Supplementary information

Quantum Tunnelling Effect in the Cis-Trans Isomerization of Uranyl Tetra Hydroxide

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Table of contents

Uranyl Tetra Hydroxide (UTH) conformers:

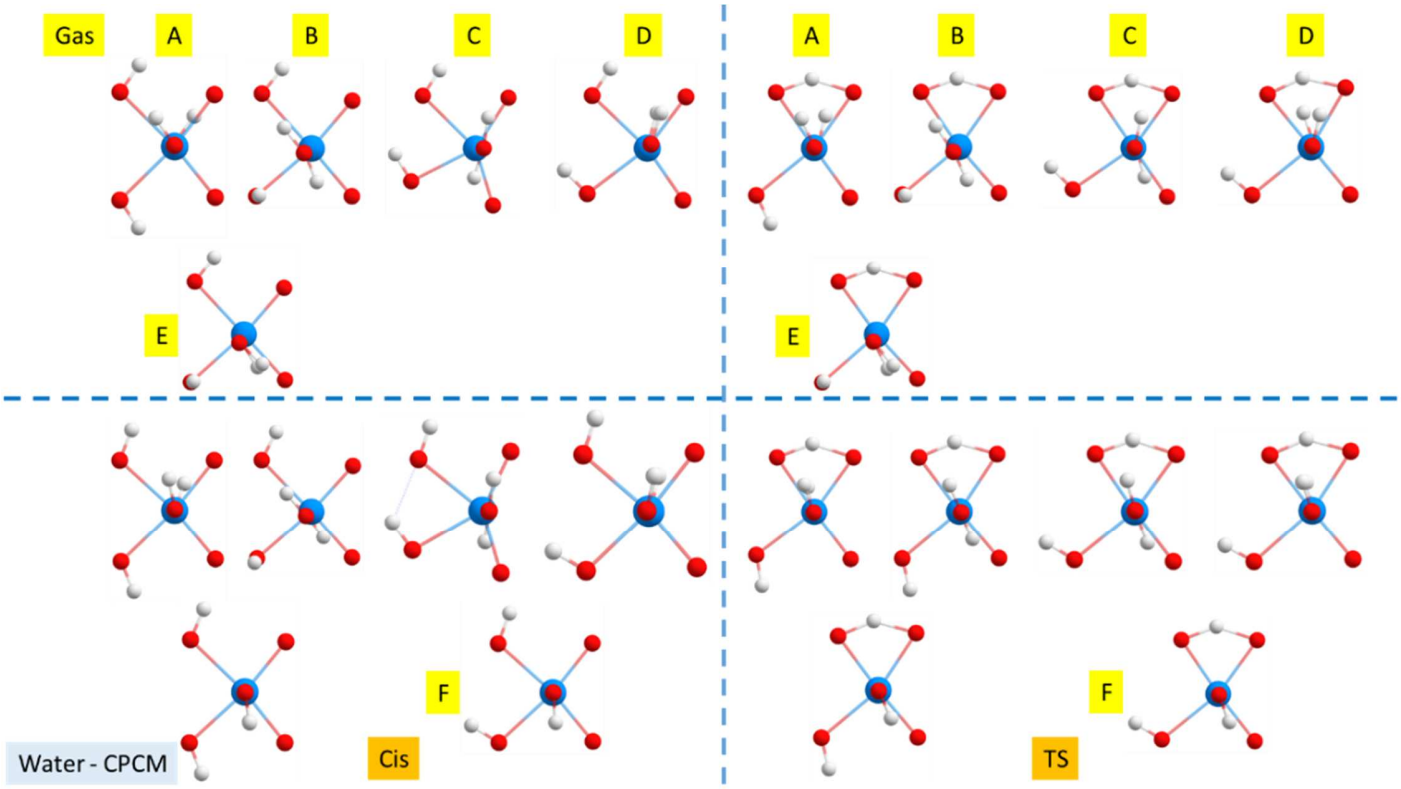

Figure S1: Cis and transition states conformations of the studied UTH: $[UO_2(OH)_4]^{2-}$ complexes, in gas phase (upper icons) and in water solution (lower icons).

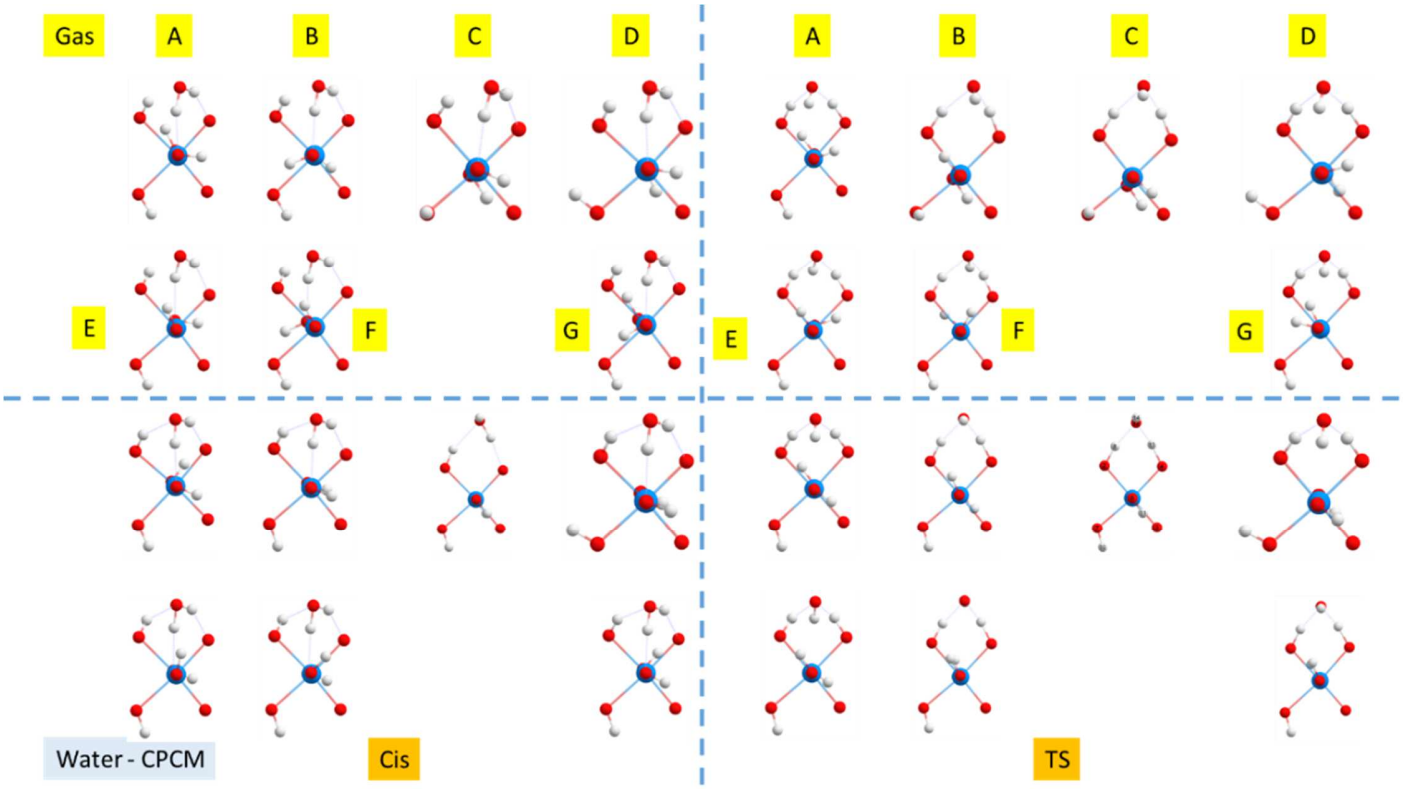

Figure S2: Cis and transition state conformations of the studied UTH···H_2O: $[UO_2(OH)_4]^{2-}$···H_2O complexes in gas phase (upper icons) and in water solution (lower icons)

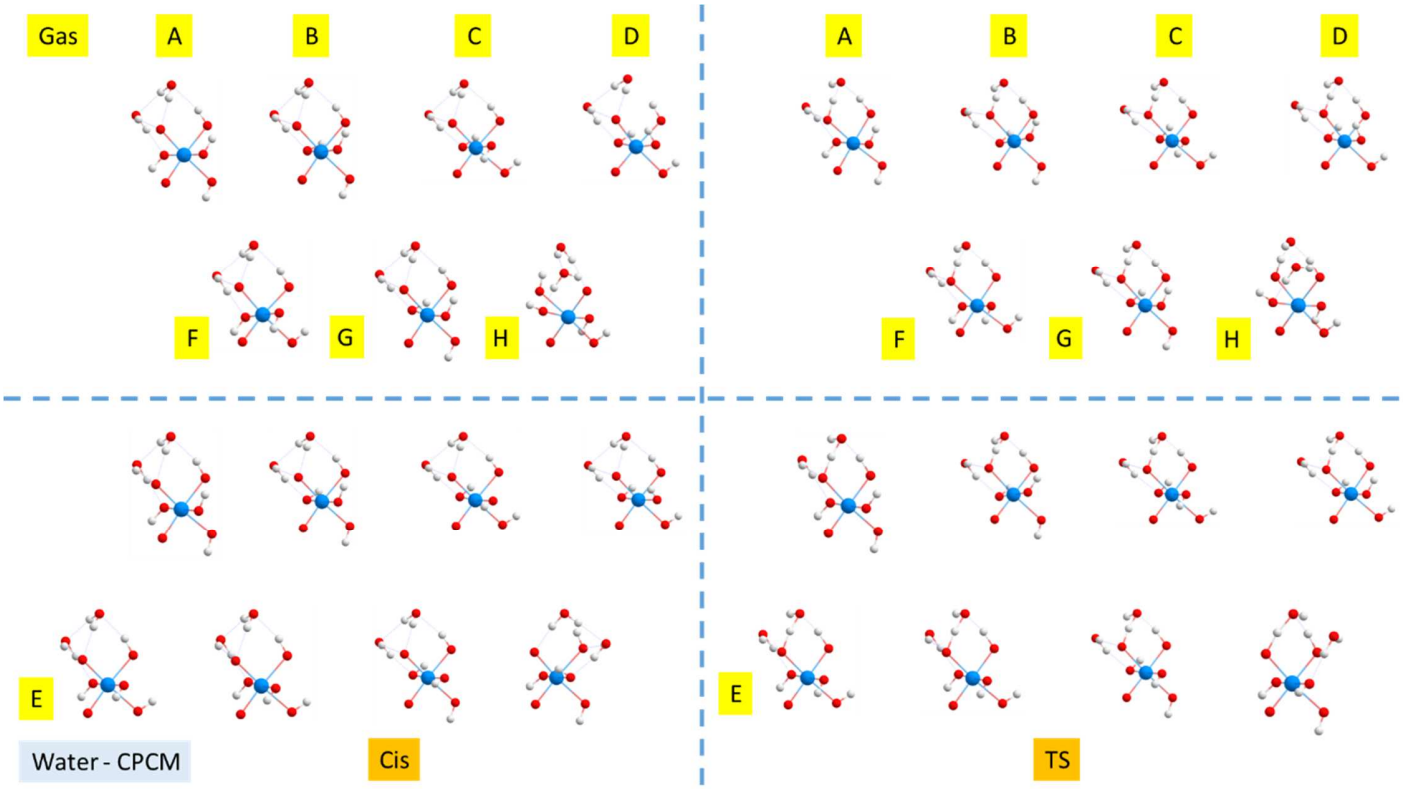

Figure S3: Cis and transition state conformations of the studied UTH···$(H_2O)_2$: $[UO_2(OH)_4]^{2-}$···$(H_2O)_2$ complexes in gas phase (upper icons) and in water solution (lower icons)

Activation barrier and reaction energy of isomerization reaction of UTH conformers:

UTH	Gas				Water - CPCM			
	$\Delta E^{\ddagger}$ (kJ·mol^{-1})		ΔE_r (kJ·mol-1)		$\Delta E^{\ddagger}$ (kJ·mol^{-1})		ΔE_r (kJ·mol-1)	
Conformer	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)
A	64	79	-102	-92	74	88	-101	-92
B	66	75	-101	-96	68	79	-107	-102
C	69	73	-100	-100	75	64	-104	-121
D	64	79	-101	-87	76	90	-104	-95
E	68	77	-98	-92	74	89	-101	-93
F					75	89	-104	-95

UTH···H_2O	Gas				Water - CPCM			
	$\Delta E^{\ddagger}$ (kJ·mol^{-1})		ΔE_r (kJ·mol-1)		$\Delta E^{\ddagger}$ (kJ·mol^{-1})		ΔE_r (kJ·mol-1)	
Conformer	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)
A	51	51	-90	-88	51	54	-88	-86
B	58	56	-86	-83	50	38	-81	-81
C	51	44	-89	-98	26	34	-111	-88
D	54	54	-91	-89	50	52	-90	-90
E	51	51	-90	-88	51	54	-88	-86
F	57	55	-82	-80	51	38	-82	-82
G	57	59	-84	-81	51	40	-82	-80

UTH···$(H_2O)_2$	Gas				Water - CPCM			
	$\Delta E^{\ddagger}$ (kJ·mol^{-1})		ΔE_r (kJ·mol-1)		$\Delta E^{\ddagger}$ (kJ·mol^{-1})		ΔE_r (kJ·mol-1)	
Conformer	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)	DFT	DLPNO-CCSD(T1)
A	36	40	-108	-102	36	41	-100	-94
B	37	40	-111	-104	37	40	-105	-98
C	38	40	-115	-108	37	39	-107	-102
D	39	42	-110	-103	38	41	-107	-101
E	36	40	-108	-102	36	40	-103	-97
F	39	42	-109	-103	36	40	-103	-97
G	37	40	-111	-104	37	39	-104	-99
H	55	57	-73	-68	48	49	-74	-77

Thermodynamic data:

	Gas			CPCM - Water		
	UTH					
	Electronic Energy (DLPNO-CCSD(T1))	Thermal Correction Enthalpy	Entropy	Electronic Energy (DLPNO-CCSD(T1))	Thermal Correction Enthalpy	Entropy
Conf.	Ha	Ha	J/mol-kelvin	Ha	Ha	J/mol-kelvin
A	-929.87519	0.06781	438.56311	-930.200359	0.06681	450.26159
B	-929.87357	0.06818	436.53934	-930.196728	0.06676	448.55207
C	-929.87211	0.06876	436.99605	-930.18966	0.06844	428.56996
D	-929.87469	0.06780	451.40127	-930.199288	0.06689	452.01301
E	-929.87366	0.06808	436.27956	-930.200327	0.06691	451.49764
F				-930.199301	0.06593	452.30212
	UTH···H_2O					
A	-1006.27558	0.09697	472.15434	-1006.58315	0.09565	479.91841
B	-1006.27636	0.09698	472.09149	-1006.58261	0.09571	473.66693
C	-1006.27249	0.09671	482.21872	-1006.58232	0.09484	504.87405
D	-1006.27579	0.09697	476.20188	-1006.58169	0.09571	478.26755
E	-1006.27558	0.09697	472.1711	-1006.58313	0.09567	477.02312
F	-1006.27734	0.09711	469.24229	-1006.58249	0.09567	476.97703
G	-1006.27735	0.09710	469.38056	-1006.58314	0.09567	477.01893
	UTH···$(H_2O)_2$					
A	-1082.67057	0.12545	516.71499	-1082.96505	0.12402	519.81140
B	-1082.67040	0.12542	519.72341	-1082.96319	0.12396	522.69412
C	-1082.66879	0.12540	521.06840	-1082.96170	0.12401	523.70391
D	-1082.66984	0.12556	513.80713	-1082.96196	0.12405	525.49304
E				-1082.96380	0.12390	525.08661
F	-1082.67077	0.12544	519.87844	-1082.96376	0.12391	525.00700
G	-1082.67041	0.12542	519.60609	-1082.96298	0.12396	521.87288
H	-1082.67452	0.12574	517.78763	-1082.96687	0.12428	518.55859

	ΔG(T) (J/mole)									
	Gas					CPCM - Water				
	Cis - UTH									
T(k)	20	77.36	194.7	273.15	298.15	20	77.36	194.7	273.15	298.15
A	0.0E+00	0.0E+00	1.2E+03	2.2E+03	2.5E+03	0.0E+00	0.0E+00	0.0E+00	8.3E+01	1.3E+02
B	5.3E+03	5.4E+03	6.8E+03	8.0E+03	8.3E+03	9.4E+03	9.5E+03	9.7E+03	1.0E+04	1.0E+04
C	1.1E+04	1.1E+04	1.2E+04	1.3E+04	1.4E+04	3.3E+04	3.4E+04	3.7E+04	3.8E+04	3.9E+04
D	1.0E+03	3.1E+02	0.0E+00	0.0E+00	0.0E+00	3.0E+03	2.9E+03	2.7E+03	2.6E+03	2.6E+03
E	4.8E+03	4.9E+03	6.4E+03	7.5E+03	7.9E+03	3.2E+02	2.4E+02	9.9E+01	8.5E+01	1.1E+02
F						4.3E+02	3.2E+02	7.7E+01	0.0E+00	0.0E+00
	Cis - UTH···H_2O									
A	4.3E+03	4.1E+03	3.8E+03	3.6E+03	3.5E+03	4.7E+02	1.9E+03	4.8E+03	6.8E+03	7.4E+03
B	2.2E+03	2.1E+03	1.8E+03	1.5E+03	1.5E+03	2.1E+03	3.9E+03	7.6E+03	1.0E+04	1.1E+04
C	1.1E+04	1.1E+04	9.2E+03	8.2E+03	7.9E+03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
D	3.6E+03	3.2E+03	2.4E+03	1.9E+03	1.7E+03	4.5E+03	6.0E+03	9.1E+03	1.1E+04	1.2E+04
E	4.3E+03	4.1E+03	3.8E+03	3.5E+03	3.5E+03	6.2E+02	2.2E+03	5.5E+03	7.7E+03	8.4E+03
F	5.2E+01	6.0E+01	7.6E+01	8.7E+01	9.0E+01	2.3E+03	3.9E+03	7.2E+03	9.3E+03	1.0E+04
G	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.7E+02	2.2E+03	5.4E+03	7.6E+03	8.3E+03
	Cis - UTH···$(H_2O)_2$									
A	9.9E+03	1.0E+04	1.0E+04	1.0E+04	1.0E+04	3.7E+03	3.6E+03	3.5E+03	3.4E+03	3.3E+03
B	9.4E+03	9.3E+03	9.0E+03	8.9E+03	8.8E+03	7.5E+03	7.3E+03	6.8E+03	6.5E+03	6.4E+03
C	1.3E+04	1.3E+04	1.3E+04	1.2E+04	1.2E+04	1.1E+04	1.1E+04	1.0E+04	9.9E+03	9.8E+03
D	1.3E+04	1.3E+04	1.4E+04	1.4E+04	1.4E+04	1.0E+04	9.7E+03	8.9E+03	8.3E+03	8.2E+03
E						5.0E+03	4.6E+03	3.9E+03	3.3E+03	3.2E+03
F	8.4E+03	8.3E+03	8.0E+03	7.9E+03	7.8E+03	5.1E+03	4.8E+03	4.0E+03	3.5E+03	3.3E+03
G	9.4E+03	9.3E+03	9.1E+03	8.9E+03	8.9E+03	8.3E+03	8.1E+03	7.7E+03	7.5E+03	7.4E+03
H	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

