Multi-Site CO_2 Fixation in Triazolates: Cooperative O,N Binding Enhanced by Solvation and Counter-Ion Effects

Puthiyavalappil K. Arathi[ab], D. Sudha[a] and Cherumuttathu H. Suresh[abc]*

[a]Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram, 695019, India.

[b]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India.

[c]Srinivasa Ramanujan Institute for Basic Sciences, Kerala State Council for Science, Technology and Environment, Kottayam, Kerala 686501, India

Email: sureshch@gmail.com; sureshch@niist.res.in

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Table S1. Benchmark study of adsorption energy. All values in kcal mol^{-1}.

Molecule	adsorption energy ΔE_{ad} using M06-2X method and basis set				
	6-311++G(d,p)	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pV5Z
1	-5.3	-6.1	-5.0	-4.6	-4.5
2	-5.7	-6.5	-5.4	-5.0	-4.9
$\mathbf{1_{OH}}$	-6.2	-7.4	-5.9	-5.5	-5.3
$\mathbf{2_{OH}}$	-7.3	-8.8	-7.1	-6.6	-6.5
$\mathbf{1_{OH2}}$	-6.1	-7.3	-5.9	-5.4	-5.2
$\mathbf{2_{OH2}}$	-7.6	-9.2	-7.4	-6.9	-6.7
$\mathbf{1_{O-}}$	-18.4	-23.3	-20.5	-19.1	-18.6
$\mathbf{2_{O-}}$	-19.9	-23.8	-21.0	-19.7	-19.1
$\mathbf{1_{O2-}}$	-44.4	-53.1	-48.3	-45.7	-44.2
$\mathbf{2_{O2-}}$	-44.5	-53.7	-48.4	-45.8	-44.4

Table S2. Benchmark adsorption energies (ΔE_{ad}) in kcal mol^{-1} for selected triazole-CO_2 complexes computed with non-augmented and augmented correlation-consistent basis sets, with and without dispersion.

Triazole–CO_2 complex	cc-pvqz	*aug*-cc-pvtz	*aug*-cc-pvtz+gd3	*aug*-cc-pvqz	*aug*-cc-pvqz+gd3
1…CO_2	-4.6	-4.7	-4.8	-4.5	-4.6
$\mathbf{1_{OH}}$ …CO_2	-5.5	-5.5	-5.7	-5.3	-5.5
$\mathbf{1_{OH2}}$…CO_2	-5.4	-5.5	-5.6	-5.3	-5.4
1_{OCO2-}	-19.1	-19.0	-19.1	-18.3	-18.4
$1_{(NCO2-)O-}$	-45.7	-43.8	-43.9	-43.0	-43.1

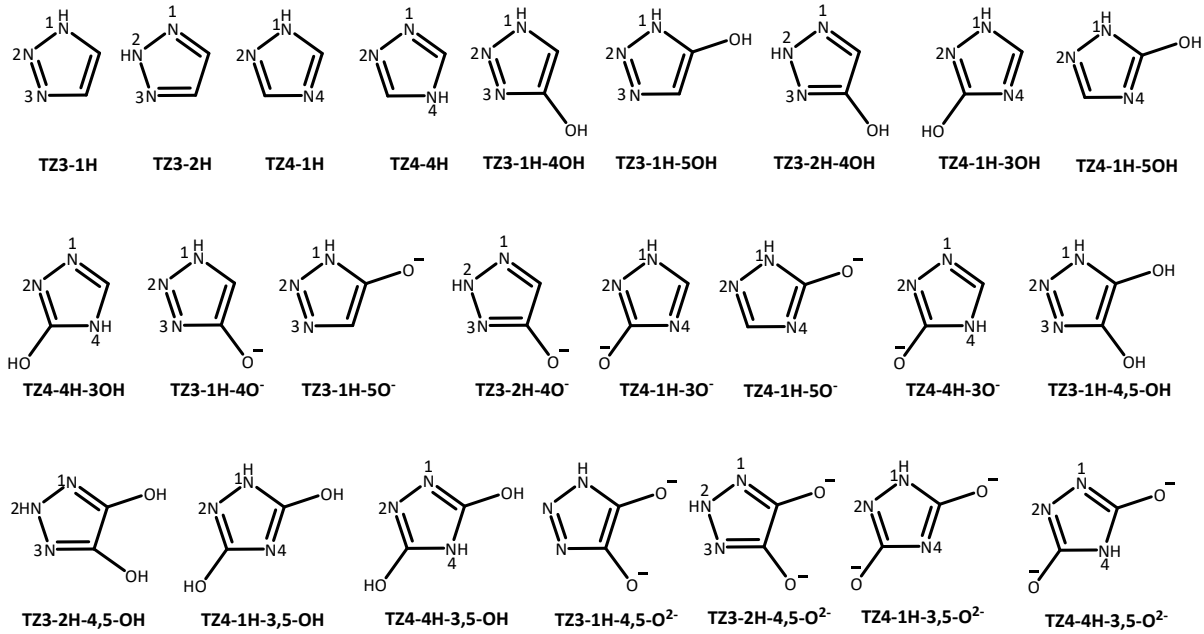

Figure S1. All neutral, anionic, and dianionic systems used for CO_2 capture.

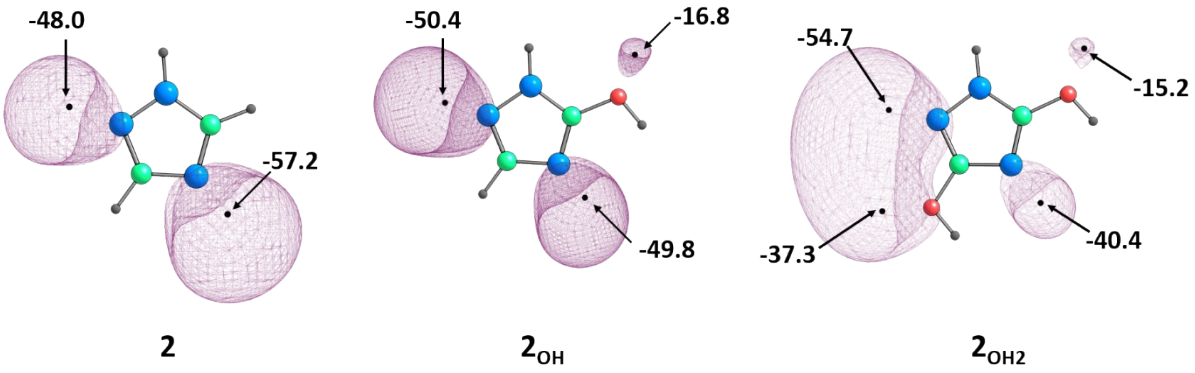

Figure S2. MESP isosurfaces of **2**, $\mathbf{2_{OH}}$, and $\mathbf{2_{OH2}}$ computed at the M06-2X/cc-pVQZ level of theory. Black dots mark V_{min} positions. Isosurface value: -12.0 kcal mol^{-1}. Color key: gray – H, blue – N, green – C, red – O.

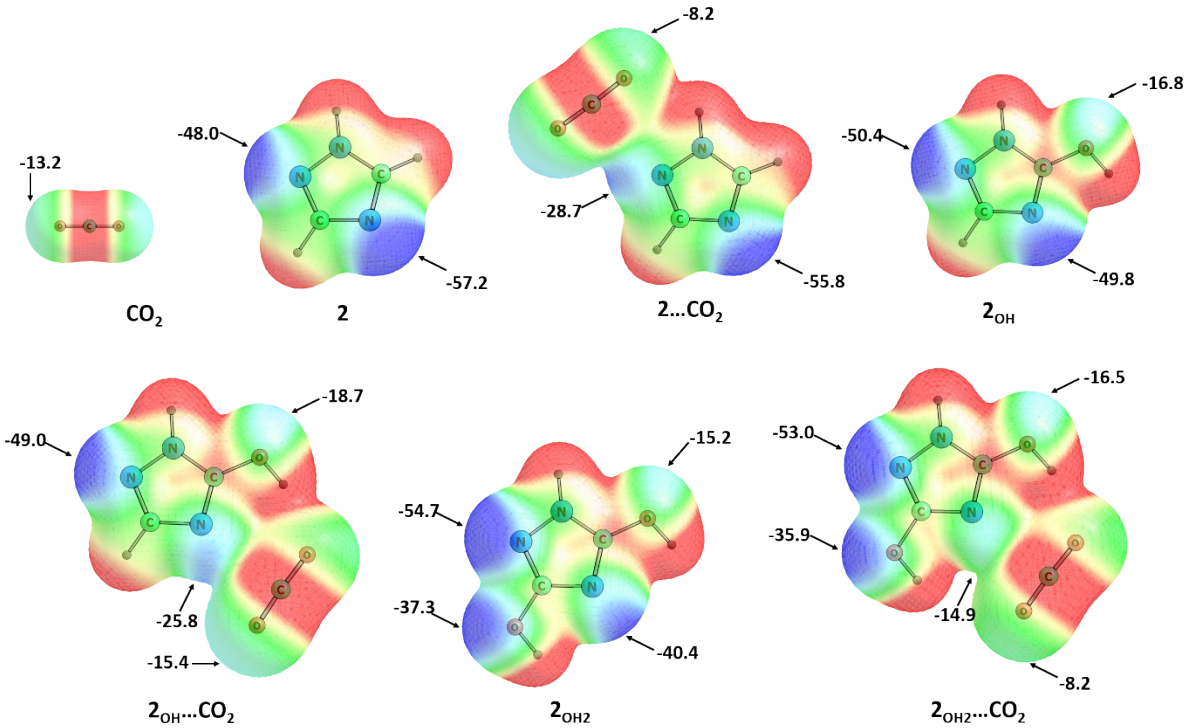

Figure S3. MESP on the 0.005 a.u. isodensity surface for CO_2, **2**, **2_{OH}**, **2_{OH2}**, and their CO_2 complexes. V_{min} values (kcal kcal mol^{-1}) and N···C, O–H···O distances (Å) at the M06-2X/cc-pVQZ level of theory. Color gradient: blue (electron-rich) to red (electron-deficient).

Table S3. BSSE-corrected adsorption energies (ΔE_{ad}) and Gibbs free energies (ΔG_{ad}) for anionic triazolate–1CO_2 adducts at the M06-2X/cc-pVQZ level of theory (kcal mol^{-1}).

Anionic systems	ΔE_{ad}	ΔG_{ad}
1_{OCO2-}	-17.8	-5.7
$1_{(CO2-)N3}$	-13.7	-0.9
$1_{(CO2-)N1}$	-8.4	4.3
2_{OCO2-}	-12.9	-1.1
$2_{(CO2-)N2}$	-18.7	-6.6
$2_{(CO2-)N4}$	-11.5	0.9

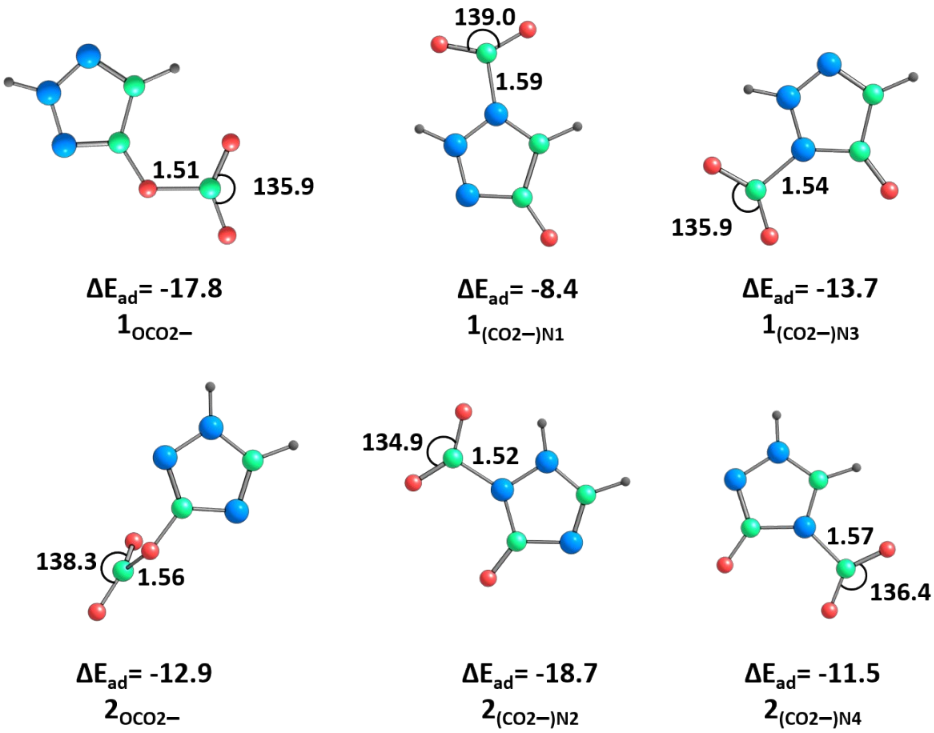

Figure S4. Optimized geometries of the anionic CO_2 adduct at the M06-2X/cc-pVQZ level of theory. Bond lengths in Å and bond angles in degrees. Color key: gray – H, blue – N, green – C, red – O.

Table S4. BSSE-corrected adsorption energies (ΔE_{ad}) and Gibbs free energies (ΔG_{ad}) for anionic triazolate–2CO_2 adducts at the M06-2X/cc-pVQZ level of theory (kcal mol^{-1}).

Anionic systems	ΔE_{ad}	ΔG_{ad}
$\mathbf{1}_{(OCO2–)}\cdots(CO_2)_{N1}$	-24.1	-3.3
$\mathbf{1}_{(OCO2–)}\cdots(CO_2)_{N3}$	-24.3	-4.3
$\mathbf{1}_{(OCO2–)\cdots(CO2)O}$	-28.0	-7.1
$\mathbf{1}_{(CO2–)N3}\cdots(CO_2)_{N1}$	-18.9	0.6
$\mathbf{1}_{(CO2–)N1}\cdots(CO_2)_{N1}$	-16.0	5.4
$\mathbf{1}_{(CO2–)N3}\cdots(CO_2)_{N3}$	-22.9	-1.6
$\mathbf{2}_{(CO2–)N2}\cdots(CO_2)_{N4}$	-25.5	-5.0
$\mathbf{2}_{(CO2–)N2}\cdots(CO_2)_{N2}$	-28.3	-7.3
$\mathbf{2}_{(CO2–)N4}\cdots(CO_2)_{N4}$	-20.9	0.5
$\mathbf{2}_{(CO2–)N2}\cdots(CO_2)_{O}$	-27.7	-6.5
$\mathbf{2}_{O–}\cdots(CO_2)_{O}\cdots(CO_2)_{N4}$	-19.3	-1.5

Table S5. BSSE-corrected adsorption energies (ΔE_{ad}) and Gibbs free energies (ΔG_{ad}) for dianionic triazolate–$2CO_2$ adducts at the M06-2X/cc-pVQZ level of theory (kcal mol^{-1}).

