

## **A DFT study on the reaction mechanism between tetrachloro-*o*-benzoquinone and H<sub>2</sub>O<sub>2</sub> and an alternative reaction approach to produce the radicals**

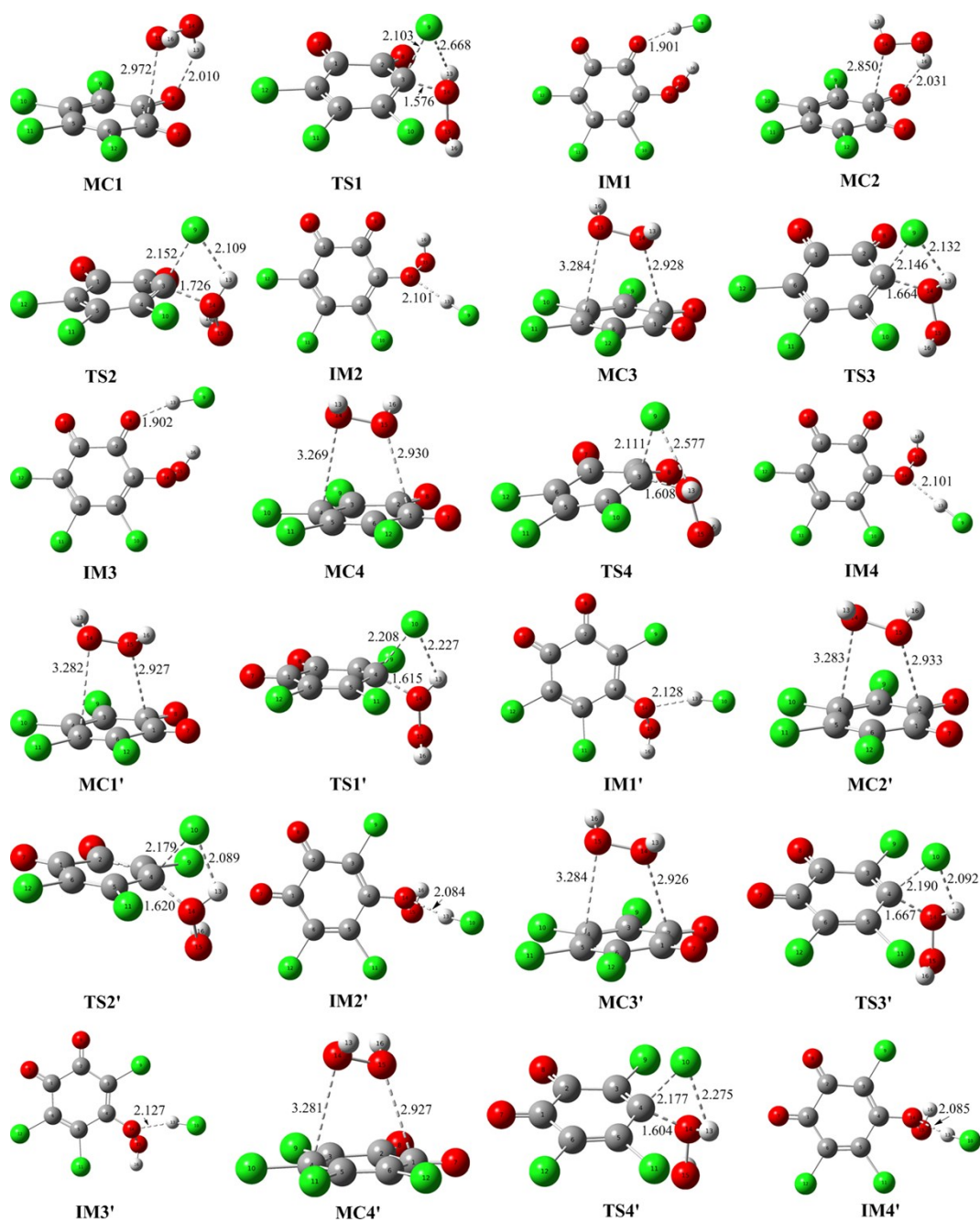
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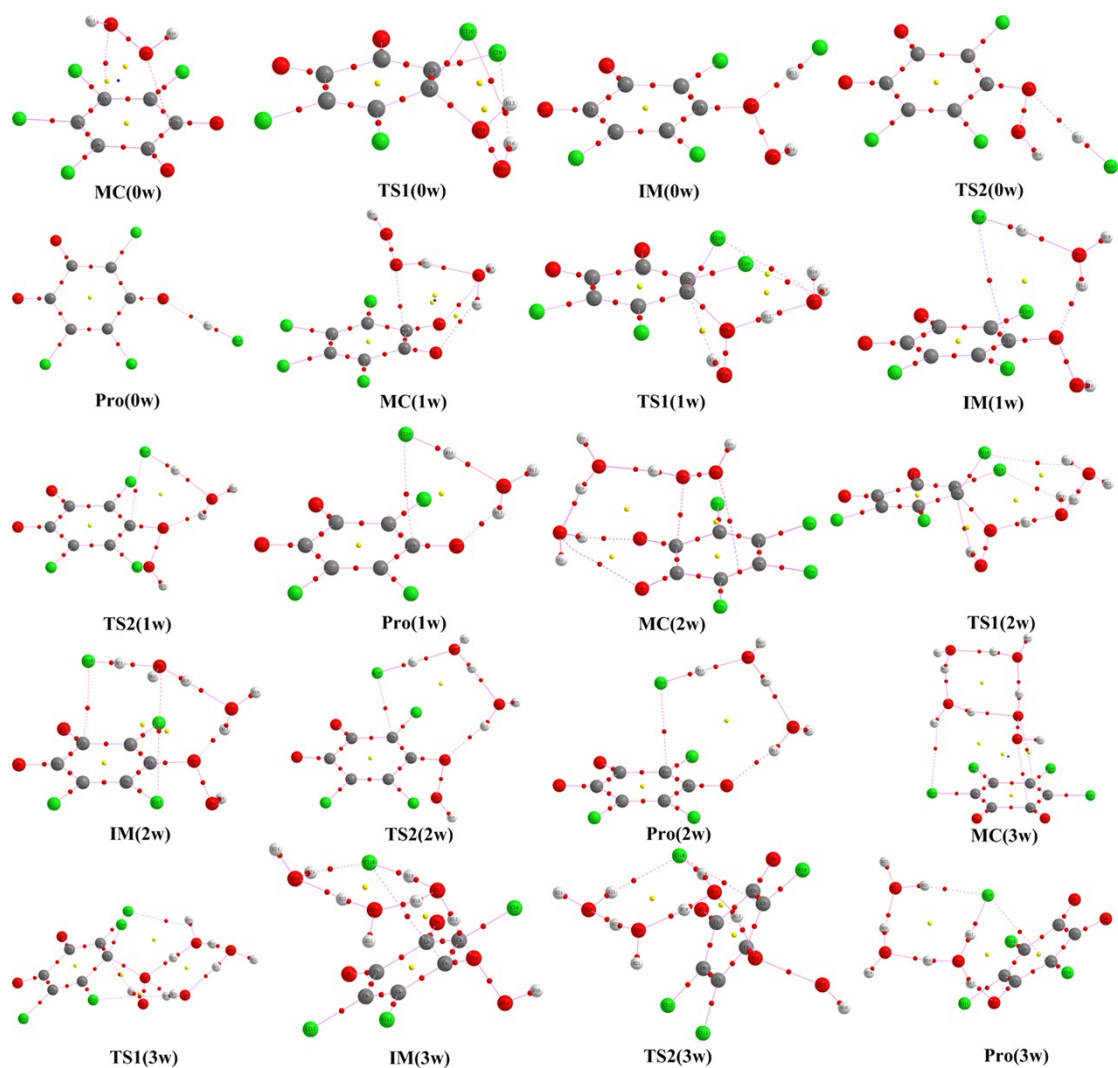
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Supplementary Material



**Figure S1.** Optimized molecular complexes (MC), transition states (TS), and intermediates (IM) in the direct nucleophilic attack process of H<sub>2</sub>O<sub>2</sub> to *o*-TCBQ. The selected interatomic distances are given in Å.



**Figure S2.** Molecular diagrams of the molecular complexes (MC), intermediates (IM), transition states (TS), and products (Pro) in different reaction paths. BCP and RCP are represented by red and small yellow dots, respectively.

