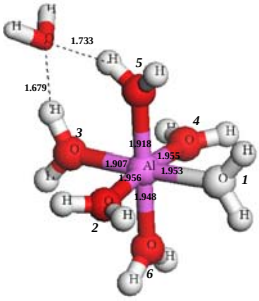


TS (-146.95 cm^{-1})

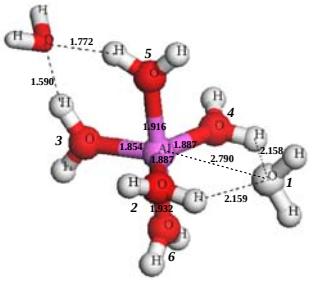
(1) N_m' = 0



P

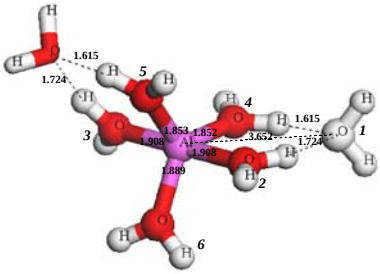


R

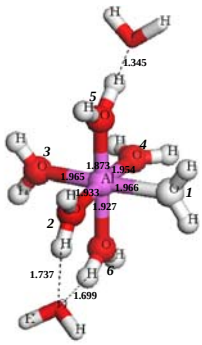


TS (-142.03 cm^{-1})

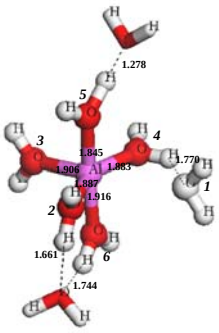
(2) N_m' = 1



P

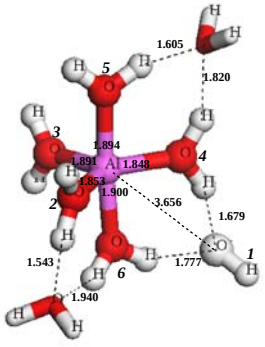


R

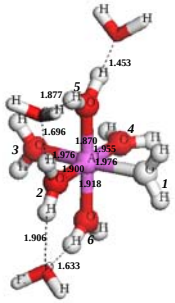


TS (-135.96 cm^{-1})

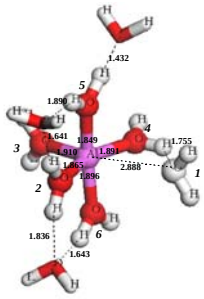
(3) N_m' = 2



P

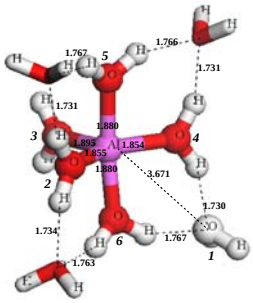


R

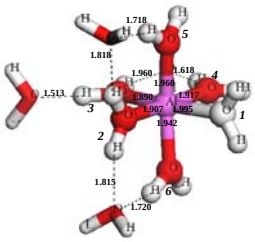


TS (-130.59 cm^{-1})

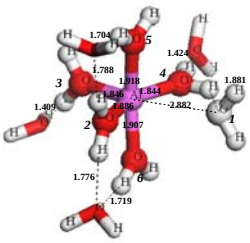
(4) N_m' = 3



P

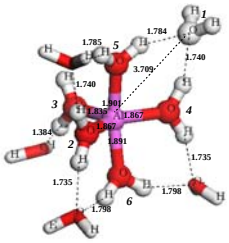


R

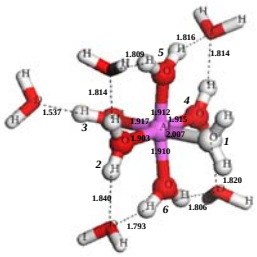


TS (-91.03 cm^{-1})

(5) N_m' = 4



P



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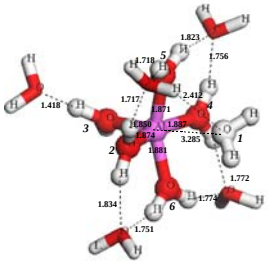
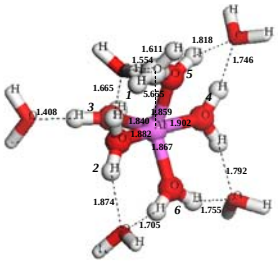


TS (-94.15 cm^{-1})

(6) N_m' = 5



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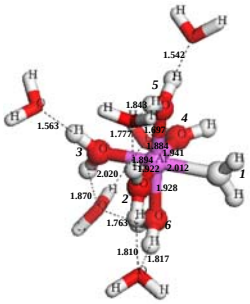
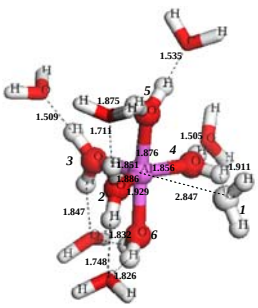
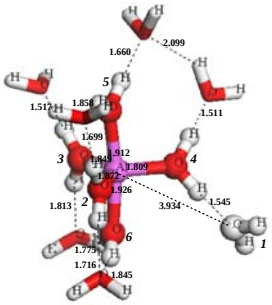


R

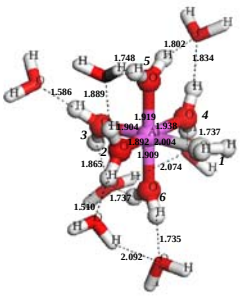


TS (-96.07 cm^{-1})

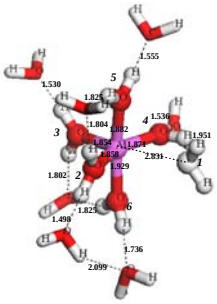
(7) N_m' = 7



P

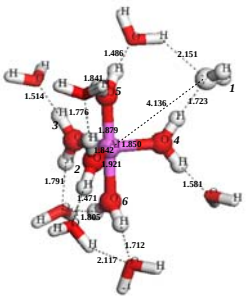


R



TS (-94.51 cm^{-1})

(8) N_m' = 7



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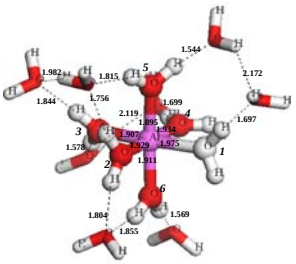
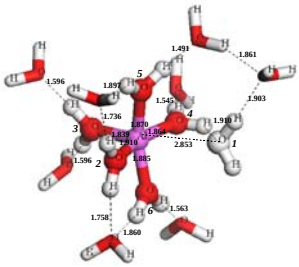
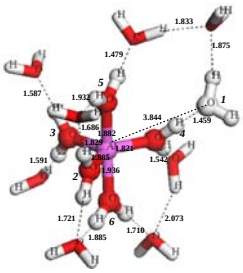


R

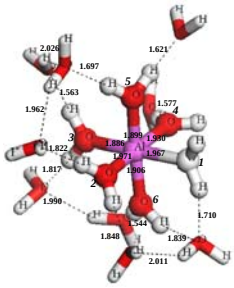


TS (-84.96 cm^{-1})

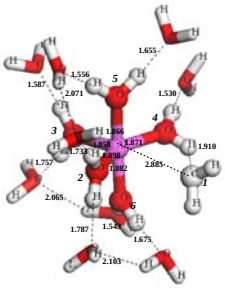
(9) N_m' = 8



P

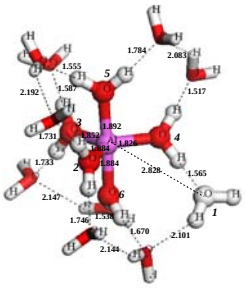


R

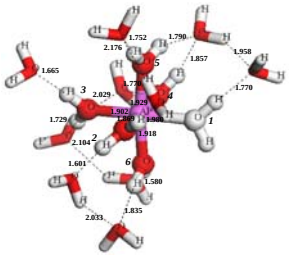


TS (-80.64 cm^{-1})

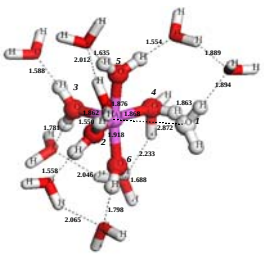
(10) N_m' = 9



P

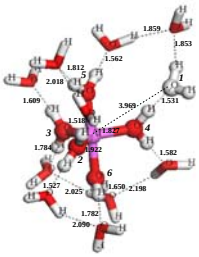


R

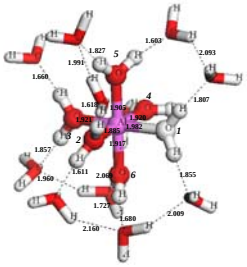


TS (-87.91 cm^{-1})

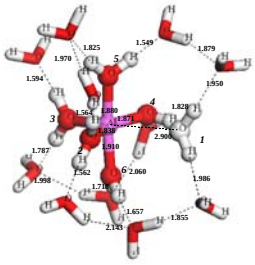
(11) N_m' = 10



P

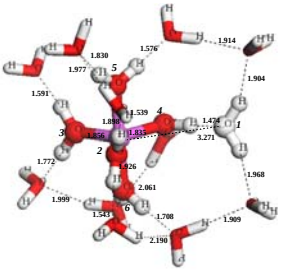


R

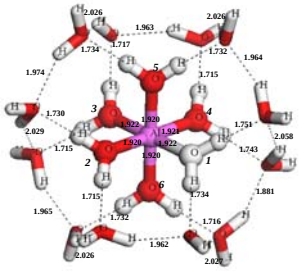


TS (-80.83 cm^{-1})

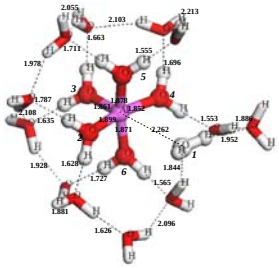
(12) N_m' = 11



P

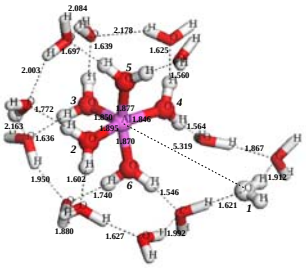


R



TS (-60.94 cm^{-1})

(13) N_m' = 12



P

Fig. S7 The optimized R,TS and P structures for the optimal pathways with N_m' = 0 ~ 12 for water-exchange reactions in $Al(H_2O)_6^{3+}$ obtained with "Independent-minimum" method (Method-II) (the leaving H_2O are colored white to differ from others and the explicit H_2O are showed by stick model)

Table S4 Selected structural and energetic parameters for the optimal pathways with N_m' = 0 ~ 12 for water-exchange reactions in $Al(H_2O)_6^{3+}$ obtained with "Independent-minimum" method (Method-II)

N_m'	Species	Bond length (Å)					Bond angle (°)			Dihedral angle (°)		$\Delta E_{elec}^{\neq}$ (kJ/mol)	$\Delta G^{\neq}$ (kJ/mol)
		r(Al-O_I)[a]	r (Al-O_I)[b]	r(Al-O_L)[c]	$\sum$r(Al-O)[d]	$\Delta\sum$r(Al-O)[e]	θ_x (O_3-Al-O_1)	θ_y (O_2-Al-O_4)	θ_z (O_5-Al-O_6)	horizontal plane D(O_2-$O_3$$O_4$-$O_1$)	axial plane D(O_5-$O_3$$O_6$-$O_1$)		
0	R	1.940, 1.940, 1.940, 1.941, 1.940, 1.939*	1.940	1.939	11.640		179.9	179.9	179.8	0.0	0.1	0.0	0.0
	TS	1.857, 1.878, 1.912, 1.920, 1.912	1.896	2.953	12.432	0.792	166.3	147.6	170.9	0.0	-13.6	121.2	111.3
	P	1.766, 1.900, 1.960, 1.893, 1.960	1.896	4.219	13.698		141.6	116.5	165.5	0.1	-42.3	148.3	129.5
1	R	1.956, 1.908, 1.917, 1.955, 1.948, 1.952*	1.939	1.952	11.636		177.7	172.6	179.2	-6.5	-1.1	0.0	0.0
	TS	1.887, 1.854, 1.916, 1.887, 1.932	1.895	2.790	12.266	0.630	158.8	153.5	172.8	0.2	-14.8	102	96.7
	P	1.908, 1.908, 1.853, 1.852, 1.889	1.882	3.652	13.062		135.5	86.8	118.7	0.8	-69.6	79.6	77.6
2	R	1.933, 1.965, 1.873, 1.954, 1.927, 1.966*	1.936	1.966	11.618		172.5	174.1	178.3	-3.2	-6.4	0.0	0.0
	TS	1.887, 1.906, 1.845, 1.883, 1.916	1.887	2.874	12.311	0.693	162.2	148.9	175.1	0.6	-16.7	87.6	81.6
	P	1.852, 1.891, 1.894, 1.848, 1.900	1.877	3.656	13.041		103.8	132.6	176.2	103.0	-84.8	60.4	64.5
3	R	1.900, 1.976, 1.870, 1.956, 1.919, 1.976*	1.933	1.976	11.597		169.9	176.8	176.1	-1.0	-9.9	0.0	0.0
	TS	1.865, 1.910, 1.849, 1.891, 1.896	1.882	2.888	12.299	0.702	158.4	154.8	171.2	1.4	-20.9	80.8	77.1
	P	1.854, 1.895, 1.880, 1.855, 1.880	1.873	3.671	13.035		102.5	142.9	172.3	101.2	-90.8	59.7	65.8
4	R	1.907, 1.890, 1.942, 1.917, 1.942, 1.995*	1.932	1.995	11.593		172.1	179.8	166.6	0.0	-10.4	0.0	0.0
	TS	1.886, 1.846, 1.918, 1.844, 1.907	1.880	2.882	12.283	0.690	165.8	150.6	166.6	-0.6	-17.1	72.8	59.5
	P	1.867, 1.835, 1.901, 1.867, 1.891	1.872	3.708	13.069		103.8	138.3	166.6	-101.2	-34.1	56.0	51.8
5	R	1.903, 1.917, 1.912, 1.915, 1.910, 2.007*	1.927	2.007	11.564		179.2	177.8	170.1	-0.4	-0.3	0.0	0.0
	TS	1.874, 1.850, 1.871, 1.887, 1.881	1.873	3.285	12.648	1.084	164.2	161.5	155.7	-9.2	10.9	83.0	75.5
	P	1.882, 1.840, 1.859, 1.902, 1.867	1.870	5.655	15.005		125.0	167.8	138.8	-26.4	33.1	82.3	73.4
6	R	1.922, 1.894, 1.884, 1.941, 1.928, 2.012*	1.930	2.012	11.581		171.3	174.9	172.7	3.5	-8.0	0.0	0.0
	TS	1.886, 1.851, 1.876, 1.856, 1.929	1.880	2.847	12.245	0.664	162.4	148.3	168.5	8.2	-18.2	72.5	56.8
	P	1.872, 1.849, 1.912, 1.809, 1.926	1.874	3.934	13.302		124.6	117.3	168.9	89.7	-63.6	66.7	50.6
7	R	1.892, 1.904, 1.919, 1.938, 1.909, 2.004*	1.928	2.004	11.566		174.7	169.7	178.6	6.2	-1.9	0.0	0.0
	TS	1.858, 1.854, 1.882, 1.871, 1.929	1.879	2.831	12.225	0.659	164.8	150.5	170.6	1.3	-14.6	77.1	55.9
	P	1.842, 1.849, 1.879, 1.850, 1.921	1.868	4.136	13.302		110.6	121.3	178.1	-117.2	-41.9	71.1	53.2
8	R	1.929, 1.907, 1.895, 1.934, 1.911, 1.975*	1.925	1.975	11.551		173.8	178.7	172.6	0.3	-7.8	0.0	0.0
	TS	1.910, 1.839, 1.870, 1.864, 1.885	1.874	2.853	12.221	0.670	162.9	158.2	160.0	-3.8	-18.2	74.5	55.8
	P	1.885, 1.829, 1.882, 1.821, 1.936	1.871	3.898	13.251		131.4	132.2	169.7	-79.0	-34.1	73.5	55.7
9	R	1.971, 1.886, 1.899, 1.930, 1.906, 1.967*	1.927	1.967	11.559		177.6	175.6	174.7	1.5	-2.9	0.0	0.0
	TS	1.898, 1.858, 1.866, 1.871, 1.882	1.875	2.885	12.260	0.701	164.0	143.3	173.2	14.2	-13.0	72.3	64.0
	P	1.884, 1.852, 1.892, 1.826, 1.884	1.868	3.828	13.166		132.3	118.6	177.5	81.9	-50.3	69.2	56.0
10	R	1.869, 1.903, 1.929, 1.952, 1.918, 1.980*	1.925	1.980	11.551		175.6	176.3	172.8	3.9	-0.9	0.0	0.0
	TS	1.843, 1.862, 1.876, 1.868, 1.918	1.873	2.872	12.239	0.688	162.2	153.9	168.2	-2.1	-14.7	71.2	59.1
	P	1.826, 1.866, 1.895, 1.827, 1.922	1.867	3.969	13.305		125.3	123.7	177.8	-94.4	-33.5	68.5	46.9
11	R	1.885, 1.921, 1.905, 1.921, 1.917, 1.982*	1.922	1.982	11.531		174.4	176.3	179.4	0.9	-3.9	0.0	0.0
	TS	1.838, 1.862, 1.880, 1.871, 1.910	1.892	2.900	12.361	0.830	163.7	147.9	173.3	1.9	-14.0	74.8	74.6
	P	1.822, 1.856, 1.898, 1.835, 1.926	1.867	3.721	13.058		151.4	124.4	179.9	-6.3	-24.9	81.3	70.5
12	R	1.920, 1.922, 1.920, 1.920, 1.921, 1.922*	1.921	1.922	11.525		180.0	180.0	180.0	0.4	0.0	0.0	0.0
	TS	1.871, 1.861, 1.899, 1.878, 1.852	1.872	3.262	12.623	1.098	172.2	164.2	161.3	0.0	-7.8	114.1	86.1
	P	1.870, 1.850, 1.895, 1.877, 1.846	1.867	5.319	14.657		141.3	158.7	159.8	-69.9	-32.2	126.0	80.6

[a] The distance between Al and O of coordinated H_2O. [b] The average bond length between Al and O of coordinated H_2O. [c] The distance between Al and O of leaving H_2O; [d] $\sum$r(Al-O) = $\sum$r(Al-O_I) + r(Al-O_L); [e] $\Delta\sum$r(Al-O) = $\sum$r(Al-O)$_{TS}$ - $\sum$r(Al-O)$_R$; *Parameters of leaving H_2O.

§S5 Cartesian coordinates

§S5.1 Cartesian coordinates for the optimized R, TS and P structures for the pathways with N_m' = 0

R

Al	-0.11806600	-0.13996300	0.10157600
O	0.84937400	-0.93896000	1.58174300
H	1.17358400	-1.85806900	1.63334100
O	1.56155800	0.40325600	-0.70311000
H	1.67244100	0.89238600	-1.54039300
H	1.10363400	-0.49860100	2.41479400
H	2.45510300	0.24373500	-0.34432400
O	-1.79779100	-0.68402300	0.90577600
H	-1.90889800	-1.16902000	1.74540900
H	-2.69121100	-0.52591600	0.54611000
O	-1.08626200	0.65666600	-1.37939200
H	-1.33943700	0.21467000	-2.21189700
H	-1.41130000	1.57539000	-1.43281200
O	-0.20303200	1.54241000	1.06295000
H	-0.90825800	1.82478400	1.67570900
H	0.45194100	2.26511300	1.02765900
O	-0.03289200	-1.82295500	-0.86002600
H	-0.68662400	-2.54667400	-0.82299100
H	0.67110100	-2.10407900	-1.47475200

TS

Al	-0.50248200	-0.22019100	0.30856300
O	0.55091200	-0.93849700	1.73760000
H	0.95641600	-1.82727100	1.74581600
O	2.03683300	0.12455700	-1.16333600
H	2.17509500	0.61082700	-1.99582600
H	0.82078200	-0.48905000	2.56164700
H	2.93842600	-0.01828800	-0.82379100
O	-2.12166500	-0.79213500	1.06493400
H	-2.22420300	-1.31601200	1.88509800
H	-3.01436100	-0.67202400	0.68239300
O	-1.36256800	0.62781100	-1.17769200
H	-1.53033200	0.21044400	-2.04493900
H	-1.67218800	1.55223600	-1.23629500
O	-0.18645200	1.52282700	1.03775700
H	-0.74980300	2.01546200	1.66847400
H	0.58773300	2.08590100	0.83552300
O	0.17346800	-1.51887700	-0.83183900
H	-0.10708700	-2.40484500	-1.12876200
H	1.04960400	-1.21349900	-1.23949700

P

Al	-0.67966900	-0.09387200	0.48719700
O	0.03623300	-1.04686500	2.04358600
H	0.75562300	-1.69805700	1.95222700
O	2.78070700	-0.38285200	-1.90052100
H	2.77202200	-0.15160400	-2.85176200
H	-0.21277200	-1.02323600	2.98686600
H	3.50124000	-1.01082000	-1.68872000
O	-2.32453900	-0.97170400	0.84892800
H	-2.45860900	-1.70504600	1.47851900
H	-3.16185800	-0.84948500	0.36301300
O	-1.69339100	1.05501200	-0.73469200
H	-1.52131300	1.05051500	-1.69400000
H	-2.42739600	1.67839700	-0.57662000
O	-0.09536400	1.49806000	1.32810800
H	0.46506400	1.55530200	2.12448800
H	-0.23048000	2.40578700	0.99744800
O	0.40649800	-0.79304700	-0.71729400
H	0.12217700	-1.61083800	-1.15368600
H	1.87443500	-0.55998600	-1.46332800

§S5.2 Cartesian coordinates for the optimized R, TS and P structures for seventeen possible pathways with N_m' = 1

1.*cis*-2 (a)

R

O	1.22887600	0.00000100	-0.82074800
H	2.32699300	0.00000300	-0.43479300
O	0.30944100	-0.00265800	1.78369700
H	0.59911800	0.78020800	2.28442400
O	-0.50695000	1.95028500	0.00366000
H	0.19149700	2.52800100	-0.35157100
O	-2.20517900	0.00003100	0.84065900
H	-2.37608800	-0.00097500	1.79953400
O	-1.39635100	0.00256000	-1.73437500
H	-1.64457900	-0.78024000	-2.25815500
O	-0.50923800	-1.95024400	-0.00108200
H	0.18883700	-2.52794000	-0.35708200
H	-1.21632800	2.52211400	0.34809900
H	0.59748400	-0.78712500	2.28285400
H	1.28930400	0.00027700	-1.78868800
H	-1.21944300	-2.52205400	0.34167700
H	-1.64331500	0.78688000	-2.25647200
H	-3.06816100	0.00119600	0.38916100
Al	-0.43956900	0.00000200	-0.01685500
O	3.51919100	0.00002000	-0.01749700
H	4.08555900	0.78478000	-0.10775700
H	4.08520000	-0.78512400	-0.10663000

TS

O	-1.15443300	0.74093900	-0.00163300
H	-2.64989400	0.67035100	-0.00106400
O	-0.24158900	-2.13705800	0.00231600
H	-0.41346900	-2.68478800	-0.78529700
O	0.38270500	-0.31892400	-1.94342400
H	-0.30921600	0.05755500	-2.51362100
O	2.18050600	-0.42796800	0.00079900
H	2.83498400	-1.14776300	0.00170400
O	1.86985700	2.09294200	-0.00152300
H	2.07913100	2.65409300	0.76401700
O	0.38153500	-0.31388300	1.94382000
H	-0.31041700	0.06464700	2.51261300
H	1.13780800	-0.56081600	-2.50859200
H	-0.41431800	-2.68280100	0.79112100
H	-0.97074800	1.69305600	-0.00369000
H	1.13602800	-0.55510100	2.51008900
H	2.08015900	2.65266000	-0.76783500
H	2.59931600	0.47558900	0.00022000
Al	0.29348000	-0.31704300	0.00018800
O	-3.70121500	0.58276900	-0.00030700
H	-4.17709100	0.86396700	-0.80569300
H	-4.17643800	0.87035400	0.80320900