Dianionic systems	ΔE_{ad}	ΔG_{ad}
$\mathbf{1}_{(CO2-)N1(CO2-)N3}$	-71.9	-59.1
$\mathbf{1}_{(CO2-)N1(CO2-)N1}$	-61.0	-49.0
$\mathbf{1}_{(CO2-)N1(OCO2-)}$	-68.4	-56.3
$\mathbf{1}_{(CO2-)N1}...(CO_2)_O$	-61.1	-50.6
$\mathbf{1}_{(OCO2-)2}$	-63.2	-52.0
$\mathbf{2}_{(CO2-)N1(CO2-)N2}$	-64.6	-41.3
$\mathbf{2}_{(CO2-)N2(CO2-)N2}$	-66.6	-43.4
$\mathbf{2}_{(CO2-)N1(CO2-)O}$	-64.6	-41.2
$\mathbf{2}_{(CO2-)N1(CO2-)O}$	-73.6	-51.1
$\mathbf{2}_{(OCO2-)2}$	-69.0	-46.0

Table S6. SCF energies, zero-point correction, thermal correction to Gibbs, free energies and BSSE of all the systems under study. All values in au.

I. Tz system

System	SCF energy E	Zero-point correction	TC to Gibbs	E+Gibbs
CO_2	-188.60336	0.011961 (Hartree/Particle)	-0.00871	-188.61208
1	-242.23921	0.060764 (Hartree/Particle)	0.03531	-242.20390
2	-242.26156	0.060813 (Hartree/Particle)	0.03470	-242.22686
$\mathbf{1}_{OH}$	-317.47415	0.065186 (Hartree/Particle)	0.03745	-317.43670
$\mathbf{2}_{OH}$	-317.50378	0.065492 (Hartree/Particle)	0.03783	-317.46595
$\mathbf{1}_{OH2}$	-392.70433	0.069265 (Hartree/Particle)	0.03973	-392.66460
$\mathbf{2}_{OH2}$	-392.74453	0.070077 (Hartree/Particle)	0.04093	-392.70360
$\mathbf{1}_{O-}$	-316.90411	0.050817 (Hartree/Particle)	0.02202	-316.88209
$\mathbf{2}_{O-}$	-316.92844	0.050922 (Hartree/Particle)	0.02281	-316.90564
$\mathbf{1}_{O2-}$	-391.41717	0.043327 (Hartree/Particle)	0.01451	-391.40266
$\mathbf{2}_{O2-}$	-391.46778	0.042879 (Hartree/Particle)	0.01399	-391.45380

II. $1CO_2$ complex

System	SCF energy E	Zero-point correction	TC to Gibbs	E+Gibbs	BSSE
1…$(CO_2)_N$	-430.84992	0.073771 (Hartree/Particle)	0.03928	-430.81063	0.00032
2…$(CO_2)_{N2}$	-430.87285	0.073865 (Hartree/Particle)	0.03941	-430.83344	0.00032
2…$(CO_2)_{N1}$	-430.87190	0.073770 (Hartree/Particle)	0.03874	-430.83316	0.00032
$\mathbf{1_{OH}}$…$(CO_2)_{N1}$	-506.08488	0.078177 (Hartree/Particle)	0.04214	-506.04274	0.00033
$\mathbf{1_{OH}}$…$(CO_2)_{N2}$	-506.08622	0.078415 (Hartree/Particle)	0.04261	-506.04361	0.00036
$\mathbf{2_{OH}}$…$(CO_2)_{N1}$	-506.11501	0.078521 (Hartree/Particle)	0.04255	-506.07245	0.00033
$\mathbf{2_{OH}}$…$(CO_2)_{N2}$	-506.11773	0.078810 (Hartree/Particle)	0.04350	-506.07423	0.00040
$\mathbf{1_{OH2}}$…$(CO_2)_N$	-581.31739	0.082440 (Hartree/Particle)	0.04485	-581.27255	0.00037
$\mathbf{2_{OH2}}$…$(CO_2)_{N1}$	-581.35597	0.083053 (Hartree/Particle)	0.04562	-581.31035	0.00033
$\mathbf{2_{OH2}}$…$(CO_2)_{N2}$	-581.35884	0.083299 (Hartree/Particle)	0.04665	-581.31219	0.00044
$\mathbf{1_{(CO2–)N3}}$	-505.53077	0.065360 (Hartree/Particle)	0.03376	-505.49701	0.00142
$\mathbf{1_{(CO2–)N1}}$	-505.52204	0.065722 (Hartree/Particle)	0.03349	-505.48855	0.00123
$\mathbf{1_{OCO2–}}$	-505.53785	0.066565 (Hartree/Particle)	0.03254	-505.50531	0.00202
$\mathbf{2_{(CO2–)N2}}$	-505.56319	0.066163 (Hartree/Particle)	0.03338	-505.52981	0.00151
$\mathbf{2_{(CO2–)N4}}$	-505.55142	0.066334 (Hartree/Particle)	0.03375	-505.51767	0.00136
$\mathbf{2_{OCO2–}}$	-505.55412	0.066115 (Hartree/Particle)	0.03291	-505.52122	0.00173
$\mathbf{1_{(NCO2–)O–}}$	-580.09336	0.058599 (Hartree/Particle)	0.02512	-580.06823	0.00290
$\mathbf{1_{(OCO2–)O–}}$	-580.08175	0.057939 (Hartree/Particle)	0.02318	-580.05856	0.00330
$\mathbf{2_{(NCO2–)O–}}$	-580.14413	0.058088 (Hartree/Particle)	0.02325	-580.12089	0.00280
$\mathbf{2_{(OCO2–)O–}}$	-580.14103	0.058478 (Hartree/Particle)	0.02395	-580.11709	0.00378

III. $2CO_2$ complex

System	SCF energy E	Zero-point correction	TC to Gibbs	E+Gibbs	BSSE
$\mathbf{1_{(CO2–)N3}}$…$(CO_2)_{N1}$	-694.14228	0.078225 (Hartree/Particle)	0.03564	-694.10664	0.00134
$\mathbf{1_{(CO2–)N1}}$…$(CO_2)_{N1}$	-694.13681	0.078775 (Hartree/Particle)	0.03862	-694.09819	0.00054
$\mathbf{1_{(CO2–)N3}}$…$(CO_2)_{N3}$	-694.14803	0.078804 (Hartree/Particle)	0.03858	-694.10945	0.00064
$\mathbf{1_{(OCO2–)}}$…$(CO_2)_{N1}$	-694.15114	0.079511 (Hartree/Particle)	0.03763	-694.11350	0.00193
$\mathbf{1_{(OCO2–)}}$…$(CO_2)_O$	-694.15626	0.079799 (Hartree/Particle)	0.03800	-694.11826	0.00072
$\mathbf{1_{(OCO2–)}}$…$(CO_2)_{N3}$	-694.15142	0.079490 (Hartree/Particle)	0.03645	-694.11497	0.00185

$\mathbf{2}_{\mathbf{O-}}$….$(CO_2)_O$…$(CO_2)_{N4}$	-694.16686	0.077308 (Hartree/Particle)	0.03376	-694.13310	0.00089
$\mathbf{2}_{(CO2-)N2}$…$(CO_2)_{N4}$	-694.17722	0.079055 (Hartree/Particle)	0.03800	-694.13922	0.00143
$\mathbf{2}_{(CO2-)N4}$…$(CO_2)_{N4}$	-694.16906	0.079504 (Hartree/Particle)	0.03944	-694.12962	0.00066
$\mathbf{2}_{(CO2-)N2}$…$(CO_2)_{O}$	-694.17987	0.079189 (Hartree/Particle)	0.03909	-694.14078	0.00062
$\mathbf{2}_{(CO2-)N2}$…$(CO_2)_{N2}$	-694.18090	0.079127 (Hartree/Particle)	0.03881	-694.14209	0.00066
$\mathbf{1}_{(CO2-)N1(CO2-)N3}$	-768.74034	0.073132 (Hartree/Particle)	0.03487	-768.70547	0.00187
$\mathbf{1}_{(CO2-)N1(CO2-)N1}$	-768.72286	0.072467 (Hartree/Particle)	0.03368	-768.68918	0.00175
$\mathbf{1}_{(CO2-)N1(OCO2-)}$	-768.73541	0.072763 (Hartree/Particle)	0.03377	-768.70165	0.00249
$\mathbf{1}_{(CO2-)N1}$…$(CO_2)_O$	-768.72304	0.071585 (Hartree/Particle)	0.03123	-768.69181	0.00182
$\mathbf{1}_{(OCO2-)2}$	-768.72688	0.072158 (Hartree/Particle)	0.03247	-768.69441	0.00221
$\mathbf{2}_{(CO2-)N1(CO2-)N2}$	-768.77924	0.072360 (Hartree/Particle)	0.03388	-768.74536	0.00171
$\mathbf{2}_{(CO2-)N1(CO2-)O}$	-768.77956	0.072769 (Hartree/Particle)	0.03372	-768.74584	0.00207
$\mathbf{2}_{(CO2-)N1(CO2-)O}$	-768.79449	0.073069 (Hartree/Particle)	0.03237	-768.76212	0.00276
$\mathbf{2}_{(CO2-)N2(CO2-)N2}$	-768.78281	0.072550 (Hartree/Particle)	0.03351	-768.74930	0.00212
$\mathbf{2}_{(OCO2-)2}$	-768.78713	0.073069 (Hartree/Particle)	0.03321	-768.75392	0.00262

IV. $3CO_2$ complex

System	SCF energy E	Zero-point correction	TC to Gibbs	E+Gibbs	BSSE
$\mathbf{1}_{(NCO2-)2}$…$(CO_2)_O$	-957.36453	0.086261 (Hartree/Particle)	0.04126	-957.32327	0.00094
$\mathbf{1}_{(NCO2-)2}$…$(CO_2)_{N1}$	-957.36281	0.086123 (Hartree/Particle)	0.04086	-957.32194	0.00177
$\mathbf{2}_{(NCO2-)(OCO2-)}$…$(CO_2)_{N2}$	-957.41859	0.086122 (Hartree/Particle)	0.03945	-957.37914	0.00093
$\mathbf{2}_{(NCO2-)(OCO2-)}$—$(CO_2)_O$	-957.40868	0.086391 (Hartree/Particle)	0.04132	-957.36736	0.00146
$\mathbf{2}_{(NCO2-)(OCO2-)}$—$(CO_2)_N$	-957.41941	0.086938 (Hartree/Particle)	0.04257	-957.37684	0.00160

V. CO_2 complexes of anionic systems in presence of trimethyl phosphonium cation

System	SCF energy E	Zero-point correction	TC to Gibbs	E+Gibbs	BSSE
$(CH_3)_4P^+(OH)^-$	-576.79012	0.162569 (Hartree/Particle)	0.12855	-576.66157	
H_2O	-76.43698	0.021260 (Hartree/Particle)	0.00361	-76.43337	
$(CH_3)_4P^+(CO_2)_1(\mathbf{1}_{O-})$	-1006.47004	0.220566 (Hartree/Particle)	0.17260	-1006.29743	0.00554
$(CH_3)_4P^+(CO_2)_2(\mathbf{1}_{O-})$	-1195.05333	0.234884 (Hartree/Particle)	0.18200	-1194.87132	0.00400

$(CH_3)_4P^+(CO_2)_3(\mathbf{1}_{O-})$	-1383.62525	0.248688 (Hartree/Particle)	0.19009	-1383.43516	0.00266
$(CH_3)_4P^+(CO_2)_1(\mathbf{2}_{O-})$	-1006.50716	0.220216 (Hartree/Particle)	0.17327	-1006.33390	0.00286
$(CH_3)_4P^+(CO_2)_2(\mathbf{2}_{O-})$	-1195.08761	0.234047 (Hartree/Particle)	0.181811	-1194.90580	0.00267
$(CH_3)_4P^+(CO_2)_3(\mathbf{2}_{O-})$	-1383.66122	0.247786 (Hartree/Particle)	0.190127	-1383.47110	0.00257
$((CH_3)_4P^+)_2(CO_2)_2(\mathbf{1}_{O2-})$	-1770.70936	0.381620 (Hartree/Particle)	0.316919	-1770.39244	0.00672
$((CH_3)_4P^+)_2(CO_2)_3(\mathbf{1}_{O2-})$	-1959.28775	0.394775 (Hartree/Particle)	0.325118	-1958.96263	0.00669
$((CH_3)_4P^+)_2(CO_2)_4(\mathbf{1}_{O2-})$	-2147.86618	0.408157 (Hartree/Particle)	0.333119	-2147.53307	0.00638
$((CH_3)_4P^+)_2(CO_2)_5(\mathbf{1}_{O2-})$	-2336.43712	0.421917 (Hartree/Particle)	0.339162	-2336.09796	0.00665
$((CH_3)_4P^+)_2(CO_2)_2(\mathbf{2}_{O2-})$	-1770.75970	0.380422 (Hartree/Particle)	0.312593	-1770.44710	0.00742
$((CH_3)_4P^+)_2(CO_2)_3(\mathbf{2}_{O2-})$	-1959.34625	0.394389 (Hartree/Particle)	0.322213	-1959.02404	0.006552
$((CH_3)_4P^+)_2(CO_2)_4(\mathbf{2}_{O2-})$	-2147.92296	0.407969 (Hartree/Particle)	0.331892	-2147.59107	0.006398
$((CH_3)_4P^+)_2(CO_2)_5(\mathbf{2}_{O2-})$	-2336.51739	0.421413 (Hartree/Particle)	0.337951	-2336.17944	0.005047
$((CH_3)_4P^+)_2(CO_2)_6(\mathbf{2}_{O2-})$	-2525.09314	0.435394 (Hartree/Particle)	0.347599	-2524.74554	0.005373

VI. Anionic systems in presence of trimethyl phosphonium cation

System	SCF energy E	Zero-point correction	TC to Gibbs	E+Gibbs	BSSE
$(CH_3)_4P^+(\mathbf{1}_{O-})$	-817.85683	0.204896 (Hartree/Particle)	0.16190	-817.69609	0.00487
$(CH_3)_4P^+(\mathbf{2}_{O-})$	-817.89600	0.206113 (Hartree/Particle)	0.16395	-817.73205	0.00406
$((CH_3)_4P^+)_2(\mathbf{1}_{O2-})$	-1393.48364	0.352162 (Hartree/Particle)	0.29864	-1393.18500	0.01424
$((CH_3)_4P^+)_2(\mathbf{2}_{O2-})$	-1393.53285	0.350938 (Hartree/Particle)	0.29407	-1393.23878	0.01339

Table S7. Cartesian coordinates for all the systems (Given in the order Atomic number, x, y, z coordinates, respectively).

