Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Microsolvation of Dimethylphosphate: A molecular model for the interaction of cell membranes with water

Supporting Information

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Table 1: Energetic analysis for $[(H_2O)_1\,DMP]^-$ clusters. Only those structres above 2.0 kcal/mol of the global minimum are shown. See text for defintion of terms. The structures are depicted in Figure 1.

Label	Conf	ΔE CCSD(T)	ΔE MP2	ΔE B3LYP	BE CCSD(T)	BE MP2	BE B3LYP	Δ BE CCSD(T)	Δ BE MP2	Δ BE B3LYP	$\%x_i$	$\nu_a PO_2^-$ cm^{-1}
W_1S_8	aa	2.7	2.7	1.6	15.7	15.8	14.9	-0.5	-0.4	-1.0	0.65	1233
W_1S_9	ag	3.4	3.3	3.9	13.0	12.0	11.0	2.2	3.3	2.9	0.18	1303
W_1S_{10}	aa	4.5	4.2	3.3	13.9	14.3	13.2	1.4	1.0	0.7	0.03	1257
W_1S_{11}	aa	5.0	5.0	5.2	13.4	13.5	11.5	1.9	1.8	2.5	0.01	1286

Table 2: Energetic analysis for $[(H_2O)_2DMP]^-$ clusters. Only those structres above 2.0 kcal/mol of the global minimum are shown. See text for defintion of terms. The structures are depicted in Figure 2.

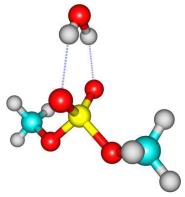
Label	Conf	ΔE CCSD(T)	ΔE MP2	ΔE B3LYP	BE CCSD(T)	BE MP2	BE B3LYP	Δ BE CCSD(T)	Δ BE MP2	Δ BE B3LYP	$\%x_i$	$\nu_a PO_2^-$ cm^{-1}
W_2S_7	ag	2.1	2.0	1.7	27.5	28.7	26.2	2.1	0.9	0.6	1.35	1288
W_2S_8	ag	2.8	2.9	2.5	26.7	27.9	25.4	2.8	1.7	1.4	0.42	1279
W_2S_9	ag	3.1	2.9	1.8	26.5	27.9	26.0	3.1	1.7	0.8	0.29	1274
W_2S_{10}	ag	3.1	3.1	2.4	26.4	27.6	25.5	3.1	2.0	1.3	0.26	1272
W_2S_{11}	aa	3.2	3.2	2.2	26.4	29.6	27.2	3.2	0.1	-0.4	0.25	1236
W_2S_{12}	ag	3.3	3.4	3.5	26.3	26.1	24.4	3.3	3.6	2.4	0.22	1305
W_2S_{13}	ag	3.4	3.4	3.3	26.2	27.4	24.5	3.4	2.2	2.3	0.16	1268
W_2S_{14}	aa	3.6	3.5	1.6	26.0	28.1	27.8	3.6	1.5	-1.0	0.13	1223
W_2S_{15}	gg	3.7	3.5	2.0	25.9	26.1	24.8	3.7	3.5	2.1	0.09	1305
W_2S_{16}	gg	4.0	3.7	2.0	25.6	25.9	24.8	4.0	3.7	2.0	0.06	1289
W_2S_{17}	gg	4.3	4.2	1.5	25.3	25.5	25.3	4.3	4.2	1.5	0.03	1273
W_2S_{18}	aa	4.6	4.9	3.9	25.0	27.9	25.5	4.6	1.7	1.3	0.02	1255
W_2S_{19}	ag	4.9	4.7	2.2	24.7	26.1	25.7	4.9	3.5	1.2	0.01	1247
W_2S_{20}	aa	4.9	4.7	4.1	24.7	29.3	25.3	4.9	0.3	1.5	0.01	1253
W_2S_{21}	ag	5.3	5.0	2.8	24.3	25.7	25.0	5.3	3.9	1.8	≈ 0.00	1277
W_2S_{22}	gg	5.7	1.7	1.7	23.9	27.9	25.1	5.7	1.7	1.7	≈ 0.00	1299
W_2S_{23}	aa	6.5	6.3	3.4	23.1	26.5	26.0	6.5	3.1	0.8	≈ 0.00	1222
W_2S_{24}	ag	8.5	8.2	7.4	21.1	22.6	20.5	8.5	7.0	6.3	≈ 0.00	1310

Table 3: Energetic analysis for $[(H_2O)_3DMP]^-$ clusters. Only those structres above 2.0 kcal/mol of the global minimum are shown. See text for defintion of terms. The structures are depicted in Figure 3.

