Supporting Information

Balanced Polarizable Drude Force Field Parameters for Molecular Anions: Phosphates, Sulfates, Sulfamates and Oxides

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Table S1. Water-model compound minimum interaction energies (E_{min}, kcal/mol) and distances (R_{min}, Å) for dimethylphosphate (DMP) from the QM and the optimized, original nucleic acid and original lipid Drude models.

Molecule	Atom	Orientation	E_{QM}	E_{OPT}	$E_{Nucleic\ Acid}$	E_{Lipid}	$E_{(QM-OPT)}$	$E_{(QM-NA)}$	$E_{(QM-LIPID)}$	R_{QM}	R_{OPT}	R_{NA}	R_{LIPID}	$R_{(QM-OPT)}$	$R_{(QM-NA)}$	$R_{(QM-LIPID)}$
dmp	O1	0	-7.86	-6.78	-6.41	-6.03	-1.08	-1.45	-1.83	1.90	1.90	2.00	2.00	0.00	-0.10	-0.10
		180	-8.30	-7.68	-7.00	-6.84	-0.61	-1.30	-1.46	1.95	1.90	1.95	1.95	-0.05	0.00	0.00
		90	-8.23	-8.03	-7.28	-7.22	-0.20	-0.94	-1.01	2.00	2.00	2.00	2.00	0.00	0.00	0.00
		270	-8.23	-8.12	-7.20	-7.35	-0.12	-1.03	-0.88	2.05	2.00	2.00	2.00	-0.05	0.05	0.05
	O2	0	-8.29	-7.32	-6.72	-6.52	-0.97	-1.57	-1.77	1.95	1.95	1.95	2.00	0.00	0.00	-0.05
		180	-7.88	-7.05	-6.60	-6.25	-0.84	-1.28	-1.64	1.95	1.90	1.95	1.95	-0.05	0.00	0.00
		90	-8.23	-8.28	-7.33	-7.49	0.05	-0.90	-0.74	2.05	1.95	2.00	2.00	-0.10	0.05	0.05
		270	-8.23	-8.17	-7.39	-7.34	-0.06	-0.84	-0.89	2.00	1.95	2.00	2.00	-0.05	0.00	0.00
	O3	0	-13.58	-13.72	-13.93	-12.39	0.13	0.34	-1.20	1.80	1.80	1.70	1.90	0.00	0.10	-0.10
		180	-12.28	-12.47	-12.26	-11.35	0.19	-0.03	-0.93	1.80	1.80	1.70	1.95	0.00	0.10	-0.15
		90	-12.75	-12.95	-13.00	-11.94	0.20	0.25	-0.81	1.75	1.80	1.70	1.95	0.05	0.05	-0.20
		270	-12.70	-12.96	-13.05	-11.87	0.25	0.35	-0.84	1.75	1.80	1.70	1.95	0.05	0.05	-0.20
	O4	0	-8.45	-7.97	-7.51	-7.91	-0.48	-0.94	-0.54	2.05	2.30	2.35	2.35	0.25	-0.30	-0.30
		180	-12.04	-11.86	-11.89	-10.83	-0.18	-0.15	-1.21	1.80	1.80	1.70	1.95	0.00	0.10	-0.15
		90	-12.62	-12.63	-12.93	-11.58	0.01	0.31	-1.04	1.75	1.80	1.70	1.95	0.05	0.05	-0.20
		270	-12.86	-12.79	-12.97	-11.78	-0.07	0.10	-1.08	1.75	1.80	1.70	1.95	0.05	0.05	-0.20

Table S2. Water-model compound minimum interaction energies (E_{min}, kcal/mol) and distances (R_{min}, Å) for methylphosphates and organic phospates from the QM and the optimized and original Drude models. The average absolute difference for all model compounds not previously available in the Drude FF (MP_0, HP_1, MSO4, NMSM, NESM, MEO, ETO) is 0.06 kcal/mol.

Molecule	Atom	Orientation	E_{QM}	E_{ORIG}	E_{OPT}	$E_{(QM-ORIG)}$	$E_{(QM-OPT)}$	R_{QM}	R_{ORIG}	R_{OPT}	$R_{(QM-ORIG)}$	$R_{(QM-OPT)}$
mp_1	O1	0	-8.10	-9.10	-7.29	1.00	-0.81	1.95	1.8	1.85	0.15	0.1
		180	-8.00	-8.58	-6.91	0.59	-1.09	1.9	1.8	1.85	0.1	0.05
		90	-8.51	-9.15	-7.70	0.64	-0.81	1.95	1.8	1.9	0.15	0.05
		270	-8.48	-9.24	-7.67	0.76	-0.81	1.95	1.8	1.9	0.15	0.05
	O2	0	-6.71	-7.29	-6.16	0.58	-0.55	2.15	1.9	2	0.25	0.15
		180	-3.96	-3.85	-3.37	-0.11	-0.59	3.2	3.3	3.3	-0.1	-0.1
		90	-6.86	-8.20	-6.97	1.34	0.11	2.05	1.9	1.95	0.15	0.1
		270	-7.69	-8.71	-7.98	1.02	0.29	2.05	1.85	1.9	0.2	0.15
	O3	0	-5.50	-3.84	-4.33	-1.66	-1.16	2	3	2.9	-1	-0.9
		180	-11.52	-11.72	-10.77	0.19	-0.75	1.8	1.7	1.85	0.1	-0.05
		90	-12.95	-13.63	-12.82	0.68	-0.13	1.75	1.65	1.8	0.1	-0.05
		270	-12.13	-12.78	-12.11	0.65	-0.02	1.75	1.7	1.8	0.05	-0.05
	O4	0	-11.55	-12.40	-12.15	0.84	0.60	1.85	1.7	1.85	0.15	0
		180	-11.78	-13.08	-12.16	1.31	0.38	1.8	1.7	1.8	0.1	0
		90	-12.53	-13.90	-13.26	1.37	0.73	1.8	1.7	1.8	0.1	0
		270	-12.59	-13.88	-13.33	1.29	0.75	1.8	1.7	1.8	0.1	0
mp_2	O1	0	-15.04	-16.49	-14.15	1.45	-0.89	1.8	1.7	1.75	0.1	0.05
		180	-15.04	-16.49	-14.15	1.45	-0.89	1.8	1.7	1.75	0.1	0.05
		90	-17.20	-19.08	-17.06	1.88	-0.14	1.75	1.65	1.65	0.1	0.1
		270	-17.20	-19.08	-17.06	1.88	-0.14	1.75	1.65	1.65	0.1	0.1
	O2	0	-19.67	-20.01	-19.00	0.35	-0.67	1.7	1.65	1.75	0.05	-0.05
		180	-20.11	-19.96	-18.88	-0.15	-1.23	1.7	1.6	1.75	0.1	-0.05
		90	-22.26	-22.58	-22.04	0.32	-0.22	1.65	1.6	1.7	0.05	-0.05
		270	-22.33	-22.74	-22.17	0.41	-0.16	1.65	1.6	1.7	0.05	-0.05
	O3	0	-6.71	-5.42	-5.47	-1.29	-1.24	3.5	3.5	3.5	0	0
		180	-19.60	-18.91	-17.79	-0.69	-1.81	1.7	1.65	1.75	0.05	-0.05
		90	-21.84	-22.89	-21.84	1.05	0.01	1.65	1.55	1.7	0.1	-0.05
		270	-21.84	-22.89	-21.84	1.05	0.01	1.65	1.55	1.7	0.1	-0.05
	O4	0	-19.67	-20.01	-19.00	0.35	-0.67	1.7	1.65	1.75	0.05	-0.05
		180	-20.11	-19.96	-18.88	-0.15	-1.23	1.7	1.6	1.75	0.1	-0.05
		90	-22.33	-22.74	-22.17	0.41	-0.16	1.65	1.6	1.7	0.05	-0.05
		270	-22.26	-22.58	-22.04	0.32	-0.22	1.65	1.6	1.7	0.05	-0.05
hp_1	O1	0	-7.02		-6.37		-0.65	2.1		2		0.1
		180	-6.93		-6.95		0.03	2.15		1.95		0.2
		90	-6.82		-6.63		-0.19	2.1		1.95		0.15

		270	-7.61		-7.68		0.07	2.05		1.95	0.1
	O2	0	-6.94		-6.96		0.02	2.15		1.95	0.2
		180	-7.02		-6.37		-0.65	2.1		2	0.1
		90	-7.61		-7.68		0.06	2.05		1.95	0.1
		270	-6.82		-6.63		-0.19	2.1		1.95	0.15
	O3	0	-11.62		-12.49		0.87	1.85		1.8	0.05
		180	-11.77		-12.41		0.65	1.8		1.8	0
		90	-12.62		-13.73		1.11	1.8		1.8	0
		270	-12.63		-13.68		1.05	1.8		1.8	0
	O4	0	-12.58		-12.12		-0.45	1.75		1.8	-0.05
		180	-11.52		-10.63		-0.89	1.8		1.85	-0.05
		90	-12.19		-12.18		-0.01	1.75		1.8	-0.05
		270	-12.94		-12.75		-0.19	1.75		1.8	-0.05
hp_2	O1	0	-12.22	-12.77	-10.76	0.55	-1.46	2.4	2.15	2.45	0.25	-0.05
		180	-12.22	-12.77	-10.76	0.55	-1.46	2.4	2.15	2.45	0.25	-0.05
		90	-13.48	-15.88	-13.60	2.40	0.11	2	1.8	1.85	0.2	0.15
		270	-13.48	-15.88	-13.60	2.40	0.11	2	1.8	1.85	0.2	0.15
	O2	0	-20.40	-20.45	-19.67	0.05	-0.73	1.7	1.6	1.75	0.1	-0.05
		180	-20.66	-20.23	-19.41	-0.42	-1.24	1.7	1.6	1.75	0.1	-0.05
		90	-22.99	-23.17	-22.79	0.17	-0.20	1.65	1.6	1.7	0.05	-0.05
		270	-22.93	-23.11	-22.74	0.18	-0.19	1.65	1.6	1.7	0.05	-0.05
	O3	0	-20.40	-20.45	-19.67	0.05	-0.73	1.7	1.6	1.75	0.1	-0.05
		180	-20.66	-20.23	-19.41	-0.42	-1.24	1.7	1.6	1.75	0.1	-0.05
		90	-22.93	-23.11	-22.75	0.18	-0.19	1.65	1.6	1.7	0.05	-0.05
		270	-22.99	-23.17	-22.79	0.17	-0.20	1.65	1.6	1.7	0.05	-0.05
	O4	0	-18.74	-20.30	-19.27	1.56	0.53	1.65	1.6	1.7	0.05	-0.05
		180	-20.52	-18.87	-18.22	-1.65	-2.31	1.7	1.65	1.75	0.05	-0.05
		90	-22.86	-22.52	-22.18	-0.34	-0.68	1.65	1.6	1.7	0.05	-0.05
		270	-22.86	-22.52	-22.18	-0.34	-0.68	1.65	1.6	1.7	0.05	-0.05

Table S3. Water-model compound minimum interaction energies (E_{min}, kcal/mol) and distances (R_{min}, Å) for for molecular ions other than phosphate from the QM and the optimized Drude models.