I. Tz system

CO_2				**1**			
6	0.000000000	0.000000000	0.000000000	6	0.000000000	0.700188000	-0.904708000
8	0.000000000	0.000000000	1.153876283	7	0.000000000	1.117374000	0.353561000
8	0.000000000	0.000000000	-1.153876283	7	0.000000000	0.000000000	1.043020000
				7	0.000000000	-1.117374000	0.353561000
				6	0.000000000	-0.700188000	-0.904708000
				1	0.000000000	1.397968000	-1.721430000
				1	0.000000000	-1.397968000	-1.721430000
				1	0.000000000	0.000000000	2.048367000
2				**1_{OH}**			
6	-0.669771000	-0.890839000	0.000000000	6	1.137632000	-0.147960000	0.000000000
7	-1.129665000	0.339577000	0.000000000	7	0.719828000	-1.405193000	0.000000000
7	0.000000000	1.064314000	0.000000000	7	-0.584327000	-1.309023000	0.000000000
6	1.070810000	0.256997000	0.000000000	7	-1.080334000	-0.080073000	0.000000000
7	0.684049000	-0.995704000	0.000000000	6	0.000000000	0.673491000	0.000000000
1	-1.328614000	-1.741147000	0.000000000	1	2.179174000	0.110797000	0.000000000
1	-0.042513000	2.067941000	0.000000000	1	-1.178694000	-2.118117000	0.000000000
1	2.084207000	0.618943000	0.000000000	8	-0.032496000	2.014776000	0.000000000
				1	-0.952467000	2.295954000	0.000000000
2_{OH}				**1_{OH2}**			
6	-0.749788000	-1.296562000	0.000000000	6	0.000000000	0.763518000	0.000000000
7	0.542670000	-1.491486000	0.000000000	7	-1.310112000	0.664319000	0.000000000
7	1.023063000	-0.221762000	0.000000000	7	-1.526183000	-0.639702000	0.000000000
6	0.000000000	0.638737000	0.000000000	7	-0.444883000	-1.399939000	0.000000000
7	-1.143869000	0.010032000	0.000000000	6	0.544427000	-0.535335000	0.000000000
8	0.205081000	1.954672000	0.000000000	1	-2.450559000	-1.027162000	0.000000000
1	-1.445872000	-2.116844000	0.000000000	8	1.845668000	-0.863245000	0.000000000
1	-0.658209000	2.381430000	0.000000000	1	1.915680000	-1.822602000	0.000000000
1	2.009116000	-0.032504000	0.000000000	8	0.678484000	1.921278000	0.000000000
				1	0.043343000	2.643657000	0.000000000
2_{OH2}				**1_{O-}**			
6	1.051586000	0.080247000	0.000000000	6	-0.102953000	1.107836000	0.000967000
7	0.755286000	-1.189093000	0.000000000	7	-1.363798000	0.710355000	0.001705000
7	-0.614163000	-1.143222000	0.000000000	7	-1.268589000	-0.600624000	-0.010785000
6	-1.018464000	0.123930000	0.000000000	7	-0.029760000	-1.120170000	0.000885000
7	0.000000000	0.947293000	0.000000000	6	0.796572000	-0.032192000	0.000797000
8	2.316567000	0.505906000	0.000000000	1	0.151030000	2.154438000	-0.000757000
8	-2.309870000	0.441996000	0.000000000	8	2.050565000	-0.044444000	0.000502000
1	-1.163966000	-1.982528000	0.000000000	1	-2.082232000	-1.179685000	0.043526000
1	2.299714000	1.466912000	0.000000000				
1	-2.375911000	1.402493000	0.000000000				
2_{O-}				**1_{O2-}**			
6	0.000000000	0.781407000	0.000000000	6	0.363228000	-0.769498000	-0.000440000
7	-1.132513000	0.023562000	0.000000000	7	-0.894643000	-1.174276000	-0.004068000
7	-0.657563000	-1.262508000	0.000000000	7	-1.700983000	-0.000047000	-0.114225000
6	0.679498000	-1.263735000	0.000000000	7	-0.894694000	1.174234000	-0.004113000
7	1.158234000	-0.055164000	0.000000000	6	0.363185000	0.769527000	-0.000433000
8	0.047832000	2.021730000	0.000000000	8	1.398780000	1.495636000	0.009790000
1	-1.287897000	-2.039009000	0.000000000	1	-2.307375000	-0.000028000	0.705657000
1	1.251148000	-2.182100000	0.000000000	8	1.398862000	-1.495578000	0.009764000

2_{O2-}			
7	0.000000000	0.717260000	-1.207023000
6	0.000000000	1.140989000	0.043364000
7	0.000000000	0.000000000	0.859949000
6	0.000000000	-1.140989000	0.043364000
7	0.000000000	-0.717260000	-1.207023000
8	0.000000000	2.321548000	0.531075000
8	0.000000000	-2.321548000	0.531075000
1	0.000000000	0.000000000	1.861102000

II. $1CO_2$ complex

1…$(CO_2)_N$			**E_{ad}**=-4.4
6	1.468640000	1.181963000	0.000479000
7	0.371288000	0.437627000	0.000210000
7	0.832563000	-0.792212000	-0.000404000
7	2.136063000	-0.925504000	-0.000453000
6	2.575944000	0.326168000	0.000044000
1	1.413644000	2.254702000	0.000829000
1	3.627233000	0.546429000	0.000044000
1	0.204770000	-1.580232000	0.000034000
6	-2.387490000	-0.051084000	0.000070000
8	-2.062074000	-1.162774000	0.000636000
8	-2.758877000	1.037455000	-0.000627000

2…$(CO_2)_{N2}$			**E_{ad}**=-4.8
6	-1.458757000	1.160381000	-0.000323000
7	-0.359135000	0.439585000	-0.000184000
7	-0.835822000	-0.814361000	0.000286000
6	-2.174460000	-0.797830000	0.000268000
7	-2.607985000	0.441675000	-0.000025000
1	-1.430854000	2.235721000	-0.000608000
1	-0.191344000	-1.587929000	-0.000157000
1	-2.776620000	-1.689570000	0.000656000
6	2.382120000	-0.063299000	0.000003000
8	2.055072000	-1.175056000	-0.000463000
8	2.760678000	1.022303000	0.000449000

2…$(CO_2)_{N1}$			**E_{ad}**=-4.2
6	1.389769000	-1.144286000	-0.001426000
7	2.558806000	-0.547129000	0.002696000
7	2.215386000	0.750868000	0.002111000
6	0.882930000	0.883100000	-0.002272000
7	0.322851000	-0.304173000	-0.004604000
1	1.298585000	-2.215970000	-0.002242000
1	2.925017000	1.462118000	0.004797000
1	0.371946000	1.830199000	-0.003469000
6	-2.428753000	0.047613000	0.000991000
8	-2.205904000	1.182710000	0.000144000
8	-2.711413000	-1.069194000	0.001824000

1_{OH}…$(CO_2)_{N1}$			**E_{ad}**=-4.4
6	-1.043760000	-1.066055000	0.001564000
7	0.086784000	-0.373642000	0.002285000
7	-0.298038000	0.876277000	0.001124000
7	-1.604385000	1.081234000	-0.000327000
6	-2.098020000	-0.141424000	-0.000300000
1	-1.059973000	-2.139151000	0.002278000
1	0.370905000	1.628222000	0.001145000
8	-3.412200000	-0.408826000	-0.001633000
1	-3.891888000	0.425145000	-0.002890000
6	2.866500000	-0.029721000	-0.000913000
8	3.183165000	-1.135257000	-0.001248000
8	2.596798000	1.096821000	-0.000147000

1_{OH}…$(CO_2)_{N2}$			**E_{ad}**=-5.2
6	2.365357000	0.346533000	-0.000262000
7	2.428574000	-0.976822000	-0.000210000
7	1.179477000	-1.358842000	0.000133000
7	0.273800000	-0.389885000	0.000355000
6	1.008171000	0.706992000	0.000109000
1	3.244051000	0.962755000	-0.000530000
1	0.915466000	-2.327838000	0.000270000
8	0.498771000	1.943026000	0.000123000
1	-0.464603000	1.881438000	0.000869000
6	-2.485383000	-0.156283000	-0.000096000
8	-2.689047000	-1.287943000	-0.000022000
8	-2.334317000	0.992296000	-0.000233000

2_{OH}…$(CO_2)_{N1}$			**E_{ad}**=-4.7
6	0.826510000	1.553652000	0.004472000
7	-0.127918000	0.658905000	0.017909000
7	0.566167000	-0.506980000	0.013961000
6	1.873798000	-0.238232000	-0.002052000
7	2.091977000	1.050911000	-0.008276000
8	2.779783000	-1.212755000	-0.009590000
1	0.613958000	2.608230000	0.004020000
1	3.649623000	-0.799534000	-0.019831000
1	0.084718000	-1.390552000	0.017858000
6	-2.732587000	-0.306876000	-0.004700000
8	-2.222282000	-1.346954000	0.004054000
8	-3.290777000	0.698552000	-0.013654000

2_{OH}…$(CO_2)_{N2}$			**E_{ad}**=-6.4
6	1.239961000	-1.429170000	0.000145000
7	2.458861000	-0.961039000	-0.000432000
7	2.250616000	0.380781000	-0.000281000
6	0.937781000	0.631817000	0.000241000
7	0.253706000	-0.485469000	0.000595000

1_{OH2}…$(CO_2)_N$			**E_{ad}**=-5.2
6	0.679119000	-0.510830000	-0.006220000
7	-0.163975000	0.499931000	-0.013477000
7	0.616799000	1.568113000	-0.008355000
7	1.914654000	1.323146000	0.001812000
6	1.988281000	0.011482000	0.003432000

8	0.471379000	1.872803000	0.000267000	1	0.246755000	2.499817000	-0.011515000
1	1.036668000	-2.485545000	0.000240000	8	3.131705000	-0.689664000	0.012678000
1	-0.495520000	1.824730000	0.000980000	1	3.867460000	-0.069978000	0.016590000
1	3.015430000	1.031489000	-0.000648000	8	0.329401000	-1.801422000	-0.008030000
6	-2.481132000	-0.150954000	-0.000199000	1	-0.634088000	-1.859494000	-0.010632000
8	-2.294790000	0.994765000	-0.000460000	6	-2.879338000	-0.054666000	0.005488000
8	-2.736404000	-1.270161000	0.000084000	8	-3.213386000	1.045632000	0.009992000
				8	-2.595325000	-1.177620000	0.001549000
2_{OH2}…$(CO_2)_{N1}$			**E_{ad}**=-4.9	**2_{OH2}…$(CO_2)_{N2}$**			**E_{ad}**=-6.6
6	-0.856645000	1.165219000	-0.000321000	6	1.240161000	0.966184000	-0.000055000
7	0.178544000	0.370119000	-0.001540000	7	2.410681000	0.394713000	-0.000120000
7	-0.423234000	-0.860388000	-0.001240000	7	2.062115000	-0.931632000	-0.000051000
6	-1.742604000	-0.706415000	0.000191000	6	0.737886000	-1.051054000	0.000131000
7	-2.075830000	0.562597000	0.000758000	7	0.163750000	0.130526000	0.000212000
8	-0.720493000	2.491328000	-0.000208000	8	1.100221000	2.292361000	-0.000190000
8	-2.565943000	-1.749570000	0.000819000	8	0.138617000	-2.232438000	0.000302000
1	0.133436000	-1.698059000	-0.001438000	1	2.759640000	-1.653150000	-0.000395000
1	-1.601807000	2.875284000	0.000526000	1	0.158430000	2.488898000	0.000500000
1	-3.467844000	-1.412491000	0.001821000	1	-0.816956000	-2.081017000	0.000252000
6	2.847771000	-0.395095000	0.000438000	6	-2.535838000	0.191180000	-0.000030000
8	3.336569000	0.645324000	0.001267000	8	-2.601639000	1.339320000	0.000364000
8	2.410957000	-1.468742000	-0.000452000	8	-2.538472000	-0.967723000	-0.000591000
$1_{(CO2–)N3}$			**E_{ad}**=-13.7	**$1_{(CO2–)N1}$**			**E_{ad}**=-8.4
6	0.648116000	0.923733000	0.000279000	6	2.106706000	-0.100795000	-0.004341000
7	-0.343729000	0.046228000	0.000118000	7	1.706325000	-1.354030000	-0.002047000
7	0.187109000	-1.148319000	-0.000766000	7	0.409785000	-1.314752000	0.009125000
7	1.504199000	-1.151620000	-0.000197000	7	-0.093794000	-0.062192000	0.006574000
6	1.889117000	0.180281000	0.000109000	6	0.980527000	0.822263000	0.000140000
1	0.446667000	1.977219000	0.000420000	1	3.149864000	0.158536000	-0.009692000
8	3.055544000	0.599639000	0.000115000	8	0.959406000	2.044184000	-0.001016000
1	-0.433784000	-1.941571000	0.001942000	1	-0.245310000	-2.079782000	-0.008237000
6	-1.923501000	0.179603000	0.000035000	6	-1.632592000	0.021045000	-0.000280000
8	-2.425834000	-0.931658000	0.000399000	8	-2.109534000	-1.118352000	-0.006294000
8	-2.270751000	1.336847000	-0.000387000	8	-2.073448000	1.147041000	0.000966000
$1_{OCO2–}$			**E_{ad}**=-17.8	**$2_{(CO2–)N2}$**			**E_{ad}**=-18.7
6	0.958198000	0.989229000	0.000033000	6	-0.978563000	0.820711000	-0.000057000
7	2.281607000	0.917536000	0.000016000	7	0.100433000	-0.066390000	-0.000687000
7	2.527380000	-0.371299000	-0.000017000	7	-0.419365000	-1.325849000	-0.000445000
7	1.470589000	-1.174259000	-0.000022000	6	-1.739663000	-1.208460000	0.000232000
6	0.438477000	-0.333972000	0.000009000	7	-2.148503000	0.028266000	0.000378000
1	0.426885000	1.917684000	0.000064000	8	-0.930157000	2.030135000	-0.000032000
8	-0.787332000	-0.824474000	0.000018000	1	0.263397000	-2.069997000	0.000046000
1	3.460608000	-0.734104000	-0.000038000	1	-2.377866000	-2.079163000	0.000541000
6	-1.996520000	0.077019000	-0.000006000	6	1.618789000	0.000941000	0.000047000
8	-1.736779000	1.272367000	-0.000045000	8	2.086252000	1.118471000	0.000183000
8	-3.006571000	-0.595527000	0.000017000	8	2.091797000	-1.146379000	0.000268000
$2_{(CO2–)N4}$			**E_{ad}**=-11.5	**$2_{OCO2–}$**			**E_{ad}**=-12.9
6	-0.968064000	0.833271000	-0.000167000	6	0.415962000	-0.182652000	-0.396132000
7	-2.138081000	0.132153000	0.000449000	7	1.143807000	-1.125464000	0.182683000
7	-1.758789000	-1.177649000	0.000437000	7	2.325845000	-0.503725000	0.383297000
6	-0.458229000	-1.337829000	-0.000110000	6	2.267655000	0.756138000	-0.070884000
7	0.104217000	-0.144075000	-0.000499000	7	1.090766000	1.001755000	-0.577714000
8	-0.823539000	2.040124000	-0.000709000	8	-0.815384000	-0.375710000	-0.798261000
1	-2.454505000	-1.898252000	0.000711000	1	3.078425000	-0.982786000	0.839078000
1	0.086957000	-2.263404000	-0.000312000	1	3.099393000	1.439075000	-0.010808000