**Table S1** The topological parameters at the BCPs for the molecular complexes, intermediates, transition states, and products in the available reaction pathways <sup>a</sup>

Species	BCP	$\rho_{\text{bcp}}$	$\nabla^2\rho_{\text{bcp}}$	$V_{\text{bcp}}$	$G_{\text{bcp}}$	$H_{\text{bcp}}$
MC(0w)	C2 - O15	0.0102	0.0367	-0.0065	0.0078	0.0014
	C4 - O14	0.0057	0.0200	-0.0034	0.0042	0.0008
IM(0w)	C4 - O14	0.2898	-0.4710	-0.7071	0.2947	-0.4124
	H13 - O14	0.0177	0.0625	-0.0111	0.0134	0.0023
	O14 - O15	0.2544	0.1215	-0.3347	0.1825	-0.1522
Pro(0w)	H13 - O14	0.0192	0.0724	-0.0122	0.0151	0.0030
MC(1w)	C1 - O14	0.0130	0.0450	-0.0082	0.0097	0.0015
	O7 - H19	0.0172	0.0642	-0.0117	0.0139	0.0022
	O14 - O15	0.2745	0.0369	-0.3666	0.1879	-0.1787
	O8 - O17	0.0072	0.0257	-0.0050	0.0057	0.0007
	H13 - O17	0.0382	0.1204	-0.0327	0.0314	-0.0013
IM(1w)	C4 - Cl10	0.0037	0.0096	-0.0015	0.0020	0.0004
	O14 - O15	0.2556	0.1189	-0.3369	0.1833	-0.1536
	H13 - O14	0.0179	0.0705	-0.0127	0.0151	0.0025
	O17 - H18	0.0368	0.1121	-0.0284	0.0282	-0.0002
Pro(1w)	C4 - Cl10	0.0047	0.0142	-0.0019	0.0027	0.0008
	H13 - O14	0.0200	0.0821	-0.0146	0.0175	0.0030
	O15 - H16	0.0413	0.1179	-0.0331	0.0313	-0.0018
MC(2w)	C4 - O14	0.4011	-0.1415	-1.3010	0.6328	-0.6682
	O8 - O20	0.0092	0.0345	-0.0065	0.0076	0.0011
	O7 - H22	0.0210	0.0785	-0.0148	0.0172	0.0024
	H13 - O14	0.3308	-2.3234	-0.7074	0.0632	-0.6441
	H18 - O20	0.0390	0.1232	-0.0339	0.0324	-0.0016
	C1 - O14	0.0148	0.0519	-0.0099	0.0114	0.0015
	C3 - O15	0.0061	0.0210	-0.0036	0.0044	0.0008
IM(2w)	H13 - O17	0.0447	0.1380	-0.0416	0.0381	-0.0036
	C2 - Cl10	0.0058	0.0188	-0.0025	0.0036	0.0011
	Cl11 - O20	0.0012	0.0040	-0.0005	0.0007	0.0003
	O14 - O15	0.2543	0.1233	-0.3347	0.1828	-0.1520
	H13 - O14	0.0197	0.0774	-0.0142	0.0168	0.0026
	O17 - H18	0.0351	0.1218	-0.0303	0.0304	0.0001
Pro(2w)	O20 - H21	0.0486	0.1303	-0.0420	0.0373	-0.0047
	C3 - Cl10	0.0071	0.0197	-0.0030	0.0039	0.0010
	H13 - O14	0.0229	0.0958	-0.0174	0.0207	0.0033
	O15 - H16	0.0384	0.1281	-0.0342	0.0331	-0.0011
	O18 - H19	0.0578	0.1338	-0.0524	0.0429	-0.0095
MC(3w)	Cl10 - H19	0.2060	-0.5255	-0.2177	0.0432	-0.1745
	Cl12 - H24	0.0060	0.0195	-0.0028	0.0038	0.0011
	C4 - O14	0.0044	0.0167	-0.0027	0.0034	0.0007
	C2 - O15	0.0101	0.0336	-0.0063	0.0073	0.0010
	O14 - O15	0.2747	0.0403	-0.3674	0.1887	-0.1787

IM(3w)	O14 - H25	0.0263	0.0902	-0.0196	0.0211	0.0015
	H13 - O17	0.0492	0.1433	-0.0471	0.0415	-0.0056
	H18 - O20	0.0405	0.1295	-0.0364	0.0344	-0.0020
	H22 - O23	0.0336	0.1189	-0.0286	0.0292	0.0005
	C4 - C110	0.0057	0.0158	-0.0024	0.0032	0.0008
	H13 - O14	0.0220	0.0866	-0.0167	0.0192	0.0025
	O14 - O15	0.2554	0.1207	-0.3370	0.1836	-0.1534
	H18 - O20	0.0588	0.1506	-0.0600	0.0488	-0.0112
	C110 - H19	0.1091	-0.0614	-0.1047	0.0447	-0.0600
	O17 - H19	0.1871	-0.4719	-0.2818	0.0819	-0.1999
Pro(3w)	H18 - O20	0.0588	0.1506	-0.0600	0.0488	-0.0112
	H22 - O23	0.0425	0.1334	-0.0389	0.0362	-0.0028
	C110 - H25	0.0231	0.0631	-0.0141	0.0149	0.0008
	C3 - C110	0.0136	0.0370	-0.0065	0.0078	0.0014
	H13 - O14	0.0355	0.1222	-0.0309	0.0307	-0.0002
	C110 - H17	0.0639	0.0472	-0.0566	0.0342	-0.0224
	C110 - H23	0.0241	0.0646	-0.0150	0.0156	0.0006
	H20 - O21	0.0457	0.1383	-0.0430	0.0388	-0.0042
H16 - O18	0.0745	0.1514	-0.0806	0.0592	-0.0214	

<sup>a</sup> Atomic numbering refers to Figure 2. The  $\rho_{\text{bcp}}$ ,  $\nabla^2\rho_{\text{bcp}}$ ,  $V_{\text{bcp}}$ ,  $G_{\text{bcp}}$ , and  $H_{\text{bcp}}$  is electron density, the Laplacian of the electron density, potential energy density, kinetic energy density, and energy density at the BCP, respectively. The electron density at the BCP of the O-O bond of  $\text{H}_2\text{O}_2$  is 0.2725.

Cartesian coordinates of all the species mentioned in this study\*

<i>o</i> -TCBQ				H <sub>2</sub> O <sub>2</sub>				HO <sub>2</sub> <sup>-</sup>			
C	-0.78016400	1.73275000	0.00008800	H	1.02761800	-0.66872100	0.41472200	H	-0.89358800	-0.86352400	0.00000000
C	0.78016400	1.73275000	0.00009900	O	0.71725800	0.11966200	-0.05192400	O	0.05584900	-0.70724000	0.00000000
C	1.45930400	0.41679500	0.00004400	O	-0.71748300	-0.11978500	-0.05171000	O	0.05584900	0.81518000	0.00000000
C	0.74117500	-0.73400400	0.00002000	H	-1.02581700	0.66969900	0.41434700				
C	-0.74117500	-0.73400400	0.00002200								
C	-1.45930400	0.41679500	0.00004100								
O	-1.36729000	2.78329400	-0.00010100								
O	1.36729000	2.78329400	-0.00009800								
Cl	3.18320400	0.45258800	0.00002000								
Cl	1.54775800	-2.26197600	-0.00003200								
Cl	-1.54775800	-2.26197600	-0.00002400								
Cl	-3.18320400	0.45258700	0.00001800								
<i>o</i> -TCBQ-PCM				H <sub>2</sub> O <sub>2</sub> -PCM				HO <sub>2</sub> <sup>-</sup> -PCM			
C	-0.00339300	-0.77955600	1.72350200	H	-1.02340500	0.61080200	0.50857900	O	0.05552100	-0.69655200	0.00000000
C	0.00339300	0.77955600	1.72350200	O	-0.71693400	-0.10898900	-0.06357100	H	-0.88833600	-0.89235400	0.00000000
C	0.00087200	1.45829400	0.41693600	O	0.71693100	0.10898500	-0.06357700	O	0.05552100	0.80809700	0.00000000
C	-0.00087200	0.74157200	-0.73461600	H	1.02343100	-0.61077300	0.50859800				
C	0.00087200	-0.74157200	-0.73461600								
C	-0.00087200	-1.45829400	0.41693600								
O	-0.00973700	-1.36053500	2.78226900								
O	0.00973700	1.36053500	2.78226900								
Cl	0.00039100	3.18486700	0.45293300								
Cl	-0.00532200	1.54679000	-2.25840800								
Cl	0.00532200	-1.54679000	-2.25840800								
Cl	-0.00039100	-3.18486700	0.45293300								
MCI				TSI				IMI			
C	0.33220500	-1.42101400	-0.78237500	C	0.94224300	-1.74121000	-0.11005400	C	0.44250600	-1.74739100	-0.09449700
C	1.37530200	-0.26755300	-0.73431900	C	-0.58741800	-1.55549500	-0.27167500	C	-0.84914800	-0.88991000	0.05025900
C	0.88380500	1.08329200	-0.40725800	C	-1.16646800	-0.22690500	0.08099700	C	-0.69855400	0.57306300	0.03812100
C	-0.41238000	1.27710000	-0.05432300	C	-0.37644300	0.88183000	-0.04169600	C	0.54108200	1.13547900	0.04961200
C	-1.38588800	0.16145800	0.00249300	C	1.06342400	0.71947900	-0.02163700	C	1.77867700	0.32367800	0.05998400
C	-1.04097200	-1.10704800	-0.32972300	C	1.69852200	-0.50166200	-0.03058400	C	1.73941900	-1.03044000	-0.02128000
O	0.66887700	-2.50311500	-1.19001100	O	1.39004200	-2.86536500	-0.10924400	O	0.34817200	-2.93742400	-0.24627600
O	2.53523800	-0.51358800	-0.97014900	O	-1.31455900	-2.40469700	-0.73514000	O	-1.90958300	-1.45991800	0.18724800
Cl	2.04659900	2.35402500	-0.46648400	Cl	-2.22164300	-0.61574600	1.85799600	Cl	-4.95484000	-0.55211200	0.29873200
Cl	-0.97193700	2.85754800	0.35514100	Cl	-1.13287200	2.45457800	0.03458600	Cl	0.67930400	2.85103900	0.07551200
Cl	-2.99874200	0.52131100	0.50536000	Cl	2.00497200	2.16711400	0.04713200	Cl	3.28930900	1.15294400	0.15364300
Cl	-2.14855600	-2.42872300	-0.28911600	Cl	3.42375500	-0.66402600	0.04079600	Cl	3.15161000	-2.01510000	-0.04910900
H	3.27612900	-1.53593000	0.59388900	H	-2.75272300	-1.15755700	-0.69976700	H	-3.76045400	-1.07128600	0.37581700
O	3.22600000	-1.72507700	1.54932600	O	-2.56325400	-0.17129100	-0.64760700	O	-1.80096300	1.35127900	0.14633300
O	1.80637500	-1.57151400	1.79423700	O	-2.43591500	0.16160800	-2.08044900	O	-2.55686400	1.23612300	-1.11676900
H	1.55434900	-2.48586000	1.98857800	H	-2.56257500	1.12662100	-2.02146700	H	-3.42105400	0.93880500	-0.77251900