Molecule	Atom	Orientation	E_{QM}	E_{OPT}	$E_{(QM-OPT)}$	R_{QM}	R_{OPT}	$R_{(QM-OPT)}$
mso4	O1	0	-7.90	-7.45	-0.45	1.95	1.9	0.05
		180	-7.90	-7.45	-0.45	1.95	1.9	0.05
		90	-8.06	-8.20	0.14	2	1.95	0.05
		270	-8.06	-8.20	0.14	2	1.95	0.05
	O2	0	-9.38	-9.41	0.03	1.9	1.9	0
		180	-9.46	-9.73	0.28	1.9	1.9	0
		90	-10.01	-10.82	0.82	1.85	1.85	0
		270	-10.01	-10.82	0.82	1.85	1.85	0
	O3	0	-9.67	-9.22	-0.45	1.85	1.9	-0.05
		180	-9.47	-8.91	-0.56	1.9	1.9	0
		90	-10.05	-10.22	0.17	1.85	1.85	0
		270	-10.28	-10.60	0.32	1.85	1.85	0
	O4	0	-9.32	-8.39	-0.93	1.9	1.95	-0.05
		180	-9.70	-9.69	-0.01	1.85	1.9	-0.05
		90	-10.28	-10.60	0.32	1.85	1.85	0
		270	-10.05	-10.22	0.17	1.85	1.85	0
so4	O1	0	-19.14	-17.33	-1.81	1.7	1.8	-0.1
		180	-19.24	-17.47	-1.77	1.7	1.75	-0.05
		90	-20.78	-20.77	-0.01	1.65	1.7	-0.05
		270	-20.76	-20.77	0.01	1.7	1.7	0
	O2	0	-19.12	-17.32	-1.80	1.7	1.8	-0.1
		180	-19.22	-17.46	-1.76	1.7	1.75	-0.05
		90	-20.77	-20.76	0.00	1.65	1.7	-0.05
		270	-20.77	-20.76	0.00	1.65	1.7	-0.05
	O3	0	-19.13	-17.32	-1.81	1.7	1.8	-0.1
		180	-19.22	-17.46	-1.76	1.7	1.75	-0.05
		90	-20.77	-20.77	-0.01	1.65	1.7	-0.05
		270	-20.77	-20.77	-0.01	1.65	1.7	-0.05
	O4	0	-19.13	-17.32	-1.80	1.7	1.8	-0.1
		180	-19.23	-17.46	-1.77	1.7	1.75	-0.05
		90	-20.77	-20.77	-0.01	1.65	1.7	-0.05
		270	-20.77	-20.77	-0.01	1.65	1.7	-0.05
msna	O1	0	-10.26	-9.66	-0.61	1.85	1.9	-0.05
		180	-10.85	-10.02	-0.83	1.85	1.85	0
		90	-11.12	-11.50	0.39	1.8	1.85	-0.05
		270	-10.57	-11.01	0.45	1.85	1.85	0

	O2	0	-10.26	-9.66	-0.60	1.85	1.9	-0.05
		180	-10.85	-10.02	-0.82	1.85	1.85	0
		90	-10.56	-11.01	0.45	1.85	1.85	0
		270	-11.11	-11.50	0.39	1.8	1.85	-0.05
	O3	0	-10.26	-9.66	-0.60	1.85	1.9	-0.05
		180	-10.85	-10.02	-0.83	1.85	1.85	0
		90	-11.12	-11.50	0.39	1.8	1.85	-0.05
		270	-10.56	-11.01	0.45	1.85	1.85	0
nmsm	N	0	-8.86	-8.16	-0.71	2	1.9	0.1
		180	-10.94	-10.37	-0.57	1.95	1.85	0.1
	O2	0	-11.53	-10.77	-0.76	1.9	1.95	-0.05
		180	-10.33	-11.38	1.04	1.9	1.9	0
		90	-10.34	-11.12	0.78	1.85	1.85	0
		270	-10.64	-11.39	0.75	1.85	1.85	0
	O3	0	-12.33	-11.89	-0.45	1.85	1.9	-0.05
		180	-10.21	-10.67	0.47	1.85	1.85	0
		90	-10.37	-11.28	0.91	1.85	1.85	0
		270	-10.58	-11.33	0.75	1.85	1.85	0
	O4	0	-12.71	-11.72	-0.98	1.85	1.9	-0.05
		180	-10.20	-10.21	0.01	1.85	1.85	0
		90	-10.97	-11.10	0.12	1.8	1.85	-0.05
		270	-10.36	-10.56	0.20	1.85	1.85	0
nesm	N	0	-8.51	-8.63	0.12	2	1.9	0.1
		180	-11.00	-10.75	-0.25	1.95	1.85	0.1
	O2	0	-10.08	-9.13	-0.95	1.85	1.9	-0.05
		180	-10.19	-9.30	-0.88	1.85	1.9	-0.05
		90	-10.29	-10.63	0.34	1.85	1.85	0
		270	-10.88	-11.19	0.31	1.8	1.85	-0.05
	O3	0	-9.92	-9.90	-0.02	1.85	1.9	-0.05
		180	-9.80	-9.94	0.14	1.85	1.9	-0.05
		90	-10.13	-11.20	1.07	1.85	1.85	0
		270	-10.53	-11.45	0.92	1.85	1.85	0
	O4	0	-9.88	-9.62	-0.26	1.85	1.9	-0.05
		180	-9.75	-9.76	0.01	1.9	1.9	0
		90	-10.54	-11.19	0.64	1.85	1.85	0
		270	-10.10	-10.96	0.86	1.85	1.85	0
eto	O	0	-19.12	-19.20	0.08	2.3	2.25	0.05
		180	-19.37	-17.78	-1.59	2.3	2.25	0.05
		90	-18.03	-17.84	-0.19	1.7	1.6	0.1
		270	-18.07	-17.88	-0.19	1.7	1.6	0.1
meo	O	0	-20.77	-20.58	-0.19	1.65	1.6	0.05
		180	-20.44	-19.69	-0.75	1.65	1.6	0.05
		90	-18.91	-19.37	0.47	1.65	1.6	0.05
		270	-18.91	-19.37	0.47	1.65	1.6	0.05

Table S4. Dipole moments from the QM and Drude models for dimethylphosphate (DMP). For the Drude model the optimized values and those from the original nucleic acid and lipid parameter sets are shown.

		Dipole Moment				Error		
		QM	**Opt**	**Nucleic Acid**	**Lipid**	**QM-Opt**	**QM-NA**	**QM-Lipid**
DMP	XX	3.55	3.36	2.96	3.64	0.19	0.59	-0.09
	YY	-4.35	-4.12	-3.52	-4.47	-0.23	-0.83	0.12
	ZZ	0.37	0.14	0.31	0.39	0.23	0.07	-0.02
	Total	5.63	5.32	4.61	5.78	0.31	1.01	-0.15
AVG_Difference						**0.12**	**0.21**	**-0.04**
ABS_AVG_Difference						**0.03**	**0.30**	**0.04**
STDEV_Difference						**0.24**	**0.79**	**0.12**
RMSD_Difference						**0.28**	**0.83**	**0.12**

Table S5. Dipole moments of QM and Drude force field for molecular ions excluding DMP. For molecules in which the electrostatic parameters were not updated only the optimized, final values are shown.

		Dipole Moment			Error	
		QM	**Opt**	**Orig**	**QM-Opt**	**QM-Orig**
MP_0	XX	-1.18	-1.28		0.10	
	YY	1.62	1.21		0.41	
	ZZ	1.66	1.83		-0.17	
	Total	2.60	2.54		0.06	
MP_1	XX	-0.46	-0.46	-1.02	0.00	0.56
	YY	3.61	3.50	2.66	0.11	0.94
	ZZ	2.74	2.88	3.13	-0.13	-0.39
	Total	4.55	4.55	4.23	0.00	0.32
MP_2	XX	-0.39	-0.87	-1.20	0.48	0.81
	YY	3.88	3.74	3.90	0.14	-0.02
	ZZ	0.00	0.00	0.00	0.00	0.00
	Total	3.90	3.84	4.07	0.06	-0.18
HP_1	XX	-3.24	-3.22		-0.03	
	YY	0.22	-0.16		0.37	
	ZZ	1.01	1.36		-0.36	
	Total	3.40	3.50		-0.09	
HP_2	XX	-1.54	-1.43	-1.09	-0.11	-0.45
	YY	-1.19	-1.35	-0.66	0.16	-0.53
	ZZ	0.84	0.77	0.61	0.08	0.23

	Total	2.12	2.11	1.42	0.01	0.70
SO4	XX	0.00	0.00		0.00	
	YY	0.00	0.00		0.00	
	ZZ	0.00	0.00		0.00	
	Total	0.00	0.00		0.00	
MSO4	XX	-2.90	-2.52		-0.38	
	YY	-1.92	-2.54		0.61	
	ZZ	-0.34	-0.22		-0.12	
	Total	3.50	3.58		-0.08	
NMSM	XX	0.93	1.05		-0.12	
	YY	3.44	2.96		0.48	
	ZZ	-2.04	-2.49		0.45	
	Total	4.10	4.01		0.10	
NESM	XX	-11.50	-11.46		-0.04	
	YY	0.35	-0.04		0.39	
	ZZ	0.58	1.12		-0.54	
	Total	11.52	11.52		0.01	
MEO	XX	-4.60	-4.50		-0.10	
	YY	-0.43	-0.42		-0.01	
	ZZ	-0.36	-0.35		-0.01	
	Total	4.64	4.53		0.10	
ETO	XX	-4.44	-4.70		0.26	
	YY	2.19	2.04		0.16	
	ZZ	-3.45	-3.17		-0.27	
	Total	6.03	6.02		0.01	
AVG_Difference					**0.05**	**0.17**
ABS_AVG_Difference					**0.16**	**0.43**
STDEV_Difference					**0.23**	**0.30**
RMSD_Difference					**0.24**	**0.54**

Table S6. Calculated hydration free energies with individual contributions and corrections for each species. All values are in kcal/mol.

RESID	$\Delta G_{aqueous}$	ΔG_{gas}	Interfacial Correction ($zf\Phi$)	Entropic Correction	Long Range Correction	ΔG_{Drude} (opt)
DMP	-204.26 ± 0.06	-109.55 ± 0.01	12.45	1.90	-0.68	-81.04 ± 0.08
MP_0	-156.15 ± 0.17	-144.32 ± 0.10	0.00	1.90	-0.51	-10.47 ± 0.22
MP_1	-208.26 ± 0.27	-116.47 ± 0.03	12.45	1.90	-0.56	-77.99 ± 0.29
MP_2	-369.87 ± 0.25	-78.38 ± 0.02	24.90	1.90	-0.59	-265.27 ± 0.25
HP_1	-215.58 ± 0.17	-121.44 ± 0.01	12.45	1.90	-0.39	-80.25 ± 0.18
HP_2	-388.02 ± 0.16	-86.16 ± 0.01	24.90	1.90	-0.48	-275.54 ± 0.16
SO4	-289.49 ± 0.31	0.00 ± 0.00	24.90	1.90	-0.50	-263.19 ± 0.31
MSO4	-146.80 ± 0.00	-65.21 ± 0.03	12.45	1.90	-0.59	-67.83 ± 0.03
MSNA	-109.26 ± 0.10	-24.91 ± 0.00	12.45	1.90	-0.51	-70.51 ± 0.10
NMSM	-237.62 ± 0.09	-151.04 ± 0.01	12.45	1.90	-0.61	-72.83 ± 0.09
NESM	-231.51 ± 0.29	-145.08 ± 0.04	12.45	1.90	-0.59	-72.77 ± 0.26
MEO	-114.76 ± 0.11	0.00 ± 0.00	12.45	1.90	-0.23	-100.64 ± 0.11
ETO	-117.24 ± 0.32	-7.60 ± 0.00	12.45	1.90	-0.33	-95.62 ± 0.32

Table S7. Molecular polarizability tensors from the QM and Drude models.