	K_{eq}									
	Gas					CPCM - Water				
	Cis - UTH									
T(k)	20	77.36	194.7	273.15	298.15	20	77.36	194.7	273.15	298.15
A	1.0E+00	1.0E+00	4.8E-01	3.8E-01	3.6E-01	1.0E+00	1.0E+00	1.0E+00	9.6E-01	9.5E-01
B	1.9E-14	2.4E-04	1.5E-02	3.0E-02	3.5E-02	2.3E-25	3.7E-07	2.4E-03	1.3E-02	1.7E-02
C	2.0E-28	6.0E-08	5.8E-04	3.0E-03	4.2E-03	1.9E-86	1.0E-23	1.5E-10	4.6E-08	1.5E-07
D	1.8E-03	6.2E-01	1.0E+00	1.0E+00	1.0E+00	1.5E-08	1.1E-02	1.9E-01	3.1E-01	3.4E-01
E	3.6E-13	5.0E-04	2.0E-02	3.6E-02	4.1E-02	1.5E-01	6.8E-01	9.4E-01	9.6E-01	9.6E-01
F						7.4E-02	6.1E-01	9.5E-01	1.0E+00	1.0E+00
	Cis - UTH···H_2O									
A	7.3E-12	1.7E-03	9.7E-02	2.1E-01	2.4E-01	6.0E-02	5.2E-02	5.1E-02	5.0E-02	5.0E-02
B	1.5E-06	3.9E-02	3.4E-01	5.1E-01	5.5E-01	2.4E-06	2.2E-03	9.1E-03	1.2E-02	1.3E-02
C	9.8E-31	5.5E-08	3.3E-03	2.7E-02	4.1E-02	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1.0E+00
D	3.9E-10	6.8E-03	2.3E-01	4.4E-01	5.0E-01	1.8E-12	8.6E-05	3.5E-03	7.1E-03	8.2E-03
E	7.8E-12	1.7E-03	9.8E-02	2.1E-01	2.5E-01	2.5E-02	3.2E-02	3.4E-02	3.4E-02	3.4E-02
F	7.3E-01	9.1E-01	9.5E-01	9.6E-01	9.6E-01	1.1E-06	2.4E-03	1.2E-02	1.6E-02	1.7E-02
G	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1.0E+00	3.1E-02	3.4E-02	3.5E-02	3.5E-02	3.5E-02
	Cis - UTH···$(H_2O)_2$									
A	1.0E-26	1.7E-07	1.9E-03	1.1E-02	1.6E-02	2.3E-10	3.6E-03	1.2E-01	2.3E-01	2.6E-01
B	3.2E-25	5.5E-07	3.8E-03	2.0E-02	2.8E-02	2.4E-20	1.2E-05	1.5E-02	5.8E-02	7.7E-02
C	5.0E-35	1.8E-09	4.3E-04	4.4E-03	7.2E-03	5.3E-30	4.3E-08	1.7E-03	1.3E-02	1.9E-02
D	6.4E-35	1.0E-09	2.0E-04	2.0E-03	3.3E-03	4.7E-27	2.9E-07	4.2E-03	2.6E-02	3.7E-02
E						8.8E-14	7.5E-04	9.2E-02	2.3E-01	2.8E-01
F	1.1E-22	2.5E-06	7.0E-03	3.1E-02	4.3E-02	3.7E-14	6.0E-04	8.4E-02	2.1E-01	2.6E-01
G	3.0E-25	5.4E-07	3.7E-03	2.0E-02	2.8E-02	1.9E-22	3.3E-06	8.4E-03	3.7E-02	5.1E-02
H	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1.0E+00

	C_i									
	Gas					CPCM - Water				
	Cis - UTH									
T(k)	20	77.36	194.7	273.15	298.15	20	77.36	194.7	273.15	298.15
A	1.0E+00	6.2E-01	3.2E-01	2.6E-01	2.5E-01	8.2E-01	4.3E-01	3.2E-01	3.0E-01	2.9E-01
B	1.9E-14	1.5E-04	9.9E-03	2.1E-02	2.4E-02	1.9E-25	1.6E-07	7.9E-04	3.8E-03	5.3E-03
C	2.0E-28	3.7E-08	3.8E-04	2.1E-03	2.9E-03	1.6E-86	4.3E-24	4.9E-11	1.4E-08	4.5E-08
D	1.8E-03	3.8E-01	6.6E-01	6.9E-01	6.9E-01	1.2E-08	4.8E-03	6.1E-02	9.6E-02	1.1E-01
E	3.6E-13	3.1E-04	1.3E-02	2.5E-02	2.8E-02	1.2E-01	3.0E-01	3.0E-01	3.0E-01	2.9E-01
F						6.0E-02	2.7E-01	3.1E-01	3.1E-01	3.1E-01
	Cis - UTH···H_2O									
A	4.2E-12	8.6E-04	3.6E-02	6.2E-02	6.9E-02	5.4E-02	4.6E-02	4.4E-02	4.4E-02	4.3E-02
B	8.4E-07	2.0E-02	1.2E-01	1.5E-01	1.6E-01	2.2E-06	1.9E-03	8.0E-03	1.0E-02	1.1E-02
C	5.7E-31	2.8E-08	1.2E-03	7.9E-03	1.2E-02	9.0E-01	8.9E-01	8.7E-01	8.7E-01	8.6E-01
D	2.3E-10	3.5E-03	8.3E-02	1.3E-01	1.4E-01	1.6E-12	7.6E-05	3.1E-03	6.2E-03	7.1E-03
E	4.5E-12	8.8E-04	3.6E-02	6.3E-02	6.9E-02	2.2E-02	2.9E-02	3.0E-02	3.0E-02	3.0E-02
F	4.2E-01	4.6E-01	3.5E-01	2.9E-01	2.7E-01	9.7E-07	2.1E-03	1.0E-02	1.4E-02	1.5E-02
G	5.8E-01	5.1E-01	3.7E-01	3.0E-01	2.8E-01	2.8E-02	3.0E-02	3.0E-02	3.0E-02	3.0E-02
	Cis - UTH···$(H_2O)_2$									
A	1.0E-26	1.7E-07	1.9E-03	1.0E-02	1.4E-02	2.3E-10	3.6E-03	8.9E-02	1.3E-01	1.3E-01
B	3.2E-25	5.5E-07	3.7E-03	1.8E-02	2.5E-02	2.4E-20	1.2E-05	1.1E-02	3.2E-02	3.9E-02
C	5.0E-35	1.8E-09	4.2E-04	4.0E-03	6.3E-03	5.3E-30	4.2E-08	1.3E-03	7.1E-03	9.8E-03
D	6.4E-35	1.0E-09	2.0E-04	1.8E-03	2.8E-03	4.7E-27	2.9E-07	3.2E-03	1.4E-02	1.9E-02
E						8.8E-14	7.5E-04	7.0E-02	1.3E-01	1.4E-01
F	1.1E-22	2.5E-06	6.8E-03	2.8E-02	3.7E-02	3.7E-14	6.0E-04	6.3E-02	1.2E-01	1.3E-01
G	3.0E-25	5.4E-07	3.6E-03	1.8E-02	2.4E-02	1.9E-22	3.2E-06	6.3E-03	2.1E-02	2.6E-02
H	1.0E+00	1.0E+00	9.8E-01	9.1E-01	8.8E-01	1.0E+00	1.0E+00	7.6E-01	5.5E-01	5.1E-01

Thermodynamic data of the most stable conformers of the three reaction pathways:

		Gas					
		Cis - UTH		Cis - UTH··H_2O		Cis - UTH··$(H_2O)_2$	H_2O
		A+2H_2O	D+2H_2O	F+H_2O	G+H_2O	H	
Electronic Energy (DLPNO-CCSD(T1))	Ha	-1082.59487	-1082.59437	-1082.63718	-1082.63719	-1082.67452	-76.35984
Thermal Correction. Enthalpy	Ha	0.11853	0.11853	0.12247	0.12246	0.12574	0.02536
Entropy	J/mole-K	528.771	541.609	514.346	514.485	517.788	45.104
		CPCM -Water					
		Cis - UTH		Cis - UTH··H_2O		Cis - UTH··$(H_2O)_2$	H_2O
		A+2H_2O	F+2H_2O	C+H_2O	G+H_2O	H	
Electronic Energy (DLPNO-CCSD(T1))	Ha	-1082.93927	-1082.93821	-1082.95178	-1082.9526	-1082.96687	-76.36946
Thermal Correction. Enthalpy	Ha	0.11731	0.11643	0.12009	0.12092	0.12428	0.02525
Entropy	J/mole-K	540.500	542.540	549.993	522.138	518.559	45.119

	Gas				
	Cis - UTH		Cis - UTH··H_2O		Cis - UTH··$(H_2O)_2$
T(k)	ΔG(T) (J/mole)				
20	189982	191030	89520	89468	0
77.36	189352	189663	89717	89657	0
194.7	188064	186868	90121	90045	0
273.15	187202	184999	90391	90304	0
298.15	186927	184404	90477	90387	0
	K_{eq}				
20	0.0E+00	0.0E+00	1.5E-234	2.1E-234	1.0E+00
77.36	1.4E-128	8.5E-129	2.6E-61	2.9E-61	1.0E+00
194.7	3.5E-51	7.3E-51	6.6E-25	6.9E-25	1.0E+00
273.15	1.6E-36	4.2E-36	5.2E-18	5.4E-18	1.0E+00
298.15	1.8E-33	4.9E-33	1.4E-16	1.5E-16	1.0E+00
	C_i				
20	0.0E+00	0.0E+00	1.5E-234	2.1E-234	1.0E+00
77.36	1.4E-128	8.5E-129	2.6E-61	2.9E-61	1.0E+00
194.7	3.5E-51	7.3E-51	6.6E-25	6.9E-25	1.0E+00
273.15	1.6E-36	4.2E-36	5.2E-18	5.4E-18	1.0E+00
298.15	1.8E-33	4.9E-33	1.4E-16	1.5E-16	1.0E+00

	CPCM -Water				
	Cis - UTH		Cis - UTH··H_2O		Cis - UTH··$(H_2O)_2$
T(k)	DG(T) (J/mole)				
20	53718	54152	27987	28562	0
77.36	52460	52776	26184	28357	0
194.7	49885	49962	22496	27937	0
273.15	48164	48081	20030	27656	0
298.15	47616	47482	19244	27567	0
	K_{eq}				
20	5.0E-141	3.7E-142	8.0E-74	2.5E-75	1.0E+00
77.36	3.8E-36	2.3E-36	2.1E-18	7.1E-20	1.0E+00
194.7	4.1E-14	3.9E-14	9.2E-07	3.2E-08	1.0E+00
273.15	6.2E-10	6.4E-10	1.5E-04	5.1E-06	1.0E+00
298.15	4.5E-09	4.8E-09	4.3E-04	1.5E-05	1.0E+00
	C_i				
20	5.0E-141	3.7E-142	8.0E-74	2.5E-75	1.0E+00
77.36	3.8E-36	2.3E-36	2.1E-18	7.1E-20	1.0E+00
194.7	4.1E-14	3.9E-14	9.2E-07	3.2E-08	1.0E+00
273.15	6.2E-10	6.4E-10	1.5E-04	5.1E-06	1.0E+00
298.15	4.5E-09	4.8E-09	4.2E-04	1.5E-05	1.0E+00

Conformers' geometries

Gas

UTH: [UO2(OH)4]2-

A, 0Ag

Cis:
-2 1

U	-0.01591500	-0.02210600	-0.05866300
O	0.46089200	1.54508300	1.46331700
O	-0.22159700	-1.46902200	-1.24397500
O	-0.31080300	1.46362100	-1.19613700
O	-2.28948400	0.10131100	0.36860400
O	2.26551300	0.00552400	-0.43800000
O	0.22636700	-1.58350800	1.49566500
H	0.26315700	2.32680800	0.93486400
H	-2.51877100	0.82904600	-0.21878700
H	0.19129900	-2.37540200	0.94724900
H	2.48138200	0.74918900	0.13785600

Trans:
-2 1

U	-0.00449100	-0.00004900	-0.02546600
O	-0.27095700	-0.00388900	1.78357400
O	0.26804000	0.00370000	-1.81960400
O	-2.29602600	-0.04729500	-0.28347600
O	0.07593100	-2.30774700	0.02940100
O	-0.01854000	2.30918900	0.02686200
O	2.27451800	0.04632000	0.30773500
H	-2.58453400	-0.05159900	0.63544300
H	0.12114500	-2.46878700	0.97816400
H	2.59124700	0.04968300	-0.60208700
H	0.02157500	2.47295700	0.97538500

Transition state:
-2 1

U	0.00882300	-0.02510400	-0.04860400
O	-0.39781400	1.20581600	1.52099800
O	0.43428200	-1.07754900	-1.50454600
O	-0.96399200	1.66646400	-0.70545100
O	-2.07861700	-0.97401400	0.05142600
O	2.05124900	1.00770600	-0.23691800
O	0.89224200	-1.66935300	1.22846800
H	-0.82285400	1.76783100	0.60510100
H	-2.61546800	-0.17485000	0.09613300
H	1.19374700	-2.30771900	0.57403900
H	1.93405100	1.75171100	0.36451400

B, 0Bg

Cis:
-2 1

U	-0.05466300	0.00333300	-0.07530900
O	0.71963200	1.57584300	1.30621500
O	-0.61134200	-1.37940700	-1.21901400
O	-0.33860800	1.47839400	-1.22007300
O	-2.18011100	0.06616600	0.82039100
O	2.23721600	-0.33182800	-0.54435500
O	0.55267400	-1.49842700	1.42631500
H	0.49790000	2.34676500	0.77086700
H	-2.52250500	-0.78865800	0.53761800
H	1.45329100	-1.54255500	1.05959100
H	2.56465300	0.39187900	0.00453800

Trans:
-2 1

U	-0.00002900	-0.00001000	-0.00002100
O	-0.00012100	-0.40198700	-1.77668400
O	0.00010800	0.40194800	1.77663900
O	-1.65022400	-1.58249000	0.31116000
O	-1.64961400	1.58307200	-0.31100800
O	1.64980600	-1.58277900	0.31133100
O	1.65035500	1.58233200	-0.31124200
H	-1.86760900	-1.80164300	-0.60133300
H	-1.86726600	1.80226100	0.60140600
H	1.86740600	1.80114500	0.60142500
H	1.86766400	-1.80159600	-0.60113400

Transition state:
-2 1

U	-0.03898100	0.00037200	-0.05530200
O	0.25102300	1.28960200	1.48595300
O	-0.30974200	-1.01060800	-1.57951200
O	-0.46220300	1.91087500	-0.66145700
O	-2.19670300	-0.47510200	0.54975500
O	2.25774500	0.11437000	-0.43895200
O	0.70799400	-1.80954300	1.07906300
H	-0.10782400	1.96246600	0.61170000
H	-2.41165300	-1.20596300	-0.03932400
H	1.62130400	-1.68387700	0.77927900
H	2.49947600	0.73636400	0.25736600

C, 0Cg

Cis:

-2 1

U	0.00324700	-0.06078500	-0.10304200
O	0.39440300	1.79656000	1.21182800
O	-0.53450600	-1.81301300	-0.31708000
O	0.60529700	1.17987100	-1.35591800
O	-2.15146200	0.55346300	-0.65359000
O	2.19619500	-0.78432900	-0.00409300
O	-0.56511400	-0.56377100	2.01017000
H	0.49656900	2.47668200	0.54024100
H	-2.63172200	-0.18092500	-0.25407100
H	-0.36910400	0.32531400	2.34424800
H	2.64706600	0.02092000	-0.28111600

Trans:

-2 1

U	-0.00443600	0.00004900	0.02548300
O	-0.27051600	0.00306600	-1.78367600
O	0.26756300	-0.00291900	1.81974800
O	0.06417400	2.30825500	-0.03017300
O	2.27509300	-0.03525500	-0.30641300
O	-2.29613000	0.03572900	0.28422500
O	-0.00752700	-2.30914200	-0.02838100
H	0.10740000	2.46856000	-0.97915800
H	2.59127600	-0.03717300	0.60358800
H	0.03330700	-2.47233700	-0.97695900
H	-2.58512200	0.03854400	-0.63456300

Transition state:

-2 1

U	-0.01223500	-0.01206500	-0.06148100
O	0.59664600	0.88571000	1.65789400
O	-0.61308900	-0.79489300	-1.62013700
O	0.98054400	1.73155800	-0.49561900
O	-2.03939900	1.06021400	0.02958600
O	2.03182000	-1.03821400	-0.27239200
O	-0.85692200	-1.75336600	1.13300600
H	0.95119100	1.60256000	0.82296800
H	-2.56695000	0.51014700	-0.55912700
H	-0.65980800	-1.44700500	2.02740400
H	2.60442700	-0.28380300	-0.09367100

D, 0Dg

Cis:

-2 1

U	-0.00004000	-0.04899500	-0.08039300
O	-0.00332000	1.47418600	1.57468800
O	-0.00009100	-1.56663200	-1.16266200
O	0.00489300	1.48934300	-1.19271700
O	-2.31044300	0.07564100	-0.14636400
O	2.31105600	0.07349400	-0.13864000
O	-0.00220000	-1.42366800	1.66563800
H	0.00509900	2.28431700	1.05510500
H	-2.41865000	0.99841800	-0.40105500
H	-0.00086000	-0.74480600	2.35545600
H	2.41894700	0.99065000	-0.41290000

Trans:

-2 1

U	0.02759300	-0.00479800	0.03815400
O	0.14224100	0.13189400	-1.78298000
O	-0.02443300	-0.05302600	1.84526200
O	-1.83944400	1.38540400	-0.04276800
O	1.54496100	1.73495700	0.11498800
O	-1.65797600	-1.57579400	-0.15431000
O	1.63449800	-1.64854600	-0.05909000
H	-1.94848400	1.47614100	-0.99597600
H	1.68537500	1.89510100	-0.82417300
H	1.69052800	-1.80516200	-1.00790500
H	-2.36471100	-0.92378400	-0.05089700

Transition state:

-2 1

U	-0.00321200	-0.03834500	-0.07626900
O	-0.00477500	1.06677300	1.64148600
O	-0.07290500	-1.02180800	-1.62533100
O	0.34864900	1.94623700	-0.50413800
O	-2.26503400	0.32991200	-0.21241800
O	2.28524900	-0.22172000	0.00300700
O	-0.27048100	-1.92370500	1.16391500
H	0.19960000	1.83841700	0.80802100
H	-2.35155600	1.11196300	0.34427300
H	-0.21694100	-1.54330600	2.04991400
H	2.49880600	0.71517900	0.08237200

E, 0Eg

Cis:

-2 1

U	-0.03881500	0.00553000	-0.05694500
O	-0.14846700	1.85731100	1.15183100
O	0.10509300	-1.57960300	-1.07091600
O	-0.57489900	1.12699700	-1.47730500
O	-2.18329400	-0.62742900	0.51482700
O	2.29614000	0.24466500	-0.32115700
O	0.76691400	-1.03705500	1.71489100
H	-0.44149300	2.46473400	0.46233500
H	-2.20474600	-1.51991300	0.15321200
H	1.68304500	-0.84092000	1.45163200
H	2.44223800	-0.49177000	-0.92556400

Trans:

-2 1

U	-0.02666100	0.00646200	-0.01166000
O	-0.14175900	-0.20320700	-1.81200500
O	0.02342800	0.12508000	1.80578200
O	-1.50895500	-1.75179900	0.18386300
O	-1.67634600	1.60873200	-0.02754100
O	1.84915600	-1.36812800	0.06649900
O	1.64415600	1.59359400	-0.19851700
H	-1.65448000	-1.97609000	-0.74137300
H	-1.75661400	1.81842200	0.90911800
H	2.35073800	0.93586600	-0.25793300
H	1.99575900	-1.40687600	1.01832000

Transition state:

-2 1

U	-0.03347300	0.00619700	-0.03683800
O	-0.41181300	1.21656800	1.53241400
O	0.25635300	-0.93849900	-1.60769400
O	-0.91053500	1.73046000	-0.70300000
O	-2.00105300	-1.14605900	0.20233900
O	2.17786900	0.74200000	-0.20196000
O	1.06306100	-1.56261300	1.17183100
H	-0.79588000	1.81441600	0.61451500
H	-1.88999200	-1.86182600	-0.43237100
H	1.92002500	-1.12597400	1.04968600
H	2.45433600	0.26843300	-0.99421100

UTH···H2O: [UO2(OH)4]2- ···H2O

A, 1Ag

Cis:

-2 1

U	-0.24408300	-0.02119300	-0.05642600
O	0.80173100	1.09153700	1.46972200
O	-1.23564500	-1.07457700	-1.24075100
O	0.95569500	0.76396800	-1.32004600
O	-1.73777500	1.71269300	-0.20884000
O	1.49247100	-1.66100100	0.17877000
O	-1.48154300	-0.96824600	1.51642100
H	1.74058400	1.06228500	1.20895900
H	-1.25071700	2.44019000	0.19499600
H	-2.11457000	-1.46352400	0.98452600
H	1.63330300	-1.90436800	-0.74393000
O	3.32387400	0.33806500	0.08515900
H	2.67959500	0.69768000	-0.56237700
H	2.81699100	-0.50206000	0.26557000

Trans:

-2 1

U	-0.25196100	-0.00019900	-0.03397700
O	0.61157700	0.45068600	1.51562200
O	-1.11759300	-0.47445000	-1.55575500
O	1.13430800	1.36529400	-1.19500700
O	-1.80191600	1.63556600	0.38172500
O	1.52652700	-1.51077500	-0.52318300
O	-1.48051700	-1.58105600	1.07000800
H	2.61036800	0.44002600	1.16256300
H	-1.52953600	1.98462300	1.23701700
H	-2.05671300	-1.92342600	0.37835700
H	1.57247300	-1.37275900	-1.47710300
O	3.34915200	0.13323300	0.60978400
H	1.97809300	1.31206900	-0.72299800
H	2.83339900	-0.57017000	0.12247700

