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Formation of large clusters of CO_2 around anions: DFT study reveals cooperative CO_2 adsorption

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1. Table S1. Average X^-…CO_2 distances (Å) in the $X^-(CO_2)_n$ complexes at M06L/6-311++G** level.

n	Cl^-	Br^-	CN^-	NO_2^-	$NCCOO^-$	$ClOCOO^-$	$HOCOO^-$	H_2NCOO^-
1	2.888	3.158	2.559	2.109	2.637	2.621	2.542	2.127
2	2.955	3.202	2.710	2.721	2.725	2.733	2.601	2.329
3	2.997	3.239	2.788	2.974	2.722	2.715	2.588	2.648
4	3.022	3.262	3.098	3.195	2.726	2.810	2.752	2.602
5	3.022	3.253	3.109	3.148	2.743	2.752	2.666	2.708
6	3.037	3.279	3.181	3.407	2.782	2.916	2.691	2.734
7	3.087	3.282	3.270	3.348	2.839	2.828	2.663	2.750
8	3.123	3.264	3.260	3.366	2.836	2.906	2.738	2.717
9	3.241	3.546	-	-	2.761	3.041	2.759	2.738
10	-	-	-	-	2.836	3.055	2.814	2.780
11	-	-	-	-	2.926	3.000	2.819	2.800

2. Table S2. Lowest frequencies in cm^{-1} for all the $X^-(CO_2)_n$ complexes at M06L/6-311++G** level

n	F^-	Cl^-	Br^-	CN^-	NO_2^-	$NCCOO^-$	$ClOCOO^-$	$HOCOO^-$	H_2NCOO^-
0	-	-	-	2102.9	800.8	193.2	169.2	541.3	412.7
1	446.1	119.1	81.9	58.6	71.0	21.6	17.1	7.1	44.5
2	28.5	7.1	6.3	11.5	22.1	29.6	37.6	12.1	19.1
3	28.5	44.3	30.4	9.8	14.4	17.8	13.9	18.5	20.8
4	24.1	41.2	33.5	27.3	14.0	17.8	26.9	19.1	19.1
5	36.0	39.0	23.8	22.9	16.4	17.9	23.3	17.9	16.8
6	63.7	27.8	27.2	17.2	13.5	20.7	18.3	14.0	28.3
7	-	23.5	24.4	9.3	29.1	20.7	18.3	24.1	22.1
8	-	29.5	36.6	23.0	24.1	28.3	16.8	24.5	19.5
9	-	18.7	10.9	-	-	21.6	24.7	23.4	18.5
10	-	-	-	-	-	19.3	7.6	25.1	17.7
11	-	-	-	-	-	30.4	7.8	21.0	12.3

3. Table S3. Zero point energy correction in Hartree/particle for all the $X^-(CO_2)_n$ complexes at M06L/6-311++G** level.

n	F^-	Cl^-	Br^-	CN^-	NO_2^-	$NCCOO^-$	$ClOCOO^-$	$HOCOO^-$	H_2NCOO^-
0	-	-	-	0.00479	0.00783	0.01942	0.01493	0.02630	0.03850
1	0.01312	0.01205	0.01194	0.01740	0.02072	0.03202	0.02763	0.03865	0.05187
2	0.02581	0.02446	0.02434	0.02999	0.03357	0.04493	0.04055	0.05157	0.06454
3	0.03817	0.03723	0.03687	0.04242	0.04606	0.05776	0.05299	0.06474	0.07721
4	0.05041	0.05005	0.04966	0.05571	0.05888	0.07088	0.06581	0.07736	0.09024
5	0.06391	0.06286	0.06241	0.06855	0.07175	0.08346	0.07894	0.09086	0.10275
6	0.07710	0.07544	0.07516	0.08116	0.08477	0.09681	0.09137	0.10315	0.11567
7	-	0.08817	0.08792	0.09377	0.09811	0.11012	0.10484	0.11643	0.12891
8	-	0.10087	0.10112	0.10703	0.11024	0.12316	0.11702	0.12982	0.14135
9	-	0.11402	0.11315	-	-	0.13574	0.12998	0.14265	0.15451
10	-	-	-	-	-	0.14848	0.14276	0.15587	0.16816
11	-	-	-	-	-	0.16115	0.15558	0.16860	0.18076

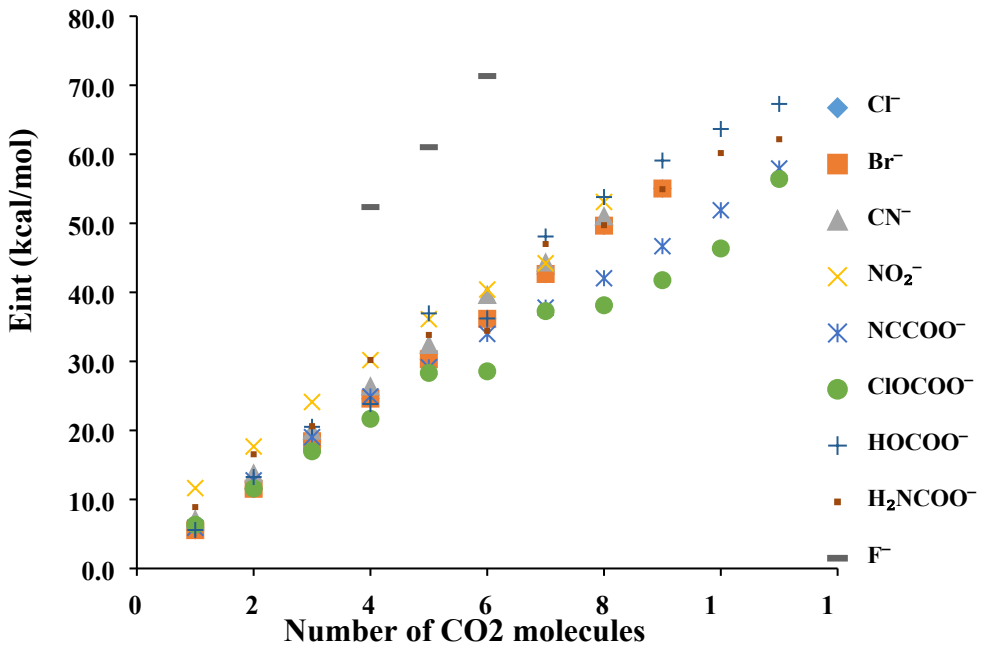
4. Table S4. BSSE energy in kcal/mol for all the $X^-(CO_2)_n$ complexes at M06L/6-311++G** level.

n	F^-	Cl^-	Br^-	CN^-	NO_2^-	$NCCOO^-$	$ClOCOO^-$	$HOCOO^-$	H_2NCOO^-
1	1.2	0.3	0.1	0.2	0.7	0.8	1.8	1.8	2.6
2	1.7	0.7	0.4	0.5	1.2	1.2	2.4	2.3	3.4
3	2.2	1.3	0.9	0.9	1.5	1.6	3.4	3.0	3.9
4	2.7	2.0	1.4	1.5	2.1	2.4	4.0	3.9	5.1
5	3.4	2.6	1.9	2.0	2.8	3.3	4.9	4.7	5.4
6	4.3	3.4	2.4	2.7	3.6	3.6	6.0	4.1	6.2
7		4.2	3.1	3.3	4.4	4.4	6.4	3.4	6.2
8		5.1	3.8	4.3	5.2	5.4	7.9	4.5	8.0
9		6.1	4.9			6.3	8.4	8.1	7.2
10						7.0	9.9	7.7	10.2
11						7.5	10.7	7.6	11.2
						8.5	11.5	8.2	11.0

5. Table S5. ZPE- and BSSE- corrected $E_{int/CO2}$ values are given in kcal/mol of the benchmark study for the representative case, $Cl^-(CO_2)_n$ complexes

n	B3LYP-D3	BP86-D3	wB97XD	M06L
1	7.7	7.0	6.2	6.9
2	7.6	6.3	6.2	7.0
3	7.8	6.1	6.2	7.2
4	7.7	5.8	6.1	7.2
5	7.7	5.7	6.1	7.1
6	7.6	5.6	6.0	7.0
7	7.6	5.5	5.9	7.0
8	7.7	5.5	5.9	7.1
9	7.4	5.0	5.5	6.7

6. Fig. S1. Variation of E_{int} values of $X^-(CO_2)_n$ complexes with number of CO_2 molecules



7. Table S6. ZPE- and BSSE- corrected ΔG_{int} and $\Delta G_{int/CO2}$, in kcal/mol, for the CO_2 complexes of NC^-, ClO^-, OH^-, and NH_2^-, at M06L/6-311++G**level.

n	$NCCOO^-(CO_2)_n$		$ClOCOO^-(CO_2)_n$		$HOCOO^-(CO_2)_n$		$H_2NCOO^-(CO_2)_n$	
	ΔG_{int}	$\Delta G_{int/CO2}$	ΔG_{int}	$\Delta G_{int/CO2}$	ΔG_{int}	$\Delta G_{int/CO2}$	ΔG_{int}	$\Delta G_{int/CO2}$
0	-6.9	-6.9	-15.0	-15.0	-34.7	-34.7	-40.2	-40.2
1	1.6	1.6	1.3	1.3	0.4	0.4	-0.4	-0.4
2	3.4	1.7	5.2	2.6	1.9	0.9	-0.3	-0.2
3	5.9	2.0	7.0	2.3	4.2	1.4	4.4	1.5
4	9.9	2.5	12.5	3.1	9.3	2.3	4.4	1.1
5	13.5	2.7	14.7	2.9	6.7	1.3	8.6	1.7
6	19.0	3.2	23.4	3.9	14.7	2.5	18.8	3.1
7	25.9	3.7	25.0	3.6	14.2	2.0	15.5	2.2
8	31.8	4.0	32.2	4.0	18.6	2.3	20.9	2.6
9	35.5	3.9	39.6	4.4	22.6	2.5	25.0	2.8
10	39.3	3.9	42.4	4.2	28.8	2.9	30.5	3.1
11	43.4	3.9	41.4	3.8	33.6	3.1	36.0	3.3

8. Table S7. ZPE- and BSSE-corrected ΔG_{int} and $\Delta G_{int/CO2}$, in kcal/mol, for the CO_2 complexes of Cl^-, Br^-, CN^-, NO_2^-, and F^- at M06L/6-311++G**level.

n	Cl^-		Br^-		CN^-		O_2N^-		F^-	
	ΔG_{int}	$\Delta G_{int/CO2}$	ΔG_{int}	$\Delta G_{int/CO2}$	ΔG_{int}	$\Delta G_{int/CO2}$	ΔG_{int}	$\Delta G_{int/CO2}$	ΔG_{int}	$\Delta G_{int/CO2}$
1	-2.4	-2.4	-1.2	-1.2	-1.4	-1.4	-3.8	-3.8	-23.4	-23.4
2	-2.6	-1.3	-0.2	-0.1	-0.7	-0.3	-2.2	-1.1	0.1	0.0
3	-0.4	-0.1	2.2	0.7	0.2	0.1	-1.1	-0.4	2.1	0.7
4	1.7	0.4	5.3	1.3	5.3	1.3	2.0	0.5	-22.0	-5.5
5	3.8	0.8	8.7	1.7	8.0	1.6	5.1	1.0	-19.6	-3.9
6	5.7	0.9	11.9	2.0	9.4	1.6	11.1	1.9	-19.7	-3.3
7	7.8	1.1	14.4	2.1	12.7	1.8	17.8	2.5	-14.4	-2.1
8	9.4	1.2	18.2	2.3	17.2	2.1	16.8	2.1	-	-
9	15.6	1.7	28.3	3.1	-	-	-	-	-	-

9. Table S8. QTAIM parameters of F ...CO_2 bond for CO_2 complexes of F^- at M06L/6-311++G** level

n	ρ	$\nabla^2\rho$	$\nabla\rho$	λ_1	a	λ_2	b	λ_3	c
1	0.1755	-0.0285	-0.1688	-0.3165	0.5334	0.5927	0.2849	0.5927	0.2849
2	0.1648	0.0251	0.1585	-0.2928	0.5412	-0.2808	0.5644	0.5987	0.2647
	0.0139	0.0540	0.2324	-0.0128	18.1347	-0.0078	29.7630	0.0746	3.1143
3	0.0181	0.0653	0.2556	-0.0182	14.0299	-0.0108	23.5577	0.0944	2.7080
	0.1072	0.1983	0.4453	-0.1691	2.6332	-0.1555	2.8646	0.5229	0.8517
	0.0199	0.0718	0.2679	-0.0199	13.4437	-0.0128	20.9716	0.1045	2.5644
4	0.0339	0.1076	0.3280	-0.0369	8.8955	-0.0271	12.1214	0.1715	1.9124
	0.0246	0.0823	0.2868	-0.0253	11.3531	-0.0168	17.0296	0.1244	2.3060
	0.0270	0.0898	0.2997	-0.0283	10.5846	-0.0194	15.4864	0.1375	2.1797
	0.0270	0.0899	0.2998	-0.0283	10.5813	-0.0194	15.4789	0.1376	2.1790
5	0.0263	0.0859	0.2931	-0.0269	10.9022	-0.0182	16.0900	0.1310	2.2371
	0.0196	0.0676	0.2601	-0.0191	13.5944	-0.0120	21.6928	0.0988	2.6335
	0.0222	0.0742	0.2724	-0.0222	12.2913	-0.0145	18.8490	0.1108	2.4580
	0.0222	0.0741	0.2722	-0.0221	12.3032	-0.0144	18.8723	0.1107	2.4600
	0.0195	0.0674	0.2597	-0.0191	13.6287	-0.0119	21.7713	0.0984	2.6384
6	0.0196	0.0676	0.2600	-0.0189	13.7413	-0.0117	22.2883	0.0982	2.6482
	0.0196	0.0674	0.2597	-0.0189	13.7559	-0.0116	22.3085	0.0979	2.6512
	0.0193	0.0668	0.2585	-0.0186	13.8696	-0.0114	22.5769	0.0969	2.6677
	0.0193	0.0667	0.2582	-0.0186	13.8894	-0.0114	22.6153	0.0967	2.6710
	0.0194	0.0669	0.2586	-0.0187	13.8433	-0.0115	22.5049	0.0971	2.6644
	0.0195	0.0672	0.2593	-0.0188	13.8005	-0.0116	22.4302	0.0976	2.6573

Here a, b and c are the principal axes of the ellipsoids aligned with the eigenvectors λ_1, $\lambda_2$and λ_3 respectively and are obtained as;

$$a = |\nabla\rho\ |/|\lambda_1| \qquad \text{(S1)}$$

$$b = |\nabla\rho\ |/|\lambda_2| \qquad \text{(S2)}$$

and

$$c = |\nabla\rho\ |/|\lambda_3| \qquad \text{(S3)}$$

Covalent nature of the F-C interactions are confirmed when,

$|\lambda_3| > |\lambda_{1,2}|$ and $c < a, b$

whereas non-covalent interactions are giving $|\lambda_3| >> |\lambda_{1,2}|$ and $c << a, b$

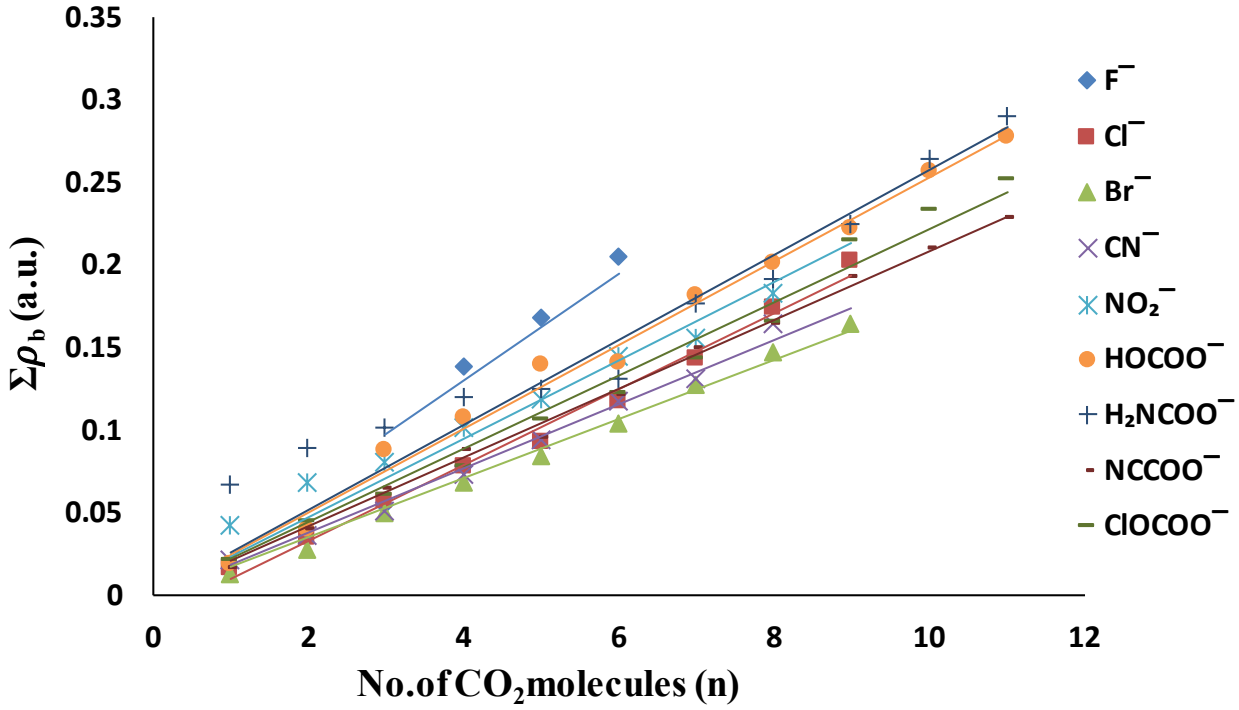
10. Table S9. Average $\nabla^2 \rho$ values (a. u.) of X^- ...CO_2 bond in complexes optimized at M06L/6-311++G** level

n	F^-	Cl^-	Br^-	CN^-	NO_2^-	$NCCOO^-$	$ClOCOO^-$	$HOCOO^-$	H_2NCOO^-
1	-0.0285	0.0481	0.0338	0.0661	0.1209	0.0560	0.0268	0.0686	0.0695
2	0.0540	0.1372	0.0648	0.1028	0.1848	0.1385	0.0736	0.0537	0.1040
3	0.1371	0.1276	0.0932	0.1345	0.2324	0.1888	0.1050	0.2902	0.1147
4	0.3693	0.1652	0.1211	0.1615	0.3013	0.2386	0.1388	0.3146	0.1174
5	0.3693	0.2094	0.1554	0.1963	0.3161	0.2748	0.2628	0.0999	0.1089
6	0.4026	0.2471	0.1791	0.2327	0.3086	0.3279	0.2150	0.1107	0.0437
7	-	0.2651	0.2094	0.2632	0.4361	0.3591	0.1416	0.4669	0.1202
8	-	0.2854	0.2485	0.2769	0.4244	0.3832	0.2357	0.1418	0.0894
9	-	0.2594	0.2294	-	-	0.4244	0.3389	0.1528	0.5591
10	-	-	-	-	-	0.5037	0.5688	0.5073	0.6033
11	-	-	-	-	-	0.4634	0.5932	0.5415	0.5290

11. Table S10. $\nabla^2\rho$ (a. u.) and H (a. u.) values for the CO_2 complexes of F^-, NC^-, ClO^-, OH^-, and NH_2^-, at M06L/6-311++G**level.