Molecule	QM				Drude_opt			
	XX	YY	ZZ	total	XX	YY	ZZ	total
DMP	10.61	9.67	8.86	29.13	7.63	7.24	6.59	21.46
MP_0	6.78	7.94	6.70	21.42	5.57	7.25	5.82	18.63
MP_1	7.34	8.56	7.49	23.39	6.24	6.59	5.54	18.37
MP_2	7.94	10.37	8.44	26.74	5.95	5.68	6.06	17.69
HP_1	6.21	5.85	5.72	17.78	5.64	5.19	4.98	15.81
HP_2	6.83	6.36	6.60	19.79	5.08	4.73	5.12	14.93
SO4	5.81	5.81	5.81	17.44	4.10	4.10	4.10	12.29
MSO4	7.74	7.65	6.95	22.34	5.32	5.90	5.67	16.88
MSNA	7.56	6.92	6.92	21.41	4.98	5.03	5.04	15.05
NMSM	7.56	8.31	8.51	24.38	6.56	6.47	6.93	19.97
NESM	11.78	9.32	9.10	30.20	8.89	7.63	7.61	24.13
MEO	5.03	4.13	4.12	13.28	2.81	2.33	2.33	7.47
ETO	6.99	6.27	6.83	20.09	6.96	3.84	4.03	14.82

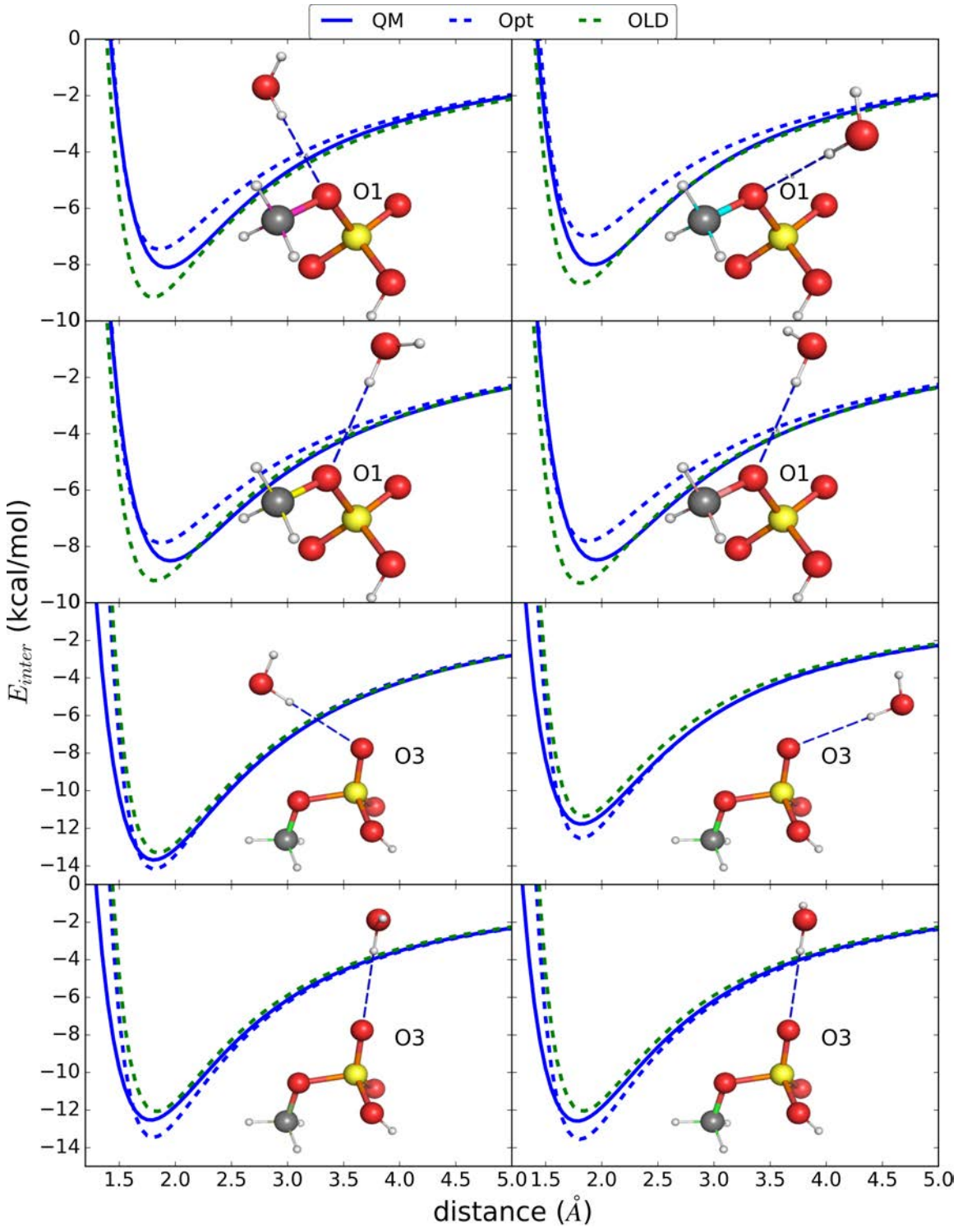

Figure S1. Water interaction energy surfaces as a function of distance from the QM and Drude models with Methylphosphate (anionic) (MP_1). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

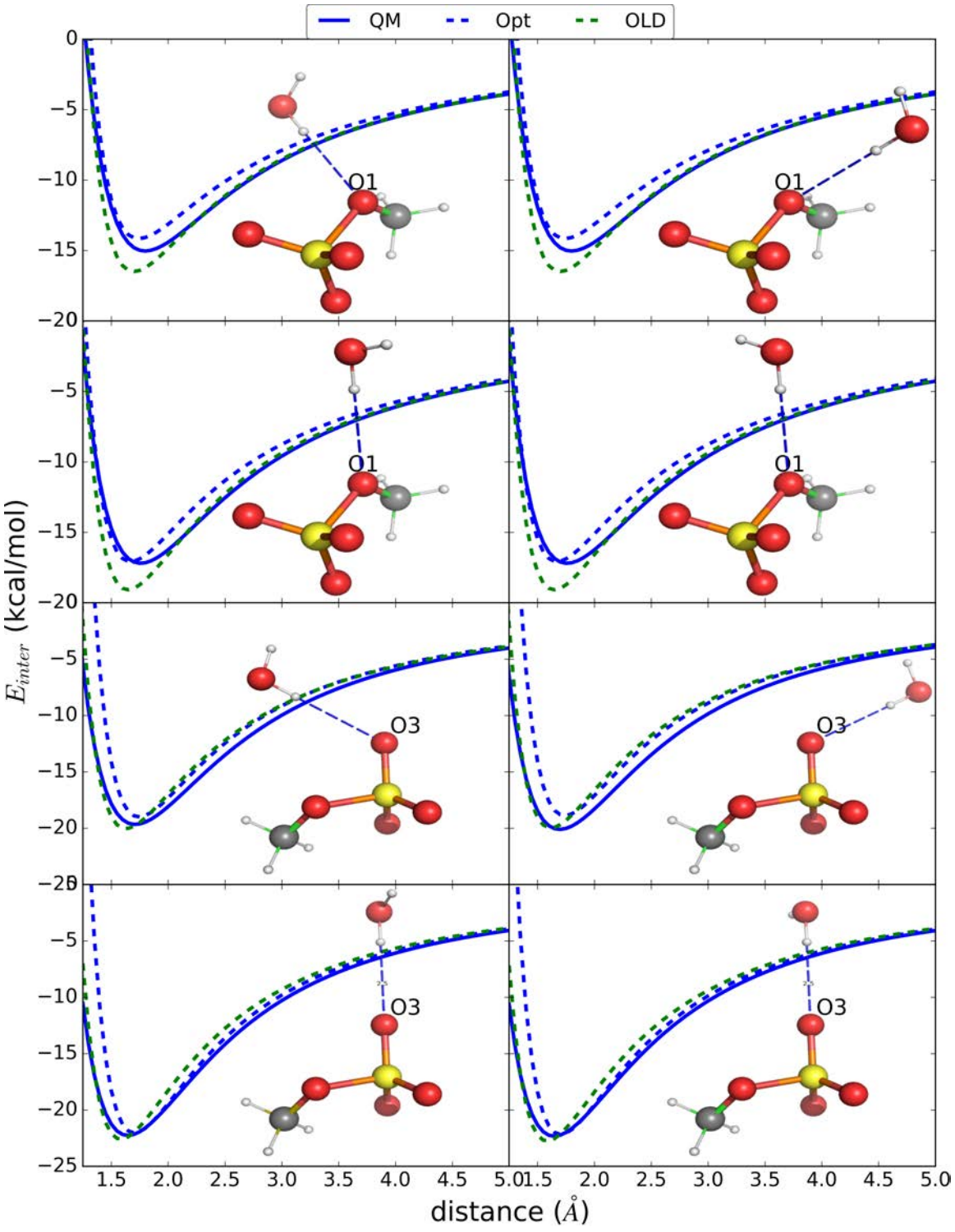

Figure S2. Water interaction energy surfaces as a function of distance from the QM and Drude models with Methylphosphate (dianionic)(MP_2). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

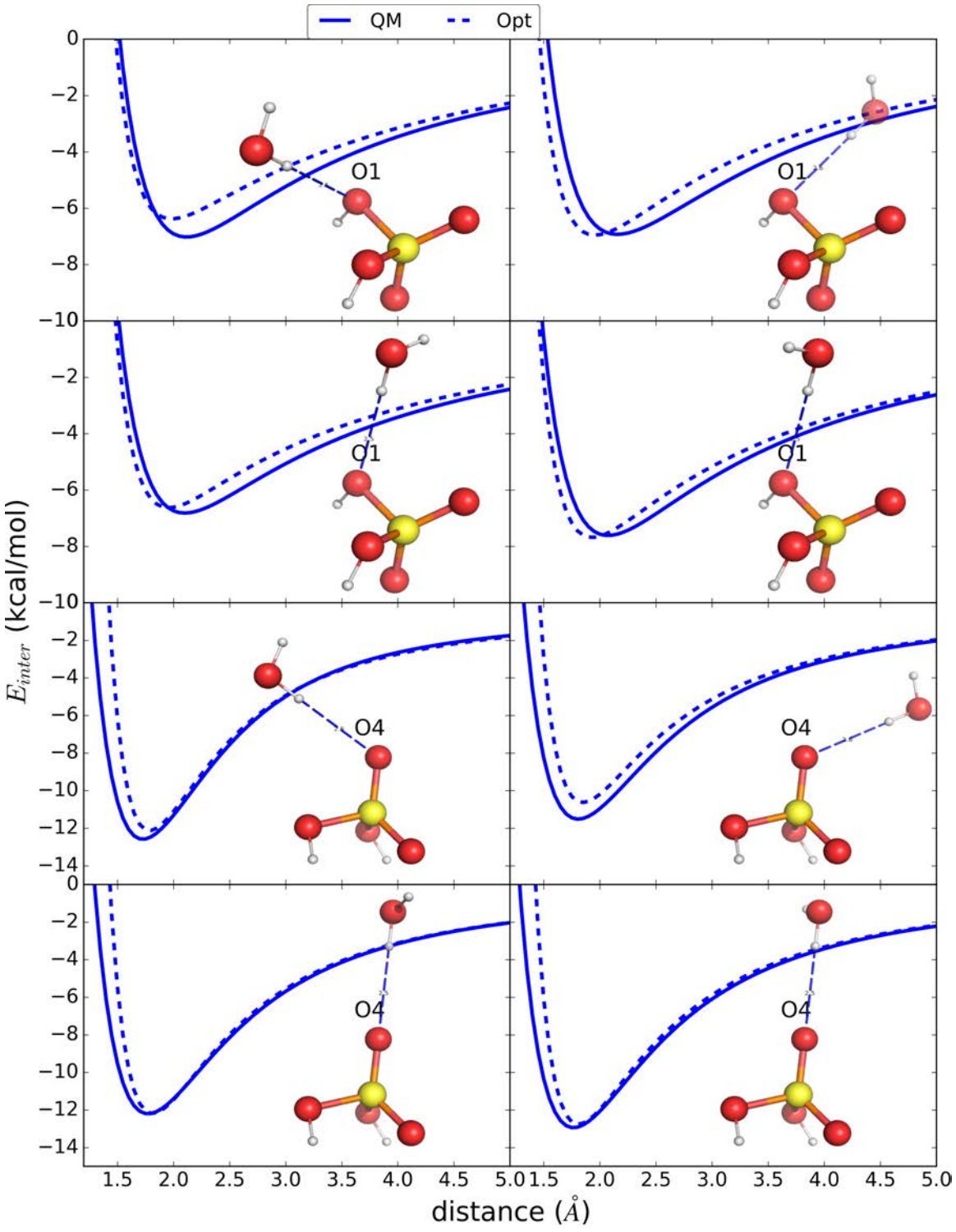

Figure S3. Water interaction energy surfaces as a function of distance from the QM and Drude models with Phosphate (anionic) (HP_1). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