Transition state:

-2 1

U	-0.23697300	-0.02007900	-0.04852000
O	0.92674300	0.81850700	1.40187000
O	-1.35121600	-0.72458700	-1.32562900
O	1.32470700	0.49977100	-1.31043300
O	-1.30911200	1.97486800	-0.23046900
O	1.00824600	-1.95191900	0.11127000
O	-1.72882500	-0.72721800	1.46829300
H	1.91214000	0.73052100	1.08383300
H	-0.78004100	2.54760000	0.33672900
H	-2.45576300	-1.06542900	0.93465700
H	1.46526100	-1.94636400	-0.73801500
O	3.18670000	0.32252700	0.27391000
H	2.26573300	0.48655300	-0.68873200
H	2.93623800	-0.60117000	0.42489100

B, 1Bg

Cis:

-2 1

U	0.23565200	-0.02115600	-0.04609500
O	-0.92576500	-0.32902300	1.74447900
O	1.34941400	0.39487800	-1.49895000
O	-0.83360500	-1.33488000	-0.91223000
O	1.84782700	-1.51855200	0.62048000
O	-1.51148900	1.53090000	-0.55746200
O	1.23540500	1.68455400	0.97495200
H	-1.84147300	-0.46458500	1.43826600
H	2.41080400	-1.57606800	-0.15837600
H	1.85871300	1.95835000	0.29237400
H	-1.35312900	2.16927100	0.14859200
O	-3.32204800	-0.38198800	0.01220600
H	-2.64331100	-0.97440200	-0.37371900
H	-2.82949800	0.46665100	-0.17423300

Trans:

-2 1

U	0.24621000	-0.01662300	0.01616700
O	-0.71992900	-0.05392500	-1.53483900
O	1.24895600	0.05197700	1.53078200
O	-1.51589400	1.34012500	0.88612500
O	1.21906300	1.95982300	-0.62632900
O	-0.97150200	-1.72691400	0.83167700
O	1.87379400	-1.36866200	-0.86302500
H	-2.66974200	-0.27074700	-1.05890000
H	1.73844700	2.19410400	0.15049900
H	2.42389300	-1.57309900	-0.09975500
H	-1.85762500	-1.60699200	0.46098000
O	-3.37505400	-0.15994800	-0.39834600
H	-1.51489100	2.03948100	0.22039300
H	-2.84690500	0.40673900	0.23108700

Transition State:

-2 1

U	0.23171200	-0.03116000	-0.04850100
O	-1.08901500	0.14202900	1.52611200
O	1.37164200	-0.14952500	-1.48482800
O	-1.30995700	-1.06629000	-0.94289700
O	1.24272300	-1.87242900	0.79475400
O	-0.59541400	2.01654100	-0.68431800
O	1.71060700	1.28817700	1.00958700
H	-2.02600600	-0.04356000	1.17104500
H	1.93241400	-2.07979800	0.15593000
H	1.41759200	2.11994700	0.61104100
H	-1.21756800	2.20508800	0.02814100
O	-3.32117500	-0.25083100	0.18248000
H	-2.30064800	-0.80397400	-0.47049100
H	-3.19862300	0.60760100	-0.24068900

C, 1Cg

Cis:

-2 1

U	0.24189500	-0.02476300	-0.04025100
O	-0.83025100	-0.50734500	1.77260900
O	1.12292100	0.50143200	-1.60374500
O	-0.83691000	-1.33575700	-0.91801400
O	2.01442100	-1.39120000	0.43617300
O	-1.49190600	1.59556900	-0.36535000
O	1.22540500	1.64023400	1.05252400
H	-1.74092200	-0.67191600	1.46932400
H	2.63084300	-1.17995600	-0.27292700
H	0.51737500	2.29132800	0.94047400
H	-1.47773000	1.71346800	-1.32204700
O	-3.29851600	-0.42060800	0.04128800
H	-2.60868300	-0.97671400	-0.38081700
H	-2.81653900	0.44339500	-0.05476000

Trans:

-2 1

U	-0.25007500	-0.00736100	-0.02158500
O	0.76121900	-0.35312500	1.45561200
O	-1.30475000	0.34371000	-1.45648900
O	1.70759500	0.36082200	-1.30839700
O	0.00062700	2.26042800	0.27253800
O	-0.30563400	-2.21468600	-0.57292300
O	-2.12045000	-0.12347100	1.29151600
H	2.82752100	-0.39974600	1.15158100
H	-0.56207400	2.62768000	-0.41786200
H	-1.77123700	-0.31093500	2.16912600
H	-0.82300300	-2.23466700	-1.38499500
O	3.58208600	-0.30194700	0.55009000
H	1.72666200	1.31161900	-1.12923700
H	3.04346600	-0.09063000	-0.25834700

Transition state:

-2 1

U	0.21680400	-0.03266300	-0.03545800
O	-1.09791600	-0.07441400	1.52838100
O	1.35382200	0.01861800	-1.48365500
O	-1.38185400	-0.72964300	-1.13961200
O	1.07017200	-2.07522900	0.44823100
O	-0.32826800	2.16855700	-0.40885000
O	1.77758500	0.94478900	1.24941700
H	-2.04964800	-0.14998800	1.15229100
H	1.74509200	-2.21389000	-0.22429800
H	1.48639100	1.85263100	1.08091000
H	0.06762100	2.34426900	-1.26965500
O	-3.34659500	-0.13782600	0.19568700
H	-2.35100300	-0.54617300	-0.59819100
H	-3.21998000	0.79934500	0.00423400

D, 1Dg

Cis:

-2 1

U	0.24374500	0.00008000	-0.06507400
O	-0.81517000	-0.43335400	1.77770600
O	1.23511400	0.57427800	-1.53801600
O	-0.86772400	-1.25250200	-0.97903000
O	1.88507500	-1.53634200	0.39487700
O	-1.56267900	1.52999700	-0.45655200
O	1.30227700	1.49695800	1.17949400
H	-1.74595800	-0.55291400	1.51398300
H	2.61677100	-1.22373800	-0.14768900
H	0.82868400	1.36169900	2.01161000
H	-1.65840600	1.46663300	-1.41404600
O	-3.30230600	-0.44027600	0.16036500
H	-2.63176200	-0.99517900	-0.29157800
H	-2.83055500	0.42610100	0.00377400

Trans:

-2 1

U	0.25324400	-0.00406700	-0.02946300
O	-0.63224200	0.27202700	1.54879600
O	1.13985500	-0.24810700	-1.59237600
O	-1.05139800	-1.79457000	-0.49870900
O	1.86088100	-1.25409600	1.01520000
O	-1.56834700	1.08297400	-1.11190600
O	1.37944000	1.95774600	0.31527800
H	-2.61967500	0.00013300	1.23270300
H	2.44312100	-1.51968500	0.29589000
H	1.04368300	2.26515400	1.16399700
H	-1.58026300	0.58346700	-1.93712000
O	-3.35632300	0.00675800	0.59818800
H	-1.90715000	-1.58495200	-0.09709700
H	-2.85309500	0.44818700	-0.14354100

Transition State:

-2 1

U	0.23517200	0.01114000	-0.05509100
O	-0.89775000	-0.27652200	1.61399000
O	1.31606700	0.25856900	-1.51650300
O	-1.24738500	-1.03701400	-1.05176100
O	1.50057300	-1.81161500	0.42958600
O	-1.15196400	1.77964700	-0.57269300
O	1.57219600	1.32247800	1.18697300
H	-1.87873000	-0.38469700	1.27882400
H	2.20085100	-1.79256900	-0.23057900
H	1.13761300	1.29307500	2.04827700
H	-1.56492300	1.46323900	-1.38468700
O	-3.14024000	-0.39590800	0.36819800
H	-2.19987900	-0.85126700	-0.46641100
H	-2.94271500	0.53023800	0.16063000

E, 1Eg

Cis:

-2 1

U	0.24411600	-0.02117700	-0.05641300
O	-0.80153200	1.09206800	1.46985800
O	1.23574800	-1.07480500	-1.24042300
O	-0.95578600	0.76390900	-1.31996200
O	-1.49221700	-1.66105600	0.17841300
O	1.73778100	1.71258600	-0.20935000
O	1.48133800	-0.96821100	1.51666100
H	-1.74036800	1.06192300	1.20925600
H	-1.63406100	-1.90382200	-0.74428200
H	2.11400200	-1.46415200	0.98496400
H	1.25046600	2.44040500	0.19359900
O	-3.32429400	0.33785000	0.08512000
H	-2.67937800	0.69761800	-0.56170000
H	-2.81762100	-0.50240100	0.26562000

Trans:

-2 1

U	0.25202200	-0.00020200	-0.03396900
O	-0.61200600	0.45106500	1.51533700
O	1.11827900	-0.47461600	-1.55532900
O	-1.13400500	1.36515000	-1.19557100
O	-1.52631100	-1.51055600	-0.52404000
O	1.80188600	1.63568900	0.38208200
O	1.47975100	-1.58137700	1.07059300
H	-2.61020700	0.44043400	1.16203800
H	-1.57250400	-1.37155700	-1.47780800
H	2.05587000	-1.92413000	0.37907200
H	1.52889000	1.98481500	1.23715400
O	-3.34955000	0.13308500	0.61025500
H	-1.97824900	1.31162400	-0.72445900
H	-2.83413100	-0.57016500	0.12258100

Transition state:

-2 1

U	0.23697300	-0.02007800	-0.04851900
O	-0.92675200	0.81848800	1.40187400
O	1.35122300	-0.72456600	-1.32563300
O	-1.32471000	0.49977400	-1.31042900
O	-1.00823000	-1.95192900	0.11124700
O	1.30910100	1.97487600	-0.23044700
O	1.72882900	-0.72722500	1.46828700
H	-1.91214600	0.73049300	1.08383700
H	-1.46522300	-1.94637800	-0.73804900
H	2.45577800	-1.06540800	0.93464900
H	0.78000500	2.54761000	0.33672600
O	-3.18670800	0.32252000	0.27390600
H	-2.26573600	0.48655500	-0.68873600
H	-2.93624500	-0.60117900	0.42487400

F, 1Fg

Cis:

-2 1

U	0.24570200	0.00360000	-0.08252900
O	-0.87211100	0.73915800	1.61946300
O	1.35714400	-0.74527400	-1.38546000
O	-0.88757400	1.08543800	-1.16520000
O	-1.48882900	-1.64642800	-0.16832200
O	1.76118400	1.67973600	0.32888500
O	1.29192800	-1.38698400	1.30189800
H	-1.80118600	0.76618300	1.32561100
H	-1.25755000	-2.15227200	0.61996300
H	1.97772800	-1.73915100	0.72342900
H	1.25515600	2.26747400	0.90195000
O	-3.32296400	0.30902200	0.03117000
H	-2.67153800	0.80177200	-0.51066900
H	-2.81739200	-0.55256800	0.03287100

Trans:

-2 1

U	-0.24625400	-0.01681400	0.01608700
O	0.71944200	-0.05685500	-1.53514500
O	-1.24934400	0.05372300	1.53036300
O	1.51686600	1.33923400	0.88554100
O	0.97033800	-1.72710600	0.83314100
O	-1.21390300	1.96220100	-0.62656100
O	-1.87618700	-1.36669600	-0.86241900
H	2.67026000	-0.27375900	-1.05941900
H	1.85637000	-1.60659700	0.46212100
H	-2.42764700	-1.56936500	-0.09968500
H	-1.73384400	2.19843500	0.14927200
O	3.37461300	-0.16115900	-0.39818400
H	1.51028700	2.04356000	0.22515100
H	2.84535400	0.40785100	0.22867000

Transition state:

-2 1

U	0.24271300	0.00121900	-0.04915300
O	-1.06037300	-0.01323300	1.54375300
O	1.41368600	-0.13829100	-1.45892100
O	-1.31153700	0.97756900	-1.00407900
O	-0.70291900	-2.02805200	-0.52302600
O	1.03360200	2.06882100	0.45297600
O	1.84411200	-0.95327900	1.18597400
H	-2.00992600	0.08588800	1.17338500
H	-1.21320900	-2.20640700	0.27529500
H	2.57286500	-1.06851700	0.56704800
H	0.27053300	2.61611900	0.23382400
O	-3.28717600	0.14682300	0.17589500
H	-2.29315000	0.70611300	-0.52453000
H	-3.09190300	-0.72816800	-0.18352300

G, 1Gg

Cis:

-2 1

U	-0.24550300	0.00342000	-0.08232900
O	0.87080700	0.74132100	1.62008800
O	-1.35509300	-0.74756700	-1.38551800
O	0.88925400	1.08345700	-1.16525000
O	-1.76086300	1.68081700	0.32390900
O	1.48787000	-1.64707700	-0.16661800
O	-1.29484000	-1.38362900	1.30304600
H	1.80023200	0.76702500	1.32747600
H	-1.25446900	2.27092000	0.89421300
H	-1.98017800	-1.73620300	0.72427200
H	1.25817700	-2.15521300	0.62059500
O	3.32241300	0.30901900	0.03068700
H	2.66806400	0.80136700	-0.50814400
H	2.81806400	-0.55324400	0.03310900

Trans:

-2 1

U	0.25388900	-0.02075400	-0.04859700
O	-0.66715300	-0.24774800	1.51988300
O	1.21885900	0.22834000	-1.56034400
O	-1.02674500	-1.61811200	-0.99406700
O	1.86662100	-1.44670500	0.74030100
O	-1.51150100	1.44893300	-0.70827600
O	1.23656100	1.85782500	0.82400100
H	-2.63421600	-0.35152400	1.08730400
H	1.54191800	-1.67433300	1.61806900
H	1.81594900	2.14361900	0.10947300
H	-1.41418500	2.11483200	-0.01569600
O	-3.35788600	-0.13819200	0.47363100
H	-1.90140000	-1.49611200	-0.59663900
H	-2.83589200	0.49817000	-0.09266000

Transition state:

-2 1

U	0.23359900	-0.00224900	-0.06743500
O	-0.99441200	-0.28529000	1.54025000
O	1.38811600	0.29917900	-1.46273600
O	-1.25782500	-0.97954300	-1.10215800
O	1.31401600	-1.94699900	0.40418500
O	-0.98567800	1.94302900	-0.36306600
O	1.67749600	1.13964000	1.21280900
H	-1.96617700	-0.31652700	1.16034900
H	0.70653200	-2.39571100	1.00349200
H	2.42629200	1.29402600	0.62719100
H	-1.17786200	2.19687500	0.54754700
O	-3.18133600	-0.23244500	0.20737400
H	-2.23346600	-0.74021400	-0.57757600
H	-2.92942000	0.66787200	-0.05026900

⋯ O	-1.30028200	-1.11223100	-1.29211000
O	1.06478700	0.54022900	-1.16455900
O	-1.68652800	1.78126200	-0.66257600
O	0.97547900	-1.76323300	0.78768300
O	-2.00149400	-0.66354500	1.35514300
H	1.37642600	1.30334200	1.33966100
H	-1.23663400	2.53141700	-0.25779300
H	-2.59386800	-1.18270000	0.80000200
H	1.07719000	-1.44546400	1.69300200
O	3.10036200	1.47449800	0.37021400
H	3.32485100	0.52106700	0.30596800
H	2.36073500	1.45445400	-0.28273100
O	3.20124700	-1.18782800	-0.52445600
H	2.61277700	-0.64571200	-1.08859100
H	2.46224500	-1.54672800	0.05501200

Trans:
-2 1

U	-0.45094800	-0.02183800	-0.03364500
O	0.14265900	1.17337700	1.21754900
O	-0.99293100	-1.22201200	-1.26609700
O	1.25878000	0.75587500	-1.42049500
O	-1.91514600	1.53876000	-0.80943500
O	1.15191900	-1.52326700	0.80385100
O	-2.00299800	-0.83646000	1.41172900
H	2.12784000	1.22332500	1.18120300
H	-1.82825300	2.28745300	-0.20996600
H	-2.43173700	-1.55055600	0.92849300
H	1.49442000	-1.09882000	1.59911400
O	3.09310900	1.22114100	1.05010100
H	3.22497900	0.45035700	0.45723300
H	1.73939900	1.42208500	-0.91248500
O	3.25892200	-0.97653600	-0.79608800
H	2.62780200	-0.38175500	-1.27438500
H	2.57827100	-1.39003900	-0.20277500

Transition state:
-2 1

U	-0.41544000	-0.03659400	-0.05106100
O	0.36211000	1.12418300	1.40988800
O	-1.13283100	-1.14682400	-1.31182700
O	1.22190900	0.66383500	-1.13523700
O	-1.71236200	1.67170600	-0.76856100
O	0.98452400	-1.71173600	0.80587000
O	-2.04823400	-0.72949200	1.30342700
H	1.36561600	1.37682600	1.18338300
H	-1.30796600	2.47083800	-0.41285000
H	-2.58984200	-1.31567000	0.76468000
H	1.25123900	-1.32405700	1.64826800
O	2.68383900	1.59296800	0.54691100
H	3.11243400	0.72445000	0.59849300
H	1.95938800	1.23668000	-0.42844200
O	3.28520600	-1.17823800	-0.54872600
H	2.73890600	-0.54315400	-1.05519100
H	2.53739100	-1.55045800	-0.01474200

C, 2Cg

Cis:
-2 1

U	-0.42831000	0.04866000	0.05787300
O	0.35905300	-1.25693700	-1.46779900
O	-1.21173200	1.27523500	1.20464300
O	1.02984700	-0.46966000	1.22887600
O	-1.79741200	-1.58433200	0.86716800
O	1.09309300	1.58438100	-0.95848200
O	-1.95470900	0.54077100	-1.47109800
H	1.29074000	-1.46702000	-1.26744300
H	-2.35518700	-1.13178900	1.50815400
H	-1.74649600	-0.10643700	-2.15798500
H	1.30360700	1.07004600	-1.74749800
O	3.01768400	-1.56760400	-0.27557500
H	3.28210300	-0.62307100	-0.24192000
H	2.28424000	-1.49813500	0.37974800
O	3.23892800	1.12646400	0.52279300
H	2.62032200	0.64004800	1.10567600
H	2.52718400	1.45307100	-0.10720800

Trans:
-2 1

U	-0.45100800	0.02193400	-0.03361700
O	0.14307300	-1.17404800	1.21659500
O	-0.99330100	1.22284000	-1.26520500
O	1.15248500	1.52250500	0.80416700
O	-2.00284500	0.83540200	1.41253600
O	1.25847400	-0.75485900	-1.42156900
O	-1.91499500	-1.53847600	-0.80997600
H	2.12763300	-1.22383700	1.18083300
H	-2.43172300	1.54992100	0.93005500
H	-1.82801700	-2.28742600	-0.21084700
H	1.73834600	-1.42174600	-0.91372800
O	3.09297100	-1.22089100	1.05031600
H	3.22468500	-0.45043800	0.45692900
H	1.49582200	1.09606300	1.59801400
O	3.25911500	0.97599700	-0.79589800
H	2.57901200	1.39005800	-0.20237900
H	2.62715100	0.38172800	-1.27384600

Transition state:
-2 1

U	-0.41036800	-0.05418900	-0.04725600
O	0.27956300	1.24800600	1.34242300
O	-1.03364100	-1.28022300	-1.24608400
O	1.20117000	0.61267500	-1.18832200
O	-1.81261100	1.47276400	-0.94409000
O	1.07887400	-1.54797300	0.96524700
O	-2.02163500	-0.63951500	1.39881800
H	1.27811600	1.50156800	1.10509700
H	-2.30260800	1.00851000	-1.63023600
H	-1.92534000	0.00930200	2.10690300
H	1.42906600	-1.01131700	1.68660200
O	2.60861400	1.68469000	0.45970900
H	3.07290900	0.83942000	0.55646100
H	1.90559300	1.25084600	-0.50346500
O	3.31906400	-1.12587600	-0.53273000
H	2.74416900	-0.53309800	-1.05990000
H	2.59676500	-1.47627000	0.04631500

D, 2Dg

Cis:

-2 1

U	0.44355800	-0.05575700	0.06840000
O	-0.36392200	1.09823200	-1.58010900
O	1.18110800	-1.24677000	1.27342100
O	-1.02258400	0.57757100	1.18032500
O	1.65724300	1.73104000	0.80560800
O	-1.04235300	-1.67456600	-0.86768400
O	2.01939300	-0.54589300	-1.39255500
H	-1.29343100	1.32771700	-1.39660600
H	1.03791800	2.21950400	1.35788000
H	1.77625000	0.04156500	-2.12105700
H	-1.24813900	-1.20139600	-1.68341900
O	-3.02713400	1.51726700	-0.41433400
H	-3.28155800	0.57426800	-0.31853700
H	-2.29104500	1.49720200	0.24142300
O	-3.20466800	-1.11507200	0.56351600
H	-2.59884800	-0.57963100	1.11541600
H	-2.48515700	-1.48403100	-0.03340500