6	1.673307000	-0.038647000	0.000064000	6	-1.936885000	0.072776000	0.188481000
8	2.163356000	-1.166604000	-0.000590000	8	-1.489840000	0.485777000	1.240170000
8	2.089438000	1.094965000	0.001069000	8	-3.017417000	-0.102796000	-0.326274000
$1_{(NCO2–)O–}$			E_{ad}=-43.9	**$1_{(OCO2–)O–}$**			E_{ad}=-36.3
6	0.602344000	0.740806000	-0.029514000	6	-0.297494000	-0.060077000	0.273901000
7	-0.446485000	-0.116172000	-0.160669000	7	-0.631661000	-1.296542000	0.406596000
7	0.034232000	-1.443048000	-0.296388000	7	-1.953797000	-1.354248000	0.001135000
7	1.426452000	-1.427990000	-0.056438000	7	-2.504383000	-0.079944000	-0.173414000
6	1.832287000	-0.176377000	0.030612000	6	-1.483996000	0.776452000	-0.090513000
8	3.000299000	0.257708000	0.159017000	8	-1.501903000	2.019231000	-0.256405000
1	-0.437969000	-1.975862000	0.427532000	1	-2.485775000	-1.891070000	0.675293000
8	0.591089000	1.960509000	0.042262000	8	0.916325000	0.433029000	0.566645000
6	-1.902654000	0.052302000	0.018348000	6	2.123617000	-0.034030000	-0.110203000
8	-2.482446000	-1.013010000	0.305685000	8	3.136513000	0.346001000	0.482253000
8	-2.340601000	1.193036000	-0.125682000	8	1.956804000	-0.684242000	-1.136822000
$2_{(NCO2–)O–}$			E_{ad}=-44.0	**$2_{(OCO2–)O–}$**			E_{ad}=-41.5
7	-0.639087000	-1.130318000	0.031579000	7	-2.231479000	1.009948000	0.077232000
6	-1.794717000	-0.499112000	0.023095000	6	-2.108068000	-0.314250000	-0.020182000
7	-1.525770000	0.887910000	-0.004707000	7	-0.726712000	-0.590456000	-0.099869000
6	-0.166067000	1.126421000	-0.030135000	6	-0.095535000	0.609820000	-0.011694000
7	0.364483000	-0.132327000	0.007869000	7	-0.941378000	1.579929000	0.082425000
8	-2.974245000	-0.935954000	0.037739000	8	-2.981538000	-1.219967000	-0.046522000
8	0.335537000	2.251341000	-0.089336000	8	1.243945000	0.809815000	-0.074266000
1	-2.214103000	1.612887000	-0.058514000	1	-0.244398000	-1.469857000	-0.065686000
6	1.804406000	-0.509818000	0.010355000	6	2.219344000	-0.240913000	0.015679000
8	2.584515000	0.438029000	0.170322000	8	1.803466000	-1.397776000	0.160682000
8	2.023567000	-1.715252000	-0.144295000	8	3.364994000	0.201176000	-0.071849000

III. $2CO_2$ complex

$1_{(CO2–)N3}...(CO_2)_{N1}$			E_{ad}=-18.9	**$1_{(CO2–)N1}...(CO_2)_{N1}$**			E_{ad}=-16.0
6	-0.230852000	1.718739000	0.001919000	6	-1.833902000	-0.929660000	0.000124000
7	-0.948709000	0.616564000	-0.004176000	7	-0.894157000	0.005833000	0.000192000
7	-0.104511000	-0.369028000	-0.015763000	7	-1.491644000	1.170113000	0.000323000
7	1.182567000	0.029846000	-0.008434000	7	-2.803673000	1.095979000	-0.000035000
6	1.194898000	1.421955000	0.000512000	6	-3.113844000	-0.257872000	-0.000028000
1	-0.689490000	2.690650000	0.007695000	1	-1.570282000	-1.969113000	0.000273000
8	2.157782000	2.173176000	0.005477000	8	-4.253839000	-0.739765000	-0.000125000
1	-0.300402000	-1.358257000	0.002843000	1	-0.916626000	1.997697000	-0.000723000
6	-3.442167000	-0.403447000	0.002770000	6	0.653551000	-0.042872000	-0.000153000
8	-2.970795000	-1.458524000	0.004348000	8	1.121157000	1.089050000	-0.000518000
8	-3.999044000	0.607500000	0.001524000	8	1.085177000	-1.176685000	0.000014000
6	2.224894000	-1.117999000	0.000819000	6	3.641569000	-0.087719000	0.000098000
8	1.639205000	-2.202775000	0.004812000	8	3.694515000	-0.087992000	-1.153548000
8	3.373330000	-0.743071000	0.002832000	8	3.694113000	-0.087523000	1.153782000
$1_{(CO2–)N3}...(CO_2)_{N3}$			E_{ad}=-22.9	**$1_{(OCO2–)}...(CO_2)_{N1}$**			E_{ad}=-24.1
6	3.263733000	-0.061449000	-0.105235000	6	0.098653000	0.511090000	0.002364000
7	2.899236000	-1.317927000	-0.079984000	7	-1.148168000	0.059812000	0.002905000
7	1.606288000	-1.324736000	0.108410000	7	-1.019077000	-1.245980000	0.001356000
7	1.072324000	-0.075304000	0.106552000	7	0.221168000	-1.709270000	-0.000072000
6	2.116525000	0.836317000	0.002397000	6	0.972850000	-0.608864000	0.000457000
1	4.294206000	0.228584000	-0.205194000	1	0.339877000	1.553263000	0.003280000
8	2.069330000	2.053817000	0.004847000	8	2.285642000	-0.728773000	-0.000653000
1	0.976678000	-2.080257000	-0.116250000	1	-1.819042000	-1.850946000	0.001548000

6	-0.435266000	-0.010432000	0.069036000	6	-3.789998000	0.481176000	-0.001320000
8	-0.921737000	-1.147756000	-0.009027000	8	-3.923057000	-0.669550000	-0.001812000
8	-0.909612000	1.106959000	0.112528000	8	-3.767163000	1.632840000	-0.000979000
6	-3.401649000	0.009524000	-0.056297000	6	3.188223000	0.486058000	-0.000670000
8	-3.519613000	-0.049796000	1.091523000	8	4.347096000	0.130203000	-0.002195000
8	-3.415353000	0.065986000	-1.210223000	8	2.592899000	1.553903000	0.000745000
1$_{(OCO2-)}$...$(CO_2)_O$			E_{ad}=-28.0	**1**$_{(OCO2-)}$...$(CO_2)_{N3}$			E_{ad}=-24.3
6	2.327010000	0.984557000	0.000161000	6	0.884656000	1.725160000	-0.001819000
7	3.651148000	0.924871000	0.000189000	7	-0.224841000	2.450987000	-0.000805000
7	3.908778000	-0.361380000	0.000109000	7	-1.188162000	1.564614000	-0.002057000
7	2.860759000	-1.173688000	0.000014000	7	-0.810062000	0.291095000	-0.003817000
6	1.823225000	-0.342846000	0.000003000	6	0.521154000	0.350773000	-0.003821000
1	1.787354000	1.908111000	0.000196000	1	1.862326000	2.159019000	-0.000738000
8	0.600475000	-0.851968000	-0.000173000	8	1.213963000	-0.768800000	-0.006796000
1	4.845477000	-0.715727000	0.000117000	1	-2.159738000	1.813514000	-0.001450000
6	-0.595685000	0.024140000	-0.000158000	6	-3.126095000	-1.057022000	0.002789000
8	-0.369335000	1.223517000	-0.000248000	8	-3.655859000	-0.024866000	0.001511000
8	-1.608071000	-0.662499000	-0.000036000	8	-2.703434000	-2.126746000	0.004352000
6	-4.033393000	0.052223000	0.000049000	6	2.733183000	-0.758885000	0.001550000
8	-3.834687000	1.189683000	-0.000003000	8	3.143027000	-1.898850000	-0.006057000
8	-4.376453000	-1.052414000	0.000107000	8	3.224989000	0.359317000	0.014083000
2$_{O-}$...$(CO_2)_O$...$(CO_2)_{N4}$			E_{ad}=-19.3	**2**$_{(CO2-)N2}$...$(CO_2)_{N4}$			E_{ad}=-25.5
6	-0.346811000	0.013637000	0.007194000	6	0.224939000	0.794504000	-0.000796000
7	-1.056557000	1.171811000	-0.007403000	7	1.325154000	-0.064139000	-0.000223000
7	-0.092634000	2.139952000	-0.011517000	7	0.839452000	-1.336848000	0.000193000
6	1.121380000	1.590908000	-0.000456000	6	-0.480542000	-1.263106000	-0.000184000
7	1.045647000	0.288216000	0.011423000	7	-0.921021000	-0.034029000	-0.000769000
8	-0.835284000	-1.130785000	0.015829000	8	0.236259000	2.003458000	-0.001200000
1	-0.342855000	3.108704000	-0.022191000	1	1.543530000	-2.061608000	0.000621000
1	2.030178000	2.173851000	-0.001698000	1	-1.102111000	-2.145043000	-0.000038000
6	3.368147000	-0.819205000	-0.001558000	6	-3.570024000	0.011706000	0.000530000
8	3.882363000	0.221400000	0.008390000	8	-3.568417000	-1.147582000	-0.001196000
8	3.023656000	-1.919539000	-0.012596000	8	-3.703232000	1.155862000	0.002013000
6	-3.312104000	-0.571087000	-0.001813000	6	2.846761000	0.042932000	0.000436000
8	-3.413077000	-0.560916000	1.150718000	8	3.344961000	-1.092284000	0.000826000
8	-3.400931000	-0.581150000	-1.155320000	8	3.281264000	1.172490000	0.000194000
2$_{(CO2-)N4}$...$(CO_2)_{N4}$			E_{ad}=-20.9	**2**$_{(CO2-)N2}$...$(CO_2)_O$			E_{ad}=-27.7
6	2.124635000	0.844216000	-0.000109000	6	0.142372000	-0.121906000	0.000226000
7	3.302098000	0.156716000	-0.000168000	7	-1.227044000	0.112265000	-0.001534000
7	2.941458000	-1.157026000	0.000002000	7	-1.397457000	1.462920000	-0.001206000
6	1.646130000	-1.341472000	0.000160000	6	-0.194451000	2.017087000	0.000391000
7	1.065973000	-0.153066000	0.000106000	7	0.770260000	1.140093000	0.001091000
8	1.959731000	2.045876000	-0.000210000	8	0.709965000	-1.196257000	0.000421000
1	3.648596000	-1.866867000	-0.000005000	1	-2.359092000	1.772544000	-0.000898000
1	1.116008000	-2.275490000	0.000307000	1	-0.068878000	3.088672000	0.000934000
6	-0.465099000	-0.060158000	0.000245000	6	-2.522856000	-0.702960000	0.000326000
8	-0.973580000	-1.186232000	0.000403000	8	-2.369465000	-1.902492000	0.001301000
8	-0.912940000	1.067174000	0.000172000	8	-3.494488000	0.064827000	0.000208000
6	-3.420715000	0.007036000	-0.000197000	6	3.230220000	-0.309126000	-0.000354000
8	-3.488896000	0.006007000	-1.153686000	8	3.292517000	-0.307106000	-1.154003000
8	-3.489440000	0.006956000	1.153260000	8	3.295964000	-0.304813000	1.153070000
2$_{(CO2-)N2}$...$(CO_2)_{N2}$			E_{ad}=-28.3	**1**$_{(CO2-)N1(CO2-)N3}$			E_{ad}=-71.9
6	-2.136382000	0.825539000	0.000122000	6	-0.768898000	1.232551000	0.001310000
7	-1.062169000	-0.073348000	0.000067000	7	-1.119544000	-0.065314000	-0.139602000
7	-1.591337000	-1.329911000	-0.000215000	7	0.000003000	-0.891875000	-0.368293000
6	-2.910887000	-1.198872000	-0.000314000	7	1.119551000	-0.065327000	-0.139521000