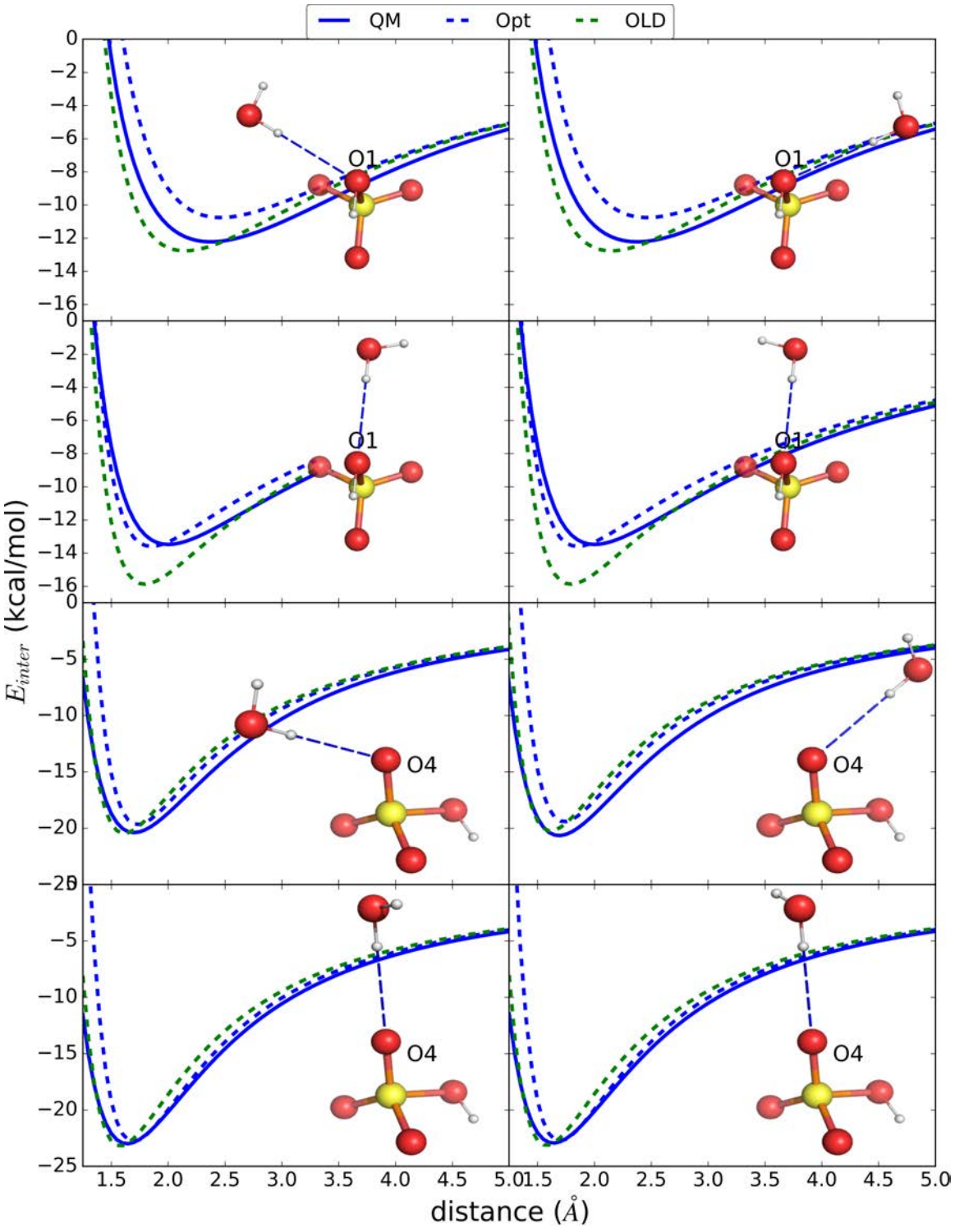

Figure S4. Water interaction energy surfaces as a function of distance from the QM and Drude models with Phosphate (dianionic) (HP_2). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

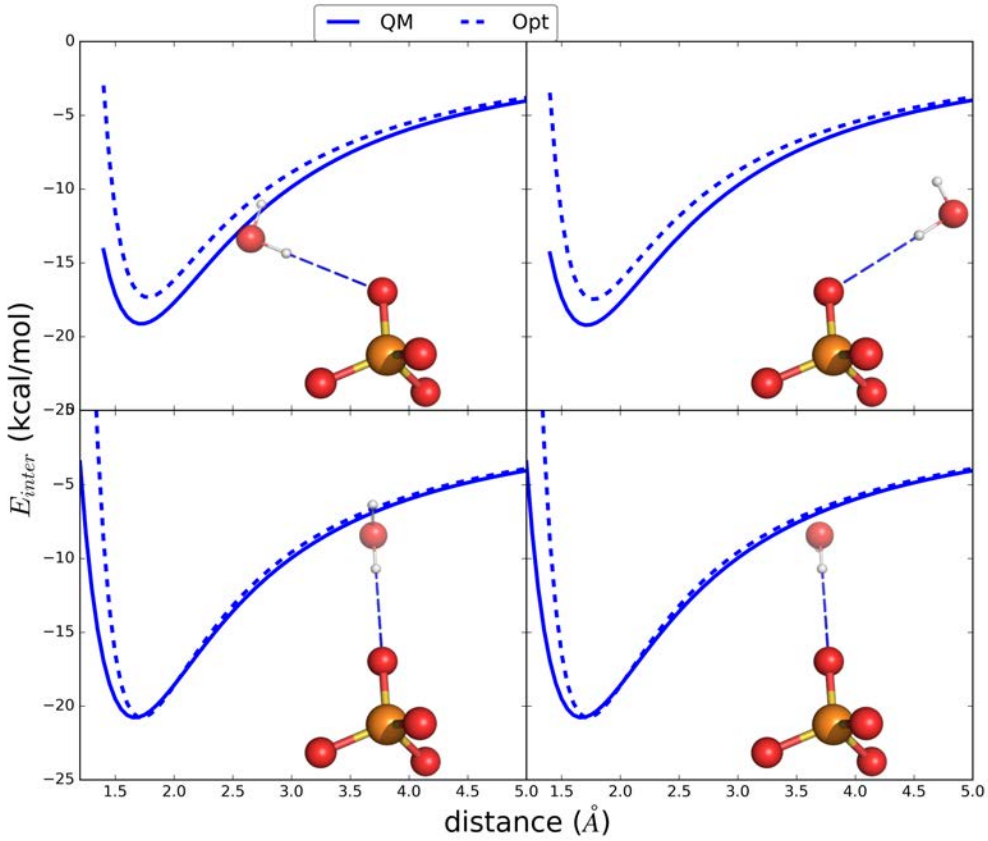

Figure S5. Water interaction energy surfaces as a function of distance from the QM and Drude models with the sulfate ion (SO4). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

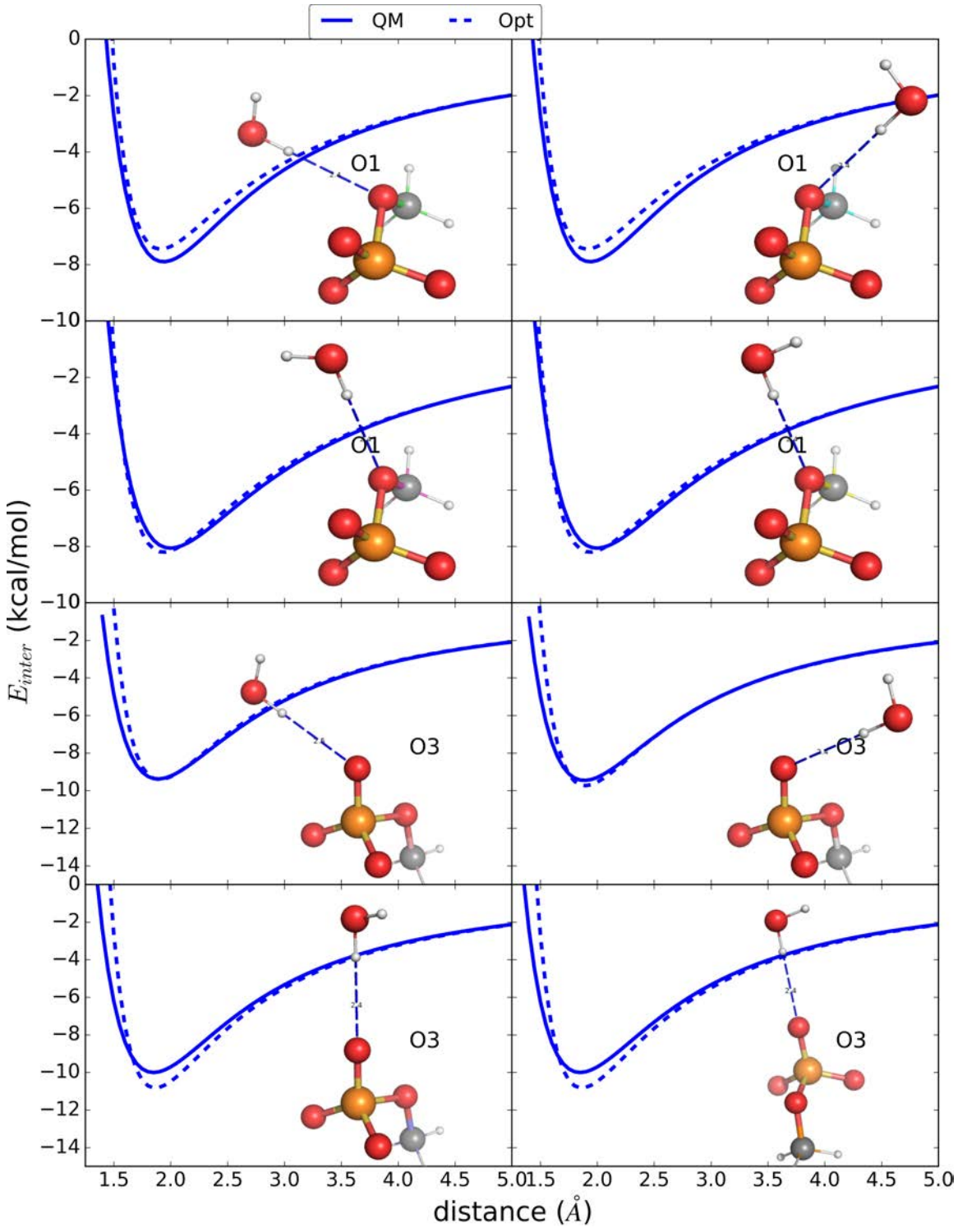

Figure S6. Water interaction energy surfaces as a function of distance from the QM and Drude models with Methylsulfate (anionic) (MSO4). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

