Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for

Theoretical Insight into 7,8-Dihydrogen-8-oxo-guanine Radical Cation Deprotonation

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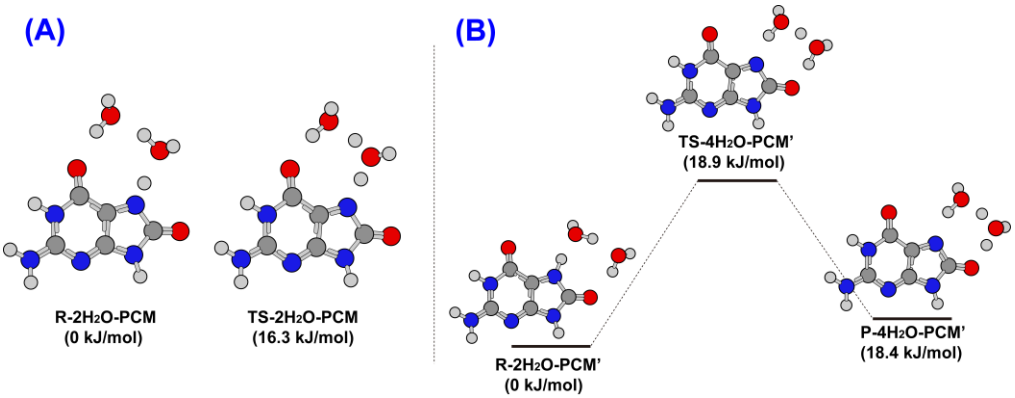

Figure S1 Optimized structures and relative energies obtained at (A) IEFPCM/M06-2X/6-31+G(d) and (B) IEFPCM/M06-2X/6-31+G(d) (structure) and IEFPCM/M06-2X/6-311++G(d,p) (energy) level for 8-oxoG$^{\bullet+}$ deprotonation under the 2H_2O-PCM-N7-1 and 2H_2O-PCM-N7-2 hydration model, respectively (all energies given are relative to the reactant complex. Carbon, oxygen, nitrogen and hydrogen atoms are denoted with gray, red, blue and white balls, respectively)

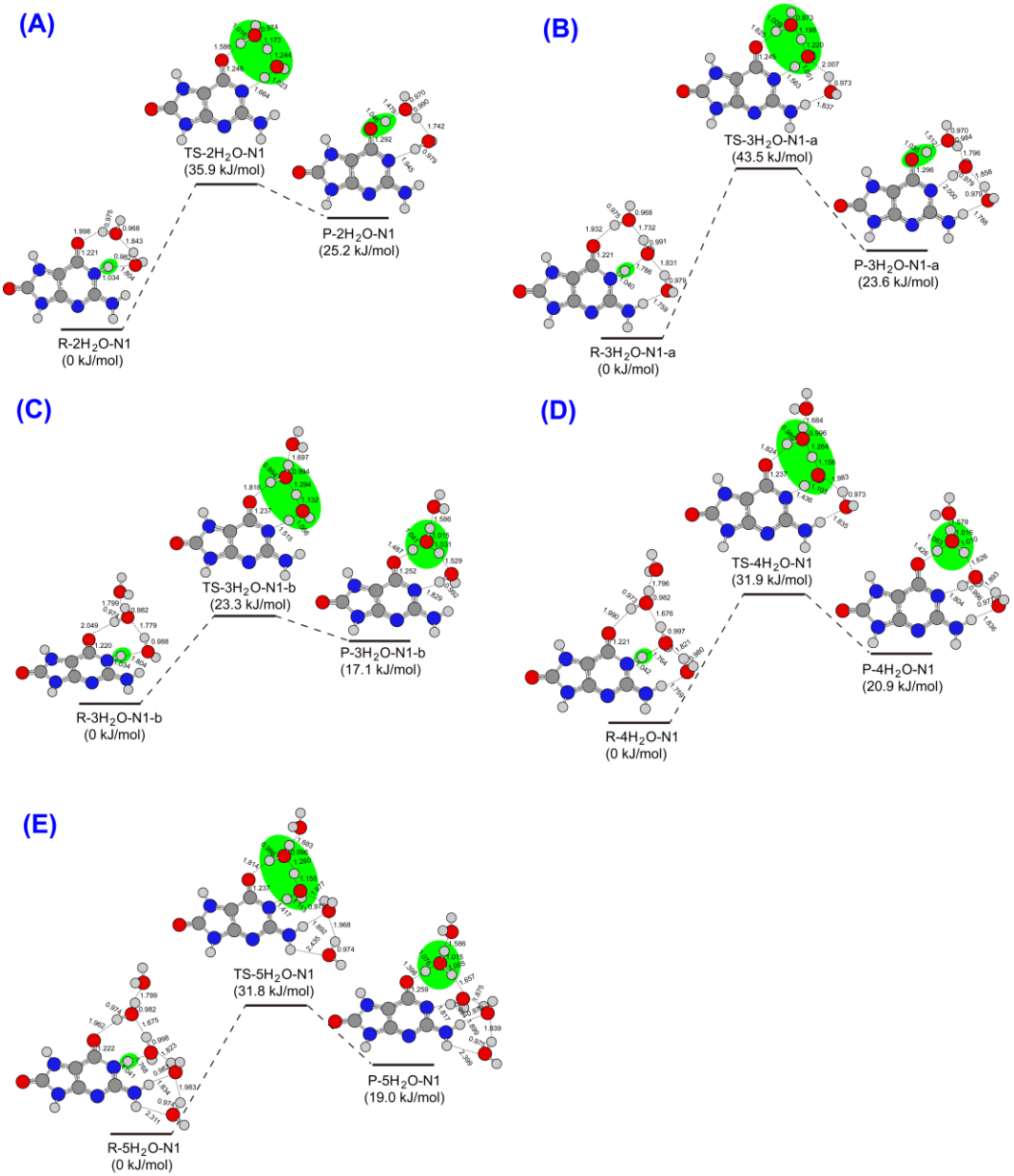

Figure S2 Potential energy profiles for 8-oxoG$^{\bullet+}$ deprotonation under (A) $2H_2O$-PCM-N1; (B) $3H_2O$-PCM-N1-a; (C) $3H_2O$-PCM-N1-b; (D) $4H_2O$-PCM-N1 and (E) $5H_2O$-PCM-N1 hydration models. The optimized geometries and energies are obtained at the IEFPCM/M06-2X/6-31+G(d) and IEFPCM/M06-2X/6-311++G(d,p) level of theory, respectively (all energies given are relative to the reactant complex. Carbon, oxygen, nitrogen and hydrogen atoms are denoted with gray, red, blue and white balls, respectively)

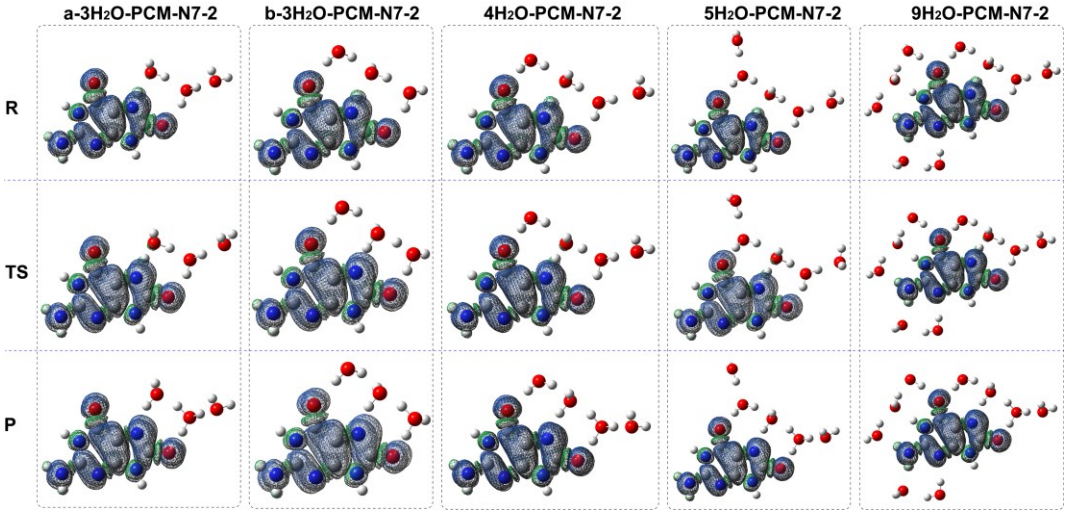

Figure S3 Spin density distribution for optimized structures in the a-3H_2O-PCM-N7-2, b-3H_2O-PCM-N7-2, 4H_2O-PCM-N7-2, 5H_2O-PCM-N7-2 and 9H_2O-PCM-N7-2 hydration model at IEFPCM/M06-2X/6-31+G(d) level of theory

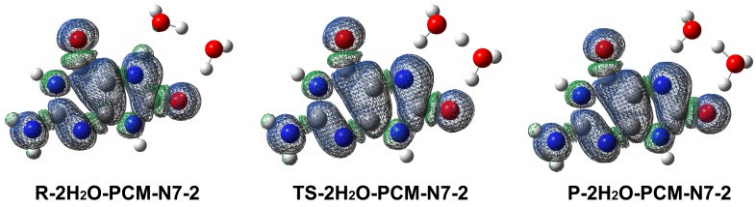

Figure S4 Spin density distribution for optimized structures in the 2H_2O-PCM-N7-2 hydration model at IEFPCM/M06-2X/6-31+G(d) level of theory

Table S1 The calculated pK_a of active protons in 8-oxoG and 8-oxoG$^{\bullet+}$ with and without ribose

	8-oxoG (with ribose)		8-oxoG$^{\bullet+}$ (with ribose)	8-oxoG (without ribose)	8-oxoG$^{\bullet+}$ (without ribose)
	pK_a (cal.)	pK_a (exp.)	pK_a (cal.)	pK_a (cal.)	pK_a (cal.)
N1-H	9.16	8.6	5.90	9.65	3.42
N2-H_a	-	-	-	14.86	6.43
N2-H_b	15.26	-	8.02	15.31	5.91
N7-H	11.37	11.7	2.36	12.57	0.23

Table S2 The calculated pK_a of active protons in 8-oxoG (without ribose) using other basis set and DFT functionals

	B3LYP 6-31+G(d,p)	B3LYP 6-311++G(d,p)	B3LYP-D3 6-31+G(d,p)	B3LYP-D3 6-311++G(d,p)	M06-2X 6-31+G(d,p)	M06-2X 6-311++G(d,p)
N1-H	9.65	9.73	52.48	14.80	9.08	9.01
N2-H_a	14.86	14.82	16.95	16.95	15.83	15.50
N2-H_b	15.31	15.40	15.72	15.81	14.77	14.62
N7-H	12.57	12.51	12.27	12.24	11.41	11.18

Table S3 The calculated pK_a of active protons in 8-oxo-dG at M06-2X/6-31+G(d,p) level of theory

	N1-H	N2-H_a	N2-H_b	N7-H
6-31+G(d,p)	6.57	-	12.86	9.03

Table S4 The calculated pK_a of active protons in 8-oxoG$^{\bullet+}$ by using M06-2X functional

	N1-H	N2-H_a	N2-H_b	N7-H
6-31+G(d,p)	1.03	6.47	5.80	-1.80
6-311++G(d,p)	0.65	5.90	5.32	-2.31

Table S5 The calculated pK_a of N1-H in G$^{\bullet+}$ by using 6-31+G(d,p) basis set

	B3LYP	M06-2X
without ribose	3.58	1.55

Table S6 Relative reaction energies (Δ E) in kJ/mol for 8-oxoG$^{\bullet+}$ deprotonation in different model with different DFT

		M06-2X		B3LYP	BVP86	WB97XD
		6-31+G(d)	6-311++G(d,p)	6-311++G(d,p)	6-311++G(d,p)	6-311++G(d,p)
a-3H_2O-PCM-N7-1	R	0	0	0	0	0
	TS	10.8	6.9	18.5	7.0	4.7
	P	5.0	3.0	15.1	4.8	3.6
b-3H_2O-PCM-N7-1	R	0	0	0	0	0
	TS	2.8	0.8	8.0	0	8.2
	P	-0.7	-2.0	8.4	-0.6	7.7
4H_2O-PCM-N7-1	R	0	0	0	0	0
	TS	15.4	10.9	24.1	11.2	25.6
	P	5.0	3.6	15.9	5.1	15.4
5H_2O-PCM-N7-1	R	0	0	0	0	0
	TS	16.1	11.6	24.9	11.6	26.4
	P	5.1	3.8	16.0	4.9	15.5
9H_2O-PCM-N7-1	R	0	0	0	0	0
	TS	16.1	11.7	24.5	11.2	26.1
	P	6.1	4.4	17.4	6.7	16.7