n	$FCOO^-(CO_2)_n$		$NCCOO^-(CO_2)_n$		$ClOCOO^-(CO_2)_n$		$HOCOO^-(CO_2)_n$		$H_2NCOO^-(CO_2)_n$	
	$\nabla^2\rho$	H	$\nabla^2\rho$	H	$\nabla^2\rho$	H	$\nabla^2\rho$	H	$\nabla^2\rho$	H
0	-0.0285	-0.1330	-0.5483	-0.2078	-0.3603	-0.2495	-0.4483	-0.2773	-0.6419	-0.2803
1	0.0251	-0.1116	-0.5585	-0.2104	-0.3901	-0.2665	-0.3959	-0.2516	-0.7783	-0.3330
2	0.1983	-0.0304	-0.5946	-0.2196	-0.3314	-0.2342	-0.4198	-0.2638	-0.8028	-0.3433
3	0.1078	-0.0004	-0.6068	-0.2223	-0.2982	-0.2186	-0.4693	-0.2992	-0.7784	-0.3375
4			-0.6199	-0.2254	-0.2386	-0.1927	-0.4541	-0.2849	-0.7750	-0.3321
5			-0.6228	-0.2263	-0.3626	-0.2481	-0.5046	-0.3516	-0.7490	-0.3187
6			-0.6277	-0.2272	-0.3203	-0.2295	-0.4931	-0.3218	-0.7311	-0.3154
7			-0.6380	-0.2291	-0.3571	-0.2450	-0.5110	-0.3611	-0.7845	-0.3333
8			-0.6254	-0.2264	-0.2838	-0.2116	-0.5043	-0.3565	-0.7712	-0.3295
9			-0.6277	-0.2266	-0.2588	-0.2026	-0.5027	-0.3577	-0.7866	-0.3358
10			-0.6254	-0.2278	-0.3215	-0.2297	-0.5011	-0.3409	-0.7732	-0.3320
11			-0.6177	-0.2255	-0.3295	-0.2324	-0.4996	-0.3343	-0.7744	-0.3338

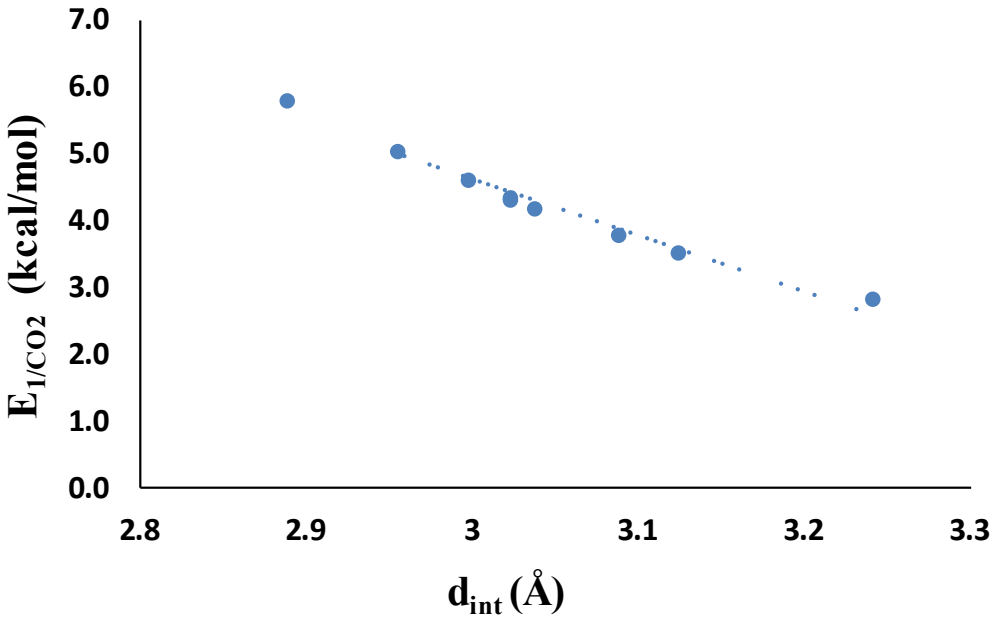
12. Fig. S2. Variation of $\Sigma\rho_b$ values of $X^-(CO_2)_n$ complexes with number of CO_2 molecules



13. Table S11. Slope (m) and correlation coefficient (R) of the plots between E_{int} and $\Sigma\rho_b$ of $X^-(CO_2)_n$ complexes at the M06L/6-311++G** level.

Anion	Slope	Correlation coefficient (R)
F^-	358.67	0.9678
Cl^-	332.34	0.9801
Br^-	342.76	0.9969
CN^-	332.64	0.9902
NO_2^-	288.44	0.9959
$NCCOO^-$	256.85	0.9878
$ClOCOO^-$	221.78	0.9667
$HOCOO^-$	254.24	0.9933
H_2NCOO^-	235.63	0.9668

14. Fig. S3. Correlation between $E_{1/CO2}$ and dint values of $Cl^{-}(CO_2)_n$ at M06L/6-311++G** level



.

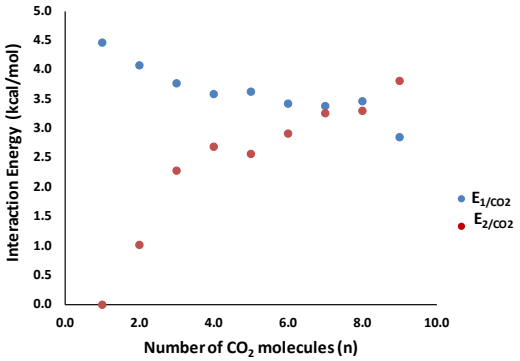
15. Table S12. $\Sigma\rho_1$ values (a.u.) of X^{-}…CO_2 bond in complexes at the M06L/6-311++G** level of theory.

n	F^{-}	Cl^{-}	Br^{-}	CN^{-}	NO_2^{-}	$NCCOO^{-}$	$ClOCOO^{-}$	$HOCOO^{-}$	H_2NCOO^{-}
1	0.1755	0.0164	0.0122	0.0210	0.0427	0.0160	0.0216	0.0186	0.0669
2	0.0139	0.0450	0.0222	0.0307	0.0679	0.0394	0.0435	0.0339	0.0894
3	0.0380	0.0391	0.0309	0.0392	0.0746	0.0523	0.0539	0.0808	0.0903
4	0.1125	0.0493	0.0392	0.0484	0.0888	0.0648	0.0610	0.0853	0.1024
5	0.1099	0.0611	0.0495	0.0575	0.0942	0.0739	0.0800	0.1096	0.0859
6	0.1166	0.0708	0.0559	0.0676	0.0832	0.0845	0.0877	0.0971	0.0684
7	-	0.0749	0.0644	0.0763	0.1152	0.0946	0.0813	0.1252	0.1246
8	-	0.0797	0.0754	0.0788	0.1136	0.0970	0.1047	0.1406	0.1224
9	-	0.0722	0.0700	-	-	0.1097	0.1242	0.1445	0.1506
10	-	-	-	-	-	0.1286	0.1416	0.1306	0.1597
11	-	-	-	-	-	0.1159	0.1470	0.1381	0.1409

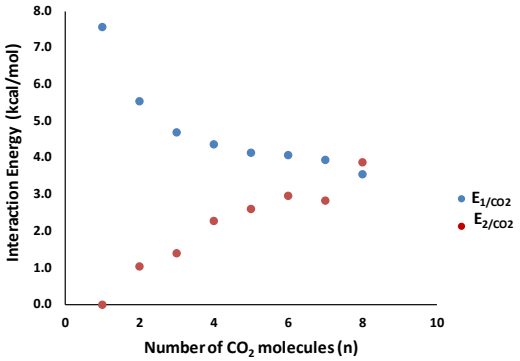
16. Table S13. $\Sigma\rho_2$ values (a.u.) of X^-…CO_2 bond in complexes at the M06L/6-311++G** level of theory.

n	F^-	Cl^-	Br^-	CN^-	NO_2^-	$NCCOO^-$	$ClOCOO^-$	$HOCOO^-$	H_2NCOO^-
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0146	0.0061	0.0056	0.0058	0.0000	0.0000	0.0013	0.0056	0.0000
3	0.0169	0.0184	0.0186	0.0118	0.0059	0.0116	0.0067	0.0071	0.0113
4	0.0265	0.0285	0.0294	0.0252	0.0127	0.0231	0.0173	0.0216	0.0176
5	0.0587	0.0318	0.0351	0.0363	0.0250	0.0218	0.0258	0.0300	0.0383
6	0.0884	0.0467	0.0475	0.0493	0.0618	0.0362	0.0349	0.0433	0.0628
7	-	0.0678	0.0624	0.0551	0.0399	0.0555	0.0626	0.0560	0.0522
8	-	0.0943	0.0719	0.0861	0.0690	0.0678	0.0608	0.0607	0.0684
9	-	0.1302	0.0938	-	-	0.0831	0.0906	0.0781	0.0737
10	-	-	-	-	-	0.0808	0.0911	0.1261	0.1050
11	-	-	-	-	-	0.1129	0.1049	0.1399	0.1492

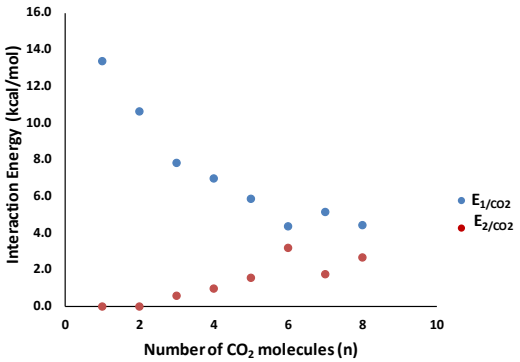
17. Fig. S4. Correlation plot for $E_{1/CO2}$ and $E_{2/CO2}$ vs number of CO_2 molecules (n) for $X^-(CO_2)_n$ at M06L/6-311++G** level.

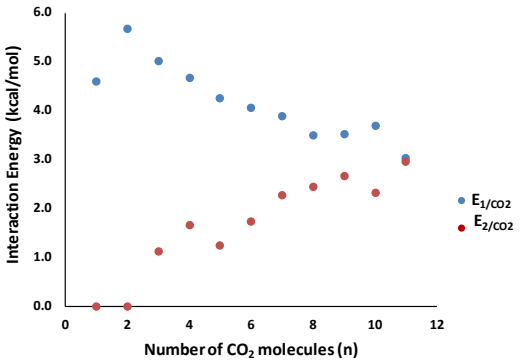


(a) $Br^-(CO_2)_n$

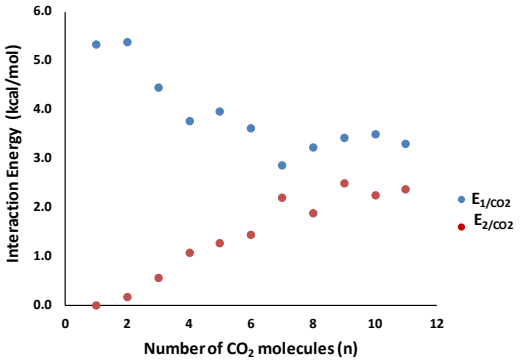


(b) $CN^-(CO_2)$

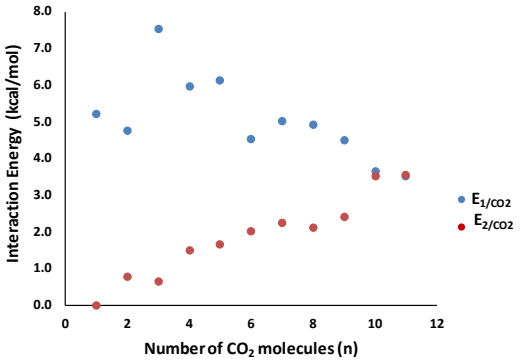




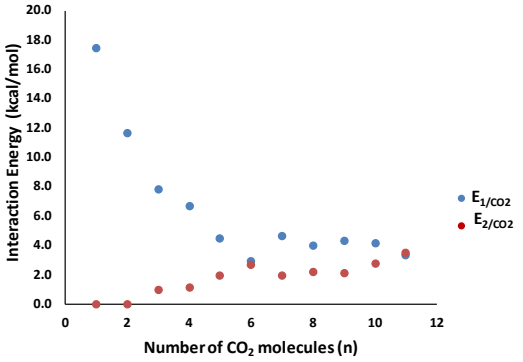
(c) $NO_2^-(CO_2)_n$



(d) $NCCOO^-(CO_2)_n$



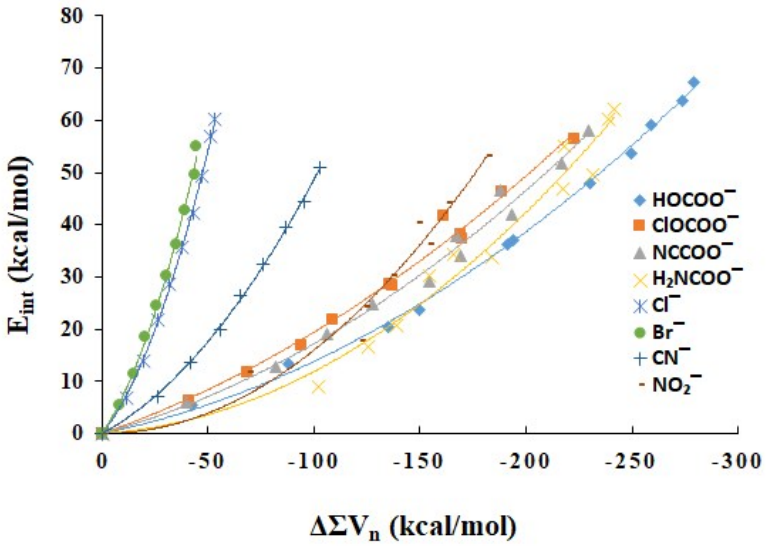
(e) $ClOCOO^-(CO_2)_n$



(f) $HOCOO^-(CO_2)_n$

(g) $H_2NCOO^-(CO_2)_n$

18. Fig. S5. Correlation between E_{int} and $\Sigma(\Delta V_n)$ of $X^-(CO_2)_n$ complexes at the M06L/6-311++G** level.



The best fitting for the data E_{int} vs $\Sigma(\Delta V_n)$ gives the second degree polynomial equation in the form;

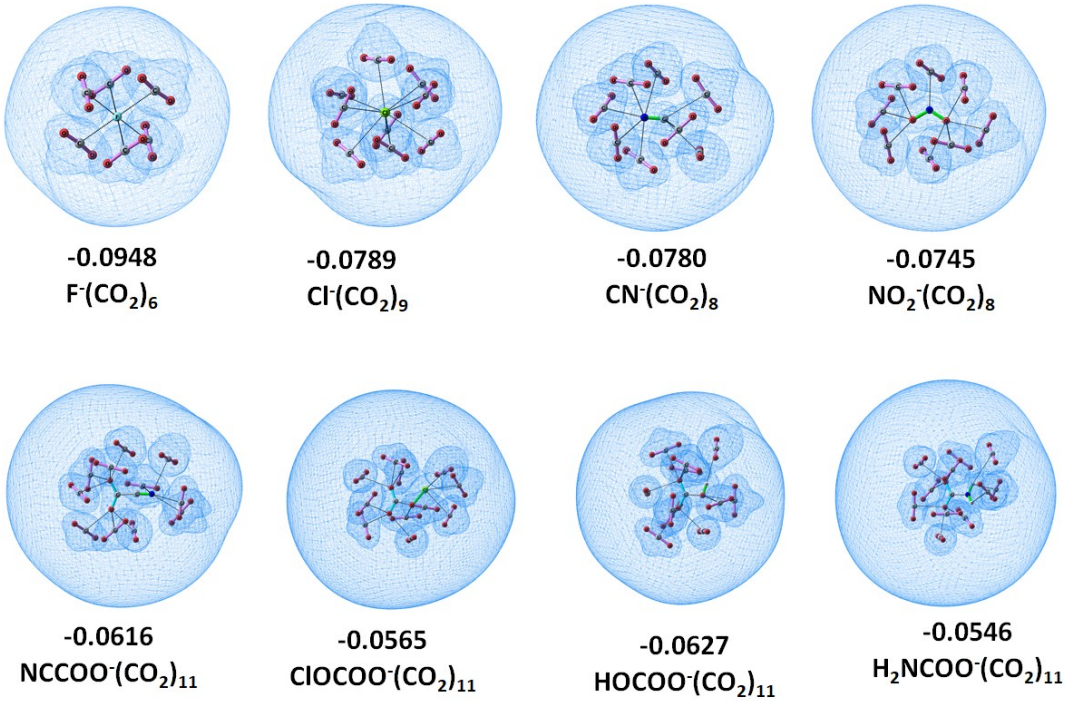
$$y = ax^2 + bx + c \quad \text{(S4)}$$

the values of a, b and the corresponding correlation coefficient (R) for each anion are given in Table S6

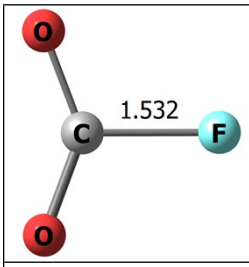
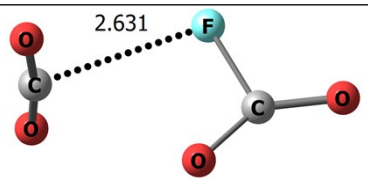
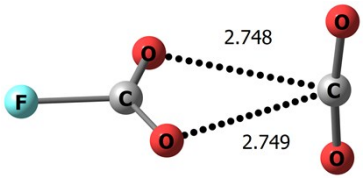
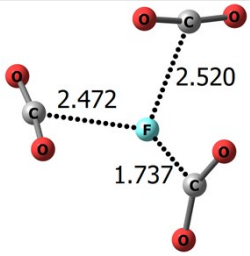
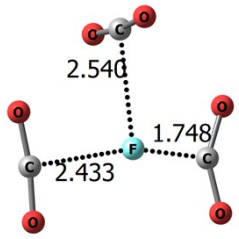
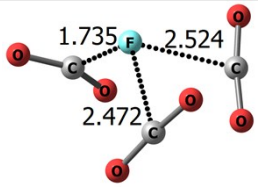
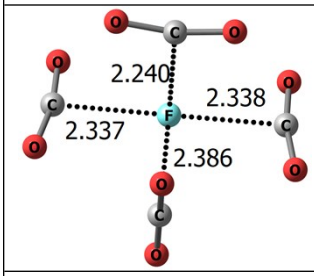
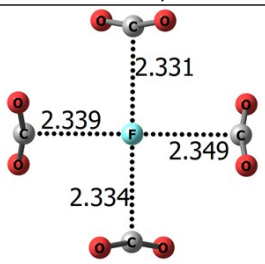
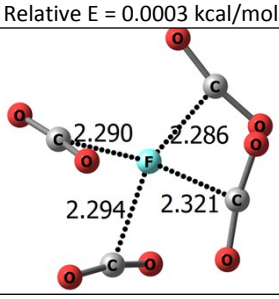
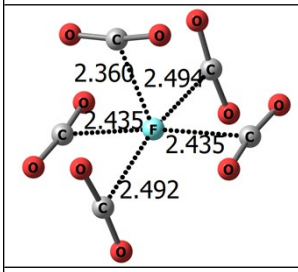
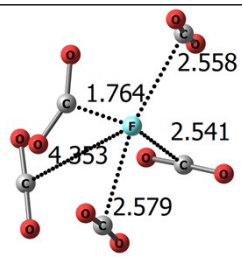
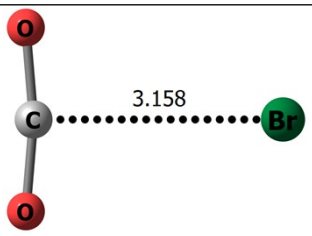
19. Table S14. Polynomial co-efficient a, b and correlation coefficient (R) of the plots between E_{int} and $\Sigma\rho_b$ of $X^-(CO_2)_n$ complexes at the M06L/6-311++G** level.