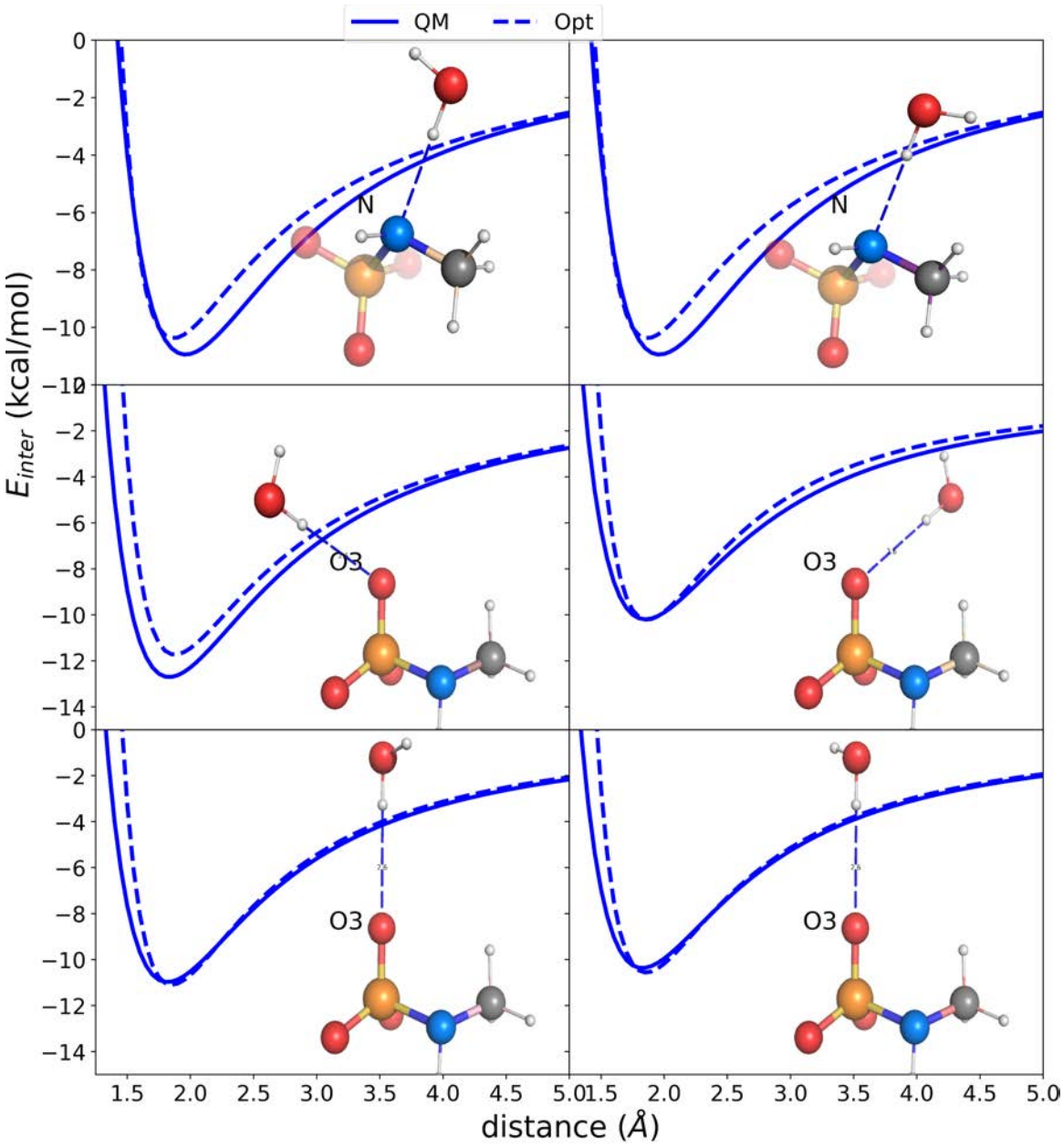

Figure S7. Water interaction energy surfaces as a function of distance from the QM and Drude models with N-methylsulfamate (anionic) (NMSM). Distances are labeled between the oxygen/Nitrogen (O/N) on the model compound and hydrogen (H) on the water.

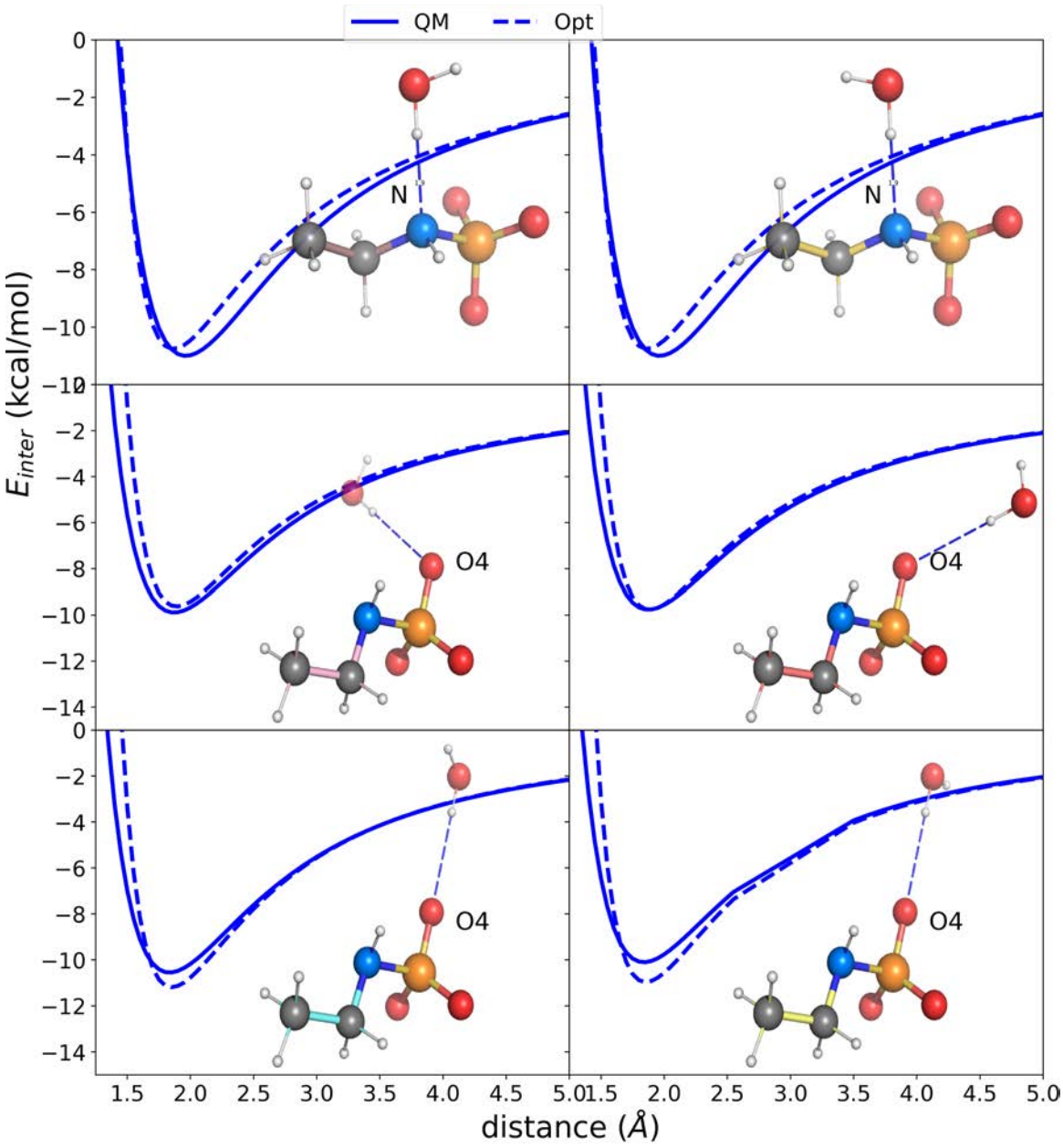

Figure S8. Water interaction energy surfaces as a function of distance from the QM and Drude models with N-ethylsulfamate (anionic) (NESM). Distances are labeled between the oxygen/Nitrogen (O/N) on the model compound and hydrogen (H) on the water.

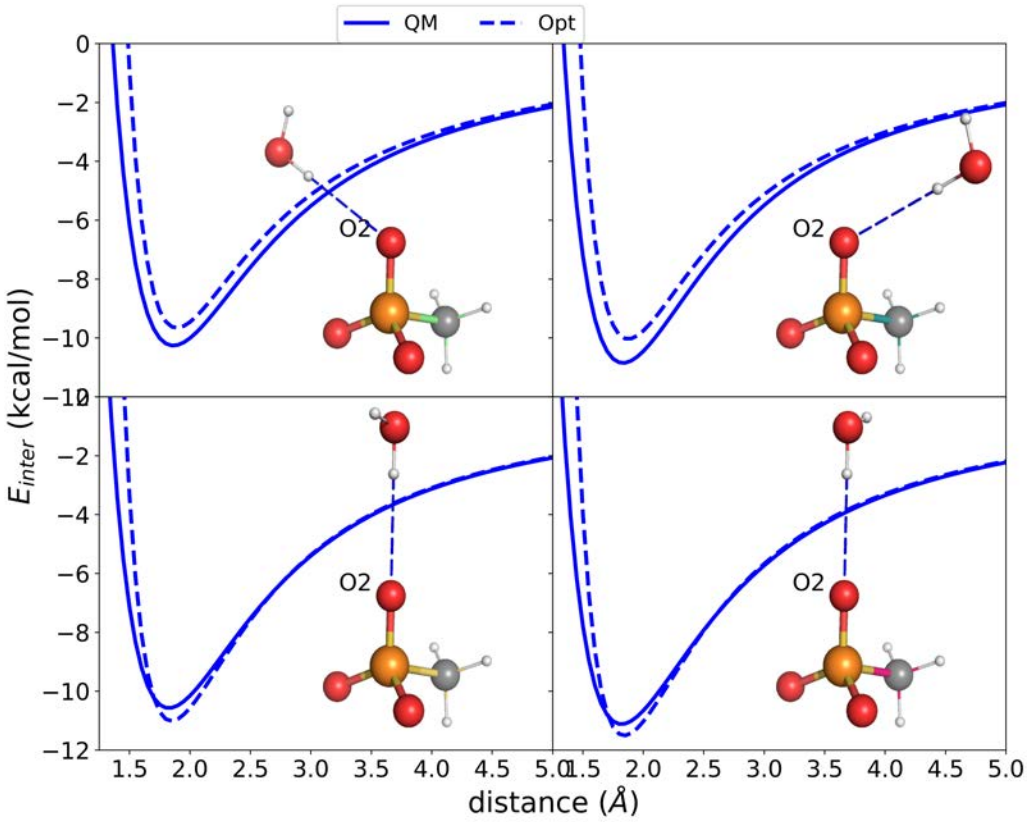

Figure S9. Water interaction energy surfaces as a function of distance from the QM and Drude models with Methylsulfonate (anionic) (MSNA). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