Table S7 Relative reaction energies (ΔE) in kJ/mol for 8-oxoG$^{\bullet+}$ deprotonation in different model with different DFT

		M06-2X		B3LYP	BVP86	WB97XD
		6-31+G(d)	6-311++G(d,p)	6-311++G(d,p)	6-311++G(d,p)	6-311++G(d,p)
2H_2O-PCM-N7-2	R	0	0	0	0	0
	TS	21.6	18.9	33.2	19.9	33.9
	P	21.2	18.4	33.4	21.2	33.7
a-3H_2O-PCM-N7-2	R	0	0	0	0	0
	TS	11.9	7.9	19.9	8.0	21.0
	P	1.8	0.3	13.6	3.5	12.9
b-3H_2O-PCM-N7-2	R	0	0	0	0	0
	TS	26.5	23.5	38.2	23.6	38.8
	P	24.5	21.8	37.0	24.6	36.5
4H_2O-PCM-N7-2	R	0	0	0	0	0
	TS	16.9	12.6	26.2	12.5	27.4
	P	3.2	2.2	15.3	4.5	14.1
5H_2O-PCM-N7-2	R	0	0	0	0	0
	TS	18.5	13.9	27.7	13.8	29.0
	P	3.4	2.4	15.6	4.8	14.2
9H_2O-PCM-N7-2	R	0	0	0	0	0
	TS	17.7	13.1	27.6	14.2	28.3
	P	4.1	2.7	16.9	6.5	15.0

Table S8 Charge distribution (|e|) of reactant, transient state and product in 8-oxoG$^{\bullet+}$ deprotonation model

		R	TS	P
a-3H_2O-PCM-N7-2	8-oxoG	0.932	0.231	0.125
	W1···H^+···W3	-	0.730	-
	W3	0.004	0.053	0.734
b-3H_2O-PCM-N7-2	8-oxoG	0.958	0.174	0.189
	W1···H^+···W3	-	0.85	-
	W3	0.028	0.164	0.768
4H_2O-PCM-N7-2	8-oxoG	0.954	0.241	0.151
	W1···H^+···W3	-	0.739	-
	W3	0.010	0.074	0.748
5H_2O-PCM-N7-2	8-oxoG	0.958	0.242	0.153
	W1···H^+···W3	-	0.745	-
	W3	0.011	0.080	0.751
9H_2O-PCM-N7-2	8-oxoG	0.863	0.162	0.077
	W1···H^+···W3	-	0.738	-
	W3	0.011	0.074	0.747

Table S9 NBO analysis of the reactant, transient state as well as product in different model at M06-2X/6-31+G(d) level after one-electron oxidative 8-oxoguanine

1. NBO analysis of reactant, transient state and product in a-3H_2O-PCM-N7-1 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.22189	0.16485	0.10918
C	2	0.25514	0.26714	0.27440
C	3	0.35310	0.35674	0.35938
C	4	0.33825	0.34910	0.36575
O	5	-0.23237	-0.25423	-0.27715
N	6	-0.33522	-0.33671	-0.33457
N	7	-0.23220	-0.25495	-0.27063
N	8	-0.31976	-0.32168	-0.32424
H	9	0.24809	0.24576	0.24504
N	10	-0.33767	-0.34885	-0.35453
H	11	0.24069	0.23893	0.23807
H	12	0.23760	0.23590	0.23500
H	13	0.25249	0.24872	0.24639
O	14	-0.53257	-0.52146	-0.48731
H	15	0.27078	0.27689	0.28687
H	16	0.26603	0.27365	0.28596
O	17	-0.52606	-0.49473	-0.51281
H	18	0.26629	0.27965	0.27296
H	19	0.27427	0.28261	0.28401
C	20	0.41352	0.40702	0.39667
N	21	-0.18062	-0.16896	-0.14373
H	22	0.25581	0.26645	0.27346
O	23	-0.21289	-0.21112	-0.20631
O	24	-0.51753	-0.51662	-0.50944
H	25	0.26649	0.26795	0.27379
H	26	0.26646	0.26794	0.27377

2. NBO analysis of reactant, transient state and product in b-3H_2O-PCM-N7-1 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.22165	0.18649	0.15165
C	2	0.25536	0.26366	0.27035
C	3	0.35309	0.35554	0.35758
C	4	0.33883	0.34503	0.35072
O	5	-0.23388	-0.24689	-0.25860
N	6	-0.33480	-0.33592	-0.33688
N	7	-0.22624	-0.24083	-0.25268
N	8	-0.32080	-0.32224	-0.32450
H	9	0.24836	0.24689	0.24562

N	10	-0.33400	-0.34110	-0.34696
H	11	0.24100	0.23985	0.23886
H	12	0.23781	0.23667	0.23566
H	13	0.25315	0.25083	0.24882
O	14	-0.52175	-0.51955	-0.51581
H	15	0.26488	0.26765	0.27112
H	16	0.26733	0.27033	0.27407
O	17	-0.52697	-0.50502	-0.48892
H	18	0.27420	0.28229	0.28692
H	19	0.27448	0.28222	0.28643
O	20	-0.52334	-0.52185	-0.51913
H	21	0.26661	0.26935	0.27229
H	22	0.26493	0.26747	0.27056
C	23	0.42433	0.42188	0.41805
N	24	-0.18699	-0.18123	-0.17380
H	25	0.25442	0.26075	0.27174
O	26	-0.23168	-0.23228	-0.23315

3. NBO analysis of reactant, transient state and product in $4H_2O$-PCM-N7-1 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23256	0.17232	0.12155
C	2	0.25241	0.26618	0.27353
C	3	0.35230	0.35640	0.35896
C	4	0.33604	0.34802	0.36480
O	5	-0.22847	-0.25245	-0.27447
N	6	-0.33482	-0.33635	-0.33420
N	7	-0.22285	-0.24756	-0.26299
N	8	-0.32027	-0.32254	-0.32474
H	9	0.24872	0.24630	0.24576
N	10	-0.33292	-0.34461	-0.34954
H	11	0.24115	0.23932	0.23860
H	12	0.23816	0.23624	0.23545
H	13	0.25370	0.24983	0.24772
O	14	-0.53094	-0.51591	-0.48408
H	15	0.27211	0.27940	0.28794
H	16	0.26637	0.27565	0.28711
O	17	-0.53405	-0.50485	-0.52216
H	18	0.27099	0.28327	0.27518
H	19	0.27829	0.28481	0.28604
O	20	-0.53097	-0.52725	-0.53095
H	21	0.25590	0.25799	0.25777
H	22	0.26076	0.25623	0.25728
C	23	0.42265	0.41818	0.40904
N	24	-0.18881	-0.17802	-0.15432

H	25	0.25449	0.26660	0.27174
O	26	-0.22839	-0.22853	-0.22345
O	27	-0.51761	-0.51618	-0.50754
H	28	0.26673	0.26869	0.27493
H	29	0.26678	0.26882	0.27504

4. NBO analysis of reactant, transient state and product in $5H_2O$-PCM-N7-1 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23443	0.17492	0.12350
C	2	0.25200	0.26588	0.27337
C	3	0.35218	0.35632	0.35894
C	4	0.33569	0.34781	0.36464
O	5	-0.22775	-0.25162	-0.27388
N	6	-0.33471	-0.33622	-0.33393
N	7	-0.22115	-0.24587	-0.26152
N	8	-0.32031	-0.32252	-0.32482
H	9	0.24881	0.24637	0.24585
N	10	-0.33218	-0.34373	-0.34871
H	11	0.24130	0.23950	0.23871
H	12	0.23818	0.23627	0.23558
H	13	0.25391	0.25011	0.24796
O	14	-0.53098	-0.51559	-0.48273
H	15	0.27214	0.27945	0.28790
H	16	0.26645	0.27593	0.28695
O	17	-0.53457	-0.50624	-0.52309
H	18	0.27169	0.28336	0.27534
H	19	0.27873	0.28486	0.28607
O	20	-0.53224	-0.52917	-0.53246
H	21	0.26296	0.26478	0.26445
H	22	0.26741	0.26335	0.26414
C	23	0.42406	0.42001	0.41101
N	24	-0.18981	-0.17944	-0.15581
H	25	0.25429	0.26613	0.27152
O	26	-0.23057	-0.23073	-0.22577
O	27	-0.51745	-0.51596	-0.50724
H	28	0.26679	0.26878	0.27516
H	29	0.26675	0.26877	0.27515
O	30	-0.53382	-0.53323	-0.53399
H	31	0.26471	0.26449	0.26468
H	32	0.25306	0.25325	0.25305

5. NBO analysis of reactant, transient state and product in $9H_2O$-PCM-N7-1 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23798	0.17805	0.12660

C	2	0.24853	0.26331	0.27133
C	3	0.34643	0.35219	0.35549
C	4	0.34719	0.35904	0.37373
O	5	-0.26718	-0.28712	-0.30646
N	6	-0.34007	-0.34146	-0.33878
N	7	-0.22987	-0.25630	-0.27311
N	8	-0.32369	-0.32575	-0.32797
H	9	0.25049	0.24885	0.24842
N	10	-0.32542	-0.33927	-0.34530
H	11	0.24015	0.23880	0.23826
H	12	0.24027	0.23897	0.23829
H	13	0.25277	0.24914	0.24703
O	14	-0.53379	-0.53409	-0.53398
H	15	0.27163	0.27110	0.27108
H	16	0.27771	0.27723	0.27712
O	17	-0.52451	-0.52515	-0.52531
H	18	0.26500	0.26429	0.26396
H	19	0.27139	0.27099	0.27077
O	20	-0.51845	-0.51944	-0.51949
H	21	0.26695	0.26653	0.26650
H	22	0.26659	0.26692	0.26691
O	23	-0.53105	-0.51610	-0.48363
H	24	0.26522	0.27454	0.28598
H	25	0.27174	0.27904	0.28761
O	26	-0.53465	-0.50535	-0.52171
H	27	0.27046	0.28276	0.27538
H	28	0.27781	0.28438	0.28569
O	29	-0.53036	-0.52690	-0.53081
H	30	0.25583	0.25799	0.25798
H	31	0.26074	0.25626	0.25725
O	32	-0.53053	-0.53216	-0.53294
H	33	0.25354	0.25420	0.25453
H	34	0.26031	0.26008	0.25996
O	35	-0.52138	-0.52139	-0.52131
H	36	0.27185	0.27142	0.27121
H	37	0.27189	0.27145	0.27124
C	38	0.42344	0.41883	0.41000
N	39	-0.19100	-0.17930	-0.15662
H	40	0.25420	0.26589	0.27160
O	41	-0.23418	-0.23388	-0.22888
O	42	-0.51770	-0.51609	-0.50773
H	43	0.26685	0.26875	0.27503
H	44	0.26686	0.26876	0.27508

6. NBO analysis of reactant, transient state and product in $2H_2O$-PCM-N7-2 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23500	0.15049	0.14951
C	2	0.25165	0.27109	0.27103
C	3	0.35186	0.35727	0.35724
C	4	0.32381	0.33560	0.33536
O	5	-0.20809	-0.23537	-0.23501
N	6	-0.33773	-0.34132	-0.34135
N	7	-0.22018	-0.24770	-0.24386
N	8	-0.32121	-0.32688	-0.32732
H	9	0.24790	0.24418	0.24429
N	10	-0.33605	-0.34984	-0.34809
H	11	0.24066	0.23810	0.23822
H	12	0.23776	0.23513	0.23525
H	13	0.25324	0.24841	0.24888
O	14	-0.52267	-0.49749	-0.50580
H	15	0.26740	0.28051	0.27652
H	16	0.27393	0.28437	0.28525
O	17	-0.52275	-0.48754	-0.48178
H	18	0.26801	0.28384	0.28349
H	19	0.26559	0.28481	0.28700
C	20	0.42646	0.43053	0.43680
N	21	-0.19342	-0.18524	-0.18657
H	22	0.25594	0.27838	0.27704
O	23	-0.23712	-0.25133	-0.25610