MC2				TS2			IM2				
C	0.70613900	-1.26276400	-0.74321500	C	0.84114100	-1.75631400	0.10444300	C	1.78573500	-1.56078000	0.16459300
C	1.40532100	0.12707500	-0.69911700	C	-0.68330200	-1.47478400	-0.10398000	C	0.26136400	-1.84903100	0.06217200
C	0.57047600	1.29764500	-0.37760100	C	-1.13189700	-0.08901900	0.08208200	C	-0.63366600	-0.70247200	-0.15919300
C	-0.73780300	1.14130000	-0.05010900	C	-0.25236200	0.93275500	-0.08422200	C	-0.15132900	0.56469800	-0.21452500
C	-1.38520600	-0.19088200	-0.00521600	C	1.19107000	0.66247700	-0.08626200	C	1.29101600	0.85462000	-0.04616700
C	-0.71075100	-1.32425600	-0.31881300	C	1.72016900	-0.59184900	0.02298000	C	2.20324200	-0.13642300	0.12557300
O	1.32965500	-2.21611900	-1.13005500	O	1.18847200	-2.89932200	0.26743600	O	2.55695300	-2.47853100	0.27060400
O	2.58816300	0.19626200	-0.94145600	O	-1.41835900	-2.36567300	-0.47357600	O	-0.15117200	-2.98220100	0.16283300
CI	1.35755500	2.83335400	-0.41730700	CI	-2.45295100	-0.05395900	1.78027200	CI	-4.88542600	0.51105500	0.76202500
CI	-1.70176300	2.51908600	0.34156900	CI	-0.84024600	2.56003000	-0.09304000	CI	-1.24444100	1.87461100	-0.44960100
CI	-3.04685700	-0.26717500	0.46394000	CI	2.23903600	2.02884500	-0.19107000	CI	1.78674700	2.50637500	-0.09061200
CI	-1.42776600	-2.88924400	-0.29092700	CI	3.42032300	-0.90576400	0.08764600	CI	3.88954200	0.16081600	0.31013700
H	2.44512600	-0.32003700	2.49981000	H	-3.27296100	-0.17957700	-0.15898700	H	-3.79300500	-0.01811000	0.31663100
O	2.19580400	-0.95700500	1.81556300	O	-2.59035600	0.11302500	-0.81844800	O	-1.97293000	-0.94341800	-0.17800500
O	3.50084400	-1.36127400	1.33090300	O	-2.74740800	-0.60956400	-2.05182300	O	-2.29562100	-1.86853200	-1.27087200
H	3.47024900	-1.03594100	0.41127400	H	-2.51949600	-1.52332100	-1.76470900	H	-2.13217700	-2.72268400	-0.83096600
MC3				TS3			IM3				
C	-0.77894100	-1.61326600	-0.54657800	C	1.12343300	-1.71016500	-0.10621500	C	0.44304800	-1.74742100	-0.09465200
C	0.77835900	-1.61690100	-0.57875400	C	-0.43868700	-1.69397600	-0.26361800	C	-0.84903400	-0.89028900	0.04984700
C	1.46070400	-0.31121400	-0.42597400	C	-1.11368400	-0.38948200	0.01742800	C	-0.69868600	0.57272900	0.03803700
C	0.74882800	0.83518500	-0.30889300	C	-0.39300400	0.76379000	-0.02136900	C	0.54085400	1.13532400	0.04953700
C	-0.73077800	0.84278700	-0.32535100	C	1.06609100	0.74323500	0.00460300	C	1.77867100	0.32388600	0.05992500
C	-1.45067500	-0.29953100	-0.43729600	C	1.79342500	-0.41086800	-0.02698200	C	1.73977100	-1.03026600	-0.02105700
O	-1.37290500	-2.65893600	-0.61986100	O	1.67705500	-2.78105900	-0.09739200	O	0.34897400	-2.93746000	-0.24667300
O	1.36315400	-2.65723800	-0.73386700	O	-1.02175200	-2.67567700	-0.62418900	O	-1.90931100	-1.46052400	0.18635100
CI	3.18615700	-0.35597700	-0.40487900	CI	-2.41556300	-0.72240300	1.69021600	CI	-4.95509200	-0.55215400	0.29885400
CI	1.56325500	2.35134600	-0.12794600	CI	-1.25729100	2.28331500	0.14298800	CI	0.67865400	2.85098000	0.07568900
CI	-1.53247500	2.36771000	-0.18763500	CI	1.87052400	2.27112200	0.09446400	CI	3.28919200	1.15348800	0.15307900
CI	-3.17733500	-0.32827800	-0.43798800	CI	3.52360900	-0.43871900	0.02429400	CI	3.15213100	-2.01470500	-0.04837400
H	-0.65708100	-1.86815900	2.65815000	H	-3.22993800	-0.13645700	-0.19112400	H	-3.76130100	-1.07259000	0.37572800
O	0.06756000	-1.37014600	2.25100900	O	-2.52711300	-0.35409800	-0.85930900	O	-1.80115400	1.35083000	0.14669100
O	-0.16068500	-0.04221300	2.78520900	O	-2.61893800	0.47176500	-2.03362400	O	-2.55704500	1.23604200	-1.11642000
H	0.64187600	0.08243000	3.31261800	H	-2.33125800	1.34744000	-1.69920500	H	-3.42119600	0.93835200	-0.77236000
MC4				TS4			IM4				
C	-0.77940200	-1.61992200	-0.57288900	C	0.96826700	-1.73170100	-0.00351000	C	1.78624600	-1.56069400	0.16459700
C	0.77807100	-1.61549800	-0.54429400	C	-0.56435900	-1.57719200	-0.24736000	C	0.26187300	-1.84906400	0.06230300
C	1.44934000	-0.30139600	-0.43829200	C	-1.15521700	-0.25470600	0.09553400	C	-0.63334000	-0.70253300	-0.15831500
C	0.72906900	0.84080400	-0.32725300	C	-0.37152500	0.85189900	-0.08422400	C	-0.15114500	0.56468600	-0.21355600
C	-0.75050100	0.83284000	-0.30966600	C	1.07443700	0.72144400	-0.07190900	C	1.29127900	0.85468000	-0.04601300
C	-1.46206800	-0.31414000	-0.42277800	C	1.72377000	-0.48526800	-0.00592500	C	2.20366500	-0.13632700	0.12511100
O	-1.36397100	-2.66106200	-0.72338500	O	1.42340200	-2.84655200	0.09846600	O	2.55750900	-2.47836600	0.27091700
O	1.37213800	-2.66120600	-0.61668000	O	-1.20144100	-2.44259700	-0.79362900	O	-0.15050800	-2.98233300	0.16254400
CI	3.17612100	-0.32943200	-0.44045000	CI	-2.23267700	-0.43506800	1.90213000	CI	-4.88729700	0.51076700	0.75942600