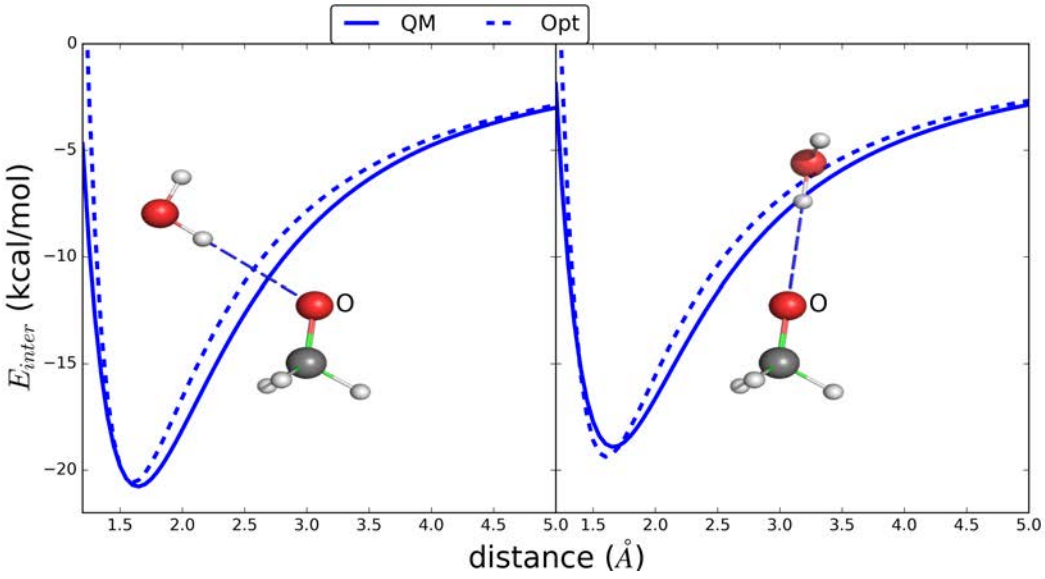

Figure S10. Water interaction energy surfaces as a function of distance from the QM and Drude models with Methoxide (anionic) (MEO). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

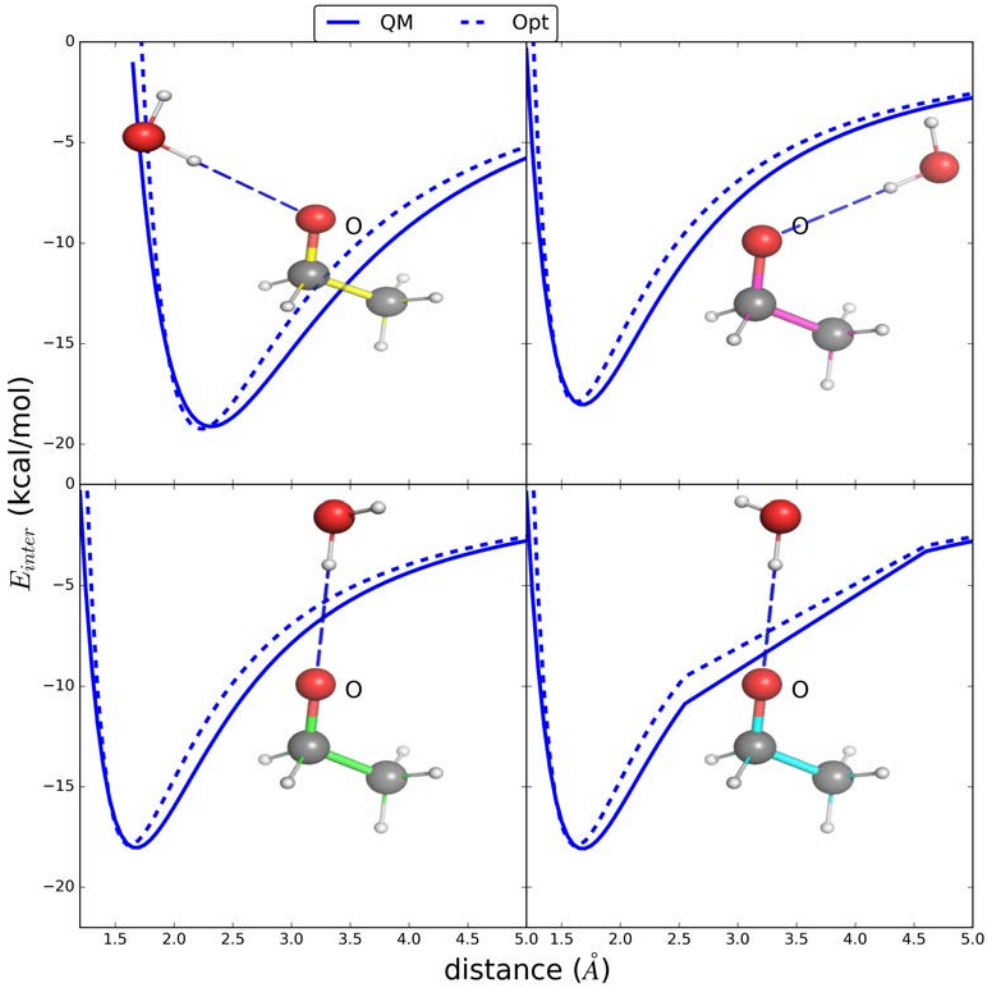

Figure S11. Water interaction energy surfaces as a function of distance from the QM and Drude models with Ethoxide (anionic) (ETO). Distances are labeled between the oxygen (O) on the model compound and hydrogen (H) on the water.