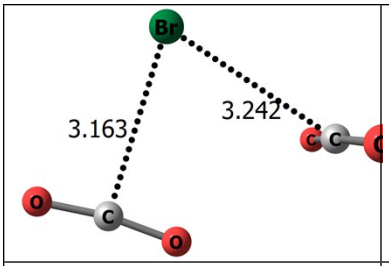
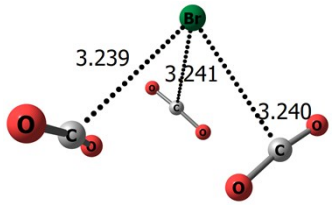
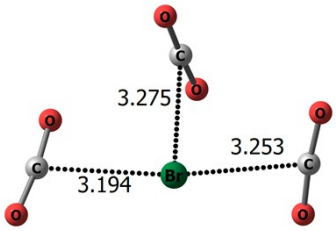
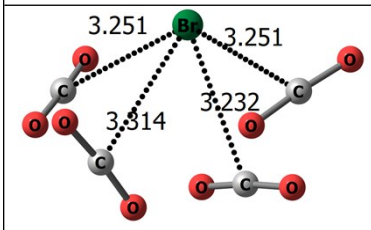
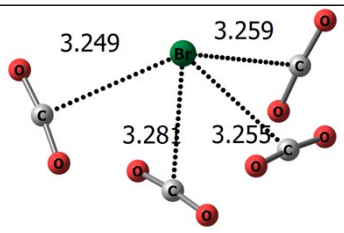
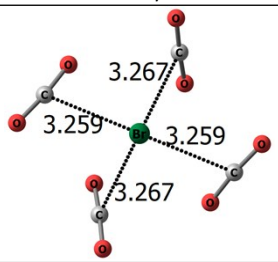
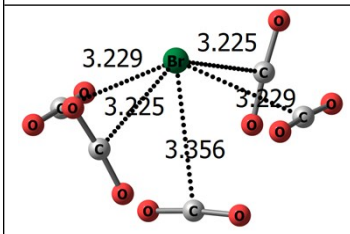
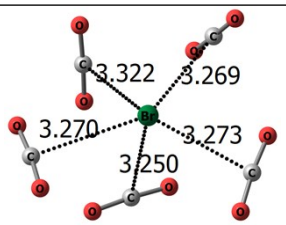
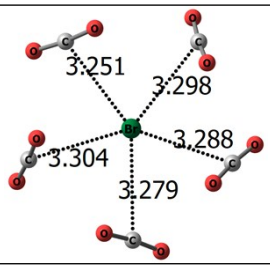
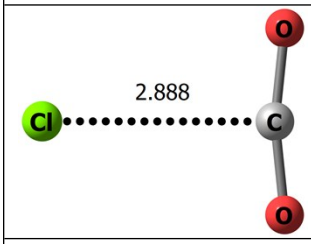
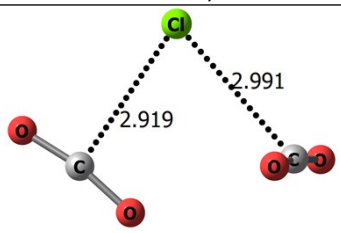
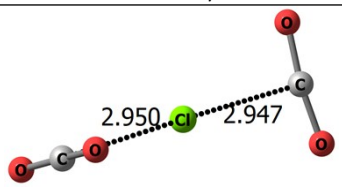
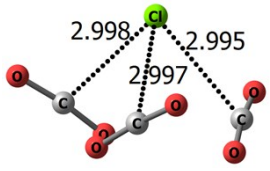
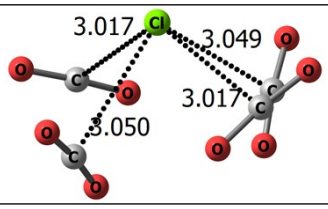
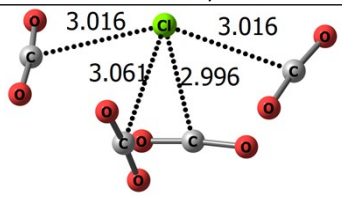
Anion	a	b	R
Cl^-	0.0115	-0.5085	0.9995
Br^-	0.0130	-0.6031	0.9986
CN^-	0.0027	-0.2189	0.9995
NO_2^-	0.0016	0.0033	0.9817
$NCCOO^-$	0.0006	-0.1114	0.9945
$ClOCOO^-$	0.0005	-0.1417	0.9941
$HOCOO^-$	0.0006	-0.0831	0.9992
H_2NCOO^-	0.0009	-0.0255	0.9860

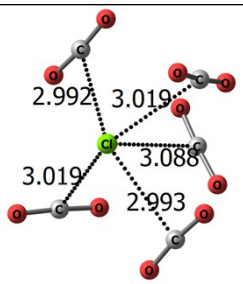
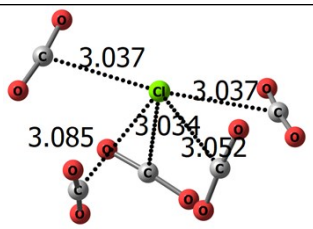
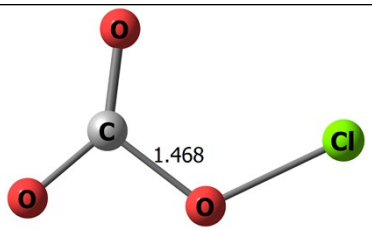
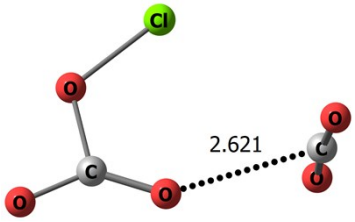
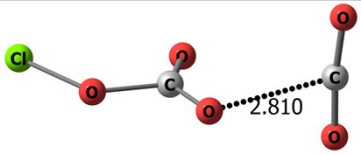
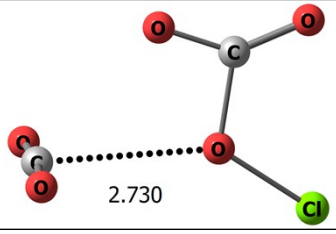
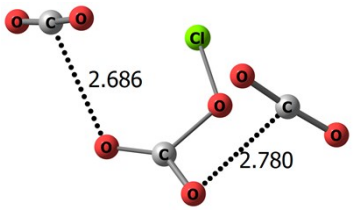
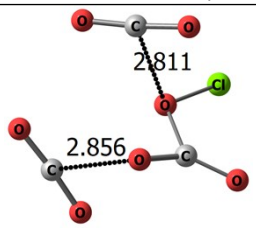
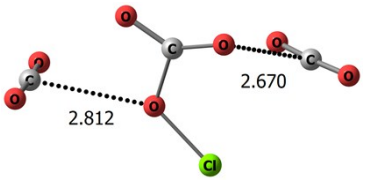
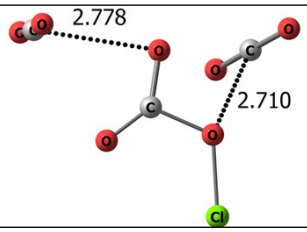
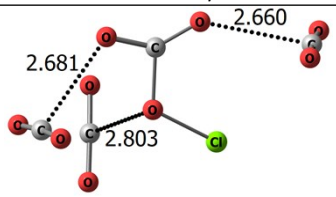
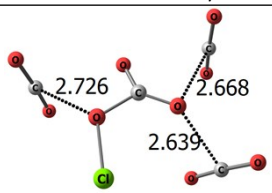
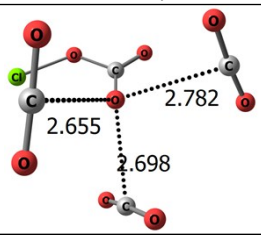
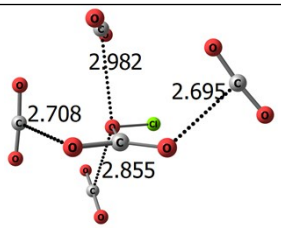
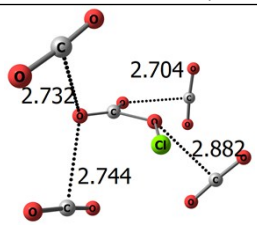
20. Fig. S6. MESP of $X^-(CO_2)_{nmax}$ at the M06L/6-311++G** level. The minimum value of MESP that engulfs the whole anion (V_m) is also depicted in a.u.

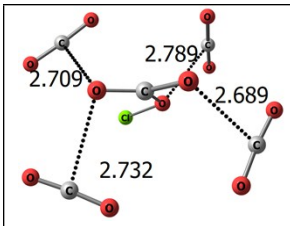
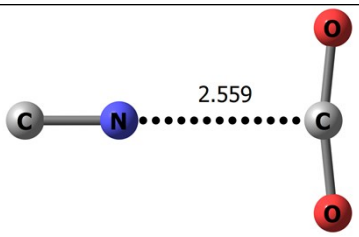
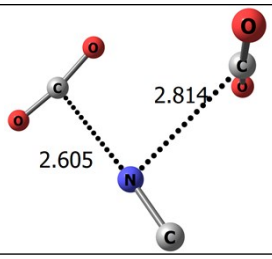
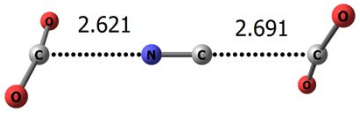
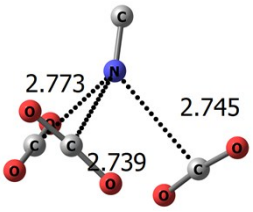
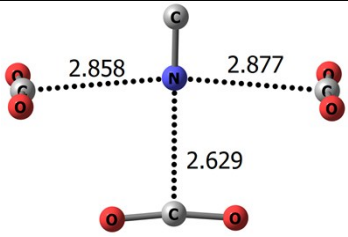
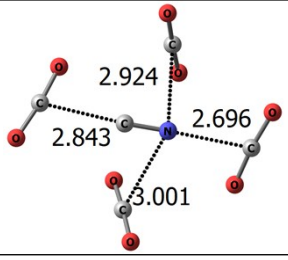
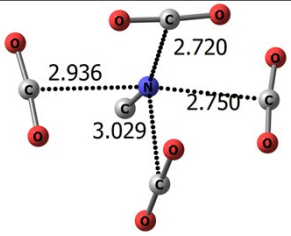
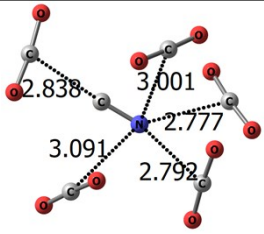
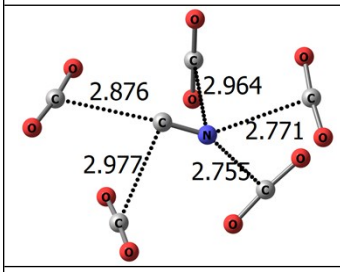
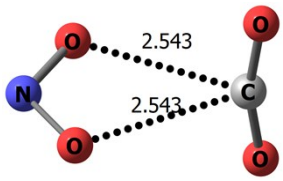
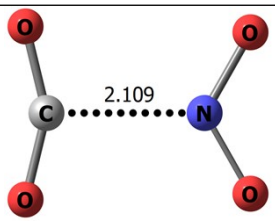
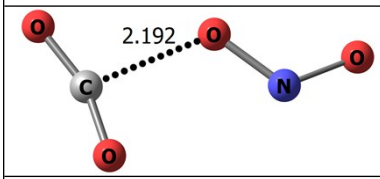
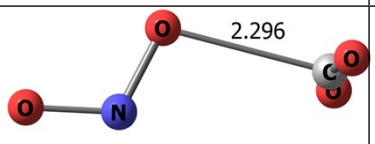
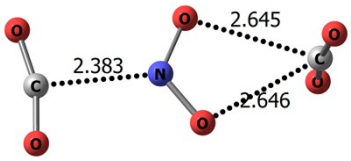


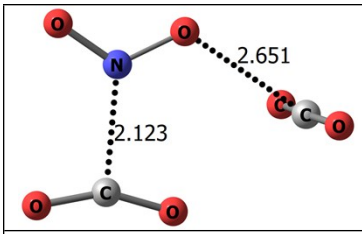
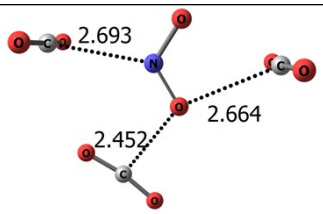
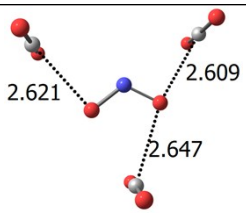
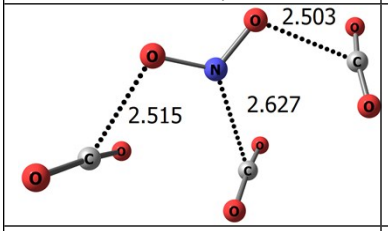
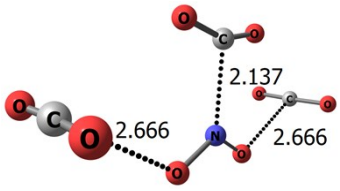
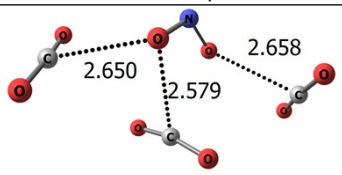
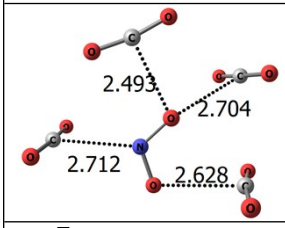
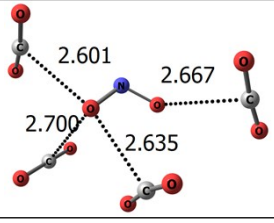
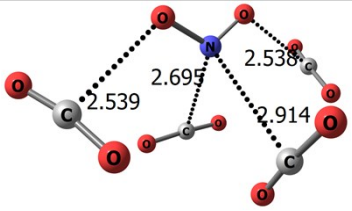
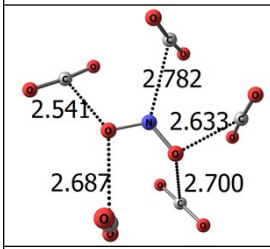
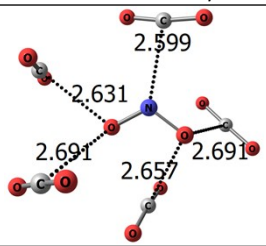
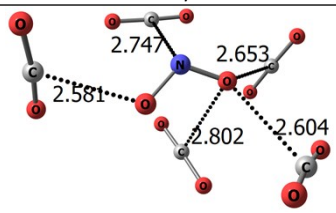
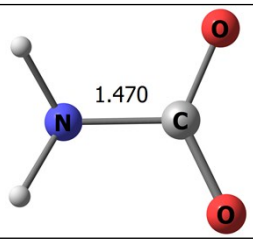
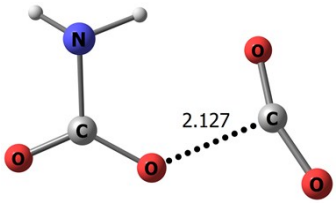
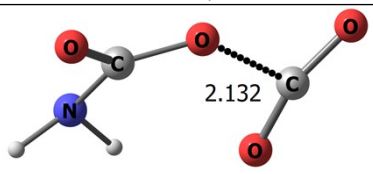
21. Table S15. Optimized geometries of $X^{-}(CO_2)_n$ complexes at M06L/6-311++G**level and their respective SCF energy in a.u.

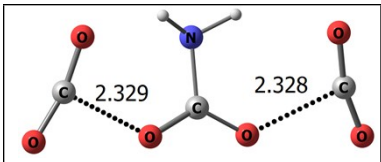
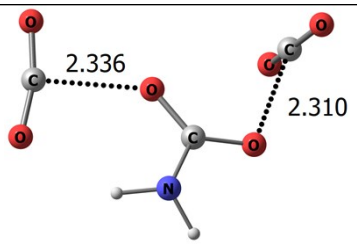
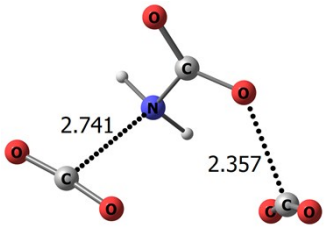
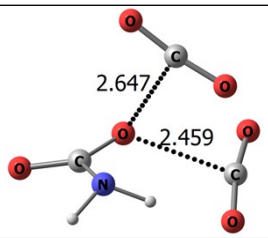
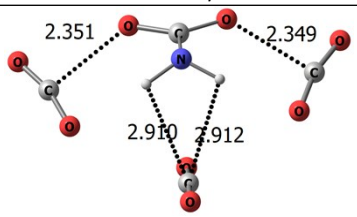
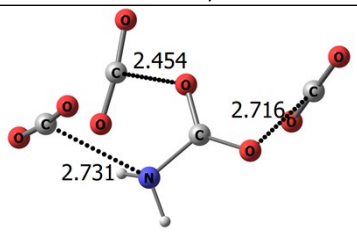
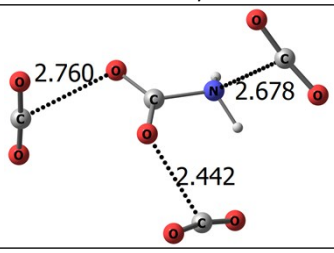
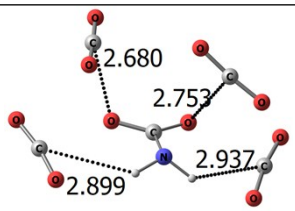
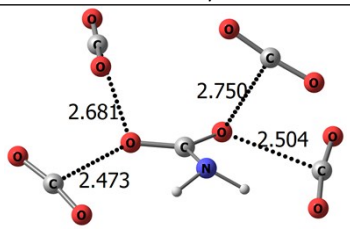
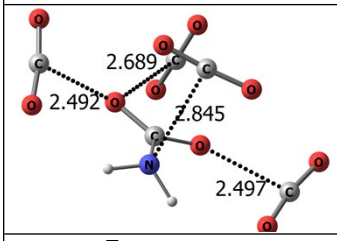
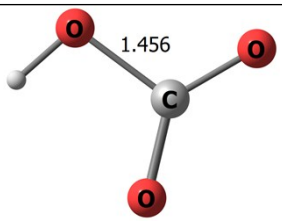
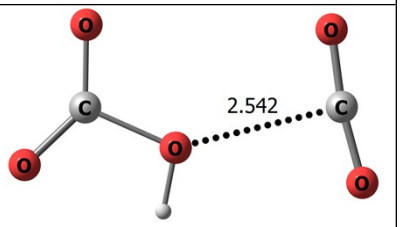
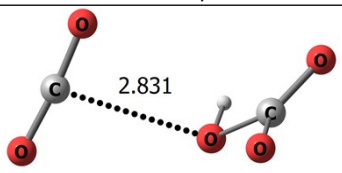
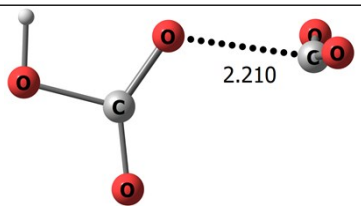
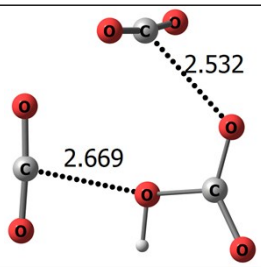
		
$FCOO^{-}$ (SCF E = -288.54171 a.u.)	$FCOO^{-}(CO_2)$ (SCF E = -477.18699 a.u.)	$FCOO^{-}(CO_2)$ (SCF E = -288.54171 a.u.) Relative E = 0.51 kcal/mol
		
$FCOO^{-}(CO_2)_2$ (SCF E = -665.83005 a.u.)	$FCOO^{-}(CO_2)_2$ (SCF E = -665.82851 a.u.) Relative E = 0.96 kcal/mol	$FCOO^{-}(CO_2)_2$ (SCF E = -665.83004 a.u.) Relative E = 0.0003 kcal/mol
		
$F^{-}(CO_2)_4$ (SCF E = -854.47699 a.u.)	$F^{-}(CO_2)_4$ (SCF E = -854.47451 a.u.) Relative E = 1.56 kcal/mol	$F^{-}(CO_2)_4$ (SCF E = -854.47591 a.u.) Relative E = 0.68 kcal/mol
		
$F^{-}(CO_2)_5$ (SCF E = -1043.12494 a.u.)	$F^{-}(CO_2)_5$ (SCF E = - 1043.11635 a.u.) Relative E = 5.38 kcal/mol	$Br^{-}(CO_2)$ (SCF E = -2762.73215 a.u.)