CI	1.53036500	2.36610300	-0.19210000	CI	-1.14755800	2.41677200	-0.02930500	CI	-1.24453600	1.87458000	-0.44753600
CI	-1.56518600	2.34935800	-0.13288200	CI	1.98862300	2.18795600	-0.09878000	CI	1.78687800	2.50646200	-0.09062800
CI	-3.18745700	-0.35944300	-0.40024500	CI	3.44893700	-0.62727800	0.07934300	CI	3.89007200	0.16100200	0.30862300
H	-0.61987100	0.10304700	3.31623000	H	-3.03334500	0.60960900	-0.31330900	H	-3.79319500	-0.01778200	0.31756700
O	0.17314100	-0.02495900	2.77533300	O	-2.60010300	-0.22242000	-0.60940900	O	-1.97261000	-0.94363200	-0.17658500
O	-0.06265500	-1.35771000	2.25647500	O	-2.54969600	-0.10345600	-2.07130900	O	-2.29600600	-1.86839200	-1.26943500
H	0.66825900	-1.85164800	2.65735900	H	-2.57071400	-1.05676600	-2.28286700	H	-2.13233700	-2.72269700	-0.82990800
<b>MC1'</b>				<b>TS1'</b>				<b>IM1'</b>			
C	0.77889500	1.61360600	-0.54652400	C	1.33824300	1.69724000	-0.06821300	C	-2.23976600	1.18270300	0.13092900
C	-0.77843300	1.61741400	-0.57720000	C	-0.18276100	2.04602200	-0.02394900	C	-0.91193600	2.00825000	0.03874700
C	-1.46067200	0.31168100	-0.42503900	C	-1.10114000	0.92477000	0.04527700	C	0.35071700	1.24699300	-0.13778300
C	-0.74885900	-0.83493000	-0.30905900	C	-0.64539900	-0.35579300	-0.05055600	C	0.33059200	-0.10718100	-0.17287400
C	0.73074400	-0.84239600	-0.32510300	C	0.78235100	-0.71086300	0.05169200	C	-0.91647900	-0.88435800	-0.01839300
C	1.45061500	0.29991400	-0.43741500	C	1.72509900	0.25394300	0.00049100	C	-2.12914100	-0.29660600	0.10925800
O	1.37285800	2.65927000	-0.62029000	O	2.15455100	2.57653300	-0.13608900	O	-3.28513100	1.76903600	0.22998400
O	-1.36327700	2.65794200	-0.73092300	O	-0.51639800	3.20911900	-0.04279900	O	-0.95996200	3.20809300	0.08925200
CI	-3.18616800	0.35631400	-0.40431800	CI	-2.80723200	1.25077700	0.06222300	CI	1.80128900	2.15173500	-0.31591300
CI	-1.56329700	-2.35130300	-0.13045600	CI	-1.45668000	-1.49028900	-1.76288500	CI	4.71882000	-0.64627800	0.79897400
CI	1.53253400	-2.36719700	-0.18660200	CI	1.18984500	-2.38340300	0.21876900	CI	-0.74429100	-2.60645400	0.04941200
CI	3.17728600	0.32858300	-0.43840600	CI	3.41323700	-0.08662100	0.03711600	CI	-3.59667800	-1.18048300	0.29284800
H	-0.64183700	-0.08554000	3.31084800	H	-2.37164600	-1.49664300	0.26795400	H	3.52090300	-0.48188300	0.34267700
O	0.16093400	0.03968700	2.78390000	O	-1.51745500	-1.44116500	0.76831200	O	1.50656100	-0.78978300	-0.26979400
O	-0.06738700	1.36802700	2.25089000	O	-1.82154500	-1.07318400	2.15439900	O	1.60735600	-1.35346100	-1.63020500
H	0.65704100	1.86565700	2.65887800	H	-1.28583000	-1.74359200	2.61421300	H	1.57919800	-2.30285200	-1.42635700
<b>MC2'</b>				<b>TS2'</b>				<b>IM2'</b>			
C	0.77840200	1.61737300	-0.57766300	C	-1.33719200	1.69650500	0.08149600	C	-2.47167600	0.16345800	0.33669800
C	-0.77892100	1.61372300	-0.54625600	C	0.18722700	2.02843400	0.06857400	C	-1.77661800	1.56744500	0.31496700
C	-1.45075200	0.29999200	-0.43724900	C	1.08155100	0.89452700	-0.01664400	C	-0.33322000	1.60081600	-0.03059400
C	-0.73096000	-0.84238900	-0.32534200	C	0.62357900	-0.39109400	0.04531400	C	0.33504700	0.45103200	-0.28153800
C	0.74864300	-0.83488200	-0.30918500	C	-0.81248100	-0.72169000	-0.08354600	C	-0.31354400	-0.87586400	-0.23639600
C	1.46056100	0.31159200	-0.42554700	C	-1.73830300	0.26024200	-0.02899000	C	-1.63117900	-1.02154400	0.04645700
O	1.36327100	2.65783900	-0.73168800	O	-2.14204500	2.58494100	0.16178300	O	-3.64607800	0.10323700	0.59151000
O	-1.37283900	2.65941300	-0.61954300	O	0.54081300	3.18502700	0.11924400	O	-2.42131300	2.55242300	0.55737000
CI	-3.17740400	0.32889400	-0.43794700	CI	2.80697600	1.20467900	-0.01333500	CI	0.42868800	3.14365600	-0.11674300
CI	-1.53277200	-2.36720500	-0.18726000	CI	1.37491800	-1.56222700	1.72199900	CI	4.30537600	-0.70544700	1.21434800
CI	1.56295100	-2.35131800	-0.13001800	CI	-1.24225200	-2.38022900	-0.27481400	CI	0.70881400	-2.22971000	-0.53353600
CI	3.18606500	0.35609900	-0.40486300	CI	-3.42990500	-0.05368600	-0.09982400	CI	-2.41621200	-2.55407600	0.10953500
H	0.64380500	-0.08508900	3.31122400	H	2.18931200	-1.76405700	-0.19095900	H	3.28618500	-0.35233900	0.50118300
O	-0.15976300	0.03979300	2.78540500	O	1.49651500	-1.43612400	-0.83227100	O	1.68020900	0.50087900	-0.51716800
O	0.06805700	1.36756400	2.25065700	O	2.05123400	-0.98424900	-2.08307500	O	1.91522200	0.30676700	-1.96238800
H	-0.65573300	1.86577700	2.65906200	H	2.54675800	-0.17936900	-1.81013200	H	2.18330100	1.20864100	-2.20461600
<b>MC3'</b>				<b>TS3'</b>				<b>IM3'</b>			
C	0.77884400	1.61370200	-0.54641600	C	1.29367100	1.75179200	-0.03568000	C	-2.23972100	1.18199400	0.13241800
C	-0.77848800	1.61722500	-0.57774600	C	-0.22596500	2.09344800	0.06033100	C	-0.91238900	2.00819600	0.03919500



C	-1.46049500	0.31138100	-0.42562600	C	-1.15480900	0.97139700	0.09549800	C	0.35048000	1.24760300	-0.13886600
C	-0.74852400	-0.83505800	-0.30929600	C	-0.70055100	-0.30207200	-0.05298700	C	0.33091500	-0.10657200	-0.17446500
C	0.73110100	-0.84242900	-0.32525300	C	0.73085400	-0.64898600	-0.01284800	C	-0.91562800	-0.88440500	-0.01924100
C	1.45074900	0.30002700	-0.43725400	C	1.68222800	0.30477900	-0.04190300	C	-2.12844200	-0.29724700	0.10974700
O	1.37270100	2.65941600	-0.61979800	O	2.11115200	2.62999400	-0.08321300	O	-3.28524600	1.76778300	0.23303300
O	-1.36345300	2.65763900	-0.73174400	O	-0.55456800	3.25609800	0.10216400	O	-0.96092400	3.20800000	0.09016200
Cl	-3.18604300	0.35574900	-0.40491700	Cl	-2.84758800	1.32049000	0.15954900	Cl	1.80039000	2.15311000	-0.31819200
Cl	-1.56269600	-2.35154200	-0.13007700	Cl	-1.55379500	-1.43767300	-1.71951100	Cl	4.71665800	-0.64714600	0.80317500
Cl	1.53305900	-2.36712600	-0.18675100	Cl	1.14698400	-2.34138200	0.06703400	Cl	-0.74260800	-2.60643500	0.04761000
Cl	3.17743800	0.32906600	-0.43787900	Cl	3.36736600	-0.04311800	-0.06832300	Cl	-3.59542900	-1.18188500	0.29419200
H	0.65443900	1.86683200	2.65872700	H	-1.75232300	-2.15723800	0.23521900	H	3.51875400	-0.48301000	0.34666600
O	-0.06892900	1.36799200	2.25034000	O	-1.59614100	-1.38296000	0.84588000	O	1.50715500	-0.78856800	-0.27276500
O	0.15971000	0.04048900	2.78533800	O	-1.16277700	-1.77000300	2.16533400	O	1.60736000	-1.35139300	-1.63350100
H	-0.64367800	-0.08472000	3.31134300	H	-0.30199300	-2.20132300	1.99026300	H	1.58000500	-2.30091100	-1.43016700
<b>MC4'</b>				<b>TS4'</b>				<b>IM4'</b>			
C	0.77815600	1.61790200	-0.57710800	C	-1.24376000	1.75614500	0.07723700	C	-2.47204300	0.16209700	0.33613800
C	-0.77916700	1.61420600	-0.54539800	C	0.28629700	2.05488900	0.00299600	C	-1.77764600	1.56645400	0.31553500
C	-1.45093300	0.30041300	-0.43696100	C	1.17044600	0.90685700	-0.05688500	C	-0.33437800	1.60082200	-0.03030600
C	-0.73106700	-0.84197500	-0.32551600	C	0.68078500	-0.36175100	0.07336900	C	0.33470200	0.45154700	-0.28139400
C	0.74852100	-0.83446500	-0.30961900	C	-0.76446900	-0.66457500	-0.02717800	C	-0.31301800	-0.87580100	-0.23607500
C	1.46038600	0.31209500	-0.42540100	C	-1.67750600	0.32528700	0.01862200	C	-1.63062400	-1.02238600	0.04637700
O	1.36297100	2.65840200	-0.73107100	O	-2.03158500	2.65983700	0.15530300	O	-3.64664500	0.10120800	0.58981000
O	-1.37310300	2.65993600	-0.61795300	O	0.65211800	3.20893400	-0.01195500	O	-2.42276400	2.55089400	0.55903200
Cl	-3.17760100	0.32929300	-0.43726400	Cl	2.88457800	1.19374600	-0.12094000	Cl	0.42651900	3.14421100	-0.11640800
Cl	-1.53283000	-2.36688200	-0.18785000	Cl	1.38808500	-1.52755200	1.77020500	Cl	4.30666500	-0.70447200	1.21344000
Cl	1.56294200	-2.35095400	-0.13146400	Cl	-1.22314100	-2.32905500	-0.18175600	Cl	0.71042300	-2.22898500	-0.53270000
Cl	3.18587600	0.35668900	-0.40464900	Cl	-3.37509600	0.03520200	-0.00917000	Cl	-2.41466900	-2.55541600	0.10922400
H	0.64592400	-0.08812800	3.30984500	H	1.39963600	-2.30496500	-0.36728200	H	3.28654200	-0.35031000	0.50220200
O	-0.15756600	0.03619700	2.78377300	O	1.56370300	-1.41058500	-0.75886200	O	1.67971100	0.50224600	-0.51729400
O	0.06805400	1.36535000	2.25154700	O	1.24701100	-1.48214700	-2.18694100	O	1.91436100	0.30848600	-1.96274000
H	-0.65674700	1.86150500	2.66066300	H	1.97437300	-0.93425900	-2.53379800	H	2.18222300	1.21048100	-2.20476300
<b>TS1-PCM</b>				<b>TS2-PCM</b>				<b>TS3-PCM</b>			
C	-0.93810200	-1.73866700	-0.00063300	C	0.87919000	-1.74526200	0.08477400	C	-1.08046100	-1.70778600	0.09060700
C	0.60377000	-1.57281300	0.14514000	C	-0.65292200	-1.51217100	-0.10245800	C	0.48155400	-1.66569100	0.21147700
C	1.17957900	-0.20932900	-0.08346900	C	-1.16187600	-0.13406600	0.10204600	C	1.14193300	-0.34934300	-0.04899000
C	0.36494300	0.88471500	0.03941800	C	-0.30672700	0.91559600	-0.06729000	C	0.39855100	0.79410700	0.00830100
C	-1.06959500	0.70909200	0.02875400	C	1.13062100	0.68310100	-0.07352700	C	-1.05210300	0.73779300	-0.00742700
C	-1.69954500	-0.51679600	-0.00480400	C	1.70453600	-0.56062600	0.02082900	C	-1.76315200	-0.43404100	0.02251900
O	-1.38021600	-2.87163400	-0.05465400	O	1.26434300	-2.88953900	0.21267700	O	-1.61039100	-2.80003800	0.09662500
O	1.30184300	-2.49760600	0.47328700	O	-1.36543600	-2.41539200	-0.47245700	O	1.08398200	-2.65423700	0.52971800
Cl	2.36553500	-0.39047100	-1.77518600	Cl	-2.38927600	-0.16872100	1.79287200	Cl	2.39523900	-0.64733600	-1.71732700
Cl	1.08305200	2.47044600	-0.03743200	Cl	-0.94604300	2.53058400	-0.04468200	Cl	1.23481300	2.32344800	-0.11119400
Cl	-2.02911700	2.14466600	0.03133200	Cl	2.14404400	2.07563800	-0.16295700	Cl	-1.89243400	2.24246700	-0.09028900
Cl	-3.43235500	-0.68326900	-0.05384100	Cl	3.42406200	-0.80810200	0.07673100	Cl	-3.50045400	-0.48481400	-0.02258200