Trans:

-2 1

U	0.46100600	-0.06804000	-0.00230900
O	-0.10596500	1.67643900	0.05315000
O	0.97283700	-1.79040500	-0.05775300
O	-1.22143300	-0.51421500	1.57030900
O	1.94870500	0.40147800	1.65250400
O	-1.22336700	-0.41015600	-1.59902100
O	1.94859900	0.50730300	-1.62327100
H	-2.07927500	1.71468800	0.05514400
H	1.78305000	1.31785900	1.89731900
H	1.78483900	1.43847800	-1.80555400
H	-1.64857400	0.44841200	-1.71487600
O	-3.05172800	1.65645900	0.05277000
H	-3.20951100	0.68841500	0.02212000
H	-1.64567700	0.33496100	1.74393600
O	-3.28561500	-1.20839000	-0.03807100
H	-2.62654700	-1.13960400	0.70005700
H	-2.62708900	-1.09168000	-0.77062800

Transition state:

-2 1

U	-0.42483700	-0.06445700	-0.06153800
O	0.30274300	1.07985300	1.44782400
O	-1.03716700	-1.22329400	-1.32218000
O	1.20127800	0.71673300	-1.12234900
O	-1.64358400	1.66087600	-0.87107800
O	1.00915100	-1.67620700	0.84967400
O	-2.09926900	-0.63319800	1.30571500
H	1.29776300	1.36538200	1.23316100
H	-0.97401500	2.26024200	-1.22033900
H	-1.96370300	-0.04869200	2.06205500
H	1.33048800	-1.21573700	1.63431600
O	2.62140700	1.62559500	0.61021600
H	3.07324500	0.76818800	0.63994400
H	1.91427200	1.27948700	-0.38966800
O	3.28640600	-1.11218200	-0.55167700
H	2.72947600	-0.47617600	-1.04559300
H	2.54974600	-1.50802600	-0.02148500

F, 2Fg

Cis:

-2 1

U	0.41789900	0.02462000	-0.04971200
O	-0.42396600	-1.21489000	1.47819400
O	1.28016800	1.20187600	-1.19960200
O	-1.07608900	-0.46594200	-1.19136700
O	1.72068300	-1.67002600	-0.84430700
O	-0.90983900	1.81299500	0.76293700
O	1.97081800	0.49377700	1.46002100
H	-1.35190400	-1.43815000	1.27566700
H	2.40744000	-1.21546900	-1.34324100
H	1.64190300	-0.01866900	2.21102600
H	-0.56571000	2.57078900	0.27750100
O	-3.07393600	-1.58766500	0.28126600
H	-3.30889600	-0.63631800	0.31844700
H	-2.34200000	-1.49734400	-0.37362100
O	-3.21636200	1.15443200	-0.37201500
H	-2.63191900	0.65581300	-0.98000600
H	-2.46742000	1.51783200	0.18674400

Trans:

-2 1

U	0.44712800	0.01420000	-0.02154400
O	-0.25198800	-1.04510500	1.28994000
O	1.10470200	1.08860200	-1.32072800
O	-1.30236700	-0.62971800	-1.41454900
O	1.75116100	-1.68625000	-0.77864500
O	-0.97326400	1.75319700	0.67089500
O	2.06890000	0.72821100	1.40614700
H	-2.18101900	-1.33505400	1.14948300
H	2.19466600	-1.32803900	-1.55473800
H	1.89020200	0.26594000	2.23205800
H	-0.71647500	2.48253500	0.09519000
O	-3.11928700	-1.41994700	0.89719600
H	-3.28689100	-0.54960100	0.47597900
H	-1.80321300	-1.30407900	-0.93420200
O	-3.27802600	1.03093800	-0.54991200
H	-2.66713000	0.48888900	-1.11074200
H	-2.56459800	1.41353800	0.02622600

Transition state:

-2 1

U	0.40566100	0.03380100	-0.04301800
O	-0.39247200	-1.09925100	1.41293400
O	1.14901400	1.11907400	-1.31647000
O	-1.22200800	-0.62092700	-1.15994200
O	1.72698800	-1.65586000	-0.76875600
O	-0.93036300	1.81127500	0.67763700
O	2.01511700	0.67409100	1.38216300
H	-1.37474300	-1.41996900	1.14186600
H	2.30332500	-1.25969500	-1.43031400
H	1.77388700	0.20533700	2.19089500
H	-0.67735200	2.54484200	0.10642400
O	-2.63743600	-1.69914400	0.46997600
H	-3.11307700	-0.86026600	0.57706600
H	-1.94105300	-1.27083700	-0.47007300
O	-3.32714900	1.09177200	-0.36952700
H	-2.77233600	0.52235100	-0.94146100
H	-2.57299800	1.46029800	0.15915500

G, 2Gg

Cis:

-2 1

U	-0.43151100	-0.02730100	-0.06221300
O	0.43644900	1.12113900	1.52702200
O	-1.30075300	-1.11156300	-1.29231100
O	1.06482100	0.54147600	-1.16382800
O	-1.68599500	1.78193200	-0.66170200
O	0.97445600	-1.76461500	0.78670400
O	-2.00193900	-0.66352300	1.35449700
H	1.37720300	1.30269800	1.34044300
H	-1.23459800	2.53290300	-0.26016700
H	-2.59389100	-1.18304000	0.79926500
H	1.07900500	-1.44472800	1.69097700
O	3.10133300	1.47386300	0.37032800
H	3.32569700	0.52042700	0.30602000
H	2.36146700	1.45388000	-0.28239400
O	3.20045500	-1.18835500	-0.52513500
H	2.61234500	-0.64546700	-1.08884700
H	2.46120600	-1.54785200	0.05368200

Trans:

-2 1

U	-0.45097100	-0.02187400	-0.03352100
O	0.14325900	1.17456700	1.21626600
O	-0.99343900	-1.22305000	-1.26475800
O	1.25898300	0.75437700	-1.42129000
O	-1.91439800	1.53872500	-0.81066300
O	1.15140800	-1.52295700	0.80493900
O	-2.00380500	-0.83491600	1.41168200
H	2.12799300	1.22415600	1.18022100
H	-1.82654900	2.28788700	-0.21191500
H	-2.43260400	-1.54918600	0.92878900
H	1.49584100	-1.09662200	1.59837900
O	3.09338500	1.22120700	1.04993000
H	3.22519700	0.45106500	0.45623900
H	1.73938800	1.42119800	-0.91386500
O	3.25886800	-0.97698200	-0.79583500
H	2.62692000	-0.38266300	-1.27380300
H	2.57903900	-1.39121200	-0.20231400

Transition state:

-2 1

U	-0.41539100	-0.03661300	-0.05107300
O	0.36183800	1.12462800	1.40975400
O	-1.13267900	-1.14720900	-1.31161300
O	1.22184100	0.66359200	-1.13521200
O	-1.71243000	1.67145400	-0.76901600
O	0.98462200	-1.71154900	0.80627200
O	-2.04821300	-0.72925400	1.30353000
H	1.36510100	1.37765300	1.18316700
H	-1.30823200	2.47060400	-0.41311700
H	-2.58931500	-1.31620200	0.76510900
H	1.25097600	-1.32394300	1.64881300
O	2.68358500	1.59333200	0.54670100
H	3.11210100	0.72482100	0.59913400
H	1.95955100	1.23654400	-0.42846300
O	3.28514500	-1.17838600	-0.54867300
H	2.73888600	-0.54331800	-1.05517300
H	2.53727500	-1.55064300	-0.01474300

H, 2Hg

Cis:

-2 1

U	-0.46568600	-0.02284000	-0.07507800
O	1.05310000	0.04504600	1.57113400
O	-1.82060900	0.18736000	-1.33570100
O	0.35079900	-1.64924600	-0.61708100
O	1.20587900	0.96395800	-1.45071400
O	-1.96323900	-1.07745700	1.27512500
O	-1.03984700	1.92684200	0.75969300
H	1.63932300	-0.72018000	1.46159300
H	1.54193000	0.19169700	-1.91967100
H	-0.41465800	2.00059700	1.49459700
H	-2.80996200	-0.70183200	1.01098900
O	3.08321500	-1.56324000	0.08356300
H	3.21224900	-0.59342400	0.05127200
H	2.16591800	-1.66951400	-0.25215500
O	3.18549300	1.31779300	0.28478200
H	2.53565800	1.05974100	0.97148400
H	2.53435100	1.32575000	-0.47730000

Trans:

-2 1

U	0.45457000	0.00643200	0.03368700
O	-0.83094200	-0.05596300	-1.29555600
O	1.73719700	0.05338800	1.30500100
O	-0.61285300	-1.60420600	1.20322900
O	-1.06762800	1.27826200	1.36117100
O	1.76131400	-1.43740200	-1.14398500
O	1.33569800	1.85445900	-0.95384000
H	-2.30778000	-1.32782600	-0.93358700
H	-1.22968400	0.54944200	1.97622700
H	0.83170600	1.98087800	-1.76475000
H	2.52980500	-1.57886100	-0.58167100
O	-3.16585500	-1.46853700	-0.49204900
H	-3.32509600	-0.54282600	-0.20687900
H	-1.49814000	-1.75948700	0.84325100
O	-3.13912600	1.33242500	-0.23134600
H	-2.53318300	1.07516400	-0.94579400
H	-2.43048400	1.39238600	0.49296900

Transition state:

-2 1

U	0.43449600	0.01924600	0.05697000
O	-0.99196200	-0.23876900	-1.38591300
O	1.75135500	0.26094300	1.30462400
O	-0.51328900	-1.54842600	0.99061800
O	-1.14181900	1.24745800	1.29851100
O	1.88914000	-1.28062000	-1.08719200
O	1.11998700	1.84318200	-1.03545900
H	-1.70626600	-0.96324700	-1.04057200
H	-1.40702800	0.54716400	1.90777100
H	0.57478100	1.84907900	-1.83217400
H	2.71970400	-1.21323500	-0.60551400
O	-2.61247500	-1.73348200	-0.22025000
H	-3.05991800	-0.92697300	0.07794900
H	-1.54191100	-1.73351000	0.49895000
O	-3.28415600	1.25371100	-0.31730300
H	-2.71471000	0.86688700	-1.00204200
H	-2.57249600	1.37118200	0.37326800

CPCM - Water

UTH: $[UO_2(OH)_4]^{2-}$

A, 0Aw

Cis:
-2 1

U	0.00380600	0.00992300	-0.06164000
O	-0.12302300	-1.45754500	1.55990200
O	0.05037300	1.45471300	-1.27078900
O	0.06874000	-1.46958400	-1.22494500
O	2.28986700	-0.01026100	0.03756700
O	-2.28197800	0.03794500	-0.17324200
O	-0.03307000	1.53434200	1.51623600
H	-0.09574300	-2.35695300	1.21360300
H	2.66982300	-0.85614900	-0.21938900
H	-0.03616600	2.41867000	1.13232000
H	-2.65530900	-0.83536300	-0.01344500

Trans:
-2 1

U	0.00034100	0.00002300	0.01063200
O	-0.17866000	0.04844800	-1.79866800
O	0.17816600	-0.05033400	1.81939600
O	-2.20507000	0.53206700	0.24552900
O	0.54294900	2.21757500	0.03707600
O	-0.53127900	-2.21980900	0.02766000
O	2.20325500	-0.53157100	-0.23867100
H	-2.62785200	0.64508500	-0.61229300
H	0.57549800	2.57809800	-0.85547100
H	2.63211200	-0.64848400	0.61563700
H	-0.68602900	-2.54780100	-0.86459800

Transition state:
-2 1

U	-0.00006600	-0.01731200	-0.05332900
O	0.00747400	1.20010800	1.55855500
O	-0.00704900	-1.05843800	-1.57722100
O	0.02111500	1.94105600	-0.66662100
O	-2.26913300	-0.02841100	-0.10387000
O	2.26837200	-0.06983600	-0.09697100
O	-0.02060800	-1.85231400	1.21234400
H	0.01728400	1.93170300	0.66433900
H	-2.64523100	0.67126500	0.44102800
H	-0.02173000	-2.69683600	0.74953800
H	2.65442200	0.62929300	0.44166600

B, 0Bw

Cis:
-2 1

U	-0.03150800	0.00201300	-0.07136100
O	0.35923000	1.57746800	1.39423500
O	-0.31881000	-1.41663900	-1.27521900
O	-0.34294200	1.39547000	-1.31063700
O	-2.21000000	-0.08028000	0.59425900
O	2.22951500	-0.14077300	-0.43766900
O	0.44809000	-1.43581200	1.52989300
H	0.21843700	2.43295000	0.97068800
H	-2.73530500	-0.77967700	0.19376300
H	1.39503400	-1.57399800	1.38578600
H	2.69990900	0.54002400	0.05609900

Trans:
-2 1

U	0.00002200	-0.00001400	0.00005000
O	-0.00191200	0.28196600	-1.79705700
O	0.00191400	-0.28181600	1.79719600
O	1.60611600	1.59678700	0.25177300
O	1.62660300	-1.57589700	-0.25217500
O	-1.62680300	1.57590500	0.25136700
O	-1.60622300	-1.59663700	-0.25147000
H	1.87387800	1.95389000	-0.60169000
H	1.90172500	-1.92893400	0.60062000
H	-1.87448800	-1.95410000	0.60167800
H	-1.90068500	1.92795500	-0.60224200

Transition state:
-2 1

U	-0.00799700	-0.00698100	-0.04484400
O	0.54691100	1.08882100	1.56038200
O	-0.48707000	-0.93279900	-1.56823800
O	0.64175900	1.84042900	-0.65963200
O	-2.12605000	0.78911100	0.09244700
O	2.09146200	-0.83761400	-0.26659300
O	-0.56316900	-1.76642300	1.20844100
H	0.73619100	1.79636500	0.66624200
H	-2.74245100	0.30591200	-0.46706900
H	-0.82080300	-2.56078400	0.72860800
H	2.73209200	-0.35145800	0.26344900

C, 0Cw

Cis:

-2 1

U	-0.00463600	-0.05240300	-0.13427300
O	0.30753600	1.67074900	1.36505200
O	-0.38878700	-1.83845400	-0.31411700
O	0.36717100	1.38871800	-1.21674800
O	-2.22348100	0.42099900	-0.42892500
O	2.21851000	-0.59801600	-0.19559500
O	-0.27084500	-0.74546900	2.00282100
H	0.47317200	2.48582000	0.88264600
H	-2.75723400	-0.33869900	-0.17291700
H	-0.10554600	0.11788000	2.41038900
H	2.73528500	0.16788400	-0.46694400

Trans:

-2 1

U	-0.00001300	-0.00027300	0.01064300
O	0.15604300	-0.07855200	-1.79963200
O	-0.15742400	0.07667900	1.82053900
O	-0.94953000	-2.07246500	0.03039900
O	-2.06260000	0.93815700	-0.22510300
O	2.06589800	-0.93449400	0.24406100
O	0.93828700	2.07739100	0.02163500
H	-1.07075900	-2.41413900	-0.86192200
H	-2.45822500	1.12604300	0.63260700
H	1.14313700	2.37711900	-0.87039000
H	2.46163300	-1.11763700	-0.61463400

Transition state:

-2 1

U	-0.00855300	-0.00938800	-0.05293000
O	0.49296800	1.00638800	1.62005300
O	-0.44230300	-0.85295300	-1.63463100
O	0.61146200	1.87721800	-0.55860900
O	-2.14589800	0.72673000	0.09785700
O	2.11851500	-0.76415100	-0.27334200
O	-0.56308300	-1.88953200	1.04424500
H	0.68450000	1.76404800	0.77027900
H	-2.74355300	0.24703100	-0.48471900
H	-0.46946000	-1.75280800	1.99548500
H	2.74210600	-0.22417300	0.22392500

D, 0Dw

Cis:

-2 1

U	0.00041000	-0.02140900	-0.07208300
O	-0.01587100	1.43632500	1.56788800
O	0.00976800	-1.47817600	-1.26439200
O	0.00099600	1.43816500	-1.25794700
O	-2.28956500	-0.01731000	-0.08113900
O	2.29053000	0.00068800	-0.06271300
O	0.00251600	-1.51591100	1.54280500
H	-0.01920500	2.34391700	1.24338300
H	-2.65202600	0.85602500	-0.26154600
H	-0.00141000	-1.00988000	2.36713400
H	2.64788200	0.86932100	-0.27337400

Trans:

-2 1

U	-0.00000200	-0.00001800	0.02167300
O	-0.00287700	0.00207200	-1.79688800
O	0.00259400	-0.00194700	1.83931700
O	-1.03710500	-2.03333100	0.03439700
O	-2.03296300	1.03730700	0.03725200
O	2.03353000	-1.03730900	0.03247500
O	1.03744900	2.03310500	0.03516500
H	-1.20059100	-2.34430900	-0.86233400
H	-2.34628500	1.19889900	-0.85898700
H	1.19731700	2.34575400	-0.86163500
H	2.34467600	-1.19787200	-0.86474400

Transition state:

-2 1

U	0.00000000	-0.02034900	-0.06131300
O	0.00000000	1.10688900	1.61335200
O	-0.00000300	-0.98466400	-1.63236700
O	0.00000800	1.96344800	-0.57281000
O	-2.26821200	-0.03396600	-0.10759000
O	2.26821100	-0.03397900	-0.10758500
O	-0.00000300	-1.96704800	1.06235700
H	0.00000600	1.88492400	0.76086900
H	-2.63978500	0.68658800	0.41264000
H	0.00000300	-1.79142300	2.01181500
H	2.63978000	0.68660300	0.41261000

E, 0Ew

Cis:

-2 1

U	0.00000100	0.01080100	-0.06089300
O	0.00001100	1.53819700	1.51193000
O	-0.00000300	-1.47286700	-1.21904300
O	0.00002300	1.45971000	-1.26791200
O	-2.28792000	0.00887300	-0.06858800
O	2.28792200	0.00882400	-0.06855300
O	-0.00003600	-1.45707800	1.56782100
H	0.00001800	2.42042400	1.12318500
H	-2.65613400	-0.87176300	-0.19259200
H	-0.00004100	-2.35579800	1.21890100
H	2.65612500	-0.87180700	-0.19262000

Trans:

-2 1

U	-0.00024900	-0.00006700	-0.01075000
O	-0.17994000	-0.00607700	-1.82016500
O	0.17913600	0.00734300	1.79910600
O	-2.26306200	-0.11343500	0.23257200
O	-0.11908800	2.27840900	-0.02778400
O	0.10754500	-2.27889200	-0.03082100
O	2.26524800	0.11229500	-0.24403100
H	-2.70626600	-0.13341500	-0.62215600
H	-0.08048400	2.63757300	0.86501800
H	2.70287700	0.13676900	0.61345900
H	0.18810800	-2.63187400	0.86170500

Transition state:

-2 1

U	0.00000200	-0.00073900	-0.03869300
O	0.00008300	1.24111700	1.55553500
O	-0.00006300	-1.04890500	-1.55787700
O	0.00027300	1.94994100	-0.68120800
O	-2.26922900	-0.01959800	-0.06203400
O	2.26921700	-0.02011900	-0.06191500
O	-0.00027400	-1.82724800	1.23281000
H	0.00021300	1.95813500	0.64933400
H	-2.62511800	-0.70940600	-0.63146200
H	-0.00030600	-2.67227100	0.77073700
H	2.62501300	-0.70995300	-0.63136900

F, 0Fw

Cis:

-2 1

U	-0.04691600	0.05658300	0.00000000
O	2.13690800	-0.16977600	0.00000000
O	-1.92416900	-0.04230700	0.00000000
O	0.24510100	1.91722100	0.00000000
O	-0.05350200	0.06213300	2.28944000
O	-0.05350200	0.06213300	-2.28944000
O	-0.05350200	-2.14323600	0.00000000
H	2.57613900	0.68839800	0.00000000
H	-0.75786800	-0.48823200	2.64710600
H	0.87722400	-2.40690700	0.00000000
H	-0.75786800	-0.48823200	-2.64710600

Trans:

-2 1

U	0.00000000	0.00000000	0.00000000
O	0.00000600	-0.00000700	1.81845000
O	-0.00000200	0.00000900	-1.81845000
O	1.58965000	1.63448900	-0.03392100
O	-1.63448900	1.58964800	0.03392900
O	1.63448700	-1.58965300	0.03391700
O	-1.58965200	-1.63448700	-0.03392500
H	1.84223200	1.89266000	0.85897600
H	-1.89267300	1.84223500	-0.85896400
H	-1.84224000	-1.89266700	0.85896900
H	1.89265400	-1.84223700	-0.85898100

Transition state:

-2 1

U	-0.04080400	0.02103200	0.00000000
O	1.97605900	0.14587500	0.00000000
O	-1.88519400	0.02058300	0.00000000
O	0.52308300	1.99264700	0.00000000
O	-0.07341900	0.02175100	2.26793000
O	-0.07341900	0.02175100	-2.26793000
O	-0.07341900	-2.22017900	0.00000000
H	1.63192800	1.24789900	0.00000000
H	-0.92914100	-0.24173200	2.62155500
H	0.83083700	-2.55882200	0.00000000
H	-0.92914100	-0.24173200	-2.62155500

UTH···H_2O: $[UO_2(OH)_4]^{2-}$ ···H_2O

A, 1Aw

Cis:

-2 1

U	-0.23270100	-0.01241700	-0.05155400
O	0.85831200	0.74303100	1.64646300
O	-1.18703000	-0.84618000	-1.42851000
O	0.84631500	1.08103200	-1.18201800
O	-1.76413200	1.65892400	0.14819500
O	1.45333100	-1.63898100	-0.10410500
O	-1.41226600	-1.19082700	1.36491300
H	1.79224000	0.79504600	1.36315800
H	-1.58584000	2.44972900	-0.37002400
H	-2.05109600	-1.74522300	0.90058100
H	1.53942000	-2.11906100	-0.93444200
O	3.24446400	0.36888700	0.08314000
H	2.62848000	0.86030300	-0.49527200
H	2.77331700	-0.50548300	0.05435300

Trans:

-2 1

U	-0.23933600	-0.00052200	0.03415500
O	0.59008000	-0.27584200	-1.57084400
O	-1.06690100	0.30697600	1.61894300
O	1.14540200	-1.48860500	1.01549200
O	-1.75536500	-1.62807900	-0.42382800
O	1.43834700	1.54724600	0.51106800
O	-1.53308400	1.58744600	-0.93550200
H	2.63051000	-0.36477100	-1.17470900
H	-1.61879200	-2.02112800	-1.29262300
H	-2.14426400	1.98764900	-0.30747600
H	1.45545700	1.80406800	1.43960100
O	3.29548100	-0.12057000	-0.51182200
H	2.01132600	-1.36165800	0.59819300
H	2.77299200	0.57532400	-0.03332300

Transition state:

-2 1

U	-0.22156900	-0.01092000	-0.05111500
O	0.91277800	0.57782800	1.51471200
O	-1.26162100	-0.58474000	-1.44785400
O	1.24796800	0.87087100	-1.21076600
O	-1.42304000	1.89708200	0.02524600
O	1.09115700	-1.87007100	-0.10123900
O	-1.64716400	-0.97353200	1.35235800
H	1.91407500	0.52491000	1.14457400
H	-1.06353400	2.54379400	0.64276200
H	-2.41382300	-1.37324300	0.92637500
H	1.02550100	-2.44086800	-0.87397600
O	3.06199300	0.29770000	0.27766600
H	2.21297800	0.67486900	-0.59391000
H	2.85259100	-0.64588000	0.17580100

B, 1Bw

Cis:

-2 1

U	0.22896400	0.00809800	-0.04941600
O	-0.85284200	-0.72353000	1.65402600
O	1.21935500	0.76159100	-1.44090300
O	-0.85519500	-1.07872300	-1.18923800
O	1.75092500	-1.65695700	0.23035800
O	-1.45891700	1.63267800	-0.16168700
O	1.36142100	1.26816300	1.35027200
H	-1.78812900	-0.78804700	1.37548700
H	2.28107000	-1.90498700	-0.53328700
H	2.00290800	1.81255000	0.87817300
H	-1.58844000	2.02403600	-1.03231100
O	-3.23715600	-0.39009700	0.09363200
H	-2.61894300	-0.88103400	-0.48421500
H	-2.77384800	0.48743900	0.05071200

Trans:

-2 1

U	-0.23808600	-0.00711700	0.02506400
O	0.63833300	-0.01628000	-1.57908300
O	-1.13200800	0.01256900	1.60341100
O	1.07493500	-1.66935700	0.79447700
O	-1.75681600	-1.47315200	-0.79987900
O	1.44582500	1.41767100	0.83852400
O	-1.40910900	1.79737300	-0.66718600
H	2.65870700	-0.20982600	-1.14087500
H	-2.38774800	-1.78148200	-0.14102800
H	-2.01238100	2.12358600	0.00965300
H	1.61036800	2.14029000	0.22147300
O	3.30295400	-0.13495900	-0.41904700
H	1.94708300	-1.53925700	0.39218900
H	2.77499900	0.45053800	0.18300900

Transition state:

-2 1

U	0.23274000	0.00451400	-0.04762000
O	-1.08000200	-0.09806100	1.50490800
O	1.44557000	0.12348500	-1.42043900
O	-1.36210700	-0.67737100	-1.17755700
O	0.91325300	-2.10503200	0.34708500
O	-0.47168200	2.10551400	-0.43590600
O	1.78571100	0.77715200	1.33305400
H	-2.04979500	-0.16847000	1.12927400
H	1.56815900	-2.44550100	-0.27108300
H	2.61357500	1.03174800	0.91041300
H	-1.33310100	2.27544700	-0.03810400
O	-3.27889400	-0.27826100	0.24766000
H	-2.33447500	-0.52929100	-0.59309700
H	-3.49125300	0.64134800	0.05317300

C, 1Cw

Cis:

-2 1

U	0.23318300	0.00143200	-0.04736300
O	-1.15568200	-0.11435200	1.57630900
O	1.56339700	0.11457800	-1.35195700
O	-1.27541000	-0.13659600	-1.25590000
O	0.44498000	-2.26670700	-0.00613900
O	0.04089800	2.27114900	-0.03124900
O	1.82225000	0.15371600	1.47060200
H	-2.07958900	-0.16353400	1.26239200
H	1.09202500	-2.61128300	-0.62961900
H	2.69277700	0.23099800	1.06324500
H	0.61094400	2.71245400	-0.66884100
O	-3.58783800	-0.13863100	0.06858900
H	-2.79347900	-0.16772200	-0.53252200
H	-3.79628800	0.80207200	0.10069800

Trans:

-2 1

U	0.23719900	-0.00208100	-0.02013600
O	-0.62537400	-0.10960700	1.58729400
O	1.09948800	0.13906600	-1.60969600
O	-1.11108300	-1.59542700	-0.87487100
O	1.73042700	-1.56609900	0.66700100
O	-1.44660000	1.46645500	-0.69037700
O	1.48498600	1.70861700	0.79454000
H	-2.64593700	-0.26779600	1.16736100
H	2.33941100	-1.84279500	-0.02580400
H	2.07461400	2.06994900	0.12357800
H	-1.44332900	1.61390500	-1.64270600
O	-3.30446500	-0.10319200	0.47402100
H	-1.98487000	-1.44258800	-0.48348500
H	-2.78118400	0.54227200	-0.06972700

Transition state:

-2 1

U	0.22458400	0.00082300	-0.04183100
O	-1.13598600	-0.06795100	1.46695000
O	1.47440700	0.06328800	-1.38369000
O	-1.43704000	-0.13451000	-1.26860400
O	0.39445100	-2.24687100	0.01359000
O	0.06596300	2.24667900	-0.07005600
O	1.86033900	0.15187600	1.44514300
H	-2.10779000	-0.09718800	1.08248600
H	1.05213100	-2.61082300	-0.58814600
H	2.74432400	0.21517600	1.06649500
H	0.67293100	2.68410500	-0.67615700
O	-3.34418600	-0.12715600	0.22173600
H	-2.40546200	-0.13906300	-0.65604400
H	-3.64147900	0.78926500	0.21922800

D, 1Dw

Cis:

-2 1

U	0.23361500	0.01396700	-0.06495400
O	-0.81468300	-0.63749900	1.69033400
O	1.21442600	0.70334800	-1.49450900
O	-0.82203700	-1.14966400	-1.15317600
O	1.78673700	-1.59175500	0.33257200
O	-1.49985200	1.58564000	-0.25563500
O	1.33027700	1.37953800	1.26997500
H	-1.75374100	-0.72858400	1.43125900
H	2.43198800	-1.77074100	-0.35814000
H	1.00672100	1.23238500	2.16866500
H	-1.66598400	1.90555100	-1.14891700
O	-3.21277900	-0.46184900	0.14320400
H	-2.59465000	-0.96959700	-0.41938000
H	-2.77360100	0.42391100	0.04012900

Trans:

-2 1

U	-0.23988800	-0.00248600	0.03228700
O	0.58944400	0.05775200	-1.59507900
O	-1.06602000	-0.02909500	1.64689100
O	1.09710000	-1.70245400	0.68076000
O	-1.77655400	-1.44959900	-0.79271000
O	1.47109500	1.37273200	0.81699400
O	-1.49493900	1.79777500	-0.53902600
H	2.63309400	-0.17319500	-1.21684200
H	-2.40717000	-1.75630100	-0.13274700
H	-1.31291300	2.09565900	-1.43698200
H	1.47834300	1.44918900	1.77747400
O	3.29557100	-0.09309900	-0.51271300
H	1.96864400	-1.51787100	0.29848300
H	2.78417000	0.49910800	0.09930100

Transition state:

-2 1

U	0.22070000	0.00808200	-0.05318000
O	-0.89117500	-0.31349300	1.60463100
O	1.23316600	0.33980600	-1.54368200
O	-1.19516000	-1.12786900	-1.04380900
O	1.46642300	-1.80435000	0.41368300
O	-1.17323100	1.77387800	-0.42426200
O	1.62001500	1.29186000	1.11304900
H	-1.89010100	-0.36789300	1.22712500
H	2.17583700	-2.00729700	-0.20459800
H	1.35419800	1.32124200	2.04081500
H	-1.14025600	2.17913700	-1.29738400
O	-3.03275400	-0.35603200	0.32312800
H	-2.17062500	-0.85790900	-0.46227600
H	-2.85175300	0.55880400	0.04695100

E, 1Ew

Cis:

-2 1

U	0.23273800	-0.01243400	-0.05164700
O	-0.85818300	0.74502400	1.64548300
O	1.18713300	-0.84831600	-1.42721600
O	-0.84694200	1.07991000	-1.18277100
O	-1.45337700	-1.63920400	-0.10222700
O	1.76436600	1.65889700	0.14539000
O	1.41249200	-1.18923000	1.36592500
H	-1.79222600	0.79676900	1.36244600
H	-1.53913300	-2.11930000	-0.93259500
H	2.05191800	-1.74362100	0.90243300
H	1.57756700	2.45489900	-0.36174400
O	-3.24419200	0.36827500	0.08300100
H	-2.62751500	0.85854800	-0.49568800
H	-2.77288800	-0.50618800	0.05597000

Trans:

-2 1

U	0.23933100	-0.00052400	0.03415900
O	-0.59007200	-0.27582600	-1.57085100
O	1.06687100	0.30698600	1.61895900
O	-1.14541200	-1.48860500	1.01546900
O	-1.43833700	1.54727200	0.51100900
O	1.75534000	-1.62810700	-0.42382200
O	1.53311600	1.58742800	-0.93549800
H	-2.63047800	-0.36475800	-1.17474200
H	-1.45544000	1.80417000	1.43952100
H	2.14427100	1.98757500	-0.30741200
H	1.61872100	-2.02107900	-1.29264500
O	-3.29541000	-0.12058300	-0.51179800
H	-2.01135200	-1.36159800	0.59821400
H	-2.77291900	0.57535100	-0.03332800

Transition state:

-2 1

U	0.22156900	-0.01092100	-0.05111600
O	-0.91278000	0.57783500	1.51470800
O	1.26162400	-0.58474700	-1.44784900
O	-1.24797400	0.87084500	-1.21077900
O	-1.09114000	-1.87008200	-0.10122100
O	1.42302300	1.89709400	0.02522200
O	1.64717600	-0.97349800	1.35237000
H	-1.91407500	0.52492100	1.14457200
H	-1.02546000	-2.44089700	-0.87394400
H	2.41382600	-1.37322200	0.92638200
H	1.06355300	2.54377100	0.64279700
O	-3.06200000	0.29770500	0.27766700
H	-2.21298200	0.67485500	-0.59391800
H	-2.85261100	-0.64587900	0.17581300

F, 1Fw

Cis:

-2 1

U	0.23276300	-0.01244000	-0.05167800
O	-0.85858100	0.74479200	1.64526700
O	1.18799000	-0.84833300	-1.42679100
O	-0.84683400	1.07991400	-1.18264400
O	-1.45303100	-1.63931100	-0.10236100
O	1.76383100	1.65951200	0.14548100
O	1.41268300	-1.18898500	1.36607700
H	-1.79266300	0.79622500	1.36234500
H	-1.53936100	-2.12149200	-0.93144200
H	2.05188500	-1.74329100	0.90216800
H	1.57588800	2.45572900	-0.36091000
O	-3.24457000	0.36797100	0.08290800
H	-2.62882500	0.85914000	-0.49596600
H	-2.77305600	-0.50626400	0.05469200

Trans:

-2 1

U	-0.24169000	-0.00658400	-0.03862500
O	0.61393700	-0.15263600	1.56954100
O	-1.12074900	0.14607400	-1.61767500
O	1.10931700	-1.57463800	-0.92968700
O	1.44168000	1.49507100	-0.70453800
O	-1.76836900	-1.55814300	0.60763200
O	-1.45098200	1.71001300	0.79087900
H	2.64215300	-0.28707900	1.15773700
H	1.56733600	2.19087900	-0.04870700
H	-2.07509300	2.05941800	0.14521500
H	-1.61030400	-1.87139800	1.50478000
O	3.29631400	-0.13157700	0.45818700
H	1.97387800	-1.46094100	-0.50608500
H	2.76833700	0.50157000	-0.09415200

Transition state:

-2 1

U	0.23942700	-0.00672500	-0.05596600
O	-1.08480700	0.23384800	1.46539600
O	1.47694300	-0.23665900	-1.39306500
O	-1.39431300	0.42298500	-1.24766400
O	-0.31136700	-2.18637800	-0.17775100
O	0.80416500	2.17745000	0.02928600
O	1.82300700	-0.48038300	1.42057400
H	-2.06288400	0.23930800	1.09394100
H	-1.16322400	-2.37628700	0.23141600
H	2.68888700	-0.67538600	1.04532600
H	0.21722600	2.69006800	0.59632400
O	-3.29455500	0.20995900	0.23355000
H	-2.36442400	0.34554200	-0.64145400
H	-3.49544600	-0.73111000	0.18067900

G, 1Gw

Cis:

-2 1

U	-0.23280700	-0.01245000	-0.05168500
O	0.85845800	0.74524800	1.64514000
O	-1.18776700	-0.84861600	-1.42681200
O	0.84660100	1.07954600	-1.18302400
O	-1.76418900	1.65921800	0.14546500
O	1.45340200	-1.63919900	-0.10205700
O	-1.41232900	-1.18895500	1.36635000
H	1.79242900	0.79660700	1.36182600
H	-1.57674500	2.45532500	-0.36128600
H	-2.05168400	-1.74337600	0.90278500
H	1.53983000	-2.11974500	-0.93209400
O	3.24482100	0.36806700	0.08309600
H	2.63004800	0.85988600	-0.49616800
H	2.77242500	-0.50574300	0.05470000

Trans:

-2 1

U	0.24169300	-0.00658900	-0.03862400
O	-0.61384300	-0.15248400	1.56959100
O	1.12058100	0.14602600	-1.61774800
O	-1.10920600	-1.57489600	-0.92942500
O	1.76852200	-1.55796200	0.60767200
O	-1.44176300	1.49494300	-0.70468900
O	1.45083300	1.71023500	0.79072500
H	-2.64210700	-0.28673900	1.15780200
H	1.61054600	-1.87124100	1.50482500
H	2.07486900	2.05952700	0.14492700
H	-1.56794500	2.19017000	-0.04834100
O	-3.29626400	-0.13155700	0.45817200
H	-1.97372700	-1.46126800	-0.50573400
H	-2.76826400	0.50132000	-0.09449000

Transition state:

-2 1

U	-0.23881000	-0.00802100	-0.05650400
O	1.06977600	0.26725100	1.47360500
O	-1.46005500	-0.27539400	-1.40160400
O	1.37950800	0.49453100	-1.24163700
O	-0.89150600	2.14900100	0.05365600
O	0.41342400	-2.15920600	-0.18593500
O	-1.81068700	-0.55719200	1.40474600
H	2.04700600	0.26691000	1.10369500
H	-0.32971200	2.67705900	0.63188000
H	-2.66770500	-0.77423000	1.02127000
H	1.27802200	-2.30002700	0.21639500
O	3.27808000	0.22933400	0.23464900
H	2.34852000	0.39477500	-0.63842700
H	3.46605800	-0.71316600	0.16370300

UTH···(H2O)2: [UO2(OH)4]2- ···$(H_2O)_2$

A, 2Aw

Cis:

-2 1

U	-0.41544000	-0.01782200	-0.04829700
O	0.56508300	1.03184400	1.50933900
O	-1.39087600	-1.01754300	-1.27505000
O	1.06712200	0.46554400	-1.21110700
O	-1.55602400	1.84519800	-0.64912700
O	0.75588600	-1.93070200	0.61422300
O	-1.98701200	-0.47600600	1.40910400
H	1.48340900	1.28964900	1.28230900
H	-1.10288900	2.67448600	-0.46369700
H	-2.71476600	-0.97343500	1.01779700
H	0.51788700	-2.72398100	0.12223700
O	3.07577400	1.49736600	0.32447500
H	3.32139800	0.54839800	0.35897700
H	2.38861300	1.42652900	-0.37506700
O	3.13912400	-1.20359500	-0.31123100
H	2.61065200	-0.70343200	-0.96241900
H	2.36358700	-1.59540900	0.17822400

Trans:

-2 1

U	-0.43496700	-0.01217500	-0.02627500
O	0.28102100	1.00182900	1.31355600
O	-1.11221700	-1.03299900	-1.35580800
O	1.31392500	0.62710800	-1.39785100
O	-1.66578400	1.74013800	-0.73484200
O	0.87727600	-1.80119600	0.66583800
O	-2.09525100	-0.67316000	1.34352900
H	2.15858600	1.32393000	1.14691700
H	-1.56851200	2.53452100	-0.19872700
H	-2.71324300	-1.28749600	0.93276200
H	0.67412400	-2.59233700	0.15315200
O	3.07878800	1.40195900	0.83787800
H	3.25803600	0.50008500	0.49547500
H	1.88021400	1.24325200	-0.90866000
O	3.22102600	-1.08553700	-0.45154800
H	2.65340900	-0.55323500	-1.05573700
H	2.48407700	-1.47372000	0.08607300

Transition state:

-2 1

U	-0.40565600	-0.03007300	-0.04418300
O	0.48312300	1.00169500	1.42750700
O	-1.22750500	-1.00778400	-1.35337800
O	1.21871400	0.60171400	-1.17776700
O	-1.59431400	1.77998800	-0.65682200
O	0.82338200	-1.88203300	0.59216400
O	-2.02577700	-0.61285600	1.34421600
H	1.47759800	1.31093600	1.13754800
H	-1.30780400	2.59744600	-0.23479100
H	-2.72238300	-1.15365100	0.95502700
H	0.62544600	-2.67457100	0.08079600
O	2.67687800	1.59155600	0.45563900
H	3.17297900	0.76084700	0.55189500
H	1.99710200	1.20831700	-0.45568400
O	3.25355400	-1.11970600	-0.28646000
H	2.73333700	-0.58412000	-0.91628100
H	2.47961700	-1.51907500	0.18553700

B, 2Bw

Cis:

-2 1

U	-0.41821100	-0.03002400	-0.05061900
O	0.38579300	1.19652300	1.48306100
O	-1.21024900	-1.20550900	-1.25497200
O	1.03044300	0.54628800	-1.20894400
O	-1.74698900	1.64906100	-0.78688400
O	0.98186800	-1.71623800	0.81289200
O	-1.96500700	-0.60714000	1.38401100
H	1.33820900	1.37565900	1.33436500
H	-1.39308400	2.53786000	-0.67649200
H	-2.60932600	-1.21276100	0.99829100
H	1.22672600	-1.44814600	1.70686300
O	2.99518100	1.47234700	0.43216200
H	3.27170800	0.53525300	0.35256200
H	2.32182600	1.46573900	-0.28336900
O	3.18512700	-1.13599100	-0.56813600
H	2.60939200	-0.58696700	-1.13433500
H	2.46061100	-1.49918900	0.01357200