P

O	1.23558900	-0.42514000	-0.81838500
H	2.27507100	-1.16869900	-0.53800000
O	0.36908100	2.27369700	0.74066400
H	0.22797300	3.12342600	0.28689500
O	-0.49074300	1.51025500	-1.64000600
H	0.08492600	1.94727700	-2.29212300
O	-1.71458900	0.01791300	0.31235900
H	-2.32050200	0.65004600	0.72765900
O	-3.11341000	-2.02179200	-0.11949400
H	-3.47037500	-2.49767300	0.65400600
O	0.60004900	-0.13028900	1.78853200
H	1.50142500	-0.33672600	2.08826800
H	-1.40119100	1.56986700	-1.97583100
H	0.70790100	2.46104300	1.63398200
H	1.17654400	-0.44707100	-1.78478000
H	-0.01424900	-0.45624100	2.46763800
H	-3.77726000	-1.97992600	-0.83341400
H	-2.52739500	-1.14299800	0.06635700
Al	-0.01791900	0.53993400	0.03935000
O	3.18481400	-1.79042200	-0.27130400
H	4.06187600	-1.46105300	-0.54122600
H	3.14188000	-2.75417800	-0.40989600

2.*cis*-2 (b)

R

O	-0.96392000	0.99667700	0.07258300
H	-1.79750700	0.50100300	0.07522200
O	-0.24077200	-1.68527500	-0.00060600
H	-0.54897600	-2.16599300	-0.78970700
O	0.66268600	0.07298300	-1.92754700
H	-0.03436500	0.46107300	-2.48548900
O	2.34141000	-0.90669900	-0.02887200
H	2.45043900	-1.87419900	-0.05313800
O	1.70743200	1.70434500	0.04105600
H	1.97191800	2.20662900	0.83176000
O	0.73174100	-0.01466700	1.97030100
H	0.05431100	0.34653300	2.56898300
H	1.33706100	-0.30686500	-2.51897100
H	-0.51948200	-2.20200300	0.77664300
H	-1.26532200	2.12130300	0.10402500
H	1.42611600	-0.41986200	2.52027500
H	1.94401200	2.24194600	-0.73511900
H	3.23152000	-0.51128200	-0.03488500
Al	0.63991800	0.07222600	0.02328800
O	-1.59448100	3.33950200	0.13805900
H	-2.00082600	3.77421500	-0.63049700
H	-1.97544700	3.73711900	0.93900800

TS

O	-1.02133400	0.91624700	0.07039000
H	-1.89595300	0.49810100	0.08086600
O	-0.32769700	-1.98479100	-0.00830300
H	-0.57206100	-2.49396800	-0.80310100
O	0.46240500	-0.11427300	-1.90834300
H	-0.21881700	0.31272400	-2.45586000
O	2.23024700	-0.61424300	-0.01742500
H	2.75222200	-1.43458300	-0.04655700
O	2.35736600	1.90354100	0.04591800
H	2.66089700	2.40406900	0.82114500
O	0.52401400	-0.20604200	1.95126700
H	-0.13709200	0.19748600	2.53973800
H	1.17917700	-0.41430800	-2.49518300
H	-0.54796600	-2.53027000	0.76925900
H	-1.33993800	2.34569700	0.10249000
H	1.25771600	-0.53556800	2.50013200
H	2.63722500	2.44491900	-0.71056100
H	2.79389100	0.20780500	-0.00532300
Al	0.38305700	-0.21271800	0.02187000
O	-1.56464100	3.38629500	0.12411900
H	-1.99953100	3.76858900	-0.66211500
H	-1.95966500	3.74391900	0.94234100

P

O	-1.27065000	0.86325400	0.02745900
H	-2.13589100	0.45325700	-0.12255000
O	-0.27794000	-2.08172900	-0.01048900
H	-0.40344100	-2.62374300	-0.80977400
O	0.16704600	-0.31997600	-1.95433000
H	-0.55621300	-0.04710700	-2.54329000
O	1.94625300	0.08705800	0.04503800
H	2.52858000	-0.67918100	0.15937200
O	3.50269700	2.02352400	-0.10384900
H	3.99813800	2.27273300	0.69846600
O	0.10982500	-0.37604300	1.99622600
H	-0.66556000	-0.18248000	2.54918400
H	0.95065900	-0.47982000	-2.50645100
H	-0.41850600	-2.64844100	0.76892200
H	-1.56200400	2.22591800	0.16428500
H	0.87364000	-0.48230100	2.58758700
H	4.07567500	2.08896300	-0.89050300
H	2.83202700	1.17227000	-0.03777600
Al	0.16876100	-0.22615800	0.02358100
O	-1.77149600	3.28698700	0.27194200
H	-2.08266300	3.76928500	-0.51656400
H	-2.26654000	3.57365800	1.06193500

3.*trans*-3 (a)

R

O	-0.50741600	1.95032100	0.00938900
H	0.18971400	2.52997400	-0.34536700
O	1.22761300	0.00209600	-0.82458900
H	2.32186300	0.00107600	-0.43790500
O	0.31216600	-0.00376700	1.78090200
H	0.60176800	0.77866100	2.28232100
O	-0.50643400	-1.95007700	0.00226900
H	0.19085900	-2.52795300	-0.35503200
O	-2.20519600	-0.00157200	0.84064700
H	-3.06846900	-0.00116200	0.38967300
O	-1.39710900	0.00248200	-1.73489100
H	-1.64527200	0.78658000	-2.25685400
H	0.60139700	-0.78871000	2.27857200
H	1.28902600	0.00427100	-1.79248300
H	-1.21832300	2.52027900	0.35379500
H	-1.64484700	-0.78054500	-2.25864600
H	-2.37558500	-0.00347300	1.79963400
H	-1.21680700	-2.52180500	0.34482500
Al	-0.44034000	0.00037100	-0.01848300
O	3.51764700	0.00017500	-0.01764500
H	4.08448200	0.78501400	-0.10365700
H	4.08444200	-0.78428700	-0.10725900

TS

O	-0.61362600	0.56447000	1.82676800
H	-0.03829500	0.97830200	2.49606400
O	1.56460000	0.62973600	-0.22159200
H	2.94153600	0.06516900	-0.16577000
O	0.11876800	-1.65905500	0.58834500
H	0.30262500	-1.95789100	1.49560700
O	-0.89636900	-0.55220200	-1.57641700
H	-0.57280000	-0.69167200	-2.48299500
O	-2.94626400	-0.71506700	-0.03462700
H	-3.73319800	-0.15666300	-0.15146600
O	-1.00122500	1.84681900	-0.46174600
H	-1.18297800	2.59300900	0.13622600
H	0.15802300	-2.43627700	0.00442600
H	1.72453400	1.53852300	-0.51687100
H	-1.48404200	0.39535600	2.23273600
H	-1.26843100	2.11776200	-1.35784100
H	-3.30836500	-1.56580500	0.26525700
H	-1.85152300	-0.80546900	-1.46002700
Al	-0.13432500	0.16340500	-0.00323500
O	3.91823900	-0.33509500	-0.12587500
H	4.51729700	0.01438200	0.56194100
H	4.38885300	-0.44983800	-0.97408600

P

O	0.84951300	1.86804100	-0.64677700
H	1.61009700	1.82057300	-1.25134700
O	1.35989800	-0.76828200	-0.42121200
H	2.86040600	-0.93075900	-0.28175800
O	0.06219600	1.08485000	1.76847200
H	0.65062600	1.80829900	2.05044500
O	-1.12657900	-1.11353900	0.85128500
H	-0.82346500	-1.86850300	1.38330300
O	-3.51691000	-0.88539200	-0.37630300
H	-3.84892700	-1.57103000	-0.98339700
O	-1.50810100	0.63041100	-0.99830200
H	-1.54905300	1.25627500	-1.74067200
H	-0.47570200	0.81932100	2.53656800
H	1.12370900	-1.59314500	-0.87197100
H	0.58570600	2.80372100	-0.58256200
H	-2.39622100	0.13950000	-0.91567300
H	-4.31022600	-0.52494900	0.05911900
H	-2.08161800	-1.25475700	0.60281200
Al	-0.01521400	0.25814200	0.05887300
O	3.90421300	-1.00883800	-0.20952700
H	4.39594300	-1.17601900	-1.03766000
H	4.26266300	-1.54237600	0.52635600

4. *trans*-3 (b)

R				TS				P			
O	0.48968000	0.53720800	1.89903900	O	0.64384700	0.47018800	1.83532500	O	-0.48019400	0.94272800	1.94443100
H	-0.26641300	0.94232400	2.35960500	H	0.09052500	0.85239700	2.54099300	H	-1.22975500	1.56270600	1.94048000
O	-1.24417700	0.62928100	-0.21944100	O	-1.56891100	0.64373000	-0.19087900	O	-1.48296400	0.31533700	-0.47880300
H	-1.41786400	1.55062700	-0.46768000	H	-1.72625500	1.56537700	-0.44503200	H	-1.40233800	0.61456500	-1.39715600
O	1.25591000	1.82225500	-0.42424800	O	0.98966100	1.87084400	-0.39119000	O	1.59989000	0.99836500	0.24395500
H	1.40884500	2.55431300	0.19985500	H	1.16773400	2.59360300	0.23597200	H	1.76431500	1.83107200	0.71730200
O	0.65724000	-0.44887900	-1.86992200	O	0.90317300	-0.48264700	-1.59771400	O	0.88090600	-1.09899700	-1.05861800
H	-0.05201200	-0.34116200	-2.52812800	H	0.58603800	-0.58705000	-2.51132300	H	0.43580900	-1.73601500	-1.64254900
O	2.35485800	-0.54985700	0.25026800	O	2.94606200	-0.71196900	-0.04794100	O	3.28168100	0.05500000	-1.48835600
H	2.63425700	-1.44876800	0.50064000	H	3.30612500	-1.57645600	0.21269900	H	4.12466400	-0.34736200	-1.21209200
O	-0.03621000	-1.75958500	0.46046100	O	-0.13593600	-1.68300900	0.50653200	O	0.12411300	-1.59407900	1.44341100
H	-0.30774400	-2.07271500	1.34119300	H	-0.31654900	-2.02155100	1.40036900	H	-0.32203300	-1.73128100	2.29856100
H	1.47493300	2.15343300	-1.31367900	H	1.25530400	2.17924800	-1.27554800	H	2.37883600	0.80040400	-0.38136500
H	-2.28317100	0.12322500	-0.13441500	H	-2.94527800	0.08430100	-0.15360900	H	-2.98843700	0.21503100	-0.33617400
H	1.21070300	0.43749000	2.54625500	H	1.52642500	0.27929100	2.20379000	H	-0.04206400	1.02020500	2.81121100
H	-0.22580600	-2.47531500	-0.17144100	H	-0.18392800	-2.43290100	-0.11143600	H	0.59532500	-2.41621400	1.21578400
H	3.16000700	-0.01249200	0.14197200	H	3.73478400	-0.15179700	-0.14300400	H	3.48421200	0.52770700	-2.31566100
H	1.42643600	-0.83563000	-2.32557900	H	1.85708800	-0.74156900	-1.48458100	H	1.79340400	-0.91505200	-1.41504400
Al	0.50406800	0.05901600	0.00800400	Al	0.12922200	0.16443300	-0.00125300	Al	0.05678000	-0.04722600	0.34127300
O	-3.42262000	-0.42892200	-0.04140300	O	-3.91820200	-0.32765500	-0.12239300	O	-4.02903900	0.17399800	-0.20824600
H	-4.03053800	-0.21453500	0.68599800	H	-4.51367700	-0.01044100	0.58404600	H	-4.53451900	0.98591800	-0.41026400
H	-3.96011300	-0.61524400	-0.82943000	H	-4.39578300	-0.40595200	-0.97096500	H	-4.48969500	-0.61989600	-0.54318900

5. *cis*-4

R				TS				P			
Al	-0.44013500	0.00034100	-0.01826600	Al	-0.45492900	-0.21995800	-0.06149900	Al	0.01939300	0.53911000	0.03914100
O	-0.50861800	1.95005600	0.02060700	O	-0.71066800	0.76512900	1.59767300	O	-0.60287800	-0.12199600	1.79070700
H	0.18850000	2.53205200	-0.33031700	H	0.01897500	1.15359100	2.10981100	H	-1.50571000	-0.32376200	2.08909000
O	-1.39653900	0.01410100	-1.73497300	O	-0.94606300	2.21914500	-1.50787700	O	3.10974500	-2.02525500	-0.11770500
H	-1.64468400	-0.76512700	-2.26416100	H	-0.85391900	2.36036100	-2.46513000	H	3.77943400	-1.98030100	-0.82591800
H	-1.21955400	2.51766600	0.36879700	H	-1.54757600	1.07025600	1.99083400	H	0.00850400	-0.44770400	2.47253800
H	-1.64418200	0.80196600	-2.25145000	H	-0.98807100	3.11796500	-1.14044600	H	3.45886900	-2.50889100	0.65451400
O	0.31128700	-0.01423700	1.78153000	O	-0.66118800	-1.86220700	0.86464900	O	-0.36211700	2.27700100	0.73350100
H	0.59897300	0.76563900	2.28801100	H	-0.77967400	-1.96486100	1.82659600	H	-0.69992700	2.46915200	1.62617800
H	0.60198200	-0.80165400	2.27443400	H	-0.64098200	-2.75211900	0.46770600	H	-0.21973100	3.12432500	0.27568000
O	-0.50608200	-1.94994700	-0.01142600	O	-0.36755300	-1.16417000	-1.76126600	O	0.49636400	1.50104000	-1.64447200
H	0.19181200	-2.52558100	-0.37114400	H	0.46243000	-1.34713800	-2.23383000	H	-0.07786100	1.93637200	-2.29895300
H	-1.21675000	-2.52375400	0.32702400	H	-1.10532400	-1.42090700	-2.34253300	H	1.40757200	1.56029700	-1.97825100
O	-2.20525500	-0.00877300	0.84086800	O	-2.22713500	0.25560300	-0.51568800	O	1.71472200	0.01457500	0.31632000
H	-3.06856800	-0.00430900	0.38995300	H	-2.25922900	1.11727200	-1.01277500	H	2.52497400	-1.14515600	0.07081400
H	-2.37564800	-0.01714200	1.79981900	H	-3.10775200	-0.13611800	-0.38276800	H	2.31998500	0.64485000	0.73540600
O	1.22813300	0.00815500	-0.82363500	O	1.27898400	0.22816400	-0.14039200	O	-1.23548500	-0.42539500	-0.81583100
H	2.32260600	0.00392900	-0.43680400	H	2.63047600	-0.25154600	0.28232500	H	-2.28324300	-1.16776500	-0.53645900
H	1.28959800	0.01459000	-1.79150600	H	1.46542000	1.05742000	-0.60732300	H	-1.17364000	-0.45257300	-1.78189000
O	3.51809400	-0.00002900	-0.01726400	O	3.56851700	-0.61813400	0.59776300	O	-3.19208300	-1.78438100	-0.27004300
H	4.08413500	0.78602300	-0.09715500	H	4.04389500	-0.10922900	1.28270800	H	-3.15026300	-2.74855800	-0.40672000
H	4.08536900	-0.78334300	-0.11369400	H	4.18420900	-0.93343100	-0.09186800	H	-4.06720600	-1.45342800	-0.54467900

6. *cis*-5 (a)

R				TS				P			
O	0.50328300	-0.48209200	1.63934000	O	0.59535200	-0.69053900	1.62656300	O	0.80675600	-1.41403100	1.25966900
H	0.85545300	-1.36728300	1.83905000	H	1.14809400	-1.47577700	1.79063000	H	1.66798200	-1.70966300	0.91303400
O	-0.32174400	-1.77827500	-0.65647700	O	-0.26152400	-2.05073000	-0.78711000	O	-0.62043500	-1.70705700	-0.96233800
H	-0.92920300	-2.52880600	-0.53192500	H	-0.87480300	-2.80463400	-0.70989100	H	-0.28504200	-2.61951600	-0.89882200
O	-2.16719800	-0.52527000	0.93020600	O	-2.00856000	-0.65063800	1.01474800	O	-1.71350800	-0.62025100	1.78251300
H	-2.43633300	-0.96831800	1.97058200	H	-2.45557200	-1.18993000	2.25526300	H	-2.35609900	-1.68254100	2.65396400
O	-1.51601700	0.54860900	-1.54692600	O	-1.39005400	0.59422900	-1.34953500	O	-1.79980900	0.66790200	-0.71742500
H	-1.73237800	-0.02277700	-2.30553200	H	-1.85711400	0.34691800	-2.16589500	H	-2.75825400	0.54367700	-0.82141700
O	-0.75527900	1.81913700	0.78347500	O	-1.08620800	2.50744600	0.30743800	O	-0.39770900	2.88457600	-1.34643700
H	-0.14820300	2.56740100	0.64069600	H	-0.47729700	3.25258700	0.17324000	H	-0.03184600	3.05231200	-2.23350600
O	1.07180600	0.55105600	-0.77579900	O	1.09539900	0.39321400	-0.66677600	O	0.57545600	1.04156400	0.19467600
H	1.96461600	0.50437500	-0.38926800	H	1.95600700	0.46584200	-0.21690100	H	1.43054200	1.14771600	0.64420600
H	-3.00816500	-0.43972200	0.45475400	H	-2.83084800	-0.36972800	0.58682800	H	-2.17211500	0.17599400	2.09083000
H	0.41056300	-2.08187100	-1.22250100	H	0.43456900	-2.29796400	-1.42424300	H	-1.00180400	-1.58891600	-1.85137600
H	0.67462800	0.07887600	2.41609300	H	0.57896900	-0.17073600	2.44981600	H	0.78729800	-1.62408500	2.20927100
H	1.15978500	0.92239500	-1.67190200	H	1.16148800	0.84546100	-1.52707000	H	0.37904900	1.86795300	-0.36671500
H	-1.49309900	2.13863000	1.33245400	H	-1.81235200	2.89156700	0.82526500	H	-0.64356200	3.76212300	-1.00234000
H	-1.90702300	1.42266800	-1.72547300	H	-1.53380600	1.54902900	-1.10023300	H	-1.54051000	1.54238300	-1.11956900
Al	-0.59627500	-0.00164800	0.10057600	Al	-0.52253500	-0.36455000	0.05072500	Al	-0.61714300	-0.38017400	0.39843200
O	-2.73280100	-1.45280100	3.10138400	O	-2.77812500	-1.59330600	3.20248200	O	-2.76303600	-2.42564000	3.27242300
H	-3.20346800	-0.92634400	3.76924800	H	-3.23452100	-0.99073600	3.82016400	H	-2.71373400	-2.27741600	4.23738800
H	-3.02243800	-2.37589500	3.19463800	H	-3.21112200	-2.46819800	3.19959300	H	-3.63115200	-2.79398800	3.01670100

7. *cis*-5 (b)

R				TS				P			
O	1.30883900	-0.56644900	1.71859900	O	1.25791700	-0.69110500	1.73126900	O	1.07604500	-1.65907900	1.37072500
H	1.55889200	-1.48584100	1.92095800	H	1.53101200	-1.56344800	2.07115200	H	2.01464000	-1.85323200	1.54738400
O	0.57051700	-1.72604400	-0.67454600	O	0.62617700	-2.02134200	-0.85208200	O	1.14244700	-1.62451700	-1.28913900
H	-0.12178000	-2.40655300	-0.60097700	H	-0.06189000	-2.71178000	-0.85856000	H	1.49366400	-2.52282200	-1.14924900
O	-1.26925500	-0.26059000	0.72656100	O	-1.22534000	-0.50367800	0.63050200	O	-1.40552200	-0.98418800	0.41977900
H	-1.37708300	-0.62408400	1.61923700	H	-1.30128400	-0.86075600	1.52727000	H	-1.66747000	-1.90629100	0.27760500
O	-0.22781800	0.73980700	-1.63113600	O	-0.05849400	0.86673000	-1.40506700	O	-0.17039000	0.67644600	-1.46953400
H	-0.46949200	0.19923400	-2.40364200	H	-0.51065000	0.76426300	-2.25882200	H	-0.93062000	0.58595100	-2.06799500
O	0.43393100	1.88318800	0.79331400	O	0.33054400	2.63321400	0.38186700	O	1.22070000	2.94406700	-0.91501500
H	1.13939100	2.55195900	0.73068800	H	1.05932300	3.27478800	0.33985300	H	2.03629600	3.19954500	-1.38231200
O	2.23797200	0.41963000	-0.61656400	O	2.24545900	0.16882700	-0.50540200	O	1.18690700	0.92742200	0.69828600
H	3.07864700	0.26263600	-0.15046500	H	3.04975800	0.04409600	0.02903200	H	1.62528600	0.96237100	1.56472000
H	-2.34390500	-0.13401800	0.30382700	H	-2.57536400	-0.28039800	0.25416900	H	-2.66479200	-0.37190500	0.97582000
H	1.31551200	-2.11474800	-1.16724300	H	1.38348900	-2.34678400	-1.37373700	H	1.26613800	-1.39810500	-2.22905000
H	1.50396100	-0.03507900	2.51126800	H	1.35158500	-0.05500000	2.46446100	H	0.55580600	-2.10660700	2.06109800
H	2.45319600	0.78155700	-1.49481400	H	2.49212000	0.63614900	-1.32364200	H	1.30264800	1.81919400	0.21450600
H	-0.29980400	2.27464700	1.29955400	H	-0.37054900	3.10625700	0.85879900	H	0.77601400	3.78414800	-0.70307500
H	-0.51767400	1.65085500	-1.81420600	H	-0.08151900	1.80910600	-1.06498400	H	0.21834400	1.58537300	-1.57036300
Al	0.43428800	0.06830700	0.07706100	Al	0.43760200	-0.32431900	-0.02660000	Al	0.25800900	-0.52003600	-0.01700900
O	-3.51512700	0.00213300	-0.15735400	O	-3.59973500	-0.10901800	-0.04643100	O	-3.53888700	0.07707200	1.34919700
H	-4.11538300	0.68676800	0.18286600	H	-4.12042300	0.53901900	0.46469400	H	-3.74696800	-0.06913200	2.29240100
H	-4.05448900	-0.76873700	-0.40135000	H	-4.14666300	-0.88839800	-0.26113400	H	-4.34294700	0.00919500	0.79823000

8. *cis*-6 (a)

R				TS				P			
O	0.30842400	0.01236600	1.78181800	O	0.40072800	-0.80919500	1.66559000	O	0.84518500	1.87306800	-0.64143400
H	0.59731900	-0.76785100	2.28699900	H	0.63368200	-1.70379200	1.97311500	H	0.57533200	2.80705300	-0.57714600
O	-0.50221000	-1.95026700	0.02052100	O	-0.27419000	-2.06293500	-0.87239200	O	0.06480600	1.07819700	1.77062700
H	-1.21268900	-2.52023700	0.36567600	H	-0.95922700	-2.75700700	-0.84859300	H	-0.46755400	0.80554000	2.54007300
O	-2.20686200	0.00173200	0.83635800	O	-2.02839900	-0.66737400	0.79315700	O	-1.51014400	0.62850300	-0.99567900
H	-2.37819400	0.00800200	1.79513800	H	-2.16228400	-0.93903100	1.71864400	H	-1.55342700	1.25471200	-1.73758500
O	-1.39463600	-0.01271400	-1.73742600	O	-1.39408300	0.60481800	-1.36618200	O	-1.12168900	-1.11807600	0.85153600
H	-1.63788900	-0.80016800	-2.25660800	H	-1.63989500	0.45669800	-2.29536000	H	-0.81355500	-1.87674300	1.37533900
O	-0.51014600	1.95050900	-0.00364900	O	-1.25260600	2.41602300	0.42197200	O	-3.51746300	-0.88245300	-0.37674000
H	0.18707700	2.52897600	-0.36007000	H	-0.70165100	3.21138200	0.33932800	H	-3.85135900	-1.56606100	-0.98511000
O	1.22865100	-0.00180600	-0.82230100	O	1.22537800	0.36727800	-0.59153000	O	1.36004400	-0.76528800	-0.42745100
H	2.32721800	-0.00076200	-0.43505800	H	2.60194000	0.41267500	-0.23308400	H	2.85986300	-0.92898500	-0.28532700
H	-3.06969000	-0.00364800	0.38458700	H	-2.90198200	-0.50757700	0.39271800	H	-2.39826600	0.13582200	-0.91063900
H	0.19670100	-2.52984600	-0.33074200	H	0.44438900	-2.37416500	-1.45313200	H	0.64907700	1.80497600	2.05270300
H	0.59452300	0.79951600	2.27773700	H	0.74503400	-0.17819800	2.32252400	H	1.60718300	1.83095200	-1.24465800
H	1.28992500	-0.00367000	-1.79015100	H	1.18747300	0.91224300	-1.39142300	H	1.12494700	-1.58477200	-0.88848600
H	-1.22381000	2.52142500	0.33331000	H	-2.00711500	2.71072800	0.95857200	H	-4.30981800	-0.52092300	0.05956200
H	-1.64571500	0.76690200	-2.26466600	H	-1.59570100	1.53219600	-1.05919200	H	-2.07721000	-1.25987500	0.60773400
Al	-0.44016700	0.00010500	-0.01963500	Al	-0.34553300	-0.33585500	-0.08282200	Al	-0.01528600	0.25832400	0.05796900
O	3.51798800	-0.00001500	-0.01720600	O	3.64169900	0.44553200	0.05514600	O	3.90364300	-1.00727700	-0.21088400
H	4.08297700	0.78586500	-0.10654300	H	4.02377500	1.31600400	0.27680500	H	4.39808700	-1.16398100	-1.03943400
H	4.08475400	-0.78430600	-0.10927500	H	4.27528000	-0.07921200	-0.47032100	H	4.26037000	-1.54932200	0.51958600