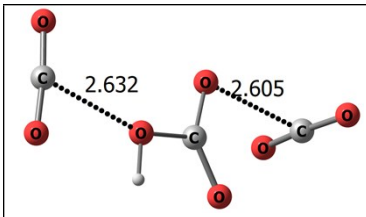
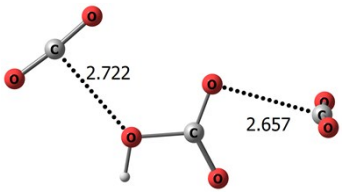
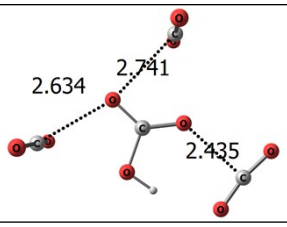
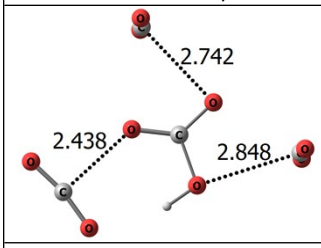
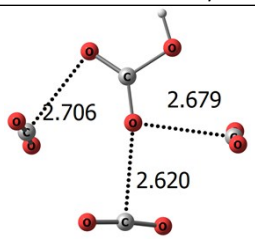
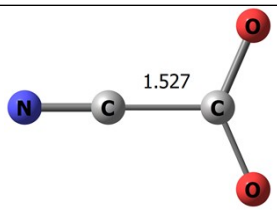
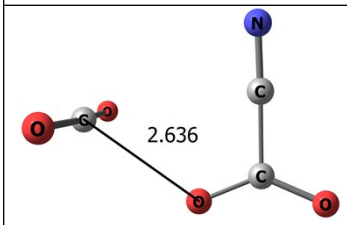
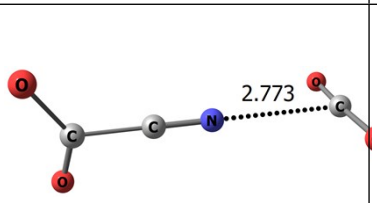
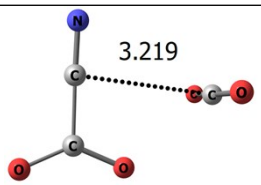
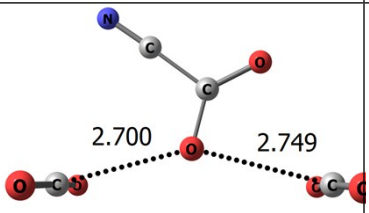
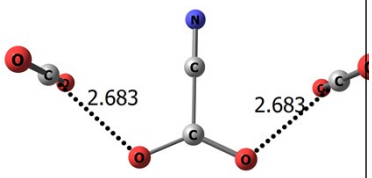
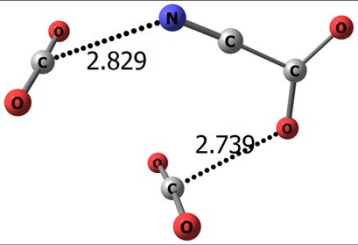
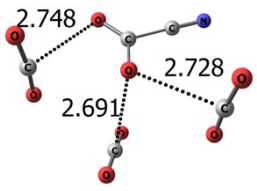
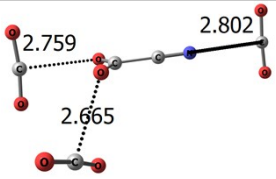
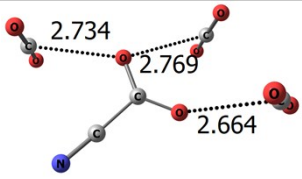
		
$Br^-(CO_2)_2$ (SCF E = -2951.37405 a.u.)	$Br^-(CO_2)_3$ (SCF E = -3140.01782 a.u.)	$Br^-(CO_2)_3$ (SCF E = -3140.01551 a.u.) Relative E = 1.44 kcal/mol
		
$Br^-(CO_2)_4$ (SCF E = -3328.66067 a.u.)	$Br^-(CO_2)_4$ (SCF E = -3328.65885 a.u.) Relative E = 1.15 kcal/mol	$Br^-(CO_2)_4$ (SCF E = -3328.65939 a.u.) Relative E = 0.80 kcal/mol
		
$Br^-(CO_2)_5$ (SCF E = -3517.30283 a.u.)	$Br^-(CO_2)_5$ (SCF E = -3517.30199 a.u.) Relative E = 0.52 kcal/mol	$Br^-(CO_2)_5$ (SCF E = -3517.29922 a.u.) Relative E = 2.26 kcal/mol
		
$Cl^-(CO_2)$ (SCF E = -648.91598 a.u.)	$Cl^-(CO_2)_2$ (SCF E = -837.5598484 a.u.)	$Cl^-(CO_2)_2$ (SCF E = -837.55788 a.u.) Relative E = 1.23 kcal/mol
		
$Cl^-(CO_2)_3$ (SCF E = -1026.20529 a.u.)	$Cl^-(CO_2)_4$ (SCF E = -1214.84983 a.u.)	$Cl^-(CO_2)_4$ (SCF E = -1214.848396 a.u.) Relative E = 0.89 kcal/mol

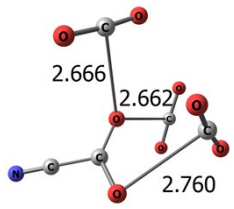
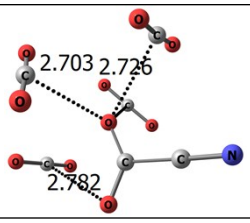
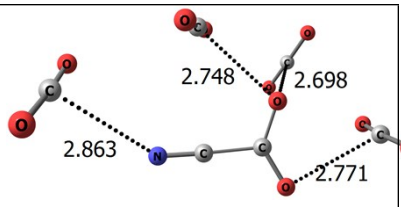
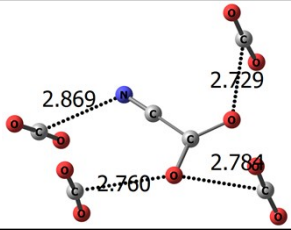
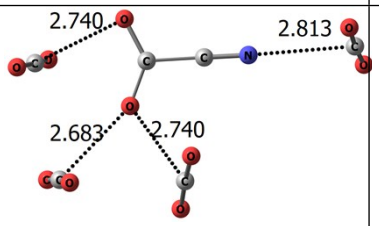
		
$Cl^-(CO_2)_5$ (SCF E = -1403.49437 a.u.)	$Cl^-(CO_2)_5$ (SCF E = -1403.49263 a.u.) Relative E = 1.09 kcal/mol	$ClCOO^-$ (SCF E = -724.06028 a.u.)
		
$ClCOO^-(CO_2)$ (SCF E = -912.70338 a.u.)	$ClCOO^-(CO_2)$ (SCF E = -912.70337 a.u.) Relative E = 0.03 kcal/mol	$ClCOO^-(CO_2)$ (SCF E = -912.70331 a.u.) Relative E = 0.04 kcal/mol
		
$ClCOO^-(CO_2)_2$ (SCF E = -1101.34536 a.u.)	$ClCOO^-(CO_2)_2$ (SCF E = -1101.34432 a.u.) Relative E = 0.65 kcal/mol	$ClCOO^-(CO_2)_2$ (SCF E = -1101.34533 a.u.) Relative E = 0.02 kcal/mol
		
$ClCOO^-(CO_2)_2$ (SCF E = -1101.34531 a.u.) Relative E = 0.03 kcal/mol	$ClCOO^-(CO_2)_3$ (SCF E = -1289.98681 a.u.)	$ClCOO^-(CO_2)_3$ (SCF E = -1289.98666 a.u.) Relative E = 0.09 kcal/mol
		
$ClCOO^-(CO_2)_3$ (SCF E = -1101.34531 a.u.) Relative E = 0.29 kcal/mol	$ClCOO^-(CO_2)_4$ (SCF E = -1101.34531 a.u.)	$ClCOO^-(CO_2)_4$ (SCF E = -1101.34531 a.u.) Relative E = 0.0007 kcal/mol

		
$ClCOO^-(CO_2)_4$ (SCF E = -1101.34531 a.u.) Relative E = 0.01 kcal/mol	$CN^-(CO_2)$ (SCF E = -281.5088534 a.u.)	$CN^-(CO_2)_2$ (SCF E = -470.15206 a.u.)
		
$CN^-(CO_2)_2$ (SCF E = -470.15112 a.u.) Relative E = 0.58 kcal/mol	$CN^-(CO_2)_3$ (SCF E = -658.79574 a.u.)	$CN^-(CO_2)_3$ (SCF E = -658.79441 a.u.) Relative E = 0.84kcal/mol
		
$CN^-(CO_2)_4$ (SCF E = -847.43836 a.u.)	$CN^-(CO_2)_4$ (SCF E = -847.43812 a.u.) Relative E = 0.15 kcal/mol	$CN^-(CO_2)_5$ (SCF E = -1036.08113 a.u.)
		
$CN^-(CO_2)_5$ (SCF E = -1036.08051 a.u.) Relative E = 0.39 kcal/mol	$NO_2^-(CO_2)$ (SCF E = -393.84510 a.u.)	$NO_2^-(CO_2)$ (SCF E = -393.84152 a.u.) Relative E = 2.24 kcal/mol
		
$NO_2^-(CO_2)$ (SCF E = -393.83986 a.u.) Relative E = 3.29 kcal/mol	$NO_2^-(CO_2)$ (SCF E = -393.83949 a.u.) Relative E = 3.52 kcal/mol	$NO_2^-(CO_2)_2$ (SCF E = -582.48781 a.u.)

		
$NO_2^-(CO_2)_2$ (SCF E = -582.48555 a.u.) Relative E = 1.42 kcal/mol	$NO_2^-(CO_2)_3$ (SCF E = -771.13062 a.u.)	$NO_2^-(CO_2)_3$ (SCF E = -771.12964 a.u.) Relative E = 0.61 kcal/mol
		
$NO_2^-(CO_2)_3$ (SCF E = -771.12767 a.u.) Relative E = 1.85 kcal/mol	$NO_2^-(CO_2)_3$ (SCF E = -771.12869 a.u.) Relative E = 1.29 kcal/mol	$NO_2^-(CO_2)_3$ (SCF E = -771.12989 a.u.) Relative E = 0.46 kcal/mol
		
$NO_2^-(CO_2)_4$ (SCF E = -959.77354 a.u.)	$NO_2^-(CO_2)_4$ (SCF E = -959.77324 a.u.) Relative E = 0.18 kcal/mol	$NO_2^-(CO_2)_4$ (SCF E = -959.7709524a.u.) Relative E = 1.62 kcal/mol
		
$NO_2^-(CO_2)_5$ (SCF E = -1148.41639 a.u.)	$NO_2^-(CO_2)_5$ (SCF E = -1148.41589 a.u.) Relative E = 0.31 kcal/mol	$NO_2^-(CO_2)_5$ (SCF E = -1148.41395 a.u.) Relative E = 1.53 kcal/mol
		
NH_2COO^- (SCF E = -244.62351 a.u.)	$NH_2COO^-(CO_2)$ (SCF E = -433.27144 a.u.)	$NH_2COO^-(CO_2)$ (SCF E = -433.27144 a.u.) Relative E = -0.0003 kcal/mol

		
$NH_2COO^-(CO_2)_{2\ a}$ (SCF E = -621.91635 a.u.)	$NH_2COO^-(CO_2)_{2\ 3}$ (SCF E = -621.91514 a.u.) Relative E = 0.76 kcal/mol	$NH_2COO^-(CO_2)_{2\ 1}$ (SCF E = -621.91215 a.u.) Relative E = 2.64 kcal/mol
		
$NH_2COO^-(CO_2)_{2\ 1a}$ (SCF E = -621.91565 a.u.) Relative E = 0.44 kcal/mol	$NH_2COO^-(CO_2)_{3\ a}$ (SCF E = -810.55615 a.u.)	$NH_2COO^-(CO_2)_{3\ 2}$ (SCF E = -810.55497 a.u.) Relative E = 0.74 kcal/mol
		
$NH_2COO^-(CO_2)_{3\ 3}$ (SCF E = --810.55593 a.u.) Relative E = 0.14 kcal/mol	$NH_2COO^-(CO_2)_{4\ a}$ (SCF E = -999.20445 a.u.)	$NH_2COO^-(CO_2)_{4\ 1}$ (SCF E = -999.20445 a.u.) Relative E = -0.0005 kcal/mol
		
$NH_2COO^-(CO_2)_{4\ 2}$ (SCF E = -999.20442 a.u.) Relative E = 0.02 kcal/mol	$HOCOO^-$ (SCF E = -264.50836 a.u.)	$HOCOO^-(CO_2)$ (SCF E = -453.14955 a.u.)
		
$HOCOO^-(CO_2)$ (SCF E = -453.14907 a.u.) Relative E = 0.31 kcal/mol	$HOCOO^-(CO_2)$ (SCF E = -453.13867 a.u.) Relative E = 6.83 kcal/mol	$HOCOO^-(CO_2)_2$ (SCF E = -641.79492 a.u.)

		
$HOCOO^-(CO_2)_2$ (SCF E = -641.79487 a.u.) Relative E = 0.03 kcal/mol	$HOCOO^-(CO_2)_2$ (SCF E = -641.79475 a.u.) Relative E = 0.10 kcal/mol	$HOCOO^-(CO_2)_3$ (SCF E = -830.44437 a.u.)
		
$HOCOO^-(CO_2)_3$ (SCF E =-830.44437 a.u.) Relative E = 0.001 kcal/mol	$HOCOO^-(CO_2)_3$ (SCF E = -830.44369 a.u.) Relative E = 0.43 kcal/mol	$NCCOO^-$ (SCF E = -281.52385 a.u.)
		
$NCCOO^-(CO_2)$ (SCF E = -470.16586 a.u.)	$NCCOO^-(CO_2)$ (SCF E = -470.16232 a.u.) Relative E = 2.23 kcal/mol	$NCCOO^-(CO_2)$ (SCF E = -470.16577 a.u.) Relative E = 0.06 kcal/mol
		
$NCCOO^-(CO_2)_2$ (SCF E = -658.80966 a.u.)	$NCCOO^-(CO_2)_2$ (SCF E = -658.80685 a.u.) Relative E = 1.76 kcal/mol	$NCCOO^-(CO_2)_2$ (SCF E = -658.80534 a.u.) Relative E = 2.71 kcal/mol
		
$NCCOO^-(CO_2)_3$ (SCF E = --847.45309 a.u.)	$NCCOO^-(CO_2)_3$ (SCF E = -847.44821a.u.) Relative E = 3.07 kcal/mol	$NCCOO^-(CO_2)_3$ (SCF E = -847.45092 a.u.) Relative E = 1.37 kcal/mol

		
$NCCOO^{-}(CO_2)_3$ (SCF E = -847.45207 a.u.) Relative E = 0.65 kcal/mol	$NCCOO^{-}(CO_2)_4$ (SCF E = -1036.09634 a.u.)	$NCCOO^{-}(CO_2)_4$ (SCF E = -1036.09201 a.u.) Relative E = 2.72 kcal/mol
		
$NCCOO^{-}(CO_2)_4$ (SCF E = -1036.08876 a.u.) Relative E = 4.76 kcal/mol	$NCCOO^{-}(CO_2)_4$ (SCF E = -1036.08929 a.u.) Relative E = 4.42 kcal/mol	

22. Table S16. Cartesian coordinates of optimized geometry of complexes at M06L/6-311++G**level. Atomic number followed by X, Y, Z coordinates in Å.

$FCOO^{-}$			
9	0.000007000	-1.308378000	0.000000000
6	0.000000000	0.224366000	0.000000000
8	-1.139064000	0.651815000	0.000000000
8	1.139056000	0.651837000	0.000000000

$FCOO^{-}(CO_2)$			
9	0.603582000	1.135429000	0.000712000
6	1.423053000	-0.191347000	-0.000179000
8	2.609384000	0.042758000	-0.000023000
8	0.658348000	-1.137741000	-0.000799000
6	-1.761791000	-0.016832000	0.000043000
8	-1.846603000	-0.012327000	-1.160274000
8	-1.846105000	-0.013914000	1.160397000

$FCOO^{-}(CO_2)_2$			
9	-0.113646000	-0.374057000	0.907530000
6	-0.948312000	1.773555000	-0.113560000
8	-0.062383000	1.825324000	-0.867106000
8	-1.859434000	1.883885000	0.600331000
6	-1.056723000	-1.485920000	-0.036597000
8	-0.840069000	-2.577838000	0.393361000
8	-1.644297000	-0.818656000	-0.840234000
6	2.141174000	-0.044812000	-0.050719000
8	1.957925000	-0.767664000	-0.942367000
8	2.474005000	0.693645000	0.785701000

$F^{-}(CO_2)_4$			
9	0.002424000	-0.151571000	-0.456527000
6	0.005103000	-1.470139000	1.354598000
8	1.164534000	-1.554872000	1.475275000
8	-1.153866000	-1.566324000	1.470972000
6	-0.011967000	2.001359000	0.572202000
8	-0.008373000	2.617120000	-0.416469000
8	-0.016291000	1.578196000	1.658514000
6	-2.288048000	-0.243476000	-0.914165000
8	-2.552458000	0.722073000	-0.314882000
8	-2.260012000	-1.209647000	-1.565276000
6	2.293947000	-0.230018000	-0.909961000
8	2.551822000	0.738042000	-0.311912000
8	2.272641000	-1.197366000	-1.559633000

$F^{-}(CO_2)_5$			
9	0.000630000	0.000403000	-0.295781000
6	0.000549000	0.000463000	2.064295000

$F^{-}(CO_2)_6$			
9	-0.644129000	-0.001561000	0.002883000
6	4.146414000	-0.007031000	0.009625000

8	0.002154000	-1.159604000	2.179526000
8	-0.000847000	1.160552000	2.179231000
6	2.481352000	0.000482000	-0.537166000
8	2.476743000	0.002842000	-1.700494000
8	2.662149000	-0.001796000	0.613139000
6	-0.001044000	2.429129000	-0.463836000
8	1.158704000	2.534595000	-0.470916000
8	-1.160904000	2.532271000	-0.481236000
6	0.000520000	-2.429062000	-0.463261000
8	1.160306000	-2.533192000	-0.479079000
8	-1.159311000	-2.533444000	-0.471916000
6	-2.481862000	-0.001209000	-0.535562000
8	-2.660796000	0.001355000	0.615014000
8	-2.478542000	-0.003886000	-1.698869000