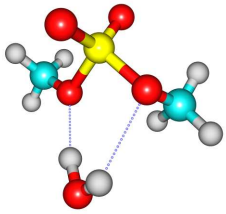
Label	Conf	ΔE CCSD(T)	ΔE MP2	ΔE B3LYP	BE CCSD(T)	BE MP2	BE B3LYP	Δ BE CCSD(T)	Δ BE MP2	Δ BE B3LYP	$\%x_i$	$\nu_a PO_2^-$ cm^{-1}
W_3S_{13}	ag	2.1	1.9	0.3	41.3	41.3	40.3	0.9	0.8	-2.2	1.16	1253
W_3S_{14}	ag	2.1	1.8	0.8	41.3	41.5	39.7	0.9	0.6	-1.7	1.16	1298
W_3S_{15}	gg	2.4	2.0	0.7	40.1	40.1	37.3	2.0	2.0	0.8	0.74	1294
W_3S_{16}	ag	2.5	2.8	0.5	40.9	40.5	40.1	1.3	1.7	-2.0	0.70	1246
W_3S_{17}	aa	2.5	2.4	0.3	42.9	42.9	40.3	-0.7	-0.8	-2.2	0.61	1212
W_3S_{18}	ag	2.5	2.1	1.3	40.9	41.2	39.3	1.3	0.9	-1.2	0.61	1287
W_3S_{19}	ag	2.8	2.7	0.9	40.6	40.6	39.7	1.6	1.5	-1.6	0.37	1244
W_3S_{20}	aa	3.1	3.0	2.1	42.3	42.3	38.5	-0.1	-0.2	-0.4	0.23	1227
W_3S_{21}	ag	3.2	2.9	3.6	40.2	40.3	37.0	2.0	1.8	1.0	0.17	1279
W_3S_{22}	gg	3.3	3.1	2.4	39.5	39.1	35.6	2.7	3.0	2.5	0.16	1289
W_3S_{23}	ag	3.3	3.0	2.2	40.1	40.2	38.4	2.1	1.9	-0.3	0.16	1268
W_3S_{24}	ag	3.4	3.1	2.3	40.0	40.2	38.3	2.2	1.9	-0.2	0.14	1268
W_3S_{25}	gg	3.4	3.2	1.3	39.1	39.0	36.6	3.1	3.1	1.4	0.12	1280
W_3S_{26}	ag	3.6	3.3	3.6	39.8	39.9	37.0	2.4	2.2	1.0	0.10	1291
W_3S_{27}	aa	3.7	3.5	1.7	41.7	41.8	38.8	0.5	0.3	-0.8	0.08	1215
W_3S_{28}	gg	4.0	3.7	1.6	38.6	38.4	36.4	3.6	3.7	1.7	0.05	1282
W_3S_{29}	gg	4.1	3.6	1.5	39.0	38.6	36.4	3.2	3.6	1.6	0.04	1290
W_3S_{30}	aa	4.1	3.9	3.4	41.3	41.4	37.2	0.9	0.8	0.9	0.04	1251
W_3S_{31}	ag	4.4	4.0	1.5	39.0	39.2	39.1	3.2	2.9	-1.1	0.03	1241
W_3S_{32}	gg	4.5	3.9	1.9	38.4	38.3	36.1	3.6	3.9	2.0	0.02	1308
W_3S_{33}	aa	4.6	4.2	1.9	40.8	41.1	38.7	1.4	1.0	-0.6	0.02	1216
W_3S_{34}	aa	4.6	4.3	3.1	40.8	41.0	37.5	1.4	1.1	0.6	0.02	1247
W_3S_{35}	aa	4.7	4.4	1.9	40.6	40.9	38.7	1.5	1.2	-0.6	0.01	1213
W_3S_{36}	gg	4.8	4.4	2.6	38.3	37.7	35.3	3.9	4.4	2.7	0.01	1297
W_3S_{37}	gg	4.8	4.5	2.5	37.7	37.7	35.5	4.5	4.4	2.6	0.01	1300

Table 4: Energetic analysis for $[(H_2O)_3DMP]^-$ clusters Part II. The structures are depicted in Figure 3.