9. *cis*-6 (b)

R				TS				P			
O	0.36313600	-0.53697400	1.62610100	O	0.46876200	-0.65739800	1.57353000	O	0.76025400	-1.43769100	1.03938700
H	0.78238200	-1.40504400	1.76545700	H	0.90986400	-1.48878000	1.82881300	H	0.43507300	-1.98686400	1.77596300
O	-0.32359300	-1.71684900	-0.77252900	O	-0.34302500	-2.03646900	-0.90542100	O	-1.09383600	-2.01837600	-0.77994900
H	-0.90654600	-2.49096500	-0.67403700	H	-0.98432600	-2.76537900	-0.81016700	H	-1.90401300	-2.08367200	-1.31787400
O	-2.21235200	-0.58951000	0.82016100	O	-2.02324000	-0.75918400	0.87200000	O	-0.96152500	0.60643500	1.10633100
H	-2.29805600	-1.00566900	1.69657100	H	-2.05745600	-1.09917200	1.78377200	H	-0.63899400	0.63092500	2.02257000
O	-1.64859500	0.58154200	-1.53439300	O	-1.64878200	0.64241700	-1.25035300	O	-1.53728100	0.52750600	-1.39714800
H	-1.79157300	0.05511300	-2.34053600	H	-1.93056200	0.55556200	-2.17596800	H	-1.46689500	0.65967600	-2.35727400
O	-0.89672400	1.78921800	0.83382200	O	-1.46696700	2.40227900	0.57672000	O	-3.01212300	1.98676700	0.35685700
H	-0.31339600	2.56466600	0.75465700	H	-0.95751900	3.22618000	0.51180600	H	-3.00588400	2.96058700	0.35002700
O	1.00980200	0.67680200	-0.78627900	O	1.03029700	0.43763400	-0.85224100	O	1.21715200	0.04752800	-1.22001300
H	1.84644700	0.59707800	-0.30224600	H	1.84986100	0.34074900	-0.34584700	H	1.69806200	-0.66861900	-1.66158000
H	-3.10147800	-0.55614600	0.42383100	H	-2.93673000	-0.63541600	0.55743000	H	-1.77035500	1.22136100	1.00631000
H	0.42985100	-1.98388700	-1.32824000	H	0.35681600	-2.33141900	-1.51660100	H	-0.78224900	-2.92369400	-0.59782300
H	0.54975000	0.00175900	2.41586300	H	0.66491900	-0.00349300	2.26985900	H	1.73253300	-1.44178000	1.08623700
H	1.27805300	1.17866500	-1.79858700	H	1.44073200	1.16716500	-2.00031800	H	2.02909200	1.26141600	-1.59309400
H	-1.64616600	2.04034100	1.40315100	H	-2.20491000	2.62962000	1.16676400	H	-3.91258900	1.74079100	0.63522400
H	-2.02832900	1.46345500	-1.69415800	H	-1.83879700	1.54936300	-0.87104200	H	-2.25187700	1.11670600	-1.03702800
Al	-0.55412400	0.06280600	-0.00559300	Al	-0.44444400	-0.30198600	-0.14277700	Al	-0.24295400	-0.38683200	-0.29611300
O	1.57348200	1.72682500	-2.90126200	O	1.74097300	1.71969000	-2.87906600	O	2.57223800	2.12193900	-1.85605500
H	1.83274200	2.66244100	-2.94680800	H	2.09098300	2.62150400	-2.75021300	H	3.39926600	2.29394800	-1.36534200
H	2.07057600	1.24888000	-3.58621200	H	2.26206900	1.24804500	-3.55633100	H	2.68698700	2.30010600	-2.80989000

10. *cis*-2//*trans*-3

R				TS				P			
O	-0.96741000	0.00005300	-1.27806400	O	1.00202300	-0.00012800	-1.33333600	O	1.76422800	0.80694500	0.59480500
H	-1.94386900	0.00003900	-1.02444100	H	2.00118300	-0.00016800	-1.17327600	H	2.56995200	0.21540600	0.48303300
O	-0.95140000	-0.00032800	1.33602300	O	1.26120900	0.00007300	1.32591500	O	0.87448700	-1.26439700	-0.60073000
H	-1.91838500	-0.00018200	1.06727400	H	2.20691800	0.00014500	0.97336400	H	1.85872300	-1.45598700	-0.49579900
O	0.55912800	-1.95212100	-0.05520300	O	-0.49576400	1.85557700	-0.16453800	O	-0.61182400	0.51453000	1.73150200
H	-0.02477400	-2.53732600	-0.56948200	H	-0.05093600	2.41247700	-0.82901600	H	-0.06400000	0.55187000	2.53614900
O	1.83245100	-0.00003800	1.37839800	O	-1.64288000	-0.00010900	1.33617000	O	-1.63153100	-0.16554900	-0.64852100
H	1.76367300	-0.00006000	2.35057400	H	-1.78242700	-0.00010900	2.30013200	H	-1.73665300	-0.20780300	-1.61106200
O	1.81779800	0.00031400	-1.36085900	O	-2.85889200	0.00002600	-0.88406200	O	-3.89622100	-0.90964500	0.15845300
H	2.20515900	0.78733100	-1.78516500	H	-3.33875200	-0.76441200	-1.24616800	H	-4.66494200	-0.37174600	-0.11455900
O	0.55872200	1.95215000	-0.05467000	O	-0.49588400	-1.85545100	-0.16444800	O	0.05952800	1.88659200	-1.11656400
H	-0.02519100	2.53737100	-0.56891400	H	-0.05098200	-2.41248700	-0.82875900	H	0.84088800	2.41246400	-1.36645200
H	1.06661000	-2.52015900	0.55167400	H	-1.05810500	2.43594100	0.38086300	H	-1.54351900	0.58328600	2.00383100
H	-0.91494600	-0.00088100	2.30648400	H	1.28232900	0.00013600	2.29940900	H	0.42816900	-2.02756800	-1.00410200
H	-0.88410800	0.00013700	-2.24689000	H	0.82065500	-0.00048900	-2.29054100	H	2.03807100	1.63072800	1.03289000
H	1.06597600	2.52012400	0.55245700	H	-1.05833900	-2.43569800	0.38095700	H	-0.71997900	2.30024700	-1.52978000
H	2.20529200	-0.78650100	-1.78541600	H	-3.33881200	0.76461300	-1.24577500	H	-4.11649100	-1.86095500	0.13296300
H	2.78497900	0.00004900	1.16894600	H	-2.50424000	-0.00024100	0.82396200	H	-2.93362000	-0.61419900	-0.20635400
Al	0.43525800	-0.00001000	0.01360500	Al	-0.18573900	0.00007100	0.15087600	Al	0.01158900	0.30322000	-0.04974400
O	-3.26434800	-0.00000700	0.00729900	O	3.39410500	-0.00005200	-0.23285400	O	3.43408100	-1.15654400	-0.01565300
H	-3.85913300	0.77192500	0.01140900	H	3.98738500	-0.77253300	-0.28454200	H	4.11871900	-1.06036200	-0.70208700
H	-3.85916400	-0.77191600	0.01123600	H	3.98739500	0.77240500	-0.28478600	H	3.83204200	-1.73270100	0.66166400

11. *cis*-2//*cis*-5

R				TS				P			
O	0.90250500	0.10334500	1.37734200	O	0.82955700	0.09444100	1.37593100	O	0.96636000	-0.11301600	1.46952600
H	1.78233900	0.51520200	1.38420800	H	1.65073100	0.61230300	1.32147400	H	1.88169500	0.19998400	1.37807700
O	-0.30963600	-1.83326800	-0.28517400	O	-0.29208100	-2.15165600	-0.36766000	O	-0.49738700	-2.25441500	-0.46253600
H	-0.79604800	-2.52564500	0.19596800	H	-0.76545800	-2.85804700	0.11082600	H	-1.05229400	-2.90245600	0.00876700
O	-1.70228600	-0.20995700	1.43248600	O	-1.65511100	-0.57464200	1.40480300	O	-1.51753600	-0.77213100	1.49071600
H	-1.41530600	-0.34961400	2.38916400	H	-1.40649700	-0.58978700	2.37433600	H	-1.28536200	-0.80647600	2.45613100
O	-1.84643500	0.08766300	-1.33903900	O	-1.68643900	0.30357400	-1.18154200	O	-1.14842100	0.79098500	-0.80404200
H	-2.16910300	-0.69219200	-1.82616300	H	-2.27060300	-0.12784200	-1.83130200	H	-1.45756300	0.57022800	-1.69555000
O	-0.73191600	2.02696700	0.11079900	O	-1.06344300	2.45885000	-0.05901200	O	-2.03343300	3.16776100	-0.46648400
H	-0.25042200	2.71182100	-0.38708400	H	-0.56844100	3.17598300	-0.49086700	H	-1.53921000	3.90033400	-0.88300000
O	0.88227800	0.37201000	-1.37430500	O	0.97235600	0.09640700	-1.29478000	O	1.28827800	-0.41227200	-1.16902400
H	1.85480700	0.37171500	-1.30921400	H	1.93833300	-0.02967100	-1.23928700	H	2.08656200	-0.97040800	-1.20285800
H	-2.66953800	-0.28769700	1.36893800	H	-2.62287900	-0.63023100	1.31669700	H	-2.48249100	-0.70858500	1.39556900
H	0.37484900	-2.28153400	-0.81345400	H	0.25354600	-2.57924600	-1.05457100	H	-0.16472900	-2.67992600	-1.27381200
H	0.68810200	-0.17053800	2.31788500	H	0.60691200	-0.06479200	2.35911900	H	0.73715800	-0.23122900	2.45756400
H	0.66715300	0.49172900	-2.31797200	H	0.78079500	0.43772700	-2.18831100	H	1.37468900	0.25440500	-1.87310400
H	-1.25388800	2.48523600	0.79335200	H	-1.63120600	2.92037000	0.58106000	H	-2.99741700	3.29847600	-0.55818000
H	-2.38078000	0.85302200	-1.61870600	H	-1.85282300	1.28454100	-1.09182800	H	-1.66698100	2.19474900	-0.61949200
Al	-0.45312300	0.09249400	0.02216200	Al	-0.38692600	-0.29878700	0.01851300	Al	-0.23322700	-0.45178200	0.08577700
O	-0.33139700	-0.52247400	3.66390300	O	-0.24558800	-0.42456900	3.67774600	O	-0.07306500	-0.58447900	3.78600400
H	-0.36704300	0.12821500	4.38848400	H	-0.39778800	0.27896800	4.33533100	H	-0.22897600	0.12207900	4.43781800
H	-0.24701300	-1.38451500	4.11012400	H	0.00684700	-1.20751000	4.20110900	H	0.20191200	-1.35769500	4.31073000

12. *cis*-2//*cis*-6

R

O	-0.93934700	-0.23388900	1.32351800
H	-1.90552500	-0.12669000	1.07795600
O	0.40694500	1.94672100	0.13256300
H	0.82556900	2.48431700	0.82846000
O	1.81365600	-0.02813100	1.39034800
H	1.71834900	-0.03516900	2.36026200
O	1.83161400	0.21866300	-1.33437900
H	2.18976400	1.06684500	-1.65358300
O	0.68913900	-1.92802800	-0.24222600
H	0.11042700	-2.50514400	-0.77178500
O	-0.96130500	0.03936000	-1.28997200
H	-1.93689600	0.02524800	-1.03314700
H	2.76995900	0.01884200	1.20537700
H	-0.16423400	2.54329000	-0.38253900
H	-0.90299800	-0.62883200	2.21033700
H	-0.88039900	0.11037400	-2.25646700
H	1.28460200	-2.50946500	0.26379900
H	2.25219100	-0.49273100	-1.85072700
Al	0.43546600	-0.00432600	0.00643900
O	-3.25567200	-0.00296800	0.00712300
H	-3.86287300	-0.76343700	-0.04525200
H	-3.83923100	0.77496200	0.06780300

TS

O	0.92519200	0.00096500	1.27795300
H	1.90780900	0.13833900	1.03821100
O	-0.32428100	-2.18261900	-0.45745700
H	-0.87640200	-2.88736800	-0.06905300
O	-1.67149400	-0.64054700	1.36413800
H	-1.54746800	-1.01244600	2.25767600
O	-1.72560100	0.31250100	-1.12774600
H	-2.28891200	-0.07598800	-1.82149800
O	-1.08355200	2.40890200	0.09177200
H	-0.58939800	3.14112200	-0.31405300
O	0.98896100	0.06816200	-1.29329100
H	1.94740900	0.20811500	-1.04083100
H	-2.62584100	-0.46889600	1.25749200
H	0.28122100	-2.60443500	-1.09578900
H	0.79524000	0.24031800	2.21138800
H	0.87099800	0.26069600	-2.24009300
H	-1.63941700	2.84509300	0.76000800
H	-1.86439800	1.29505300	-1.01133700
Al	-0.36460400	-0.33816200	-0.02481900
O	3.23235500	0.34078100	0.14512600
H	3.70607800	1.19056900	0.20814600
H	3.93029500	-0.33922200	0.17841100

P

O	1.06790400	-0.20233700	1.35312700
H	2.04651600	-0.02634700	1.12072200
O	-0.39420000	-2.24452800	-0.68492500
H	-1.07031800	-2.92042100	-0.49542200
O	-1.41969900	-1.17135400	1.52430600
H	-1.29118100	-1.91542800	2.14052200
O	-1.44077100	0.70068000	-0.47810600
H	-2.26551800	0.37438400	-0.86855100
O	-1.69992000	3.24204200	-0.63607600
H	-1.84813500	3.61773200	-1.52580500
O	1.12894500	-0.13622500	-1.21574400
H	2.08687600	-0.01437400	-0.98195500
H	-2.25439400	-0.73545700	1.77088000
H	0.18357700	-2.58915400	-1.39019900
H	0.94836400	-0.17901200	2.31715000
H	0.97986600	0.17142100	-2.12534100
H	-2.26275600	3.68361600	0.02916500
H	-1.60813000	2.19757200	-0.56831500
Al	-0.25496300	-0.50708500	0.07782600
O	3.38400000	0.16526500	0.27097300
H	3.85277900	1.01702100	0.32692300
H	4.08073300	-0.51254400	0.33381400

13. *trans*-3//*cis*-4

R

Al	-0.44046700	0.00028500	-0.01838800
O	0.31219100	-0.00464300	1.78087800
H	0.60229300	0.77768800	2.28216600
O	-2.20520300	-0.00411700	0.84105900
H	-3.06871900	-0.00440400	0.39052000
H	0.60182400	-0.78964500	2.27823600
H	-2.37518900	-0.00664600	1.80013400
O	1.22764500	0.00458500	-0.82457000
H	2.32143100	0.00234600	-0.43785200
H	1.28915700	0.00878400	-1.79245800
O	-1.39690200	0.00340600	-1.73500700
H	-1.64575000	0.78800800	-2.25588400
H	-1.64362200	-0.77912500	-2.25997900
O	-0.50474400	-1.94997000	0.00014400
H	0.19296000	-2.52680600	-0.35803000
H	-1.21441900	-2.52261400	0.34259400
O	-0.50955000	1.95019000	0.01073000
H	0.18737100	2.53070600	-0.34302200
H	-1.22055600	2.51928600	0.35634400
O	3.51782600	0.00012500	-0.01737100
H	4.08408100	0.78570100	-0.10025100
H	4.08509000	-0.78358900	-0.11036700

TS

Al	-0.36727000	-0.37235000	-0.07376600
O	0.74560000	-1.27078100	1.22840700
H	1.28212500	-2.06384400	1.05607500
O	2.22581000	0.85773500	-0.77268400
H	2.38200200	1.60037600	-1.38019100
H	0.81353400	-1.06536400	2.17673400
H	3.07940300	0.74434200	-0.32161800
O	-1.87798900	-1.26442800	0.19268600
H	-2.43696700	-2.40211200	0.96940900
H	-2.63255500	-0.99326300	-0.35122500
O	-0.98042800	0.88192700	-1.43692000
H	-0.96482400	0.72489900	-2.39759600
H	-1.41489100	1.74019100	-1.28844000
O	-0.32631600	1.14590200	1.11933200
H	-1.01869600	1.41452800	1.75075700
H	0.40396600	1.79050300	1.16814900
O	0.72914900	-1.14191100	-1.40450600
H	0.63616700	-1.90429000	-2.00145100
H	1.57163300	-0.63381200	-1.55122500
O	-2.82118500	-3.21243000	1.52857500
H	-3.04911400	-4.02463400	1.03595900
H	-3.50315900	-3.00810700	2.19747200

P

Al	0.01527500	0.25837400	0.05907000
O	-0.06327000	1.08619300	1.76797200
H	0.47454700	0.82132000	2.53635900
O	3.51679000	-0.88563200	-0.37686300
H	3.84851000	-1.57170900	-0.98361300
H	-0.65220700	1.80944000	2.04942800
H	4.31036200	-0.52459900	0.05760600
O	-1.35932900	-0.76878000	-0.42085300
H	-2.85985900	-0.93180800	-0.28219300
H	-1.12283200	-1.59346500	-0.87178400
O	1.50782300	0.62892800	-0.99892000
H	2.39594900	0.13784500	-0.91594600
H	1.54878100	1.25447000	-1.74155300
O	-0.84921800	1.86790700	-0.64796200
H	-1.60991300	1.82033700	-1.25237100
H	-0.58533600	2.80360600	-0.58405400
O	1.12672100	-1.11208900	0.85402900
H	0.82316600	-1.86658100	1.38648400
H	2.08146100	-1.25429100	0.60545600
O	-3.90370700	-1.00949700	-0.20978800
H	-4.26202500	-1.54413900	0.52537200
H	-4.39566100	-1.17553500	-1.03802700

14. *trans*-3//*cis*-5

R

O	-0.40324400	1.94564000	0.14426500
H	0.16836200	2.54333500	-0.36899800
O	0.95958800	0.04220900	-1.28849900
H	1.93509500	0.02549500	-1.03347600
O	0.94027800	-0.24087900	1.32082200
H	1.90568100	-0.12811300	1.07417600
O	-0.69390400	-1.92687500	-0.24930000
H	-0.11508000	-2.50125800	-0.78173000
O	-1.81751100	-0.03285600	1.38989900
H	-2.77391900	0.01633700	1.20574300
O	-1.82323300	0.22946700	-1.34072600
H	-2.17980500	1.08040500	-1.65425600
H	0.90751500	-0.64897100	2.20186500
H	0.87731600	0.11947600	-2.25434300
H	-0.81998500	2.48103200	0.84297800
H	-2.24723900	-0.47794900	-1.85972300
H	-1.72141900	-0.04347200	2.35977000
H	-1.29059200	-2.51074100	0.25249200
Al	-0.43810900	-0.00519100	0.00920700
O	3.25628900	-0.00404300	0.00750200
H	3.83899700	0.77438900	0.06951500
H	3.86431200	-0.76378900	-0.04542400

TS

O	-0.87464600	-0.26837800	1.60789900
H	-0.40961300	-0.39278300	2.45669700
O	1.36838900	1.17852500	0.01450200
H	2.31399500	0.78424400	0.04385500
O	1.00090700	-1.36756200	-0.08459100
H	1.99436100	-1.27214900	-0.04041400
O	-0.70238300	-0.13756600	-1.88020200
H	-0.16386500	-0.18741500	-2.69229000
O	-2.64654100	-1.12561100	-0.28580600
H	-3.52325800	-0.70403300	-0.31557800
O	-1.29624900	1.71851600	-0.08709900
H	-1.64566400	2.17241400	0.70218300
H	0.77940100	-2.31410400	-0.12306200
H	1.41365300	2.15030100	0.04970000
H	-1.77209100	-0.65626700	1.66132500
H	-1.57739800	2.22647800	-0.87070700
H	-2.84943700	-2.07683400	-0.32553600
H	-1.58311500	-0.53871000	-2.03529400
Al	-0.16996900	0.14902100	-0.09376600
O	3.47440500	-0.30158600	0.05760000
H	4.03085400	-0.37955700	0.85451000
H	4.09967500	-0.32644700	-0.69018200

P

O	-1.49054600	0.30093000	1.19233500
H	-1.55777100	0.65231300	2.09813400
O	1.48981700	0.29759700	-1.19344800
H	2.36612800	-0.12257900	-0.93994200
O	1.09738100	-0.59498900	1.19911300
H	2.07103900	-0.82242900	0.99418100
O	-1.09638100	-0.60001000	-1.19755300
H	-0.84302900	-0.98805200	-2.05340400
O	-3.43781300	-0.93135500	-0.14437800
H	-4.22389300	-0.45520400	-0.47081500
O	-0.00065900	2.18184300	-0.00277400
H	-0.72708200	2.75894800	0.30044100
H	0.84543900	-0.97926200	2.05706100
H	1.55663200	0.64594100	-2.10042600
H	-2.36680300	-0.12086100	0.94046100
H	0.72429400	2.75897000	-0.30930000
H	-3.76122500	-1.81807700	0.10089700
H	-2.07005500	-0.82663700	-0.99271900
Al	-0.00025900	0.29230700	-0.00023900
O	3.43856300	-0.93057400	0.14695000
H	4.22400400	-0.45297800	0.47261000
H	3.76279900	-1.81763300	-0.09601500

15. *trans*-3//*cis*-6

R

O	-0.65287200	-0.20938900	1.87395400
H	-0.06655800	0.22839900	2.51662100
O	1.03970800	1.04534800	0.06449400
H	1.95122500	0.71122800	0.12058900
O	0.38418400	-1.65973900	-0.10768400
H	0.66978000	-2.17907100	0.66579600
O	-0.43301800	0.03282100	-2.01555600
H	0.28016600	0.44102100	-2.53721000
O	-2.25900000	-0.93509900	-0.23248200
H	-3.16041100	-0.58998400	-0.36817000
O	-1.49622100	1.71564500	-0.00945100
H	-2.40030900	1.92650800	0.27689100
H	0.70938400	-2.11477000	-0.90566400
H	1.05061900	2.05371900	0.04945600
H	-1.37061300	-0.62764400	2.38254300
H	-0.99303100	2.57952200	-0.08710900
H	-2.32822300	-1.90776300	-0.24629100
H	-1.13543700	-0.21867500	-2.64152100
Al	-0.57346500	0.03602000	-0.06521700
O	0.39829100	3.60064700	-0.05916000
H	0.50606600	4.19812700	0.70314200
H	0.59646800	4.15404700	-0.83622800

TS

O	-0.96446900	-0.22074500	1.63811300
H	-0.87768300	0.25186500	2.48742500
O	1.25343900	1.23926200	0.02734300
H	2.15887700	0.88260700	0.05126400
O	0.65473900	-1.41296100	-0.08100600
H	0.93517600	-1.92047100	0.70311200
O	-0.81598500	-0.10274800	-1.85167200
H	-0.65261800	0.41394700	-2.66300500
O	-2.48994200	-1.48560900	-0.24634500
H	-3.44182500	-1.28385200	-0.27478000
O	-1.22196800	1.94706400	-0.04490500
H	-2.17676200	2.13144800	-0.07474300
H	0.99404300	-1.87441800	-0.87032300
H	1.28103000	2.26433000	0.06215500
H	-1.68334800	-0.88262400	1.69941900
H	-0.72931800	2.81409800	0.00100900
H	-2.46182500	-2.45788500	-0.27891100
H	-1.54127700	-0.74490800	-2.00113300
Al	-0.31584300	0.25785800	-0.06965400
O	0.77557000	3.76413700	0.09076000
H	0.94366600	4.29777100	0.88934200
H	1.00457900	4.34807700	-0.65578200