8	4.227815000	-1.165963000	0.041330000
8	4.117424000	1.152478000	-0.023380000
6	-2.088499000	-0.400079000	-2.004283000
8	-2.991256000	0.200002000	-1.581841000
8	-1.282387000	-1.027310000	-2.561950000
6	0.267704000	2.077545000	-1.061071000
8	-0.371543000	1.970893000	-2.027619000
8	0.968598000	2.319945000	-0.164809000
6	-1.559368000	-2.073407000	1.066872000
8	-2.264914000	-2.324210000	0.176373000
8	-0.914660000	-1.962665000	2.029369000
6	0.787120000	0.407376000	1.984156000
8	1.692148000	-0.194937000	1.564661000
8	-0.012149000	1.035463000	2.548152000
6	-2.482451000	1.339179000	1.052945000
8	-2.121438000	2.345395000	0.593759000
8	-2.965475000	0.422997000	1.583310000
6	1.166091000	-1.340999000	-1.053270000
8	0.789498000	-2.354272000	-0.626570000
8	1.675226000	-0.417997000	-1.550259000

$Cl^-(CO_2)$

17	-0.000109000	-1.679408000	0.000000000
6	0.000000000	1.210214000	0.000000000
8	-1.159934000	1.331831000	0.000000000
8	1.160166000	1.329251000	0.000000000

$Cl^-(CO_2)_2$

17	0.229069000	1.673689000	-0.002211000
6	-1.943167000	-0.382693000	0.008514000
8	-2.029101000	-0.429937000	-1.151452000
8	-1.995492000	-0.452834000	1.169357000
6	1.777073000	-0.801494000	-0.006926000
8	2.825132000	-0.294352000	0.015996000
8	0.837258000	-1.491327000	-0.030393000

$Cl^-(CO_2)_3$

17	-0.001989000	-0.001700000	1.679464000
6	-1.652830000	-1.400343000	-0.391362000
8	-1.821721000	-0.424585000	-1.004580000
8	-1.585925000	-2.447987000	0.108911000
6	2.039985000	-0.728645000	-0.391413000
8	2.914390000	-0.153349000	0.115340000
8	1.279388000	-1.356607000	-1.011077000
6	-0.385807000	2.130189000	-0.391458000
8	0.538806000	1.783424000	-1.009215000
8	-1.321722000	2.601815000	0.112436000

$Cl^-(CO_2)_4$

17	0.000344000	0.238303000	1.336983000
6	0.001133000	1.665913000	-1.296505000
8	1.162087000	1.708998000	-1.362719000
8	-1.159858000	1.708456000	-1.362269000
6	-0.001636000	-2.003165000	-0.747736000
8	-0.003381000	-2.855723000	0.041740000
8	0.000212000	-1.250220000	-1.635350000
6	-2.909751000	0.086288000	0.559304000
8	-2.753377000	-0.890883000	-0.053818000
8	-3.213269000	1.046875000	1.139322000
6	2.909933000	0.084027000	0.559531000
8	2.753028000	-0.892973000	-0.053741000
8	3.214070000	1.044278000	1.139801000

$Cl^-(CO_2)_5$

17	0.000194000	-0.000714000	-1.060317000
6	0.000039000	0.002035000	2.027424000
8	-0.542436000	-1.024272000	2.090462000
8	0.542466000	1.028476000	2.089877000
6	2.631744000	-1.270518000	-0.300217000
8	3.001985000	-1.362551000	-1.397913000

$Cl^-(CO_2)_6$

17	-0.062028000	-0.110360000	-0.599096000
6	1.663713000	-0.236864000	1.976888000
8	2.421048000	-0.973036000	1.491941000
8	0.970342000	0.492058000	2.559251000
6	1.870281000	2.211754000	-0.848685000
8	1.449111000	2.561701000	-1.873310000

8	2.382614000	-1.239572000	0.836287000
6	1.395219000	2.549805000	-0.349625000
8	2.442728000	2.044342000	-0.318563000
8	0.416982000	3.179142000	-0.358517000
6	-1.395226000	-2.549322000	-0.347609000
8	-0.416754000	-3.178304000	-0.354124000
8	-2.442955000	-2.044248000	-0.318495000
6	-2.631947000	1.268618000	-0.300745000
8	-2.382567000	1.240189000	0.835805000
8	-3.002346000	1.357852000	-1.398568000

8	2.375892000	1.958616000	0.168174000
6	-1.423457000	1.750715000	1.390422000
8	-0.873802000	2.681865000	0.963164000
8	-2.028003000	0.894600000	1.894285000
6	2.339642000	-1.755986000	-1.385844000
8	2.943004000	-0.813660000	-1.705079000
8	1.837976000	-2.768152000	-1.111850000
6	-1.574013000	-2.047446000	1.096070000
8	-0.682494000	-2.201409000	1.827166000
8	-2.532289000	-1.987973000	0.439496000
6	-2.832425000	0.155512000	-1.816993000
8	-3.117264000	1.011506000	-1.082101000
8	-2.664517000	-0.679864000	-2.606952000

$Cl^-(CO_2)_7$

17	0.023050000	-0.100060000	-0.290839000
6	-0.377039000	2.968759000	-0.046092000
8	-1.162829000	2.971196000	-0.902654000
8	0.394316000	3.074686000	0.816777000
6	-2.055832000	0.276589000	1.962473000
8	-2.231813000	-0.868798000	2.054119000
8	-1.953373000	1.434217000	1.956992000
6	1.900975000	0.701693000	1.990230000
8	1.131550000	0.377459000	2.798789000
8	2.741199000	1.056000000	1.268732000
6	-2.675951000	0.331057000	-1.739329000
8	-3.247542000	0.456206000	-0.733754000
8	-2.205368000	0.222784000	-2.795361000
6	2.461656000	1.057420000	-1.724834000
8	2.002624000	2.124790000	-1.765865000
8	3.013773000	0.034628000	-1.750663000
6	2.096378000	-2.429586000	-0.253824000
8	2.542583000	-2.062417000	0.754621000
8	1.719439000	-2.877897000	-1.257820000
6	-1.366773000	-2.838370000	0.010648000
8	-0.582890000	-3.235053000	0.771941000
8	-2.198209000	-2.545847000	-0.747274000

$Cl^-(CO_2)_8$

17	-0.000606000	-0.000967000	-0.004971000
6	-1.777664000	-2.030585000	-1.582799000
8	-0.923567000	-2.239763000	-2.342461000
8	-2.690584000	-1.889191000	-0.877505000
6	2.688687000	0.175486000	1.590525000
8	2.228559000	0.927521000	2.347665000
8	3.236205000	-0.570324000	0.887144000
6	-2.691036000	-0.174839000	1.583511000
8	-2.233397000	-0.928442000	2.340545000
8	-3.236454000	0.571601000	0.879279000
6	1.776185000	2.025057000	-1.586662000
8	2.690128000	1.882561000	-0.882961000
8	0.920894000	2.234904000	-2.344818000
6	-2.023194000	1.769053000	-1.590173000
8	-2.231408000	0.911184000	-2.345958000
8	-1.883231000	2.685873000	-0.889683000
6	-0.184041000	2.681342000	1.591326000
8	-0.933700000	2.216442000	2.347972000
8	0.559306000	3.233439000	0.889050000
6	2.025722000	-1.765706000	-1.596340000
8	2.228138000	-0.907627000	-2.353516000
8	1.890777000	-2.682472000	-0.894884000
6	0.186314000	-2.678396000	1.595835000
8	0.932597000	-2.211846000	2.354842000
8	-0.553705000	-3.232864000	0.891935000

$Cl^-(CO_2)_9$

17	-0.007538000	0.004425000	0.004225000
6	2.424702000	0.487936000	-2.080898000
8	1.841274000	1.394155000	-2.514539000
8	3.073182000	-0.400290000	-1.706071000
6	-2.432995000	1.530168000	1.477704000
8	-3.075960000	0.576355000	1.640792000
8	-1.857309000	2.532135000	1.356829000
6	2.421443000	-2.038179000	0.620321000
8	3.073119000	-1.268300000	1.196830000
8	1.835791000	-2.869954000	0.059217000
6	-2.414899000	0.513810000	-2.078453000
8	-3.069657000	1.129854000	-1.342569000
8	-1.825634000	-0.089421000	-2.877576000
6	0.006939000	-2.358945000	-2.242866000
8	0.776717000	-1.792944000	-2.903255000
8	-0.762788000	-2.993667000	-1.648147000

6	-2.418288000	-2.056202000	0.580521000
8	-1.837515000	-2.443279000	1.509299000
8	-3.065631000	-1.730010000	-0.327398000
6	-0.004666000	3.129502000	-0.907285000
8	-0.768872000	2.932953000	-1.759636000
8	0.760258000	3.418349000	-0.082309000
6	2.424047000	1.557585000	1.457972000
8	1.843205000	1.481387000	2.461224000
8	3.070997000	1.677401000	0.500381000
6	-0.000102000	-0.769430000	3.169082000
8	-0.773108000	0.060087000	3.420632000
8	0.773314000	-1.621401000	3.010243000

$Br^-(CO_2)$

35	0.000000000	1.246340000	0.000000000
6	-0.000013000	-1.912109000	0.000000000
8	-1.160629000	-2.009577000	0.000000000
8	1.160639000	-2.009077000	0.000000000

$Br^-(CO_2)_2$

35	0.423074000	-1.391357000	-0.000462000
6	1.526321000	1.572618000	-0.000906000
8	2.650665000	1.272759000	0.003961000
8	0.460284000	2.042117000	-0.005491000
6	-2.174218000	0.548737000	0.001506000
8	-2.236558000	0.591497000	1.162423000
8	-2.239415000	0.589798000	-1.159321000

$Br^-(CO_2)_3$

35	0.006982000	0.011985000	1.582839000
6	-0.514624000	-2.135442000	-0.788381000
8	-1.219177000	-1.409177000	-1.364067000
8	0.155748000	-2.958300000	-0.314843000
6	2.102145000	0.617385000	-0.812040000
8	2.483681000	1.612545000	-0.348513000
8	1.821167000	-0.359791000	-1.379122000
6	-1.598523000	1.499554000	-0.805698000
8	-0.618624000	1.741698000	-1.385776000
8	-2.645090000	1.334468000	-0.328009000

$Br^-(CO_2)_4$

35	-0.000028000	-0.594100000	-1.282878000
6	-0.000174000	-1.181845000	1.895098000
8	1.160951000	-1.200653000	1.959977000
8	-1.161299000	-1.199953000	1.960182000
6	0.000183000	2.235590000	0.442759000
8	-0.000071000	2.896238000	-0.512371000
8	0.000463000	1.677388000	1.463691000
6	-3.019901000	-0.076649000	-0.197026000
8	-2.771206000	1.016578000	0.115072000
8	-3.395570000	-1.141066000	-0.473485000
6	3.019951000	-0.076714000	-0.196997000
8	2.771167000	1.016498000	0.115072000
8	3.395643000	-1.141129000	-0.473422000

$Br^-(CO_2)_5$

35	0.000001000	-0.000001000	-1.215232000
6	-0.000016000	-0.000089000	2.141040000
8	0.716278000	0.913281000	2.196214000
8	-0.716311000	-0.913463000	2.196100000
6	-2.522644000	1.669304000	-0.098496000
8	-3.034525000	1.759393000	-1.137721000
8	-2.109320000	1.649042000	0.989144000
6	-1.935581000	-2.309492000	-0.054432000
8	-2.852350000	-1.594328000	-0.013582000
8	-1.098015000	-3.115641000	-0.063900000
6	1.935565000	2.309581000	-0.054413000
8	1.097941000	3.115671000	-0.063795000
8	2.852382000	1.594474000	-0.013654000
6	2.522679000	-1.669304000	-0.098494000
8	2.109390000	-1.648937000	0.989158000
8	3.034524000	-1.759487000	-1.137728000

$Br^-(CO_2)_6$

35	-0.024399000	-0.196429000	-0.776352000
6	1.532710000	-0.698350000	2.084305000
8	2.316014000	-1.381788000	1.563814000
8	0.799920000	-0.037388000	2.698081000
6	2.099391000	2.262093000	-0.208954000
8	1.861586000	2.782968000	-1.219324000
8	2.407395000	1.822650000	0.822992000
6	-1.444907000	1.605328000	1.580901000
8	-0.826759000	2.543999000	1.285182000
8	-2.110787000	0.727539000	1.951960000
6	2.968800000	-1.351656000	-1.418400000
8	3.430645000	-0.287100000	-1.334247000
8	2.611826000	-2.450707000	-1.535671000
6	-2.063667000	-2.063352000	0.917901000
8	-1.237394000	-2.411025000	1.658091000
8	-2.963093000	-1.792976000	0.231991000

	6 -3.054435000 0.542559000 -1.783496000 8 -3.176547000 1.339835000 -0.945203000 8 -3.034480000 -0.219098000 -2.660321000
$Br^-(CO_2)_7$ 35 -0.018627000 0.110016000 0.572668000 6 1.480247000 2.937332000 -0.004918000 8 0.584754000 3.356058000 -0.616155000 8 2.423643000 2.617722000 0.595048000 6 -2.862246000 -1.103927000 1.608813000 8 -2.428442000 -2.175774000 1.724956000 8 -3.387177000 -0.068537000 1.538840000 6 3.111679000 -0.334469000 1.515250000 8 2.853102000 -0.243216000 2.643568000 8 3.469412000 -0.441242000 0.413742000 6 -1.853782000 -0.784958000 -2.017274000 8 -2.729819000 -1.154034000 -1.348660000 8 -1.035118000 -0.443917000 -2.768423000 6 1.940943000 -0.253848000 -2.075633000 8 2.055144000 0.897557000 -2.183846000 8 1.885488000 -1.414387000 -2.049188000 6 0.519314000 -3.055007000 0.028454000 8 1.402405000 -3.074136000 0.784446000 8 -0.348622000 -3.140543000 -0.739888000 6 -2.307239000 2.428247000 0.082871000 8 -2.559376000 1.995101000 -0.966310000 8 -2.125587000 2.933000000 1.113277000	$Br^-(CO_2)_8$ 35 -0.001335000 -0.001288000 0.001589000 6 2.656469000 1.022716000 1.597661000 8 2.596814000 0.137015000 2.347761000 8 2.794320000 1.940812000 0.898236000 6 -1.152169000 -2.599141000 -1.601577000 8 -1.733269000 -1.927569000 -2.351230000 8 -0.604046000 -3.349712000 -0.903566000 6 1.156257000 2.603630000 -1.593922000 8 1.740788000 1.932490000 -2.341244000 8 0.604661000 3.353077000 -0.897503000 6 -2.659800000 -1.023663000 1.596257000 8 -2.796818000 -1.941080000 0.895873000 8 -2.601625000 -0.139061000 2.347805000 6 -1.023967000 2.656962000 1.594452000 8 -0.137747000 2.599710000 2.344153000 8 -1.943089000 2.793404000 0.896138000 6 -2.601726000 1.154348000 -1.596781000 8 -1.931879000 1.739543000 -2.344799000 8 -3.350245000 0.601788000 -0.900086000 6 1.021626000 -2.660411000 1.594517000 8 0.136057000 -2.601160000 2.344794000 8 1.939740000 -2.798514000 0.895247000 6 2.605859000 -1.151958000 -1.593024000 8 1.936260000 -1.732933000 -2.344431000 8 3.354005000 -0.604037000 -0.892287000
$Br^-(CO_2)_9$ 35 0.000400000 -0.001170000 0.001372000 6 -2.511255000 -1.120424000 -1.879052000 8 -3.133784000 -1.508009000 -0.977669000 8 -1.953672000 -0.760601000 -2.833040000 6 -0.020437000 1.707942000 2.862004000 8 0.747180000 2.481667000 2.459497000 8 -0.789607000 0.982384000 3.343561000 6 0.022308000 1.627215000 -2.904196000 8 -0.744620000 2.414004000 -2.526043000 8 0.789712000 0.885272000 -3.363491000 6 2.508036000 -1.073618000 1.915787000 8 1.947090000 -0.692788000 2.859489000 8 3.134171000 -1.481416000 1.025890000 6 2.545606000 -1.108356000 -1.853297000 8 1.995945000 -2.121984000 -1.996736000 8 3.161324000 -0.127385000 -1.760049000 6 2.527774000 2.176236000 -0.009474000 8 1.982720000 2.801293000 -0.823446000 8 3.138070000 1.611747000 0.802309000 6 -2.542801000 -1.052696000 1.889288000 8 -1.992675000 -2.061231000 2.062641000 8 -3.159073000 -0.075502000 1.767069000 6 -2.525544000 2.175082000 -0.059795000 8 -1.980737000 2.828267000 0.732036000 8 -3.135758000 1.580561000 -0.850042000	

6	-0.003750000	-3.329763000	0.036252000
8	0.754923000	-3.367548000	0.915546000
8	-0.762911000	-3.384828000	-0.841663000

$CN^-(CO_2)$			
6	-2.640907000	-0.000374000	-0.000077000
7	-1.461285000	0.000431000	0.000062000
6	1.098139000	-0.000032000	0.000881000
8	1.217819000	1.159517000	-0.000328000
8	1.217882000	-1.159590000	-0.000328000

$CN^-(CO_2)_2$			
6	0.445258000	2.418128000	-0.000547000
7	-0.233290000	1.452994000	-0.001922000
6	1.835937000	-0.454655000	0.001777000
8	1.883770000	-0.506376000	1.162503000
8	1.889251000	-0.503726000	-1.158789000
6	-1.873417000	-0.571104000	-0.001149000
8	-1.029499000	-1.374836000	-0.005987000
8	-2.845226000	0.069292000	0.003894000

$CN^-(CO_2)_3$			
6	-0.010612000	-1.981884000	-0.010031000
7	0.007691000	-0.802121000	-0.008196000
6	2.855544000	-0.557772000	-0.002615000
8	2.920032000	-0.564966000	1.158041000
8	2.918046000	-0.534555000	-1.163240000
6	-2.858189000	-0.553761000	0.009237000
8	-2.910394000	-0.530985000	1.170356000
8	-2.931173000	-0.559908000	-1.150877000
6	0.002625000	1.827256000	-0.001769000
8	-1.157477000	1.917740000	-0.032236000
8	1.162209000	1.924151000	0.029010000

$CN^-(CO_2)_4$			
6	0.586937000	-0.078882000	1.630770000
7	-0.559767000	0.119226000	1.445245000
6	-2.770378000	0.568964000	-0.031780000
8	-3.334656000	-0.371909000	0.355200000
8	-2.332023000	1.539208000	-0.499750000
6	2.834654000	-0.618905000	-0.023493000
8	2.326871000	-1.577270000	-0.444566000
8	3.460907000	0.304956000	0.305334000
6	0.636379000	2.198561000	-0.357475000
8	0.430760000	3.044889000	0.411330000
8	0.874990000	1.430594000	-1.197664000
8	-0.550566000	-2.987045000	0.430746000
6	-0.681159000	-2.163368000	-0.377546000
8	-0.841310000	-1.417524000	-1.255577000

$CN^-(CO_2)_5$			
6	-0.547442000	-0.461468000	1.260857000
7	0.476861000	0.059705000	1.000827000
6	1.545853000	1.759113000	-0.939312000
8	1.648384000	2.644627000	-0.193347000
8	1.484663000	0.947802000	-1.769283000
6	-3.084704000	-1.352252000	0.352948000
8	-3.495155000	-0.265541000	0.282659000
8	-2.817081000	-2.484215000	0.371946000
6	0.122816000	-1.628527000	-1.455227000
8	1.111938000	-2.163133000	-1.160040000
8	-0.866912000	-1.151623000	-1.834210000
8	-1.954282000	2.467593000	1.458114000
6	-1.669234000	2.192030000	0.366363000
8	-1.426958000	2.002918000	-0.755095000
8	2.835927000	-1.732876000	1.836202000
6	3.091045000	-0.871857000	1.100266000
8	3.468473000	-0.045573000	0.372908000