7. NBO analysis of reactant, transient state and product in a-3H_2O-PCM-N7-2 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23267	0.17977	0.14006
C	2	0.25249	0.26547	0.27286
C	3	0.35211	0.35571	0.35779
C	4	0.32412	0.33227	0.33657
O	5	-0.20896	-0.22725	-0.23792
N	6	-0.33788	-0.34018	-0.34164
N	7	-0.22233	-0.24441	-0.25006
N	8	-0.32105	-0.32362	-0.32748
H	9	0.24772	0.24520	0.24379
N	10	-0.33701	-0.34786	-0.35125
H	11	0.24058	0.23877	0.23786
H	12	0.23763	0.23576	0.23489
H	13	0.25299	0.24933	0.24796
O	14	-0.52532	-0.49330	-0.51438
H	15	0.26665	0.28048	0.27198
H	16	0.27404	0.28290	0.28427

O	17	-0.53382	-0.52311	-0.48784
H	18	0.26491	0.27244	0.28271
H	19	0.27066	0.27695	0.28701
C	20	0.42496	0.42165	0.43040
N	21	-0.19217	-0.18585	-0.17904
H	22	0.25594	0.26673	0.27386
O	23	-0.23425	-0.23708	-0.25080
O	24	-0.51759	-0.51670	-0.50932
H	25	0.26640	0.26791	0.27382
H	26	0.26652	0.26802	0.27389

8. NBO analysis of reactant, transient state and product in b-3H_2O-PCM-N7-2 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23640	0.15369	0.15124
C	2	0.25144	0.27017	0.27022
C	3	0.35201	0.35744	0.35739
C	4	0.33323	0.34619	0.34537
O	5	-0.22431	-0.25161	-0.25060
N	6	-0.33492	-0.33789	-0.33822
N	7	-0.21944	-0.24726	-0.24009
N	8	-0.32049	-0.32544	-0.32644
H	9	0.24875	0.24543	0.24555
N	10	-0.33191	-0.34583	-0.34259
H	11	0.24136	0.23887	0.23905
H	12	0.23824	0.23573	0.23590
H	13	0.25400	0.24927	0.25009
O	14	-0.53073	-0.50395	-0.51758
H	15	0.27191	0.28460	0.27805
H	16	0.27804	0.28599	0.28738
O	17	-0.52147	-0.48820	-0.47724
H	18	0.26852	0.28453	0.28390
H	19	0.26688	0.28475	0.28905
C	20	0.42589	0.42781	0.43984
N	21	-0.19123	-0.18191	-0.18607
H	22	0.25464	0.27521	0.27442
O	23	-0.23387	-0.24608	-0.25591
O	24	-0.53018	-0.52603	-0.52810
H	25	0.25639	0.25871	0.25800
H	26	0.26085	0.25583	0.25739

9. NBO analysis of reactant, transient state and product in 4H_2O-PCM-N7-2 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23439	0.17599	0.14188
C	2	0.25205	0.26592	0.27206

C	3	0.35219	0.35627	0.35804
C	4	0.33355	0.34356	0.34678
O	5	-0.22490	-0.24565	-0.25329
N	6	-0.33503	-0.33707	-0.33876
N	7	-0.22122	-0.24483	-0.24844
N	8	-0.32046	-0.32310	-0.32671
H	9	0.24866	0.24610	0.24502
N	10	-0.33273	-0.34428	-0.34686
H	11	0.24123	0.23935	0.23852
H	12	0.23801	0.23610	0.23543
H	13	0.25373	0.24992	0.24885
O	14	-0.53091	-0.52636	-0.53040
H	15	0.25640	0.25833	0.25812
H	16	0.26110	0.25673	0.25807
O	17	-0.53362	-0.50445	-0.52384
H	18	0.27114	0.28376	0.27444
H	19	0.27794	0.28462	0.28608
O	20	-0.53230	-0.51721	-0.48421
H	21	0.26547	0.27478	0.28328
H	22	0.27189	0.27924	0.28777
C	23	0.42440	0.42142	0.43096
N	24	-0.19021	-0.18221	-0.17781
H	25	0.25465	0.26670	0.27217
O	26	-0.23139	-0.23498	-0.24931
O	27	-0.51743	-0.51598	-0.50759
H	28	0.26669	0.26863	0.27484
H	29	0.26671	0.26871	0.27489

10. NBO analysis of reactant, transient state and product in $5H_2O$-PCM-N7-2 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23491	0.17501	0.14108
C	2	0.25194	0.26613	0.27228
C	3	0.35214	0.35625	0.35811
C	4	0.33517	0.34530	0.34840
O	5	-0.22696	-0.24804	-0.25566
N	6	-0.33463	-0.33661	-0.33809
N	7	-0.22109	-0.24503	-0.24884
N	8	-0.32036	-0.32309	-0.32659
H	9	0.24884	0.24629	0.24512
N	10	-0.33203	-0.34379	-0.34651
H	11	0.24135	0.23940	0.23865
H	12	0.23814	0.23621	0.23550
H	13	0.25393	0.25003	0.24891
O	14	-0.53249	-0.52873	-0.53210

H	15	0.26366	0.26538	0.26497
H	16	0.26781	0.26392	0.26510
O	17	-0.53417	-0.50568	-0.52431
H	18	0.27183	0.28418	0.27489
H	19	0.27843	0.28484	0.28621
O	20	-0.53206	-0.51563	-0.48348
H	21	0.26555	0.27535	0.28380
H	22	0.27215	0.27986	0.28790
C	23	0.42418	0.42122	0.43025
N	24	-0.18960	-0.18134	-0.17667
H	25	0.25448	0.26688	0.27210
O	26	-0.23093	-0.23478	-0.24821
O	27	-0.51740	-0.51595	-0.50728
H	28	0.26674	0.26875	0.27510
H	29	0.26679	0.26885	0.27524
O	30	-0.53410	-0.53310	-0.53382
H	31	0.26479	0.26470	0.26491
H	32	0.25301	0.25323	0.25304

11. NBO analysis of reactant, transient state and product in $9H_2O$-PCM-N7-2 model

Atom	Number	Natural charge		
		R	TS	P
C	1	0.23911	0.17966	0.14565
C	2	0.24807	0.26342	0.26957
C	3	0.34637	0.35218	0.35435
C	4	0.34530	0.35512	0.35835
O	5	-0.26391	-0.28079	-0.28687
N	6	-0.34018	-0.34220	-0.34417
N	7	-0.22809	-0.25386	-0.25800
N	8	-0.32379	-0.32600	-0.32904
H	9	0.25044	0.24873	0.24787
N	10	-0.32516	-0.33925	-0.34264
H	11	0.24014	0.23872	0.23811
H	12	0.24027	0.23893	0.23840
H	13	0.25287	0.24922	0.24821
O	14	-0.53410	-0.53468	-0.53491
H	15	0.27135	0.27071	0.27050
H	16	0.27762	0.27710	0.27692
O	17	-0.52437	-0.52512	-0.52547
H	18	0.26494	0.26428	0.26402
H	19	0.27135	0.27097	0.27085
O	20	-0.51998	-0.52155	-0.52223
H	21	0.26664	0.26607	0.26585
H	22	0.26730	0.26792	0.26818
O	23	-0.53023	-0.52510	-0.52913

H	24	0.25487	0.25665	0.25661
H	25	0.26142	0.25731	0.25859
O	26	-0.53459	-0.50468	-0.52414
H	27	0.27080	0.28384	0.27471
H	28	0.27749	0.28449	0.28611
O	29	-0.53199	-0.51691	-0.48416
H	30	0.26577	0.27505	0.28346
H	31	0.27174	0.27919	0.28772
O	32	-0.53042	-0.53212	-0.53273
H	33	0.25356	0.25427	0.25452
H	34	0.26037	0.26011	0.25999
O	35	-0.52139	-0.52142	-0.52143
H	36	0.27181	0.27142	0.27123
H	37	0.27194	0.27152	0.27132
C	38	0.42552	0.42236	0.43166
N	39	-0.19222	-0.18377	-0.17847
H	40	0.25424	0.26630	0.27211
O	41	-0.23677	-0.23947	-0.25319
O	42	-0.51751	-0.51598	-0.50786
H	43	0.26663	0.26862	0.27476
H	44	0.26675	0.26873	0.27485

Table S10 The cartesian coordinates for the optimized structure of reactant, transient state and product in a-3H_2O-PCM-N7-1 model at M06-2X/6-31+G(d) level

1. R-a-3H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.618377	0.241752	0.040454
2	6	0	-2.009183	0.557019	-0.104078
3	6	0	-2.620973	-1.594282	-0.086510
4	6	0	-0.214429	-1.142566	0.132438
5	8	0	0.916909	-1.573690	0.262825
6	7	0	-1.320492	-1.994096	0.051344
7	7	0	-2.995919	-0.300920	-0.167891
8	7	0	-2.080853	1.907848	-0.161146
9	1	0	-1.104321	-2.987509	0.111270
10	7	0	-3.565287	-2.513283	-0.142987
11	1	0	-4.527601	-2.210840	-0.244548
12	1	0	-3.378705	-3.507530	-0.088720
13	1	0	-2.927014	2.459182	-0.264096
14	8	0	3.612115	-0.708487	0.813673
15	1	0	4.310275	-1.062979	0.221596
16	1	0	2.791484	-1.182931	0.595724
17	8	0	2.714615	1.761855	0.299898
18	1	0	3.102984	2.116086	-0.514194
19	1	0	3.162787	0.890682	0.470979
20	6	0	-0.803663	2.469706	-0.061668
21	7	0	0.079489	1.378489	0.064608
22	1	0	1.134112	1.505317	0.148027
23	8	0	-0.506147	3.636789	-0.079345
24	8	0	5.618895	-1.671581	-0.856118
25	1	0	6.231369	-2.287988	-0.427503
26	1	0	6.178115	-0.977217	-1.235598

2. TS-a-3H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.804849	0.087630	-0.021112
2	6	0	2.070730	0.742953	0.143910
3	6	0	3.228577	-1.166253	0.095481
4	6	0	0.787076	-1.350972	-0.143528
5	8	0	-0.184505	-2.076353	-0.297263
6	7	0	2.076014	-1.886846	-0.065044
7	7	0	3.253863	0.172635	0.203688
8	7	0	1.782966	2.059727	0.225721
9	1	0	2.124659	-2.900348	-0.144682
10	7	0	4.379006	-1.818380	0.146419

11	1	0	5.230850	-1.282527	0.263590
12	1	0	4.452683	-2.825743	0.077669
13	1	0	2.447484	2.815966	0.349651
14	8	0	-2.939529	-1.753070	-0.761702
15	1	0	-3.542463	-2.248843	-0.156895
16	1	0	-2.031181	-2.072235	-0.594896
17	8	0	-2.651062	0.681829	-0.263071
18	1	0	-3.095731	0.936643	0.564271
19	1	0	-2.855196	-0.332251	-0.452669
20	6	0	0.392930	2.244581	0.120114
21	7	0	-0.184159	0.977818	-0.035074
22	1	0	-1.511653	0.812890	-0.144656
23	8	0	-0.191118	3.305636	0.158125
24	8	0	-4.618639	-3.111438	0.918157
25	1	0	-4.946139	-3.950741	0.560924
26	1	0	-5.409568	-2.617565	1.182518

3. P-a-3H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.516101	0.221889	0.080099
2	6	0	-1.899281	0.508595	-0.188651
3	6	0	-2.527227	-1.630385	-0.106449
4	6	0	-0.146767	-1.156758	0.272389
5	8	0	0.966632	-1.623115	0.514663
6	7	0	-1.238028	-2.014303	0.156535
7	7	0	-2.891659	-0.354230	-0.284717
8	7	0	-1.956315	1.848042	-0.320681
9	1	0	-1.023708	-3.000828	0.284095
10	7	0	-3.457543	-2.571696	-0.187222
11	1	0	-4.410809	-2.289614	-0.380678
12	1	0	-3.264040	-3.558672	-0.074900
13	1	0	-2.781906	2.402649	-0.517438
14	8	0	3.376305	-0.594090	0.820688
15	1	0	4.010816	-0.991181	0.130129
16	1	0	2.462859	-0.992212	0.699768
17	8	0	2.914389	1.827577	0.535045
18	1	0	3.330817	2.239464	-0.238884
19	1	0	3.274925	0.454955	0.681776
20	6	0	-0.660576	2.381204	-0.142535
21	7	0	0.219889	1.327779	0.108528
22	1	0	1.938475	1.774050	0.347249
23	8	0	-0.381206	3.563466	-0.202957
24	8	0	4.977708	-1.654958	-0.912342
25	1	0	5.750501	-2.076500	-0.504178