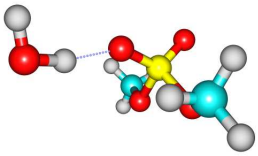
Label	Conf	ΔE CCSD(T)	ΔE MP2	ΔE B3LYP	BE CCSD(T)	BE MP2	BE B3LYP	Δ BE CCSD(T)	Δ BE MP2	Δ BE B3LYP	$\%x_i$	$\nu_a PO_2^-$ cm^{-1}
W_3S_{38}	ag	4.9	4.3	3.2	38.5	38.9	37.4	3.7	3.2	0.7	0.01	1289
W_3S_{39}	ag	5.0	4.5	2.3	38.4	38.8	38.3	3.8	3.3	-0.2	0.01	1288
W_3S_{40}	ag	5.5	4.9	3.1	37.9	38.4	37.5	4.3	3.8	0.6	≈ 0.00	1274
W_3S_{41}	ag	5.6	5.1	3.3	37.8	38.2	37.3	4.4	3.9	0.7	≈ 0.00	1280
W_3S_{42}	aa	5.6	5.0	1.3	39.8	40.3	39.3	2.4	1.8	-1.2	≈ 0.00	1221
W_3S_{43}	ag	6.5	6.1	4.4	36.8	37.1	36.2	5.3	5.0	1.8	≈ 0.00	1281
W_3S_{44}	ag	6.6	6.3	6.0	36.8	37.0	34.6	5.4	5.1	3.5	≈ 0.00	1283
W_3S_{45}	gg	7.1	6.8	3.2	35.4	35.4	34.8	6.8	6.8	3.3	≈ 0.00	1286
W_3S_{46}	gg	7.2	2.6	2.2	35.4	39.5	35.8	6.8	2.6	2.3	≈ 0.00	1298
W_3S_{47}	gg	7.2	6.8	3.2	37.7	35.4	34.8	4.5	6.8	3.3	≈ 0.00	1265
W_3S_{48}	ag	7.3	6.9	5.6	36.1	36.4	35.0	6.1	5.8	3.1	≈ 0.00	1281
W_3S_{49}	ag	7.5	7.1	3.4	35.9	36.2	37.2	6.3	5.9	0.9	≈ 0.00	1236
W_3S_{50}	ag	8.1	7.6	4.6	35.2	35.7	36.0	6.9	6.4	2.0	≈ 0.00	1277
W_3S_{51}	ag	10.2	9.4	5.7	33.2	33.8	34.9	9.0	8.3	3.1	≈ 0.00	1278
W_3S_{52}	aa	10.2	9.6	4.8	35.1	35.7	35.8	7.0	6.4	2.3	≈ 0.00	1217



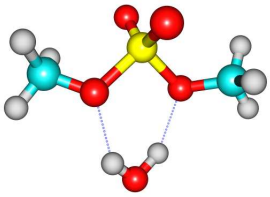
$W_1S_8(aa)$; $\Delta E = 2.7$



$W_1S_9(ag)$; $\Delta E = 3.4$



$W_1S_{10}(aa)$; $\Delta E = 4.5$



$W_1S_{11}(aa)$; $\Delta E = 5.0$

Figure 1: Local minima on the $[(H_2O)_1\,DMP]^-$ MP2/6–311++G** PES. CCSD(T)//MP2 relative energies in kcal/mol with respect to W_1S_1, only structures above 2.0 kcal/mol of the global minimum are included. Explicit $(CH_3O)_2\,PO_2^- \leftrightarrow H_2O$ interactions are represented by dotted lines.