$CN^-(CO_2)_6$			
6	-0.683106000	0.079230000	-0.925223000
7	0.462202000	-0.146123000	-0.769617000
6	1.116128000	0.182821000	2.070100000
8	2.087329000	-0.438842000	1.925044000
8	0.169206000	0.812679000	2.304657000
6	-1.865227000	2.296502000	0.556978000
8	-2.709546000	1.650216000	1.027536000
8	-1.067329000	3.028476000	0.135443000
6	1.950657000	2.257133000	-0.876833000
8	1.834259000	2.369956000	-2.026322000
8	2.127185000	2.233716000	0.272570000
8	-3.287425000	-1.411382000	-0.052746000
6	-3.503563000	-0.559503000	-0.814446000
8	-3.852854000	0.250365000	-1.572542000
8	2.417026000	-2.418762000	-0.511913000
6	2.883491000	-1.384946000	-0.766578000
8	3.466801000	-0.414747000	-1.033061000
6	-0.544353000	-2.763559000	0.266188000
8	-0.718328000	-3.244757000	-0.776424000
8	-0.386272000	-2.369821000	1.348535000

$CN^-(CO_2)_7$			
6	-0.450721000	-0.205536000	0.004939000
7	0.707231000	-0.200038000	-0.204808000
6	1.622459000	1.408190000	2.032240000

$CN^-(CO_2)_8$			
6	-0.598612000	0.043269000	0.308538000
7	0.562415000	-0.088195000	0.161292000
6	0.334712000	2.683791000	1.711933000

8	1.397034000	0.590125000	2.824891000	8	-0.248877000	2.298570000	2.639342000
8	1.882528000	2.279871000	1.308169000	8	0.924181000	3.141128000	0.821575000
6	-2.242633000	1.307764000	-1.843177000	6	-1.616550000	-0.423523000	-2.453643000
8	-2.731228000	1.900351000	-0.969960000	8	-2.319932000	0.499257000	-2.388655000
8	-1.808788000	0.765501000	-2.773543000	8	-0.942724000	-1.358278000	-2.598490000
6	1.508744000	2.124206000	-1.623673000	6	1.717844000	1.836674000	-1.704322000
8	2.563259000	1.663316000	-1.787393000	8	2.754068000	1.813650000	-1.178208000
8	0.483970000	2.661204000	-1.519393000	8	0.715499000	1.912230000	-2.285915000
8	-3.024049000	0.471624000	1.880997000	8	-3.682996000	1.199892000	0.387454000
6	-2.165384000	1.255941000	1.860184000	6	-2.829081000	1.955675000	0.160356000
8	-1.363230000	2.094298000	1.921068000	8	-2.055314000	2.793451000	-0.063430000
8	3.181472000	-1.623198000	-1.231197000	8	3.571215000	-0.737454000	0.533172000
6	3.352236000	-0.933580000	-0.311075000	6	3.121334000	0.046310000	1.264282000
8	3.638313000	-0.284437000	0.609660000	8	2.770763000	0.834420000	2.042548000
6	0.647119000	-3.153093000	-0.111858000	6	0.400454000	-2.648503000	1.696659000
8	1.253128000	-3.110425000	0.879000000	8	1.325679000	-2.260594000	2.282931000
8	0.053934000	-3.285957000	-1.101971000	8	-0.521420000	-3.109109000	1.160658000
6	-2.821476000	-1.899216000	0.050206000	6	-3.045787000	-1.601133000	0.850143000
8	-3.359249000	-1.316557000	-0.800288000	8	-3.165631000	-1.837467000	-0.281807000
8	-2.373678000	-2.559192000	0.895828000	8	-3.004703000	-1.425824000	1.997786000
				6	1.901822000	-1.834543000	-1.644240000
				8	1.687628000	-2.760336000	-0.976368000
				8	2.160852000	-0.969877000	-2.376002000

$NO_2^-(CO_2)$				$NO_2^-(CO_2)_2$			
7	-1.750895000	-0.000063000	0.000024000	7	-0.360415000	0.000744000	0.001208000
8	-1.084276000	0.002870000	-1.066187000	8	0.277896000	-1.071109000	0.000862000
8	-1.084149000	-0.002880000	1.066219000	8	0.279473000	1.071690000	0.002488000
6	1.224967000	0.000014000	-0.000095000	6	2.697921000	-0.000099000	-0.001059000
8	1.390782000	1.159594000	0.002653000	8	2.814057000	0.002371000	-1.162045000
8	1.390952000	-1.159539000	-0.002635000	8	2.819461000	-0.002798000	1.159397000
				6	-2.743767000	-0.000165000	-0.000275000
				8	-2.919570000	-1.160082000	-0.002214000
				8	-2.921570000	1.159473000	0.001455000
$NO_2^-(CO_2)_3$				$NO_2^-(CO_2)_4$			
7	0.051810000	-0.646876000	0.002488000	7	0.710713000	-0.856457000	0.092509000
8	0.822300000	-1.627458000	0.000819000	8	0.323153000	-2.009839000	0.352816000
8	0.596321000	0.493506000	0.003619000	8	-0.183234000	-0.026794000	-0.251940000
6	-2.543088000	-1.367794000	-0.000130000	6	-2.365176000	1.336629000	0.580309000
8	-2.619303000	-1.402139000	-1.161109000	8	-2.891192000	1.214870000	-0.449411000
8	-2.622634000	-1.398781000	1.160730000	8	-1.917892000	1.515910000	1.637153000
6	3.128650000	-0.333642000	-0.001218000	6	3.404856000	-0.679516000	0.349767000
8	3.240644000	-0.320083000	-1.162177000	8	3.358614000	-0.266030000	1.436659000
8	3.244402000	-0.322859000	1.159368000	8	3.604442000	-1.100629000	-0.716095000
6	-1.089352000	2.273542000	-0.000706000	6	-2.217696000	-1.877532000	-0.306373000
8	-0.300973000	3.132799000	0.001671000	8	-2.602603000	-1.626828000	0.766350000
8	-2.028247000	1.581953000	-0.003557000	8	-2.027874000	-2.186024000	-1.413042000
				6	0.914835000	2.170218000	-0.680769000
				8	-0.093792000	2.755872000	-0.672039000
				8	2.005889000	1.766543000	-0.728597000
$NO_2^-(CO_2)_5$				$NO_2^-(CO_2)_6$			
7	0.295844000	0.088515000	0.320769000	7	-0.133022000	0.273242000	1.301386000
8	-0.884755000	-0.199696000	0.651727000	8	-1.320590000	-0.066749000	1.068030000

8	0.544439000	1.309593000	0.196317000
6	-1.778898000	2.303714000	1.109059000
8	-2.274345000	2.420370000	0.059874000
8	-1.410858000	2.324376000	2.213271000
6	2.506515000	-1.600969000	0.341767000
8	2.968084000	-1.024699000	1.239873000
8	2.144514000	-2.260889000	-0.545655000
6	-2.736230000	-0.164367000	-1.313295000
8	-3.578508000	-0.437345000	-0.558843000
8	-1.958953000	0.097368000	-2.134736000
6	2.774172000	1.863052000	-0.889707000
8	2.984435000	0.786164000	-1.279898000
8	2.708026000	2.982556000	-0.579376000
6	-0.753837000	-2.814744000	0.375723000
8	-1.295888000	-2.781163000	-0.652829000
8	-0.213844000	-2.984101000	1.391941000

8	0.687978000	0.023027000	0.378489000
6	-1.512706000	-2.769649000	0.774405000
8	-2.649235000	-2.735558000	1.018035000
8	-0.382384000	-2.906800000	0.542316000
6	2.954688000	0.269958000	1.752502000
8	3.284571000	1.207310000	1.145626000
8	2.738403000	-0.650104000	2.427465000
6	-1.541830000	-0.134501000	-1.606418000
8	-1.251057000	0.988405000	-1.712832000
8	-1.893797000	-1.242224000	-1.642605000
6	1.925052000	-1.538416000	-1.410456000
8	2.816925000	-1.591642000	-0.667151000
8	1.090068000	-1.541661000	-2.218235000
6	-3.043506000	1.927166000	0.667116000
8	-3.781352000	1.176066000	0.172256000
8	-2.374976000	2.747022000	1.145663000
6	1.468105000	2.170747000	-1.044906000
8	2.018311000	1.459441000	-1.783131000
8	0.946178000	2.950402000	-0.361823000

$NO_2^-(CO_2)_7$

7	0.677527000	0.731018000	0.397237000
8	0.148016000	1.342618000	1.349155000
8	0.348603000	-0.481599000	0.264215000
6	-1.253606000	-0.789602000	2.252259000
8	-0.427348000	-1.188146000	2.969665000
8	-2.213974000	-0.478653000	1.665815000
6	2.609639000	-1.700587000	1.138394000
8	2.259004000	-2.713513000	0.684235000
8	3.030404000	-0.733871000	1.621687000
6	-2.037199000	2.503090000	0.297357000
8	-1.820704000	2.006596000	-0.730570000
8	-2.314790000	3.041445000	1.289252000
6	-0.203999000	-2.918612000	-0.848079000
8	-0.799936000	-3.205159000	0.106613000
8	0.372023000	-2.706667000	-1.834687000
6	2.379396000	2.787114000	-0.228092000
8	3.174959000	2.461674000	0.552726000
8	1.648694000	3.195674000	-1.036943000
6	1.437632000	0.097969000	-2.228964000
8	2.509270000	-0.158216000	-1.852283000
8	0.406967000	0.366752000	-2.689965000
6	-3.301942000	-0.493434000	-1.076287000
8	-4.219494000	0.077388000	-0.645556000
8	-2.416970000	-1.080418000	-1.540883000

$NO_2^-(CO_2)_8$

7	-0.024192000	0.489020000	-0.276640000
8	-0.969705000	-0.323292000	-0.131839000
8	1.124390000	-0.017464000	-0.331957000
6	1.770368000	-1.785141000	1.587035000
8	0.708926000	-1.802405000	2.058598000
8	2.864168000	-1.822230000	1.192227000
6	0.389777000	-2.370737000	-1.685228000
8	-0.156982000	-1.797820000	-2.536144000
8	0.946356000	-3.030539000	-0.906161000
6	1.991880000	1.938227000	1.513829000
8	2.222050000	1.084419000	2.266986000
8	1.790124000	2.843590000	0.814683000
6	-2.146508000	1.371374000	1.738028000
8	-3.160923000	1.397485000	1.170669000
8	-1.168538000	1.388682000	2.364361000
6	-0.424163000	3.095075000	-1.160031000
8	0.269190000	2.918026000	-2.075167000
8	-1.135923000	3.381141000	-0.284826000
6	3.619818000	-0.049837000	-1.211091000
8	3.331333000	-0.871066000	-1.979773000
8	3.993435000	0.770527000	-0.476890000
6	-2.184881000	-2.374609000	1.099558000
8	-2.533861000	-1.642469000	1.931468000
8	-1.890052000	-3.171909000	0.307686000
6	-3.050421000	0.141776000	-1.630239000
8	-2.635655000	1.125645000	-2.089408000
8	-3.551568000	-0.832808000	-1.241346000

$NCCOO^-$

6	-0.952458000	0.000227000	0.000052000
7	-2.117772000	0.000176000	-0.000036000
6	0.574196000	-0.000002000	0.000054000
8	1.068740000	1.137944000	-0.000005000

$NCCOO^-(CO_2)$

6	1.094522000	1.001295000	0.000034000
7	0.815999000	2.132223000	0.000189000
6	1.420627000	-0.486689000	-0.000102000
8	2.630613000	-0.743522000	0.000132000

8	1.068007000	-1.138267000	-0.000043000

8	0.404387000	-1.206235000	-0.000444000
6	-2.000439000	-0.124589000	0.000063000
8	-2.067437000	-0.104583000	1.160848000
8	-2.067595000	-0.103867000	-1.160698000

$NCCOO^-(CO_2)_2$

6	-1.045484000	1.734242000	-0.000305000
7	-2.059622000	2.305165000	-0.001195000
6	0.249217000	0.953593000	0.000886000
8	1.278273000	1.644093000	0.000923000
8	0.082240000	-0.282003000	0.001690000
6	-2.437554000	-1.252428000	0.000167000
8	-2.489583000	-1.280028000	1.161036000
8	-2.488834000	-1.280919000	-1.160729000
6	2.805130000	-0.659172000	-0.000794000
8	2.868635000	-0.699726000	-1.161706000
8	2.872955000	-0.700613000	1.159866000

$NCCOO^-(CO_2)_3$

6	1.243121000	-1.839235000	0.828943000
7	2.287182000	-2.197202000	1.196676000
6	-0.091483000	-1.347119000	0.326999000
8	-1.072907000	-1.997501000	0.706204000
8	-0.006671000	-0.336536000	-0.405097000
6	2.499605000	0.596104000	-0.945851000
8	2.458040000	1.339946000	-0.052810000
8	2.633868000	-0.100930000	-1.865005000
6	-2.753117000	-0.291479000	-0.642030000
8	-2.782312000	-0.960425000	-1.592271000
8	-2.854227000	0.432230000	0.264209000
6	-0.379440000	2.044167000	0.793315000
8	-0.513851000	2.587530000	-0.226110000
8	-0.252239000	1.586410000	1.852756000

$NCCOO^-(CO_2)_4$

6	-1.346192000	0.109763000	2.153031000
7	-2.412287000	0.150583000	2.616060000
6	0.018028000	0.056463000	1.520478000
8	0.974759000	0.065202000	2.300547000
8	-0.015867000	0.012256000	0.266717000
6	-2.446311000	-0.314950000	-0.922831000
8	-2.404573000	-1.467057000	-0.776454000
8	-2.571867000	0.823375000	-1.119921000
6	2.721953000	0.251532000	0.144178000
8	2.664336000	1.413134000	0.149404000
8	2.901935000	-0.895731000	0.079860000
6	0.470418000	-2.404495000	-0.842752000
8	0.559927000	-1.943338000	-1.906544000
8	0.388348000	-2.944818000	0.181686000
6	0.018313000	2.347731000	-1.075623000
8	0.317825000	1.814424000	-2.064060000
8	-0.281229000	2.956259000	-0.132648000

$NCCOO^-(CO_2)_5$

6	-1.284472000	-1.521319000	-0.076514000
7	-1.716398000	-2.599756000	-0.128000000
6	-0.736017000	-0.123410000	0.000088000
8	-1.590603000	0.770934000	0.044493000
8	0.513735000	-0.059271000	0.010185000
6	1.917970000	-2.373424000	0.222012000
8	1.809551000	-2.375613000	1.379024000
8	2.083710000	-2.451065000	-0.925554000
6	0.382503000	2.732476000	-0.212096000
8	0.323243000	2.678508000	-1.372030000
8	0.487236000	2.903389000	0.933119000
6	1.638252000	0.530134000	2.406497000
8	2.677378000	0.711230000	1.917244000
8	0.637348000	0.360605000	2.969889000
6	1.749843000	0.198904000	-2.398150000
8	2.713750000	0.606902000	-1.892528000
8	0.827640000	-0.206682000	-2.975554000
6	-4.232958000	-0.083553000	0.024550000
8	-4.272981000	-0.136434000	1.184599000
8	-4.284499000	-0.047573000	-1.135676000

$NCCOO^-(CO_2)_6$

6	-0.139191000	-2.051031000	-0.518851000
7	-0.093494000	-3.189383000	-0.750740000
6	-0.187044000	-0.582397000	-0.205504000
8	-1.318785000	-0.075772000	-0.221231000
8	0.930239000	-0.075072000	0.025697000
6	3.032374000	-1.819098000	0.435726000
8	2.752888000	-1.933796000	1.557569000
8	3.381306000	-1.755756000	-0.670582000
6	0.004382000	2.539437000	-0.227366000
8	0.198575000	2.493019000	-1.371700000
8	-0.189671000	2.691462000	0.909265000

$NCCOO^-(CO_2)_7$

6	0.717267000	0.841589000	1.838568000
7	1.005143000	0.920881000	2.961657000
6	0.425207000	0.747395000	0.370852000
8	1.393108000	1.041698000	-0.353722000
8	-0.731770000	0.394374000	0.064395000
6	-2.785228000	-0.258883000	1.760135000
8	-3.139354000	-1.122405000	1.067171000
8	-2.504381000	0.587252000	2.503880000
6	-0.161967000	1.051766000	-2.629809000
8	-0.556283000	2.129602000	-2.453097000
8	0.201778000	-0.015542000	-2.918572000

6	1.598473000	0.839105000	2.474896000
8	2.552059000	1.337161000	2.033292000
8	0.674266000	0.362107000	2.990849000
6	2.458294000	0.671475000	-2.136033000
8	3.184984000	1.274250000	-1.458238000
8	1.776454000	0.089808000	-2.874382000
6	-3.379341000	-2.036721000	-0.057176000
8	-3.069675000	-2.332310000	1.021743000
8	-3.748262000	-1.790493000	-1.131895000
6	-3.458977000	1.558606000	0.006074000
8	-3.003089000	2.372320000	-0.686102000
8	-3.986209000	0.794249000	0.703787000

6	3.779284000	1.282452000	1.041201000
8	3.895178000	0.125333000	1.044852000
8	3.746100000	2.442484000	1.069536000
6	-2.278399000	2.678229000	0.130324000
8	-3.212946000	2.078577000	-0.215295000
8	-1.389099000	3.333849000	0.485929000
6	2.566142000	-1.170581000	-1.401787000
8	1.910452000	-1.855275000	-0.731309000
8	3.261581000	-0.551964000	-2.098044000
6	-1.984429000	-1.443554000	-1.586313000
8	-2.669146000	-0.616413000	-2.030240000
8	-1.333170000	-2.320335000	-1.192150000
6	0.014554000	-3.356712000	1.269646000
8	-0.230359000	-2.380511000	1.844819000
8	0.259488000	-4.355271000	0.725787000

$NCCOO^{-}(CO_2)_8$

6	-0.057820000	1.426856000	-1.245800000
7	-0.040716000	2.314783000	-1.996320000
6	-0.082181000	0.313998000	-0.234763000
8	-1.203553000	0.077576000	0.241963000
8	1.026692000	-0.212150000	-0.013339000
6	2.602016000	-0.300655000	-2.227657000
8	1.732798000	-0.754349000	-2.851448000
8	3.516447000	0.144852000	-1.665968000
6	0.355236000	-1.493824000	2.344700000
8	0.423376000	-0.484874000	2.917951000
8	0.302010000	-2.546301000	1.855871000
6	0.852093000	-2.979008000	-0.921526000
8	2.000769000	-3.102175000	-0.794758000
8	-0.295747000	-2.913891000	-1.080794000
6	3.323081000	-0.066508000	1.525398000
8	3.321152000	-1.226995000	1.555383000
8	3.384887000	1.093179000	1.542491000
6	-2.951953000	2.282039000	-0.437104000
8	-3.453625000	1.651326000	-1.274745000
8	-2.495138000	2.961105000	0.385981000
6	-3.233560000	-0.597350000	1.924984000
8	-2.677439000	-1.521376000	2.355228000
8	-3.850543000	0.311837000	1.548660000
6	-2.535177000	-1.203730000	-1.823131000
8	-3.307889000	-1.638727000	-1.071321000
8	-1.796069000	-0.801728000	-2.623236000
6	1.708651000	3.226950000	0.554840000
8	2.545360000	3.521743000	-0.195248000
8	0.876851000	2.958936000	1.319154000