Trans:

-2 1

U	-0.43648300	-0.01531400	-0.02727000
O	0.10919400	1.01439400	1.37607500
O	-0.91994800	-1.05292900	-1.42524900
O	1.25869900	0.91014800	-1.30524500
O	-1.87289700	1.58093200	-0.71970300
O	1.09049400	-1.63060300	0.66723900
O	-2.01944700	-0.96081300	1.26077800
H	2.08013900	1.08678500	1.32196800
H	-1.89101200	2.36879300	-0.16564800
H	-2.53444100	-1.63933500	0.81062200
H	1.44129700	-1.41977000	1.54074000
O	3.01800300	1.17341100	1.08031400
H	3.17473800	0.39756800	0.50331000
H	1.80113300	1.46920500	-0.73036400
O	3.20591900	-0.93211300	-0.83710700
H	2.59922000	-0.28389200	-1.26637100
H	2.52525300	-1.38984900	-0.28219500

Transition state:

-2 1

U	-0.40619000	-0.03761700	-0.04694300
O	0.32292400	1.11590600	1.42384000
O	-1.05635900	-1.13753500	-1.35456800
O	1.19868600	0.69503000	-1.15365600
O	-1.74087300	1.61095800	-0.79045200
O	0.98056600	-1.71623500	0.76089300
O	-2.00580800	-0.73755000	1.30204200
H	1.35156500	1.35460400	1.20709000
H	-1.55855800	2.47752600	-0.41046900
H	-2.63019900	-1.36015700	0.91220800
H	1.27608000	-1.47301200	1.64683100
O	2.61115100	1.55843400	0.58536600
H	3.07790000	0.70918700	0.64643400
H	1.95093000	1.24328500	-0.37917100
O	3.27067300	-1.08187100	-0.55015100
H	2.71710100	-0.46566600	-1.06865300
H	2.53699500	-1.48213800	-0.02205700

C, 2Cw

Cis:

-2 1

U	-0.41647100	-0.04708700	-0.05094100
O	0.29194100	1.33143000	1.40686900
O	-1.09159000	-1.35049900	-1.18946300
O	0.99957300	0.47038600	-1.27506400
O	-1.79485800	1.54266900	-0.86996900
O	1.06418100	-1.55665000	0.97118500
O	-1.96121400	-0.59436700	1.41009700
H	1.24946700	1.49504400	1.27298200
H	-2.08718700	1.48787200	-1.78492400
H	-1.88565900	-0.01788700	2.18225500
H	1.34107200	-1.16986900	1.81070500
O	2.91328300	1.55095100	0.35650400
H	3.23171500	0.62488500	0.31576000
H	2.25074400	1.48844700	-0.36573900
O	3.21465100	-1.08952900	-0.52587100
H	2.61594500	-0.59998700	-1.12239100
H	2.51149800	-1.41167600	0.10357100

Trans:

-2 1

U	-0.43646500	-0.01377600	-0.02884600
O	0.09972200	0.65478600	1.58147300
O	-0.91005800	-0.68999300	-1.63640800
O	1.24910500	1.18654400	-1.06933200
O	-1.84868200	1.71649800	-0.30812100
O	1.10386600	-1.72897900	0.29010900
O	-2.04371700	-1.24150300	0.96459600
H	2.07329800	0.75788500	1.54257100
H	-2.31397800	1.71405000	-1.15155300
H	-2.09639200	-1.13483000	1.92060300
H	1.46433000	-1.70531900	1.18444800
O	3.00691400	0.91352200	1.32000200
H	3.16783600	0.29364400	0.57911300
H	1.78306700	1.61510000	-0.38489100
O	3.21070500	-0.69075900	-1.03472200
H	2.59658300	0.03435900	-1.30061900
H	2.53722500	-1.26843800	-0.59659400

Transition state:

-2 1

U	-0.40520500	-0.04359000	-0.04638500
O	0.27945300	1.12243000	1.43941300
O	-0.99806700	-1.15282300	-1.37097600
O	1.18186900	0.71983400	-1.16008100
O	-1.75439300	1.59006700	-0.76806700
O	1.03372200	-1.65779000	0.78978000
O	-2.01976000	-0.81449700	1.26581200
H	1.30662700	1.36218700	1.22969800
H	-2.27896700	1.41426200	-1.55598400
H	-2.00901300	-0.38943600	2.13279300
H	1.36385300	-1.36561500	1.64827800
O	2.57172800	1.57974700	0.60268500
H	3.05754400	0.74115500	0.65462800
H	1.91992700	1.26497400	-0.37034000
O	3.28497700	-1.03218400	-0.59034000
H	2.71430700	-0.41854600	-1.09351800
H	2.56834000	-1.43697000	-0.04392200

D, 2Dw

Cis:

-2 1

U	-0.42047800	-0.04928600	-0.05538700
O	0.31361700	1.26307500	1.45920400
O	-1.09111500	-1.35085900	-1.20433600
O	0.98948500	0.52777000	-1.25016000
O	-1.78723000	1.56767500	-0.85974400
O	1.04654000	-1.59474800	0.94128300
O	-1.99516300	-0.58359700	1.36533000
H	1.26817000	1.43710300	1.32325000
H	-1.44563200	2.13723900	-1.55567000
H	-1.89093400	-0.04050800	2.15863700
H	1.33178500	-1.20608300	1.77715400
O	2.93304100	1.52626000	0.40681300
H	3.23616800	0.59706700	0.33266600
H	2.26625100	1.50146800	-0.31282900
O	3.19415500	-1.09122700	-0.55301800
H	2.60319000	-0.57851500	-1.13658600
H	2.48837300	-1.42827700	0.06596300

Trans:

-2 1

U	-0.43814500	-0.02529700	-0.03849200
O	0.06471500	0.98407900	1.39413900
O	-0.87541000	-1.04033800	-1.46820600
O	1.25746400	0.94757600	-1.28226700
O	-1.88799000	1.56170300	-0.72097800
O	1.11020300	-1.61969100	0.65418200
O	-2.03630900	-1.04081000	1.18037200
H	2.04906800	1.07398400	1.36659600
H	-1.90732300	2.34996400	-0.16756800
H	-2.08790800	-0.74965000	2.09722600
H	1.44834100	-1.41555600	1.53416300
O	2.98637300	1.17857300	1.13111500
H	3.15439000	0.41900300	0.53610900
H	1.78242800	1.50880100	-0.69358000
O	3.22071400	-0.88037200	-0.83671400
H	2.60773100	-0.22960600	-1.25377600
H	2.54457200	-1.35540600	-0.29106300

Transition state:

-2 1

U	-0.40838300	-0.04921500	-0.05751200
O	0.28669300	1.10728000	1.42546200
O	-1.02402200	-1.15710000	-1.37470800
O	1.18671200	0.70865500	-1.15300700
O	-1.75530000	1.58918500	-0.80403900
O	1.00483500	-1.69532600	0.77211100
O	-2.03315700	-0.80278600	1.25342100
H	1.31719700	1.35837400	1.21914200
H	-1.53122500	2.47212500	-0.49018600
H	-1.97174800	-0.42027500	2.13806500
H	1.29160700	-1.44302600	1.65832300
O	2.57118000	1.58285900	0.60362400
H	3.05552100	0.74274500	0.66027500
H	1.93050400	1.26904400	-0.36158500
O	3.28751800	-1.03039800	-0.53156300
H	2.72555700	-0.42859900	-1.05795200
H	2.55819800	-1.44155400	-0.00534500

E, 2Ew

Cis:

-2 1

U	-0.41275100	-0.02998100	-0.05061900
O	0.49477700	1.07735400	1.51324900
O	-1.31754400	-1.06899600	-1.29384000
O	1.04478300	0.47109500	-1.23762200
O	-1.59897500	1.80441400	-0.64218600
O	0.83497700	-1.87432500	0.66106200
O	-1.98187500	-0.54727400	1.40469600
H	1.41356400	1.34365900	1.29531000
H	-2.16200500	1.71569300	-1.41753600
H	-1.77624500	-0.10667600	2.24024200
H	0.59895700	-2.69546100	0.21566000
O	3.00201500	1.57043400	0.33249300
H	3.28499400	0.63120400	0.35100900
H	2.32668700	1.48660800	-0.37629900
O	3.17704100	-1.11540100	-0.34160600
H	2.62474000	-0.63563300	-0.98882100
H	2.42081800	-1.51954100	0.16740000

Trans:

-2 1

U	0.43473500	0.01467300	-0.02481900
O	-0.27755600	-0.91473300	1.37717600
O	1.10644200	0.95023600	-1.41761500
O	-1.29902600	-0.71119500	-1.37092100
O	1.65245200	-1.79106100	-0.60361700
O	-0.89068100	1.82980900	0.56915100
O	2.10304500	0.79360200	1.27632800
H	-2.14948700	-1.28354200	1.21501300
H	2.16401600	-1.67339700	-1.41135500
H	2.06494500	0.47803600	2.18586800
H	-0.68335700	2.59601100	0.02129000
O	-3.06517300	-1.38559000	0.89997500
H	-3.24893500	-0.50306500	0.51239000
H	-1.86113500	-1.30836900	-0.85403700
O	-3.22235100	1.03079400	-0.51730900
H	-2.64744400	0.47008000	-1.08839100
H	-2.49139000	1.45947000	-0.00277500

Transition state:

-2 1

U	-0.40461100	-0.03511200	-0.04497300
O	0.46047900	0.95878800	1.46679900
O	-1.19342100	-0.97222600	-1.40113400
O	1.19933100	0.65523200	-1.16967800
O	-1.60394900	1.78942400	-0.57102400
O	0.86616100	-1.87267000	0.55147000
O	-2.03159400	-0.72935600	1.30284200
H	1.44730100	1.29638000	1.18133600
H	-2.20168400	1.69978300	-1.32047300
H	-1.90937900	-0.37543300	2.19307600
H	0.66968700	-2.66502000	0.03907400
O	2.63689900	1.62014400	0.49862400
H	3.15244900	0.79823000	0.56458700
H	1.96708400	1.25655200	-0.42154300
O	3.27247600	-1.04914900	-0.33780500
H	2.73744200	-0.50548400	-0.94828200
H	2.51023900	-1.47621400	0.12900300

F, 2Fw

Cis:

-2 1

U	0.41284500	0.03057700	-0.05055500
O	-0.49274000	-1.07687500	1.51472500
O	1.31538800	1.06968000	-1.29538300
O	-1.04339300	-0.47197600	-1.23852000
O	1.59775100	-1.80412400	-0.64194900
O	-0.83628200	1.87417700	0.66356100
O	1.98340900	0.54626300	1.40353200
H	-1.41099800	-1.34493700	1.29686200
H	2.15095300	-1.72428700	-1.42526300
H	1.77818300	0.10565300	2.23916200
H	-0.60897000	2.68968400	0.20332500
O	-2.99919000	-1.57287100	0.33188300
H	-3.28488200	-0.63460500	0.35143300
H	-2.32339700	-1.48626500	-0.37634500
O	-3.17904300	1.11443200	-0.34027000
H	-2.62732500	0.63606900	-0.98896600
H	-2.42251200	1.51598600	0.17024400

Trans:

-2 1

U	0.43471700	0.01465600	-0.02487200
O	-0.27864600	-0.91424000	1.37695500
O	1.10748600	0.94980300	-1.41748100
O	-1.29966400	-0.71054300	-1.37104400
O	1.65129900	-1.79202300	-0.60299900
O	-0.88927200	1.83132100	0.56805700
O	2.10299100	0.79232100	1.27670000
H	-2.15015400	-1.28415700	1.21470900
H	2.16324500	-1.67573600	-1.41068600
H	2.06640100	0.47679400	2.18629300
H	-0.67949800	2.59749600	0.02110500
O	-3.06545100	-1.38619900	0.89865500
H	-3.24936300	-0.50296000	0.51272100
H	-1.86070800	-1.30727200	-0.85243600
O	-3.22193800	1.03154900	-0.51550800
H	-2.64807400	0.47120000	-1.08804700
H	-2.49021300	1.46034600	-0.00211300

Transition state:

-2 1

U	-0.40461400	-0.03510200	-0.04494900
O	0.46057000	0.95856300	1.46692600
O	-1.19349400	-0.97200000	-1.40121800
O	1.19924500	0.65544900	-1.16964800
O	-1.60403800	1.78949000	-0.57060700
O	0.86621700	-1.87274000	0.55111300
O	-2.03149100	-0.72961100	1.30285500
H	1.44737700	1.29618700	1.18145900
H	-2.20176100	1.69998300	-1.32008200
H	-1.90925200	-0.37580400	2.19313200
H	0.66967700	-2.66502200	0.03863800
O	2.63694100	1.62005100	0.49872200
H	3.15248900	0.79812100	0.56450500
H	1.96705600	1.25662400	-0.42146300
O	3.27245400	-1.04909500	-0.33825200
H	2.73737200	-0.50531000	-0.94858200
H	2.51025500	-1.47623500	0.12855000

G, 2Gw

Cis:

-2 1

U	-0.41501600	-0.02753900	-0.04097800
O	0.35611800	1.21132300	1.50551900
O	-1.14970100	-1.20877700	-1.27397200
O	1.01166400	0.55309100	-1.22538400
O	-1.75009400	1.65886200	-0.74427100
O	1.01945300	-1.67173100	0.83055300
O	-1.95351000	-0.63909300	1.39256400
H	1.31011600	1.38280500	1.35859100
H	-2.01757200	1.66590200	-1.66865800
H	-2.54974000	-1.29892000	1.01787100
H	1.29813000	-1.36868300	1.70332600
O	2.96656500	1.47810800	0.43711200
H	3.25801000	0.54742300	0.34063500
H	2.29165400	1.47310000	-0.27705100
O	3.18858500	-1.11093100	-0.61263300
H	2.60028700	-0.56208000	-1.16639200
H	2.47793200	-1.47279000	-0.01426000

Trans:

-2 1

U	0.43443900	0.00621300	-0.01426200
O	-0.11175500	-0.82085700	1.51734600
O	0.91674600	0.84290700	-1.54115800
O	-1.24522000	-1.09021600	-1.17005300
O	1.85302200	-1.68975700	-0.45135400
O	-1.10257700	1.69123100	0.44728500
O	2.01402400	1.12678400	1.13533800
H	-2.09567900	-0.88300500	1.45158800
H	2.28926700	-1.63199200	-1.30824400
H	2.49370000	1.77274200	0.60525100
H	-1.48414900	1.58485800	1.32669800
O	-3.03190200	-0.98829900	1.21173700
H	-3.16671200	-0.30861900	0.51969700
H	-1.79350400	-1.57193300	-0.53425200
O	-3.18306400	0.80734900	-1.01256800
H	-2.57466600	0.09772700	-1.32783600
H	-2.51083300	1.33545900	-0.51337100

Transition state:

-2 1

U	-0.40479500	-0.02967600	-0.03595500
O	0.32279600	1.08807000	1.46749700
O	-1.03678300	-1.09614400	-1.37795900
O	1.18958000	0.73634600	-1.14221700
O	-1.72576900	1.64848100	-0.71545500
O	1.00165100	-1.70214100	0.73355600
O	-1.99223000	-0.78568100	1.30107200
H	1.34850900	1.32157600	1.25023000
H	-2.20363500	1.52229700	-1.54173500
H	-2.56956700	-1.45515300	0.91621000
H	1.33621800	-1.44997800	1.60297700
O	2.61507600	1.53360400	0.62063600
H	3.07985700	0.68245000	0.65251500
H	1.94159800	1.24793200	-0.35675700
O	3.25954900	-1.07545800	-0.63704500
H	2.69968600	-0.43504600	-1.11812500
H	2.53752100	-1.48053800	-0.09809500

H, 2Hw

Cis:

-2 1

U	0.44008200	0.00992500	-0.05404900
O	-1.04487400	0.26613700	1.53970000
O	1.78766600	-0.30664800	-1.30729600
O	-0.33326300	1.51844200	-0.92142900
O	-1.12337900	-1.25649200	-1.25996300
O	1.86863400	1.28599500	1.14597800
O	1.05970100	-1.79788700	0.98740500
H	-1.69285400	0.94451700	1.27463700
H	-1.47382100	-0.72507500	-1.98404500
H	1.81725600	-2.23032300	0.57446100
H	2.71501200	1.47333200	0.72801700
O	-3.01236200	1.52385900	-0.13431600
H	-3.17970800	0.56153700	-0.07165300
H	-2.13001400	1.57241500	-0.56056200
O	-3.14406300	-1.25878100	0.46631800
H	-2.53189600	-0.91037700	1.14207100
H	-2.47602300	-1.39609200	-0.26159500

Trans:

-2 1

U	0.42480000	-0.00312500	0.02958700
O	-0.83665700	-0.18970400	-1.30032400
O	1.66690400	0.19717500	1.33317000
O	-0.71931600	-1.38502300	1.36434500
O	-0.83253700	1.74793100	0.90155400
O	1.58588500	-1.74840100	-0.83211200
O	1.55621500	1.46092500	-1.26990900
H	-2.35995000	-1.38287200	-0.81297100
H	-0.64196700	2.00920500	1.80794900
H	2.31706400	1.83783800	-0.81441600
H	2.33841600	-2.00286900	-0.28745700
O	-3.15312300	-1.47354700	-0.25707100
H	-3.31164400	-0.52390700	-0.06694300
H	-1.59759500	-1.59212300	1.00857300
O	-3.12434000	1.31006900	-0.29050700
H	-2.60670500	1.02717000	-1.05979000
H	-2.36350000	1.55968400	0.30987400

Transition state:

-2 1

U	0.41282500	-0.01397700	-0.04540200
O	-0.99357200	0.42963500	1.34711400
O	1.68630700	-0.43741600	-1.29329100
O	-0.66348300	1.23996500	-1.25240900
O	-0.92262700	-1.76035800	-0.76303500
O	1.67383800	1.69839600	0.69018800
O	1.40019200	-1.37813200	1.38840600
H	-1.76682000	1.05381900	0.89031700
H	-0.77373400	-2.11091100	-1.64685400
H	2.16705200	-1.84203000	1.03294100
H	2.49946200	1.84332700	0.21668200
O	-2.66562800	1.64634900	0.01758500
H	-3.14738200	0.81505500	-0.13397200
H	-1.70284600	1.51589800	-0.72355100
O	-3.26401500	-1.15365700	0.32487900
H	-2.77523400	-0.80431000	1.08472800
H	-2.48846100	-1.46321800	-0.21884800

Polyrate 17 input file example (UTH in gas phase, conformer 0Ag):

Filename: uo2_oh4_la7.dat

```
*GENERAL

TITLE
  uo2cis_oh4_la7
END

DL ISPE

ATOMS
1 U
2 O
3 O
4 O
5 O
6 O
7 O
8 H
9 H
10 H
11 H
END

NOSUPERMOL

*SECOND

HESSCAL hhook

FPRINT

*OPTIMIZATION

PRINT

OPTMIN ohook
OPTTS ohook

*REACT1
INITGEO hooks
GEOM
1
2
3
4
5
6
7
8
9
10
11
END
SPECIES nonlinrp

*PROD1
INITGEO hooks
GEOM
1
2
3
4
5
6
7
8
9
10
11
END
SPECIES nonlinrp

*START
INITGEO hooks
GEOM
1
2
3
4
5
6
7
8
9
10
11
END
SPECIES nonlints
PROJECT

*PATH
#SYMMETRY
INTMU 3
SSTEP 0.001
RPM pagem
SRANGE
  SLP 4.185
  SLM -2.35
END
#SPECSTOP
#  CURVE VMEP
#  PERCENTDOWN 99.
#END
PRPATH
  coord 1 2
  xmol
  freq 27
END

*TUNNEL
ZCT
SCT
#QRST
#  harmonic
#  mode 27
#  states all
#END

*RATE
FORWARDK
SIGMAF 1
TST
CVT
PRDELG
PRPART rtp

TEMP
4
5
6
8
10
20
30
40
50
75
77.355
100
```

```
125
150
175
194.7
200
225
250
273.15
275
298.15
300
325
350
373.15
375
400
END

ANALYSIS
4
5
6
8
10
20
30
40
50
75
77.355
100
125
150
175
194.7
200
225
250
273.15
275
298.15
300
325
350
373.15
375
400
END

EACT
6. 10.
10. 20.
20. 50.
50. 100.
200. 225.
300. 325.
END

GTLOG
```