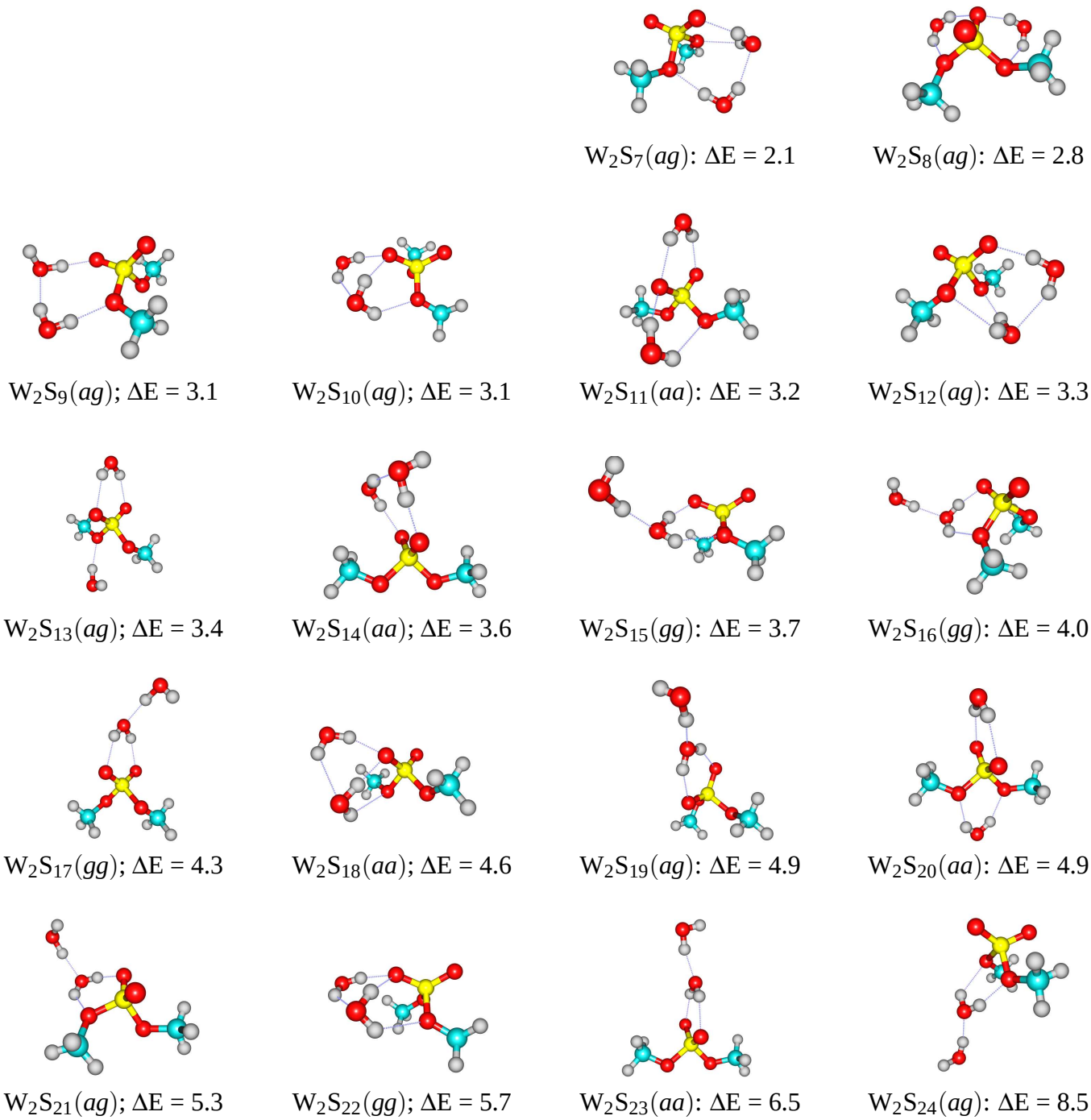
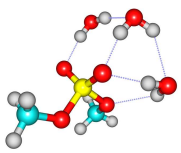
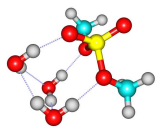


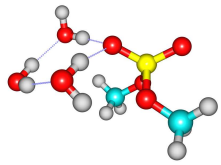
Figure 2: Local minima on the $[(H_2O)_2DMP]^-$ MP2/6–311++G** PES. CCSD(T)//MP2 relative energies in kcal/mol with respect to W_2S_1, only structures above 2.0 kcal/mol of the global minimum are included. Explicit $(CH_3O)_2PO_2^- \leftrightarrow H_2O$ interactions are represented by dotted lines.