H	3.06490800	-0.91739000	0.59129600	H	-3.30553700	-0.41673400	-0.30477100	H	3.26690400	0.05624200	0.32390800
O	2.54330100	-0.10282300	0.78909200	O	-2.57457500	0.02692200	-0.79817900	O	2.52301400	-0.31889900	0.85350600
O	2.27763800	-0.19261100	2.21246200	O	-2.55065400	-0.44175500	-2.15324100	O	2.46502600	0.28535500	2.15243700
H	2.56731600	0.69424600	2.49790700	H	-2.39820800	-1.40438100	-2.04526100	H	2.25033100	1.22208900	1.96254900
<b>TS4-PCM</b>				<b>TS1'-PCM</b>				<b>TS2'-PCM</b>			
C	-1.04201200	-1.71761900	0.04249300	C	1.21387500	1.73935700	-0.06214400	C	-1.24408900	1.72384300	0.07398600
C	0.51834000	-1.64378000	0.17240400	C	-0.31923700	2.00479100	-0.02329800	C	0.28733000	2.00190700	0.04984600
C	1.14789600	-0.31275900	-0.05741700	C	-1.16398100	0.85403400	0.05311500	C	1.13922900	0.85588200	-0.03525200
C	0.38602500	0.81673400	0.01269300	C	-0.65244800	-0.42024100	-0.03983500	C	0.64119600	-0.42425500	0.04468600
C	-1.06419300	0.72896600	0.00345400	C	0.80292800	-0.69029200	0.05957800	C	-0.81263500	-0.70177400	-0.08099200
C	-1.75162500	-0.45742400	0.00843900	C	1.68382400	0.32983000	0.00927300	C	-1.70075700	0.31248200	-0.02821500
O	-1.54773800	-2.82103300	0.01542900	O	1.97726700	2.67090000	-0.13708400	O	-2.01397500	2.64883300	0.15985600
O	1.13954600	-2.62654800	0.47756300	O	-0.70462300	3.16402900	-0.04957500	O	0.66632100	3.16138200	0.09401000
Cl	2.43035400	-0.53783400	-1.73293300	Cl	-2.89228500	1.08327500	0.07332800	Cl	2.87075500	1.09943200	-0.05546600
Cl	1.18506300	2.35968600	-0.09157100	Cl	-1.31358600	-1.50246600	-1.79400000	Cl	1.27487600	-1.52369300	1.78923000
Cl	-1.93746500	2.21703100	-0.03940900	Cl	1.30607100	-2.33104300	0.20457600	Cl	-1.30240200	-2.34147200	-0.26219700
Cl	-3.48778500	-0.54331900	-0.03362200	Cl	3.39134700	0.08808200	0.03858600	Cl	-3.40595800	0.05985300	-0.08933000
H	3.17447300	0.32397100	0.39408200	H	-2.33308800	-1.59439200	0.38997800	H	2.22878100	-1.79584200	-0.27013400
O	2.53719000	-0.27638200	0.84350000	O	-1.43109000	-1.49761000	0.78101700	O	1.44208800	-1.48312100	-0.78520100
O	2.35583300	0.26129100	2.17169800	O	-1.62318900	-1.11277500	2.17221500	O	1.78970500	-1.13191000	-2.13764900
H	2.54745500	-0.53187000	2.70609200	H	-1.15990100	-1.85026900	2.61496800	H	2.40285500	-0.37417900	-2.02037600
<b>TS3'-PCM</b>				<b>TS4'-PCM</b>							
C	1.16343600	1.78159200	-0.04476200	C	1.13629500	1.78697000	-0.05898500				
C	-0.37144700	2.02288700	0.04345500	C	-0.40249900	2.00881800	0.00782400				
C	-1.20779400	0.86176500	0.09330700	C	-1.22009100	0.83741100	0.07921600				
C	-0.68356600	-0.40254600	-0.05884400	C	-0.67836400	-0.42327700	-0.05018200				
C	0.77953700	-0.64782200	0.01134600	C	0.78980300	-0.64893700	0.02506400				
C	1.65369900	0.37532600	-0.02473000	C	1.64581400	0.38954500	-0.01806800				
O	1.91508600	2.72232700	-0.10984200	O	1.87454500	2.73870500	-0.12793200				
O	-0.76690000	3.17887500	0.06709600	O	-0.81478200	3.15960900	0.00544500				
Cl	-2.93325600	1.09249000	0.13657000	Cl	-2.95072100	1.03971800	0.12412300				
Cl	-1.34345500	-1.46201500	-1.78616600	Cl	-1.31500200	-1.51334800	-1.77900600				
Cl	1.29731100	-2.29405200	0.13241600	Cl	1.33152000	-2.28382200	0.14243100				
Cl	3.36132200	0.14838900	-0.02517600	Cl	3.35847200	0.18902300	-0.01178200				
H	-1.50027400	-2.35642000	0.35525800	H	-1.30728400	-2.38311600	0.44664000				
O	-1.49865600	-1.46406800	0.78378700	O	-1.46463900	-1.47309400	0.79903900				
O	-1.22888800	-1.54213800	2.19655000	O	-1.05376700	-1.49002200	2.19137700				
H	-0.36070400	-1.99257100	2.24541800	H	-1.86188500	-1.13838200	2.61269900				
<b>MC(0w)</b>				<b>TSI(0w)</b>				<b>IM(0w)</b>			
C	0.77840200	1.61737300	-0.57766300	C	-1.33719200	1.69650500	0.08149600	C	-2.47167600	0.16345800	0.33669800
C	-0.77892100	1.61372300	-0.54625600	C	0.18722700	2.02843400	0.06857400	C	-1.77661800	1.56744500	0.31496700
C	-1.45075200	0.29999200	-0.43724900	C	1.08155100	0.89452700	-0.01664400	C	-0.33322000	1.60081600	-0.03059400
C	-0.73096000	-0.84238900	-0.32534200	C	0.62357900	-0.39109400	0.04531400	C	0.33504700	0.45103200	-0.28153800
C	0.74864300	-0.83488200	-0.30918500	C	-0.81248100	-0.72169000	-0.08354600	C	-0.31354400	-0.87586400	-0.23639600