$NCCOO^{-}(CO_2)_9$

6	-1.107458000	0.249193000	0.007444000
7	-2.244329000	0.471039000	0.090695000
6	0.367934000	-0.005480000	-0.107756000
8	1.054089000	1.022418000	-0.220432000
8	0.695485000	-1.207671000	-0.069315000
6	0.236103000	-2.484151000	2.335165000
8	1.237579000	-3.071494000	2.273651000
8	-0.773179000	-1.923591000	2.458358000
6	2.007988000	-2.019687000	-2.326785000
8	1.761705000	-3.128407000	-2.076696000
8	2.277446000	-0.937377000	-2.648525000
6	-0.385589000	3.286041000	-0.993289000
8	-0.280255000	3.728035000	0.077247000
8	-0.523757000	2.904856000	-2.080439000
6	-1.051667000	-3.152917000	-0.905391000
8	-0.747711000	-3.885160000	-0.057215000
8	-1.407282000	-2.478176000	-1.782827000
6	3.345786000	2.153218000	-1.052237000
8	4.045838000	1.350189000	-0.589141000
8	2.716345000	2.996135000	-1.544263000
6	3.267377000	-1.029315000	0.953888000
8	3.703412000	-1.685596000	0.100559000
8	2.901783000	-0.388589000	1.851534000
6	1.454820000	2.292517000	2.171750000
8	2.375058000	2.862162000	1.747915000
8	0.547466000	1.757249000	2.659780000
6	-4.380661000	2.293680000	0.200167000
8	-4.965658000	1.662909000	0.980806000
8	-3.847539000	2.973165000	-0.576025000
8	-3.697130000	-2.177755000	0.498371000
8	-4.767713000	-0.853819000	-1.080782000
6	-4.210893000	-1.491956000	-0.285516000

$NCCOO^{-}(CO_2)_{10}$

6	-0.919282000	-0.487475000	0.116724000
7	-2.040027000	-0.785278000	0.190541000
6	0.515829000	-0.063190000	-0.024791000
8	0.657500000	1.139151000	-0.293940000

$NCCOO^{-}(CO_2)_{11}$

6	-0.670799000	-0.000915000	-0.203209000
7	-1.825239000	-0.090859000	-0.306098000
6	0.826869000	0.038563000	-0.045740000
8	1.349978000	-1.085634000	-0.022196000

8	1.350320000	-0.971621000	0.146439000
6	1.497286000	-1.913187000	2.724939000
8	2.657542000	-1.972433000	2.682826000
8	0.341630000	-1.875182000	2.833170000
6	2.817070000	-1.179658000	-2.177239000
8	2.918112000	-2.318648000	-1.964100000
8	2.752740000	-0.055223000	-2.456422000
6	-1.682036000	2.391771000	-1.169652000
8	-1.782768000	2.954263000	-0.157909000
8	-1.632707000	1.865617000	-2.203649000
6	0.631848000	-3.662384000	-0.265798000
8	1.337123000	-3.995210000	0.595373000
8	-0.092172000	-3.405776000	-1.136795000
6	2.188849000	3.100187000	-1.327846000
8	3.182550000	2.779766000	-0.818781000
8	1.236583000	3.489185000	-1.867223000
6	3.579764000	0.431128000	1.026320000
8	4.275390000	-0.097076000	0.260890000
8	2.951195000	0.984252000	1.832303000
6	-4.759108000	-0.333112000	-0.611441000
8	-4.446322000	0.646019000	-1.150281000
8	-5.133478000	-1.300485000	-0.087883000
6	-1.463653000	-1.189237000	-2.986248000
8	-2.602868000	-1.416165000	-2.953535000
8	-0.325980000	-0.969337000	-3.050175000
6	0.430952000	2.558030000	2.026401000
8	0.987826000	3.477299000	1.586497000
8	-0.134833000	1.674477000	2.526049000
6	-3.203975000	0.110069000	2.718671000
8	-2.726900000	-0.735835000	3.353471000
8	-3.710614000	0.967873000	2.119422000

8	1.322308000	1.176607000	0.040155000
6	1.549639000	2.647715000	-2.351936000
8	2.620390000	3.037181000	-2.121797000
8	0.483908000	2.286219000	-2.636309000
6	2.516640000	1.319296000	2.522594000
8	2.303922000	2.462979000	2.526925000
8	2.754815000	0.185705000	2.588560000
6	-0.404485000	-3.095719000	0.774142000
8	-0.389031000	-3.600353000	-0.271932000
8	-0.459535000	-2.638474000	1.840307000
6	-0.024737000	3.455074000	0.751693000
8	0.654440000	4.099037000	0.064815000
8	-0.747426000	2.882177000	1.459369000
6	3.367519000	-2.738469000	0.738313000
8	4.231260000	-2.072091000	0.339743000
8	2.560726000	-3.458042000	1.162885000
6	3.887409000	0.577333000	-0.923894000
8	4.381627000	1.061217000	0.008461000
8	3.462068000	0.100854000	-1.895603000
6	-4.157893000	-1.847506000	0.627332000
8	-3.434887000	-2.703926000	0.927687000
8	-4.918283000	-1.020342000	0.332204000
6	-1.583668000	0.018787000	2.986883000
8	-2.710858000	-0.229512000	2.852688000
8	-0.462836000	0.268581000	3.152738000
6	1.509541000	-2.302955000	-2.441185000
8	2.320204000	-3.038408000	-2.050393000
8	0.705603000	-1.599146000	-2.895817000
6	-3.793824000	-0.584423000	-2.424878000
8	-4.056420000	0.542771000	-2.513730000
8	-3.567587000	-1.722784000	-2.372596000
8	-2.670460000	3.031152000	-0.945915000
8	-3.933943000	2.092375000	0.761594000
6	-3.292745000	2.541698000	-0.095456000

$ClOCOO^-$			
17	1.724792000	0.009627000	0.000054000
8	0.089605000	-0.769197000	-0.000179000
8	-0.925434000	1.331076000	-0.000046000
6	-1.076135000	0.123776000	-0.000004000
8	-2.022252000	-0.675169000	0.000113000

$ClOCOO^-(CO_2)$			
17	0.275592000	1.733268000	-0.005476000
8	1.702436000	0.608724000	0.038620000
8	0.282821000	-1.231229000	-0.104676000
6	1.429025000	-0.819575000	-0.025492000
8	2.560640000	-1.316013000	0.021030000
6	-2.204669000	-0.414700000	0.025304000
8	-2.323047000	-0.371052000	-1.130534000
8	-2.226750000	-0.447917000	1.187340000

$ClOCOO^-(CO_2)_2$			
17	0.759959000	1.682651000	-0.844818000
8	-0.556434000	0.963885000	0.115142000
8	-3.512888000	0.221618000	-0.324628000
6	-2.736233000	-0.609920000	-0.565308000
8	-2.043351000	-1.486613000	-0.884124000
6	-0.169018000	0.182996000	1.311919000

$ClOCOO^-(CO_2)_3$			
17	-0.887930000	0.920798000	1.210898000
8	0.236077000	-0.117001000	0.306161000
8	2.308519000	-2.391739000	1.007122000
6	2.752845000	-1.524825000	0.374240000
8	3.309381000	-0.682071000	-0.203114000
6	-0.303764000	-0.816941000	-0.897248000

8	-1.252005000	-0.212676000	1.751674000
8	1.009156000	0.089313000	1.605152000
6	2.491257000	-1.004447000	-0.349222000
8	3.470117000	-0.457118000	-0.039998000
8	1.580987000	-1.620514000	-0.726022000

8	0.671124000	-1.444877000	-1.313871000
8	-1.467758000	-0.650413000	-1.202410000
6	-3.773889000	-0.163487000	0.029715000
8	-3.954125000	0.824063000	-0.556253000
8	-3.710621000	-1.143109000	0.652061000
6	1.982139000	1.985038000	-0.319766000
8	1.644604000	1.957364000	-1.429855000
8	2.356654000	2.081248000	0.776796000

$ClOCOO^{-}(CO_2)_4$

17	-0.611185000	-1.147782000	1.278333000
8	0.290703000	-0.187580000	0.092723000
6	-0.170606000	-0.261940000	-1.350193000
8	0.679583000	0.397604000	-1.941801000
8	-1.184106000	-0.882715000	-1.592915000
8	-3.356408000	0.367824000	0.020755000
6	-3.457630000	-0.777917000	-0.149353000
8	-3.668794000	-1.912897000	-0.282057000
6	2.567296000	1.510418000	-0.351293000
8	1.916010000	2.429645000	-0.065588000
8	3.313941000	0.653571000	-0.595648000
6	-0.973209000	2.454657000	0.652685000
8	-0.784747000	2.302988000	1.790155000
8	-1.190898000	2.661145000	-0.467818000
6	2.459348000	-2.011777000	0.440434000
8	2.183059000	-2.506439000	-0.572287000
8	2.781528000	-1.569189000	1.466311000

$ClOCOO^{-}(CO_2)_5$

17	-0.713796000	1.107120000	1.850946000
8	-1.288689000	-0.216547000	0.820501000
6	2.338409000	-0.146055000	2.056621000
8	2.841108000	0.827599000	1.666478000
8	1.901820000	-1.115101000	2.524376000
6	-0.316630000	-0.806565000	-0.111333000
8	0.817654000	-0.345657000	-0.150124000
8	-0.936670000	-1.701527000	-0.681339000
8	-1.637093000	1.495537000	-1.736384000
6	-2.443263000	1.818669000	-0.967286000
8	-3.266456000	2.185271000	-0.232304000
6	2.050623000	1.910084000	-1.052334000
8	1.284971000	2.663578000	-0.612867000
8	2.861693000	1.228528000	-1.531759000
6	2.770407000	-1.739057000	-1.347930000
8	2.262241000	-1.791696000	-2.390322000
8	3.360700000	-1.746401000	-0.345216000
6	-3.588443000	-1.671424000	-0.072534000
8	-3.493733000	-2.498513000	0.737443000
8	-3.799056000	-0.861937000	-0.880647000

$ClOCOO^{-}(CO_2)_6$

17	0.150390000	0.388362000	0.708659000
8	-1.204509000	-0.735475000	0.454830000
6	2.941219000	1.140757000	2.062315000
8	2.916556000	1.693838000	1.040269000
8	2.992298000	0.623246000	3.099750000
6	-0.861067000	-2.039952000	-0.164558000
8	0.295940000	-2.250083000	-0.486107000
8	-1.938077000	-2.632515000	-0.200647000
8	-2.129271000	1.907557000	-1.210498000
6	-2.537109000	1.840595000	-0.124916000
8	-2.970799000	1.826800000	0.952703000
6	1.152270000	-0.311060000	-2.265874000
8	0.073866000	-0.178998000	-2.673954000
8	2.261797000	-0.403134000	-1.927400000
6	0.664779000	3.190350000	-0.830884000
8	0.176315000	3.721978000	0.080548000
8	1.167750000	2.701552000	-1.754930000
6	2.969183000	-2.445766000	0.016660000
8	3.059675000	-3.255480000	-0.810591000
8	2.969611000	-1.657117000	0.870193000
6	-4.049174000	-1.184147000	0.731896000
8	-3.964043000	-1.626446000	1.802347000
8	-4.236763000	-0.704074000	-0.310892000

$ClOCOO^{-}(CO_2)_7$

17	-0.676775000	0.075500000	-2.035933000
8	-1.068877000	0.277376000	-0.325204000
6	3.388724000	-0.733201000	-1.438862000
8	2.861879000	-0.666599000	-2.470836000
8	3.977327000	-0.819972000	-0.440305000
6	2.100165000	2.566112000	-0.708952000
8	3.097475000	2.135123000	-1.125274000
8	1.127070000	3.064910000	-0.322144000
6	0.080442000	0.306633000	0.595622000
8	1.197409000	0.096348000	0.133572000
8	-0.391219000	0.541930000	1.703463000
8	-2.683234000	-1.378053000	1.857453000
6	-2.996887000	-0.259034000	1.845546000
8	-3.402808000	0.829677000	1.860298000
6	0.982644000	-2.766146000	0.348431000
8	0.343027000	-2.669164000	1.310615000
8	1.622051000	-2.923218000	-0.611088000
6	-2.724907000	-2.186247000	-0.989955000
8	-3.658067000	-1.497218000	-1.050274000
8	-1.822898000	-2.916258000	-0.944556000
6	2.720449000	0.408120000	2.329239000
8	2.639747000	-0.707622000	2.640863000
8	2.868689000	1.536767000	2.090419000
6	-2.871722000	2.503266000	-0.526334000

	8 -3.622278000 1.838708000 -1.115315000 8 -2.156328000 3.217198000 0.043621000
$ClOCOO^{-}(CO_2)_8$ 17 0.802545000 0.285966000 1.192630000 8 0.537438000 -0.665088000 -0.279738000 6 1.732506000 -2.533539000 -2.040659000 8 1.511890000 -3.396817000 -1.294030000 8 2.029633000 -1.725380000 -2.820586000 6 1.619011000 3.370169000 1.324733000 8 1.416893000 3.240694000 2.460835000 8 1.844788000 3.542136000 0.198562000 6 1.618873000 1.403379000 -1.895777000 8 0.532911000 1.722993000 -2.152071000 8 2.725132000 1.129788000 -1.669162000 8 -0.534793000 -3.004718000 1.352470000 6 0.604103000 -2.949950000 1.571768000 8 1.736122000 -2.933219000 1.832126000 8 -1.718035000 -0.076986000 -0.210636000 6 -0.866746000 -0.719163000 -0.804071000 8 -0.783895000 -1.453401000 -1.780032000 6 -4.337214000 0.204581000 -0.802358000 8 -4.305760000 -0.390694000 -1.797015000 8 -4.460238000 0.815439000 0.181440000 6 -2.986275000 -1.298118000 1.945341000 8 -2.396314000 -0.679448000 2.730455000 8 -3.617327000 -1.948363000 1.216950000 6 -1.897772000 2.683489000 -0.604105000 8 -2.543436000 2.502223000 -1.552726000 8 -1.266931000 2.942356000 0.336012000 6 3.971259000 -0.124594000 0.612415000 8 4.148296000 0.883725000 1.165277000 8 3.844908000 -1.140108000 0.067064000	$ClOCOO^{-}(CO_2)_9$ 17 0.452673000 0.080836000 -0.345190000 8 -0.732673000 -0.645736000 0.751331000 6 -0.206678000 -1.570518000 1.818724000 8 0.994993000 -1.753837000 1.875517000 8 -1.228703000 -1.918847000 2.399890000 6 0.657773000 -0.354305000 -3.479012000 8 1.462880000 -1.182457000 -3.348350000 8 -0.129285000 0.480919000 -3.653392000 6 -3.214230000 1.727349000 -1.221358000 8 -3.696820000 2.759611000 -0.986595000 8 -2.762269000 0.689666000 -1.472845000 8 3.375272000 -1.424489000 -0.206412000 6 2.576493000 -2.239017000 -0.434263000 8 1.834426000 -3.085719000 -0.714988000 8 -1.437270000 2.270031000 1.267532000 6 -1.390974000 1.717676000 2.291386000 8 -1.361776000 1.225103000 3.339557000 6 3.330378000 1.501702000 -0.741887000 8 3.861128000 1.623287000 0.281220000 8 2.824397000 1.404775000 -1.785537000 6 2.511361000 0.360682000 2.733371000 8 1.640298000 1.110953000 2.562134000 8 3.422770000 -0.327960000 2.941678000 6 0.280962000 3.278986000 -0.865670000 8 1.162013000 3.464321000 -0.130341000 8 -0.585628000 3.138504000 -1.624508000 6 -1.199554000 -3.055849000 -1.219387000 8 -1.266086000 -2.261769000 -2.066802000 8 -1.141243000 -3.880306000 -0.406336000 8 -3.487247000 -2.034936000 0.317571000 6 -3.492146000 -1.054245000 0.938658000 8 -3.601144000 -0.057235000 1.527784000
$ClOCOO^{-}(CO_2)_{10}$ 17 -0.558411000 -0.602514000 0.255523000 8 0.234800000 0.896046000 -0.239034000 6 1.687827000 0.812665000 -0.530592000 8 2.237405000 -0.274394000 -0.438342000 8 2.000461000 1.965753000 -0.814538000 6 -1.931633000 -1.098249000 3.094220000 8 -0.972494000 -1.613862000 3.500101000 8 -2.915148000 -0.608207000 2.719465000 6 -3.453590000 2.300759000 -0.064257000 8 -4.272238000 2.501181000 -0.866002000 8 -2.648506000 2.127965000 0.752286000 8 1.651672000 -2.873005000 1.230729000 6 1.876880000 -1.901891000 1.830369000 8 2.115213000 -0.979219000 2.492554000 8 -1.937115000 0.845488000 -2.392606000 6 -0.927791000 1.114733000 -2.906761000 8 0.047021000 1.386162000 -3.470707000 6 -0.917505000 -3.794888000 -0.090541000	$ClOCOO^{-}(CO_2)_{11}$ 17 1.567952000 0.499668000 0.110500000 8 0.296331000 -0.723070000 0.140265000 6 -1.092174000 -0.229609000 0.188563000 8 -1.297786000 0.970284000 0.120852000 8 -1.769203000 -1.255304000 0.281164000 6 4.171796000 0.217934000 2.163351000 8 3.681504000 0.963984000 2.905173000 8 4.698746000 -0.519969000 1.437029000 8 1.238315000 -1.142495000 -2.916411000 6 0.075812000 -1.132855000 -2.916338000 8 -1.082943000 -1.125616000 -2.960894000 6 3.623920000 2.194826000 -1.529792000 8 3.165360000 2.246576000 -2.594358000 8 4.098677000 2.172452000 -0.468746000 6 -0.024492000 2.588754000 -1.739851000 8 -0.212439000 1.810855000 -2.581052000 8 0.199910000 3.415004000 -0.953265000 6 3.531572000 -1.695698000 -1.107212000

8	-0.261593000	-4.188290000	-0.961242000
8	-1.595187000	-3.431803000	0.783188000
6	1.652758000	-2.170394000	-2.295680000
8	0.719912000	-1.585568000	-2.668892000
8	2.573168000	-2.806248000	-1.985059000
6	-3.322653000	-1.405795000	-1.170182000
8	-2.766910000	-2.172905000	-1.844090000
8	-3.918655000	-0.667889000	-0.501558000
6	0.867452000	1.748939000	2.708872000
8	-0.226451000	1.433492000	2.951092000
8	1.961310000	2.074004000	2.505911000
8	0.180641000	3.870522000	0.800653000
6	-0.224008000	3.684163000	-0.270911000
8	-0.688439000	3.579148000	-1.332140000
6	4.761804000	0.844067000	-0.364309000
8	4.948134000	0.722595000	-1.505570000
8	4.667465000	0.978795000	0.785644000
8	4.134486000	-0.876515000	-1.671322000
8	2.961885000	-2.541379000	-0.554210000
8	-0.024179000	-3.682825000	1.087539000
6	-0.122458000	-3.531537000	-0.060102000
8	-0.193115000	-3.462245000	-1.217354000
6	-0.953745000	2.808497000	2.076980000
8	-1.862805000	3.406374000	1.667302000
8	-0.039400000	2.264980000	2.541552000
6	-3.822416000	-0.552187000	2.009751000
8	-4.563683000	-1.206466000	1.397358000
8	-3.133901000	0.102130000	2.676611000
6	-3.611461000	2.293730000	-0.516888000
8	-3.029744000	2.818759000	-1.374373000
8	-4.260027000	1.817510000	0.320395000
6	-3.687104000	-1.671494000	-1.577530000
8	-3.896721000	-0.537043000	-1.714145000
8	-3.534817000	-2.820175000	-1.494389000
6	0.912863000	-1.496766000	2.872667000
8	2.013854000	-1.739971000	2.584235000
8	-0.171788000	-1.262826000	3.208532000

$HOCOO^-$

8	1.045252000	-0.740812000	-0.000105000
1	1.735773000	-0.070428000	0.000760000
6	-0.165162000	0.069082000	0.000003000
8	0.062450000	1.295148000	-0.000035000
8	-1.200802000	-0.597344000	0.000043000