26	1	0	5.329235	-1.041383	-1.576763

Table S11 The cartesian coordinates for the optimized structure of reactant, transient state and product in b-3H_2O-PCM-N7-1 model at M06-2X/6-31+G(d) level

1. R-b-3H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.420311	-0.025517	-0.125773
2	6	0	-1.209606	-1.207819	0.051398
3	6	0	-3.128927	-0.061377	0.092349
4	6	0	-1.074839	1.261746	-0.172481
5	8	0	-0.544041	2.353056	-0.283541
6	7	0	-2.461102	1.121906	-0.068866
7	7	0	-2.512602	-1.260884	0.157886
8	7	0	-0.328186	-2.238279	0.082502
9	1	0	-2.986687	1.993483	-0.104279
10	7	0	-4.443049	-0.038775	0.192935
11	1	0	-4.933965	-0.917850	0.312427
12	1	0	-4.988170	0.814739	0.162312
13	1	0	-0.555477	-3.220735	0.200880
14	8	0	2.048959	3.393082	0.465370
15	1	0	2.116356	3.569526	1.415120
16	1	0	1.114350	3.172193	0.299336
17	8	0	2.992245	1.080014	-0.618543
18	1	0	3.705595	0.550533	-0.196099
19	1	0	2.887126	1.931139	-0.134938
20	8	0	4.470474	-0.973880	0.407082
21	1	0	3.789931	-1.645760	0.216686
22	1	0	5.265538	-1.255470	-0.068685
23	6	0	0.974103	-1.761262	-0.061641
24	7	0	0.865711	-0.368667	-0.198054
25	1	0	1.730907	0.271952	-0.371996
26	8	0	1.998112	-2.407607	-0.063086

2. TS-b-3H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.433125	-0.085403	-0.185823
2	6	0	-1.218625	-1.274285	-0.029631
3	6	0	-3.147086	-0.149168	0.037998
4	6	0	-1.102372	1.194437	-0.203602
5	8	0	-0.586386	2.297825	-0.290567
6	7	0	-2.487588	1.042515	-0.101485
7	7	0	-2.524229	-1.342509	0.078695

8	7	0	-0.327214	-2.293766	-0.019040
9	1	0	-3.019684	1.910395	-0.116740
10	7	0	-4.463785	-0.132710	0.141792
11	1	0	-4.951011	-1.015199	0.246218
12	1	0	-5.011147	0.719237	0.130297
13	1	0	-0.539353	-3.280849	0.083420
14	8	0	2.006277	3.253503	0.440444
15	1	0	2.113276	3.393512	1.393068
16	1	0	1.057816	3.071748	0.295634
17	8	0	2.866732	1.009825	-0.661571
18	1	0	3.608800	0.474282	-0.266984
19	1	0	2.748433	1.872475	-0.172543
20	8	0	4.397076	-0.933270	0.298492
21	1	0	3.743465	-1.638332	0.122910
22	1	0	5.198010	-1.176518	-0.189248
23	6	0	0.968055	-1.784150	-0.154990
24	7	0	0.857922	-0.395479	-0.269087
25	1	0	1.858561	0.346490	-0.473569
26	8	0	1.998470	-2.430573	-0.163497

3. P-b-3H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.401788	-0.036023	-0.127441
2	6	0	-1.205868	-1.210410	0.048569
3	6	0	-3.120490	-0.064702	0.097723
4	6	0	-1.057914	1.249732	-0.158006
5	8	0	-0.532860	2.351195	-0.251222
6	7	0	-2.445234	1.117402	-0.056480
7	7	0	-2.515276	-1.263137	0.156960
8	7	0	-0.324173	-2.236300	0.077976
9	1	0	-2.966274	1.991616	-0.078849
10	7	0	-4.439414	-0.025519	0.197829
11	1	0	-4.940445	-0.898145	0.314955
12	1	0	-4.972491	0.834561	0.173123
13	1	0	-0.541678	-3.219317	0.202121
14	8	0	2.087935	3.221026	0.395979
15	1	0	2.202379	3.358219	1.348889
16	1	0	1.135619	3.040104	0.253132
17	8	0	3.000116	1.069881	-0.648756
18	1	0	3.691704	0.489106	-0.183074
19	1	0	2.827288	1.952248	-0.164604
20	8	0	4.327577	-0.840964	0.453115
21	1	0	3.663892	-1.542606	0.281400
22	1	0	5.151174	-1.129671	0.031238

23	6	0	0.974739	-1.726237	-0.063205
24	7	0	0.887220	-0.344483	-0.208423
25	1	0	2.107763	0.521691	-0.534850
26	8	0	2.000250	-2.390128	-0.046436

Table S12 The cartesian coordinates for the optimized structure of reactant, transient state and product in $4H_2O$-PCM-N7-1 model at M06-2X/6-31+G(d) level

1. R-$4H_2O$-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.802668	0.083106	0.096009
2	6	0	2.095620	0.693301	0.006573
3	6	0	3.148517	-1.279196	-0.063658
4	6	0	0.696506	-1.358560	0.084219
5	8	0	-0.324262	-2.020384	0.128278
6	7	0	1.960320	-1.952009	0.012844
7	7	0	3.241419	0.068637	-0.070772
8	7	0	1.878196	2.031983	0.024936
9	1	0	1.956528	-2.970398	0.005423
10	7	0	4.268813	-1.968685	-0.136778
11	1	0	5.144165	-1.460084	-0.193726
12	1	0	4.302338	-2.981291	-0.141753
13	1	0	2.588648	2.755883	-0.023286
14	8	0	-3.078007	-1.554377	-0.669920
15	1	0	-3.777720	-2.158833	-0.338570
16	1	0	-2.222680	-1.938423	-0.410571
17	8	0	-2.802409	0.830323	0.444887
18	1	0	-3.072415	0.789657	1.375532
19	1	0	-3.043706	-0.051274	0.040086
20	8	0	-2.918383	3.513203	-0.527470
21	1	0	-1.986457	3.665498	-0.299778
22	1	0	-3.076272	2.586407	-0.269793
23	6	0	0.514219	2.301320	0.123235
24	7	0	-0.119247	1.045707	0.166968
25	1	0	-1.163340	0.935099	0.288400
26	8	0	-0.026123	3.381163	0.160093
27	8	0	-5.157544	-3.160910	0.211150
28	1	0	-5.130718	-3.432754	1.140660
29	1	0	-5.294687	-3.977442	-0.291993

2. TS-$4H_2O$-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.802389	-0.200939	-0.296845

2	6	0	-0.182476	-1.487415	-0.161885
3	6	0	1.887220	-0.649209	-0.186013
4	6	0	0.043788	0.967250	-0.375372
5	8	0	-0.305678	2.134000	-0.474169
6	7	0	1.397050	0.621175	-0.326540
7	7	0	1.104922	-1.740384	-0.104372
8	7	0	-1.205513	-2.370437	-0.106769
9	1	0	2.043960	1.404728	-0.387704
10	7	0	3.197131	-0.817475	-0.124708
11	1	0	3.557282	-1.758858	-0.021084
12	1	0	3.859353	-0.052576	-0.162711
13	1	0	-1.130316	-3.377138	-0.005261
14	8	0	-2.701553	3.469878	0.156054
15	1	0	-2.930337	4.316584	-0.303971
16	1	0	-1.775067	3.246193	-0.061685
17	8	0	-3.875605	1.443943	-0.605734
18	1	0	-4.129305	1.523054	-1.543031
19	1	0	-3.433902	2.377492	-0.292119
20	8	0	-5.802046	-0.495808	0.526211
21	1	0	-5.116157	-1.140957	0.278184
22	1	0	-5.413469	0.363667	0.298545
23	6	0	-2.421241	-1.680145	-0.197764
24	7	0	-2.127742	-0.319896	-0.320559
25	1	0	-3.074093	0.635638	-0.500778
26	8	0	-3.528817	-2.183136	-0.170338
27	8	0	-3.461905	5.772690	-1.051896
28	1	0	-3.255662	5.852229	-1.995489
29	1	0	-3.127761	6.585541	-0.643263

3. P-4H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.689478	0.071907	0.005127
2	6	0	2.008778	0.629573	0.127281
3	6	0	3.031515	-1.344750	-0.045287
4	6	0	0.579349	-1.352860	-0.181854
5	8	0	-0.440229	-2.024490	-0.334162
6	7	0	1.823446	-1.978054	-0.183869
7	7	0	3.154476	-0.018706	0.109924
8	7	0	1.811226	1.956889	0.268171
9	1	0	1.797869	-2.987262	-0.314899
10	7	0	4.131799	-2.081393	-0.067994
11	1	0	5.025335	-1.615055	0.033193
12	1	0	4.125919	-3.088185	-0.171224
13	1	0	2.525423	2.668962	0.374050

14	8	0	-3.002672	-1.460702	-0.639464
15	1	0	-3.587386	-2.134508	-0.132510
16	1	0	-2.032869	-1.694571	-0.525893
17	8	0	-2.983082	0.890940	0.262584
18	1	0	-3.292093	0.957776	1.181173
19	1	0	-3.121965	-0.500109	-0.253962
20	8	0	-2.786044	3.642706	-0.677469
21	1	0	-1.878467	3.626638	-0.322981
22	1	0	-3.128924	2.752144	-0.491695
23	6	0	0.429395	2.216924	0.232424
24	7	0	-0.248345	1.010512	0.073074
25	1	0	-1.987338	0.974046	0.284493
26	8	0	-0.070911	3.326802	0.323463
27	8	0	-4.524768	-3.107889	0.599522
28	1	0	-4.081216	-3.656155	1.266339
29	1	0	-4.978186	-3.725304	0.003523

Table S13 The cartesian coordinates for the optimized structure of reactant, transient state and product in $5H_2O$-PCM-N7-1 model at M06-2X/6-31+G(d) level

1. R-$5H_2O$-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.127812	-0.281466	0.107208
2	6	0	-1.975740	-1.432782	0.023340
3	6	0	-3.841568	-0.198379	0.019432
4	6	0	-1.720170	1.036754	0.132028
5	8	0	-1.135360	2.103446	0.175170
6	7	0	-3.115327	0.957738	0.098115
7	7	0	-3.282210	-1.428011	-0.019953
8	7	0	-1.146053	-2.506215	0.000170
9	1	0	-3.597140	1.854875	0.113125
10	7	0	-5.156184	-0.123564	-0.022880
11	1	0	-5.686714	-0.985691	-0.082275
12	1	0	-5.666093	0.751747	0.002402
13	1	0	-1.426697	-3.480227	-0.061132
14	8	0	1.489504	3.009479	-0.688438
15	1	0	1.823413	3.865983	-0.341877
16	1	0	0.564345	2.927300	-0.398356
17	8	0	2.424447	0.764331	0.352297
18	1	0	2.674642	0.915167	1.277259
19	1	0	2.205032	1.660988	-0.032916
20	8	0	3.714550	-1.510203	-0.707911
21	1	0	2.976135	-2.093737	-0.460388
22	1	0	3.431336	-0.621637	-0.415417

23	6	0	0.183022	-2.093261	0.060035
24	7	0	0.142863	-0.689264	0.130758
25	1	0	1.010903	-0.099118	0.235116
26	8	0	1.174830	-2.783942	0.048527
27	8	0	2.483152	5.410955	0.277197
28	1	0	2.687741	6.062153	-0.410501
29	1	0	3.296600	5.321365	0.795988
30	8	0	6.135456	-2.283425	0.416688
31	1	0	5.284527	-2.014755	0.006981
32	1	0	6.735307	-2.455537	-0.322127