C	1.46056100	0.31159200	-0.42554700	C	-1.73830300	0.26024200	-0.02899000	C	-1.63117900	-1.02154400	0.04645700
O	1.36327100	2.65783900	-0.73168800	O	-2.14204500	2.58494100	0.16178300	O	-3.64607800	0.10323700	0.59151000
O	-1.37283900	2.65941300	-0.61954300	O	0.54081300	3.18502700	0.11924400	O	-2.42131300	2.55242300	0.55737000
Cl	-3.17740400	0.32889400	-0.43794700	Cl	2.80697600	1.20467900	-0.01333500	Cl	0.42868800	3.14365600	-0.11674300
Cl	-1.53277200	-2.36720500	-0.18726000	Cl	1.37491800	-1.56222700	1.72199900	Cl	4.30537600	-0.70544700	1.21434800
Cl	1.56295100	-2.35131800	-0.13001800	Cl	-1.24225200	-2.38022900	-0.27481400	Cl	0.70881400	-2.22971000	-0.53353600
Cl	3.18606500	0.35609900	-0.40486300	Cl	-3.42990500	-0.05368600	-0.09982400	Cl	-2.41621200	-2.55407600	0.10953500
H	0.64380500	-0.08508900	3.31122400	H	2.18931200	-1.76405700	-0.19095900	H	3.28618500	-0.35233900	0.50118300
O	-0.15976300	0.03979300	2.78540500	O	1.49651500	-1.43612400	-0.83227100	O	1.68020900	0.50087900	-0.51716800
O	0.06805700	1.36756400	2.25065700	O	2.05123400	-0.98424900	-2.08307500	O	1.91522200	0.30676700	-1.96238800
H	-0.65573300	1.86577700	2.65906200	H	2.54675800	-0.17936900	-1.81013200	H	2.18330100	1.20864100	-2.20461600
<b>TS2(0w)</b>				<b>Pro(0w)</b>				<b>MC(1w)</b>			
C	2.46487300	-0.05615200	0.23583900	C	2.41235500	-0.17748400	0.00008700	C	0.84162000	1.09451700	0.77822200
C	1.94178600	1.40202500	0.08826700	C	2.01389200	1.32146300	0.00006800	C	1.13407800	-0.42414100	0.94461700
C	0.50912400	1.57778000	-0.27902100	C	0.58930900	1.62486800	-0.00007800	C	0.06529900	-1.36766500	0.56178500
C	-0.36433000	0.46014000	-0.44099500	C	-0.45239300	0.58871600	-0.00014300	C	-1.14397000	-0.90862700	0.15653300
C	0.20599500	-0.91783200	-0.31038800	C	0.00686300	-0.83990800	-0.00012900	C	-1.44272900	0.53857000	0.06782500
C	1.50669700	-1.16101200	-0.01314600	C	1.31677800	-1.19456400	0.00002300	C	-0.51584100	1.48481100	0.36060500
O	3.61730300	-0.22754600	0.53221600	O	3.57467000	-0.48054700	0.00012700	O	1.72165300	1.88951800	1.01651500
O	2.68590000	2.33145600	0.25879800	O	2.88290200	2.16713800	0.00016600	O	2.20043100	-0.76563600	1.39371600
Cl	-0.05917300	3.13234200	-0.53800900	Cl	0.09780100	3.24299900	-0.00007700	Cl	0.44613900	-3.04245600	0.68765000
Cl	-4.58127700	-0.53249000	0.30319400	Cl	-4.80653500	-0.09753100	0.00026700	Cl	-2.39483300	-2.02009400	-0.27613700
Cl	-0.92356200	-2.17864600	-0.57700300	Cl	-1.25879500	-1.99917300	-0.00028100	Cl	-3.02838500	1.00649000	-0.43291900
Cl	2.15147400	-2.75121400	0.11687000	Cl	1.83027600	-2.83283400	0.00011200	Cl	-0.82591700	3.17814500	0.25400500
H	-3.39784300	-0.14410800	-0.05363100	H	-3.55606100	0.24179100	0.00005400	H	2.65531700	0.52861800	-1.45104600
O	-1.58236900	0.64580000	-0.57683200	O	-1.63650500	0.87476300	-0.00021800	O	1.73441600	0.35417100	-1.76704500
O	-1.47152200	1.09614000	1.53272100					O	1.85127700	-0.99549100	-2.28659300
H	-2.16837800	1.15776200	2.20919800					H	1.70319800	-0.84197700	-3.22998900
								O	4.05985300	0.92890600	-0.44486100
								H	4.51297400	0.14486000	-0.11591400
								H	3.60765200	1.29651200	0.33139400
<b>TS1(1w)</b>				<b>IM(1w)</b>				<b>TS2(1w)</b>			
C	1.84014800	1.46837700	-0.05886700	C	-1.82633100	1.30864400	0.12743900	C	2.22753200	0.53802000	-0.49026700
C	0.40865200	2.08157800	-0.02661300	C	-0.48799500	2.11933700	0.06394600	C	1.29486800	1.78239200	-0.46315700
C	-0.67271800	1.14342100	0.09045900	C	0.71830300	1.39175700	-0.40309200	C	-0.08248800	1.58987400	0.06992300
C	-0.50455900	-0.23662700	-0.06038800	C	0.64220900	0.08026400	-0.72375700	C	-0.51928400	0.33168300	0.58152800
C	0.87335800	-0.81292800	0.04134200	C	-0.61430600	-0.69050900	-0.64628900	C	0.42807100	-0.82538800	0.53112400
C	1.96299600	-0.02171100	0.00049600	C	-1.77963300	-0.12241900	-0.25392100	C	1.68362400	-0.74090600	0.02558900
O	2.80364000	2.18493900	-0.11518300	O	-2.82891400	1.87362300	0.47845700	O	3.34120000	0.66243200	-0.92635500
O	0.29332600	3.28960900	-0.08120700	O	-0.48177700	3.28241600	0.36653800	O	1.69058800	2.84478000	-0.86503500
Cl	-2.30445200	1.82288700	0.00683500	Cl	2.18904800	2.28393500	-0.52224800	Cl	-1.14250900	2.88487400	0.00772100
Cl	-1.29832600	-1.04933200	-1.77420700	Cl	0.76558600	-0.69212900	3.01458500	Cl	-2.08717600	-0.99932600	-2.44733300
Cl	0.99145200	-2.52903400	0.18809400	Cl	-0.50727500	-2.36319700	-1.04711600	Cl	-0.20638600	-2.28901900	1.15599200
Cl	3.56876700	-0.65021700	0.04065900	Cl	-3.26125400	-0.99398100	-0.14532000	Cl	2.75124100	-2.08833100	-0.04678200