P

O	-1.51169100	-0.58573000	1.07809100
H	-1.65204600	-0.63465600	2.04051700
O	1.17389300	1.27923700	-0.89166200
H	1.80751600	0.93894000	-1.54835500
O	1.16293100	-0.70171200	0.91593000
H	1.02207200	-1.53655200	1.40162700
O	-0.99469900	-0.29734200	-1.43692100
H	-0.79028500	-0.06469300	-2.35959800
O	-3.02837100	-1.75707200	-0.76784000
H	-3.94140700	-1.46985900	-0.95471800
O	-0.60452900	1.98831000	0.84142500
H	-1.35481200	2.18915500	1.42790100
H	2.11962600	-0.50916900	0.93465900
H	1.30192000	2.27073400	-0.79999700
H	-2.23494300	-1.10837900	0.61554200
H	-0.10625900	2.85060200	0.61384600
H	-3.03516200	-2.72407100	-0.89472600
H	-1.81267300	-0.90581200	-1.40957300
Al	-0.17302300	0.35033100	0.09250700
O	0.95120400	3.82073700	-0.10965600
H	1.63111700	4.25577800	0.43763800
H	0.60931700	4.52151200	-0.69546000

16. *cis*-4//*cis*-5

R				TS				P			
Al	-0.44028700	-0.00018100	-0.01816300	Al	-0.48515500	-0.33595100	0.40175300	Al	0.02472800	0.23026600	0.10498400
O	-2.20516500	0.00302200	0.84102000	O	0.60493300	-0.70817100	1.99302400	O	-0.46312400	0.89999500	1.82046700
H	-2.37530100	0.00892900	1.80003400	H	1.03860000	-1.55587900	2.19719000	H	-0.33271500	0.43449500	2.66527000
O	-0.50979000	1.95019800	-0.00766000	O	2.16820100	0.26666200	-0.71457600	O	3.85957300	-0.70950000	-0.54261200
H	0.18810900	2.52744000	-0.36482200	H	2.35869800	0.59555000	-1.60963600	H	4.13159400	-1.20581800	-1.33670300
H	-3.06857400	-0.00111600	0.39031500	H	0.83773700	-0.07718600	2.69712000	H	-0.89385500	1.75284500	2.00574300
H	-1.22150600	2.52253000	0.33110300	H	3.04078300	0.25064400	-0.28477000	H	4.62315200	-0.22254500	-0.18031700
O	-0.50473900	-1.95009600	0.01718000	O	-1.98057100	-0.83634600	1.45210700	O	-0.53051800	2.02566600	-0.56167900
H	0.19318900	-2.53015000	-0.33533500	H	-2.89900200	-0.81571700	1.12720800	H	-1.23779000	2.13478200	-1.21928400
H	-1.21434000	-2.51969200	0.36486000	H	-1.98853800	-1.14593100	2.37677200	H	-0.11476500	2.89733800	-0.43930100
O	1.22776400	-0.00297900	-0.82412800	O	-1.48425600	-0.00340700	-1.06768700	O	-1.34030800	-0.58506100	-0.73369000
H	2.32132100	-0.00197700	-0.43777800	H	-1.96855500	-0.65158600	-2.22472900	H	-2.75828300	-0.77045100	-0.60928200
H	1.28926200	-0.00639700	-1.79203000	H	-1.77902400	0.90971500	-1.19796600	H	-1.11148200	-1.08553500	-1.53197900
O	-1.39684300	-0.01224500	-1.73475400	O	0.03446300	1.48722300	0.69966900	O	1.68249600	0.42296700	-0.56654300
H	-1.64313200	-0.79942500	-2.25292500	H	-0.46464300	2.26312700	1.01433200	H	1.81082700	1.16920500	-1.17014300
H	-1.64674100	0.76769000	-2.26209200	H	0.89846400	1.77329800	0.33965500	H	2.87211300	-0.18793900	-0.56652400
O	0.31184300	0.01254000	1.78131500	O	0.48014300	-1.78020800	-0.35814500	O	0.58018500	-1.39940700	1.07312200
H	0.60392200	-0.76729900	2.28532600	H	0.20983200	-2.65298200	-0.69257700	H	0.05553700	-2.21742900	1.07783800
H	0.59883600	0.80002200	2.27630100	H	1.35005300	-1.50703700	-0.73452100	H	1.44581800	-1.60727200	1.46331200
O	3.51807400	-0.00019600	-0.01743700	O	-2.32881400	-1.16597400	-3.10851200	O	-3.82174700	-0.87938200	-0.50546800
H	4.08527700	-0.78474800	-0.10339500	H	-3.28249200	-1.36679200	-3.16213800	H	-4.38352400	-0.56322200	-1.23825400
H	4.08425000	0.78460200	-0.10773400	H	-1.99764900	-0.86523900	-3.97582400	H	-4.16054700	-1.72414000	-0.15393600

17. *cis*-4//*cis*-6

R				TS				P			
O	0.83579600	-0.02733600	1.27784600	O	0.63716200	0.27584900	1.16774800	O	0.16515200	0.48832800	1.20293600
H	1.18474900	0.75867900	1.73523000	H	0.46298900	1.19871600	1.44779500	H	-0.15862700	1.34722900	1.64310600
O	-0.41152200	-1.98583200	-0.21635800	O	-0.37128500	-2.33273800	-0.32663400	O	0.46268200	-1.86679900	-0.05403800
H	-0.79212500	-2.70349300	0.32116500	H	-0.76212900	-3.04189300	0.21670300	H	0.47162600	-2.49879600	0.68743000
O	-1.81593900	-0.45888500	1.53806000	O	-1.68989000	-0.87285000	1.44107700	O	-2.14345900	-1.34419500	-0.07119200
H	-1.53365900	-0.55367400	2.46538400	H	-1.38268800	-0.97547600	2.35935500	H	-2.20354700	-2.31174500	-0.16816500
O	-2.27287900	-0.14316300	-1.09259300	O	-2.18481800	0.24442100	-0.84114900	O	-1.78462200	1.28642600	-0.26950300
H	-2.59296200	-0.91981100	-1.58431100	H	-2.72620300	-0.00592000	-1.61011000	H	-2.34537400	1.61426900	-0.99267000
O	-0.97508500	1.83107100	0.33843500	O	-1.24070600	2.27543900	0.68470800	O	-1.04368800	2.66488800	1.92629300
H	-0.58626100	2.55549200	-0.18294600	H	-0.93387200	3.09557700	0.26171000	H	-0.61085700	3.53537300	1.86456000
O	0.42971100	0.30713800	-1.45213200	O	0.44038900	-0.07703600	-1.56865200	O	-0.00586200	-0.05312900	-1.99048000
H	1.38232700	0.42837600	-1.31601300	H	1.37761900	0.10499500	-1.40694400	H	0.26425500	0.84665300	-2.22886500
H	-2.77978000	-0.59655000	1.50999200	H	-2.65788000	-0.97893800	1.43673400	H	-3.03156300	-1.00954600	0.15024500
H	0.14698100	-2.39406900	-0.90134700	H	0.17793100	-2.74348000	-1.01879000	H	1.19635000	-2.10388900	-0.64715400
H	1.41315700	-0.77578300	1.51271800	H	1.50581600	-0.01738700	1.49834800	H	0.96060400	0.16746800	1.65987400
H	0.25300100	0.44869600	-2.59126900	H	0.32256600	0.12835500	-2.96080300	H	0.15000600	-0.76433400	-3.32006500
H	-1.52241500	2.23119300	1.03783300	H	-1.77457700	2.58947200	1.43493000	H	-1.57957500	2.70407000	2.73879700
H	-2.81811200	0.61588800	-1.36459100	H	-2.36654400	1.17297100	-0.57146600	H	-1.75357100	1.97260400	0.45306300
Al	-0.65854300	-0.06363700	0.00105700	Al	-0.57353000	-0.45990200	-0.12163200	Al	-0.61025300	-0.25060400	-0.32606500
O	0.06242300	0.60213900	-3.83381800	O	0.21088900	0.28653000	-4.02748300	O	0.28472100	-1.27990600	-4.22380800
H	0.36304000	-0.06223700	-4.47641900	H	0.56260800	-0.39675100	-4.62926000	H	1.16636500	-1.22156600	-4.64198400
H	0.14112500	1.47544600	-4.25314700	H	0.40455600	1.17675700	-4.37724100	H	-0.42633600	-1.20699000	-4.88997500

§S5.3 Cartesian coordinates for the optimized R, TS and P structures for the optimal pathways with N_m' = 2 ~ 7

1.N_m'= 2

R				TS				P			
O	-0.60921100	0.26609100	1.95413700	O	-0.76872800	-0.02388700	1.75986500	O	-0.83652900	-0.11947400	1.29461400
H	0.07795700	0.63464500	2.53481200	H	-0.24609800	-0.08361200	2.57940300	H	-0.54583400	0.07760300	2.20132300
O	1.09812400	1.19853700	-0.02442000	O	1.30318100	1.36795200	-0.04038500	O	1.48135000	1.19742200	0.67413900
H	1.99238900	0.79534000	-0.06120400	H	2.20341100	0.97727300	-0.03546500	H	2.36719600	0.77818300	0.79505000
O	0.68447000	-1.42957600	0.09835800	O	0.96394600	-1.25046000	0.00225600	O	1.29564600	-0.88128600	-0.88980700
H	1.69329500	-1.35137300	-0.03120800	H	1.98691300	-1.16441400	0.00020200	H	2.27762500	-0.88286500	-0.58319500
O	-0.50517500	0.10797800	-1.96030800	O	-0.78196100	-0.08545000	-1.77969600	O	-1.37290300	-0.48807100	-1.23119100
H	0.14609900	0.54066900	-2.53743800	H	-0.26223100	-0.17896300	-2.59797600	H	-1.50090800	-0.59106100	-2.18988700
O	-2.02411200	-1.02747100	-0.00310500	O	-2.56373500	-1.13619800	0.02460700	O	-3.03475200	-1.39285400	0.63794500
H	-2.93361600	-0.67956800	0.00507300	H	-3.45734400	-0.75320300	0.02163400	H	-3.91565900	-1.00127500	0.77859100
O	-1.65050500	1.63846200	-0.08100300	O	-1.41632500	1.75040700	-0.03980600	O	-0.35487800	2.00897400	-0.98025400
H	-1.90960200	2.19730300	0.67169500	H	-1.72011200	2.24620700	0.74012100	H	0.13648400	2.86774500	-0.70746000
H	0.49587800	-2.31511200	0.44507800	H	0.72094900	-2.18957300	0.01676700	H	1.11970200	-1.66113900	-1.44208200
H	1.21056900	2.26389500	-0.01437800	H	1.41293400	2.49295500	-0.05997000	H	1.57078700	2.18014300	0.73498700
H	-1.25472100	-0.18842100	2.52249000	H	-1.61977200	-0.49060800	1.87671000	H	-1.71180300	-0.62185300	1.30588500
H	-1.94812400	2.07961500	-0.89507600	H	-1.72208600	2.22081400	-0.83454300	H	-1.10387500	2.22591800	-1.55994700
H	-2.09289500	-1.99581100	-0.07242400	H	-2.72496900	-2.09505000	0.04002900	H	-3.15036500	-2.34470500	0.81029300
H	-1.04219400	-0.47929600	-2.51961000	H	-1.63685900	-0.54839100	-1.87941700	H	-2.14187100	-0.91657900	-0.74845900
Al	-0.42263500	0.11930800	0.00266000	Al	-0.15129100	0.28306700	-0.01762700	Al	0.05706400	0.34714800	-0.26855200
O	3.16668200	-0.78731200	-0.17323100	O	3.43045200	-0.58936900	-0.01064500	O	3.59364800	-0.55398000	0.18192400
H	3.79306400	-0.94180300	0.55469900	H	4.00065300	-0.73755600	0.76337500	H	3.94054200	-1.20446500	0.81810200
H	3.67150000	-0.98119600	-0.98149000	H	3.99883500	-0.76303900	-0.78070000	H	4.36633000	-0.27185900	-0.33906900
O	1.35149700	3.66557800	0.00879800	O	1.53071400	3.78959500	-0.08419300	O	1.08447100	3.86817700	0.03924700
H	1.59326000	4.19044900	-0.77001200	H	1.83402300	4.25999100	-0.87760900	H	1.73676600	4.36064700	-0.48998900
H	1.67699600	4.15362600	0.78109500	H	1.83646300	4.28927200	0.69016300	H	0.69131400	4.52950800	0.63617100

2.N_m'= 3

R				TS				P			
O	-0.56135300	0.25627500	1.94601800	O	-0.63279800	0.21817100	1.92455400	O	-0.48541500	0.12930100	2.26282800
H	-1.11380000	0.91474400	2.44458700	H	-1.22732000	0.83572200	2.44210900	H	-1.19893000	0.74287300	2.65625700
O	1.10578100	1.21026700	-0.18091200	O	1.31115600	1.38228400	-0.10848800	O	1.54574500	1.19668300	-0.16734600
H	1.98983200	0.78692500	-0.20043100	H	2.18432500	0.93599700	-0.09429500	H	2.46732600	0.83633100	-0.24254500
O	0.64429100	-1.38239600	0.12604900	O	0.75804600	-1.22139700	0.20063600	O	1.30899800	-1.21108300	0.75875500
H	1.65771000	-1.31988400	0.07945800	H	1.77796100	-1.21261500	0.14641000	H	2.28987300	-1.12708800	0.54400200
O	-0.62613000	0.13622200	-1.94589200	O	-0.75930000	0.13515600	-1.71494800	O	-0.93662500	-0.65475500	-0.71774100
H	-0.00621500	0.59492200	-2.53629100	H	-0.25936500	0.21345500	-2.54371800	H	-0.61676300	-1.48313400	-1.10596500
O	-2.04446800	-1.02116900	-0.01938500	O	-2.45576900	-1.28005200	-0.41717900	O	-3.13377800	-0.26238800	-1.69298300
H	-2.91436300	-0.76810900	-0.37174900	H	-3.36544500	-0.98136500	-0.26016300	H	-3.24228700	0.05065400	-2.60460500
O	-1.62253600	1.70747200	0.04619300	O	-1.47805600	1.83438200	0.15351100	O	-0.92556500	1.86531600	0.37274200
H	-1.97069600	2.11372900	0.89135300	H	-1.87952900	2.19865400	0.99096800	H	-1.60541500	2.13572800	1.02970500
H	0.38780400	-2.30280200	-0.03803500	H	0.43587100	-2.13364900	0.14354100	H	1.12638200	-2.11449100	1.06338000
H	1.24737100	2.24625400	-0.12217900	H	1.47335800	2.44699600	-0.21222200	H	1.47662900	2.13651600	-0.51051600
H	-0.03258900	-0.26417000	2.56952700	H	-0.28228900	-0.47463700	2.50587400	H	-0.14541900	-0.46581300	2.94949700
H	-1.88685000	2.25299900	-0.71038400	H	-1.80846600	2.32532000	-0.61554900	H	-0.60229900	2.65430300	-0.13118500
H	-2.19921500	-1.77353300	0.57631700	H	-2.53854000	-2.24612500	-0.46845200	H	-3.87314600	-0.85923000	-1.49690600
H	-1.13469100	-0.49107600	-2.48632600	H	-1.54018700	-0.45905800	-1.81395200	H	-1.94268500	-0.45511400	-1.16667000
Al	-0.45649300	0.18171000	0.01822900	Al	-0.22295500	0.40385100	0.08949600	Al	0.08668600	0.25119700	0.48902600
O	3.15581700	-0.78526900	-0.06162000	O	3.27239500	-0.71966400	0.03568200	O	3.70123200	-0.43425000	0.00383600
H	3.76161700	-0.86788500	0.69393800	H	3.86056600	-0.83524300	0.80122100	H	4.41385200	-0.27294500	0.64610200

H	3.68059700	-1.05423500	-0.83440800
O	1.47685900	3.69279100	-0.06360100
H	1.65456100	4.23671500	-0.84552000
H	1.92734700	4.12790100	0.67527900
O	-2.22963300	2.28235100	2.57478900
H	-1.92060200	3.09157000	3.01610600
H	-3.12005900	2.12760500	2.93403600

H	3.80143700	-0.99340500	-0.73280300
O	1.68491400	3.80412700	-0.35709600
H	1.92077800	4.21281400	-1.20401700
H	2.07751400	4.35002700	0.34101700
O	-2.24822900	2.17694300	2.69270000
H	-1.93515000	2.90204900	3.26031100
H	-3.16747600	2.01994900	2.96963500

H	4.14144700	-0.82061600	-0.77282700
O	0.73865900	3.59260900	-0.93198500
H	0.66443600	3.82631100	-1.87272600
H	1.04925400	4.40417500	-0.49568800
O	-2.28942300	1.88228400	2.82522000
H	-2.11762800	2.58337300	3.47709100
H	-3.21806200	1.62970500	2.96416900

3.N_m'= 4

R			
O	-0.62121400	0.27181900	1.99388000
H	-1.12993500	0.96110400	2.47657900
O	1.11522000	1.23547600	-0.11456800
H	1.97971900	0.80151800	-0.27442900
O	0.65261500	-1.39610100	0.32480100
H	1.57028200	-1.41693900	-0.06662100
O	-0.43546400	0.05647700	-1.87802400
H	0.16358800	0.54769300	-2.46164700
O	-1.96114000	-1.09802800	-0.08251200
H	-2.90132600	-0.87241600	-0.00016800
O	-1.65899200	1.62810400	0.02716500
H	-1.99286800	2.10309000	0.84759900
H	0.67997600	-1.85350300	1.20193300
H	1.27075900	2.24837100	0.03877900
H	-0.30777100	-0.44272900	2.60505300
H	-1.94015500	2.10614600	-0.76720400
H	-1.88750000	-2.06425800	-0.13983700
H	-0.99682400	-0.51551400	-2.42583400
Al	-0.42730200	0.16288100	0.09388900
O	3.08168900	-0.78536800	-0.61101900
H	3.85812900	-0.89090700	-0.03768200
H	3.40382300	-1.01939100	-1.49647500
O	1.51170000	3.70764400	0.26047500
H	1.59096900	4.35014800	-0.45972100
H	2.06199700	4.04514500	0.98202000
O	-2.26364300	2.45832700	2.45010900
H	-1.93448900	3.30022300	2.80547600
H	-3.16314400	2.37044800	2.80716700
O	0.42870400	-2.00292900	3.00482400
H	1.20999700	-1.99491700	3.58176200
H	-0.12450000	-2.72098300	3.35390300

TS			
O	-0.65245700	0.23345500	2.00107700
H	-1.26141300	0.84590300	2.48307000
O	1.34018100	1.38922200	-0.08060500
H	2.18854000	0.91692900	-0.23874900
O	0.77636300	-1.22650300	0.38778800
H	1.69411800	-1.29375900	0.00322700
O	-0.60223400	0.05299900	-1.63336800
H	-0.14135300	0.25482600	-2.46188100
O	-2.28751100	-1.37461400	-0.36972100
H	-3.23834700	-1.18775100	-0.33206800
O	-1.44035000	1.82426400	0.16272300
H	-1.88704300	2.19607900	0.97862900
H	0.72048100	-1.77986100	1.20356300
H	1.51135700	2.43345800	-0.09749100
H	-0.38696800	-0.54445600	2.56845300
H	-1.74749800	2.29130700	-0.62911000
H	-2.23078500	-2.34261600	-0.36214400
H	-1.32576000	-0.60394400	-1.75567600
Al	-0.18455300	0.39667500	0.19211100
O	3.22262000	-0.66467800	-0.53525100
H	3.99227200	-0.78818500	0.04415800
H	3.54841000	-0.89054500	-1.42181600
O	1.74948100	3.84426200	-0.12295700
H	1.90833800	4.34698800	-0.93551700
H	2.20624400	4.31467000	0.58980500
O	-2.34846500	2.28414900	2.60075200
H	-2.06526000	3.04460100	3.13537000
H	-3.28502000	2.15314300	2.82494600
O	0.28490700	-2.05421400	2.97300400
H	0.99788400	-2.07943300	3.63245500
H	-0.30011800	-2.79244700	3.21050800

P			
O	-1.03427900	-0.08061800	1.84504500
H	-1.68749300	0.52860100	2.27374800
O	1.52807200	1.18411000	-0.60714600
H	2.41152800	0.74290400	-0.70337500
O	1.36180600	-0.78208100	1.09728300
H	2.28303600	-0.88565000	0.73454100
O	-0.82154300	-0.23055300	-0.94892600
H	-0.47904100	-0.14352100	-1.85122000
O	-2.96419400	-1.43219500	-1.13207200
H	-3.75524200	-1.02028900	-1.51056500
O	-0.40304700	2.22199900	0.80430100
H	-1.13203700	2.46367500	1.43836200
H	1.15780500	-1.44022200	1.81605000
H	1.57965900	2.14541300	-0.84792000
H	-0.86699700	-0.88034400	2.40576000
H	-0.01312300	3.01680400	0.34938800
H	-3.01373700	-2.37960500	-1.32852000
H	-1.76179200	-0.75823700	-1.00894500
Al	0.12785200	0.46529600	0.45848000
O	3.63379400	-0.48898100	-0.29014100
H	4.45555600	-0.19458800	0.13693700
H	3.91744400	-1.11980500	-0.97266600
O	1.07583700	3.84936700	-0.72746600
H	0.72183900	4.29496100	-1.51506300
H	1.69979600	4.48473200	-0.33840400
O	-2.36722100	2.15739100	2.61634700
H	-2.24187400	2.52705100	3.50625000
H	-3.29435100	2.34477100	2.39500100
O	0.17713800	-2.20186100	3.02985600
H	0.47764800	-2.14766800	3.95237000
H	-0.09609700	-3.12622500	2.90897700

4.N_m'= 5

R			
O	-0.66378400	0.29195500	1.98563100
H	-1.16619500	0.96630300	2.49369500
O	1.03719200	1.31431400	-0.05384500
H	1.88097300	0.89963200	-0.34034500
O	0.57639700	-1.34386500	0.24381700
H	1.42828400	-1.35322400	-0.26760700
O	-0.53826400	0.12997800	-1.86009200
H	0.21275800	0.25152200	-2.52050100
O	-2.07339500	-1.01118300	-0.05531200
H	-3.00099300	-0.78737900	0.11698500
O	-1.73497500	1.69963300	0.05977800
H	-2.05901100	2.15836600	0.88892000
H	0.72138700	-1.76812900	1.12551200
H	1.19920100	2.28579400	0.22154800
H	-0.27595600	-0.39796600	2.57900800
H	-1.96223300	2.22360900	-0.72242600
H	-2.00324000	-1.97696200	-0.11549900
H	-1.25538200	-0.33266700	-2.31774500
Al	-0.50052900	0.22987000	0.07273500
O	2.77140300	-0.55204600	-1.09389000
H	3.68476700	-0.80070600	-0.88352800
H	2.72153700	-0.47409300	-2.06432400
O	1.44678200	3.73760200	0.66595800
H	1.47478600	4.48806600	0.05556400
H	2.05132700	3.96158700	1.38779700
O	-2.29832700	2.46716300	2.52724400
H	-1.95303400	3.29564500	2.89730300
H	-3.19027700	2.37790500	2.90134000
O	0.59933400	-1.91465400	2.93208900
H	1.41489600	-1.85400000	3.45528900
H	0.11878900	-2.66775300	3.31262200
O	1.47898000	0.17790500	-3.59019300
H	1.43113000	-0.48182100	-4.30102100
H	1.77440200	0.99135300	-4.02893100