2. TS-5H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.885895	0.110728	0.008472
2	6	0	2.182645	0.723562	0.022253
3	6	0	3.257558	-1.228248	0.166088
4	6	0	0.803456	-1.330862	0.051460
5	8	0	-0.205045	-2.019866	0.017498
6	7	0	2.071568	-1.911329	0.137225
7	7	0	3.342325	0.112842	0.099997
8	7	0	1.947579	2.053781	-0.054032
9	1	0	2.078357	-2.928777	0.167407
10	7	0	4.380388	-1.918957	0.263443
11	1	0	5.258127	-1.413032	0.281019
12	1	0	4.407054	-2.929044	0.328830
13	1	0	2.644412	2.791129	-0.072485
14	8	0	-2.882082	-1.521142	-0.693914
15	1	0	-3.588238	-2.046260	-0.238440
16	1	0	-2.018537	-1.920766	-0.466891
17	8	0	-2.547053	0.783284	0.095645
18	1	0	-2.826669	0.870903	1.025042
19	1	0	-2.783046	-0.219980	-0.236896
20	8	0	-2.737712	3.496319	-0.984666
21	1	0	-1.802405	3.554796	-0.711330
22	1	0	-2.994501	2.581381	-0.780539
23	6	0	0.567155	2.279008	-0.112390
24	7	0	-0.067845	1.035957	-0.066125
25	1	0	-1.406419	0.895211	0.037311
26	8	0	0.025916	3.366515	-0.193372
27	8	0	-4.819442	-2.955576	0.546152
28	1	0	-5.338540	-3.514906	-0.051443
29	1	0	-5.468207	-2.427793	1.036090
30	8	0	-4.358600	5.351674	0.316602
31	1	0	-3.786747	4.709560	-0.156104

32	1	0	-4.679010	5.961565	-0.362156

3. P-5H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.014025	-0.210968	0.000609
2	6	0	-1.888428	-1.344169	0.133725
3	6	0	-3.748832	-0.116100	0.068290
4	6	0	-1.619505	1.089513	-0.137636
5	8	0	-1.063443	2.175471	-0.297131
6	7	0	-3.008754	1.028227	-0.080073
7	7	0	-3.203970	-1.336982	0.173887
8	7	0	-1.063406	-2.409389	0.214157
9	1	0	-3.483466	1.922294	-0.184964
10	7	0	-5.068094	-0.008949	0.106486
11	1	0	-5.616529	-0.854017	0.212627
12	1	0	-5.557576	0.874986	0.043558
13	1	0	-1.335419	-3.381820	0.307166
14	8	0	1.428747	2.932407	-0.721813
15	1	0	1.623849	3.803069	-0.212305
16	1	0	0.473955	2.658789	-0.568778
17	8	0	2.594342	0.860842	0.140563
18	1	0	2.913927	0.959309	1.052852
19	1	0	2.017893	2.155167	-0.366213
20	8	0	3.738378	-1.617840	-0.778467
21	1	0	2.928199	-2.052225	-0.447140
22	1	0	3.598402	-0.670731	-0.597991
23	6	0	0.265968	-1.960803	0.131651
24	7	0	0.263915	-0.574169	0.006296
25	1	0	1.761579	0.309044	0.184011
26	8	0	1.247215	-2.687899	0.161344
27	8	0	1.862926	5.131235	0.513339
28	1	0	2.240094	5.816408	-0.061447
29	1	0	2.458886	5.064285	1.276619
30	8	0	6.032925	-2.580933	0.456405
31	1	0	5.225278	-2.249304	0.006754
32	1	0	6.563786	-2.995366	-0.237671

Table S14 The cartesian coordinates for the optimized structure of reactant, transient state and product in 9H_2O-PCM-N7-1 model at M06-2X/6-31+G(d) level

1. R-9H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.396719	-0.780031	-0.293817

2	6	0	0.722431	-1.650568	-0.088917
3	6	0	2.188379	0.055855	-0.070935
4	6	0	-0.170694	0.645696	-0.368657
5	8	0	-1.033215	1.508558	-0.497073
6	7	0	1.174007	0.958587	-0.273066
7	7	0	1.971333	-1.285743	0.025071
8	7	0	0.211858	-2.908053	-0.027593
9	1	0	1.398931	1.965148	-0.412680
10	7	0	3.413676	0.501783	0.036814
11	1	0	4.185091	-0.160689	0.182704
12	1	0	3.646533	1.511552	0.032424
13	1	0	0.733204	-3.766535	0.120531
14	8	0	1.541947	3.705189	-0.763595
15	1	0	1.437718	3.898254	-1.708097
16	1	0	0.749194	4.086329	-0.310760
17	8	0	4.060418	3.230599	0.180143
18	1	0	4.807273	3.521195	-0.363447
19	1	0	3.269286	3.693100	-0.164672
20	8	0	-0.800787	4.226137	0.461201
21	1	0	-0.799841	4.406791	1.412831
22	1	0	-1.088548	3.301556	0.359654
23	8	0	-3.915070	1.733817	-0.740817
24	1	0	-2.943094	1.763413	-0.699240
25	1	0	-4.238573	2.163249	0.081704
26	8	0	-4.098697	-0.901246	-0.881386
27	1	0	-4.322045	-1.134840	-1.796027
28	1	0	-4.178450	0.092533	-0.817462
29	8	0	-4.705458	-3.176731	0.725633
30	1	0	-3.864597	-3.586779	0.464145
31	1	0	-4.699681	-2.317661	0.265349
32	8	0	4.101702	-3.369138	0.618489
33	1	0	3.381745	-2.743573	0.426775
34	1	0	4.891816	-2.800281	0.624571
35	8	0	5.793996	-1.090269	0.465281
36	1	0	6.423566	-1.019090	-0.269080
37	1	0	6.279255	-0.796533	1.252062
38	6	0	-1.172279	-2.877047	-0.176403
39	7	0	-1.507446	-1.521804	-0.343294
40	1	0	-2.495749	-1.217888	-0.548222
41	8	0	-1.940267	-3.810100	-0.161380
42	8	0	-4.786906	2.967310	1.585381
43	1	0	-5.233476	3.815399	1.443216
44	1	0	-5.396465	2.443531	2.126639

2. TS-9H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.440092	-0.741862	-0.241221
2	6	0	0.659739	-1.646734	-0.064833
3	6	0	2.191591	-0.004519	-0.068126
4	6	0	-0.152024	0.671083	-0.314305
5	8	0	-0.973570	1.582755	-0.423609
6	7	0	1.205212	0.935486	-0.241493
7	7	0	1.929569	-1.332032	0.024530
8	7	0	0.101540	-2.879145	-0.003778
9	1	0	1.465757	1.931738	-0.374471
10	7	0	3.436620	0.403766	0.013006
11	1	0	4.186710	-0.284027	0.139708
12	1	0	3.702390	1.402578	0.014371
13	1	0	0.584965	-3.761745	0.125243
14	8	0	1.687046	3.691060	-0.693314
15	1	0	1.563489	3.914801	-1.628507
16	1	0	0.920365	4.084226	-0.207875
17	8	0	4.210015	3.115455	0.178650
18	1	0	4.946179	3.382278	-0.390907
19	1	0	3.423001	3.603968	-0.138805
20	8	0	-0.605787	4.236833	0.613634
21	1	0	-0.570935	4.363102	1.573358
22	1	0	-0.915524	3.324163	0.469183
23	8	0	-3.762216	1.740625	-0.768492
24	1	0	-2.795372	1.837366	-0.649571
25	1	0	-4.199752	2.156091	0.017306
26	8	0	-3.918583	-0.710611	-0.857293
27	1	0	-4.117761	-0.993393	-1.768287
28	1	0	-3.944534	0.367716	-0.822176
29	8	0	-4.825917	-3.070546	0.663193
30	1	0	-3.944711	-3.388857	0.397788
31	1	0	-4.864439	-2.166089	0.314121
32	8	0	3.988757	-3.488292	0.478660
33	1	0	3.286895	-2.829067	0.333650
34	1	0	4.799250	-2.948960	0.491873
35	8	0	5.780558	-1.280778	0.387572
36	1	0	6.411339	-1.207350	-0.345386
37	1	0	6.276707	-1.030289	1.182343
38	6	0	-1.287639	-2.765717	-0.130324
39	7	0	-1.591522	-1.411389	-0.281690
40	1	0	-2.843370	-1.019575	-0.596741
41	8	0	-2.082862	-3.686897	-0.107138
42	8	0	-4.942522	2.889049	1.387203

43	1	0	-5.422556	3.706676	1.185835
44	1	0	-5.577507	2.323427	1.852407

3. P-9H_2O-PCM-N7-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.460520	-0.699018	-0.211469
2	6	0	0.653809	-1.588850	-0.030696
3	6	0	2.171982	0.062625	-0.052205
4	6	0	-0.175787	0.708849	-0.297079
5	8	0	-0.998714	1.630697	-0.413630
6	7	0	1.173458	0.991830	-0.229531
7	7	0	1.924426	-1.262619	0.051888
8	7	0	0.104632	-2.821028	0.040668
9	1	0	1.424742	1.988385	-0.375039
10	7	0	3.413313	0.490563	0.020160
11	1	0	4.171450	-0.186239	0.152739
12	1	0	3.666211	1.491456	0.016553
13	1	0	0.590858	-3.700818	0.174598
14	8	0	1.651892	3.744891	-0.714370
15	1	0	1.520530	3.961969	-1.650045
16	1	0	0.889618	4.141405	-0.225064
17	8	0	4.181053	3.213691	0.168709
18	1	0	4.914845	3.473775	-0.406922
19	1	0	3.389907	3.687608	-0.160202
20	8	0	-0.627047	4.284384	0.618596
21	1	0	-0.579049	4.412835	1.577423
22	1	0	-0.927223	3.367502	0.480501
23	8	0	-3.617683	1.730459	-0.712111
24	1	0	-2.621141	1.663807	-0.597559
25	1	0	-4.026077	2.174467	0.117705
26	8	0	-4.178537	-0.705545	-0.969696
27	1	0	-4.379810	-0.945675	-1.889295
28	1	0	-3.973125	0.757583	-0.830035
29	8	0	-4.849873	-3.073884	0.588159
30	1	0	-3.941626	-3.360357	0.381484
31	1	0	-4.927444	-2.208709	0.151890
32	8	0	3.993875	-3.397764	0.480818
33	1	0	3.286571	-2.742082	0.343025
34	1	0	4.799771	-2.851908	0.503472
35	8	0	5.773367	-1.177478	0.416180
36	1	0	6.412288	-1.098709	-0.309071
37	1	0	6.258681	-0.925734	1.217157
38	6	0	-1.290664	-2.703444	-0.087459
39	7	0	-1.613984	-1.359317	-0.250772

40	1	0	-3.246250	-1.014037	-0.784167
41	8	0	-2.071726	-3.641481	-0.053581
42	8	0	-4.581698	2.900430	1.353343
43	1	0	-5.111460	3.682608	1.130763
44	1	0	-5.145613	2.346241	1.916259

Table S15 The cartesian coordinates for the optimized structure of reactant, transient state and product in $2H_2O$-PCM-N7-2 model at M06-2X/6-31+G(d) level

1. R-$2H_2O$-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.316418	0.270132	0.019060
2	6	0	0.924804	-1.024653	0.027426
3	6	0	2.995744	-0.177210	-0.003988
4	6	0	1.151002	1.452009	0.000066
5	8	0	0.777798	2.606510	-0.005332
6	7	0	2.509684	1.099222	-0.011605
7	7	0	2.207956	-1.276141	0.016531
8	7	0	-0.098696	-1.916226	0.049173
9	1	0	3.157056	1.885757	-0.026340
10	7	0	4.300153	-0.367990	-0.017178
11	1	0	4.646610	-1.320704	-0.011700
12	1	0	4.975905	0.386285	-0.033102
13	1	0	-0.014211	-2.927790	0.058337
14	8	0	-3.040620	1.876297	-0.006100
15	1	0	-3.119943	2.416985	0.794296
16	1	0	-3.825081	1.276484	-0.019611
17	8	0	-4.816768	-0.175035	-0.167849
18	1	0	-4.161761	-0.883038	-0.024355
19	1	0	-5.495159	-0.291163	0.513516
20	6	0	-1.320794	-1.248493	0.053581
21	7	0	-1.009944	0.120814	0.035248
22	1	0	-1.756365	0.875229	0.035587
23	8	0	-2.426784	-1.740056	0.069032

2. TS-$2H_2O$-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.428550	-0.045699	0.095813
2	6	0	1.213343	-1.226040	-0.114050
3	6	0	3.158821	-0.139230	0.000874
4	6	0	1.116592	1.215623	0.277494
5	8	0	0.616959	2.308386	0.467492
6	7	0	2.511143	1.046806	0.209199