H	-2.53263400	-1.02968400	0.53153800	H	2.57179500	-1.94997300	0.28104200	H	-3.16448100	-0.97506700	0.77267500
O	-1.44547500	-1.05716000	0.82261900	O	1.79217600	-0.58783400	-1.04898100	O	-1.62291800	0.23905900	1.13952600
O	-1.36603800	-0.64289300	2.20750400	O	1.81235000	-0.84220400	-2.50211600	O	-0.58324200	1.22849400	2.75627800
H	-1.17910700	0.31790000	2.10484400	H	2.42078200	-0.13881400	-2.78358900	H	-0.79941900	1.29395300	3.70210600
O	-3.79561000	-1.09331000	0.18605700	O	2.67024400	-2.30823200	1.17496000	O	-3.71554500	-1.43839400	0.12280900
H	-3.77853200	-1.38113000	-0.74105800	H	1.60203000	-1.42798200	2.31204900	H	-2.86934400	-1.23877300	-1.40752800
H	-4.15220400	-0.19239200	0.18431500	H	3.61549800	-2.33649800	1.35534700	H	-4.59926800	-1.06449400	0.20336800
<b>Pro(1w)</b>				<b>MC(2w)</b>				<b>TS1(2w)</b>			
C	-1.93390700	0.99426900	0.34314300	C	-0.77728900	0.92119700	-0.86672500	C	2.45898700	1.00867300	-0.12610200
C	-0.80351500	2.02592300	0.09329800	C	-0.85597100	-0.62479300	-1.00630500	C	1.24145300	1.97619600	-0.15623300
C	0.41850700	1.52773400	-0.52251000	C	0.32759300	-1.40426500	-0.60252500	C	-0.04430200	1.35958300	-0.05534200
C	0.61013600	0.12374600	-0.90285100	C	1.46295600	-0.77725500	-0.20914800	C	-0.26889300	-0.03285400	-0.11861900
C	-0.53458100	-0.81137600	-0.65554500	C	1.56023200	0.69765200	-0.14721600	C	0.92632300	-0.94175200	-0.03652800
C	-1.69998100	-0.41849800	-0.08384800	C	0.51309000	1.50178700	-0.45602200	C	2.18350700	-0.46332800	-0.06401800
O	-2.95797800	1.35202600	0.85932800	O	-1.75269300	1.58606600	-1.13351700	O	3.58128800	1.43936200	-0.14553000
O	-0.97563800	3.18420900	0.40766900	O	-1.85877700	-1.11845700	-1.46402000	O	1.45752300	3.17025800	-0.25673500
Cl	1.68694000	2.60990400	-0.80928900	Cl	0.17600100	-3.11848300	-0.68734500	Cl	-1.43678400	2.44716100	-0.23135400
Cl	1.82725100	-0.71148900	2.35605100	Cl	2.85222800	-1.69920800	0.24120300	Cl	-1.41168200	-0.63532700	-1.48655700
Cl	-0.25578100	-2.43218500	-1.14968200	Cl	3.06449900	1.38865800	0.35081800	Cl	0.60227700	-2.63563700	0.10878300
Cl	-3.00094000	-1.50171900	0.20177400	Cl	0.58475700	3.22294900	-0.37430200	Cl	3.57041700	-1.48987800	0.00167300
H	3.00343200	-1.54108300	-0.69417000	H	-2.15605100	-0.00105000	1.88081700	H	-2.37096000	-0.10376100	1.05508300
O	1.65078600	-0.27058800	-1.40274900	O	-1.20790800	0.25462000	1.72182700	O	-1.23546300	-0.51048400	1.11335100
O	3.44456000	-1.94758800	0.06822800	O	-0.46408000	-0.71166600	2.50152800	O	-0.70830800	0.00937400	2.34156000
H	2.60207000	-1.29240200	1.45200500	H	-0.13843600	-0.15718500	3.22429100	H	-0.33917100	0.87287800	2.03720400
H	4.38371500	-1.75845300	-0.02828400	O	-3.83834000	-0.21197200	1.84170700	O	-3.50846400	0.29238300	1.01905300
				H	-4.15719500	-0.00441800	0.93231100	H	-4.05507200	-0.31017100	0.44349100
				H	-4.43795500	0.22511100	2.45295600	H	-3.46769000	1.16787300	0.60192700
				O	-4.39066600	0.34847800	-0.77523400	O	-4.79015600	-1.38510400	-0.56955600
				H	-4.30606300	-0.47477400	-1.26989700	H	-4.18673100	-1.82120700	-1.18334800
				H	-3.60548500	0.85325300	-1.04751800	H	-5.44607500	-2.03846700	-0.30371500
<b>IM(2w)</b>				<b>TS2(2w)</b>				<b>Pro(2w)</b>			
C	2.22176500	0.24885400	0.26216700	C	-1.91464800	1.31684100	-0.31258100	C	2.01513000	-1.21749300	0.17188600
C	1.49689500	1.62829500	0.12070800	C	-0.55755400	1.67287000	-0.98038500	C	0.74498900	-1.97082400	-0.30069700
C	0.03909800	1.65503400	0.40935100	C	0.50522600	0.62627200	-0.95870700	C	-0.34140800	-1.15792800	-0.83088600
C	-0.60591600	0.52604300	0.78025400	C	0.24152500	-0.69822000	-0.49281100	C	-0.25786300	0.29875300	-0.97151000
C	0.07481500	-0.77539000	0.90703300	C	-1.12115200	-1.00400800	0.04023800	C	1.02389900	0.95169100	-0.55376900
C	1.39695500	-0.92065200	0.65620200	C	-2.10778300	-0.08050700	0.14473300	C	2.06652000	0.26262700	-0.02834600
O	3.40746300	0.19167200	0.07161400	O	-2.75114000	2.17443000	-0.21048200	O	2.91970000	-1.83395900	0.66661300
O	2.12867700	2.60817200	-0.16847100	O	-0.39901400	2.74301000	-1.50335500	O	0.70597800	-3.17933300	-0.22354400
Cl	-0.76723300	3.17326200	0.28529600	Cl	2.02282500	1.03908800	-1.53722400	Cl	-1.76122300	-1.92982400	-1.33922700
Cl	0.63236000	0.16084900	-2.88230400	Cl	0.93802700	1.55193700	2.14745100	Cl	-1.10821600	-0.17904100	2.39863700
Cl	-0.92144200	-2.11590100	1.34849200	Cl	-1.33126200	-2.62600400	0.55721200	Cl	1.06788000	2.65412000	-0.77752700
Cl	2.21758700	-2.43082400	0.77582300	Cl	-3.65422400	-0.43900500	0.81130100	Cl	3.52479000	1.02432200	0.46488100
H	-3.24401200	-0.49301100	-0.17563000	H	2.94555600	-1.78441800	-0.21029400	H	-3.04291100	1.32465000	-1.21008400

O	-1.96347200	0.56534600	0.96067100	O	1.09155900	-1.59368800	-0.60687900	O	-1.17614500	0.96454700	-1.42199500
O	-2.26302400	0.54925600	2.40715000	O	0.48000800	-1.57105000	-2.68343400	O	-3.93114400	1.46180400	-0.84146000
H	-2.44537600	1.49317100	2.54850700	H	0.52571200	-2.27000600	-3.35721300	H	-3.95627200	1.01531900	0.85023300
O	-3.64003800	-0.95116500	-0.93188200	O	3.78837100	-1.71758400	0.26978800	H	-4.54746600	1.07833700	-1.47273900
H	-2.46830900	-1.43503400	-2.18781400	H	3.72063800	-0.45427900	1.46736600	O	-3.85798000	0.73632200	1.78909400
H	-4.41340700	-0.43725300	-1.18482000	H	4.48411000	-1.77878000	-0.39169000	H	-2.36674500	0.23564600	2.13694300
O	-1.77577100	-1.64363100	-2.84964000	O	3.59447300	0.27186300	2.12156300	H	-4.17240000	1.46723600	2.33092700
H	-0.42913300	-0.64906000	-2.87771900	H	2.15816800	0.96034000	2.13677400				
H	-1.63374400	-2.59468100	-2.81655600	H	3.87685000	-0.07047700	2.97596000				
<b>MC(3w)</b>				<b>TS1(3w)</b>				<b>IM(3w)</b>			
C	0.74731200	-0.83478400	1.85059500	C	2.80972500	0.65284500	0.19319200	C	-2.36077100	-1.27768500	0.56527000
C	1.59540200	0.45580900	1.65349500	C	1.82276400	1.84914800	0.09243200	C	-2.63844400	0.24464500	0.80706300
C	1.99286300	0.80110700	0.26905100	C	0.45399300	1.50715700	-0.12222500	C	-1.73710400	1.20973700	0.12949500
C	1.62131100	0.02691200	-0.77869500	C	-0.02967100	0.20164200	-0.34806800	C	-0.72395900	0.76489300	-0.64626100
C	0.80615300	-1.19484500	-0.59323200	C	0.94717700	-0.93207400	-0.21733800	C	-0.47393300	-0.66736200	-0.89023800
C	0.38497800	-1.59224200	0.63168700	C	2.25583100	-0.73025700	0.01534000	C	-1.23294700	-1.63572000	-0.32686500
O	0.43869700	-1.17781600	2.96182300	O	3.97712900	0.83694600	0.41359900	O	-3.07171000	-2.08792500	1.09954300
O	1.90205600	1.11430300	2.61435800	O	2.27571600	2.97637200	0.19419200	O	-3.55945600	0.57818800	1.50328300
Cl	2.92290200	2.24442600	0.08723600	Cl	-0.65073100	2.87080000	-0.37488500	Cl	-2.03577300	2.88876400	0.37482900
Cl	2.08918400	0.44994900	-2.38631200	Cl	-1.12373600	-0.04003900	-1.81376900	Cl	1.53016100	0.27886900	2.06977300
Cl	0.39723200	-2.11307600	-1.99854200	Cl	0.30569100	-2.54177800	-0.35341900	Cl	0.85935900	-1.04119900	-1.92062100
Cl	-0.57594900	-3.01108000	0.88043500	Cl	3.39152300	-2.02341300	0.15987200	Cl	-0.95593300	-3.31722300	-0.57888100
H	-2.20683600	2.05458600	-0.40425800	H	-2.34795200	0.68291200	0.71377200	H	2.02932200	1.86186900	-0.59966500
O	-1.39231300	1.47709700	-0.35480100	O	-1.23625300	-0.15883100	0.77724700	O	0.15926200	1.67069400	-1.17482600
O	-1.09027100	1.46883400	1.06382300	O	-0.69951400	0.03959300	2.09311500	O	-0.18059100	1.92591400	-2.58763000
H	-0.64298300	2.31984100	1.18852500	H	-0.19619800	0.87522100	1.97502000	H	-0.65010400	2.77182100	-2.49432000
O	-3.64201100	2.89181200	-0.45353200	O	-3.25230700	1.26617800	0.67465000	O	2.69559300	1.85618600	0.10969000
H	-4.37035700	2.23798000	-0.32618100	H	-4.05203800	0.63459900	0.44245500	H	3.51273500	1.33874800	-0.19098200
H	-3.88769200	3.43756100	-1.20630600	H	-3.11036600	1.96397300	0.01618900	H	2.21093000	1.24134100	0.98608900
O	-5.34440200	0.81068400	-0.15629500	O	-4.99249800	-0.45012600	0.18216600	O	4.77817100	0.39461400	-0.34636500
H	-5.81843600	0.63538900	0.66181900	H	-5.75468500	-0.55558000	0.76130700	H	5.03757200	-0.04124900	-1.16317300
H	-4.68681500	0.08981700	-0.25811600	H	-4.45301400	-1.28164500	0.23479500	H	4.70767200	-0.30300400	0.35261500
O	-3.14673100	-0.79402000	-0.56232700	O	-3.19406900	-2.39529700	0.44793000	O	4.21923200	-1.33785700	1.62950300
H	-2.83072000	-1.61141500	-0.16415300	H	-3.01396300	-3.09162500	-0.19207200	H	4.73089200	-1.44015300	2.43809600
H	-2.41177200	-0.15637100	-0.50102900	H	-2.34303700	-1.95196700	0.60272400	H	3.33708500	-1.01554000	1.90826200
<b>TS2(3w)</b>				<b>Pro(3w)</b>				<b>OH-</b>			
C	-2.13555300	-0.34801500	-1.04489200	C	2.36317200	-0.25466300	0.76413400	O	0.00000000	0.00000000	0.10840800
C	-1.31049800	-1.64666200	-0.83750400	C	1.73075900	-1.62573700	0.41190300	H	0.00000000	0.00000000	-0.86726100
C	-0.14792500	-1.56002900	0.09676400	C	0.59929800	-1.60568200	-0.50763500				
C	0.05395000	-0.41394900	0.93382700	C	0.10468100	-0.38321000	-1.13256000				
C	-0.92774400	0.70295500	0.84842300	C	0.88284400	0.87121100	-0.89219400				
C	-1.91565800	0.75684200	-0.07826300	C	1.91166500	0.94076400	-0.01455700				
O	-2.94159300	-0.30259900	-1.93609700	O	3.20980900	-0.18734100	1.61307400				
O	-1.63840900	-2.66908400	-1.37454100	O	2.19907600	-2.63618200	0.88516900				