TS			
O	-0.66705200	0.22851900	1.92719400
H	-1.28225200	0.82919000	2.41540800
O	1.37429300	1.44945900	-0.00898700
H	2.22791500	0.99154800	-0.18714300
O	0.81837200	-1.18529400	0.32682900
H	1.73578600	-1.23369800	-0.04438100
O	-0.56842400	0.14975500	-1.66023700
H	-0.07010600	0.27815100	-2.56604800
O	-2.32378300	-1.30359700	-0.37801400
H	-3.27052600	-1.11009800	-0.30961300
O	-1.39564900	1.90967200	0.14991500
H	-1.84687600	2.26857900	0.96187900
H	0.76155600	-1.74852300	1.13435100
H	1.53394400	2.47480200	0.06155800
H	-0.41439600	-0.56101000	2.47810100
H	-1.70470700	2.37348400	-0.64187800
H	-2.27776400	-2.27006100	-0.42530300
H	-1.32847300	-0.45823600	-1.76443900
Al	-0.16443500	0.44283100	0.12536500
O	3.30163900	-0.49081200	-0.51843900
H	4.06210100	-0.63275300	0.06783600
H	3.65227200	-0.62961900	-1.41232200
O	1.78213200	3.92639300	0.18240600
H	1.93549600	4.51590700	-0.56950900
H	2.23255300	4.32565500	0.94025400
O	-2.33644600	2.26875100	2.61783700
H	-2.04327500	2.98854300	3.20011600
H	-3.27755200	2.14522200	2.82378200
O	0.27651300	-2.08440800	2.87670300
H	0.96544200	-2.11491500	3.56024700
H	-0.30147900	-2.84013400	3.07011200
O	0.61169700	0.41225000	-3.86641300
H	0.76253900	-0.34372600	-4.45231600
H	0.49580600	1.18150300	-4.44251400

P			
O	-0.50163000	-0.33924100	1.86369500
H	-1.27392300	-0.00250000	2.38786300
O	1.47163200	1.83053500	-0.23188200
H	2.40065700	1.60294900	-0.49613100
O	1.66704500	-0.65431300	0.49475100
H	2.55798200	-0.48076900	0.09899100
O	-0.65825800	-0.05090800	-1.08390200
H	-0.74881800	-1.03382900	-1.35925600
O	-1.85157200	1.40552500	-2.81413600
H	-2.81311700	1.50000800	-2.86486800
O	-0.85134500	2.03894100	0.88086900
H	-1.57716900	1.98136400	1.55198700
H	1.67785500	-1.44553100	1.09072500
H	1.29557500	2.80596200	-0.28160100
H	-0.12621000	-1.17554500	2.24398800
H	-0.65123700	2.97755900	0.63544000
H	-1.52671200	1.49543700	-3.72114500
H	-1.15029700	0.52535500	-1.77388400
Al	0.21990400	0.56152000	0.37577100
O	3.79941900	0.55009500	-0.66354700
H	4.59296300	0.76461600	-0.14615600
H	4.12809200	0.32923700	-1.55008000
O	0.36628500	4.27430200	-0.02978000
H	0.04912400	4.77561700	-0.79833500
H	0.72119000	4.94181600	0.58000300
O	-2.49141600	1.17879000	2.85746200
H	-2.43551200	1.55765100	3.75005500
H	-3.43155000	0.97281500	2.72903900
O	1.04721600	-2.47272800	2.39679700
H	1.55561800	-2.53509100	3.22200500
H	0.78038000	-3.38380900	2.19347400
O	-0.90302700	-2.51144200	-1.73660100
H	-1.75678800	-2.96609000	-1.71057200
H	-0.40051600	-2.92901400	-2.45018400

5.N_m'= 6 (without PCM)

R			
O	-0.67583600	0.33254400	1.94009800
H	-1.15356000	1.04060600	2.43687600
O	1.10270000	1.32277000	-0.04277200
H	1.94585000	0.88825400	-0.29577700
O	0.57132500	-1.31441500	0.22506100
H	1.44194000	-1.33717400	-0.25000800
O	-0.43191400	0.14316800	-1.90553600
H	0.34289200	0.20582800	-2.53516000
O	-2.05136200	-0.96029400	-0.13928400
H	-2.96386100	-0.76058800	0.11634200
O	-1.67960900	1.74301600	-0.03617000
H	-1.96024700	2.21875200	0.77789300
H	0.67972500	-1.74083100	1.10978500
H	1.27963200	2.27783100	0.25583100
H	-0.31181200	-0.35803500	2.54178600
H	-2.09050700	2.19564200	-0.85523500
H	-1.97307800	-1.91856800	-0.26388100
H	-1.20164500	-0.15576100	-2.40935400
Al	-0.48259300	0.28910800	0.02865000
O	2.83989300	-0.57993900	-1.02385900
H	3.74081800	-0.84636400	-0.78625200
H	2.81228000	-0.51699100	-1.99688700
O	1.58209200	3.72148600	0.77236600

TS			
O	-0.69609100	0.26464100	1.90758100
H	-1.33326300	0.87342600	2.36835100
O	1.38208200	1.41353200	-0.04118900
H	2.22810100	0.93528700	-0.20209900
O	0.79586200	-1.19267700	0.38367100
H	1.69727000	-1.27660400	-0.00874200
O	-0.49912400	0.01151300	-1.67914100
H	-0.02435200	0.19119700	-2.57470700
O	-2.29565700	-1.40714100	-0.40693900
H	-3.24666700	-1.22895700	-0.37773300
O	-1.40706600	1.86560000	0.02994800
H	-1.85320800	2.22369000	0.82740900
H	0.75936900	-1.70555600	1.22493000
H	1.56253200	2.42581200	0.01711600
H	-0.43004700	-0.48962800	2.49201400
H	-1.73657800	2.37950800	-0.79281700
H	-2.22848800	-2.37281400	-0.38646100
H	-1.24002800	-0.61732300	-1.78465000
Al	-0.18701700	0.44313700	0.09976100
O	3.30082800	-0.53259000	-0.50964400
H	4.06045900	-0.67065400	0.07782700
H	3.64969200	-0.68348700	-1.40169600
O	1.88515700	3.89637300	0.11899100

P			
O	-1.16160300	-0.06768300	1.71821400
H	-1.92072300	0.44895000	2.09798400
O	1.40321800	1.49047700	-0.47130000
H	2.28335300	1.05220700	-0.53908000
O	1.23488500	-0.61845100	1.01296900
H	2.17876200	-0.65556100	0.71133600
O	-0.74432800	-0.30375300	-1.13276400
H	-0.67185500	-0.01332900	-2.10869400
O	-2.11981700	-2.47606000	-1.04368600
H	-3.08518000	-2.50456600	-1.09378900
O	-0.98175500	2.18201200	0.45141800
H	-1.70219300	2.29952100	1.10996800
H	1.05354500	-1.28418800	1.72300400
H	1.51719000	2.45260300	-0.74066200
H	-0.93764400	-0.84173400	2.29059100
H	-1.00857300	2.98160300	-0.22159800
H	-1.80899500	-3.29982700	-1.44400700
H	-1.30313300	-1.15521300	-1.09600200
Al	-0.06306200	0.57541900	0.30562200
O	3.60404000	-0.15324500	-0.14134400
H	4.36268900	0.14535100	0.38519900
H	3.98015500	-0.72676400	-0.82756400
O	1.84796300	4.01048300	-1.21498500

H	1.62350200	4.49856500	0.19822300
H	2.20036100	3.89547900	1.49574600
O	-2.13918300	2.50561500	2.59357400
H	-1.73837700	3.30096000	2.97723300
H	-3.01445300	2.44196600	3.00721400
O	0.53033200	-1.91935400	2.91014600
H	1.33587600	-1.88610900	3.45000100
H	0.02279100	-2.66393100	3.27036100
O	1.67554500	0.03900500	-3.57197600
H	1.63698800	-0.66097300	-4.24311900
H	2.01162200	0.81670700	-4.04399400
O	-2.78722300	2.82481300	-2.07684900
H	-2.46022500	3.60317300	-2.54836600
H	-3.74492800	2.81334500	-2.21473300

H	2.17571200	4.43749800	-0.62800500
H	2.25721300	4.30617200	0.91225300
O	-2.38418500	2.19796000	2.62647500
H	-2.10924700	2.91049600	3.22461500
H	-3.31789500	2.03791600	2.83556100
O	0.30590500	-2.00550200	2.96465500
H	0.99480700	-1.99556800	3.64801000
H	-0.25362300	-2.76767000	3.18289300
O	0.67341500	0.37247700	-3.89927200
H	0.86624900	-0.36647400	-4.49357700
H	0.54435000	1.14647500	-4.46442700
O	-2.26493300	3.20756300	-1.96936500
H	-2.10223400	4.15622800	-2.06367200
H	-3.09913100	3.03128600	-2.42580200

H	2.23678600	4.15044900	-2.09222800
H	2.33754500	4.60010200	-0.62094200
O	-2.91709100	1.81722000	2.41587100
H	-2.86092000	2.25304400	3.28110700
H	-3.86425300	1.78105700	2.20921800
O	0.11727500	-2.11200900	2.96529000
H	0.40804200	-2.03649700	3.88830100
H	-0.12690700	-3.04397000	2.85004600
O	-0.58393500	0.40267900	-3.59403900
H	-0.09821700	-0.09756600	-4.26384000
H	-1.30653800	0.84452100	-4.06025300
O	-1.01369100	4.05569000	-1.19936400
H	-0.17882400	4.53096300	-1.33259800
H	-1.74678200	4.65987700	-1.37932000

6.N_m'= 6 (with PCM)

R

O	-0.61961600	0.31301700	1.95732700
H	-1.11672700	1.01111400	2.44601100
O	1.06586000	1.22687800	-0.07853400
H	1.93526600	0.80326800	-0.23108500
O	0.49212300	-1.40576500	0.21664600
H	1.37437100	-1.41196400	-0.23722800
O	-0.51717000	0.08715000	-1.86621100
H	0.27305600	0.22472200	-2.45945600
O	-2.10799700	-0.92582600	-0.03473000
H	-3.01746100	-0.62880000	0.17071800
O	-1.63340800	1.73127100	-0.01466400
H	-1.93287500	2.20179400	0.79551000
H	0.58183500	-1.83142600	1.10433800
H	1.17224200	2.20708100	0.14125500
H	-0.33654500	-0.42349200	2.54608700
H	-1.82200000	2.28488000	-0.84183600
H	-2.09592500	-1.90472500	-0.05301700
H	-1.17796600	-0.44609700	-2.34959900
Al	-0.53035800	0.21109200	0.04644300
O	2.75579700	-0.71254900	-0.98764100
H	3.65008300	-1.05068100	-0.79974500
H	2.69757600	-0.54917100	-1.94856700
O	1.25774200	3.72755800	0.49730300
H	1.49820500	4.33877100	-0.22211400
H	1.82190600	3.97234000	1.25290900
O	-2.08372200	2.45002300	2.55756800
H	-1.69172500	3.24367600	2.97015200
H	-2.97609600	2.36188800	2.94480500
O	0.38566500	-2.00647800	2.83560000
H	1.20187900	-2.03386900	3.37184500
H	-0.17988400	-2.72883400	3.17142600
O	1.66328200	0.23610000	-3.36652300
H	1.60801700	-0.30337500	-4.17929700
H	1.97977300	1.11336600	-3.65734100
O	-2.07133300	3.15115100	-2.11465400
H	-2.30441700	4.08602400	-1.96980400
H	-2.72469100	2.81273100	-2.75320500

TS

O	-0.67582300	0.13433000	1.85224000
H	-1.36190200	0.65631200	2.35186400
O	1.33626400	1.58013800	-0.06417500
H	2.20300100	1.17387200	-0.30285500
O	0.90345600	-1.05205200	0.17628500
H	1.81816800	-1.01340000	-0.20266700
O	-0.67372300	0.18063700	-1.62924100
H	-0.01642800	-0.18884300	-2.31136600
O	-2.69199400	-0.97013900	-0.48792800
H	-3.58828600	-0.59498600	-0.41838500
O	-1.35180600	1.97479600	0.18316000
H	-1.87851900	2.20687100	0.97906700
H	0.89818400	-1.65069100	0.96193200
H	1.38549700	2.60682400	-0.07417400
H	-0.37910700	-0.67603600	2.34471100
H	-1.56361500	2.60241400	-0.59335900
H	-2.80805100	-1.93528500	-0.42452200
H	-1.52786300	-0.31474900	-1.64895700
Al	-0.16439300	0.54122000	0.11596700
O	3.25212600	-0.18809100	-0.72902500
H	4.04674800	-0.30946800	-0.17296200
H	3.55491100	-0.28343100	-1.65139200
O	1.41623000	4.10369800	-0.06838600
H	1.67245100	4.53832300	-0.90274800
H	1.95228800	4.52294600	0.63002800
O	-2.43683600	1.88590000	2.66085100
H	-2.19716400	2.52559300	3.36004500
H	-3.37532800	1.65828900	2.81135100
O	0.41673300	-2.14001400	2.57627100
H	1.11227200	-2.17132400	3.26281300
H	-0.11670600	-2.95124700	2.69157600
O	1.13677100	-0.65620100	-3.22234700
H	1.13356800	-1.59478700	-3.48747100
H	1.26051100	-0.14796400	-4.04552500
O	-1.81238500	3.53782800	-1.77190300
H	-1.87725200	4.48873500	-1.56846700
H	-2.57182900	3.33512600	-2.34818200

P

O	-0.37263800	-0.02461700	1.99276400
H	-1.11217100	0.37494300	2.52997400
O	1.34838600	1.82355400	-0.14740200
H	2.26156200	1.56236300	-0.41841500
O	1.44419300	-0.76225400	0.29078400
H	2.34133300	-0.57415100	-0.08409300
O	-0.73858700	-0.21234100	-1.12884500
H	-0.43251600	-1.07370100	-1.58428000
O	-2.76904800	0.80605200	-2.47572900
H	-2.69315200	0.65093000	-3.43762000
O	-1.20659600	1.90795200	0.47912600
H	-1.79183300	1.97058400	1.26593400
H	1.49683600	-1.46541400	0.98163800
H	1.24808300	2.84755500	-0.11743000
H	0.02656800	-0.82953900	2.41869900
H	-1.52153900	2.54325600	-0.26506900
H	-3.65455100	0.47483400	-2.22866200
H	-1.53618100	0.15326900	-1.61034500
Al	0.08392300	0.57139700	0.29977800
O	3.56333100	0.44280600	-0.74672700
H	4.38379900	0.54325000	-0.22496800
H	3.84633100	0.30921700	-1.67268700
O	1.09275100	4.33296300	-0.04209500
H	1.09182000	4.81628700	-0.88872700
H	1.72347100	4.80161200	0.53536100
O	-2.33434300	1.43141700	2.89652600
H	-2.19943700	2.03609400	3.65263800
H	-3.23593700	1.06724100	2.99595000
O	1.01050900	-2.19534800	2.50709300
H	1.68246100	-2.22488500	3.21683200
H	0.57725900	-3.07188000	2.50610800
O	-0.01800400	-2.36954400	-2.27862900
H	-0.68090400	-3.08308300	-2.31674500
H	0.35495900	-2.30040100	-3.17638500
O	-1.94734600	3.29501100	-1.49125800
H	-2.44315100	4.12723900	-1.39063100
H	-2.48982500	2.69286300	-2.03245100

7.N_m'= 7

R

O	-0.74781600	0.32372600	1.88173900
H	-1.24611600	1.02383400	2.36547200
O	1.05587500	1.28341700	-0.06598200
H	1.90751500	0.85320600	-0.29309500
O	0.53417700	-1.34010200	0.17605800
H	1.41714100	-1.35027400	-0.27259900
O	-0.42228000	0.14965500	-1.97892000
H	0.36658300	0.23212100	-2.58119600
O	-2.06461800	-0.94754000	-0.23988000
H	-3.04625600	-0.83069100	0.00254700
O	-1.66936300	1.77421900	-0.11954800
H	-2.00416300	2.21903500	0.68955500
H	0.62407500	-1.76614100	1.06116300
H	1.22178000	2.22453100	0.26065500
H	-0.40689100	-0.37119300	2.48817000
H	-2.01721900	2.25738600	-0.94021100
H	-1.91089900	-1.88764900	-0.40609300
H	-1.16673800	-0.18207700	-2.49890700
Al	-0.55321800	0.25446700	-0.03666800
O	2.83644300	-0.59039700	-1.01774400
H	3.73413400	-0.85828300	-0.77172700
H	2.82131600	-0.50930800	-1.98995000
O	1.53154400	3.67552600	0.83379500
H	1.59409100	4.46824700	0.28406800
H	2.13502800	3.82316600	1.57482600
O	-2.23846000	2.49892700	2.50043100
H	-1.84592000	3.28977800	2.90042200
H	-3.13018700	2.44119300	2.87610200
O	0.44693500	-1.94521800	2.86918600
H	1.24367200	-1.90378900	3.42065800
H	-0.05436100	-2.69951600	3.21603200
O	1.76129900	0.07021100	-3.58733200
H	1.74242000	-0.61720200	-4.27159700
H	2.11812700	0.85362100	-4.03326000
O	-2.62369400	2.99398100	-2.18751700
H	-2.22343200	3.75872400	-2.62225100
H	-3.57016400	3.04765900	-2.37724400
O	-4.56588900	-0.74806000	0.34759700
H	-4.97320800	-1.20646800	1.09532400
H	-5.25339200	-0.68750700	-0.32984900

TS

O	-0.65354800	0.28916300	1.94458700
H	-1.29082000	0.88607100	2.41843100
O	1.40776800	1.45420400	-0.03125000
H	2.24943300	0.97597100	-0.20970700
O	0.82640100	-1.14079300	0.38069800
H	1.72365600	-1.21920300	-0.02085800
O	-0.57085500	0.08496200	-1.62176900
H	-0.07866700	0.12261400	-2.51395800
O	-2.30770500	-1.31256200	-0.40391000
H	-3.29430100	-1.17061100	-0.40624300
O	-1.33760100	1.96599700	0.12004600
H	-1.78744300	2.30109900	0.92409600
H	0.79017400	-1.67691200	1.20612900
H	1.58463900	2.46441700	0.00057900
H	-0.39742300	-0.48481000	2.50534700
H	-1.67044800	2.49237900	-0.69022100
H	-2.20009900	-2.27264600	-0.38377500
H	-1.33578100	-0.54475200	-1.62466800
Al	-0.17245800	0.49786600	0.13302900
O	3.31309000	-0.48568100	-0.56464800
H	4.09422200	-0.63195800	-0.00857200
H	3.62454200	-0.62578200	-1.47196200
O	1.91614600	3.94844700	0.06072400
H	2.20285200	4.46968400	-0.70142100
H	2.29143200	4.37916600	0.84097700
O	-2.32558200	2.21963300	2.71907100
H	-2.04698600	2.90499200	3.34610500
H	-3.26546800	2.07019000	2.90443300
O	0.33535300	-2.01950200	2.94172600
H	1.02480100	-2.02814000	3.62419200
H	-0.22473500	-2.78654900	3.13872400
O	0.67526800	0.12180500	-3.85927100
H	0.76653500	-0.67199100	-4.40457800
H	0.63782200	0.86544800	-4.47616100
O	-2.20047300	3.35843100	-1.84561900
H	-2.02931500	4.30600900	-1.93058500
H	-3.02784100	3.18876100	-2.31532500
O	-4.96450600	-0.98115500	-0.46553100
H	-5.57254400	-1.27062000	0.22681300
H	-5.46319400	-1.05439100	-1.28970700

P

O	-0.20570400	0.02613300	2.26193500
H	-0.92471400	0.43350800	2.82158700
O	1.17293500	1.72168200	-0.28152400
H	2.09553500	1.50981900	-0.55301800
O	1.61764100	-0.70077100	0.56855500
H	2.45880300	-0.51066100	0.08552400
O	-0.76046900	-0.64903200	-0.75689500
H	-0.31491800	-1.36930300	-1.31082700
O	-3.25120100	-0.67307100	-1.24594300
H	-3.74821200	-0.04972300	-1.81415300
O	-1.35838200	1.64637000	0.58334700
H	-1.85398100	1.77568000	1.41597500
H	1.78419100	-1.31343300	1.31979000
H	0.98557400	2.71264300	-0.47389100
H	0.32114500	-0.64709200	2.76422500
H	-1.84966900	2.14952800	-0.19279400
H	-3.75051900	-1.49878600	-1.21435900
H	-1.76626800	-0.63739100	-0.97488900
Al	0.05720600	0.43341000	0.45066600
O	3.60176700	0.50776300	-0.80824900
H	4.42023100	0.78949400	-0.37041600
H	3.86966400	0.24491900	-1.70236200
O	0.80535600	4.19321900	-0.79196900
H	0.89117000	4.54084800	-1.69041600
H	1.10579600	4.89541400	-0.19828700
O	-2.20711300	1.41341100	3.28283900
H	-2.05497500	2.11340600	3.93674400
H	-3.05026500	1.00582100	3.53431400
O	1.50496000	-1.89303900	3.05162000
H	2.19859900	-1.72952100	3.71011800
H	1.20919400	-2.80228900	3.21565500
O	0.35295500	-2.45861600	-2.24620900
H	0.39477800	-3.40220400	-2.04119300
H	0.33956200	-2.39763500	-3.21084200
O	-2.52226300	2.82589500	-1.28314100
H	-2.58737300	3.78817700	-1.31912800
H	-3.28732800	2.44859100	-1.77025800
O	-4.53676700	1.43418400	-2.61994500
H	-5.46114400	1.58500300	-2.37140600
H	-4.52826800	1.46871200	-3.58810700

§S5.4 Cartesian coordinates for the optimized R, TS and P structures for the optimal pathway with N_m' = 0 ~ 12 obtained with "Independent-minimum" method (Method-II)

1.N_m'= 0

R				TS				P			
O	-1.27394300	1.29836300	0.67519500	O	0.84053000	0.00112900	-1.48764500	O	-1.07469000	-0.00014700	-0.72360100
H	-1.91872700	1.15920600	1.39437500	H	0.75963300	0.00145700	-2.45977400	H	-1.13838700	-0.00036400	-1.69104100
O	-0.65293300	-1.30478700	1.27644000	O	-2.09716200	-0.00056900	-0.71183300	O	2.04052400	0.00031400	-1.18705900
H	-1.37850600	-1.94197200	1.13474500	H	-2.62855800	-0.78869900	-0.94462800	H	2.45947100	0.78636200	-1.58548700
O	-1.31265200	-0.61400100	-1.29050600	O	-0.21321300	-1.90551800	0.03217800	O	0.76956700	1.94449500	0.08402100
H	-2.21856500	-0.26984900	-1.40557900	H	0.14010400	-2.47730200	-0.67679600	H	0.08404300	2.55194300	-0.24911800
O	1.27538600	-1.29531900	-0.67898600	O	-0.57334100	-0.00079200	1.85267600	O	0.64130000	-0.00016600	1.87308700
H	1.91922900	-1.15326800	-1.39853600	H	0.14136500	0.00004000	2.52108000	H	0.62974400	0.78676200	2.44940700
O	0.65164300	1.30849100	-1.27511900	O	2.59305000	0.00028900	0.29818100	O	-3.67508600	-0.00010200	-0.04515600
H	1.38112800	1.94158500	-1.13497400	H	3.16159100	0.76695400	0.49149400	H	-4.18857600	-0.81008500	-0.24181300
O	1.31113700	0.60610300	1.29503000	O	-0.21491700	1.90554400	0.03354300	O	0.77018100	-1.94440400	0.08372800
H	1.19147500	1.31589400	1.95416700	H	0.13797000	2.47810300	-0.67502300	H	0.08491300	-2.55207500	-0.24953100
H	-1.18846200	-1.32025200	-1.95271700	H	-0.44675900	-2.48404900	0.78366900	H	1.50748100	2.49360900	0.41005200
H	-0.31761000	-1.44885800	2.18154200	H	-2.62933300	0.78728500	-0.94379400	H	2.45956600	-0.78561800	-1.58561400
H	-1.39012200	2.21475600	0.35956600	H	1.79983300	0.00084100	-1.16012400	H	-2.69326600	-0.00009500	-0.32596500
H	2.21867400	0.26415300	1.40388500	H	-0.44916400	2.48335900	0.78536700	H	1.50823200	-2.49326500	0.40987300
H	0.32057200	1.44959600	-2.18225500	H	3.16144800	-0.76658800	0.49104900	H	-4.18872300	0.80968000	-0.24226300
H	1.39327000	-2.21226300	-0.36627100	H	-1.42318700	-0.00219800	2.33801600	H	0.62965900	-0.78723900	2.44920500
Al	-0.00011200	0.00080600	-0.00033700	Al	-0.33880800	0.00001100	-0.05287200	Al	0.54396000	0.00003600	-0.01752800