7	-3.309417000	0.040430000	-0.000123000	6	0.768802000	1.232587000	0.001258000
8	-2.074689000	2.031898000	0.000293000	8	1.459273000	2.224338000	0.128637000
1	-0.920506000	-2.084080000	-0.000275000	1	-0.000085000	-1.642340000	0.317632000
1	-3.556565000	-2.063849000	-0.000520000	8	-1.459417000	2.224263000	0.128888000
6	0.429992000	-0.005707000	0.000230000	6	-2.445073000	-0.769529000	0.007328000
8	0.915425000	1.109169000	0.000536000	8	-2.302128000	-1.980141000	0.205232000
8	0.923993000	-1.148227000	0.000007000	8	-3.424867000	-0.041528000	-0.076972000
6	3.395724000	0.002807000	-0.000177000	6	2.445158000	-0.769517000	0.007259000
8	3.464091000	0.001012000	-1.153659000	8	2.302300000	-1.980218000	0.204466000
8	3.464537000	-0.000711000	1.153264000	8	3.424849000	-0.041289000	-0.076332000
$1_{(CO2–)N1(CO2–)N1}$			E_{ad}=-61.0	**$1_{(CO2–)N1(OCO2–)}$**			E_{ad}=-68.4
6	-1.417342000	-0.758674000	-0.066011000	6	-0.303013000	0.655311000	0.158453000
7	-0.613326000	0.359998000	-0.128449000	7	-1.418232000	-0.082563000	-0.152986000
7	-1.419108000	1.529791000	-0.197512000	7	-1.063456000	-1.430999000	-0.228069000
7	-2.755992000	1.134492000	0.031681000	7	0.217757000	-1.584232000	0.225675000
6	-2.834431000	-0.181756000	0.045304000	6	0.724535000	-0.411265000	0.371994000
8	-3.842463000	-0.907367000	0.140909000	8	1.961160000	-0.189616000	0.806769000
1	-1.113163000	2.123495000	0.568416000	1	-1.755530000	-1.978712000	0.269894000
8	-1.079839000	-1.920366000	-0.088887000	8	-0.178131000	1.858474000	0.272820000
6	0.777903000	0.561707000	-0.040222000	6	-2.884499000	0.210897000	-0.092573000
8	1.196222000	1.691089000	0.130870000	8	-3.555956000	-0.826749000	0.040748000
8	1.468033000	-0.525003000	-0.144281000	8	-3.190886000	1.390950000	-0.167908000
6	3.032734000	-0.360131000	0.037414000	6	3.025759000	0.082672000	-0.206140000
8	3.577293000	-0.274876000	-1.040438000	8	2.643370000	0.029034000	-1.366121000
8	3.340624000	-0.421019000	1.205905000	8	4.098736000	0.292605000	0.342113000
$1_{(CO2–)N1}...(CO_2)_O$			E_{ad}=-61.1	**$1_{(OCO2–)2}$**			E_{ad}=-63.2
6	0.087277000	-0.140302000	-0.042399000	6	0.725142000	0.434530000	-0.330793000
7	1.417829000	0.083917000	-0.156555000	7	1.137078000	1.669963000	-0.210722000
7	1.653951000	1.474468000	-0.269700000	7	-0.000103000	2.401948000	-0.213594000
7	0.439292000	2.145368000	-0.030941000	7	-1.137155000	1.669735000	-0.210389000
6	-0.524120000	1.254664000	0.031051000	6	-0.725002000	0.434384000	-0.330572000
8	-1.763085000	1.443013000	0.153409000	8	-1.490507000	-0.626939000	-0.540985000
1	2.332678000	1.698168000	0.451150000	1	-0.000098000	3.221460000	0.369319000
8	-0.526271000	-1.200287000	0.009290000	8	1.490880000	-0.626604000	-0.541476000
6	2.607193000	-0.788794000	0.017194000	6	-2.774235000	-0.815276000	0.214003000
8	3.629641000	-0.146391000	0.315809000	8	-2.851126000	-0.200377000	1.264780000
8	2.417666000	-1.990855000	-0.142477000	8	-3.499556000	-1.600529000	-0.381818000
6	-3.094877000	-0.604340000	0.006313000	6	2.774216000	-0.815229000	0.214157000
8	-3.244767000	-0.738889000	1.148920000	8	2.850527000	-0.200791000	1.265244000
8	-3.183562000	-0.610566000	-1.150416000	8	3.499861000	-1.600189000	-0.381639000
$2_{(CO2–)N1(CO2–)N2}$			E_{ad}=-64.6	**$2_{(CO2–)N1(CO2–)O}$**			E_{ad}=-64.6
7	-0.684919000	0.019451000	-0.160575000	7	-1.907905000	-0.873665000	-0.014812000
6	-1.136629000	1.301383000	-0.206508000	6	-1.099672000	-1.928967000	-0.032260000
7	-0.000806000	2.078397000	0.000300000	7	0.233137000	-1.434216000	-0.028917000
6	1.135969000	1.301985000	0.205670000	6	0.186252000	-0.093344000	-0.019687000
7	0.685278000	0.020010000	0.157080000	7	-1.086743000	0.250261000	-0.017660000
8	-2.256781000	1.765393000	-0.355226000	8	-1.352237000	-3.147153000	-0.052325000
8	2.255582000	1.767091000	0.354936000	8	1.202030000	0.737990000	0.041920000
1	-0.001145000	3.079477000	0.001212000	1	1.107324000	-1.932195000	-0.038077000
6	1.572067000	-1.153051000	-0.341561000	6	-1.693447000	1.671391000	-0.032437000
8	2.651278000	-1.196586000	0.232157000	8	-1.029713000	2.461050000	-0.693024000
8	1.041419000	-1.800932000	-1.232237000	8	-2.730804000	1.752339000	0.608997000
6	-1.571390000	-1.152904000	0.342019000	6	2.629888000	0.276862000	0.071727000
8	-1.040965000	-1.796662000	1.235749000	8	2.802607000	-0.930996000	-0.078294000
8	-2.650012000	-1.199424000	-0.232449000	8	3.368758000	1.224256000	0.240693000
$2_{(CO2–)N1(CO2–)O}$			E_{ad}=-73.6	**$2_{(CO2–)N2(CO2–)N2}$**			E_{ad}=-66.6

7	0.374828000	-1.071197000	-0.000067000	7	-1.679387000	1.138046000	0.000297000
6	-0.703156000	-0.368510000	-0.000061000	6	-2.816880000	0.469433000	-0.000094000
7	-0.442013000	0.970192000	-0.000065000	7	-2.510285000	-0.918043000	-0.000480000
6	0.939123000	1.148239000	0.000006000	6	-1.157605000	-1.132295000	0.000085000
7	1.413606000	-0.141691000	-0.000034000	7	-0.656775000	0.160095000	0.000381000
8	-1.920201000	-0.918164000	-0.000168000	8	-3.997828000	0.868080000	-0.000160000
8	1.493527000	2.236610000	0.000145000	8	-0.602002000	-2.218959000	0.000305000
1	-1.166523000	1.668184000	0.000161000	1	-3.185715000	-1.657100000	-0.000012000
6	2.852052000	-0.613937000	0.000004000	6	0.690628000	0.582998000	0.000115000
8	3.669360000	0.304705000	-0.000512000	8	1.522734000	-0.423730000	0.000148000
8	2.969787000	-1.836570000	0.000539000	8	0.976108000	1.755576000	-0.000100000
6	-3.166201000	-0.143095000	0.000011000	6	3.022139000	-0.066407000	-0.000118000
8	-3.051491000	1.085660000	0.000374000	8	3.467920000	0.001483000	-1.129826000
8	-4.134648000	-0.885429000	-0.000224000	8	3.468212000	0.001805000	1.129469000

2$_{(OCO2-)2}$			E_{ad}=-69.0
7	0.695423000	2.152737000	-0.041897000
6	1.076528000	0.908985000	-0.068888000
7	-0.000166000	0.073993000	-0.001766000
6	-1.076496000	0.909119000	0.068424000
7	-0.694985000	2.152849000	0.045327000
8	2.351603000	0.549782000	-0.219227000
8	-2.351941000	0.550193000	0.216346000
1	-0.000518000	-0.933535000	-0.001303000
6	2.850589000	-0.805851000	0.072685000
8	2.005245000	-1.623252000	0.425129000
8	4.059771000	-0.861243000	-0.102203000
6	-2.850565000	-0.806075000	-0.072646000
8	-2.004633000	-1.625079000	-0.420024000
8	-4.060260000	-0.860474000	0.099003000

IV. $3CO_2$ complex

1$_{(NCO2-)2}$…$(CO_2)_O$			E_{ad}=-85.6	**1**$_{(NCO2-)2}$…$(CO_2)_{N1}$			E_{ad}=-83.9
6	1.160050000	-1.249252000	0.133641000	6	0.647713000	1.522387000	-0.020177000
7	1.921925000	-0.167363000	-0.143230000	7	-0.056197000	0.373374000	-0.176617000
7	1.141308000	0.981097000	-0.382480000	7	0.787142000	-0.735965000	-0.401127000
7	-0.168005000	0.616085000	-0.013225000	7	2.089194000	-0.260112000	-0.141139000
6	-0.274435000	-0.708952000	0.216783000	6	2.120338000	1.081941000	0.010281000
8	-1.257905000	-1.383914000	0.464527000	8	3.059814000	1.835908000	0.163163000
1	1.462429000	1.729398000	0.226551000	1	0.568670000	-1.463684000	0.274743000
8	1.472100000	-2.408852000	0.312361000	8	0.262081000	2.665265000	0.097569000
6	3.419636000	0.043736000	-0.113264000	6	-1.507492000	0.093793000	-0.099200000
8	3.707985000	1.239826000	-0.017001000	8	-1.761389000	-1.113578000	0.018090000
8	4.079964000	-0.982873000	-0.172557000	8	-2.244346000	1.076483000	-0.142298000
6	-1.146315000	1.737397000	0.171115000	6	-4.341047000	-0.507417000	0.098026000
8	-2.317499000	1.382808000	0.284988000	8	-4.494972000	-0.617956000	-1.043400000
8	-0.597515000	2.838557000	0.201255000	8	-4.376042000	-0.439223000	1.252430000
6	-3.638735000	-0.707618000	-0.317213000	6	3.154100000	-1.318070000	0.043949000
8	-4.113310000	-0.800256000	0.733469000	8	4.301678000	-0.900983000	-0.009773000
8	-3.330099000	-0.689048000	-1.432088000	8	2.659263000	-2.432565000	0.234239000

2$_{(NCO2-)(OCO2-)}$…$(CO_2)_{N2}$			E_{ad}=-87.7	**2**$_{(NCO2-)(OCO2-)}$—$(CO_2)_O$			E_{ad}=-81.2
7	-0.248847000	-0.293336000	-0.000141000	7	0.263720000	1.798168000	0.023884000
6	0.996904000	0.035193000	-0.000038000	6	1.136750000	0.840104000	0.039256000
7	1.164569000	1.388354000	0.000029000	7	0.521678000	-0.387103000	0.020785000
6	-0.090149000	1.991339000	-0.000017000	6	-0.812990000	-0.151905000	-0.002469000

7	-0.945039000	0.914009000	-0.000107000	7	-0.962351000	1.169146000	0.009844000
8	1.977235000	-0.864055000	0.000058000	8	2.435613000	1.057491000	0.099253000
8	-0.280415000	3.195685000	-0.000090000	8	-1.761690000	-1.020752000	-0.088300000
1	2.072723000	1.822657000	0.000110000	1	0.980488000	-1.288378000	0.012651000
6	-2.445679000	0.913447000	-0.000240000	6	-2.291575000	2.020980000	0.024525000
8	-2.949484000	2.031400000	0.000540000	8	-3.208799000	1.417556000	0.550554000
8	-2.940462000	-0.218016000	-0.001098000	8	-2.129385000	3.113798000	-0.484442000
6	3.411573000	-0.511431000	0.000016000	6	3.467041000	-0.034314000	-0.020408000
8	3.676172000	0.692653000	0.000164000	8	3.011550000	-1.159805000	-0.173763000
8	4.097073000	-1.517623000	-0.000120000	8	4.579172000	0.445270000	0.063534000
6	-1.893151000	-2.519328000	0.000304000	6	-1.501065000	-2.590737000	-0.028307000
8	-1.899415000	-2.618277000	1.152952000	8	-2.540603000	-3.144977000	-0.265596000
8	-1.898766000	-2.619413000	-1.152248000	8	-0.352206000	-2.868315000	0.240030000

2$_{(NCO2-)(OCO2-)}$–$(CO_2)_N$			E_{ad}=-87.8
7	0.637929000	-1.079189000	0.001516000
6	1.725102000	-0.386303000	0.000594000
7	1.481466000	0.960399000	0.000324000
6	0.114292000	1.170979000	0.001246000
7	-0.382038000	-0.126469000	0.001500000
8	2.926012000	-0.939844000	-0.000181000
8	-0.442499000	2.247239000	0.000594000
1	2.224596000	1.641377000	0.000073000
6	-1.743317000	-0.577260000	0.001456000
8	-2.571863000	0.409209000	-0.000996000
8	-1.979686000	-1.759125000	0.003211000
6	4.199854000	-0.156378000	-0.000986000
8	4.073149000	1.067264000	-0.001274000
8	5.150278000	-0.910224000	-0.001172000
6	-4.131298000	0.001334000	-0.001613000
8	-4.539598000	-0.069764000	1.131401000
8	-4.537531000	-0.074604000	-1.135037000

V. CO_2 complexes of anionic systems in presence of trimethyl phosphonium cation

$(CH_3)_4P^+(OH)^-$				H_2O			
15	-0.505301000	0.001652000	-0.000621000	8	0.000000000	0.000000000	0.118293000
6	0.090396000	1.244282000	1.142422000	1	0.000000000	0.758963000	-0.473171000
1	-0.267852000	2.224070000	0.827839000	1	0.000000000	-0.758963000	-0.473171000
1	-0.274228000	1.020121000	2.144325000				
1	1.180502000	1.195954000	1.101032000				
6	-2.300157000	-0.003381000	-0.009630000				
1	-2.662037000	-0.221995000	0.994530000				
1	-2.661351000	0.974877000	-0.325267000				
1	-2.653579000	-0.766934000	-0.701719000				
6	0.109818000	0.371685000	-1.639824000				
1	-0.247893000	1.354150000	-1.946762000				
1	1.199237000	0.360116000	-1.560563000				
1	-0.241294000	-0.386427000	-2.339018000				
6	0.088834000	-1.608703000	0.504620000				
1	1.178234000	-1.552185000	0.480094000				
1	-0.277555000	-2.362617000	-0.191528000				
8	2.742253000	-0.006788000	0.002222000				
1	3.704080000	-0.005867000	0.012426000				
1	-0.268125000	-1.827043000	1.510623000				
$(CH_3)_4P^+(CO_2)_1$(**1**$_{O-}$)				$(CH_3)_4P^+(CO_2)_2$(**1**$_{O-}$)			
6	-3.176104000	0.707142000	0.932276000	6	3.779181000	-1.307370000	0.607199000