Table S8. Polarizable Drude Force Field Topology File

```
* Drude toppar file for molecular anions
*
read rtf card append
* topology for molecular anions
*
41

DEFA FIRS NONE LAST NONE
AUTOGENERATE ANGLES DIHEDRALS DRUDE PATCH

RESI DMP          -1.000 ! dimethylphosphate, aak&aah, optimized for both lipids
GROUP                    ! and nucleic acids
ATOM P    PD1AN    1.192   ALPHA -0.974  THOLE 2.098 !         H11
ATOM O13  OD2C2C  -0.856   ALPHA -0.931  THOLE 1.083 !         |
ATOM O14  OD2C2C  -0.856   ALPHA -0.931  THOLE 1.083 !    H12--C1--H13
ATOM O11  OD30BN  -0.520   ALPHA -0.901  THOLE 0.181 !         |
ATOM O12  OD30BN  -0.520   ALPHA -0.901  THOLE 0.181 !         O11
ATOM C1   CD33C    0.202   ALPHA -1.642  THOLE 0.862 !         |
ATOM H11  HDA3A    0.026                              !    O14==P--O13(-)
ATOM H12  HDA3A    0.026                              !         |
ATOM H13  HDA3A    0.026                              !         O12
ATOM C2   CD33C    0.202   ALPHA -1.642  THOLE 0.862 !         |
ATOM H21  HDA3A    0.026                              !    H22--C2--C23
ATOM H22  HDA3A    0.026                              !         |
ATOM H23  HDA3A    0.026                              !         H21

BOND P      O11    P      O12    P      O13    P      O14
BOND O11    C1     O12    C2
BOND C1     H11    C1     H12    C1     H13
BOND C2     H21    C2     H22    C2     H23

ANISOTROPY O11 O13 O12 O14 A11 1.0000  A22 0.6000
ANISOTROPY O12 O14 O11 O13 A11 1.0000  A22 0.6000
ANISOTROPY O13 P   O11 O12 A11 0.6000  A22 1.0000
ANISOTROPY O14 P   O12 O11 A11 0.6000  A22 1.0000

IC   O11 P   O12 C2      1.5837  102.73   72.47  116.87   1.4386
IC   O12 P   O11 C1      1.5843  102.73   72.47  116.85   1.4394
IC   O13 P   O11 C1      1.4910  107.70  -41.57  116.85   1.4394
IC   O14 P   O12 C2      1.4906  107.67  -41.56  116.87   1.4386
IC   H11 C1  O11 P       1.1128  110.79  -42.95  116.85   1.5837
IC   H12 C1  O11 P       1.1118  109.92   77.01  116.85   1.5837
IC   H13 C1  O11 P       1.1095  109.84 -163.26  116.85   1.5837
IC   H21 C2  O12 P       1.1125  110.79  -42.95  116.87   1.5843
IC   H22 C2  O12 P       1.1123  109.91   77.00  116.87   1.5843
IC   H23 C2  O12 P       1.1094  109.84 -163.30  116.87   1.5843
IC   O12 O11 *P  O13     1.5843  102.73 -114.04  107.70   1.4910
IC   O12 O11 *P  O14     1.5843  102.73  113.68  108.15   1.4906
IC   P   O11 C1  H11     1.5837  116.85  -42.95  110.79   1.1128
IC   H11 O11 *C1 H12     1.1128  110.79  119.96  109.92   1.1118
IC   H11 O11 *C1 H13     1.1128  110.79 -120.31  109.84   1.1095
IC   P   O12 C2  H21     1.5843  116.87  -42.95  110.79   1.1125
IC   H21 O12 *C2 H22     1.1125  110.79  119.95  109.91   1.1123
IC   H21 O12 *C2 H23     1.1125  110.79 -120.35  109.84   1.1094
patch first none last none

RESI MP_0          0.000 ! Methylphosphate, neutral
GROUP
```

```
ATOM C1   CD33C    0.242  ALPHA -1.642  THOLE 0.862 !        H11
ATOM O1   OD30D   -0.520  ALPHA -0.901  THOLE 0.811 !         |
ATOM P1   PD1AN    1.376  ALPHA -0.974  THOLE 2.098 !   H13--C1--H12
ATOM O2   OD31D    0.000  ALPHA -0.927  THOLE 1.100 !         |
ATOM LP2A LPDNA1  -0.253                            !         O1
ATOM LP2B LPDNA1  -0.253                            !         |
ATOM O3   OD31D    0.000  ALPHA -0.927  THOLE 1.100 !     O4==P1--O3
ATOM LP3A LPDNA1  -0.253                            !         |    \
ATOM LP3B LPDNA1  -0.253                            !         O2    H3
ATOM O4   OD2C2C  -0.776  ALPHA -0.921  THOLE 1.083 !          \
ATOM H11  HDA3A    0.026                            !           H2
ATOM H12  HDA3A    0.026                            !
ATOM H13  HDA3A    0.026
ATOM H2   HDP1A    0.306
ATOM H3   HDP1A    0.306

BOND P1   O1     P1   O2    P1   O3    P1   O4    O1   C1
BOND C1   H11    C1   H12   C1   H13   O2   H2    O3   H3
BOND O2   LP2A   O2 LP2B
BOND O3   LP3A   O3 LP3B

LONEPAIR relative LP2A O2 P1 H2 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR relative LP2B O2 P1 H2 distance 0.35 angle 110.0 dihe 270.0
LONEPAIR relative LP3A O3 P1 H3 distance 0.35 angle 110.0 dihe  90.0
LONEPAIR relative LP3B O3 P1 H3 distance 0.35 angle 110.0 dihe 270.0
ANISOTROPY O2 P1 LP2A LP2B A11 0.76473 A22 1.16239
ANISOTROPY O3 P1 LP3A LP3B A11 0.76473 A22 1.16239

 IC    H11     C1      O1      P1          0.0000    0.00  180.00    0.00   0.0000
 IC    C1      O1      P1      O2          0.0000    0.00  180.00    0.00   0.0000
 IC    H11     O1      *C1     H12         0.0000    0.00  120.00    0.00   0.0000
 IC    H11     O1      *C1     H13         0.0000    0.00 -120.00    0.00   0.0000
 IC    O2      O1      *P1     O3          0.0000    0.00  120.00    0.00   0.0000
 IC    O2      O1      *P1     O4          0.0000    0.00 -120.00    0.00   0.0000
 IC    O1      P1      O2      H2          0.0000    0.00  180.00    0.00   0.0000
 IC    O1      P1      O3      H3          0.0000    0.00  180.00    0.00   0.0000
PATCH FIRST NONE LAST NONE

RESI MP_1         -1.000 ! Methylphosphate, anionic
GROUP                    ! Villa et al., JPCB, 2018
ATOM C1   CD33C    0.182  ALPHA -1.642  THOLE 0.862 !        H11
ATOM O1   OD30D   -0.520  ALPHA -0.901  THOLE 0.811 !         |
ATOM P1   PD1AN    1.252  ALPHA -0.974  THOLE 2.098 !   H13--C1--H12
ATOM O2   OD31D    0.000  ALPHA -0.927  THOLE 1.100 !         |
ATOM LPA  LPDNA1  -0.273                            !         O1
ATOM LPB  LPDNA1  -0.273                            !         |
ATOM O3   OD2C2C  -0.856  ALPHA -0.921  THOLE 1.083 !     O4==P1--O3(-)
ATOM O4   OD2C2C  -0.856  ALPHA -0.921  THOLE 1.083 !         |
ATOM H11  HDA3A    0.026                            !         O2
ATOM H12  HDA3A    0.026                            !           \
ATOM H13  HDA3A    0.026                            !            H2
ATOM H2   HDP1A    0.266

BOND P1     O2     P1     O3     P1     O4
BOND O1     P1     O1     C1
BOND O2     H2
BOND C1     H11    C1     H12    C1     H13
BOND O2     LPA    O2     LPB

LONEPAIR relative LPA O2 P1 H2 distance 0.35 angle 110.00 dihe 90.00
LONEPAIR relative LPB O2 P1 H2 distance 0.35 angle 110.00 dihe 270.00
ANISOTROPY O2 P1 LPA LPB A11 0.76473 A22 1.16239
PATCH FIRST NONE LAST NONE
```

```
IC    H11     C1      O1      P1          0.0000    0.00  180.00    0.00   0.0000
IC    C1      O1      P1      O2          0.0000    0.00  180.00    0.00   0.0000
IC    O1      P1      O2      H2          0.0000    0.00  180.00    0.00   0.0000
IC    O2      O1      *P1     O3          0.0000    0.00   90.00    0.00   0.0000
IC    O2      O1      *P1     O4          0.0000    0.00  180.00    0.00   0.0000
IC    H11     O1      *C1     H12         0.0000    0.00   90.00    0.00   0.0000
IC    H11     O1      *C1     H13         0.0000    0.00  180.00    0.00   0.0000
PATCH FIRST NONE LAST NONE

RESI MP_2         -2.000 ! Methylphosphate, dianionic
GROUP                    ! Villa et al., JPCB, 2018
ATOM C1   CD33C    0.161  ALPHA -1.642  THOLE 0.862 !       H11
ATOM O1   OD30D   -0.740  ALPHA -0.901  THOLE 0.181 !       |
ATOM P1   PD1AN    1.792  ALPHA -0.974  THOLE 2.098 !  H13--C1--H12
ATOM O2   OD2C2C  -1.087  ALPHA -0.931  THOLE 1.083 !       |
ATOM O3   OD2C2C  -1.087  ALPHA -0.931  THOLE 1.083 !       O1
ATOM O4   OD2C2C  -1.087  ALPHA -0.931  THOLE 1.083 !       |
ATOM H11  HDA3A    0.016                            !   O4==P1--O3(-)
ATOM H12  HDA3A    0.016                            !       |
ATOM H13  HDA3A    0.016                            !       O2(-)

BOND O1  P1   O1 C1
BOND P1  O2   P1 O3   P1 O4
BOND C1  H11  C1 H12  C1 H13

IC    H11     C1      O1      P1          0.0000    0.00  180.00    0.00   0.0000
IC    C1      O1      P1      O2          0.0000    0.00  180.00    0.00   0.0000
IC    O2      O1      *P1     O3          0.0000    0.00   90.00    0.00   0.0000
IC    O2      O1      *P1     O4          0.0000    0.00  180.00    0.00   0.0000
IC    H11     O1      *C1     H12         0.0000    0.00   90.00    0.00   0.0000
IC    H11     O1      *C1     H13         0.0000    0.00  180.00    0.00   0.0000
PATCH FIRST NONE LAST NONE

RESI HP_0          0.000 ! Hydrogenphosphate, neutral
GROUP
ATOM P1   PD1AN    0.827  ALPHA -1.244  THOLE 1.678 !         H1
ATOM O4   OD2C2C  -0.590  ALPHA -0.951  THOLE 1.083 !        /
ATOM O1   OD31D   -0.445  ALPHA -0.929  THOLE 1.091 !       O1
ATOM O2   OD31D   -0.445  ALPHA -0.929  THOLE 1.091 !       |
ATOM O3   OD31D   -0.445  ALPHA -0.929  THOLE 1.091 !   O4==P1--O3
ATOM H1   HDP1A    0.366                            !       |     \
ATOM H2   HDP1A    0.366                            !       O2     H3
ATOM H3   HDP1A    0.366                            !      /
                                                    !     H2
BOND P1 O1 P1 O2 P1 O3 P1 O4
BOND O1 H1 O2 H2 O3 H3

PATCH FIRST NONE LAST NONE
IC    H1      O1      P1      O2          0.0000    0.00  180.00    0.00   0.0000
IC    O2      P2      O3      H3          0.0000    0.00  180.00    0.00   0.0000
IC    H3      O3      P1      O2          0.0000    0.00  180.00    0.00   0.0000
IC    O2      O1      *P1     O3          0.0000    0.00   90.00    0.00   0.0000
IC    O1      O2      *P1     O4          0.0000    0.00  180.00    0.00   0.0000
PATCH FIRST NONE LAST NONE

RESI HP_1         -1.000 ! Hydrogenphosphate, anionic
GROUP
ATOM P1   PD1AN    1.220  ALPHA -1.244  THOLE 1.678 !        H1
ATOM O3   OD2C2C  -0.856  ALPHA -0.951  THOLE 1.083 !       /
ATOM O4   OD2C2C  -0.856  ALPHA -0.951  THOLE 1.083 !      O1
ATOM O1   OD31D    0.000  ALPHA -1.291  THOLE 1.091 !      |
ATOM O2   OD31D    0.000  ALPHA -1.291  THOLE 1.091 !  O4==P1--O3(-)
ATOM LP1A LPDNA1  -0.253                            !      |
ATOM LP1B LPDNA1  -0.253                            !      O2
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ATOM LP2A LPDNA1  -0.253                              !     /
ATOM LP2B LPDNA1  -0.253                              !    H2
ATOM H1   HDP1A    0.252                              !
ATOM H2   HDP1A    0.252                              !

BOND P1  O1   P1  O2   P1  O3   P1  O4
BOND O1  H1   O1  LP1A O1  LP1B
BOND O2  H2   O2  LP2A O2  LP2B

LONEPAIR relative LP1A O1 P1 H1 distance 0.35 angle 110.00 dihe 90.00
LONEPAIR relative LP1B O1 P1 H1 distance 0.35 angle 110.00 dihe 270.00
ANISOTROPY O1 P1 LP1A LP1B A11 0.76473 A22 1.16239

LONEPAIR relative LP2A O2 P1 H2 distance 0.35 angle 110.00 dihe 90.00
LONEPAIR relative LP2B O2 P1 H2 distance 0.35 angle 110.00 dihe 270.00
ANISOTROPY O2 P1 LP2A LP2B A11 0.76473 A22 1.16239

IC    H1      O1      P1      O3          0.0000    0.00  180.00    0.00   0.0000
IC    H2      O2      P1      O3          0.0000    0.00  180.00    0.00   0.0000
IC    O2      O1      *P1     O3          0.0000    0.00   90.00    0.00   0.0000