2.N_m'= 1

R				TS				P			
O	-2.09253700	-1.08070800	-0.03657600	O	-2.68643500	-1.06013000	0.00018600	O	3.43705400	-0.93240300	0.14575100
H	-2.16851000	-2.04657600	-0.14334700	H	-2.90579000	-2.00853100	0.00048600	H	3.75922000	-1.81977400	-0.09893300
O	-0.65375700	0.12124100	1.97156500	O	-0.80971100	-0.16345400	1.74821200	O	1.49122900	0.29920800	-1.19072300
H	0.02278800	0.48082500	2.57276600	H	-0.30887900	-0.25681600	2.58036400	H	1.55952600	0.65006200	-2.09660400
O	0.63751900	-1.51159500	0.06796400	O	0.95925400	-1.35974100	0.00032700	O	-1.09481900	-0.59851100	-1.19865600
H	0.46000000	-2.40982600	0.39288000	H	0.72064200	-2.30288900	0.00079600	H	-0.84062800	-0.98466100	-2.05513900
O	1.11053200	1.06994900	0.04840600	O	1.37345700	1.18079100	-0.00026100	O	-1.49252100	0.30231500	1.18942000
H	1.19729500	2.03811800	0.07502100	H	1.43663700	2.15217800	-0.00041600	H	-1.56126400	0.65185500	2.09579900
O	-1.62404500	1.62132900	-0.00702800	O	-1.28433200	1.76535900	-0.00060100	O	0.00032600	2.18250900	-0.00145000
H	-1.93905000	2.08593000	-0.80360200	H	-1.59148700	2.25126900	-0.78840900	H	-0.72608400	2.75964200	0.30164300
O	-0.52674600	0.11227300	-1.92984000	O	-0.80952100	-0.16470900	-1.74801500	O	1.09528100	-0.59691100	1.20038400
H	0.11569800	0.57768300	-2.49384300	H	-0.30862200	-0.25854700	-2.58010900	H	0.84181500	-0.98178100	2.05765000
H	-1.31379600	-0.33308600	2.52540000	H	-1.70569800	-0.54527300	1.85314100	H	2.36723200	-0.12278800	-0.93731200
H	-3.00242200	-0.73034500	-0.01710000	H	-3.55689000	-0.62473100	0.00022800	H	4.22398500	-0.45697200	0.47106600
H	-1.93214900	2.12352800	0.76913900	H	-1.59170800	2.25174700	0.78689300	H	0.72611800	2.75961300	-0.30604200
H	-1.07602400	-0.43645000	-2.51786100	H	-1.70561100	-0.54636600	-1.85274800	H	2.06848000	-0.82511800	0.99635900
H	2.02644100	0.65061300	-0.00129100	H	2.31250900	0.77047700	-0.00012200	H	-2.36810900	-0.12057500	0.93595700
H	1.62790800	-1.42626000	-0.06277000	H	1.95519800	-1.28083800	0.00035600	H	-2.06778100	-0.82728400	-0.99476700
Al	-0.49252800	0.03583200	0.02362900	Al	-0.18544100	0.17679900	-0.00001100	Al	0.00019400	0.29320900	0.00037500
O	3.14341000	-0.60007400	-0.13275700	O	3.45379500	-0.33614700	0.00008900	O	-3.43685300	-0.93313300	-0.14518400
H	3.68899700	-0.67652300	-0.93640800	H	4.04417100	-0.39814900	-0.77346600	H	-3.75916300	-1.81974300	0.10201300
H	3.76779000	-0.73643800	0.60296200	H	4.04420300	-0.39768000	0.77365700	H	-4.22345700	-0.45878700	-0.47290000

3.N_m'= 2

R				TS				P			
O	1.22273800	-0.97258400	-1.03449000	O	-1.14814500	-0.22597800	-1.37644800	O	-1.11536900	-1.49722800	-0.75666700
H	2.21338500	-0.85804500	-0.97966000	H	-2.15298700	-0.14821400	-1.31908100	H	-2.12017700	-1.28587400	-0.86255800
O	0.01792300	1.60119900	-1.14609700	O	-0.08386300	-2.07951200	0.81380700	O	-0.05895900	-0.73026600	2.07687600
H	-0.53502800	1.67904900	-1.94174800	H	0.53529500	-2.79165800	0.57422600	H	0.55013300	-1.27614500	2.60658300
O	-1.51767700	-0.62633600	-0.78826000	O	1.47071400	-0.58809200	-0.88876600	O	1.49465900	-1.58988900	0.00498600
H	-1.48651700	-1.19502000	-1.57232100	H	1.42605500	-1.04251300	-1.74418600	H	1.53532500	-2.55657100	0.09772100
O	-1.06116500	1.15807900	1.27179700	O	0.94381200	0.61532200	1.47170800	O	1.15550100	0.96999900	-0.27200400
H	-1.41007400	2.04316000	1.07203900	H	1.54002500	0.32957900	2.18360300	H	2.11102200	0.85699500	-0.51411800
O	-0.11469200	-1.33903300	1.44640500	O	0.32489600	2.54962000	-0.03941900	O	-0.17598300	3.22997900	-0.05439200
H	0.54462200	-1.52566100	2.13608500	H	-0.31187400	3.23561000	0.21897100	H	0.01056000	3.86655200	0.65807100
O	1.60548300	0.72933700	0.89964400	O	-1.63200700	0.12267500	1.10744900	O	-1.38605600	0.85193000	0.34939700
H	2.53372500	0.48069100	0.61018100	H	-2.54380900	0.14298000	0.69959700	H	-2.31961900	0.65077200	0.10507600
H	-2.59243800	-0.46709700	-0.58149400	H	2.58707300	-0.37278600	-0.71318400	H	2.40593000	-1.24298600	-0.29400600
H	0.68854200	2.30353500	-1.18883200	H	-0.75697000	-2.45505800	1.40897700	H	-0.71543900	-0.33746300	2.68076300
H	1.04307500	-1.73183000	-1.61083200	H	-0.87852400	-0.11848900	-2.30290200	H	-0.89022200	-2.28970000	-1.27172700
H	1.65184200	1.36713400	1.63036500	H	-1.67436300	0.44195300	2.02405400	H	-1.21777400	1.83315600	0.29644200
H	-0.73112400	-2.09011000	1.42193800	H	0.92336000	3.00402900	-0.65373100	H	-0.39225100	3.77805900	-0.82926200
H	-1.43698700	0.87383900	2.12214700	H	1.01852800	1.58718600	1.27441500	H	0.86784300	1.93470600	-0.28099900
Al	0.00618800	0.05300300	0.06376300	Al	-0.03067600	-0.29633900	0.14267000	Al	0.02756300	-0.41071900	0.21539100
O	-3.90433900	-0.28752900	-0.34323600	O	3.83041700	-0.14371500	-0.52290000	O	3.55387100	-0.22355300	-0.76104100
H	-4.46607800	0.25888800	-0.91606100	H	4.44924100	-0.86068000	-0.30591600	H	4.33192300	-0.10418100	-0.18778200
H	-4.46726300	-0.99113700	0.01782700	H	4.31024800	0.50681200	-1.06170900	H	3.91329500	-0.31363600	-1.66167100
O	3.72088900	-0.28349500	-0.33534800	O	-3.65670800	0.03417400	-0.63851100	O	-3.50412800	-0.61035000	-0.77199000
H	4.30201200	0.25297900	-0.90276800	H	-4.28797700	-0.70590800	-0.68304500	H	-4.20773600	-1.05016300	-0.26237900
H	4.31458600	-0.92653000	0.09089700	H	-4.17745000	0.82361000	-0.87016200	H	-3.92942300	-0.32914500	-1.60156200

4.N_m'= 3

R				TS				P			
O	-0.01875500	-0.88529900	1.92531000	O	0.11743800	-1.34033100	2.35520200	O	-0.33604500	-3.17055500	1.61966800
H	-0.71814700	-1.31619300	2.44364700	H	-0.56304900	-1.80708900	2.86598400	H	-0.26282900	-4.06965600	1.25616000
O	0.86798400	-2.14672300	-0.23821000	O	0.77026400	-1.99372200	-0.01126500	O	1.13846700	-1.13829200	0.72187000
H	1.20977800	-2.49116900	-1.07976300	H	1.40082900	-2.52494000	-0.52420900	H	2.11842300	-0.97663100	0.82268200
O	-1.76527200	-1.37873700	-0.12290300	O	-1.74831600	-1.27787300	-0.33566200	O	-1.43398800	-1.11815900	0.26371900
H	-2.65563600	-0.90421000	-0.05573900	H	-2.63954300	-0.82453700	-0.19061200	H	-2.35721900	-0.76254100	0.37884400
O	-0.03119900	-0.34901300	-1.97462200	O	0.00665500	-0.35179400	-2.25524100	O	-0.01494500	-0.61144500	-2.04534200
H	0.59492100	0.19662500	-2.47773700	H	0.65721400	0.13906400	-2.78621200	H	0.58598800	-0.31158100	-2.74982000
O	1.48311300	0.55115500	0.13239200	O	1.45142800	0.63218700	-0.09186000	O	1.45758900	1.14295500	-0.50871800
H	1.43389400	1.52640300	0.26844300	H	1.41008600	1.59271000	0.12250400	H	1.33780000	2.12646700	-0.60999100
O	-1.10428600	1.13311600	0.21927900	O	-1.08851400	1.16265600	0.11384400	O	-1.10109300	1.44900000	-0.08450300
H	-2.08630300	1.18255400	0.22599100	H	-2.07317000	1.18823100	0.19312300	H	-2.07678400	1.38526500	0.11834600
H	1.20895300	-2.70808200	0.47754000	H	0.80760000	-2.19499700	0.96047100	H	0.83535800	-1.98024900	1.16519800
H	0.61180400	-0.49452600	2.55182400	H	0.72303700	-0.99354700	3.02890400	H	-0.50307400	-3.29773300	2.56933700
H	2.49437200	0.26473500	0.08638100	H	2.46421100	0.31866300	-0.08843500	H	2.38643200	0.91515000	-0.22964200
H	-0.68883900	2.03312400	0.34388200	H	-0.66976800	2.05696200	0.31504400	H	-0.79401500	2.38865200	-0.22652300
H	-0.73368100	-0.62713700	-2.58504400	H	-0.62929400	-0.76527500	-2.86493700	H	-0.63070800	-1.26323900	-2.42393000
H	-1.90509700	-2.32970400	-0.25399500	H	-1.85990400	-2.24158200	-0.36233400	H	-1.30886900	-1.97477500	0.75616400
Al	-0.08685800	-0.45601100	-0.00247500	Al	-0.09637600	-0.34695200	-0.34819500	Al	0.01038900	-0.02642200	-0.24270600
O	-3.75974100	0.29292000	0.10972500	O	-3.71839800	0.37742300	0.11304000	O	-3.54677000	0.53982100	0.46586600
H	-4.34102700	0.29426300	0.88916400	H	-4.25211900	0.33350200	0.92484900	H	-3.97487900	0.71372600	1.32167300
H	-4.34618300	0.50137200	-0.63729300	H	-4.34320000	0.63896500	-0.58502600	H	-4.26980200	0.56117800	-0.18423900
O	0.56416400	3.16884300	0.49742800	O	0.49356200	3.19562000	0.52471500	O	0.37771800	3.60945700	-0.58748200

H	0.65895100	3.85368000	-0.18530000	H	0.53941200	3.94285700	-0.09521500	H	0.28728400	4.12455000	-1.40745200
H	0.66255700	3.64442700	1.33898500	H	0.60753000	3.59166200	1.40489200	H	0.56831600	4.26846600	0.10195300
O	3.89053900	-0.13401400	0.02580800	O	3.82445600	-0.12863900	-0.11557500	O	3.58988000	-0.09592200	0.56874900
H	4.47061300	-0.18441800	0.80034400	H	4.37465400	-0.20758800	0.67845900	H	4.04174300	0.26105500	1.35251800
H	4.46767900	0.03515600	-0.73397000	H	4.42976300	0.06309600	-0.84828800	H	4.29609700	-0.49812700	0.03457000

5.N_m'= 4

R				TS				P			
O	-1.44649100	0.61100500	0.26107900	O	1.79465200	0.40416900	-0.08821000	O	0.35422500	-1.74384700	-0.56922300
H	-1.72029300	1.51685000	-0.02203900	H	2.16114500	1.11949000	0.49181900	H	-0.36897700	-2.26515200	-1.01300700
O	1.25179300	0.22682500	0.75325300	O	-0.88496600	0.86401600	-1.32971600	O	-0.43306000	-0.00181100	1.80443500
H	2.18793600	-0.05764000	0.73034400	H	-0.90883500	0.59622300	-2.26016400	H	0.21599500	-0.00280600	2.52401000
O	-0.64029700	-1.88511900	0.51444800	O	0.57976300	-1.50212400	-1.30910200	O	1.98995800	-0.00237100	0.47734800
H	-0.14356000	-2.69615500	0.69883300	H	0.07770000	-2.29715400	-1.54347300	H	2.55050200	0.81515200	0.43581800
O	1.43888900	-1.34976200	-1.30501200	O	-1.33899800	-1.25767600	0.57388600	O	0.35743800	1.74529800	-0.56431300
H	2.38536600	-1.35302600	-0.95079900	H	-2.37872000	-1.38541700	0.40747600	H	-0.36540100	2.26971900	-1.00512500
O	-1.13188500	-1.13924300	-1.98064900	O	0.73385500	-2.08013800	1.94763700	O	2.85189400	2.52418800	0.02039500
H	-1.33614400	-0.70657300	-2.82448000	H	0.84787200	-1.90658700	2.89414000	H	3.49995500	2.71954900	-0.67689600
O	0.19946100	1.13985600	-1.72743600	O	-0.20158900	1.05585700	1.38617000	O	-1.57110100	0.00258700	-0.75469400
H	0.97427300	1.32566500	-2.27854700	H	-0.98634900	1.13194500	1.94892600	H	-1.99186800	0.82068400	-1.12249500
H	-1.40888400	-1.81660400	1.14765900	H	1.49859800	-1.54565800	-1.70150100	H	2.54829800	-0.82132800	0.43480200
H	1.13722000	0.85881000	1.55915300	H	-1.43481000	1.77565300	-1.24453400	H	-1.41499600	-0.00097000	2.25380200
H	-2.07137300	0.24126800	0.93052600	H	2.49528500	0.01812000	-0.67228400	H	1.19305200	-2.26922100	-0.46161400
H	-0.36152200	1.96220300	-1.65664900	H	0.50737400	1.68773600	1.69319800	H	-1.99417400	-0.81427000	-1.12268300
H	-1.68124800	-1.93535500	-1.90754500	H	1.17088600	-2.93412500	1.81095500	H	3.05068500	3.15509400	0.73218900
H	1.37550700	-1.91516000	-2.08922200	H	-1.00347200	-1.87906400	1.25575600	H	1.19823700	2.26770000	-0.45792200
Al	-0.00944100	-0.36847700	-0.52226800	Al	-0.00498000	-0.15934100	-0.07034700	Al	0.13523200	0.00008500	0.05987600
O	-2.74399200	-1.10015200	1.95744300	O	3.12604900	-1.09145700	-1.92501600	O	2.84511100	-2.53114300	0.01792200
H	-3.63618700	-1.43595000	1.76902400	H	3.82451000	-1.72194600	-1.68183200	H	3.49324600	-2.72729800	-0.67908900
H	-2.71123000	-1.01155600	2.92416500	H	3.40014000	-0.73087400	-2.78499000	H	3.04207000	-3.16321800	0.72919300
O	-1.61585700	2.98766100	-1.08062500	O	2.08361300	2.37201900	1.74868900	O	-1.95413400	-2.52693700	-1.66862600
H	-1.37435900	3.83827300	-0.67860300	H	2.20940400	3.30218600	1.49758500	H	-2.54132400	-3.17704300	-1.24876300
H	-2.35662200	3.19498200	-1.67440700	H	2.61235000	2.25505800	2.55563700	H	-2.02488600	-2.70365600	-2.62153400
O	3.68993700	-1.05214500	-0.04223000	O	-3.77788600	-1.56253800	0.21045000	O	-1.94697700	2.53392200	-1.66679400
H	4.09578700	-1.77478900	0.46420000	H	-4.15575200	-2.22757600	-0.38351800	H	-2.53552600	3.18427900	-1.24917800
H	4.43654600	-0.56500700	-0.42786700	H	-4.43296900	-1.40582100	0.90638200	H	-2.01302500	2.71152300	-2.61987700
O	1.06240500	1.77564800	2.76107600	O	-2.17124400	2.97401300	-1.15728200	O	-2.65320300	0.00005600	2.87166600
H	1.42903700	2.67118800	2.77441700	H	-3.13790600	2.99740400	-1.21660200	H	-3.00984000	0.77984100	3.32265300
H	1.09297800	1.46237500	3.67624300	H	-1.84771200	3.81271900	-1.51852400	H	-3.01124200	-0.77922800	3.32241100

6.N_m'= 5

R				TS				P			
O	1.44646800	-0.74608300	-0.72495900	O	1.44139800	0.72526300	0.56364400	O	0.91682200	-1.14040800	-0.16740100
H	1.60797100	-1.71669500	-0.78687800	H	1.62795600	1.69231300	0.62477200	H	0.88743300	-1.90263100	-0.78902400
O	0.38368200	0.00260500	1.62911500	O	0.55126700	-0.08986500	-1.99700700	O	-1.12608500	-0.72593200	1.69940700
H	1.32570500	-0.05559300	2.02755200	H	1.52377900	-0.34393700	-2.34374200	H	-0.78528600	-1.56374700	2.26736800
O	0.44576900	1.75843600	-0.57525300	O	0.36194100	-1.64864400	0.42162500	O	0.72848600	1.35376800	0.46599500
H	-0.03519900	2.58253800	-0.31787500	H	-0.21110100	-2.44658400	0.32292600	H	0.51130800	2.29863700	0.65333800
O	-1.87234900	0.75463900	0.41674000	O	-1.84416500	-0.60454500	-0.53704000	O	-1.85956100	1.38499000	0.09272500
H	-2.04419800	1.72741700	0.44287500	H	-2.07837600	-1.56823900	-0.48381300	H	-1.66752700	2.32311400	0.36171000
O	-0.86513900	0.02974800	-2.09010900	O	-0.40426500	-0.06250000	3.00293700	O	4.90406700	0.78931500	-1.24072200
H	-1.28528200	-0.70744800	-2.55619100	H	-0.40950600	0.72512600	3.56471700	H	5.55703500	0.15184200	-1.55965100
O	-0.99413500	-1.73626000	-0.11630200	O	-0.83858300	1.75680000	-0.22266200	O	-1.39248500	-0.75163600	-1.33106000
H	-0.46064700	-2.56426400	-0.21150900	H	-0.30395900	2.56969000	-0.02207100	H	-1.03933600	-1.55028600	-1.81465800
H	1.37904700	1.93032800	-0.85240800	H	1.05353200	-1.75896500	1.12981100	H	1.72173300	1.14697600	0.51284800
H	-0.23241100	0.14800000	2.35921200	H	-0.01348100	0.03963600	-2.77227500	H	-1.89107300	-0.34986500	2.15942000
H	2.21364100	-0.21003300	-1.03979500	H	1.94698000	0.20091400	1.24334300	H	1.86091200	-0.85083500	0.03135000
H	-1.91552800	-1.90886500	0.19809200	H	-1.79675000	1.95973100	-0.37440500	H	-2.26575500	-0.44208200	-1.68868900
H	-0.77802200	0.76880400	-2.70933000	H	-1.00423400	-0.66582900	3.46345900	H	5.30542600	1.66239900	-1.34639100
H	-2.69283100	0.22164000	0.55190500	H	-2.64355400	-0.02608700	-0.63383900	H	-2.66516500	1.33340100	-0.48111500
Al	-0.21736400	0.00698300	-0.19110600	Al	-0.08895100	0.03245000	-0.26594800	Al	-0.52880100	0.02683500	0.13009100
O	3.01202400	1.37863000	-1.40157900	O	2.22098300	-1.16864000	2.24280700	O	3.04878800	0.23503200	0.45775600
H	3.27641000	1.56667700	-2.31675000	H	1.80087100	-1.03287700	3.10831600	H	3.78439500	0.45479600	-0.21573800
H	3.78629700	1.61854500	-0.86778800	H	3.09021000	-1.57076300	2.40107400	H	3.50656600	0.08558200	1.29892100
O	1.03274100	-3.45893800	-0.64194500	O	1.14030600	3.45001400	0.42999400	O	0.04005700	-2.81576000	-2.18949700
H	1.43327000	-4.03004900	0.03290600	H	1.58833900	3.98880900	-0.24220200	H	-0.24059300	-3.73627100	-2.06111200
H	1.02528100	-4.00065600	-1.44775300	H	1.10979300	4.01438700	1.21951200	H	0.46702100	-2.80217500	-3.06152200
O	-3.56210200	-1.36968300	0.70931300	O	-3.48803900	1.53092100	-0.69447300	O	-3.67200300	0.60542100	-1.77232200
H	-4.31037000	-1.54866300	0.11696600	H	-4.14778700	1.72412900	-0.00850500	H	-3.81081100	1.11330600	-2.58854100
H	-3.87995000	-1.62875800	1.58950100	H	-3.90083100	1.81483400	-1.52662200	H	-4.54722400	0.25100600	-1.54477000
O	2.70849400	-0.07780700	2.69752300	O	2.81081900	-0.68849600	-2.83028100	O	-0.37784100	-2.65984300	3.05156100
H	3.04516700	0.66192500	3.22297500	H	3.01622500	-1.55113700	-3.21887400	H	0.09440200	-2.55862000	3.89084500
H	3.10118000	-0.87367200	3.08298600	H	3.41460500	-0.04664300	-3.23129100	H	-0.88414200	-3.48344600	3.10789800
O	-1.52023000	3.45451100	0.25803500	O	-1.76124400	-3.26738300	-0.17330000	O	-0.66566700	3.67188000	0.83812800
H	-1.99707900	4.01123400	-0.37884100	H	-2.28822000	-3.71638200	0.50755600	H	-0.58265000	4.42231600	0.22736900
H	-1.45851000	3.99841800	1.05988400	H	-1.74147500	-3.88738500	-0.92048300	H	-0.79885500	4.07310900	1.71238500

7.N_m'= 6

R				TS				P			
O	-0.49706500	0.37951800	-2.40026000	O	1.01980300	0.52585200	-2.80702900	O	-1.94848900	-0.14471700	3.38582500
H	0.05260000	0.89787100	-3.00773700	H	1.61058900	-0.01269300	-3.35331300	H	-2.33393100	-0.93130800	3.79516200
O	1.18654600	-1.15033800	-1.05973600	O	-0.91991800	-0.59766400	-1.45105000	O	-0.08812300	-0.13789300	1.62068400
H	2.06641400	-1.41977600	-0.66748600	H	-1.79616200	-1.13839200	-1.48280100	H	0.80860400	-0.29994400	2.09404500
O	1.15322600	1.59251500	-0.68764500	O	1.40631000	-1.51807800	-0.39835700	O	-2.03335500	-0.71597700	-0.22679200
H	0.85811600	2.53434900	-0.64465000	H	2.38809800	-1.45816100	-0.33346400	H	-2.86460500	-0.20040700	-0.33487000
O	0.53038500	-0.10281700	1.32537700	O	-0.51023500	-0.80683600	1.37158200	O	0.33170500	-1.39408800	-1.13041000
H	0.04815200	-0.43280400	2.15672800	H	-1.07956500	-0.42059500	2.13800100	H	1.23844100	-1.56211100	-1.58815600
O	-1.48079600	-1.13206200	-0.35349500	O	-0.62737700	1.65261600	-0.01695800	O	1.38653800	0.97162600	-0.44140300
H	-2.37410900	-0.91305100	-0.00392900	H	-0.18694200	2.45978800	0.32619200	H	1.40101100	1.88201100	-0.81292300
O	-1.43422800	1.47202200	0.01168900	O	1.80795400	0.92466300	0.33976900	O	-1.10355900	1.62816900	-0.77414700
H	-1.27141200	2.44378200	-0.01665900	H	2.71814400	0.53405800	0.31588800	H	-2.08987900	1.73068600	-0.86312200
H	1.10702100	-1.56856300	-1.92833500	H	-0.59822900	-0.38112100	-2.34812500	H	-0.83822200	-0.17265000	2.31175400
H	-1.34089000	0.19289200	-2.83722600	H	0.96792100	1.37473300	-3.26935900	H	-2.01605000	0.56093500	4.04383700
H	-1.43675200	-2.12612800	-0.58600300	H	-1.58172200	1.89097400	-0.30106100	H	2.29662200	0.78290900	-0.05736700
H	-2.36021200	1.26004300	0.28256800	H	1.83500800	1.89453400	0.55735500	H	-0.62065500	2.46047200	-1.03130500
H	1.42622600	0.22008500	1.56332200	H	-0.37986900	-1.77275500	1.51317500	H	-0.24140500	-2.18908900	-1.24631400
H	2.02637600	1.50888800	-0.22345600	H	1.11406500	-2.40714900	-0.08478100	H	-2.18137600	-1.66897900	-0.44606800
Al	-0.10809900	0.15554000	-0.43894000	Al	0.23586200	-0.00969100	-0.12276200	Al	-0.27359700	0.06375400	-0.16771700
O	-3.73508600	0.17733500	0.59092500	O	1.28688800	3.48578300	0.86651000	O	0.67973600	3.48935500	-1.40213300
H	-4.04816400	0.06817700	1.50224200	H	1.33280200	3.83564800	1.77013100	H	0.81183900	3.76282700	-2.32400400
H	-4.54083800	0.27632200	0.05968300	H	1.58147100	4.21428900	0.29760900	H	0.80072700	4.29573000	-0.87587400
O	3.09521200	0.86934600	1.02466900	O	0.22587400	-3.47109500	1.11264700	O	-1.70939100	-3.24501100	-1.11295700
H	3.64962400	1.46241600	1.55385200	H	0.75532400	-3.93161500	1.78260200	H	-2.13632800	-3.54376600	-1.93164000
H	3.65862600	0.11847500	0.75960700	H	-0.40211900	-4.13805800	0.79484300	H	-1.69507800	-4.02502600	-0.53619300