Cl	0.77127700	-2.95030600	0.33724400	Cl	-0.12448400	-3.08067300	-0.93857500				
Cl	1.33246200	-0.40903900	-1.98937100	Cl	-1.35483100	-0.63779500	1.71715600				
Cl	-0.66079200	1.97886500	1.96929800	Cl	0.33540300	2.24266600	-1.77741700				
Cl	-2.98366500	2.10115800	-0.22685800	Cl	2.76272100	2.39882300	0.30438600				
H	2.56847000	-0.54821000	0.98478500	H	-2.46980200	-0.85906300	-1.21810300				
O	1.01286500	-0.35623800	1.72309700	O	-0.89389900	-0.36336300	-1.84817300				
O	-0.29167600	-1.49023500	3.06721500	O	-3.13744800	-0.95018000	-0.49503800				
H	-0.25227800	-1.57797800	4.03291000	H	-3.71216000	-0.08909600	-0.44829200				
O	3.22371800	-0.41102500	0.24851100	H	-2.54964500	-0.94929200	0.38223200				
H	3.54484100	0.58892400	0.26010100	O	-4.46429100	1.17225600	-0.13929000				
H	2.66957100	-0.51670100	-0.61080900	H	-4.54276600	1.87501900	-0.79181200				
O	3.90329200	1.99216700	0.08147800	H	-4.07114500	1.56668200	0.68419300				
H	3.82613300	2.59974800	0.82428200	O	-3.13453600	1.94233000	2.03424400				
H	3.36982900	2.36155100	-0.67181300	H	-3.50219500	2.05091200	2.91706900				
O	2.28544300	2.62404000	-1.92982300	H	-2.45625300	1.23722900	2.10592000				
H	2.50822500	3.01692600	-2.77973700								
H	1.82885500	1.78116800	-2.12389700								
Br-TS				CH <sub>2</sub> -TS				MC'			
C	2.14240000	1.83193600	0.24318000	C	2.80427000	0.72269300	-0.00173200	C	-0.77148000	-1.63658600	-0.41845900
C	0.74422100	2.51308800	0.23012800	C	1.76706500	1.86562100	-0.16895800	C	0.75756800	-1.64062000	-0.41358400
C	-0.37579600	1.64033100	0.05007600	C	0.43045300	1.45126800	-0.40846800	C	1.41797500	-0.31544800	-0.31154700
C	-0.28321400	0.25978500	-0.17365100	C	-0.02063400	0.12169300	-0.43866000	C	0.72308100	0.84670300	-0.23120200
C	1.07385100	-0.38112500	-0.09052000	C	1.00625100	-0.96128600	-0.26865700	C	-0.73536900	0.84955700	-0.22552700
C	2.19613200	0.34333400	0.07530000	C	2.30932700	-0.69094900	-0.08454200	C	-1.43067700	-0.31085400	-0.30281300
O	3.13422400	2.49325100	0.39660300	O	3.96489300	0.96865300	0.19681500	O	-1.39850200	-2.66054500	-0.61424500
O	0.69992500	3.72387400	0.35102900	O	2.16644600	3.01896200	-0.09766500	O	1.38515500	-2.66722500	-0.60058500
H	-2.50655800	-0.28174200	1.10458400	Cl	-0.73377700	2.75919300	-0.69972100	Cl	3.16231900	-0.34532900	-0.30291900
O	-1.19843000	-0.59491800	1.04777000	Cl	-1.18622200	-0.29057500	-1.83934400	Cl	1.55882200	2.38656600	-0.15156500
O	-0.69251600	-0.20986800	2.33355500	Cl	0.43407100	-2.60322600	-0.28265800	Cl	-1.56383500	2.38866700	-0.12345700
H	-0.63702900	0.76434600	2.24642500	Cl	3.50519600	-1.92424700	0.10815700	Cl	-3.16945500	-0.34062200	-0.28349000
O	-3.58581500	-0.07125200	1.17579900	H	-2.34948200	0.65336500	0.66120200	H	0.91432100	-0.03837900	2.53316900
H	-4.12052500	-0.93291600	0.97860500	O	-1.16876100	-0.21882800	0.75122400	O	-0.02739400	-0.21966100	2.39788200
H	-3.76405900	0.64691900	0.54576000	O	-0.51587900	-0.24592100	2.03780100	O	-0.01855700	-1.48206000	1.75819100
O	-4.63255400	-2.32071500	0.75736500	O	-3.21630800	1.21609000	0.47674700				
H	-5.24476000	-2.70061900	1.39608700	H	-3.96547600	0.55230300	0.13031800				
H	-3.81803500	-2.88381800	0.75141100	H	-2.93700800	1.87129600	-0.19019200				
O	-2.19905800	-3.43172600	0.84047900	O	-4.81883100	-0.53121900	-0.23033400				
H	-1.83066300	-4.02958200	0.18205800	H	-5.66324200	-0.62895000	0.22233500				
H	-1.56466200	-2.69878600	0.91156200	H	-4.28325100	-1.35615800	-0.06897000				
Br	-1.35472900	-0.49143700	-1.71182100	O	-3.08516700	-2.43658100	0.37734500				
Br	-2.06989500	2.55251800	-0.13190200	H	-2.85369700	-3.16640400	-0.20672800				
Br	1.15809500	-2.28014700	-0.18146300	H	-2.25355000	-1.95194400	0.52892800				
Br	3.93208700	-0.40485000	0.15820400	C	-0.70355700	0.99361100	2.73103000				
				H	-0.14056200	0.85152400	3.65547900				

	H	-0.29251800	1.83461500	2.17239200								
	H	-1.75897700	1.15574100	2.97031600								
	<b>TS'</b>				<b>MC'-PCM</b>		<b>TS'-PCM</b>					
C	-0.86314600	-1.71774500	-0.23161500		C	-0.76624800	-1.59923600	-0.44211700	C	-0.87737300	-1.69972900	-0.23983300
C	0.67112100	-1.66426300	-0.43028000		C	0.75824600	-1.60428200	-0.42012400	C	0.65157100	-1.64855500	-0.43578600
C	1.32376100	-0.33150400	-0.24578300		C	1.42708800	-0.29125400	-0.31310800	C	1.32207200	-0.32689100	-0.21006900
C	0.57654500	0.83411800	-0.31934500		C	0.73036000	0.86822100	-0.21772500	C	0.57323800	0.85018300	-0.29147900
C	-0.84341800	0.75390900	-0.23013100		C	-0.73302800	0.86921700	-0.21396900	C	-0.83408300	0.76710700	-0.22436700
C	-1.53592700	-0.43990200	-0.18767700		C	-1.43134800	-0.28685000	-0.32208700	C	-1.53638400	-0.43988700	-0.19403600
O	-1.42060400	-2.80417700	-0.20276400		O	-1.38430600	-2.63495100	-0.65219600	O	-1.42236400	-2.80687400	-0.20293200
O	1.28259000	-2.65840900	-0.74652100		O	1.37608700	-2.64538300	-0.60659100	O	1.25963800	-2.64710700	-0.75435700
Cl	3.04646800	-0.30144700	-0.53069200		Cl	3.16522100	-0.32688200	-0.31717900	Cl	3.03392000	-0.30325600	-0.55031200
Cl	1.37915700	2.40373700	-0.26120500		Cl	1.55822000	2.39678000	-0.11535400	Cl	1.38347100	2.40750700	-0.24658600
Cl	-1.74548600	2.25502000	-0.19497300		Cl	-1.55755000	2.39597000	-0.07453500	Cl	-1.74052800	2.25449900	-0.18609900
Cl	-3.28544400	-0.49319500	-0.06793000		Cl	-3.16885600	-0.32051600	-0.31014700	Cl	-3.28753900	-0.48060600	-0.06760600
H	1.11576000	0.77581000	2.46692500		H	0.85953300	-0.16428900	2.58732900	H	1.08335200	0.69825300	2.57863000
O	0.51315700	0.01982600	2.40447100		O	-0.07102000	-0.37818000	2.42069000	O	0.51758600	-0.07240400	2.41390000
O	1.27495600	-0.94142300	1.71152100		O	-0.01070600	-1.59668400	1.69811000	O	1.33312600	-0.92862100	1.65026900

\*: The optimized structures in aqueous solution are denoted by the PCM symbol.