IC    O1      O2      *P1     O4          0.0000    0.00  180.00    0.00   0.0000
PATCH FIRST NONE LAST NONE

RESI HP_2         -2.000 ! Hydrogenphosphate, dianionic
GROUP
ATOM O1   OD31D   -0.000  ALPHA -1.291  THOLE 1.091 !        H
ATOM P1   PD1AN    1.730  ALPHA -1.244  THOLE 1.678 !       /
ATOM O2   OD2C2C  -1.087  ALPHA -0.951  THOLE 1.083 !      O1
ATOM O3   OD2C2C  -1.087  ALPHA -0.951  THOLE 1.083 !      |
ATOM O4   OD2C2C  -1.087  ALPHA -0.951  THOLE 1.083 !  O4==P1--O3(-)
ATOM LPA  LPDNA1  -0.345                              !      |
ATOM LPB  LPDNA1  -0.345                              !      O2(-)
ATOM H    HDP1A    0.221                    !

BOND P1  O1   P1  O2   P1  O3   P1  O4
BOND O1  H    O1  LPA  O1  LPB

LONEPAIR relative LPA O1 P1 H distance 0.35 angle 110.00 dihe 90.00
LONEPAIR relative LPB O1 P1 H distance 0.35 angle 110.00 dihe 270.00
!ANISOTROPY O1 P1 LPA LPB A11 0.76473 A22 1.16239 ! need to check on this

IC    H       O1      P1      O2          1.0000    109.00  179.00    109.00   1.6000
IC    O2      O1      *P1     O3          1.60000   109.00   90.00    109.00   1.60000
IC    O1      O2      *P1     O4          1.60000   109.00  179.00    109.00   1.60000
PATCH FIRST NONE LAST NONE

RESI SO4          -2.000 ! Sulfate ion
GROUP
ATOM S    SD1A     2.000  ALPHA -0.930  THOLE 1.098 !           OS2(-1)
ATOM OS1  OD2C2C  -1.000  ALPHA -0.990  THOLE 1.083 !            |
ATOM OS2  OD2C2C  -1.000  ALPHA -0.990  THOLE 1.083 ! (-1) OS2--S(+2)--OS4 (-1)
ATOM OS3  OD2C2C  -1.000  ALPHA -0.990  THOLE 1.083 !           ||
ATOM OS4  OD2C2C  -1.000  ALPHA -0.990  THOLE 1.083 !           OS1

BOND S  OS1  S  OS2  S  OS3  S  OS4

RESI MSO4         -1.000 ! Methylsulfate
GROUP
ATOM S    SD1A     1.330  ALPHA -0.930  THOLE 1.098 !           OS2(-1)
ATOM OS1  OD30B   -0.560  ALPHA -0.670  THOLE 0.181 !            |
ATOM OS2  OD2C2C  -0.706  ALPHA -0.990  THOLE 1.083 ! (-1) OS2--S(+2)--OS4 (-1)
ATOM OS3  OD2C2C  -0.706  ALPHA -0.990  THOLE 1.083 !            |
ATOM OS4  OD2C2C  -0.706  ALPHA -0.990  THOLE 1.083 !           OS1
ATOM C1   CD33C    0.240  ALPHA -1.642  THOLE 0.862 !             \
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ATOM H11  HDA3A    0.036                            !         H11-C1-H13
ATOM H12  HDA3A    0.036                            !              |
ATOM H13  HDA3A    0.036                            !             H12

BOND  S   OS1  S   OS2  S   OS3  S   OS4  OS1  C1
BOND  C1  H11  C1  H12  C1  H13

ACCE  OS1
ACCE  OS2
ACCE  OS3
ACCE  OS4

IC    H11     C1      OS1      S          0.0000    0.00  180.00    0.00   0.0000
IC    C1      OS1     S       OS2         0.0000    0.00  180.00    0.00   0.0000
IC    OS2     OS1     *S      OS3         0.0000    0.00   90.00    0.00   0.0000
IC    OS2     OS1     *S      OS4         0.0000    0.00  180.00    0.00   0.0000
IC    H11     OS1     *C1     H12         0.0000    0.00   90.00    0.00   0.0000
IC    H11     OS1     *C1     H13         0.0000    0.00  180.00    0.00   0.0000

RESI MSNA         -1.000 ! Methylsulfonate
GROUP
ATOM S    SD1A     1.219  ALPHA -0.930  THOLE 1.098 !           OS2(-1)
ATOM OS1  OD2C2C  -0.706  ALPHA -0.990  THOLE 1.083 !             |
ATOM OS2  OD2C2C  -0.706  ALPHA -0.990  THOLE 1.083 ! (-1) OS2--S(+2)--OS4 (-1)
ATOM OS3  OD2C2C  -0.706  ALPHA -0.990  THOLE 1.083 !             |
ATOM C1   CD33C   -0.209  ALPHA -1.642  THOLE 0.862 !        H11-C1-H13
ATOM H11  HDA3A    0.036                            !            |
ATOM H12  HDA3A    0.036                            !           H12
ATOM H13  HDA3A    0.036                            !

BOND  S  OS1  S  OS2  S  OS3  S   C1
BOND  C1 H11  C1 H12  C1 H13

ACCE  OS1
ACCE  OS2
ACCE  OS3

RESI NMSM         -1.000 ! N-methyl sulfamate
GROUP
ATOM C1   CD33C    0.260  ALPHA -1.642  THOLE 0.862 !          H11
ATOM S    SD1A     1.504  ALPHA -0.930  THOLE 1.098 !          |
ATOM OS2  OD2C2C  -0.780  ALPHA -0.990  THOLE 1.083 !      H13-C1-H12
ATOM OS3  OD2C2C  -0.780  ALPHA -0.990  THOLE 1.083 !          |
ATOM OS4  OD2C2C  -0.780  ALPHA -0.990  THOLE 1.083 !          N-HN
ATOM N    ND2A2   -0.782  ALPHA -1.942  THOLE 0.250 !          |
ATOM HN   HDP1A    0.280                            !     OS3==S==OS4
ATOM H11  HDA3A    0.026                            !          |
ATOM H12  HDA3A    0.026                            !          OS2(-)
ATOM H13  HDA3A    0.026                            !

BOND  N   C1    N   S     N   HN
BOND  S   OS2   S   OS3   S   OS4
BOND  C1  H11   C1  H12   C1  H13

IC OS3    S    N   C1   1.5109    120.35    -58.37    106.61    1.4455
IC OS4    S    N   C1   2.4267     38.58    108.63    109.00    1.4111
IC OS2    S    N   C1   2.4267     38.58   -115.20    116.51    1.4439
IC C1     S   *N   HN   2.6812     29.10   -125.97    104.18    1.0300
IC H11    C1   N   S    0.0000    000.00      0.0     000.00    0.0000
IC H12    C1   N   S    0.0000    000.00    120.0     000.00    0.0000
IC H13    C1   N   S    0.0000    000.00   -120.0     000.00    0.0000

RESI NESM         -1.000 ! N-Ethyl sulfamate
GROUP
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ATOM C1   CD32C    0.240  ALPHA -1.642  THOLE 0.862 !          H23
ATOM S    SD1A     1.564  ALPHA -0.930  THOLE 1.098 !          |
ATOM OS2  OD2C2C  -0.780  ALPHA -0.990  THOLE 1.083 !      C21-C2-C22
ATOM OS3  OD2C2C  -0.780  ALPHA -0.990  THOLE 1.083 !          |
ATOM OS4  OD2C2C  -0.780  ALPHA -0.990  THOLE 1.083 !      C11-C1-C12
ATOM N    ND2A2   -0.782  ALPHA -1.942  THOLE 0.250 !          |
ATOM HN   HDP1A    0.280                            !          N-HN
ATOM H11  HDA2A    0.026                            !          |
ATOM H12  HDA2A    0.026                            !     OS3==S==OS4
ATOM C2   CD33C   -0.092  ALPHA -1.642  THOLE 0.862 !          |
ATOM H21  HDA3A    0.026                            !          OS2(-)
ATOM H22  HDA3A    0.026                            !
ATOM H23  HDA3A    0.026                            !

BOND  N  C1   N  S    N  HN
BOND  S  OS2  S  OS3  S  OS4
BOND  C1 C2   C1 H11  C1 H12
BOND  C2 H21  C2 H22  C2  H23

IC S   N   C1  H11  0.0000    0.00  -60.42    0.00   0.0000
IC N   H11 *C1 H12  0.0000    0.00   117.9    0.00   0.0000
IC N   H11 *C1 C2   0.0000    0.00  -126.1    0.00   0.0000
IC H11 C1  N   H21  0.0000    0.00  -176.0    0.00   0.0000
IC C1  N   S   O11  0.0000    0.00  -51.92    0.00   0.0000
IC N   O11 *S  O12  0.0000    0.00  -112.5    0.00   0.0000
IC N   O11 *S  O13  0.0000    0.00   110.8    0.00   0.0000
IC N   C1  C2  H21  0.0000    0.00  -58.51    0.00   0.0000
IC C1  H21 *C2 H22  0.0000    0.00   122.1    0.00   0.0000
IC C1  H21 *C2 H23  0.0000    0.00  -120.4    0.00   0.0000

RESI MEO          -1.000 ! Methoxide
GROUP
ATOM C    CD33A   -0.305  ALPHA -1.854  THOLE 1.224 !     O(-)
ATOM O    OD30E   -0.680  ALPHA -1.041  THOLE 0.347 !     |
ATOM H1   HDA3A   -0.005                            !  H1-C-H2
ATOM H2   HDA3A   -0.005                            !     |
ATOM H3   HDA3A   -0.005                            !     H3

BOND C  O    C  H1    C  H2    C  H3

RESI ETO          -1.000 ! Ethoxide
GROUP
ATOM C1   CD32A   -0.200  ALPHA -1.854  THOLE 1.224 !     O(-)
ATOM O    OD30E   -0.640  ALPHA -1.041  THOLE 0.347 !     |
ATOM H11  HDA2A   -0.030                            ! H11-C1-H12
ATOM H12  HDA2A   -0.030                            !     |
ATOM C2   CD33A   -0.190  ALPHA -1.854  THOLE 1.224 ! H21-C2-H22
ATOM H21  HDA3A    0.030                            !     |
ATOM H22  HDA3A    0.030                            !     H23
ATOM H23  HDA3A    0.030                            !

BOND C1   O    C1   C2
BOND C1   H11  C1   H12
BOND C2   H21  C2   H22  C2   H23

END

read param card append
* parameters for molecular anions
*

BONDS
OD2C2C   SD1A     525.00      1.493
OD30B    SD1A     240.00      1.701
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CD33A    OD30E    480.00      1.345
OD30E    CD32A    396.00      1.425
SD1A     ND2A2    185.00      1.700
SD1A     CD33C    218.00      1.823

ANGLES
OD2C2C   SD1A     OD2C2C    60.00    115.35
OD2C2C   SD1A     OD30B     90.00     98.44
SD1A     OD30B    CD33C     40.00    109.00
OD30B    SD1A     OD30B     40.00    109.00
OD30E    CD33A    HDA3A     61.00    117.20
OD30E    CD32A    CD33A     66.00    112.50
OD30E    CD32A    HDA2A     54.00    111.50
CD2R6A   CD2R6A   CD2R6I    50.00    118.20
CD2R6A   CD2R6I   OD30E     55.20    127.80
CD2R6A   CD2R6I   CD2R6A    50.00    111.50
CD2R6I   CD2R6A   HDR6A     30.00    116.55
SD1A     ND2A2    HDP1A     48.00    118.00
CD33C    ND2A2    SD1A      40.00    109.00
ND2A2    CD32C    CD33C     50.00    109.00
OD2C2C   SD1A     ND2A2     50.00    113.00
CD32C    ND2A2    SD1A      40.00    109.00
CD32C    CD33C    HDA3A     34.60    110.10   22.53   2.1790
HDA2A    CD32C    CD33C     34.60    110.10   22.53   2.1790
OD2C2C   SD1A     CD33C     60.00    103.55
SD1A     CD33C    HDA3A     35.00    108.80

DIHEDRALS
OD2C2C   SD1A     CD33C    HDA3A     0.280    3     0.00
SD1A     OD30B    CD33C    HDA3A     0.200    3     0.00
OD2C2C   SD1A     OD30B    CD33C     0.200    3     0.00
OD30B    SD1A     OD30B    CD33C     0.200    3     0.00
OD30E    CD32A    CD33A    HDA3A     0.175    3     0.00
CD32C    ND2A2    SD1A     OD2C2C    0.500    3     0.00
SD1A     ND2A2    CD32C    HDA2A     0.200    3     0.00
SD1A     ND2A2    CD32C    CD33C     0.500    3     0.00
OD2C2C   SD1A     ND2A2    HDP1A     0.200    3     0.00
ND2A2    CD32C    CD33C    HDA3A     0.200    3     0.00
HDP1A    ND2A2    CD32C    CD33C     0.200    3     0.00
HDA2A    CD32C    CD33C    HDA3A     0.200    3     0.00
CD33C    ND2A2    SD1A     OD2C2C    0.200    3     0.00
SD1A     ND2A2    CD33C    HDA3A     0.200    3     0.00
! New optimized dihedrals for DMP
CD33C    OD30BN   PD1AN    OD30BN       0.6417  1   180.00
CD33C    OD30BN   PD1AN    OD30BN       0.7706  2     0.00
CD33C    OD30BN   PD1AN    OD30BN       0.1118  3     0.00
CD33C    OD30BN   PD1AN    OD30BN       0.0905  4     0.00
CD33C    OD30BN   PD1AN    OD30BN       0.0532  5   180.00
CD33C    OD30BN   PD1AN    OD30BN       0.0167  6   180.00
CD33C    OD30BN   PD1AN    OD2C2C       0.8520  1     0.00
CD33C    OD30BN   PD1AN    OD2C2C       0.3200  2   180.00
CD33C    OD30BN   PD1AN    OD2C2C       0.0732  3     0.00
CD33C    OD30BN   PD1AN    OD2C2C       0.1860  4     0.00
CD33C    OD30BN   PD1AN    OD2C2C       0.0002  5     0.00
CD33C    OD30BN   PD1AN    OD2C2C       0.0151  6     0.00

IMPROPERS

NONBONDED nbxmod  5 atom vatom cdiel vdistance switch vswitch -
cutnb 16.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5

END

RETURN
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