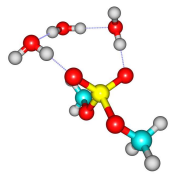
$W_3S_{13}(ag)$; ΔE = 2.1



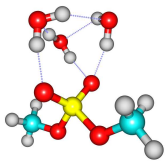
$W_3S_{14}(ag)$; ΔE = 2.1



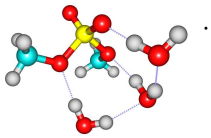
$W_3S_{15}(gg)$: ΔE = 2.4



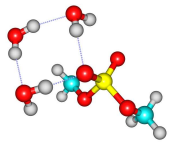
$W_3S_{16}(gg)$: ΔE = 2.5



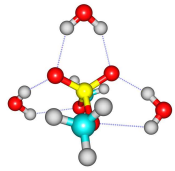
$W_3S_{17}(aa)$; ΔE = 2.5



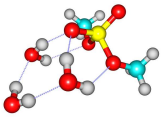
$W_3S_{18}(ag)$; ΔE = 2.5



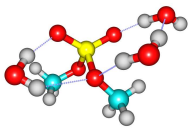
$W_3S_{19}(ag)$: ΔE = 2.8



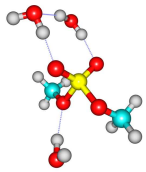
$W_3S_{20}(aa)$: ΔE = 3.1



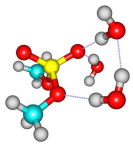
$W_3S_{21}(ag)$; ΔE = 3.2



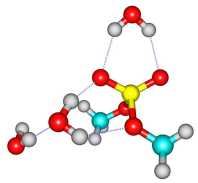
$W_3S_{22}(gg)$; ΔE = 3.3



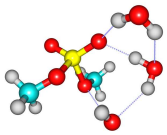
$W_3S_{23}(ag)$: ΔE = 3.3



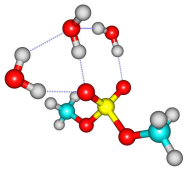
$W_3S_{24}(ag)$: ΔE = 3.4



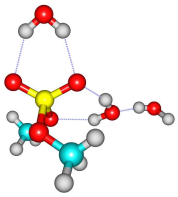
$W_3S_{25}(gg)$; ΔE = 3.4



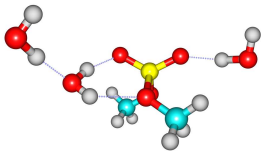
$W_3S_{26}(ag)$; ΔE = 3.6



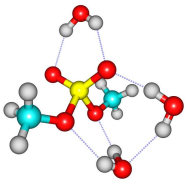
$W_3S_{27}(aa)$: ΔE = 3.7



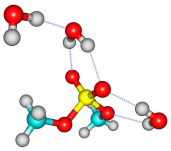
$W_3S_{28}(gg)$: ΔE = 4.0



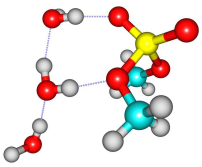
$W_3S_{29}(gg)$; ΔE = 4.1



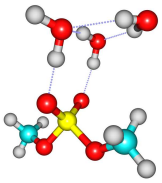
$W_3S_{30}(aa)$; ΔE = 4.1



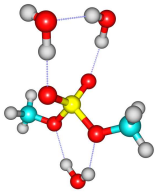
$W_3S_{31}(ag)$: ΔE = 4.4



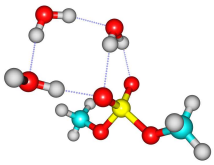
$W_3S_{32}(gg)$: ΔE = 4.5



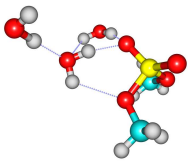