O	-0.27933300	3.92033600	-0.34960300	O	3.97841100	-0.64842000	0.05161600	O	-3.76076400	1.34800900	-0.78520200
H	-0.51869000	4.50227100	-1.08838200	H	4.62662600	-0.51527300	-0.65808700	H	-4.32050300	1.77854200	-0.11945600
H	-0.09752200	4.52233000	0.38931300	H	4.49807900	-0.95199300	0.81283600	H	-4.28284100	1.36082000	-1.60341800
O	-0.69553800	-0.87469400	3.45853900	O	-1.89924200	0.09134800	3.29700900	O	2.56030000	-1.89367000	-2.25450800
H	-0.80934300	-0.28483400	4.21677400	H	-1.52587900	0.29765600	4.16512200	H	2.73523400	-1.67719200	-3.18146300
H	-0.64952400	-1.76843200	3.82507400	H	-2.82404200	-0.14741600	3.44863200	H	3.02375100	-2.72548000	-2.08084300
O	-1.39291700	-3.60124300	-1.03232900	O	-3.00309600	2.32428500	-0.68697800	O	3.78938300	0.64154800	0.65556800
H	-1.21312000	-4.34221100	-0.43746600	H	-3.65272700	2.63217700	-0.03995600	H	4.45488200	0.07815300	0.23283900
H	-1.93773200	-3.96082600	-1.74671800	H	-3.22547400	2.76300600	-1.51977200	H	4.26769900	1.44234300	0.92054600
O	3.66264800	-1.68265700	-0.15520000	O	-3.04016500	-1.97889000	-1.58609800	O	2.15228800	-0.63649900	2.69827300
H	4.35085800	-1.72730100	-0.83802900	H	-3.10908800	-2.74404700	-2.17433300	H	2.30734800	-0.99953700	3.58008600
H	3.85516600	-2.42408000	0.43968200	H	-3.93416500	-1.62012000	-1.50273000	H	2.98133100	-0.25556500	2.37267900

8.N_m'= 7

R				TS				P			
O	-0.51662200	-1.82383200	-0.18931300	O	-0.97288600	-1.53944700	0.34620200	O	-0.79095300	-1.15567500	-1.34524900
H	-1.48067100	-2.07850600	0.05719500	H	-1.94814700	-1.52869400	0.67835300	H	-1.78666400	-1.44001400	-1.42418900
O	0.51045900	0.23222700	1.48313700	O	0.57482300	0.83145900	1.40825600	O	0.40593000	-0.88632200	1.64465900
H	0.99342000	-0.36641800	2.13913400	H	1.36033100	0.65606600	2.04092300	H	1.25014900	-1.39718900	1.93595200
O	1.87853100	-0.85282100	-0.65742800	O	1.52109300	-1.26465200	-0.23587400	O	1.68546600	-0.65765400	-0.69989700
H	2.68361300	-0.34476400	-0.90984800	H	2.47539500	-1.07208500	-0.53435000	H	2.61762200	-0.31493300	-0.41808900
O	0.91970500	1.64369500	-0.86922800	O	0.88674400	0.98728500	-1.43305500	O	0.38316900	1.62943300	-0.24050900
H	1.87976500	1.70727400	-1.08074800	H	0.76186200	0.64358100	-2.33663800	H	1.24469200	2.00731900	-0.57199900
O	-0.31411100	-0.21696300	-2.30629700	O	-0.36167800	-0.88069400	-2.80778900	O	2.71256000	2.80115500	-1.00045100
H	-0.20808000	0.49181100	-2.95668000	H	-1.07206000	-0.66492400	-3.42820800	H	2.86849500	3.05317300	-1.92283900
O	-1.56387800	0.72992000	-0.11657200	O	-1.56601300	0.94743900	-0.21592100	O	-1.73151800	0.27615500	0.67464000
H	-1.71813900	1.29639700	0.68071500	H	-1.65845600	1.73694200	0.36539100	H	-1.96529700	0.08451300	1.61244200
H	2.06110700	-1.82287700	-0.58626600	H	1.45394400	-2.20598500	0.04024900	H	1.76744800	-1.24574800	-1.48203200
H	0.03368400	0.93803700	1.96860100	H	0.04057100	1.58516700	1.75103800	H	-0.23406900	-0.86804600	2.39455500
H	0.06164700	-2.61447700	-0.17162600	H	-0.60621400	-2.45034000	0.41527000	H	-0.25753000	-1.60263700	-2.04596400
H	-2.43641800	0.49589700	-0.53275900	H	-2.46621300	0.71098600	-0.56953800	H	-2.56152100	0.54069100	0.18662400
H	-0.50223600	-1.04436300	-2.77086400	H	0.04201300	-1.68014400	-3.17360600	H	2.95649900	3.58320500	-0.48283200
H	0.60192000	2.53382200	-0.55640500	H	1.15979300	1.97181900	-1.45075400	H	-0.22561500	2.40864500	-0.01791600
Al	0.15444900	-0.06348600	-0.36375700	Al	0.06725400	-0.07429700	-0.12780000	Al	0.00760300	-0.16747900	-0.01127100
O	1.71374900	-3.51666800	-0.33203600	O	0.62714900	-3.76377700	0.51081400	O	1.15901900	-2.23647100	-2.90919200
H	1.84441400	-4.15414400	-1.05108200	H	0.59933300	-4.50404100	-0.11441100	H	1.33552000	-1.94096800	-3.81549300
H	2.08105600	-3.94557600	0.45585800	H	0.81920500	-4.16788300	1.37071800	H	1.31848500	-3.19280000	-2.91802200
O	-2.93249200	-2.35835600	0.36233000	O	-3.36922500	-1.45999100	1.14674600	O	-3.20735300	-1.81249300	-1.50051200
H	-3.31203200	-3.17657700	0.70840800	H	-3.80236900	-2.06605500	1.76230500	H	-3.57781000	-2.59438900	-1.93107000
H	-3.63040300	-1.86674100	-0.09811800	H	-4.03927700	-1.10604700	0.54155300	H	-3.87264400	-1.10756600	-1.50784300
O	-1.25018600	2.28920700	2.02729200	O	-1.27202400	2.81916100	1.78363500	O	-1.75662000	-0.55949500	3.28541600
H	-0.94165600	3.15435100	1.70275900	H	-1.04203900	3.74990800	1.63976600	H	-1.74724400	0.03768300	4.04930600
H	-1.78104100	2.45192200	2.82081400	H	-1.86829500	2.81977400	2.54833000	H	-2.27822500	-1.32693600	3.56747500
O	1.72561800	-1.31576100	3.17800400	O	2.50460300	0.44816500	3.03572000	O	2.45311500	-2.15326000	2.45862700
H	2.58762200	-1.10042900	3.55998200	H	3.24427300	1.06206100	3.13954000	H	3.05218400	-1.79205800	3.12610500
H	1.24345900	-1.78763500	3.87101500	H	2.39791800	0.00602200	3.88905600	H	2.48946800	-3.11556000	2.54677000
O	3.59394900	1.13443400	-1.39048600	O	3.96387000	-0.88651900	-0.94381300	O	3.89429100	0.32990800	-0.01647900
H	3.95217600	1.19001200	-2.29027500	H	4.32616300	-1.03369600	-1.82764600	H	4.03002100	1.22494400	-0.36272500
H	4.31368000	1.43850300	-0.81621100	H	4.70503900	-0.97962000	-0.33057700	H	4.75631400	-0.09530600	0.08186700
O	0.08700400	4.04130900	0.13494000	O	1.56922000	3.45183900	-1.50124900	O	-1.09444500	3.70557700	0.23323400
H	0.77219800	4.63577700	0.47777700	H	2.49152800	3.72882000	-1.41155900	H	-1.13704100	4.18650400	1.07064400
H	-0.47755400	4.60936000	-0.41171600	H	1.15429700	4.09444000	-2.09330400	H	-1.30269400	4.35083600	-0.45597000
O	-4.04010100	-0.00727800	-0.96467300	O	-4.12927800	0.37959600	-0.93879500	O	-4.07915400	0.77852800	-0.56902000
H	-4.77900200	0.38364400	-0.47383800	H	-4.78524700	1.04844300	-0.68987500	H	-4.87437700	0.74013000	-0.01612100
H	-4.34335600	-0.03189800	-1.88435100	H	-4.42884400	0.05243100	-1.79964500	H	-4.23306200	1.51865100	-1.17423700

9.N_m'= 8

R				TS				P			
O	0.76400000	1.44334300	1.31485500	O	0.47686100	1.99322900	0.70880900	O	-0.80813500	-1.76508100	-1.35123900
H	0.30024600	1.79955200	2.10631600	H	0.07331000	2.49064800	1.46051700	H	-1.68532100	-1.88117000	-1.79898200
O	-1.01328800	1.03913900	-0.77008300	O	-1.36009000	0.86595900	-1.25464000	O	-0.89665500	-0.61890800	1.55439400
H	-0.71470300	1.83164100	-1.27106100	H	-1.10419900	1.29071700	-2.13355300	H	-0.32413400	-1.02798300	2.28162700
O	1.60275400	0.21393400	-0.86991300	O	1.39245900	0.28173600	-0.99494000	O	1.30065400	-1.19262700	0.00687900
H	2.15311900	-0.50912400	-1.32556000	H	1.92643500	-0.56340400	-1.25400700	H	2.15149300	-0.81248000	0.46080300
O	-0.48609800	-1.59694100	-0.71430700	O	-0.37617400	-1.52293100	-0.09575000	O	0.41513700	1.26335500	-0.45189700
H	-0.11717100	-2.47312500	-0.54296200	H	0.19467700	-2.01246400	0.52768300	H	1.30347200	1.43251500	-0.93978500
O	1.22627700	-1.36843000	1.28398100	O	1.49927000	-1.27362400	1.71144400	O	2.58349700	1.67835900	-1.70038900
H	0.93332400	-1.66234600	2.15662000	H	1.39849000	-1.31291900	2.67108800	H	2.61106500	2.17897500	-2.52495500
O	-1.19430700	-0.32757100	1.64167500	O	-1.28811800	0.32845300	1.55165800	O	-2.10386800	0.35582500	-0.68309700
H	-1.98604500	-0.96150700	1.63590800	H	-1.93881900	-0.39345400	1.84778500	H	-2.42257800	1.30059500	-0.70895300
H	2.07434300	1.07565900	-0.89343900	H	1.96775100	1.06641300	-1.10355600	H	1.50927600	-2.06512000	-0.37870500
H	-1.99087200	0.86720500	-0.95973800	H	-2.36621200	0.80612600	-1.21057100	H	-1.77203600	-0.33105000	1.96977800
H	1.35571300	2.12069800	0.90513500	H	1.25027100	2.47744900	0.32624600	H	-0.19767900	-2.52743200	-1.54691700
H	-1.32322900	0.33776600	2.35233600	H	-1.37959200	1.10576200	2.14342300	H	-2.77256500	-0.19504500	-1.14193000
H	2.19047200	-1.61265300	1.18254100	H	2.39621100	-1.62627200	1.53276100	H	3.47929400	1.70479300	-1.30636000
H	-1.13749200	-1.66886500	-1.46771900	H	-0.87946900	-2.13932400	-0.73026000	H	0.05039500	2.14236600	-0.09277000
Al	0.12861600	-0.06182800	0.28905300	Al	-0.16706700	0.32501800	0.03672800	Al	-0.37453400	-0.35453100	-0.17868300
O	2.23516500	2.82637500	-0.44077000	O	2.60235500	2.81072900	-0.71087600	O	1.13542800	-3.56042100	-1.54416600
H	3.06416400	3.31689800	-0.34425700	H	3.47934900	2.93065000	-0.31634100	H	1.66020700	-3.65379700	-2.35394100
H	1.65524800	3.33791400	-1.03699000	H	2.53269100	3.49717800	-1.39135500	H	1.05856800	-4.45628400	-1.18200600
O	-0.93455300	1.80352700	3.42148700	O	-0.98759400	2.78923500	2.82993700	O	-3.32865400	-1.62182900	-2.24038900
H	-1.57409900	2.52931200	3.47916400	H	-1.64329300	3.50163300	2.78485200	H	-4.01012800	-2.24493700	-1.94487000
H	-0.63276300	1.66298000	4.33203200	H	-0.60012400	2.85628100	3.71607100	H	-3.53323200	-1.44087900	-3.17086900
O	-3.45575700	0.38845400	-1.29751300	O	-3.95896000	0.70250700	-1.19260700	O	-3.11223800	0.09678900	2.71337700
H	-3.49045700	-0.29973100	-1.98036400	H	-4.43247700	0.09174000	-1.77303700	H	-3.13642900	0.79722200	3.37880800
H	-4.23091700	0.95389500	-1.41164400	H	-4.54504900	1.46199700	-1.07490700	H	-3.80140700	-0.53210500	2.96595200
O	-0.06584900	3.38673800	-2.01945600	O	-0.71541100	2.03901300	-3.48902400	O	0.51328000	-1.64148300	3.48205300
H	0.07342100	3.39688800	-2.97838800	H	-0.54296300	1.57760600	-4.32045700	H	0.80548500	-1.11009200	4.23454500
H	-0.56403800	4.19774800	-1.83691100	H	-1.08896200	2.89577000	-3.73593000	H	0.37005300	-2.53348900	3.82571500
O	2.99323700	-1.70879300	-1.81358600	O	2.75234900	-1.77646100	-1.51650100	O	3.37775700	-0.29336200	1.10547000
H	3.64467500	-2.05131000	-1.18286500	H	3.34449200	-2.11115200	-0.81247100	H	4.06134200	0.24406100	0.65223100
H	3.33774200	-1.85415700	-2.70457600	H	3.12940900	-2.01669800	-2.37212600	H	3.79587500	-0.73582100	1.85390500
O	-2.31399300	-1.92231600	-2.66720400	O	-1.66697700	-3.09996900	-1.64847400	O	-0.62313900	3.39192200	0.50923200
H	-2.06363600	-1.85382200	-3.60057100	H	-1.31443400	-3.48391900	-2.46203000	H	-0.17708900	4.15407800	0.89964400
H	-2.83993500	-2.73423300	-2.60826500	H	-2.32525400	-3.72469200	-1.31634100	H	-1.45220000	3.69644600	0.10976400
O	-3.21841900	-1.93148800	1.68687500	O	-2.98130600	-1.42984000	2.37816800	O	-3.09691200	2.86663600	-0.84058500
H	-3.32519600	-2.64148000	2.33455500	H	-2.87378800	-1.96513700	3.17570900	H	-3.23833400	3.26307500	-1.71321000
H	-4.11053300	-1.63788200	1.46014400	H	-3.93347800	-1.33621800	2.24290300	H	-3.90225200	3.06237300	-0.33889700
O	3.76267100	-2.21713100	0.97931300	O	3.97115300	-2.48556800	0.89897300	O	5.04772400	1.41180800	-0.36026200
H	3.91555900	-3.14945200	1.19602100	H	4.03678300	-3.43180500	1.09626500	H	5.42453800	2.16961100	0.11072200
H	4.51633200	-1.74542100	1.36402000	H	4.83665800	-2.12332100	1.13871000	H	5.78225000	1.04260100	-0.87250900

10.N_m'= 9

R

O	-0.41789700	-1.75333500	0.50004400
H	-1.26749500	-2.25057800	0.51225700
O	0.53396800	0.81926200	1.07167900
H	1.52955300	0.90429800	1.23920800
O	1.53247100	-0.62703300	-1.03107900
H	2.03333800	-0.18977300	-1.78450700
O	0.03461300	1.56146100	-1.50139300
H	-0.22312600	1.58717600	-2.43161500
O	-0.94425500	-0.86509100	-2.06177200
H	-1.91598400	-1.06570200	-2.12322700
O	-1.96239700	0.42033400	0.03601300
H	-2.24641300	1.31792800	0.42567400
H	2.19303000	-1.14501400	-0.49689200
H	0.05229400	1.23545500	1.82375200
H	0.23893700	-2.27250200	1.01950900
H	-2.73329700	-0.00195200	-0.39856000
H	-0.44614300	-1.50289400	-2.58991000
H	0.18245000	2.51139400	-1.18393600
Al	-0.17771200	-0.04179200	-0.44788100
O	1.38604300	-3.28770600	2.00540100
H	1.38959300	-4.24611000	1.86232300
H	1.38897800	-3.18114400	2.96816100
O	-2.84977600	-3.19721100	0.39002300
H	-3.41202500	-3.21619100	1.17900700
H	-2.80751100	-4.12013500	0.09759500
O	-0.69000700	2.21182300	3.16477600
H	-0.19324500	2.98992600	3.45777500
H	-0.99015000	1.78676600	3.98128900
O	3.07710000	0.87864100	1.45941400
H	3.65209400	1.47993300	1.94807500
H	3.52675200	0.02228300	1.37530800
O	2.84563100	0.36692700	-3.07227300
H	3.08824500	-0.16197700	-3.84397900
H	3.45807900	1.11360100	-3.06155100
O	0.36238300	4.01751800	-0.75379500
H	1.10334700	4.57259700	-1.03083700
H	-0.39893800	4.60618000	-0.66951700
O	-2.54792500	2.68881800	1.07000800
H	-3.40743000	3.13001300	1.06180400
H	-2.17371000	2.77389200	1.96378300
O	-3.51686300	-1.21098700	-1.54109100
H	-4.30051900	-1.05937300	-2.08949500
H	-3.65929900	-2.03268300	-1.03540500
O	3.34634700	-1.81941100	0.54970300
H	4.17715000	-2.18770000	0.21712100
H	2.95621400	-2.48649600	1.14396800

TS

O	-0.91423900	1.50777900	-0.46335000
H	-1.88440800	1.56095800	-0.65411200
O	0.64861500	-0.98241300	-1.33499900
H	1.58231200	-0.88859200	-1.71057600
O	1.53213700	0.98738700	0.32333600
H	2.19285000	0.88704700	1.06757000
O	0.47212400	-1.01489300	1.66135400
H	-0.09168300	-0.79520900	2.42812100
O	-1.30370000	0.67017100	2.60673300
H	-2.26905600	0.56050500	2.54501700
O	-1.66844800	-0.92792600	0.03836400
H	-1.72992300	-1.93516400	-0.09740500
H	1.89903600	1.66279400	-0.33797600
H	0.16718200	-1.64114000	-1.89974200
H	-0.55240800	2.42828200	-0.52587200
H	-2.49237000	-0.63940600	0.51772100
H	-1.14692900	1.27900500	3.34008600
H	1.21811900	-1.66710900	1.90437000
Al	-0.00671000	-0.04975600	0.13185700
O	-0.11231900	4.11719500	-0.83711200
H	-0.12635500	4.77930200	-0.13077100
H	-0.47508000	4.56694300	-1.61431600
O	-3.63552200	1.87358200	-0.82034400
H	-4.08264500	1.58099900	-1.62814900
H	-3.96318800	2.77228500	-0.66825500
O	-0.48977000	-2.90584900	-2.92704400
H	0.12114500	-3.58994900	-3.23836700
H	-1.02719800	-2.67986100	-3.70007100
O	3.01156400	-0.81872000	-2.39712000
H	3.71603800	-1.46996100	-2.28355000
H	3.17137200	-0.39007000	-3.24804100
O	3.37285600	0.78076000	2.22338200
H	3.37742800	1.33224100	3.01718600
H	4.30236900	0.66556900	1.98504300
O	2.31881200	-2.66108400	2.28175000
H	3.02623700	-2.43042700	2.89763300
H	2.16903200	-3.61098600	2.37736900
O	-1.74386600	-3.44448000	-0.41594000
H	-2.28349800	-4.14344100	-0.02582200
H	-1.56815000	-3.67389000	-1.34161900
O	-3.77653600	-0.00032000	1.38179800
H	-4.49528300	-0.50240300	1.79173600
H	-4.18418700	0.68209900	0.82288200
O	2.34540900	2.74502400	-1.36268500
H	3.24362700	2.97990600	-1.62669100
H	1.81591600	3.55677900	-1.34251600

P

O	0.20523600	-1.57863500	-0.94413800
H	1.05264600	-2.01006400	-1.23310800
O	-0.41232500	1.56703800	-0.94163700
H	-1.30954700	2.03362400	-0.92814300
O	-1.83691600	-0.31991900	0.20892400
H	-2.29531800	-0.60700600	1.03730300
O	0.22065900	0.01048600	1.82320300
H	1.10815200	-0.21360600	2.25893800
O	2.49870700	-0.63412700	2.84022700
H	3.15614300	-1.10638600	2.30784100
O	1.84082000	0.38338800	-0.27171000
H	2.20720000	1.32495300	-0.14146300
H	-2.49914500	-0.40110300	-0.55458400
H	0.20635700	2.13393100	-1.47713800
H	-0.54555200	-2.14523300	-1.27074800
H	2.59949800	-0.24077200	-0.09635600
H	2.73202700	-0.73919100	3.77097400
H	-0.43749500	0.34747600	2.52919900
Al	0.01067100	0.03512100	0.00916200
O	-1.73182000	-3.13194100	-2.05627100
H	-2.05603500	-3.93692800	-1.62663400
H	-1.57597700	-3.38408200	-2.97841900
O	2.45574900	-2.97389700	-1.62188600
H	2.85214600	-2.89183400	-2.50212900
H	2.41855500	-3.92677500	-1.45029000
O	1.12072300	3.29947100	-2.37575700
H	0.76421400	4.19662400	-2.45133800
H	1.46609500	3.09113900	-3.25568200
O	-2.64719300	2.88579000	-0.97507200
H	-2.90283200	3.53701600	-0.30865600
H	-3.12062600	3.12206700	-1.78333400
O	-3.31108900	-1.04084800	2.43838600
H	-3.31053700	-1.93117200	2.81810200
H	-4.24204800	-0.77492800	2.42339800
O	-1.47979300	0.86765100	3.50083400
H	-2.26130200	0.30892800	3.62790700
H	-1.33373600	1.38409500	4.30347200
O	2.68097700	2.78315500	-0.01929700
H	3.35180800	3.17502300	0.55347100
H	2.58694600	3.33691500	-0.80775300
O	3.83159400	-1.28529100	0.32626800
H	4.76273100	-1.02116100	0.30862000
H	3.76214700	-2.08836800	-0.21547800
O	-3.39702000	-0.71136500	-1.78523200
H	-4.28294900	-0.39495900	-2.00146800
H	-3.29877000	-1.60245400	-2.15034200