7	-4.203249000	1.415335000	0.482089000	7	4.915749000	-1.906378000	0.273316000
7	-4.561053000	0.794779000	-0.617081000	7	5.567177000	-1.002231000	-0.416366000
7	-3.852006000	-0.268287000	-0.940121000	7	4.961337000	0.153382000	-0.577982000
6	-2.962107000	-0.346552000	0.034942000	6	3.824631000	-0.020456000	0.065607000
1	-2.647587000	0.968672000	1.831564000	1	3.016963000	-1.797338000	1.184395000
8	-2.092631000	-1.376052000	0.083547000	8	2.964849000	1.032681000	0.162033000
1	-5.339089000	1.107381000	-1.180738000	1	6.483946000	-1.178851000	-0.804816000
6	-0.691275000	-1.085307000	0.169407000	6	1.632134000	0.787715000	0.057007000
8	-0.370054000	0.104969000	0.126241000	8	1.161101000	-0.302850000	-0.143409000
8	-0.020697000	-2.112879000	0.265830000	8	0.996428000	1.910489000	0.209037000
15	3.064030000	0.302917000	-0.071319000	15	-3.825394000	-0.667369000	-0.056947000
6	2.446766000	-0.659901000	-1.450693000	6	-2.145612000	-1.183877000	-0.403846000
1	2.756475000	-1.697493000	-1.331242000	1	-1.894510000	-0.948267000	-1.437037000
1	2.871393000	-0.250834000	-2.367458000	1	-2.076665000	-2.259529000	-0.241295000
6	2.602211000	-0.417474000	1.503141000	6	-4.074320000	1.050242000	-0.499614000
1	2.922674000	-1.458446000	1.527084000	1	-3.857039000	1.181642000	-1.558963000
1	3.103398000	0.141445000	2.293485000	1	-5.113342000	1.311274000	-0.299189000
1	1.522949000	-0.355316000	1.622256000	1	-3.408572000	1.673712000	0.095037000
6	4.855088000	0.340947000	-0.170506000	6	-4.961365000	-1.680608000	-1.002744000
1	5.234864000	-0.678728000	-0.113095000	1	-4.744943000	-1.557776000	-2.063571000
1	5.152761000	0.791997000	-1.116260000	1	-4.832865000	-2.724305000	-0.718583000
1	5.249014000	0.927457000	0.658534000	1	-5.982634000	-1.363288000	-0.795161000
6	2.439076000	1.978393000	-0.178166000	6	-4.146155000	-0.876974000	1.693078000
1	2.750529000	2.412569000	-1.127685000	1	-3.995077000	-1.921672000	1.962506000
1	1.352494000	1.953670000	-0.116747000	1	-3.455492000	-0.246658000	2.253088000
1	2.847443000	2.562838000	0.645784000	1	-5.172920000	-0.583370000	1.908343000
1	1.361514000	-0.593541000	-1.477252000	1	-1.469579000	-0.667246000	0.274624000
				6	-0.524665000	1.772977000	0.079887000
				8	-1.051413000	1.641314000	1.168313000
				8	-0.887112000	1.859479000	-1.075648000
$(CH_3)_4P^+(CO_2)_3$(**1**$_{O-}$)				$(CH_3)_4P^+(CO_2)_1$(**2**$_{O-}$)			
6	-5.403500000	0.441194000	-0.693722000	6	-3.143782000	0.945735000	0.035100000
7	-5.867512000	1.489867000	-0.024694000	7	-2.338023000	-0.180869000	-0.090267000
7	-5.396487000	1.330119000	1.189109000	7	-3.145062000	-1.264859000	0.093429000
7	-4.660134000	0.263097000	1.393131000	6	-4.365185000	-0.808520000	0.311855000
6	-4.652614000	-0.309025000	0.206616000	7	-4.428987000	0.503669000	0.289168000
1	-5.613804000	0.274498000	-1.735131000	8	-2.768756000	2.109191000	-0.061953000
8	-4.029849000	-1.511982000	-0.000433000	1	-2.757916000	-2.197615000	0.044945000
1	-5.593053000	1.989147000	1.931732000	1	-5.191210000	-1.479731000	0.485827000
6	-2.708599000	-1.566696000	-0.238383000	6	-0.915796000	-0.379043000	-0.351581000
8	-2.148185000	-2.607273000	-0.367381000	8	-0.264518000	0.653637000	-0.521603000
8	-2.178269000	-0.341025000	-0.358583000	8	-0.579350000	-1.571531000	-0.357011000
15	4.787827000	-0.084144000	0.341051000	15	3.056269000	0.041329000	0.093137000
6	6.064176000	-0.166834000	1.596761000	6	2.091196000	-0.558149000	1.479541000
1	6.177634000	-1.199524000	1.924222000	1	2.528451000	-0.160582000	2.395422000
1	7.002380000	0.193974000	1.176991000	1	2.126711000	-1.646845000	1.496564000
1	5.772758000	0.457982000	2.440496000	6	2.859784000	1.815462000	-0.056756000
6	5.240980000	-1.130378000	-1.041275000	1	1.810097000	2.039914000	-0.238126000
1	6.192060000	-0.792493000	-1.450921000	1	3.188197000	2.286945000	0.869086000
1	5.330367000	-2.159723000	-0.695660000	1	3.468372000	2.171194000	-0.887552000
1	4.463741000	-1.061806000	-1.802345000	6	4.783596000	-0.326192000	0.409845000
6	3.243243000	-0.672391000	1.032723000	1	5.091200000	0.167397000	1.331020000
1	3.421277000	-1.642199000	1.497584000	1	4.906517000	-1.404189000	0.510793000
1	2.882219000	0.034523000	1.778342000	1	5.385630000	0.036866000	-0.422344000
1	2.513859000	-0.782314000	0.232688000	6	2.580777000	-0.757661000	-1.438440000
6	4.636457000	1.608584000	-0.224775000	1	2.631101000	-1.838111000	-1.307040000

1	3.891145000	1.656364000	-1.017149000
1	4.333979000	2.240237000	0.609486000
1	5.605716000	1.933193000	-0.602964000
6	-0.791095000	-0.184094000	-0.258463000
8	-0.441031000	0.785307000	-1.020712000
6	1.116129000	1.138792000	-0.899119000
8	1.301858000	1.883043000	0.030492000
8	1.725420000	0.596489000	-1.788860000
8	-0.129923000	-0.856586000	0.481963000

1	1.568320000	-0.457341000	-1.698273000
1	3.278621000	-0.447424000	-2.216090000
1	1.063834000	-0.216164000	1.379549000

$(CH_3)_4P^+(CO_2)_2(\mathbf{2_{O-}})$

6	-4.027871000	1.146918000	-0.010197000
7	-3.142229000	0.047769000	0.009296000
7	-3.910653000	-1.078250000	0.133250000
6	-5.168333000	-0.671549000	0.183795000
7	-5.298886000	0.631273000	0.104708000
8	-3.690102000	2.310080000	-0.111064000
1	-3.499596000	-2.001942000	0.166752000
1	-5.974466000	-1.381762000	0.281410000
6	-1.746970000	-0.001724000	-0.072991000
8	-1.081324000	0.998376000	-0.188802000
8	-1.320834000	-1.232342000	-0.005066000
15	3.883885000	0.337029000	0.049027000
6	2.411871000	1.244314000	-0.420210000
1	2.571845000	2.298420000	-0.193347000
1	1.564731000	0.873310000	0.152829000
6	5.317411000	1.135659000	-0.672216000
1	5.209850000	1.143763000	-1.756514000
1	5.382634000	2.157498000	-0.300672000
1	6.213791000	0.582540000	-0.394311000
6	4.030429000	0.344811000	1.834433000
1	4.072482000	1.375231000	2.185374000
1	3.160948000	-0.155531000	2.260146000
1	4.939338000	-0.182297000	2.122077000
6	3.816382000	-1.356925000	-0.529581000
1	2.980928000	-1.865848000	-0.052455000
1	3.685706000	-1.361231000	-1.611001000
1	4.754118000	-1.846850000	-0.267767000
1	2.229614000	1.119068000	-1.486681000
6	0.225938000	-1.357094000	-0.116174000
8	0.737460000	-1.377603000	0.983644000
8	0.574677000	-1.438737000	-1.272859000

$(CH_3)_4P^+(CO_2)_3(\mathbf{2_{O-}})$

6	-5.304669000	0.978263000	0.005807000
7	-4.127890000	0.181623000	0.094294000
7	-4.520893000	-1.055162000	0.536100000
6	-5.828783000	-0.980367000	0.733258000
7	-6.344117000	0.184715000	0.426878000
8	-5.325811000	2.126540000	-0.377014000
1	-3.854776000	-1.777064000	0.780726000
1	-6.374740000	-1.830558000	1.111656000
6	-2.840789000	0.487827000	-0.298977000
8	-2.497614000	1.559112000	-0.692292000
8	-2.076393000	-0.622373000	-0.203671000
15	4.835557000	0.546183000	0.222291000
6	5.198837000	1.162039000	-1.420313000
1	4.492972000	0.720817000	-2.123877000
1	6.216227000	0.883634000	-1.692473000
6	3.183229000	1.060533000	0.685168000
1	3.184947000	2.141426000	0.825566000
1	2.493233000	0.798254000	-0.114376000
1	2.892385000	0.567142000	1.611671000
6	4.976707000	-1.239366000	0.223911000
1	4.279112000	-1.656008000	-0.500849000
1	5.998960000	-1.504279000	-0.046024000
1	4.747307000	-1.616533000	1.219679000
6	6.013334000	1.223827000	1.390652000
1	7.017015000	0.903687000	1.113436000
1	5.952139000	2.311261000	1.369681000
1	5.771905000	0.859533000	2.388774000
1	5.096801000	2.246600000	-1.426656000
6	-0.686385000	-0.494450000	-0.129664000
8	-0.160296000	0.457529000	0.374584000
8	-0.161554000	-1.553771000	-0.628629000
6	1.428783000	-1.589712000	-0.483984000
8	1.739765000	-1.985116000	0.611978000
8	1.939636000	-1.240727000	-1.520873000

$((CH_3)_4P^+)_2(CO_2)_2(\mathbf{1_{O2-}})$

6	-0.261541000	-0.680487000	1.306419000
7	-0.539150000	-0.913614000	0.009717000
7	-0.173576000	0.161220000	-0.821901000
7	0.545228000	1.026109000	0.026109000
6	0.456094000	0.659200000	1.322684000
8	0.838355000	1.224179000	2.329819000
1	0.453043000	-0.192376000	-1.546231000
8	-0.506033000	-1.347224000	2.295454000
6	-1.159867000	-2.078632000	-0.652323000
8	-0.982639000	-2.089841000	-1.873403000
8	-1.749227000	-2.850354000	0.104126000

$((CH_3)_4P^+)_2(CO_2)_3(\mathbf{1_{O2-}})$

6	-0.557934000	-1.158838000	-0.943941000
7	-0.186510000	-0.287246000	0.044868000
7	-1.112994000	-0.236239000	1.108044000
7	-2.082653000	-1.201727000	0.756109000
6	-1.851783000	-1.780097000	-0.439842000
8	-2.498869000	-2.595267000	-1.062314000
1	-0.640593000	-0.565157000	1.954118000
8	-0.025746000	-1.386934000	-1.999491000
6	0.879586000	0.617278000	0.098172000
8	1.006337000	1.350702000	1.040952000
8	1.655029000	0.607909000	-0.971469000

6	1.226366000	2.170802000	-0.612920000	6	-3.201281000	-1.388859000	1.715623000
8	1.192379000	2.125310000	-1.846137000	8	-3.081385000	-0.705090000	2.733315000
8	1.738529000	2.971750000	0.168818000	8	-4.058245000	-2.189307000	1.346828000
15	4.472523000	-0.397301000	-0.116218000	15	-5.083722000	1.309123000	-0.383708000
6	3.828165000	0.374630000	1.363433000	6	-4.792663000	-0.163078000	-1.361757000
1	3.171003000	-0.327390000	1.876043000	1	-5.719310000	-0.429482000	-1.870472000
1	4.662684000	0.636972000	2.013716000	1	-4.014967000	0.038051000	-2.097963000
1	3.278203000	1.275950000	1.091376000	1	-4.494928000	-0.980759000	-0.706378000
6	3.120677000	-0.859111000	-1.198786000	6	-6.181548000	0.909853000	0.974118000
1	2.384046000	-1.432256000	-0.633416000	1	-7.120871000	0.528002000	0.575756000
1	2.678089000	0.049093000	-1.609467000	1	-5.708084000	0.150845000	1.597710000
1	3.512009000	-1.467667000	-2.013781000	1	-6.365353000	1.809172000	1.561000000
6	5.537350000	0.757897000	-0.975717000	6	-3.541784000	1.937803000	0.277308000
1	4.959911000	1.649122000	-1.221651000	1	-3.167291000	1.259803000	1.043039000
1	6.372582000	1.024569000	-0.329296000	1	-2.813824000	2.032989000	-0.528378000
1	5.908190000	0.293263000	-1.888621000	1	-3.727768000	2.915267000	0.722507000
6	5.399932000	-1.862311000	0.333148000	6	-5.833101000	2.563465000	-1.420983000
1	6.210288000	-1.580594000	1.004396000	1	-5.155655000	2.795666000	-2.242150000
1	4.732657000	-2.563348000	0.833620000	1	-6.774802000	2.184251000	-1.815802000
1	5.807286000	-2.319058000	-0.567921000	1	-6.013796000	3.458506000	-0.827100000
15	-4.571487000	0.349301000	-0.088403000	15	6.027141000	0.504365000	0.384890000
6	-5.026772000	2.025414000	-0.526311000	6	4.451222000	1.167873000	0.923281000
1	-4.136868000	2.558161000	-0.860156000	1	3.979868000	0.473871000	1.617944000
1	-5.763252000	1.997171000	-1.328613000	1	4.627517000	2.123594000	1.416924000
1	-5.448801000	2.521281000	0.347039000	1	3.814300000	1.326941000	0.054591000
6	-3.844052000	-0.462012000	-1.508886000	6	7.183306000	0.557462000	1.752836000
1	-4.535342000	-0.391062000	-2.348463000	1	7.319118000	1.592041000	2.065695000
1	-2.903990000	0.029187000	-1.761468000	1	6.781932000	-0.028394000	2.579225000
1	-3.669131000	-1.509936000	-1.266687000	1	8.136642000	0.139071000	1.432479000
6	-3.387485000	0.389654000	1.255302000	6	5.846976000	-1.189460000	-0.167237000
1	-2.536300000	1.000220000	0.952088000	1	5.453026000	-1.792702000	0.649759000
1	-3.860085000	0.832142000	2.131807000	1	5.165359000	-1.221023000	-1.016859000
1	-3.069373000	-0.628387000	1.481393000	1	6.827513000	-1.562050000	-0.463297000
6	-6.029523000	-0.554417000	0.427199000	6	6.645189000	1.503736000	-0.967080000
1	-6.485001000	-0.045910000	1.276037000	1	5.942669000	1.438430000	-1.798071000
1	-6.734533000	-0.595262000	-0.402451000	1	6.732743000	2.538145000	-0.636642000
1	-5.737358000	-1.564225000	0.713691000	1	7.620017000	1.128765000	-1.276359000
				6	2.544177000	-0.592403000	-1.171647000
				8	3.157405000	-0.494909000	-2.216784000
				8	2.507747000	-1.385615000	-0.244195000
$((CH_3)_4P^+)_2(CO_2)_4(\mathbf{1}_{O2-})$				$((CH_3)_4P^+)_2(CO_2)_5(\mathbf{1}_{O2-})$			
6	0.930328000	0.270218000	1.392993000	6	-1.607768000	-2.412586000	0.531599000
7	0.032847000	0.827761000	0.531692000	7	-2.116722000	-1.239642000	0.058513000
7	0.559343000	1.905214000	-0.218467000	7	-1.138078000	-0.351454000	-0.447579000
7	1.924689000	1.913310000	0.146840000	7	0.060973000	-1.093990000	-0.327113000
6	2.231725000	1.009282000	1.123559000	6	-0.109774000	-2.318703000	0.275881000
8	3.277608000	0.809038000	1.683629000	8	0.703893000	-3.143757000	0.579254000
1	0.507560000	1.646577000	-1.208609000	1	-1.324773000	-0.229565000	-1.447777000
8	0.785167000	-0.601417000	2.209877000	8	-2.158539000	-3.337404000	1.065804000
6	-1.339311000	0.547982000	0.322357000	6	1.214390000	-0.421787000	-0.728282000
8	-1.941565000	1.155667000	-0.530748000	8	2.278998000	-1.216733000	-0.581039000
8	-1.771848000	-0.380545000	1.105319000	8	1.180228000	0.677935000	-1.187375000
6	2.723839000	2.892992000	-0.471352000	6	3.558295000	-0.645769000	-0.538100000
8	2.232774000	3.643807000	-1.267148000	8	3.746740000	0.453604000	-0.097617000
8	3.974407000	2.913168000	-0.059933000	8	4.394809000	-1.508817000	-0.979619000
15	4.461387000	-2.457888000	-0.447594000	15	8.598065000	1.613347000	0.547538000