7	7	0	2.524375	-1.313507	-0.166362
8	7	0	0.305572	-2.223284	-0.246141
9	1	0	3.052446	1.900755	0.329300
10	7	0	4.482761	-0.142780	-0.040024
11	1	0	4.955480	-1.024935	-0.195118
12	1	0	5.047330	0.689072	0.073844
13	1	0	0.499028	-3.205343	-0.409040
14	8	0	-3.171190	1.099933	0.324445
15	1	0	-3.302809	1.533824	1.185055
16	1	0	-3.835393	0.042641	0.229012
17	8	0	-4.258947	-1.029143	0.042779
18	1	0	-3.448301	-1.629076	-0.046718
19	1	0	-4.785716	-1.336917	0.801933
20	6	0	-0.974355	-1.678875	-0.124606
21	7	0	-0.872814	-0.314098	0.089794
22	1	0	-2.223165	0.762186	0.287664
23	8	0	-2.010958	-2.341341	-0.202918

3. P-2H_2O-PCM-N7-2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.264280	0.243746	0.004986
2	6	0	0.889255	-1.045876	0.016051
3	6	0	2.959762	-0.215493	0.017915
4	6	0	1.112163	1.418600	0.001955
5	8	0	0.760205	2.582742	-0.005394
6	7	0	2.472760	1.062008	0.008821
7	7	0	2.176719	-1.310014	0.022764
8	7	0	-0.143188	-1.925364	0.016601
9	1	0	3.121272	1.846966	0.005900
10	7	0	4.271424	-0.397438	0.022303
11	1	0	4.623888	-1.346956	0.028306
12	1	0	4.940826	0.361306	0.018222
13	1	0	-0.082419	-2.937716	0.020585
14	8	0	-3.184468	1.939909	-0.106928
15	1	0	-3.300869	2.528570	0.656861
16	1	0	-3.988541	0.826013	-0.049299
17	8	0	-4.439306	-0.165169	-0.068473
18	1	0	-3.656601	-0.848627	-0.026185
19	1	0	-5.010897	-0.288727	0.711435
20	6	0	-1.333918	-1.203437	0.003616
21	7	0	-1.061185	0.150233	-0.002160
22	1	0	-2.284048	1.528521	-0.033128
23	8	0	-2.452088	-1.735395	-0.003431

Table S16 The cartesian coordinates for the optimized structure of reactant, transient state and product in a-3H_2O-PCM-N7-2 model at M06-2X/6-31+G(d) level

1. R-a-3H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.867911	0.276705	-0.070904
2	6	0	-1.441849	-1.032872	-0.012983
3	6	0	-3.520254	-0.237343	0.221793
4	6	0	-1.725603	1.437170	0.034146
5	8	0	-1.382935	2.600946	0.004554
6	7	0	-3.066740	1.050666	0.183848
7	7	0	-2.711202	-1.316227	0.127394
8	7	0	-0.404278	-1.898857	-0.134849
9	1	0	-3.727557	1.821103	0.269002
10	7	0	-4.813212	-0.458310	0.356506
11	1	0	-5.136794	-1.418632	0.382356
12	1	0	-5.502662	0.280904	0.420170
13	1	0	-0.464445	-2.912164	-0.134381
14	8	0	2.420470	1.948765	-0.504868
15	1	0	2.569177	2.515034	0.267253
16	1	0	3.212204	1.353291	-0.578589
17	8	0	4.244537	0.000471	-0.781867
18	1	0	3.630576	-0.738831	-0.626610
19	1	0	4.953757	-0.077025	-0.107725
20	6	0	0.794602	-1.201296	-0.268793
21	7	0	0.453087	0.160497	-0.221138
22	1	0	1.179489	0.934208	-0.304359
23	8	0	1.903968	-1.665811	-0.400570
24	8	0	6.271315	-0.201332	1.114734
25	1	0	6.297091	0.524684	1.755772
26	1	0	7.163223	-0.243317	0.738522

2. TS-a-3H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.894297	0.245020	-0.034263
2	6	0	-1.508343	-1.047809	0.017804
3	6	0	-3.577079	-0.213535	0.142409
4	6	0	-1.736609	1.420512	0.012878
5	8	0	-1.378765	2.582242	-0.017632
6	7	0	-3.093239	1.064483	0.102667
7	7	0	-2.793131	-1.307632	0.103460
8	7	0	-0.483453	-1.930789	-0.044601
9	1	0	-3.741052	1.849119	0.141690
10	7	0	-4.884833	-0.397350	0.223483

11	1	0	-5.235408	-1.347373	0.250842
12	1	0	-5.554480	0.360873	0.251812
13	1	0	-0.555205	-2.942547	-0.037525
14	8	0	2.307585	1.758854	-0.303096
15	1	0	2.455271	2.247239	0.525842
16	1	0	3.117880	1.111291	-0.462548
17	8	0	4.022585	-0.013688	-0.744127
18	1	0	3.473379	-0.799921	-0.551085
19	1	0	4.815457	-0.051234	-0.156719
20	6	0	0.725228	-1.231682	-0.139669
21	7	0	0.428047	0.131792	-0.126268
22	1	0	1.392704	1.068610	-0.195850
23	8	0	1.832372	-1.735616	-0.222445
24	8	0	6.263231	-0.102541	0.823482
25	1	0	6.168887	0.274534	1.711604
26	1	0	7.019369	0.356832	0.426354

3. P-a-3H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.770533	0.266867	-0.083557
2	6	0	-1.346405	-1.043410	-0.004679
3	6	0	-3.429356	-0.285530	0.246477
4	6	0	-1.652300	1.411203	0.021446
5	8	0	-1.345204	2.587842	-0.021152
6	7	0	-2.989222	1.007893	0.190202
7	7	0	-2.615853	-1.351755	0.153448
8	7	0	-0.293956	-1.886955	-0.130710
9	1	0	-3.659264	1.769589	0.273163
10	7	0	-4.726505	-0.508050	0.401366
11	1	0	-5.047935	-1.467517	0.441163
12	1	0	-5.414374	0.231093	0.466032
13	1	0	-0.320938	-2.900628	-0.123182
14	8	0	2.583467	2.124828	-0.574951
15	1	0	2.745500	2.705819	0.184811
16	1	0	3.510634	0.964272	-0.636215
17	8	0	3.969671	0.029706	-0.712959
18	1	0	3.229851	-0.660232	-0.590475
19	1	0	4.672064	-0.088496	0.015626
20	6	0	0.866723	-1.125160	-0.281914
21	7	0	0.546784	0.220006	-0.248915
22	1	0	1.727288	1.659726	-0.407295
23	8	0	1.990159	-1.617284	-0.423533
24	8	0	5.766184	-0.344593	1.107026
25	1	0	5.763303	0.299103	1.833100

26	1	0	6.670215	-0.344252	0.754496

Table S17 The cartesian coordinates for the optimized structure of reactant, transient state and product in b-3H_2O-PCM-N7-2 model at M06-2X/6-31+G(d) level

1. R-b-3H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.453072	-0.010503	0.149659
2	6	0	1.215564	-1.207988	-0.037269
3	6	0	3.160227	-0.101919	-0.044083
4	6	0	1.133827	1.261901	0.229253
5	8	0	0.622245	2.357774	0.362819
6	7	0	2.518136	1.092564	0.130655
7	7	0	2.516756	-1.287522	-0.133269
8	7	0	0.312584	-2.220090	-0.089536
9	1	0	3.062747	1.951042	0.189342
10	7	0	4.474479	-0.110469	-0.133710
11	1	0	4.944446	-0.999821	-0.262538
12	1	0	5.041429	0.728047	-0.082452
13	1	0	0.521728	-3.205506	-0.217157
14	8	0	-3.099850	1.151145	0.555815
15	1	0	-3.287181	1.355888	1.485234
16	1	0	-3.780874	0.490322	0.270004
17	8	0	-4.521441	-0.966451	-0.313849
18	1	0	-3.837151	-1.644403	-0.162567
19	1	0	-5.309191	-1.262888	0.165477
20	6	0	-0.980747	-1.724374	0.051894
21	7	0	-0.840846	-0.333331	0.202927
22	1	0	-1.664988	0.300242	0.365305
23	8	0	-2.016700	-2.347948	0.043219
24	8	0	-1.927227	3.416207	-0.732484
25	1	0	-1.045701	3.203169	-0.385686
26	1	0	-2.497086	2.707812	-0.381779

2. TS-b-3H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.438398	-0.037573	0.110783
2	6	0	1.222266	-1.225856	-0.059708
3	6	0	3.164965	-0.130701	0.003232
4	6	0	1.125753	1.228307	0.224873
5	8	0	0.623615	2.334342	0.351772
6	7	0	2.513862	1.061970	0.170065
7	7	0	2.532606	-1.311628	-0.115112

8	7	0	0.315720	-2.227809	-0.151189
9	1	0	3.055631	1.919534	0.252971
10	7	0	4.487213	-0.124005	-0.046770
11	1	0	4.969885	-1.005981	-0.171135
12	1	0	5.041350	0.720244	0.024871
13	1	0	0.510727	-3.214459	-0.283276
14	8	0	-3.090466	1.039543	0.488566
15	1	0	-3.228998	1.329416	1.408514
16	1	0	-3.800683	0.086758	0.225084
17	8	0	-4.283335	-0.958060	-0.117318
18	1	0	-3.521502	-1.608467	-0.120395
19	1	0	-4.951470	-1.273633	0.516641
20	6	0	-0.967466	-1.684618	-0.047983
21	7	0	-0.861675	-0.310434	0.123237
22	1	0	-2.149906	0.626780	0.419888
23	8	0	-2.004627	-2.340049	-0.108312
24	8	0	-1.827812	3.395227	-0.803848
25	1	0	-1.017997	3.057718	-0.381848
26	1	0	-2.519259	2.764149	-0.549913

3. P-b-3H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.393033	-0.022514	0.099284
2	6	0	1.176851	-1.207722	-0.093176
3	6	0	3.120635	-0.118164	-0.012498
4	6	0	1.083640	1.241349	0.232883
5	8	0	0.584242	2.345848	0.375779
6	7	0	2.471870	1.072472	0.174977
7	7	0	2.485690	-1.296812	-0.151254
8	7	0	0.264221	-2.205922	-0.202037
9	1	0	3.015761	1.927322	0.271910
10	7	0	4.442317	-0.114664	-0.062809
11	1	0	4.922342	-0.995869	-0.202714
12	1	0	4.999127	0.726629	0.022482
13	1	0	0.452465	-3.191352	-0.352974
14	8	0	-3.194814	1.161636	0.594360
15	1	0	-3.379248	1.434649	1.508682
16	1	0	-3.916236	-0.047467	0.218927
17	8	0	-4.195710	-1.010882	-0.111897
18	1	0	-3.319490	-1.596074	-0.127429
19	1	0	-4.835798	-1.401307	0.512080
20	6	0	-1.005846	-1.651777	-0.087091
21	7	0	-0.908246	-0.288982	0.109701
22	1	0	-2.272168	0.788972	0.574299

23	8	0	-2.050491	-2.314092	-0.163092
24	8	0	-1.893920	3.387609	-0.785893
25	1	0	-1.065590	3.077349	-0.380116
26	1	0	-2.573809	2.783949	-0.443235

Table S18 The cartesian coordinates for the optimized structure of reactant, transient state and product in $4H_2O$-PCM-N7-2 model at M06-2X/6-31+G(d) level

1. R-$4H_2O$-PCM-N7-2

Center	Atomic	Atomic		Coordinates (Angstroms)	
Number	Number	Type	X	Y	Z
1	6	0	-0.983732	-0.005493	0.146294
2	6	0	-1.606351	-1.283004	-0.030214
3	6	0	-3.666269	-0.412561	0.034543
4	6	0	-1.806226	1.177717	0.256212
5	8	0	-1.422839	2.325659	0.383239
6	7	0	-3.163926	0.848845	0.196761
7	7	0	-2.891914	-1.513635	-0.086678
8	7	0	-0.593907	-2.181530	-0.123142
9	1	0	-3.801836	1.639265	0.272968
10	7	0	-4.972642	-0.577222	-0.009067
11	1	0	-5.337057	-1.515681	-0.129871
12	1	0	-5.633336	0.186467	0.072815
13	1	0	-0.691119	-3.182728	-0.260466
14	8	0	0.958111	3.702346	-0.729800
15	1	0	0.115630	3.377377	-0.372805
16	1	0	1.612014	3.045855	-0.426629
17	8	0	2.423233	1.541893	0.418021
18	1	0	2.645584	1.736043	1.341835
19	1	0	3.150905	0.956674	0.065704
20	8	0	4.028485	-0.316069	-0.593654
21	1	0	3.468840	-1.091551	-0.412902
22	1	0	4.901027	-0.489819	-0.177255
23	6	0	0.637345	-1.537767	-0.019703
24	7	0	0.340068	-0.174009	0.153749
25	1	0	1.093555	0.551198	0.291469
26	8	0	1.738175	-2.034094	-0.071642
27	8	0	6.512468	-0.768509	0.556230
28	1	0	6.799954	-0.081957	1.176538
29	1	0	7.229345	-0.846133	-0.090931