11.N_m'= 10

R

O	-0.64587800	0.21704000	1.69157100
H	-0.04798500	0.42848700	2.47468800
O	1.41526600	-1.09754800	0.49344700
H	1.39997200	-1.90206100	1.08540200
O	-1.27855500	-1.60401100	-0.16647600
H	-1.59622100	-1.92438900	-1.03965800
O	0.36194800	-0.43336100	-1.93391500
H	-0.35880700	-0.75589800	-2.51692200
O	-1.58097200	1.02157500	-0.76641100
H	-1.39712100	1.95814800	-0.91488400
O	0.92575500	1.53838700	-0.11556100
H	1.66761500	1.71527800	-0.77579100
H	-1.77746500	-2.05126800	0.56578200
H	2.34732400	-0.92624300	0.20347700
H	-1.60618600	0.23817100	1.98216200
H	1.09443900	2.10830500	0.67213500
H	-2.43710400	0.79779500	-1.20487000
H	1.22237900	-0.74381700	-2.31030300
Al	-0.09424200	-0.08513000	-0.06870000
O	-2.74754200	-2.81702600	1.78450800
H	-3.52119600	-3.33998600	1.52880600
H	-2.29092600	-3.35432400	2.44715600
O	0.94815000	0.92212400	3.59917100
H	0.90684700	0.77711700	4.55229300
H	1.26332000	1.82759100	3.44818100
O	3.87093700	-0.63798200	-0.57685900
H	3.84872500	-1.07736900	-1.44525300
H	4.70092100	-0.89190700	-0.14996600
O	1.41240900	-3.21668600	2.07849600
H	1.58654700	-4.11576100	1.77066000
H	1.78289900	-3.16937500	2.96959900
O	-1.95283600	-1.67664500	-2.80178700
H	-2.74305400	-1.11154500	-2.90126900
H	-2.02713200	-2.38547800	-3.45601900
O	2.71320300	-1.27700100	-3.11437800
H	2.77303200	-2.15019000	-3.52884000
H	3.01976900	-0.65486100	-3.79058900
O	1.54431000	3.24424900	2.01803700
H	0.99603500	4.02840800	2.16646600
H	2.45534300	3.56972900	2.05582800
O	-3.15369500	0.03541800	2.36580700
H	-3.69935500	0.59810300	2.92958100
H	-3.39523900	-0.88457800	2.54708200
O	2.95856400	1.82789100	-1.69699600
H	3.31044300	2.62983200	-2.10456000
H	3.70145600	1.31542500	-1.34073100
O	-3.79905000	0.42371000	-2.30095200
H	-4.66564900	0.23319400	-1.91224800
H	-3.98219900	1.05003000	-3.01778100

TS

O	-0.50542500	0.31880200	1.66948400
H	0.04080800	0.71228300	2.42612000
O	1.60328100	-1.38072700	0.47179700
H	1.52973100	-2.36102400	0.70309800
O	-1.15495600	-1.56530900	-0.03179000
H	-1.65080300	-1.80876100	-0.88358200
O	0.27164600	-0.29205700	-1.80805900
H	-0.38792700	0.30789100	-2.21131200
O	-1.77594200	1.25512500	-1.40618900
H	-1.80097300	2.22008000	-1.41310600
O	1.26090800	1.33278800	0.02849000
H	2.01919900	1.44876500	-0.60991700
H	-1.64543000	-1.97200100	0.72085100
H	2.56094300	-1.13711600	0.43383400
H	-1.47672300	0.25425100	1.95817700
H	1.26032400	2.09485000	0.65725200
H	-2.66325200	0.96984500	-1.70928500
H	1.05291200	-0.49719200	-2.43124500
Al	0.18165500	-0.25259800	0.05748000
O	-2.77158300	-2.73876700	1.91678000
H	-3.54644700	-3.18906700	1.55066400
H	-2.44418400	-3.32993800	2.60926800
O	0.94260300	1.37994300	3.50747200
H	0.92807800	1.23111700	4.46111700
H	1.15555500	2.31231900	3.34796100
O	4.29265100	-0.78140600	0.21650800
H	4.79222900	-1.46878100	-0.24911300
H	4.81294300	-0.59222500	1.01137900
O	1.48842700	-3.89250000	1.12025700
H	1.50067600	-4.62920700	0.49557100
H	1.82816000	-4.23929700	1.95558200
O	-2.60014600	-2.09120400	-2.08108400
H	-3.28696500	-1.45410400	-2.35546200
H	-2.70086400	-2.89595500	-2.60249400
O	2.31225900	-0.73078200	-3.25435400
H	2.35713000	-1.14777100	-4.12471300
H	2.93523200	0.00984800	-3.23956000
O	1.42193400	3.54310900	1.71123100
H	0.77071500	4.25722100	1.65641200
H	2.27647200	3.99264400	1.78163600
O	-2.94998200	0.04731400	2.39237000
H	-3.48734500	0.61285100	2.96027700
H	-3.21491400	-0.87540800	2.53670400
O	3.42963600	1.36322700	-1.53357100
H	3.90229300	2.14862200	-1.84256000
H	4.06608000	0.82138600	-1.03424200
O	-4.18008300	0.19980500	-2.54211700
H	-5.04443400	0.27488900	-2.11314900
H	-4.33371200	0.47028600	-3.45916600

P

O	-0.29878900	0.52479300	1.98357500
H	0.30250400	0.85807000	2.73675400
O	1.46272800	-1.53401700	0.25499900
H	1.21131500	-2.50945400	0.24597600
O	-1.19299200	-1.33182500	0.32983500
H	-1.52409200	-1.83552000	-0.48705300
O	-0.26741100	0.59105000	-1.23556700
H	-1.20403500	0.58868100	-1.64139700
O	-2.59379900	0.68981900	-2.27513800
H	-3.07825200	1.52009900	-2.35299000
O	1.76511600	1.07663100	0.44516800
H	2.52660700	1.11207000	-0.20361900
H	-1.77554500	-1.57989400	1.08481500
H	2.44929600	-1.47997200	0.20576200
H	-1.27465000	0.64468300	2.26247000
H	1.79151100	1.91655700	0.96759400
H	-2.99421100	0.04949700	-2.89621000
H	0.34914300	1.11494100	-1.83932800
Al	0.25761500	-0.11321700	0.36593800
O	-3.05194800	-2.04544700	2.29664800
H	-3.89536900	-2.36382300	1.94407200
H	-2.86047700	-2.62380400	3.04860000
O	1.23905200	1.41746200	3.80550800
H	1.21066500	1.27653500	4.76001200
H	1.58444500	2.30647800	3.63363900
O	4.20413400	-1.55715000	-0.10782400
H	4.52602300	-2.28188000	-0.66417900
H	4.79759400	-1.54863900	0.65781700
O	0.99091500	-4.10303800	0.24638000
H	1.15975500	-4.68299800	-0.50733600
H	1.08209600	-4.65433900	1.03469100
O	-2.05075700	-2.66156900	-1.70414200
H	-2.63266200	-2.34309300	-2.42354100
H	-2.07190600	-3.62497100	-1.72549400
O	1.38373600	1.86968500	-2.76832800
H	1.18289300	2.35400600	-3.57874300
H	2.30185400	1.56959900	-2.82097800
O	2.05443200	3.40123500	1.91664700
H	1.50427900	4.18218200	1.76043400
H	2.95324700	3.74564200	2.01993100
O	-2.74431600	0.74600900	2.62870400
H	-3.20222600	1.44822900	3.10655900
H	-3.19736600	-0.09579200	2.79551100
O	3.77431800	1.03094700	-1.28006200
H	4.44692100	1.71753000	-1.38810500
H	4.24917300	0.19708700	-1.11749400
O	-3.61211300	-1.47781600	-3.74495100
H	-4.57229600	-1.60188400	-3.74127500
H	-3.34238100	-1.61715000	-4.66414400

12.N_m'= 11

R				TS				P			
O	-0.36215700	0.26147300	1.62791800	O	-0.40301100	0.13794100	1.71862100	O	-0.41243400	0.08215800	1.87492300
H	0.21678800	-0.07612200	2.37271200	H	0.24492900	0.06614500	2.49177100	H	0.25916400	0.13026500	2.63540200
O	0.03832100	-1.88136400	-0.13167000	O	-0.03602900	-2.26547600	-0.08285300	O	-0.08757900	-2.40661700	-0.10487700
H	-0.72825600	-2.49686100	-0.29903000	H	-0.79673300	-2.86060500	-0.37331000	H	-0.86073900	-2.93639700	-0.48122100
O	-1.91086600	-0.03153000	-0.55056400	O	-1.92618100	-0.28706300	-0.38070500	O	-1.95132100	-0.49103100	-0.21939800
H	-2.30666700	0.28845900	-1.41607300	H	-2.29892200	0.21214800	-1.18331700	H	-2.29863600	0.08149500	-0.98055200
O	0.27802800	-0.07134900	-2.10632200	O	0.22719100	0.07720600	-1.78860700	O	0.23137000	0.45870500	-1.27297400
H	0.36091600	0.72973100	-2.63668500	H	0.37210700	1.04577100	-1.85267800	H	0.21814200	1.49001700	-1.22771200
O	-0.05235100	2.00008800	-0.48290600	O	0.06258600	2.41241300	-0.67916000	O	0.10842900	2.94060800	-0.99289200
H	0.58420100	2.59955500	-0.03244200	H	0.72308300	3.00542100	-0.27696200	H	0.83902400	3.49987800	-0.67627100
O	1.85030600	0.08601700	0.12035100	O	1.78233300	-0.30361700	0.37135200	O	1.77211600	-0.66102400	0.63490600
H	2.51577200	-0.40109500	-0.43181700	H	2.46786500	-0.74525400	-0.19611300	H	2.43817100	-1.09450200	0.03529500
H	-2.64085900	-0.21187400	0.08346900	H	-2.68058700	-0.46674500	0.22616300	H	-2.71723300	-0.71184200	0.35831400
H	0.82542800	-2.42776100	0.08129600	H	0.75005700	-2.83706600	0.09504700	H	0.66690300	-3.03288800	0.03304600
H	-1.12570700	0.78510500	2.01032800	H	-1.23471800	0.61872900	2.03968900	H	-1.29069500	0.48944600	2.19133600
H	2.31964100	0.53810800	0.87316400	H	2.23903600	0.37278200	0.95194600	H	2.22220300	0.13059400	1.04198500
H	-0.82324800	2.54454400	-0.77092500	H	-0.67457400	2.97973100	-0.97656000	H	-0.57726100	3.47295800	-1.43773000
H	0.70173600	-0.84588800	-2.61203200	H	0.77979100	-0.44984300	-2.46211400	H	0.83294900	0.12159100	-2.00438700
Al	-0.03690700	0.03660500	-0.21488800	Al	-0.08713700	-0.40537800	-0.00875300	Al	-0.10371100	-0.57646300	0.20445500
O	-4.12463700	-0.33300100	1.14293800	O	-4.22728200	-0.53859400	1.19150900	O	-4.26757700	-0.83529000	1.32216100
H	-4.96996400	-0.03472600	0.77754100	H	-5.01544800	-0.19649300	0.74546700	H	-5.06605000	-0.49195400	0.89592200
H	-4.32680200	-1.17048900	1.58315300	H	-4.52423700	-1.33838900	1.64783400	H	-4.55120700	-1.64207900	1.77469300
O	1.31181600	-0.44992700	3.49432000	O	1.29753500	0.05790000	3.64578600	O	1.32087100	0.32187400	3.73875800
H	1.16363600	-0.79952000	4.38171900	H	1.18590600	-0.15986100	4.57918700	H	1.26526400	0.17622900	4.69098300
H	2.01290900	0.21569500	3.55265400	H	2.00070100	0.71846800	3.56495700	H	2.00690500	0.98097100	3.56294000
O	2.27359100	-3.57506900	0.26899500	O	2.15462000	-3.93874500	0.18465500	O	1.98796000	-4.21426700	0.01850600
H	2.19371500	-4.42963700	-0.17949100	H	2.07926000	-4.76913800	-0.30877400	H	1.86962700	-4.99668400	-0.54049500
H	2.57633600	-3.78989100	1.16299400	H	2.46964400	-4.19822800	1.06308600	H	2.29909000	-4.55826800	0.86905700
O	-1.93404300	-3.61721800	-0.51208100	O	-1.91883200	-3.91195300	-0.79332200	O	-1.96848100	-3.92764400	-1.04802600
H	-2.23425900	-3.92518000	-1.37661900	H	-2.16212900	-4.12968700	-1.70214700	H	-2.19252600	-4.03930100	-1.98068200
H	-2.14662500	-4.32576200	0.10864100	H	-2.25454500	-4.62956500	-0.24097600	H	-2.34555100	-4.68515700	-0.58244700
O	-2.82122900	1.08713700	-2.70685500	O	-2.98863700	1.11681600	-2.23484900	O	-2.93916000	1.04029500	-2.05449800
H	-2.91840000	2.04523700	-2.59619200	H	-2.85749900	2.08436100	-2.24732100	H	-2.74626600	1.98714400	-2.19680100
H	-3.38911500	0.80742500	-3.43526000	H	-3.49420000	0.86466700	-3.01591500	H	-3.53303700	0.75892900	-2.75996500
O	1.51846200	-1.97610900	-3.26851400	O	1.66327700	-1.36488000	-3.31427300	O	1.82957600	-0.63596900	-2.99459500
H	1.49695900	-2.25460900	-4.19280100	H	1.71847000	-1.40866900	-4.27690000	H	1.93289000	-0.51924600	-3.94648800
H	2.44206100	-1.96944800	-2.97016500	H	2.52815000	-1.59391800	-2.93916500	H	2.59085200	-1.13745100	-2.66384700
O	3.01427200	1.45679100	2.09592000	O	2.98122800	1.54979700	1.85081200	O	2.96699800	1.53196000	1.67321700
H	2.76478400	2.38048300	1.91243600	H	2.79518200	2.45974200	1.53405800	H	2.81260600	2.40524700	1.25500600
H	3.95982100	1.46109000	2.29855400	H	3.92855400	1.51344200	2.03989500	H	3.90985900	1.50153600	1.88404500
O	-2.46894500	1.54432800	2.49777400	O	-2.55646200	1.30136000	2.52269500	O	-2.64232600	1.05557500	2.66140000
H	-2.60012800	2.01010600	3.33276100	H	-2.68291100	1.82789500	3.32103600	H	-2.80418300	1.61808000	3.42817200
H	-3.27051800	1.02297100	2.32413100	H	-3.37361600	0.80298300	2.35477700	H	-3.43862500	0.52471900	2.49368700
O	3.51815000	-1.53966100	-1.25630700	O	3.49108900	-1.76474500	-1.12653000	O	3.45731300	-1.97466300	-0.99113800
H	4.46083700	-1.39020600	-1.41216900	H	4.44506500	-1.62437000	-1.20389900	H	4.42049500	-1.88589100	-0.99243200
H	3.43658900	-2.36627000	-0.74413000	H	3.36618100	-2.65774500	-0.75592000	H	3.26285100	-2.90967100	-0.79809700
O	1.73483300	3.74847300	0.86086100	O	2.15138800	3.98417900	0.69501600	O	2.41945800	4.04581800	0.36126000
H	1.33678700	4.40276100	1.45348500	H	1.84884700	4.66631600	1.31175800	H	2.21966300	4.76534200	0.97758000
H	2.34042500	4.25823700	0.30256300	H	2.78860000	4.43571500	0.12263100	H	3.13750000	4.38916100	-0.19015900
O	-2.09364800	3.61430900	-1.48354700	O	-2.18625000	3.80304300	-1.89315000	O	-2.20063600	3.81282400	-2.37285500
H	-2.74013200	4.03675200	-0.90040800	H	-2.79134900	4.36799300	-1.39212100	H	-2.80829300	4.44880300	-1.96913000
H	-1.81653500	4.31158600	-2.09554700	H	-1.96538000	4.31575400	-2.68396700	H	-2.08872100	4.11976100	-3.28406100

13.N_m'= 12

R				TS				P			
O	0.52809900	1.49769700	1.05190900	O	0.65505000	1.25513000	0.97979500	O	0.64625600	1.19397800	0.48497800
H	-0.06411800	2.25201000	1.29887700	H	0.12471300	2.03114800	1.30460900	H	0.23954500	2.01660500	0.86516500
O	-1.53461400	-0.32017500	1.06445700	O	-1.70203200	-0.31938200	1.28051600	O	-1.64082500	-0.35973900	1.42083100
H	-2.19003100	0.37549600	1.33138200	H	-2.34708400	0.42627600	1.46851400	H	-2.21739300	0.39628600	1.74375600
O	-1.06448700	1.21056000	-1.08648100	O	-0.98680400	1.10575700	-1.04002500	O	-1.50347200	1.11824200	-0.94801700
H	-0.79420200	2.13518500	-1.32458200	H	-0.72746200	2.07646800	-1.13628200	H	-1.22652100	2.05736000	-1.20517200
O	-0.51961400	-1.48402200	-1.13045000	O	-0.75575200	-1.52245900	-1.04097700	O	-1.27248400	-1.51268500	-1.11330700
H	0.07277100	-2.23864400	-1.37598100	H	-0.20861600	-2.32883200	-1.32439100	H	-0.83478400	-2.06835600	-1.83892300
O	1.54348800	0.33315200	-1.14268600	O	2.59048100	0.10149900	-1.46367500	O	4.67585200	0.16639200	-1.20451600
H	2.19993100	-0.36223900	-1.40839700	H	3.25123000	-0.61829900	-1.43474800	H	5.16707000	-0.45641300	-0.63868200
O	1.07326300	-1.19719600	1.00779400	O	0.94878400	-1.37909600	0.90356900	O	0.84532300	-1.40768400	0.34311000
H	2.03081100	-1.06197400	1.22162900	H	1.90462900	-1.24502200	1.22147200	H	1.69622600	-1.26570900	0.87888400
H	-2.02254800	1.07605500	-1.29889700	H	-1.91228300	1.00389600	-1.37114400	H	-2.47979700	1.02333500	-1.07069900
H	-1.88836700	-1.21724000	1.28914000	H	-2.11924500	-1.20260000	1.49270600	H	-1.99266400	-1.24966500	1.72533600
H	1.46743300	1.72039400	1.28126800	H	1.61771200	1.55554800	0.84659400	H	1.62887500	1.38808600	0.25800000
H	0.80296600	-2.12150400	1.24713600	H	0.67664800	-2.32677200	1.04728500	H	0.60705200	-2.38293100	0.38219400
H	1.89710800	1.23020900	-1.36737700	H	2.54104400	0.36834200	-2.39116900	H	5.22170100	0.34165700	-1.98018800
H	-1.45881000	-1.70731200	-1.35931600	H	-1.70644400	-1.68685400	-1.27738200	H	-2.24411500	-1.72224100	-1.07732800
Al	0.00427400	0.00680600	-0.03939200	Al	-0.23193300	-0.16769800	0.14878800	Al	-0.49754200	-0.19473500	-0.02374300
O	-0.23886500	3.75702400	-1.37235900	O	-0.45888300	3.68253800	-1.15111300	O	-0.81116600	3.59025600	-1.41485400
H	0.73631400	3.72997300	-1.42990500	H	0.49866900	3.94475000	-1.29243400	H	0.13108800	3.68355200	-1.74393400
H	-0.53819800	4.38351500	-2.04646800	H	-0.97690900	4.22039700	-1.76566400	H	-1.35789000	4.16044700	-1.97243100
O	-3.72690100	0.78257900	-1.27872400	O	-3.69570200	0.89602200	-1.32989700	O	-4.20181800	0.88017100	-0.67763300
H	-4.32577400	1.15349100	-1.94277700	H	-4.25805200	1.28621800	-2.01464600	H	-4.89584600	1.26173300	-1.23455100
H	-3.98939500	1.16123400	-0.41886100	H	-3.93817800	1.32754400	-0.49080200	H	-4.26778600	1.32132500	0.18726000
O	2.49337600	2.85862900	-1.36568100	O	2.09725900	4.21497800	-1.41098300	O	1.70997000	3.63336700	-2.13177200
H	2.98275100	2.89627800	-0.52247500	H	2.70252500	3.83637600	-0.75696700	H	2.37623200	3.18401500	-1.58665400
H	3.08949100	3.19456400	-2.05056400	H	2.51179100	5.00406300	-1.78116600	H	2.16413900	4.24371300	-2.72450400
O	3.32227300	-1.65503000	-1.50285800	O	4.73336500	-1.75162800	-0.86266200	O	5.64239500	-1.65494900	0.77308600
H	2.81023600	-2.48649800	-1.54039300	H	4.78019500	-2.66747300	-1.17094600	H	5.91139800	-2.53904900	0.48634800
H	3.98836800	-1.70861800	-2.20274900	H	5.61903300	-1.39426200	-1.02215400	H	6.36916300	-1.34041700	1.32978600
O	-3.14270200	-2.04042000	-1.39113700	O	-3.39633300	-1.95644000	-1.27432400	O	-3.87088300	-1.98996200	-0.67340900
H	-3.61114700	-1.18334500	-1.41236600	H	-3.81480500	-1.07793500	-1.35338400	H	-4.31261900	-1.12009200	-0.66482200
H	-3.54378100	-2.59107300	-2.07850800	H	-3.82285600	-2.52579900	-1.93056200	H	-4.42843200	-2.57918300	-1.20131100
O	1.17748100	-3.57153400	-1.41739600	O	0.55266600	-3.65480400	-1.60700700	O	-0.16087800	-2.90319700	-2.97089400
H	0.99287000	-4.01595900	-0.56865100	H	0.45025900	-4.29849400	-0.89075600	H	0.04838900	-3.84207200	-2.89021700
H	1.14411400	-4.25316900	-2.10400800	H	0.61683400	-4.13782700	-2.44064500	H	-0.19400500	-2.70520900	-3.91558300
O	3.73578300	-0.76835500	1.20131800	O	3.41835900	-1.11685500	1.54339500	O	3.00936400	-1.16541600	1.72227700
H	4.33459400	-1.13837500	1.86591200	H	3.79812300	-1.30440900	2.41109500	H	3.00048800	-1.27984600	2.67995100
H	3.99891600	-1.14739900	0.34187700	H	4.03421300	-1.45647800	0.86384500	H	3.90758700	-1.40882800	1.41636400
O	0.24721100	-3.74320500	1.29514200	O	-0.03018100	-3.85808600	1.22383500	O	-0.02972100	-3.86360600	0.58894700
H	0.54655600	-4.36979800	1.96916900	H	0.32103800	-4.50778700	1.84845900	H	0.44837500	-4.67891700	0.78569700
H	-0.72796700	-3.71651900	1.35267000	H	-0.98277700	-3.78225100	1.41072600	H	-0.85568900	-3.88386100	1.09672700
O	-1.16842600	3.58512500	1.34059400	O	-0.97077800	3.34958300	1.53233400	O	-0.76772400	3.36105700	1.31755900
H	-0.98366200	4.02916000	0.49165400	H	-0.86234200	3.82656000	0.68185200	H	-0.84635700	3.81456400	0.45103400
H	-1.13517100	4.26713900	2.02683100	H	-0.81613800	3.98666900	2.24456800	H	-0.46309600	4.01934800	1.95811300
O	3.15057300	2.05368700	1.31389000	O	3.00744900	2.09541000	0.36950400	O	3.01139100	1.92080900	-0.18390400

H	3.61914400	1.19662900	1.33480000
H	3.55162700	2.60402600	2.00155200
O	-3.31338400	1.66796300	1.42555400
H	-2.80176300	2.49958900	1.46419100
H	-3.97968000	1.72059300	2.12540700
O	-2.48560900	-2.84486300	1.28768800
H	-2.97493700	-2.88142000	0.44439400
H	-3.08201800	-3.18019000	1.97256400

H	3.18215100	1.43463900	-0.33529200
H	3.75416300	2.08451000	0.98310900
O	-3.30483300	1.75191700	1.47431900
H	-2.69353600	2.50731700	1.59912400
H	-4.01650400	1.85817600	2.12183100
O	-2.76363100	-2.74081900	1.45136500
H	-3.27004100	-2.77015600	0.61848000
H	-3.34827200	-3.06885100	2.15004900

H	3.65792900	1.26151500	-0.57771600
H	3.50683000	2.40022300	0.49364200
O	-3.07842500	1.77439200	1.93565200
H	-2.44263300	2.51320000	1.84380400
H	-3.58708600	1.94238400	2.74171900
O	-2.58727000	-2.77402200	1.81438900
H	-3.30223900	-2.81370100	1.15398500
H	-2.93692400	-3.14556900	2.63691300