Filename: uo2_oh4_la7.70

```
*GRGENERAL
GRRESTART

*GRSTART
CHARGE -2
MULTIPLICITY 1

*GRCOMMON

GRENER
%mem=200gb
%nproc=36
#n m06 genecp  units(au) fchk nosymm
END

GRFIRST
%mem=200gb
%nproc=36
#n m06 genecp  units(au) fchk nosymm force
END

GRSEC
%mem=200gb
%nproc=36
#n m06 genecp  units(au) fchk nosymm freq
END

GRBASIS
@/local/gaus/beneliye/uo2_oh4_la7/ulanl2dz_def2svp.gbs
END
```

Filename: uo2_oh4_la7.51

```
*ISPEGEN
ENERXN -21.87      # Corrected Reaction energy (SCF)
ENESAD 18.85   # Corrected Activation energy (SCF)
MEPTYPER one
MEPTYPEP one
RCINFO
 SRC -4.44  # Position of the reactant in Bohr (s from fu28)
END
PCINFO
 SPC 7.91   # Position of the product in Bohr
END
```

Filename: uo2_oh4_la7.71, Reactant: Cis UTH

```
%mem=200gb
%nproc=36
#n m06 genecp  fchk  nosymm

-2 1
 U            -0.01591500   -0.02210600   -0.05866300
 O             0.46089200    1.54508300    1.46331700
 O            -0.22159700   -1.46902200   -1.24397500
 O            -0.31080300    1.46362100   -1.19613700
 O            -2.28948400    0.10131100    0.36860400
 O             2.26551300    0.00552400   -0.43800000
 O             0.22636700   -1.58350800    1.49566500
 H             0.26315700    2.32680800    0.93486400
 H            -2.51877100    0.82904600   -0.21878700
 H             0.19129900   -2.37540200    0.94724900
 H             2.48138200    0.74918900    0.13785600

@/local/gaus/beneliye/uo2_oh4_la7/ulanl2dz_def2svp.gbs
```

Filename: uo2_oh4_la7.73, Product: Trans UTH

%mem=200gb
%nproc=36
#n m06 genecp fchk nosymm

-2 1

U	-0.00449100	-0.00004900	-0.02546600
O	-0.27095700	-0.00388900	1.78357400
O	0.26804000	0.00370000	-1.81960400
O	-2.29602600	-0.04729500	-0.28347600
O	0.07593100	-2.30774700	0.02940100
O	-0.01854000	2.30918900	0.02686200
O	2.27451800	0.04632000	0.30773500
H	-2.58453400	-0.05159900	0.63544300
H	0.12114500	-2.46878700	0.97816400
H	2.59124700	0.04968300	-0.60208700
H	0.02157500	2.47295700	0.97538500

@/local/gaus/beneliye/uo2_oh4_la7/ulanl2dz_def2svp.gbs

Filename: uo2_oh4_la7.75, Transition state: Trans UTH

%mem=200gb
%nproc=36
#n m06 genecp fchk nosymm

-2 1

U	0.00882300	-0.02510400	-0.04860400
O	-0.39781400	1.20581600	1.52099800
O	0.43428200	-1.07754900	-1.50454600
O	-0.96399200	1.66646400	-0.70545100
O	-2.07861700	-0.97401400	0.05142600
O	2.05124900	1.00770600	-0.23691800
O	0.89224200	-1.66935300	1.22846800
H	-0.82285400	1.76783100	0.60510100
H	-2.61546800	-0.17485000	0.09613300
H	1.19374700	-2.30771900	0.57403900
H	1.93405100	1.75171100	0.36451400

@/local/gaus/beneliye/uo2_oh4_la7/ulanl2dz_def2svp.gbs

Reaction rate constants (semi-classical -k_{SC}-, and Quantum Tunnelling -k_{QT}-)

UTH		GAS									
		A, $0A_g$		B, $0B_g$		C, $0C_g$		D, $0D_g$		E, $0E_g$	
T(K)	1/T (1/K)	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}
10	1.00E-01										
20	5.00E-02	2E-175	3E-07	2E-165	4E-06	2E-150	2E-05	1E-178	1E-07	1E-169	2E-06
30	3.33E-02	4E-113	3E-07	1E-106	4E-06	2E-96	2E-05	2E-115	1E-07	3E-109	2E-06
40	2.50E-02	6E-82	4E-07	5E-77	5E-06	2E-69	2E-05	1E-83	1E-07	4E-79	2E-06
50	2.00E-02	3E-63	5E-07	3E-59	5E-06	3E-53	3E-05	1E-64	2E-07	6E-61	3E-06
75	1.33E-02	4E-38	1E-06	1E-35	1E-05	1E-31	7E-05	3E-39	4E-07	1E-36	5E-06
77.36	1.29E-02	1E-36	1E-06	3E-34	1E-05	3E-30	8E-05	1E-37	5E-07	3E-35	5E-06
100	1.00E-02	1E-25	4E-06	9E-24	3E-05	1E-20	2E-04	2E-26	1E-06	1E-24	1E-05
125	8.00E-03	5E-18	2E-05	1E-16	1E-04	4E-14	1E-03	7E-19	1E-05	3E-17	6E-05
150	6.67E-03	6E-13	2E-04	6E-12	8E-04	9E-10	9E-03	8E-14	1E-04	2E-12	4E-04
175	5.71E-03	2E-09	2E-03	2E-08	7E-03	1E-06	9E-02	3E-10	1E-03	6E-09	4E-03
194.7	5.14E-03	4E-07	1E-02	2E-06	4E-02	1E-04	5E-01	5E-08	7E-03	7E-07	2E-02
200	5.00E-03	1E-06	2E-02	5E-06	6E-02	3E-04	8E-01	2E-07	1E-02	2E-06	3E-02
225	4.44E-03	1E-04	2E-01	5E-04	5E-01	2E-02	7E+00	2E-05	1E-01	2E-04	3E-01
250	4.00E-03	7E-03	2E+00	2E-02	4E+00	5E-01	5E+01	1E-03	8E-01	9E-03	2E+00
273.15	3.66E-03	1E-01	1E+01	3E-01	2E+01	7E+00	3E+02	2E-02	4E+00	2E-01	1E+01
275	3.64E-03	2E-01	1E+01	4E-01	2E+01	9E+00	3E+02	3E-02	5E+00	2E-01	1E+01
298.15	3.35E-03	2E+00	6E+01	4E+00	1E+02	7E+01	1E+03	3E-01	2E+01	2E+00	6E+01
300	3.33E-03	2E+00	7E+01	4E+00	1E+02	9E+01	1E+03	3E-01	2E+01	2E+00	7E+01
325	3.08E-03	2E+01	3E+02	3E+01	5E+02	6E+02	6E+03	3E+00	1E+02	2E+01	3E+02
350	2.86E-03	1E+02	1E+03	2E+02	2E+03	3E+03	2E+04	2E+01	4E+02	1E+02	1E+03
373.15	2.68E-03	6E+02	4E+03	8E+02	6E+03	1E+04	7E+04	1E+02	1E+03	5E+02	4E+03
375	2.67E-03	7E+02	5E+03	9E+02	6E+03	1E+04	7E+04	1E+02	1E+03	6E+02	4E+03
400	2.50E-03	3E+03	2E+04	4E+03	2E+04	5E+04	2E+05	5E+02	4E+03	2E+03	1E+04

UTH		CPCM -Water											
		A, $0A_w$		B, $0B_w$		C, $0C_w$		D, $0D_w$		E, $0E_w$		F, $0F_w$	
T(K)	1/T (1/K)	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}
10	1.00E-01					4E-253	5E-02						
20	5.00E-02	4E-204	2E-11	9E-179	3E-06	6E-121	5E-02	1E-205	2E-11	1E-204	7E-11	3E-166	2E-07
30	3.33E-02	3E-132	2E-11	2E-115	3E-06	7E-77	6E-02	3E-133	2E-11	1E-132	8E-11	5E-107	2E-07
40	2.50E-02	2E-96	3E-11	1E-83	3E-06	9E-55	6E-02	4E-97	3E-11	1E-96	9E-11	2E-77	2E-07
50	2.00E-02	9E-75	4E-11	1E-64	3E-06	2E-41	6E-02	2E-75	3E-11	5E-75	1E-10	1E-59	3E-07
75	1.33E-02	6E-46	1E-10	4E-39	5E-06	9E-24	9E-02	2E-46	8E-11	4E-46	3E-10	7E-36	6E-07
77.36	1.29E-02	3E-44	1E-10	1E-37	5E-06	1E-22	1E-01	1E-44	1E-10	2E-44	3E-10	2E-34	7E-07
100	1.00E-02	1E-31	8E-10	2E-26	8E-06	6E-21	7E-04	7E-32	4E-10	1E-31	9E-10	6E-24	3E-06
125	8.00E-03	6E-23	8E-09	9E-19	3E-05	3E-14	2E-03	4E-23	5E-09	4E-23	6E-09	8E-17	2E-05
150	6.67E-03	4E-17	1E-07	1E-13	1E-04	7E-10	1E-02	2E-17	8E-08	3E-17	9E-08	5E-12	1E-04
175	5.71E-03	5E-13	2E-06	5E-10	1E-03	1E-06	8E-02	3E-13	1E-06	3E-13	1E-06	1E-08	1E-03
194.7	5.14E-03	1E-10	2E-05	7E-08	6E-03	8E-05	4E-01	1E-10	1E-05	1E-10	1E-05	1E-06	1E-02
200	5.00E-03	6E-10	4E-05	2E-07	9E-03	2E-04	6E-01	4E-10	2E-05	4E-10	2E-05	4E-06	2E-02
225	4.44E-03	1E-07	5E-04	3E-05	7E-02	2E-02	5E+00	1E-07	3E-04	1E-07	3E-04	4E-04	2E-01
250	4.00E-03	1E-05	5E-03	2E-03	5E-01	5E-01	4E+01	9E-06	4E-03	8E-06	3E-03	1E-02	1E+00
273.15	3.66E-03	3E-04	4E-02	3E-02	3E+00	7E+00	2E+02	3E-04	3E-02	2E-04	3E-02	2E-01	9E+00
275	3.64E-03	4E-04	5E-02	4E-02	3E+00	9E+00	3E+02	3E-04	4E-02	3E-04	3E-02	3E-01	1E+01
298.15	3.35E-03	6E-03	3E-01	4E-01	2E+01	8E+01	1E+03	5E-03	2E-01	5E-03	2E-01	3E+00	5E+01
300	3.33E-03	8E-03	3E-01	5E-01	2E+01	9E+01	1E+03	7E-03	3E-01	6E-03	2E-01	3E+00	6E+01
325	3.08E-03	9E-02	2E+00	5E+00	8E+01	7E+02	6E+03	8E-02	2E+00	7E-02	1E+00	3E+01	3E+02
350	2.86E-03	8E-01	1E+01	3E+01	3E+02	4E+03	2E+04	7E-01	9E+00	6E-01	7E+00	2E+02	1E+03
373.15	2.68E-03	5E+00	4E+01	1E+02	1E+03	1E+04	7E+04	4E+00	3E+01	3E+00	3E+01	7E+02	4E+03
375	2.67E-03	5E+00	4E+01	2E+02	1E+03	2E+04	8E+04	5E+00	4E+01	4E+00	3E+01	7E+02	4E+03
400	2.50E-03	3E+01	2E+02	7E+02	4E+03	6E+04	2E+05	2E+01	1E+02	2E+01	1E+02	3E+03	1E+04

UTH···H_2O		GAS													
		A, $1A_g$		B, $1B_g$		C, $1C_g$		D, $1D_g$		E, $1E_g$		F, $1F_g$		G, $1G_g$	
T(K)	1/T (1/K)	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}
4	2.50E-01														
5	2.00E-01														
6	1.67E-01					2E-267	4E-31								
8	1.25E-01	4E-239	2E-07	9E-263	3E-32	7E-198	4E-31	5E-253	3E-07	4E-239	2E-07	9E-254	3E-21	1E-275	4E-09
10	1.00E-01	4E-189	2E-07	5E-208	3E-32	4E-156	4E-31	3E-200	3E-07	4E-189	2E-07	8E-201	3E-21	3E-218	4E-09
20	5.00E-02	6E-89	2E-07	2E-98	3E-32	2E-72	4E-31	2E-94	3E-07	6E-89	2E-07	8E-95	3E-21	2E-103	4E-09
30	3.33E-02	2E-55	2E-07	9E-62	4E-32	2E-44	9E-29	3E-59	3E-07	2E-55	2E-07	2E-59	8E-21	3E-65	4E-09
40	2.50E-02	1E-38	3E-07	2E-43	2E-30	2E-30	2E-20	2E-41	3E-07	9E-39	3E-07	1E-41	4E-19	5E-46	5E-09
50	2.00E-02	1E-28	5E-07	2E-32	2E-24	4E-22	3E-15	6E-31	7E-07	1E-28	5E-07	6E-31	4E-17	2E-34	1E-08
75	1.33E-02	3E-15	3E-05	1E-17	9E-15	7E-11	5E-08	1E-16	2E-05	3E-15	2E-05	1E-16	1E-11	6E-19	5E-07
77.36	1.29E-02	2E-14	4E-05	1E-16	4E-14	4E-10	2E-07	7E-16	3E-05	2E-14	4E-05	1E-15	4E-11	5E-18	8E-07
100	1.00E-02	2E-08	1E-03	3E-10	4E-09	3E-05	8E-04	1E-09	8E-04	2E-08	1E-03	2E-09	2E-07	3E-11	4E-05
125	8.00E-03	2E-04	9E-02	9E-06	4E-05	7E-02	5E-01	2E-05	3E-02	2E-04	9E-02	4E-05	5E-04	2E-06	3E-03
150	6.67E-03	1E-01	4E+00	8E-03	2E-02	1E+01	4E+01	2E-02	1E+00	1E-01	4E+00	3E-02	1E-01	2E-03	2E-01
175	5.71E-03	8E+00	1E+02	1E+00	2E+00	5E+02	1E+03	2E+00	3E+01	8E+00	1E+02	4E+00	1E+01	4E-01	8E+00
194.7	5.14E-03	1E+02	8E+02	2E+01	3E+01	5E+03	9E+03	3E+01	3E+02	1E+02	8E+02	7E+01	2E+02	8E+00	9E+01
200	5.00E-03	2E+02	1E+03	4E+01	7E+01	8E+03	1E+04	6E+01	5E+02	2E+02	1E+03	1E+02	3E+02	2E+01	2E+02
225	4.44E-03	3E+03	1E+04	7E+02	1E+03	7E+04	1E+05	9E+02	4E+03	3E+03	1E+04	2E+03	4E+03	3E+02	2E+03
250	4.00E-03	2E+04	7E+04	7E+03	9E+03	4E+05	5E+05	7E+03	3E+04	2E+04	7E+04	2E+04	3E+04	4E+03	1E+04
273.15	3.66E-03	1E+05	3E+05	4E+04	5E+04	1E+06	2E+06	4E+04	1E+05	1E+05	3E+05	1E+05	2E+05	2E+04	7E+04
275	3.64E-03	1E+05	3E+05	5E+04	6E+04	1E+06	2E+06	4E+04	1E+05	1E+05	3E+05	1E+05	2E+05	3E+04	8E+04
298.15	3.35E-03	5E+05	1E+06	2E+05	2E+05	4E+06	6E+06	2E+05	4E+05	5E+05	1E+06	6E+05	8E+05	1E+05	3E+05
300	3.33E-03	5E+05	1E+06	2E+05	3E+05	5E+06	6E+06	2E+05	4E+05	5E+05	1E+06	6E+05	8E+05	1E+05	3E+05
325	3.08E-03	2E+06	3E+06	8E+05	1E+06	1E+07	2E+07	7E+05	1E+06	2E+06	3E+06	2E+06	3E+06	6E+05	1E+06
350	2.86E-03	5E+06	8E+06	3E+06	3E+06	3E+07	3E+07	2E+06	4E+06	5E+06	8E+06	7E+06	8E+06	2E+06	3E+06
373.15	2.68E-03	1E+07	2E+07	6E+06	7E+06	5E+07	6E+07	4E+06	8E+06	1E+07	2E+07	2E+07	2E+07	5E+06	8E+06
375	2.67E-03	1E+07	2E+07	7E+06	7E+06	6E+07	7E+07	5E+06	8E+06	1E+07	2E+07	2E+07	2E+07	5E+06	9E+06
400	2.50E-03	2E+07	3E+07	2E+07	2E+07	1E+08	1E+08	1E+07	2E+07	2E+07	3E+07	4E+07	5E+07	1E+07	2E+07

UTH···H2O		CPCM -Water													
		A, $1A_w$		B, $1B_w$		C, $1C_w$		D, $1D_w$		E, $1E_w$		F, $1F_w$		G, $1G_g$	
T(K)	1/T (1/K)	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}
4	2.50E-01			1E-280	6E-26	3E-281	3E+04					9E-284	4E-28		
5	2.00E-01			1E-222	6E-26	6E-223	3E+04					7E-225	4E-28	9E-248	3E-27
6	1.67E-01			1E-183	6E-26	5E-184	3E+04					1E-185	4E-28	1E-204	3E-27
8	1.25E-01	6E-248	4E-05	6E-135	6E-26	3E-135	3E+04	1-235	1E-02	6E-246	2E-04	2E-136	4E-28	9E-151	3E-27
10	1.00E-01	4E-196	4E-05	9E-106	6E-26	5E-106	3E+04	2E-186	1E-02	1E-194	2E-04	5E-107	4E-28	2E-118	3E-27
20	5.00E-02	2E-92	4E-05	3E-47	6E-26	2E-47	3E+04	1E-87	1E-02	1E-91	2E-04	7E-48	4E-28	1E-53	3E-27
30	3.33E-02	7E-58	5E-05	1E-27	3E-20	7E-28	3E+04	1E-54	1E-02	3E-57	2E-04	4E-28	1E-21	7E-32	2E-22
40	2.50E-02	2E-40	8E-05	9E-18	9E-13	4E-18	2E+04	4E-38	1E-02	4E-40	3E-04	4E-18	7E-14	5E-21	1E-14
50	2.00E-02	4E-30	2E-04	8E-12	3E-08	3E-12	2E+04	4E-28	2E-02	1E-29	6E-04	4E-12	6E-09	2E-14	1E-09
75	1.33E-02	4E-16	5E-03	9E-04	6E-02	2E-04	3E+04	7E-15	6E-02	7E-16	1E-02	5E-04	3E-02	1E-05	5E-03
77.36	1.29E-02	3E-15	6E-03	3E-03	1E-01	7E-04	3E+04	4E-14	7E-02	5E-15	1E-02	1E-03	7E-02	4E-05	1E-02
100	1.00E-02	4E-09	8E-02	1E+01	2E+02	2E+00	4E+04	3E-08	3E-01	6E-09	1E-01	6E+00	6E+01	8E-07	1E-03
125	8.00E-03	6E-05	1E+00	3E+03	2E+04	4E+02	1E+05	3E-04	3E+00	1E-04	2E+00	2E+03	8E+03	5E-03	4E-01
150	6.67E-03	4E-02	1E+01	1E+05	5E+05	1E+04	5E+05	1E-01	4E+01	6E-02	2E+01	7E+04	2E+05	2E+00	3E+01
175	5.71E-03	4E+00	2E+02	2E+06	5E+06	2E+05	2E+06	1E+01	5E+02	6E+00	3E+02	1E+06	2E+06	1E+02	9E+02
194.7	5.14E-03	6E+01	1E+03	9E+06	2E+07	8E+05	5E+06	1E+02	3E+03	9E+01	2E+03	5E+06	1E+07	1E+03	8E+03
200	5.00E-03	1E+02	2E+03	1E+07	3E+07	1E+06	7E+06	3E+02	4E+03	2E+02	3E+03	8E+06	1E+07	3E+03	1E+04
225	4.44E-03	2E+03	1E+04	6E+07	1E+08	5E+06	2E+07	3E+03	3E+04	2E+03	2E+04	4E+07	6E+07	3E+04	1E+05
250	4.00E-03	1E+04	8E+04	2E+08	4E+08	1E+07	4E+07	3E+04	1E+05	2E+04	1E+05	1E+08	2E+08	2E+05	6E+05
273.15	3.66E-03	7E+04	3E+05	6E+08	9E+08	3E+07	8E+07	1E+05	5E+05	1E+05	4E+05	3E+08	5E+08	9E+05	2E+06
275	3.64E-03	8E+04	3E+05	6E+08	1E+09	4E+07	9E+07	1E+05	5E+05	1E+05	5E+05	4E+08	5E+08	1E+06	2E+06
298.15	3.35E-03	3E+05	1E+06	1E+09	2E+09	7E+07	2E+08	5E+05	1E+06	4E+05	1E+06	8E+08	1E+09	3E+06	7E+06
300	3.33E-03	3E+05	1E+06	1E+09	2E+09	8E+07	2E+08	5E+05	2E+06	5E+05	2E+06	8E+08	1E+09	4E+06	8E+06
325	3.08E-03	1E+06	3E+06	3E+09	4E+09	1E+08	3E+08	2E+06	4E+06	2E+06	4E+06	2E+09	2E+09	1E+07	2E+07
350	2.86E-03	3E+06	7E+06	6E+09	7E+09	3E+08	4E+08	4E+06	1E+07	4E+06	1E+07	3E+09	4E+09	3E+07	5E+07
373.15	2.68E-03	7E+06	1E+07	9E+09	1E+10	4E+08	6E+08	9E+06	2E+07	1E+07	2E+07	5E+09	6E+09	6E+07	1E+08
375	2.67E-03	7E+06	2E+07	9E+09	1E+10	4E+08	6E+08	1E+07	2E+07	1E+07	2E+07	5E+09	6E+09	7E+07	1E+08
400	2.50E-03	2E+07	3E+07	2E+10	2E+10	6E+08	9E+08	2E+07	4E+07	2E+07	4E+07	9E+09	1E+10	1E+08	2E+08