6	4.397271000	-4.213788000	-0.090875000	6	6.972447000	2.138622000	0.006467000
1	3.865331000	-4.723299000	-0.893346000	1	6.993238000	2.344794000	-1.062762000
1	5.412807000	-4.600754000	-0.016226000	1	6.244653000	1.360190000	0.226874000
1	3.874573000	-4.365623000	0.853011000	1	6.709526000	3.045057000	0.552149000
6	2.780962000	-1.846773000	-0.577142000	6	9.234353000	0.291042000	-0.479900000
1	2.261189000	-2.418721000	-1.345734000	1	8.608364000	-0.591057000	-0.360466000
1	2.284300000	-1.989005000	0.382858000	1	9.232738000	0.613263000	-1.520437000
1	2.807545000	-0.793973000	-0.855506000	1	10.253840000	0.071524000	-0.162762000
6	5.340872000	-1.634270000	0.877270000	6	9.717223000	3.010012000	0.445927000
1	4.764562000	-1.724210000	1.797431000	1	9.767216000	3.349015000	-0.588451000
1	6.308165000	-2.121871000	0.999293000	1	9.345908000	3.814343000	1.079719000
1	5.488121000	-0.584552000	0.627706000	1	10.706720000	2.701166000	0.780715000
6	5.323404000	-2.204346000	-1.996918000	6	8.498033000	1.053166000	2.246081000
1	6.333412000	-2.603380000	-1.907703000	1	8.123230000	1.865868000	2.867439000
1	4.789174000	-2.725469000	-2.790614000	1	7.817988000	0.203356000	2.298552000
1	5.361262000	-1.136703000	-2.208055000	1	9.490225000	0.755893000	2.583742000
15	-7.008159000	-0.207369000	-0.481373000	6	5.920088000	-1.021488000	-0.828945000
6	-5.604464000	0.510146000	-1.334667000	8	6.318651000	-1.266942000	0.283035000
1	-5.219364000	-0.203047000	-2.062142000	8	6.302850000	-0.555116000	-1.871046000
1	-5.943476000	1.411664000	-1.845306000	6	-3.446977000	-0.753769000	0.036830000
1	-4.831781000	0.768557000	-0.613734000	8	-3.676878000	0.306430000	-0.495516000
6	-8.373012000	-0.340682000	-1.636466000	8	-4.270244000	-1.562075000	0.610877000
1	-8.635943000	0.653343000	-1.995971000	15	-8.489221000	1.819823000	-0.070889000
1	-8.069268000	-0.967100000	-2.474653000	6	-6.829386000	1.883219000	-0.744217000
1	-9.227392000	-0.789596000	-1.131419000	1	-6.789462000	1.321873000	-1.676559000
6	-6.631345000	-1.840535000	0.150907000	1	-6.577104000	2.927427000	-0.929518000
1	-6.291753000	-2.473024000	-0.668410000	1	-6.133236000	1.464340000	-0.020492000
1	-5.855130000	-1.763663000	0.909587000	6	-9.576544000	2.792112000	-1.112765000
1	-7.540273000	-2.255762000	0.586133000	1	-9.225128000	3.822923000	-1.132774000
6	-7.485008000	0.858274000	0.877683000	1	-9.564705000	2.378792000	-2.120888000
1	-6.659616000	0.917652000	1.586342000	1	-10.588070000	2.753300000	-0.710325000
1	-7.712685000	1.850673000	0.490047000	6	-9.107184000	0.140117000	-0.001340000
1	-8.364384000	0.440724000	1.366692000	1	-9.087815000	-0.291038000	-1.001448000
6	-3.273920000	-0.776445000	0.819228000	1	-8.481955000	-0.446182000	0.669452000
8	-4.012410000	-0.194397000	1.580245000	1	-10.131726000	0.168576000	0.369679000
8	-3.336381000	-1.591810000	-0.070110000	6	-8.473238000	2.510665000	1.581943000
6	4.850112000	1.732163000	-0.408318000	1	-7.826120000	1.900310000	2.211523000
8	5.923234000	1.815910000	0.149968000	1	-8.092494000	3.530547000	1.539444000
8	4.324982000	0.958093000	-1.195747000	1	-9.486685000	2.509507000	1.981258000
				6	-5.778574000	-1.093528000	0.500239000
				8	-6.124461000	-0.561143000	1.529573000
				8	-6.242614000	-1.405246000	-0.570188000
$((CH_3)_4P^+)_2(CO_2)_2(\mathbf{2}_{O2-})$				$((CH_3)_4P^+)_2(CO_2)_3(\mathbf{2}_{O2-})$			
7	0.671250000	-0.556730000	-0.042412000	7	0.204654000	-0.644148000	-0.049348000
6	-0.541952000	-0.124716000	-0.056981000	6	1.415719000	-0.202109000	-0.020729000
7	-0.611586000	1.235231000	-0.044260000	7	1.481719000	1.161219000	0.025974000
6	0.674666000	1.731122000	-0.020852000	6	0.205229000	1.664616000	0.031049000
7	1.448770000	0.594974000	-0.020282000	7	-0.571788000	0.509934000	-0.015995000
8	-1.571346000	-0.965825000	-0.081109000	8	2.443985000	-1.029714000	-0.056277000
8	0.984412000	2.913432000	-0.004517000	8	-0.130144000	2.829060000	0.066979000
1	-1.468432000	1.769703000	-0.053563000	1	2.340781000	1.692279000	0.077862000
6	2.905843000	0.495559000	-0.007342000	6	-1.962450000	0.380609000	-0.050216000
8	3.505049000	1.578439000	0.002985000	8	-2.569801000	1.536040000	0.013271000
8	3.348282000	-0.660772000	-0.008996000	8	-2.494006000	-0.702291000	-0.125115000
6	-2.957653000	-0.531310000	-0.117111000	6	3.841036000	-0.589932000	0.035383000
8	-3.161385000	0.681023000	-0.109665000	8	4.026966000	0.610282000	0.210727000

8	-3.708417000	-1.499315000	-0.148265000	8	4.589594000	-1.548332000	-0.082578000
15	6.870710000	-0.510432000	0.033193000	15	7.837497000	-0.305014000	0.003469000
6	6.228734000	0.248069000	-1.457575000	6	9.474433000	0.425544000	0.072990000
1	6.405194000	1.322297000	-1.417450000	1	10.034987000	-0.028748000	0.889035000
1	5.161844000	0.046543000	-1.527660000	1	9.987231000	0.248289000	-0.871638000
6	8.653018000	-0.309070000	0.052630000	1	9.377542000	1.497297000	0.244548000
1	9.077718000	-0.778244000	-0.833952000	6	6.943579000	0.442447000	-1.358070000
1	8.889483000	0.754629000	0.055212000	1	5.997678000	-0.075969000	-1.496658000
1	9.058145000	-0.778104000	0.948440000	1	6.767410000	1.494463000	-1.136823000
6	6.196044000	0.250689000	1.507978000	1	7.555172000	0.352081000	-2.255834000
1	6.699963000	-0.178484000	2.373957000	6	7.994149000	-2.067185000	-0.277600000
1	6.374497000	1.324681000	1.470377000	1	6.999382000	-2.508237000	-0.315956000
1	5.127608000	0.050542000	1.554283000	1	8.511456000	-2.230482000	-1.222539000
6	6.480036000	-2.258914000	0.030307000	1	8.566561000	-2.507960000	0.537929000
1	5.397671000	-2.378169000	0.016963000	6	7.024594000	-0.014178000	1.573822000
1	6.916201000	-2.719694000	-0.855352000	1	6.075185000	-0.544525000	1.591046000
1	6.894156000	-2.717578000	0.927571000	1	7.674842000	-0.383189000	2.367079000
1	6.752091000	-0.181641000	-2.311660000	1	6.860194000	1.055433000	1.699553000
15	-6.962434000	-0.200287000	0.059860000	15	-7.477652000	-0.895615000	0.043373000
6	-7.150432000	-1.981415000	0.013833000	6	-8.642297000	-1.996050000	-0.759684000
1	-7.746511000	-2.254312000	-0.856439000	1	-8.424595000	-2.023959000	-1.826985000
1	-7.652452000	-2.309316000	0.923539000	1	-8.540563000	-2.994808000	-0.336915000
6	-6.180338000	0.359904000	-1.451684000	1	-9.654519000	-1.626938000	-0.599219000
1	-5.239211000	-0.168457000	-1.587298000	6	-7.804745000	-0.856950000	1.804617000
1	-6.854284000	0.148030000	-2.281770000	1	-7.679575000	-1.858810000	2.213831000
1	-6.001350000	1.432501000	-1.386061000	1	-7.098117000	-0.174091000	2.276136000
6	-8.582694000	0.561196000	0.172417000	1	-8.823772000	-0.511206000	1.974031000
1	-9.170564000	0.284575000	-0.701978000	6	-5.813363000	-1.501040000	-0.222966000
1	-9.080402000	0.215605000	1.077555000	1	-5.773643000	-2.547099000	0.080661000
1	-8.462838000	1.643672000	0.208175000	1	-5.554549000	-1.410872000	-1.277063000
6	-6.018212000	0.262317000	1.510846000	1	-5.124142000	-0.916999000	0.383480000
1	-6.608214000	0.012683000	2.392767000	6	-7.676692000	0.754549000	-0.624194000
1	-5.080204000	-0.288146000	1.520083000	1	-7.449401000	0.742068000	-1.689356000
1	-5.824801000	1.334063000	1.487275000	1	-8.709125000	1.067157000	-0.468559000
1	-6.163613000	-2.437363000	-0.052387000	1	-6.997857000	1.432376000	-0.108793000
				6	-4.080734000	1.433790000	-0.095672000
				8	-4.614914000	1.450203000	0.999573000
				8	-4.455317000	1.397027000	-1.252614000
$((CH_3)_4P^+)_2(CO_2)_4(\mathbf{2}_{O2-})$				$((CH_3)_4P^+)_2(CO_2)_5(\mathbf{2}_{O2-})$			
7	0.413592000	1.122506000	-0.422850000	7	-0.576481000	-0.215363000	-0.580606000
6	-0.818204000	0.807690000	-0.579114000	6	0.564478000	-0.703563000	-0.225614000
7	-1.013560000	-0.503877000	-0.883515000	7	0.487459000	-2.011442000	0.165423000
6	0.218174000	-1.120518000	-0.925103000	6	-0.811997000	-2.431153000	0.064960000
7	1.085670000	-0.069502000	-0.636700000	7	-1.457056000	-1.280044000	-0.411274000
8	-1.766828000	1.750383000	-0.503646000	8	1.657224000	0.029052000	-0.269017000
8	0.452477000	-2.284334000	-1.154472000	8	-1.270083000	-3.517500000	0.328047000
1	-1.903521000	-0.970380000	-0.992234000	1	1.274095000	-2.558225000	0.491809000
6	2.485097000	-0.081240000	-0.522146000	6	-2.789108000	-1.071177000	-0.693258000
8	2.983205000	-1.263002000	-0.749768000	8	-3.483237000	-2.221737000	-0.606441000
8	3.097134000	0.919920000	-0.238321000	8	-3.244315000	-0.013342000	-1.020202000
6	4.509597000	-1.308179000	-0.647132000	15	-5.837094000	2.806455000	0.075005000
8	4.868385000	-1.691702000	0.450692000	6	-5.506169000	4.561774000	-0.073271000
8	5.044260000	-0.988746000	-1.689850000	1	-5.607434000	5.027731000	0.906244000
15	7.940295000	0.326553000	0.715940000	1	-4.492658000	4.703215000	-0.446930000
6	8.129568000	-1.050921000	-0.413604000	1	-6.221009000	5.002172000	-0.767368000
1	8.189076000	-0.673090000	-1.433566000	6	-5.711708000	2.044998000	-1.541165000