$W_3S_{33}(aa)$; ΔE = 4.6



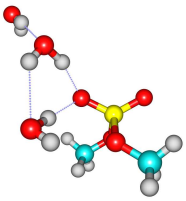
$W_3S_{34}(aa)$; ΔE = 4.6



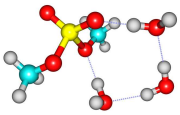
$W_3S_{35}(aa)$: ΔE = 4.7



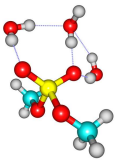
$W_3S_{36}(gg)$: ΔE = 4.8



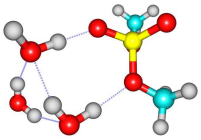
$W_3S_{37}(gg)$; ΔE = 4.8



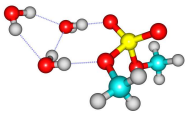
$W_3S_{38}(ag)$; ΔE = 4.9



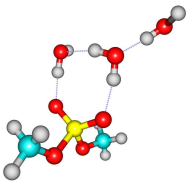
$W_3S_{39}(ag)$: ΔE = 5.0



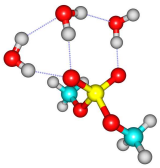
$W_3S_{40}(ag)$: ΔE = 5.5



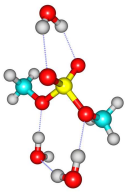
$W_3S_{41}(ga)$; ΔE = 5.6



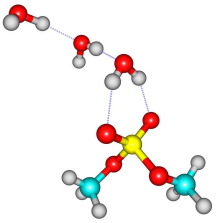
$W_3S_{42}(aa)$; ΔE = 5.6



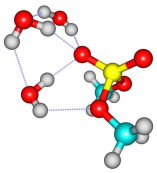
$W_3S_{43}(ag)$: ΔE = 6.5



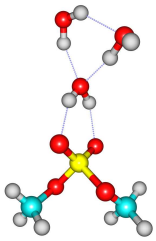
$W_3S_{44}(ag)$: ΔE = 6.6



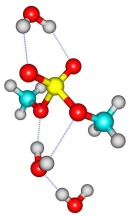
$W_3S_{45}(gg)$; ΔE = 7.1



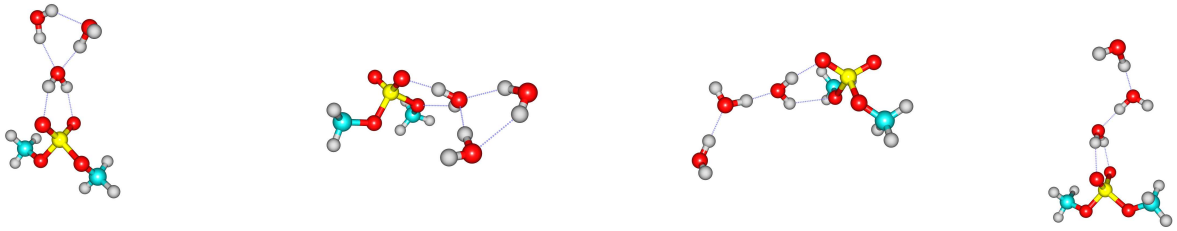
$W_3S_{46}(gg)$; ΔE = 7.2



$W_3S_{47}(gg)$: ΔE = 7.2



$W_3S_{48}(ag)$: ΔE = 7.3



$W_3S_{49}(ag)$; $\Delta E = 7.5$ $W_3S_{50}(ag)$; $\Delta E = 8.1$ $W_3S_{51}(ag)$: $\Delta E = 10.2$ $W_3S_{52}(aa)$: $\Delta E = 10.2$

Figure 3: Local minima on the $[(H_2O)_3DMP]^-$ MP2/6–311++G** PES. CCSD(T)//MP2 relative energies in kcal/mol with respect to W_3S_1, only structures above 2.0 kcal/mol of the global minimum are included. Explicit $(CH_3O)_2PO_2^- \leftrightarrow H_2O$ interactions are represented by dotted lines.