UTH···$(H_2O)_2$		GAS													
		A, $2A_g$		B, $2B_g$		C, $2C_g$		D, $2D_g$		F, $2F_g$		G, $2G_g$		H, $2H_g$	
T(K)	1/T (1/K)	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}
4	2.50E-01														
5	2.00E-01	4E-259	7E+02	1E-265	4E+02	1E-277	1E+02	2E-284	9E+01	8E-281	2E+02	1E-265	4E+02		
6	1.67E-01	4E-214	7E+02	1E-219	4E+02	2E-229	1E+02	3E-235	9E+01	3E-232	2E+02	2E-219	4E+02		
8	1.25E-01	7E-158	7E+02	6E-162	4E+02	2E-169	1E+02	1E-173	9E+01	1E-171	2E+02	6E-162	4E+02	1E-261	3E-05
10	1.00E-01	4E-124	7E+02	2-127	4E+02	2E-133	1E+02	8E-137	9E+01	6E-135	2E+02	2E-127	4E+02	5E-207	3E-05
20	5.00E-02	2E-56	8E+02	4E-58	4E+02	4E-61	1E+02	8E-63	9E+01	7E-62	2E+02	4E-58	4E+02	6E-98	3E-05
30	3.33E-02	8E-34	8E+02	6E-35	4E+02	6E-37	1E+02	4E-38	9E+01	2E-37	2E+02	6E-35	4E+02	2E-61	2E-05
40	2.50E-02	2E-22	8E+02	2E-23	3E+02	7E-25	1E+02	1E-25	9E+01	3E-25	2E+02	2E-23	4E+02	3E-43	2E-05
50	2.00E-02	1E-15	8E+02	2E-16	3E+02	1E-17	1E+02	3E-18	9E+01	7E-18	2E+02	2E-16	4E+02	3E-32	4E-05
75	1.33E-02	2E-06	1E+03	5E-07	4E+02	6E-08	1E+02	3E-08	1E+02	5E-08	3E+02	5E-07	5E+02	1E-17	8E-04
77.36	1.29E-02	6E-06	1E+03	2E-06	5E+02	2E-07	1E+02	1E-07	1E+02	2E-07	3E+02	2E-06	5E+02	8E-17	1E-03
100	1.00E-02	6E-02	4E+03	2E-02	1E+03	4E-03	4E+02	1E-01	3E+03	5E-03	8E+02	2E-02	1E+03	2E-10	1E-02
125	8.00E-03	4E+01	2E+04	2E+01	7E+03	4E+00	3E+03	7E+01	2E+04	4E+00	5E+03	2E+01	7E+03	6E-06	2E-01
150	6.67E-03	2E+03	1E+05	1E+03	5E+04	3E+02	2E+04	4E+03	1E+05	4E+02	3E+04	1E+03	5E+04	5E-03	3E+00
175	5.71E-03	5E+04	8E+05	3E+04	4E+05	7E+03	1E+05	8E+04	8E+05	1E+04	2E+05	3E+04	4E+05	6E-01	4E+01
194.7	5.14E-03	3E+05	3E+06	2E+05	1E+06	5E+04	5E+05	5E+05	3E+06	7E+04	7E+05	2E+05	1E+06	1E+01	3E+02
200	5.00E-03	5E+05	4E+06	3E+05	2E+06	8E+04	7E+05	7E+05	4E+06	1E+05	1E+06	3E+05	2E+06	2E+01	5E+02
225	4.44E-03	3E+06	1E+07	2E+06	7E+06	5E+05	3E+06	4E+06	1E+07	7E+05	4E+06	2E+06	7E+06	4E+02	4E+03
250	4.00E-03	1E+07	4E+07	6E+06	2E+07	2E+06	8E+06	1E+07	4E+07	3E+06	1E+07	6E+06	2E+07	4E+03	2E+04
273.15	3.66E-03	3E+07	9E+07	2E+07	5E+07	7E+06	2E+07	4E+07	1E+08	1E+07	3E+07	2E+07	5E+07	2E+04	8E+04
275	3.64E-03	3E+07	1E+08	2E+07	5E+07	7E+06	2E+07	4E+07	1E+08	1E+07	3E+07	2E+07	5E+07	2E+04	9E+04
298.15	3.35E-03	8E+07	2E+08	5E+07	1E+08	2E+07	5E+07	1E+08	2E+08	3E+07	7E+07	5E+07	1E+08	9E+04	3E+05
300	3.33E-03	9E+07	2E+08	5E+07	1E+08	2E+07	5E+07	1E+08	2E+08	3E+07	7E+07	5E+07	1E+08	1E+05	3E+05
325	3.08E-03	2E+08	4E+08	1E+08	2E+08	4E+07	1E+08	2E+08	5E+08	7E+07	1E+08	1E+08	2E+08	4E+05	1E+06
350	2.86E-03	4E+08	7E+08	2E+08	4E+08	9E+07	2E+08	5E+08	8E+08	1E+08	3E+08	2E+08	4E+08	1E+06	3E+06
373.15	2.68E-03	7E+08	1E+09	4E+08	7E+08	2E+08	3E+08	8E+08	1E+09	3E+08	5E+08	4E+08	7E+08	3E+06	6E+06
375	2.67E-03	7E+08	1E+09	4E+08	7E+08	2E+08	3E+08	8E+08	1E+09	3E+08	5E+08	4E+08	7E+08	3E+06	6E+06
400	2.50E-03	1E+09	2E+09	7E+08	1E+09	3E+08	5E+08	1E+09	2E+09	5E+08	7E+08	7E+08	1E+09	6E+06	1E+07

UTH···$(H_2O)_2$		CPCM -Water															
		A, $2A_w$		B, $2B_w$		C, $2C_w$		D, $2D_w$		E, $2E_w$		F, $2F_w$		G, $2G_g$		H, $2H_g$	
T(K)	1/T (1/K)	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}
4	2.50E-01																
5	2.00E-01	8E-261	2E+03	1E-262	5E+03	4E-249	5E+03	2E-264	6E+02	3E-259	5E+03	4E-249	1E+04	1E-252	5E+03		
6	1.67E-01	1E-215	2E+03	4E-217	5E+03	9E-206	5E+03	1E-218	6E+02	3E-214	5E+03	8E-206	1E+04	1E-208	5E+03	9E-260	8E+00
8	1.25E-01	4E-159	2E+03	4E-160	5E+03	1E-151	5E+03	3E-161	6E+02	6E-158	5E+03	1E-151	1E+04	8E-154	5E+03	4E-192	8E+00
10	1.00E-01	3E-126	2E+02	6E-126	4E+03	4E-119	5E+03	8E-127	6E+02	3E-124	5E+03	4E-119	1E+04	7E-121	5E+03	2E-151	8E+00
20	5.00E-02	3E-58	2E+02	2E-57	4E+03	6E-54	5E+03	8E-58	6E+02	2E-56	5E+03	5E-54	9E+03	8E-55	5E+03	4E-70	9E+00
30	3.33E-02	2E-35	2E+02	2E-34	4E+03	3E-32	4E+03	9E-35	6E+02	6E-34	5E+03	3E-32	9E+03	9E-33	5E+03	6E-43	9E+00
40	2.50E-02	5E-24	2E+02	6E-23	4E+03	3E-21	4E+03	3E-23	6E+02	1E-22	5E+03	3E-21	9E+03	1E-21	5E+03	2E-29	9E+00
50	2.00E-02	4E-17	2E+02	5E-16	4E+03	1E-14	4E+03	3E-16	5E+02	9E-16	5E+03	1E-14	8E+03	5E-15	5E+03	4E-21	9E+00
75	1.33E-02	6E-08	3E+02	8E-07	5E+03	6E-06	4E+03	6E-07	8E+02	1E-06	5E+03	6E-06	9E+03	4E-06	5E+03	4E-10	3E+01
77.36	1.29E-02	2E-07	3E+02	3E-06	5E+03	2E-05	5E+03	2E-06	9E+02	4E-06	5E+03	2E-05	9E+03	1E-05	5E+03	2E-09	4E+01
100	1.00E-02	5E-02	1E+04	3E-02	7E+03	1E-01	9E+03	2E-02	3E+03	3E+00	5E+04	1E-01	1E+04	1E-01	9E+03	1E-04	2E+02
125	8.00E-03	3E+01	5E+04	2E+01	3E+04	6E+01	4E+04	1E+01	1E+04	8E+02	2E+05	6E+01	5E+04	5E+01	4E+04	3E-01	1E+03
150	6.67E-03	2E+03	2E+05	1E+03	1E+05	3E+03	2E+05	1E+03	7E+04	3E+04	9E+05	3E+03	2E+05	3E+03	2E+05	5E+01	9E+03
175	5.71E-03	4E+04	1E+06	3E+04	6E+05	6E+04	9E+05	2E+04	3E+05	4E+05	4E+06	6E+04	1E+06	6E+04	1E+06	2E+03	6E+04
194.7	5.14E-03	3E+05	3E+06	2E+05	2E+06	3E+05	3E+06	1E+05	1E+06	2E+06	1E+07	3E+05	3E+06	3E+05	3E+06	2E+04	2E+05
200	5.00E-03	4E+05	4E+06	3E+05	2E+06	5E+05	4E+06	2E+05	1E+06	3E+06	1E+07	5E+05	4E+06	5E+05	4E+06	3E+04	3E+05
225	4.44E-03	2E+06	1E+07	2E+06	8E+06	3E+06	1E+07	1E+06	5E+06	1E+07	4E+07	3E+06	1E+07	3E+06	1E+07	2E+05	1E+06
250	4.00E-03	9E+06	3E+07	6E+06	2E+07	1E+07	3E+07	4E+06	1E+07	4E+07	9E+07	1E+07	3E+07	1E+07	4E+07	1E+06	5E+06
273.15	3.66E-03	3E+07	8E+07	2E+07	5E+07	3E+07	7E+07	1E+07	3E+07	9E+07	2E+08	3E+07	6E+07	3E+07	8E+07	4E+06	1E+07
275	3.64E-03	3E+07	8E+07	2E+07	5E+07	3E+07	7E+07	1E+07	3E+07	9E+07	2E+08	3E+07	7E+07	3E+07	8E+07	5E+06	2E+07
298.15	3.35E-03	7E+07	2E+08	5E+07	1E+08	6E+07	1E+08	3E+07	7E+07	2E+08	3E+08	6E+07	1E+08	7E+07	2E+08	1E+07	4E+07
300	3.33E-03	7E+07	2E+08	5E+07	1E+08	7E+07	1E+08	3E+07	7E+07	2E+08	4E+08	7E+07	1E+08	7E+07	2E+08	2E+07	4E+07
325	3.08E-03	2E+08	3E+08	1E+08	2E+08	1E+08	3E+08	7E+07	1E+08	4E+08	6E+08	1E+08	2E+08	2E+08	3E+08	4E+07	9E+07
350	2.86E-03	3E+08	6E+08	2E+08	4E+08	3E+08	5E+08	1E+08	2E+08	7E+08	9E+08	3E+08	4E+08	3E+08	5E+08	9E+07	2E+08
373.15	2.68E-03	5E+08	9E+08	3E+08	6E+08	4E+08	7E+08	2E+08	4E+08	1E+09	1E+09	4E+08	6E+08	5E+08	8E+08	2E+08	3E+08
375	2.67E-03	5E+08	9E+08	4E+08	6E+08	5E+08	7E+08	3E+08	4E+08	1E+09	1E+09	4E+08	7E+08	5E+08	8E+08	2E+08	3E+08
400	2.50E-03	9E+08	1E+09	6E+08	9E+08	7E+08	1E+09	4E+08	6E+08	2E+09	2E+09	7E+08	9E+08	8E+08	1E+09	4E+08	6E+08

Reaction rate constants of deuterated UTH complexes

		Gas									
		UTH				UTH···H_2O				UTH···$(H_2O)_2$	
		$0A_g$		$0D_g$		$1F_g$		$1G_g$		$2H_g$	
T(K)	1/T (1/K)	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}
5	2.00E-01										
6	1.67E-01										
8	1.25E-01					9E-277	9E-25			6E-290	2E-08
10	1.00E-01					3E-219	9E-25	1E-238	1E-12	9E-230	2E-08
20	5.00E-02	3E-182	3E-11	4E-185	1E-11	5E-104	1E-24	1E-113	1E-12	3E-109	2E-08
30	3.33E-02	1E-117	3E-11	1E-119	2E-11	2E-65	3E-24	5E-72	1E-12	4E-69	2E-08
40	2.50E-02	2E-85	4E-11	7E-87	2E-11	3E-46	2E-22	4E-51	2E-12	6E-49	2E-08
50	2.00E-02	6E-66	5E-11	4E-67	2E-11	1E-34	4E-20	2E-38	4E-12	7E-37	3E-08
75	1.33E-02	6E-40	1E-10	6E-41	7E-11	5E-19	5E-14	1E-21	4E-10	1E-20	8E-07
77.36	1.29E-02	2E-38	2E-10	2E-39	8E-11	4E-18	2E-13	1E-20	7E-10	1E-19	1E-06
100	1.00E-02	6E-27	8E-10	8E-28	4E-10	3E-11	3E-09	3E-13	8E-08	1E-12	2E-05
125	8.00E-03	4E-19	1E-08	6E-20	6E-09	1E-06	1E-05	4E-08	2E-05	9E-08	6E-04
150	6.67E-03	7E-14	2E-07	1E-14	1E-07	2E-03	8E-03	9E-05	3E-03	1E-04	2E-02
175	5.71E-03	3E-10	5E-06	5E-11	3E-06	4E-01	9E-01	2E-02	2E-01	3E-02	6E-01
194.7	5.14E-03	6E-08	7E-05	1E-08	3E-05	8E+00	2E+01	7E-01	4E+00	7E-01	7E+00
200	5.00E-03	2E-07	1E-04	3E-08	7E-05	2E+01	3E+01	2E+00	8E+00	2E+00	1E+01
225	4.44E-03	3E-05	3E-03	5E-06	1E-03	3E+02	6E+02	4E+01	1E+02	3E+01	2E+02
250	4.00E-03	2E-03	4E-02	3E-04	2E-02	4E+03	6E+03	5E+02	1E+03	4E+02	1E+03
273.15	3.66E-03	3E-02	4E-01	5E-03	1E-01	2E+04	3E+04	4E+03	8E+03	2E+03	6E+03
275	3.64E-03	4E-02	5E-01	7E-03	2E-01	3E+04	4E+04	4E+03	9E+03	3E+03	7E+03
298.15	3.35E-03	5E-01	4E+00	8E-02	1E+00	1E+05	2E+05	2E+04	4E+04	1E+04	3E+04
300	3.33E-03	6E-01	4E+00	1E-01	1E+00	1E+05	2E+05	3E+04	5E+04	1E+04	3E+04
325	3.08E-03	6E+00	3E+01	1E+00	8E+00	5E+05	7E+05	1E+05	2E+05	6E+04	1E+05
350	2.86E-03	4E+01	1E+02	7E+00	4E+01	2E+06	2E+06	4E+05	6E+05	2E+05	3E+05
373.15	2.68E-03	2E+02	6E+02	3E+01	1E+02	5E+06	5E+06	1E+06	2E+06	5E+05	8E+05
375	2.67E-03	2E+02	7E+02	4E+01	2E+02	5E+06	6E+06	1E+06	2E+06	5E+05	9E+05
400	2.50E-03	1E+03	2E+03	2E+02	6E+02	1E+07	1E+07	3E+06	4E+06	1E+06	2E+06

		CPCM - Water									
		UTH				UTH···H_2O				UTH···$(H_2O)_2$	
		$0A_w$		$0F_w$		$1C_w$		$1G_w$		$2H_w$	
T(K)	1/T (1/K)	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}	k_{SC}	k_{QT}
5	2.00E-01					3E-268	4E+01	5E-289	4E-32		
6	1.67E-01					1E-221	4E+01	5E-239	4E-32		
8	1.25E-01					1E-163	4E+01	1E-176	4E-32	2E-224	2E-02
10	1.00E-01					1E-128	4E+01	4.55-139	4E-32	2E-177	2E-02
20	5.00E-02	2E-210	2E-16	2E-172	6E-12	9E-59	3E+01	6E-64	4E-32	4E-83	2E-02
30	3.33E-02	2E-136	3E-16	3E-111	7E-12	2E-35	3E+01	9E-39	3E-24	1E-51	2E-02
40	2.50E-02	2E-99	3E-16	2E-80	9E-12	9E-24	3E+01	4E-26	3E-16	8E-36	2E-02
50	2.00E-02	3E-77	4E-16	4E-62	1E-11	1E-16	3E+01	1E-18	2E-11	3E-26	2E-02
75	1.33E-02	1E-47	2E-15	2E-37	5E-11	2E-07	4E+01	2E-08	1E-04	1E-13	9E-02
77.36	1.29E-02	7E-46	3E-15	5E-36	6E-11	8E-07	4E+01	9E-08	3E-04	8E-13	1E-01
100	1.00E-02	8E-33	3E-14	3E-25	4E-10	1E-02	9E+01	3E-03	3E-01	3E-07	8E-01
125	8.00E-03	6E-24	9E-13	7E-18	6E-09	6E+00	5E+02	4E+00	6E+01	2E-03	8E+00
150	6.67E-03	5E-18	4E-11	6E-13	2E-07	4E+02	5E+03	4E+02	3E+03	8E-01	1E+02
175	5.71E-03	8E-14	2E-09	2E-09	5E-06	8E+03	4E+04	1E+04	5E+04	5E+01	1E+03
194.7	5.14E-03	3E-11	5E-08	3E-07	8E-05	5E+04	1E+05	9E+04	3E+05	7E+02	7E+03
200	5.00E-03	1E-10	1E-07	8E-07	2E-04	7E+04	2E+05	1E+05	4E+05	1E+03	1E+04
225	4.44E-03	3E-08	3E-06	9E-05	4E-03	4E+05	9E+05	1E+06	2E+06	1E+04	7E+04
250	4.00E-03	3E-06	8E-05	4E-03	6E-02	2E+06	3E+06	5E+06	9E+06	9E+04	3E+05
273.15	3.66E-03	8E-05	1E-03	6E-02	6E-01	4E+06	7E+06	2E+07	3E+07	4E+05	1E+06
275	3.64E-03	1E-04	1E-03	8E-02	7E-01	5E+06	8E+06	2E+07	3E+07	5E+05	1E+06
298.15	3.35E-03	2E-03	1E-02	8E-01	5E+00	1E+07	2E+07	5E+07	7E+07	2E+06	3E+06
300	3.33E-03	2E-03	2E-02	1E+00	5E+00	1E+07	2E+07	5E+07	8E+07	2E+06	4E+06
325	3.08E-03	3E-02	1E-01	8E+00	3E+01	3E+07	3E+07	1E+08	2E+08	5E+06	1E+07
350	2.86E-03	3E-01	1E+00	5E+01	2E+02	5E+07	6E+07	3E+08	3E+08	1E+07	2E+07
373.15	2.68E-03	2E+00	5E+00	2E+02	6E+02	8E+07	1E+08	5E+08	6E+08	3E+07	4E+07
375	2.67E-03	2E+00	5E+00	3E+02	7E+02	8E+07	1E+08	5E+08	6E+08	3E+07	5E+07
400	2.50E-03	9E+00	2E+01	1E+03	2E+03	1E+08	2E+08	9E+08	1E+09	6E+07	9E+07