2. TS-$4H_2O$-PCM-N7-2

Center	Atomic	Atomic		Coordinates (Angstroms)	
Number	Number	Type	X	Y	Z
1	6	0	-0.910857	-0.411186	-0.275396

2	6	0	-0.011482	-1.508846	-0.072596
3	6	0	1.810031	-0.237992	-0.306177
4	6	0	-0.359111	0.904207	-0.501945
5	8	0	-0.975620	1.944146	-0.670492
6	7	0	1.039314	0.874712	-0.509277
7	7	0	1.300800	-1.463264	-0.080644
8	7	0	-0.806220	-2.586992	0.123438
9	1	0	1.488243	1.774362	-0.668957
10	7	0	3.125396	-0.107909	-0.331895
11	1	0	3.694588	-0.932504	-0.181418
12	1	0	3.593617	0.776195	-0.486796
13	1	0	-0.502693	-3.538252	0.302659
14	8	0	-3.466748	2.836301	0.564648
15	1	0	-2.633750	2.587789	0.127567
16	1	0	-4.060502	2.089587	0.387657
17	8	0	-4.402477	0.262081	-0.514470
18	1	0	-4.583993	0.452947	-1.452732
19	1	0	-5.052096	-0.537758	-0.191500
20	8	0	-5.651085	-1.692832	0.310120
21	1	0	-4.932287	-2.358015	0.293198
22	1	0	-6.392932	-2.034148	-0.250449
23	6	0	-2.147063	-2.193281	0.050193
24	7	0	-2.174122	-0.820704	-0.205194
25	1	0	-3.350395	-0.172006	-0.413050
26	8	0	-3.111630	-2.925329	0.189605
27	8	0	-7.697201	-2.633140	-1.202494
28	1	0	-8.011600	-2.028607	-1.891852
29	1	0	-8.483304	-2.869793	-0.687188

3. P-4H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.858342	0.020225	0.035786
2	6	0	-1.462360	-1.275613	-0.082112
3	6	0	-3.538660	-0.502105	0.173622
4	6	0	-1.725399	1.162694	0.220807
5	8	0	-1.399200	2.336028	0.311656
6	7	0	-3.070927	0.779473	0.286198
7	7	0	-2.742497	-1.568223	-0.019106
8	7	0	-0.421619	-2.122667	-0.266855
9	1	0	-3.730090	1.545000	0.412335
10	7	0	-4.843506	-0.708467	0.258389
11	1	0	-5.187134	-1.657449	0.172785
12	1	0	-5.515621	0.033316	0.406643
13	1	0	-0.469584	-3.127335	-0.397466

14	8	0	0.839030	3.776124	-0.895043
15	1	0	0.082082	3.324911	-0.481932
16	1	0	1.611838	3.259096	-0.609601
17	8	0	2.547188	1.751375	0.279635
18	1	0	2.736322	2.014195	1.195058
19	1	0	3.503025	0.631747	-0.221430
20	8	0	3.888942	-0.247886	-0.583796
21	1	0	3.133883	-0.931893	-0.524145
22	1	0	4.685901	-0.555959	-0.016276
23	6	0	0.759399	-1.379016	-0.264879
24	7	0	0.464775	-0.041506	-0.065997
25	1	0	1.709468	1.217704	0.297873
26	8	0	1.878560	-1.872613	-0.425962
27	8	0	5.880029	-1.078309	0.802422
28	1	0	6.138800	-0.498559	1.536567
29	1	0	6.680670	-1.208264	0.269352

Table S19 The cartesian coordinates for the optimized structure of reactant, transient state and product in $5H_2O$-PCM-N7-2 model at M06-2X/6-31+G(d) level

1. R-$5H_2O$-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.168989	-0.270323	0.146499
2	6	0	-1.984580	-1.439228	0.004028
3	6	0	-3.877310	-0.248570	-0.059269
4	6	0	-1.793637	1.032835	0.174457
5	8	0	-1.236229	2.111105	0.267300
6	7	0	-3.183459	0.921999	0.077299
7	7	0	-3.287655	-1.463940	-0.096508
8	7	0	-1.129023	-2.492380	-0.005503
9	1	0	-3.689078	1.805973	0.099035
10	7	0	-5.189570	-0.201053	-0.163389
11	1	0	-5.698504	-1.072287	-0.264603
12	1	0	-5.716447	0.664395	-0.157805
13	1	0	-1.382961	-3.471212	-0.099200
14	8	0	1.380920	3.066441	-0.639181
15	1	0	0.474749	2.869953	-0.345167
16	1	0	1.909910	2.308310	-0.321065
17	8	0	2.444409	0.718369	0.491722
18	1	0	2.703916	0.853376	1.416468
19	1	0	3.057234	0.022200	0.121444
20	8	0	3.689097	-1.377695	-0.547722
21	1	0	3.044677	-2.064888	-0.303732
22	1	0	4.560681	-1.662728	-0.195032

23	6	0	0.186442	-2.050462	0.116898
24	7	0	0.108605	-0.649372	0.217724
25	1	0	0.963721	-0.051363	0.357947
26	8	0	1.194253	-2.717179	0.129285
27	8	0	6.172627	-2.142932	0.416681
28	1	0	6.545859	-1.546126	1.082500
29	1	0	6.850263	-2.214391	-0.272238
30	8	0	2.318424	5.505423	0.299204
31	1	0	1.986768	4.647759	-0.045841
32	1	0	2.514694	6.040504	-0.482118

2. TS-5H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.123778	-0.316946	0.076690
2	6	0	-1.970259	-1.457528	-0.118455
3	6	0	-3.849260	-0.276948	0.129383
4	6	0	-1.737738	0.970233	0.305561
5	8	0	-1.172465	2.041105	0.464629
6	7	0	-3.131962	0.871910	0.328220
7	7	0	-3.283029	-1.476127	-0.099163
8	7	0	-1.125493	-2.495158	-0.324789
9	1	0	-3.625770	1.747631	0.488920
10	7	0	-5.168995	-0.208525	0.161438
11	1	0	-5.700271	-1.058309	0.012189
12	1	0	-5.676714	0.652891	0.320378
13	1	0	-1.384437	-3.460155	-0.501597
14	8	0	1.258571	3.030705	-0.726836
15	1	0	0.430729	2.755936	-0.291156
16	1	0	1.887564	2.315599	-0.532586
17	8	0	2.336368	0.520222	0.286624
18	1	0	2.532049	0.675280	1.228705
19	1	0	3.017137	-0.239461	-0.089639
20	8	0	3.652445	-1.332918	-0.638864
21	1	0	2.978677	-2.043529	-0.605221
22	1	0	4.441410	-1.634334	-0.119970
23	6	0	0.194999	-2.035125	-0.267555
24	7	0	0.157087	-0.663750	-0.008198
25	1	0	1.307568	0.039504	0.192167
26	8	0	1.194121	-2.716101	-0.422217
27	8	0	5.865763	-2.114806	0.718951
28	1	0	5.706296	-2.582795	1.552876
29	1	0	6.466200	-1.386558	0.940985
30	8	0	2.168047	5.564882	-0.014436
31	1	0	1.842364	4.676442	-0.273442

32	1	0	2.137360	6.096586	-0.821728

3. P-5H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.988187	-0.269021	0.048325
2	6	0	-1.811345	-1.426404	-0.152756
3	6	0	-3.718790	-0.312023	0.152111
4	6	0	-1.639318	0.994765	0.309322
5	8	0	-1.109584	2.083685	0.474131
6	7	0	-3.030368	0.853616	0.357317
7	7	0	-3.124071	-1.488533	-0.110460
8	7	0	-0.935279	-2.431973	-0.389763
9	1	0	-3.545160	1.711022	0.545699
10	7	0	-5.040760	-0.280861	0.214436
11	1	0	-5.551489	-1.142087	0.060700
12	1	0	-5.568578	0.564435	0.392530
13	1	0	-1.158827	-3.402290	-0.582640
14	8	0	1.311336	3.122510	-0.701101
15	1	0	0.485387	2.807766	-0.288472
16	1	0	1.987093	2.475715	-0.426866
17	8	0	2.648843	0.831417	0.381427
18	1	0	2.874431	1.016178	1.307759
19	1	0	3.411700	-0.415962	-0.163660
20	8	0	3.655537	-1.332989	-0.552917
21	1	0	2.795897	-1.879139	-0.549330
22	1	0	4.367161	-1.791759	0.029308
23	6	0	0.359902	-1.912878	-0.337210
24	7	0	0.303769	-0.558756	-0.054977
25	1	0	1.736734	0.435690	0.376990
26	8	0	1.376202	-2.585623	-0.524358
27	8	0	5.433956	-2.522982	0.849497
28	1	0	5.460628	-2.263389	1.784259
29	1	0	6.335103	-2.398983	0.510744
30	8	0	1.945846	5.760031	-0.106328
31	1	0	1.717512	4.830298	-0.324160
32	1	0	1.900610	6.240396	-0.944457

Table S20 The cartesian coordinates for the optimized structure of reactant, transient state and product in 9H_2O-PCM-N7-2 model at M06-2X/6-31+G(d) level

1. R-9H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.376253	-0.091020	0.085710

2	6	0	-0.250477	-1.376138	0.020698
3	6	0	-2.316076	-0.488655	0.092210
4	6	0	-0.448471	1.093425	0.147455
5	8	0	-0.036061	2.248438	0.175530
6	7	0	-1.795710	0.779631	0.176572
7	7	0	-1.536495	-1.603908	0.018536
8	7	0	0.760782	-2.281641	-0.045977
9	1	0	-2.437322	1.582360	0.342167
10	7	0	-3.616597	-0.632681	0.080093
11	1	0	-4.022763	-1.574854	0.031355
12	1	0	-4.272353	0.168859	0.048921
13	1	0	0.666520	-3.290493	-0.110491
14	8	0	-3.387600	3.012616	0.805896
15	1	0	-3.395370	3.139578	1.767346
16	1	0	-2.862437	3.763076	0.430104
17	8	0	-5.424616	1.501856	-0.195632
18	1	0	-6.249867	1.435742	0.306470
19	1	0	-4.938730	2.271225	0.165119
20	8	0	-1.541684	4.670239	-0.219408
21	1	0	-1.628888	4.952913	-1.141788
22	1	0	-0.881587	3.952933	-0.214932
23	8	0	2.376293	3.437605	-1.065747
24	1	0	1.565776	3.089930	-0.659137
25	1	0	3.076601	2.854441	-0.719931
26	8	0	3.838658	1.410769	0.263396
27	1	0	4.032989	1.657214	1.180966
28	1	0	4.563552	0.788031	-0.025043
29	8	0	5.457426	-0.523130	-0.568970
30	1	0	4.857171	-1.269033	-0.393455
31	1	0	6.278041	-0.691000	-0.055889
32	8	0	-2.567171	-4.465279	-0.155990
33	1	0	-2.178747	-3.575194	-0.101356
34	1	0	-3.524736	-4.289949	-0.136647
35	8	0	-5.075369	-3.132239	-0.032314
36	1	0	-5.628857	-3.256206	0.754464
37	1	0	-5.685629	-3.158602	-0.785817
38	6	0	1.993305	-1.634042	-0.027361
39	7	0	1.701144	-0.261425	0.058263
40	1	0	2.462138	0.460563	0.147429
41	8	0	3.091898	-2.136098	-0.076997
42	8	0	7.789022	-0.950651	0.873951
43	1	0	8.001219	-0.245457	1.503591
44	1	0	8.583679	-1.056551	0.329787