1	9.048954000	-1.578270000	-0.159270000
1	7.274134000	-1.716315000	-0.312726000
6	7.772985000	-0.298462000	2.386824000
1	8.662624000	-0.871817000	2.644959000
1	7.661187000	0.540563000	3.072703000
1	6.891908000	-0.937603000	2.437341000
6	9.400393000	1.361643000	0.613962000
1	10.279196000	0.766796000	0.859800000
1	9.489731000	1.750207000	-0.400031000
1	9.303351000	2.187113000	1.318102000
6	6.497842000	1.308801000	0.310280000
1	6.512808000	1.561063000	-0.749154000
1	5.600331000	0.742969000	0.550390000
1	6.525390000	2.219603000	0.908634000
6	-3.095437000	1.422052000	-0.330819000
8	-3.773711000	2.510484000	-0.297265000
8	-3.481867000	0.284172000	-0.230423000
6	-5.334439000	2.278848000	-0.110730000
8	-5.635147000	2.419051000	1.050203000
8	-5.859132000	2.054876000	-1.175014000
15	-7.092551000	-1.197384000	0.639589000
6	-8.274241000	0.149189000	0.631812000
1	-9.058613000	-0.073533000	-0.090956000
1	-8.706059000	0.247883000	1.627365000
1	-7.765100000	1.071616000	0.354897000
6	-5.835645000	-0.893642000	1.879167000
1	-6.311450000	-0.884267000	2.859667000
1	-5.093840000	-1.690665000	1.836013000
1	-5.363422000	0.068615000	1.689921000
6	-7.943645000	-2.723396000	1.040510000
1	-8.403810000	-2.626933000	2.023202000
1	-8.710399000	-2.912742000	0.290331000
1	-7.224820000	-3.542135000	1.048576000
6	-6.349551000	-1.351495000	-0.983151000
1	-7.132483000	-1.595878000	-1.700838000
1	-5.880221000	-0.407278000	-1.255003000
1	-5.606193000	-2.147986000	-0.961234000

1	-4.716120000	2.223622000	-1.944511000
1	-5.893525000	0.974592000	-1.449654000
1	-6.461834000	2.492604000	-2.193186000
6	-4.644909000	2.086537000	1.202932000
1	-3.642289000	2.234177000	0.803018000
1	-4.735829000	2.586330000	2.167202000
1	-4.843118000	1.021984000	1.321692000
6	-7.495326000	2.580407000	0.715442000
1	-7.553980000	3.017545000	1.711656000
1	-8.198553000	3.080647000	0.050059000
1	-7.728110000	1.517249000	0.763509000
6	-4.869852000	-2.166009000	-0.461647000
8	-5.532697000	-2.923876000	-1.102054000
8	-5.209145000	-1.328218000	0.466101000
6	2.981984000	-0.459217000	0.146372000
8	3.025922000	-1.600384000	0.594132000
8	3.822737000	0.404712000	-0.040454000
15	8.715254000	1.261133000	-0.157813000
6	9.496471000	1.505209000	-1.750950000
1	9.062973000	0.810584000	-2.469636000
1	9.325544000	2.530110000	-2.078164000
1	10.565889000	1.320399000	-1.656222000
6	9.416075000	2.401683000	1.032208000
1	9.247220000	3.421994000	0.689874000
1	8.932507000	2.250378000	1.996690000
1	10.485350000	2.212875000	1.120617000
6	6.955549000	1.560091000	-0.304668000
1	6.798694000	2.583888000	-0.643586000
1	6.532559000	0.866222000	-1.030506000
1	6.485726000	1.421444000	0.668534000
6	9.003948000	-0.420189000	0.390816000
1	8.587118000	-1.113305000	-0.339635000
1	10.078004000	-0.583392000	0.476334000
1	8.534283000	-0.566322000	1.363220000
6	5.792929000	-1.476429000	0.649631000
8	5.796159000	-1.124498000	1.750404000
8	5.846427000	-1.848551000	-0.443328000
6	-6.691489000	-0.918538000	0.648650000
8	-6.900373000	-0.727913000	1.827595000
8	-7.297447000	-0.816612000	-0.395580000

$((CH_3)_4P^+)_2(CO_2)_6(\mathbf{2}_{O2-})$

7	0.281159000	-0.695551000	-1.241224000
6	1.249996000	-1.169301000	-0.549470000
7	0.918846000	-1.452831000	0.740456000
6	-0.403033000	-1.124887000	0.929424000
7	-0.771552000	-0.657063000	-0.340532000
8	2.431376000	-1.417923000	-1.124140000
8	-1.057401000	-1.221455000	1.937101000
1	1.541387000	-1.779718000	1.467395000
15	-8.777391000	0.740073000	0.842806000
6	-9.508729000	0.002372000	-0.616247000
1	-10.005548000	-0.926244000	-0.336842000
1	-10.234862000	0.699039000	-1.034449000
1	-8.726738000	-0.198910000	-1.347664000
6	-7.890007000	2.225177000	0.379899000
1	-8.603369000	2.935858000	-0.037338000

1	-7.418238000	2.651170000	1.264727000
1	-7.135188000	1.975704000	-0.363747000
6	-10.076041000	1.174924000	1.999701000
1	-10.743894000	1.897812000	1.532807000
1	-10.631973000	0.277137000	2.267728000
1	-9.626101000	1.610493000	2.891297000
6	-7.684585000	-0.437107000	1.638658000
1	-8.285669000	-1.270928000	2.001493000
1	-6.945782000	-0.805672000	0.929856000
1	-7.185121000	0.049893000	2.475519000
6	-1.996434000	-0.190647000	-0.791585000
8	-2.204936000	0.138598000	-1.920774000
8	-2.873496000	-0.120973000	0.221188000
6	-4.230199000	0.041537000	-0.090476000
8	-4.634347000	-0.870451000	-0.905616000
8	-4.834953000	0.902513000	0.477593000
6	-6.056179000	-0.723330000	-1.558150000
8	-6.624869000	-1.789048000	-1.504979000
8	-6.245119000	0.387007000	-1.998344000
15	6.378720000	2.692045000	-0.225814000
6	6.630147000	3.307326000	1.437753000
1	7.450338000	4.024470000	1.433202000
1	5.716603000	3.792149000	1.780369000
1	6.873019000	2.471636000	2.093351000
6	5.029733000	1.513202000	-0.218927000
1	4.121907000	2.022773000	0.104254000
1	4.896967000	1.114787000	-1.224703000
1	5.270810000	0.710934000	0.476207000
6	5.967167000	4.057612000	-1.310246000
1	5.054361000	4.533479000	-0.954132000
1	6.785948000	4.776200000	-1.305869000
1	5.815670000	3.676294000	-2.319524000
6	7.886877000	1.917860000	-0.805641000
1	8.670061000	2.674596000	-0.848771000
1	8.179550000	1.125781000	-0.117876000
1	7.718463000	1.502879000	-1.798533000
6	3.588547000	-1.470362000	-0.366401000
8	3.596746000	-1.270515000	0.817647000
8	4.561753000	-1.732101000	-1.168526000
6	5.964240000	-1.977609000	-0.521387000
8	5.943432000	-2.870270000	0.293903000
8	6.775888000	-1.228769000	-1.019198000
6	7.762988000	-1.166128000	1.691282000
8	8.669976000	-1.828842000	1.426166000
8	6.873622000	-0.486409000	1.982522000

VI. Anionic systems in presence of trimethyl phosphonium cation

$(CH_3)_4P^+(\mathbf{1}_{O-})$				$(CH_3)_4P^+(\mathbf{2}_{O-})$			
6	-2.930850000	1.100762000	0.007050000	6	-1.927917000	0.565129000	0.046692000
7	-4.227309000	0.820582000	-0.002625000	7	-1.830468000	-0.777639000	0.105170000
7	-4.269110000	-0.487260000	-0.008572000	7	-3.129880000	-1.188858000	0.017753000
7	-3.089427000	-1.112532000	-0.004767000	6	-3.938951000	-0.142127000	-0.086618000
6	-2.177778000	-0.114728000	0.006408000	7	-3.253840000	0.980625000	-0.075394000
1	-2.576411000	2.118359000	0.014395000	8	-0.939007000	1.364210000	0.094245000
8	-0.904460000	-0.285183000	0.014548000	1	-3.370937000	-2.166757000	0.036936000

1	-5.142208000	-0.990793000	-0.019405000	1	-5.009924000	-0.243164000	-0.167648000
15	2.478508000	0.013283000	-0.001997000	15	2.113105000	-0.079130000	-0.012869000
6	1.984987000	-1.474175000	-0.866818000	6	1.283715000	-0.610619000	1.482528000
1	2.419686000	-2.337562000	-0.363982000	1	1.913503000	-0.359095000	2.335797000
1	2.343274000	-1.425745000	-1.894498000	1	1.129256000	-1.688394000	1.441200000
6	1.901683000	-0.057068000	1.691576000	6	2.331984000	1.698868000	0.011957000
1	2.356418000	-0.915160000	2.185476000	1	1.350268000	2.167218000	0.047860000
1	2.187814000	0.860109000	2.205387000	1	2.913711000	1.972802000	0.891671000
1	0.817468000	-0.160943000	1.674680000	1	2.862637000	2.002910000	-0.889896000
6	4.267672000	0.137391000	-0.008964000	6	3.727841000	-0.859821000	-0.079076000
1	4.689008000	-0.734819000	0.489738000	1	4.301053000	-0.576142000	0.802867000
1	4.620284000	0.178603000	-1.038860000	1	3.599356000	-1.941543000	-0.101665000
1	4.565113000	1.042745000	0.519070000	1	4.248484000	-0.532740000	-0.978364000
6	1.790461000	1.448947000	-0.821770000	6	1.191720000	-0.554972000	-1.472802000
1	2.158483000	1.482099000	-1.846701000	1	1.027736000	-1.631928000	-1.457216000
1	0.705245000	1.357091000	-0.811404000	1	0.239208000	-0.029147000	-1.461989000
1	2.100740000	2.346811000	-0.288298000	1	1.773621000	-0.281684000	-2.352948000
1	0.897018000	-1.530887000	-0.845177000	1	0.326464000	-0.096718000	1.543696000
$((CH_3)_4P^+)_2(\mathbf{1}_{O2-})$				$((CH_3)_4P^+)_2(\mathbf{2}_{O2-})$			
6	-0.138851000	1.984159000	0.588620000	7	0.042023000	-0.831608000	-0.524389000
7	0.638062000	1.968098000	-0.472855000	6	-0.480007000	-0.986855000	0.680479000
7	-0.215232000	2.000334000	-1.583697000	7	-0.304852000	0.204911000	1.376976000
7	-1.541783000	2.218386000	-1.190556000	6	0.374928000	1.088486000	0.546923000
6	-1.551664000	2.155035000	0.124013000	7	0.583000000	0.478715000	-0.608594000
8	-2.569235000	2.215147000	0.893176000	8	-1.063043000	-2.005072000	1.176660000
1	0.081432000	2.717404000	-2.238165000	8	0.711631000	2.261880000	0.904388000
8	0.221004000	1.864302000	1.808623000	1	-0.564472000	0.374118000	2.335413000
15	-2.350461000	-1.425770000	-0.023910000	15	3.925414000	-0.104819000	-0.242063000
6	-1.865317000	-0.991540000	1.646037000	6	3.682476000	1.626428000	-0.633981000
1	-1.501189000	0.035407000	1.683843000	1	2.624481000	1.802143000	-0.815998000
1	-2.737507000	-1.092664000	2.292445000	1	4.270031000	1.862345000	-1.521348000
1	-1.087269000	-1.679622000	1.976822000	6	5.684892000	-0.364390000	0.009460000
6	-3.745564000	-0.437720000	-0.556255000	1	6.226376000	-0.061262000	-0.885950000
1	-3.455415000	0.611233000	-0.592447000	1	6.013946000	0.235112000	0.858051000
1	-4.055107000	-0.783339000	-1.542557000	1	5.868093000	-1.418785000	0.212478000
1	-4.560118000	-0.575284000	0.154843000	6	3.064343000	-0.580102000	1.260380000
6	-0.973246000	-1.213562000	-1.152974000	1	3.060769000	0.256735000	1.958155000
1	-0.546424000	-0.217695000	-1.033771000	1	2.045316000	-0.867870000	1.008765000
1	-0.226177000	-1.977745000	-0.941455000	1	3.587304000	-1.427038000	1.704042000
1	-1.338170000	-1.334728000	-2.173303000	6	3.374610000	-1.137609000	-1.597955000
6	-2.843731000	-3.151417000	-0.038179000	1	2.300599000	-0.997758000	-1.719295000
1	-2.011903000	-3.766764000	0.302570000	1	3.906568000	-0.852158000	-2.504989000
1	-3.695887000	-3.284075000	0.627582000	1	3.590798000	-2.178102000	-1.355598000
1	-3.121552000	-3.435759000	-1.052538000	1	4.027891000	2.228932000	0.205837000
15	3.063448000	-0.574076000	0.002801000	15	-3.901931000	0.074483000	-0.304703000
6	4.364355000	-1.802525000	0.143295000	6	-2.721324000	1.281343000	-0.901413000
1	3.971113000	-2.776665000	-0.145311000	1	-2.978217000	1.526045000	-1.932480000
1	5.187800000	-1.528865000	-0.515480000	1	-1.714784000	0.862368000	-0.870808000
1	4.714264000	-1.837352000	1.174389000	6	-3.774616000	-0.138971000	1.469971000
6	2.509526000	-0.530963000	-1.702013000	1	-3.796165000	0.837549000	1.952463000
1	3.348886000	-0.232777000	-2.330540000	1	-4.626154000	-0.732857000	1.803032000
1	2.177568000	-1.528018000	-1.990877000	1	-2.850145000	-0.668257000	1.700742000
1	1.696232000	0.187444000	-1.798929000	6	-5.558552000	0.641419000	-0.694997000
6	1.718072000	-1.036710000	1.092303000	1	-5.732521000	1.595016000	-0.196977000
1	1.348760000	-2.020225000	0.803567000	1	-5.650305000	0.767196000	-1.773127000
1	2.097499000	-1.073301000	2.113767000	1	-6.281859000	-0.094089000	-0.345125000

1	0.932817000	-0.284289000	1.024770000	6	-3.599886000	-1.493925000	-1.115706000
6	3.719364000	1.017212000	0.496744000	1	-3.711602000	-1.364290000	-2.191843000
1	4.059563000	0.948137000	1.529706000	1	-2.584482000	-1.814829000	-0.879203000
1	4.557612000	1.271476000	-0.151544000	1	-4.318428000	-2.228365000	-0.753053000
1	2.929226000	1.760630000	0.405050000	1	-2.776365000	2.179614000	-0.286993000