2. TS-9H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.448250	-0.140364	-0.008425
2	6	0	-0.198479	-1.417342	-0.071493
3	6	0	-2.254567	-0.528030	0.083787
4	6	0	-0.372786	1.040193	0.106855
5	8	0	0.040170	2.199027	0.147150
6	7	0	-1.722034	0.735775	0.174651
7	7	0	-1.490049	-1.642658	-0.035332
8	7	0	0.807079	-2.318995	-0.184254
9	1	0	-2.352619	1.535657	0.374995
10	7	0	-3.561031	-0.655628	0.113267
11	1	0	-3.979167	-1.590145	0.056475
12	1	0	-4.204181	0.153176	0.109108
13	1	0	0.717709	-3.326764	-0.259388
14	8	0	-3.286346	2.978805	0.920498
15	1	0	-3.271548	3.071472	1.885588
16	1	0	-2.753804	3.731316	0.560192
17	8	0	-5.354472	1.521127	-0.094161
18	1	0	-6.172372	1.457420	0.419950
19	1	0	-4.846977	2.269633	0.280765
20	8	0	-1.425411	4.631296	-0.090117
21	1	0	-1.528006	4.938194	-1.003046
22	1	0	-0.791826	3.889297	-0.120333
23	8	0	2.257389	3.255425	-1.433164
24	1	0	1.541864	2.901038	-0.877320
25	1	0	3.046710	2.775671	-1.136497
26	8	0	3.739468	1.246089	0.084354
27	1	0	3.861340	1.588360	0.988433
28	1	0	4.543860	0.561472	-0.143023
29	8	0	5.382257	-0.487374	-0.509830
30	1	0	4.808684	-1.278294	-0.439443
31	1	0	6.149008	-0.613324	0.104491
32	8	0	-2.548186	-4.467350	-0.237759
33	1	0	-2.150806	-3.580514	-0.177661
34	1	0	-3.503437	-4.286912	-0.182710
35	8	0	-5.058658	-3.149170	-0.015299
36	1	0	-5.598101	-3.286712	0.778796
37	1	0	-5.682609	-3.159303	-0.757733
38	6	0	2.033269	-1.645242	-0.193273
39	7	0	1.770174	-0.279487	-0.078557
40	1	0	2.793790	0.607726	0.041941
41	8	0	3.129896	-2.169444	-0.287616
42	8	0	7.498174	-0.825942	1.153704

43	1	0	7.558498	-0.181537	1.875152
44	1	0	8.356606	-0.793916	0.704799

3. P-9H_2O-PCM-N7-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.479987	-0.094055	0.003935
2	6	0	-0.128583	-1.388078	-0.098192
3	6	0	-2.213588	-0.585179	0.098095
4	6	0	-0.387242	1.050006	0.158185
5	8	0	-0.024943	2.224833	0.229095
6	7	0	-1.725634	0.693459	0.223544
7	7	0	-1.411638	-1.665770	-0.061589
8	7	0	0.911951	-2.244510	-0.246760
9	1	0	-2.383615	1.463536	0.445507
10	7	0	-3.516202	-0.760551	0.134661
11	1	0	-3.899796	-1.706857	0.047661
12	1	0	-4.187308	0.023631	0.155445
13	1	0	0.868000	-3.251854	-0.357661
14	8	0	-3.372368	2.872570	1.020120
15	1	0	-3.352687	2.957358	1.985742
16	1	0	-2.867908	3.644986	0.661913
17	8	0	-5.388700	1.361059	-0.018585
18	1	0	-6.203110	1.260632	0.495088
19	1	0	-4.903668	2.116051	0.372906
20	8	0	-1.573539	4.591531	0.006988
21	1	0	-1.689962	4.903305	-0.902535
22	1	0	-0.919309	3.867363	-0.032444
23	8	0	2.232351	3.405463	-1.205417
24	1	0	1.497849	2.996238	-0.715222
25	1	0	3.027708	2.986606	-0.834157
26	8	0	3.917529	1.595880	0.277251
27	1	0	4.077695	1.922227	1.177443
28	1	0	4.882255	0.449885	-0.133545
29	8	0	5.272361	-0.446842	-0.446072
30	1	0	4.496836	-1.110111	-0.419618
31	1	0	6.018513	-0.754975	0.185469
32	8	0	-2.353576	-4.512403	-0.338589
33	1	0	-1.995278	-3.610641	-0.252885
34	1	0	-3.315853	-4.375445	-0.281359
35	8	0	-4.920437	-3.308957	-0.081362
36	1	0	-5.457323	-3.494621	0.704575
37	1	0	-5.540867	-3.316357	-0.826730
38	6	0	2.096654	-1.506290	-0.235192
39	7	0	1.805663	-0.163891	-0.071134

40	1	0	3.071473	1.076074	0.299633
41	8	0	3.214970	-2.012389	-0.360391
42	8	0	7.151273	-1.279334	1.090080
43	1	0	7.230723	-0.813223	1.937587
44	1	0	8.027582	-1.232477	0.675597

Table S21 The cartesian coordinates for the optimized structure of reactant, transient state and product in $9H_2O$-PCM-N1 model at M06-2X/6-31+G(d) level

1. R-$9H_2O$-PCM-N1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.932586	-0.531348	-0.197359
2	6	0	-0.307095	-1.792972	0.054189
3	6	0	1.756627	-0.907515	-0.069776
4	6	0	-0.110462	0.637623	-0.408960
5	8	0	-0.530017	1.770278	-0.619684
6	7	0	1.238063	0.333405	-0.348777
7	7	0	0.978759	-2.011225	0.120144
8	7	0	-1.320042	-2.687101	0.207061
9	1	0	1.885234	1.110107	-0.604877
10	7	0	3.055280	-1.037700	0.024220
11	1	0	3.457828	-1.956893	0.243941
12	1	0	3.705158	-0.231812	-0.016463
13	1	0	-1.228870	-3.676689	0.414742
14	8	0	2.845280	2.446196	-1.241726
15	1	0	2.926232	2.392107	-2.206555
16	1	0	2.270764	3.238963	-1.051948
17	8	0	4.813836	1.153364	0.119959
18	1	0	5.674289	1.041402	-0.309628
19	1	0	4.339159	1.847328	-0.382511
20	8	0	0.980114	4.250366	-0.715448
21	1	0	1.020597	4.722631	0.144972
22	1	0	0.292525	3.567603	-0.626023
23	8	0	1.145035	5.639622	1.681292
24	1	0	1.055017	5.103724	2.483497
25	1	0	0.489743	6.347703	1.770956
26	8	0	-2.902226	3.003760	0.674696
27	1	0	-2.095490	2.666171	0.252550
28	1	0	-3.606461	2.426970	0.326883
29	8	0	-4.390919	0.956931	-0.611097
30	1	0	-4.575158	1.145494	-1.544333
31	1	0	-5.127893	0.379221	-0.286628
32	8	0	-6.009053	-0.943159	0.402977
33	1	0	-5.384200	-1.685780	0.307813

34	1	0	-6.815989	-1.203845	-0.065033
35	8	0	2.088102	-4.862689	0.023420
36	1	0	1.657932	-3.991016	0.045991
37	1	0	3.013308	-4.659258	0.248693
38	8	0	4.483669	-3.473686	0.660655
39	1	0	5.281803	-3.563883	0.116882
40	1	0	4.792174	-3.496535	1.579892
41	6	0	-2.550892	-2.054008	0.066231
42	7	0	-2.257746	-0.703775	-0.189960
43	1	0	-3.010740	0.000691	-0.387302
44	8	0	-3.650161	-2.552272	0.148670

2. TS-9H_2O-PCM-N1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.963333	-0.460008	-0.183913
2	6	0	-0.419303	-1.763304	0.019044
3	6	0	1.671700	-0.952366	-0.084224
4	6	0	-0.057173	0.658091	-0.356551
5	8	0	-0.463826	1.819371	-0.531007
6	7	0	1.261600	0.321240	-0.316802
7	7	0	0.850949	-2.047836	0.071217
8	7	0	-1.488481	-2.603525	0.141972
9	1	0	2.145214	1.336876	-0.805795
10	7	0	2.967018	-1.181707	0.007872
11	1	0	3.312706	-2.125202	0.202309
12	1	0	3.648391	-0.411627	0.009946
13	1	0	-1.458386	-3.603027	0.313780
14	8	0	2.751257	2.177591	-1.188992
15	1	0	2.878283	2.056837	-2.147582
16	1	0	2.112167	3.103047	-1.014959
17	8	0	4.832479	0.981242	0.254402
18	1	0	5.744769	0.855738	-0.045090
19	1	0	4.468723	1.710238	-0.276933
20	8	0	1.214706	3.994216	-0.786752
21	1	0	1.397627	4.532899	0.030150
22	1	0	0.429141	3.428927	-0.613995
23	8	0	1.778174	5.482634	1.373926
24	1	0	1.495823	5.106535	2.221754
25	1	0	1.395544	6.372870	1.344160
26	8	0	-2.669019	3.033277	0.941869
27	1	0	-1.902774	2.670494	0.464822
28	1	0	-3.429773	2.570798	0.546046
29	8	0	-4.346063	1.268907	-0.514088
30	1	0	-4.519910	1.532393	-1.430704

31	1	0	-5.112911	0.711837	-0.227087
32	8	0	-6.059569	-0.605093	0.394258
33	1	0	-5.451038	-1.359243	0.276561
34	1	0	-6.859849	-0.819726	-0.107154
35	8	0	1.787586	-4.919411	-0.002165
36	1	0	1.423238	-4.016500	0.014160
37	1	0	2.726782	-4.784086	0.216491
38	8	0	4.291023	-3.723079	0.610910
39	1	0	5.073681	-3.863885	0.055947
40	1	0	4.610842	-3.764729	1.525391
41	6	0	-2.674531	-1.891099	0.028191
42	7	0	-2.299783	-0.554886	-0.178829
43	1	0	-3.003529	0.199124	-0.345190
44	8	0	-3.805253	-2.324840	0.095099

3. P-9H_2O-PCM-N1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.922605	-0.463329	-0.196264
2	6	0	-0.316114	-1.738733	0.004173
3	6	0	1.720773	-0.804430	-0.074146
4	6	0	-0.064702	0.690752	-0.346177
5	8	0	-0.570935	1.835546	-0.510960
6	7	0	1.254490	0.451476	-0.305107
7	7	0	0.966308	-1.951601	0.069755
8	7	0	-1.343626	-2.633129	0.109315
9	1	0	2.331355	1.638206	-1.184481
10	7	0	3.026776	-0.961151	0.028334
11	1	0	3.430424	-1.883088	0.212720
12	1	0	3.659144	-0.149600	0.014790
13	1	0	-1.265573	-3.632012	0.268927
14	8	0	2.834279	2.439380	-1.488396
15	1	0	2.927959	2.370510	-2.451946
16	1	0	1.742585	3.532860	-1.018937
17	8	0	4.782156	1.312102	0.121348
18	1	0	5.696752	1.165029	-0.160156
19	1	0	4.393888	1.939114	-0.518620
20	8	0	0.862658	3.885766	-0.665253
21	1	0	1.001932	4.310055	0.251099
22	1	0	0.252803	3.033175	-0.576983
23	8	0	1.234418	4.984864	1.643160
24	1	0	1.052795	4.398416	2.394706
25	1	0	0.688246	5.774312	1.784459
26	8	0	-2.784077	2.777601	1.147098
27	1	0	-2.002855	2.529228	0.623720

28	1	0	-3.522168	2.339619	0.685896
29	8	0	-4.371475	1.119826	-0.524416
30	1	0	-4.516841	1.450936	-1.423868
31	1	0	-5.123894	0.509765	-0.318804
32	8	0	-6.033656	-0.889583	0.172128
33	1	0	-5.360665	-1.594096	0.108303
34	1	0	-6.751317	-1.144947	-0.426050
35	8	0	2.043931	-4.759214	0.240915
36	1	0	1.641624	-3.874058	0.180522
37	1	0	2.987091	-4.566005	0.387103
38	8	0	4.527714	-3.419723	0.579777
39	1	0	5.246740	-3.556135	-0.056357
40	1	0	4.951738	-3.409217	1.451737
41	6	0	-2.561831	-1.979999	-0.013246
42	7	0	-2.252848	-0.624586	-0.205231
43	1	0	-2.990062	0.096865	-0.369445
44	8	0	-3.670325	-2.470509	0.036617