$HOCOO^-(CO_2)$

8	-0.354543000	-0.541589000	0.085316000
1	-0.540511000	-1.485466000	0.051449000
6	2.114063000	0.058178000	-0.016215000
8	1.966126000	1.208886000	-0.033993000
8	2.416346000	-1.068293000	-0.004120000
6	-1.697487000	0.061191000	0.004268000
8	-2.598084000	-0.791030000	-0.072389000
8	-1.674714000	1.288182000	0.027715000

$HOCOO^-(CO_2)_2$

8	-0.262365000	-1.061576000	-0.000462000
1	-0.131235000	-2.015469000	-0.000777000
6	-1.722978000	-0.943389000	0.000068000
8	-2.303889000	-2.036480000	-0.000164000
8	-2.110292000	0.227920000	0.000651000
6	2.373366000	-0.642228000	-0.000027000
8	2.495862000	-1.799770000	0.000511000
8	2.365550000	0.518244000	-0.000582000
6	-0.280432000	1.978651000	0.000057000
8	-0.223450000	2.054472000	-1.160421000
8	-0.222479000	2.054348000	1.160492000

$HOCOO^-(CO_2)_3$

8	0.007584000	-0.036335000	-0.479922000
1	-0.795242000	0.287206000	-0.906022000
8	2.187078000	-2.223743000	-1.059538000
6	2.528172000	-1.302927000	-0.436501000
8	3.019852000	-0.394891000	0.101883000
8	1.798220000	2.330139000	-0.867651000
6	1.529615000	2.116793000	0.244603000
8	1.295871000	2.000277000	1.375141000
8	-1.676648000	-0.923264000	0.755594000
6	-0.438727000	-0.885936000	0.594170000
8	0.486008000	-1.443876000	1.184138000
8	-2.823969000	0.761491000	-1.200397000
6	-3.474887000	0.217727000	-0.394041000
8	-4.302720000	-0.214942000	0.297829000

$HOCOO^-(CO_2)_4$

8	0.222649000	-0.378785000	-0.386557000
1	-0.643920000	-0.278542000	-0.797609000
8	2.702477000	-1.875663000	-1.615599000

$HOCOO^-(CO_2)_5$

8	-0.912676000	1.870876000	-0.357017000
1	-1.862646000	2.021209000	-0.283027000
8	-0.653925000	-2.729049000	-1.428442000

6	2.951873000	-1.058519000	-0.826928000
8	3.334058000	-0.207152000	-0.130827000
8	1.551949000	2.328009000	0.086624000
6	1.480098000	1.691226000	1.059671000
8	1.421967000	1.131929000	2.072582000
8	-1.059860000	-2.005757000	0.545668000
6	0.103031000	-1.569183000	0.433784000
8	1.180402000	-1.952865000	0.883341000
8	-2.803899000	-0.188633000	-0.748597000
6	-3.209056000	-1.048299000	-0.065328000
8	-3.816933000	-1.820471000	0.553732000
8	-1.495126000	2.440604000	0.560181000
6	-1.317915000	2.347088000	-0.584354000
8	-1.163217000	2.291867000	-1.733479000
6	-0.511260000	-2.566501000	-0.286552000
8	-0.352557000	-2.543155000	0.866250000
8	2.152333000	-0.667784000	1.886954000
6	1.130712000	-0.190078000	2.173642000
8	0.141370000	0.276878000	2.561203000
8	-1.797127000	-0.204684000	-0.338963000
6	-0.750951000	0.475390000	-0.379927000
8	0.436011000	0.106712000	-0.425337000
8	-3.951408000	1.648637000	-0.124339000
6	-4.166159000	0.500469000	-0.097837000
8	-4.562791000	-0.589698000	-0.054654000
8	1.953231000	2.398409000	0.762242000
6	1.831403000	2.474985000	-0.392345000
8	1.791648000	2.648204000	-1.540290000
8	3.336306000	-0.034073000	-0.973875000
6	2.818851000	-1.072338000	-0.911087000
8	2.387969000	-2.150369000	-0.877774000

$HOCOO^-(CO_2)_6$

1	-0.464577000	0.043581000	-1.260173000
8	0.350241000	0.393693000	-0.878197000
6	-3.839560000	0.807591000	-0.790491000
8	-2.980415000	1.580268000	-0.893971000
8	-4.725923000	0.061291000	-0.699515000
6	0.793056000	-0.588635000	0.054557000
8	0.032689000	-1.567797000	0.207207000
8	1.872066000	-0.309479000	0.586838000
8	2.530067000	2.494636000	0.192801000
6	2.971297000	1.719491000	-0.553946000
8	3.500620000	1.064952000	-1.357659000
6	-1.589432000	-0.667421000	2.155214000
8	-0.823625000	-0.808581000	3.013024000
8	-2.433640000	-0.500365000	1.368770000
6	-0.440872000	2.729357000	0.413140000
8	-0.328893000	3.381352000	-0.541868000
8	-0.593913000	2.142884000	1.404275000
6	-2.059368000	-2.242717000	-1.002188000
8	-2.181880000	-3.214015000	-0.379978000
8	-2.080118000	-1.317460000	-1.715629000
6	3.979185000	-1.694693000	-0.118063000
8	3.417222000	-2.271740000	-0.955418000
8	4.642844000	-1.182317000	0.688174000

$HOCOO^-(CO_2)_7$

1	1.346652000	1.497775000	-1.493208000
8	0.431529000	1.197562000	-1.436334000
6	-2.847714000	-0.362058000	-1.765351000
8	-2.150327000	-0.492631000	-2.685413000
8	-3.626993000	-0.260954000	-0.908898000
6	3.448728000	1.876903000	0.310587000
8	4.033978000	1.242450000	1.088055000
8	2.973834000	2.594875000	-0.474081000
6	0.359750000	0.427642000	-0.270226000
8	1.423815000	0.266673000	0.363648000
8	-0.781601000	-0.005949000	-0.019855000
8	3.360609000	-2.051232000	0.155401000
6	3.374219000	-1.266888000	-0.698819000
8	3.473845000	-0.522334000	-1.588775000
6	0.269660000	-1.253383000	2.284035000
8	0.453706000	-2.246658000	1.708829000
8	0.070324000	-0.333263000	2.967449000
6	-0.460407000	-2.545074000	-1.082259000
8	-1.516569000	-2.864970000	-0.716938000
8	0.596111000	-2.298785000	-1.497817000
6	-2.764103000	0.011937000	1.834754000
8	-2.723986000	-1.143678000	1.944566000
8	-2.868815000	1.168408000	1.788975000
6	-1.570255000	2.843248000	-0.350235000
8	-2.361707000	2.567832000	-1.155923000
8	-0.813494000	3.196188000	0.456895000

$HOCOO^-(CO_2)_8$

8	1.068433000	0.357291000	1.127987000
1	1.862196000	-0.180757000	1.238178000
8	-1.877057000	-2.533420000	-0.981056000
6	-1.413652000	-1.856242000	-1.805465000
8	-1.024203000	-1.239467000	-2.711091000
8	-1.261367000	2.179404000	-2.215323000
6	-0.186123000	1.744322000	-2.132681000
8	0.910189000	1.363026000	-2.121060000
8	0.761901000	-1.342498000	-0.320961000

$HOCOO^-(CO_2)_9$

8	-0.080316000	1.587794000	-0.001729000
1	0.815149000	1.948645000	-0.002030000
8	0.471207000	-2.883565000	1.160150000
6	0.465464000	-2.828781000	-0.001277000
8	0.471908000	-2.882389000	-1.162753000
8	-2.181957000	-1.412004000	-2.623982000
6	-1.300891000	-0.661263000	-2.725295000
8	-0.429990000	0.083655000	-2.914528000
8	1.268529000	-0.209235000	0.000276000

6	0.268472000	-0.323559000	0.199695000
8	-0.847343000	0.200297000	0.018672000
8	3.463864000	-0.256885000	-0.711227000
6	3.005073000	-0.816914000	-1.623766000
8	2.651467000	-1.369974000	-2.580621000
8	-0.351220000	2.994765000	0.998981000
6	-0.831650000	2.273133000	1.774431000
8	-1.323527000	1.643258000	2.618217000
8	-3.319151000	1.925511000	0.177147000
6	-3.413645000	1.059169000	-0.590942000
8	-3.582009000	0.219130000	-1.374760000
8	-1.230819000	-1.870863000	2.230650000
6	-2.223225000	-1.400928000	1.852790000
8	-3.256600000	-0.973055000	1.536400000
8	3.247256000	2.234996000	1.900929000
6	2.955214000	2.599058000	0.835857000
8	2.710365000	3.003214000	-0.223267000
8	0.982676000	-4.057579000	0.731798000
6	1.583866000	-3.231504000	1.282437000
8	2.236122000	-2.489458000	1.899546000

6	0.086837000	0.196820000	-0.000487000
8	-0.978260000	-0.446506000	-0.000734000
8	2.296505000	1.860318000	-1.908146000
6	2.492463000	0.761745000	-2.234739000
8	2.740775000	-0.302308000	-2.629823000
8	-3.002455000	1.443998000	-1.160688000
6	-2.960175000	1.412749000	0.000475000
8	-3.001906000	1.443239000	1.161680000
8	-3.935856000	-1.363654000	0.000084000
6	-3.193751000	-2.257332000	-0.000485000
8	-2.510062000	-3.195505000	-0.000903000
8	-0.430688000	0.083320000	2.913941000
6	-1.301276000	-0.662001000	2.724872000
8	-2.182190000	-1.412884000	2.623417000
8	0.504949000	4.411810000	-0.004200000
6	-0.651844000	4.302600000	-0.000738000
8	-1.811937000	4.254629000	0.002783000
8	2.739669000	-0.304341000	2.631219000
6	2.490208000	0.760254000	2.238320000
8	2.292970000	1.859157000	1.913657000
8	4.253897000	-0.233634000	0.000334000
6	3.814900000	-1.311288000	0.000046000
8	3.446864000	-2.410604000	-0.000322000

$HOCOO^{-}(CO_2)_{10}$

8	0.744897000	-1.216829000	0.143603000
1	0.168897000	-1.989602000	0.206306000
8	-2.105166000	2.298559000	1.101467000
6	-2.067730000	2.283063000	-0.060750000
8	-2.093259000	2.350943000	-1.220364000
8	1.187480000	2.268830000	-2.669965000
6	0.423162000	1.402381000	-2.798324000
8	-0.335880000	0.550394000	-3.009073000
8	-1.347324000	-0.402545000	-0.028573000
6	-0.133485000	-0.118642000	0.013175000
8	0.441968000	0.980823000	-0.043307000
8	-0.877517000	-2.496046000	-2.140808000
6	-1.822743000	-1.843614000	-2.323161000
8	-2.789923000	-1.251144000	-2.572222000
8	3.421487000	0.223039000	-0.414245000
6	3.082619000	0.479593000	0.667093000
8	2.838154000	0.730042000	1.774895000
8	2.510013000	3.289559000	0.009369000
6	1.421581000	3.668327000	-0.134563000
8	0.359287000	4.113706000	-0.280825000
8	-0.043712000	0.612617000	2.974176000
6	0.295430000	1.691611000	2.711261000
8	0.636595000	2.786658000	2.526827000
8	1.611574000	-3.816021000	1.380908000
6	2.491301000	-3.069090000	1.511279000
8	3.396840000	-2.359905000	1.671366000
8	-2.842763000	-0.651569000	2.630815000
6	-2.021090000	-1.453809000	2.454229000
8	-1.228094000	-2.296139000	2.342735000
8	-3.928156000	-1.974216000	0.139991000
6	-4.116517000	-0.834770000	-0.001477000
8	-4.374228000	0.287278000	-0.139031000

$HOCOO^{-}(CO_2)_{11}$

8	-0.274028000	1.241993000	-0.006162000
1	-1.234175000	1.196020000	0.099587000
8	0.961094000	-3.107535000	-1.180726000
6	1.073688000	-3.060392000	-0.023924000
8	1.219857000	-3.111809000	1.127268000
8	3.339558000	-0.119568000	2.259694000
6	2.266829000	-0.421697000	2.589914000
8	1.224301000	-0.728906000	2.995669000
8	-0.742034000	-0.952731000	0.147926000
6	0.160738000	-0.101118000	0.015134000
8	1.390006000	-0.236612000	-0.100574000
8	-1.536667000	0.449504000	2.807144000
6	-1.618911000	-0.709120000	2.802140000
8	-1.741252000	-1.862665000	2.871214000
8	2.444231000	2.689412000	0.151311000
6	2.312830000	2.266634000	-0.922572000
8	2.222359000	1.924209000	-2.029540000
8	4.461195000	0.201892000	-0.609814000
6	4.177135000	-0.896421000	-0.361602000
8	3.958741000	-2.010862000	-0.118262000
8	0.500163000	-0.465120000	-3.034531000
6	1.610632000	-0.772194000	-2.891024000
8	2.726917000	-1.087593000	-2.830270000
8	-2.143344000	3.324205000	-1.187661000
6	-1.052295000	3.694659000	-1.334911000
8	0.018063000	4.109939000	-1.507334000
8	-2.010685000	-2.144794000	-2.416007000
6	-2.174083000	-1.004777000	-2.267591000
8	-2.393044000	0.133134000	-2.174650000
8	-3.466431000	-2.086825000	0.287847000
6	-2.645415000	-2.911863000	0.326161000
8	-1.886255000	-3.786568000	0.361903000

6	2.399165000	-1.962249000	-2.064658000
8	2.736031000	-2.847266000	-1.389174000
8	2.096814000	-1.114169000	-2.794931000

6	0.240513000	2.925601000	2.180293000
8	-0.521326000	3.638522000	1.665184000
8	1.000609000	2.261843000	2.750968000
8	-3.450953000	1.142610000	0.598315000
8	-5.182197000	0.548579000	-0.830632000
6	-4.304470000	0.839016000	-0.126319000

H_2NCOO^-

7	-1.283712000	-0.002978000	-0.108363000
1	-1.667325000	0.830210000	0.323166000
1	-1.664819000	-0.836835000	0.324036000
6	0.182911000	0.000322000	-0.008504000
8	0.704260000	-1.134967000	0.010128000
8	0.698324000	1.138160000	0.010168000

$H_2NCOO^-(CO_2)$

7	1.319000000	-1.169931000	0.355011000
1	0.455696000	-1.624552000	0.085227000
1	2.137132000	-1.651741000	0.008916000
6	1.354511000	0.216970000	0.005549000
8	2.470678000	0.724480000	-0.179689000
8	0.224994000	0.806798000	-0.032092000
6	-1.727727000	-0.035660000	-0.035061000
8	-1.565598000	-1.178556000	-0.292207000
8	-2.328390000	0.944523000	0.203720000

$H_2NCOO^-(CO_2)_2$

7	-0.000434000	1.041618000	0.549658000
1	0.842729000	1.531019000	0.281626000
1	-0.843408000	1.530452000	0.280010000
6	3.247699000	0.081862000	-0.107939000
8	2.969944000	1.213725000	-0.237260000
8	3.810533000	-0.933879000	-0.003129000
6	-3.247564000	0.081636000	-0.107843000
8	-2.970507000	1.213604000	-0.237807000
8	-3.810003000	-0.934208000	-0.001989000
6	0.000074000	-0.320437000	0.135056000
8	1.124223000	-0.867914000	-0.003928000
8	-1.123883000	-0.867723000	-0.006497000

$H_2NCOO^-(CO_2)_3$

7	-0.000412000	-0.397980000	1.552355000
1	0.841094000	0.155016000	1.642335000
1	-0.842909000	0.153454000	1.642714000
6	3.054223000	-0.275090000	-0.155940000
8	2.634565000	0.708012000	0.325362000
8	3.707123000	-1.095896000	-0.661828000
6	-3.053000000	-0.275718000	-0.155239000
8	-2.634893000	0.706040000	0.330298000
8	-3.704868000	-1.094420000	-0.665901000
6	-0.000310000	-1.261125000	0.415159000
8	1.126959000	-1.613615000	-0.013194000
8	-1.127763000	-1.614320000	-0.012480000
6	-0.000434000	2.042511000	-0.406948000
8	-0.001778000	1.450732000	-1.404169000
8	0.000884000	2.690209000	0.560197000

$H_2NCOO^-(CO_2)_4$

7	-0.274150000	-0.876367000	-1.020406000
1	-1.170859000	-1.288503000	-1.245646000
1	0.501578000	-1.407814000	-1.394073000
6	2.250373000	1.685789000	0.241073000
8	2.453321000	1.322862000	-0.846465000
8	2.115728000	2.143395000	1.299309000
6	-3.538962000	-0.995929000	0.466670000
8	-3.272379000	-1.762765000	-0.371752000
8	-3.988376000	-0.293680000	1.276591000
6	-0.134233000	-0.601974000	0.377558000
8	1.035134000	-0.627592000	0.836175000
8	-1.191884000	-0.291612000	0.979350000
6	-1.620310000	1.747907000	-0.820042000
8	-2.615793000	1.282578000	-1.204922000
8	-0.662271000	2.318255000	-0.495012000
6	3.109374000	-1.555976000	-0.136780000

$H_2NCOO^-(CO_2)_5$

7	-0.571018000	-0.464779000	-1.218345000
1	-1.436888000	-0.084733000	-1.582632000
1	-0.146817000	-1.101828000	-1.882677000
6	2.343619000	2.330425000	0.595835000
8	2.600411000	3.054167000	-0.279355000
8	2.186859000	1.704960000	1.564094000
6	-0.075258000	-2.310796000	1.018418000
8	-0.734341000	-3.130703000	0.516755000
8	0.588781000	-1.544777000	1.580164000
6	2.998706000	-1.685406000	-0.525371000
8	3.874683000	-1.019856000	-0.153546000
8	2.224968000	-2.485821000	-0.874308000
6	-2.510421000	2.286327000	-0.119738000
8	-2.987172000	1.472990000	-0.812554000
8	-2.249401000	3.167795000	0.590593000
6	-3.075787000	-1.270367000	0.211802000

8	2.629116000	-2.122007000	-1.037677000	8	-3.481578000	-1.681584000	-0.796570000
8	3.771263000	-1.075434000	0.690866000	8	-2.728611000	-0.881014000	1.249699000
				6	0.343699000	0.582866000	-0.839044000
				8	-0.176699000	1.630184000	-0.386872000
				8	1.561286000	0.318874000	-0.955312000
$H_2NCOO^-(CO_2)_6$				$H_2NCOO^-(CO_2)_7$			
7	-2.703126000	-1.134655000	-1.507194000	7	-0.682838000	-0.854074000	-1.184189000
1	-3.587329000	-0.674567000	-1.328893000	1	-1.428850000	-0.551944000	-1.798594000
1	-2.776704000	-1.815329000	-2.252259000	1	-0.142386000	-1.607820000	-1.592235000
6	1.846096000	-0.946760000	-2.027475000	6	2.815934000	2.071117000	-0.772353000
8	1.684893000	-1.565213000	-1.054310000	8	3.199934000	2.005841000	0.324657000
8	2.149411000	-0.373443000	-2.990759000	8	2.533216000	2.240211000	-1.886844000
6	1.830983000	-1.662075000	1.813774000	6	-0.917606000	-2.423893000	1.305116000
8	1.682896000	-2.813389000	1.819202000	8	-2.071510000	-2.559292000	1.235928000
8	2.008171000	-0.515057000	1.857711000	8	0.233364000	-2.357778000	1.429591000
6	3.769322000	1.449423000	0.496130000	6	2.532249000	-0.502127000	1.813781000
8	4.115324000	0.613525000	-0.231058000	8	1.820344000	0.160318000	2.448820000
8	3.467656000	2.295254000	1.233224000	8	3.298939000	-1.193415000	1.278946000
6	0.234337000	1.656549000	0.268569000	6	-2.762316000	1.996523000	-1.091032000
8	1.065793000	1.420474000	-0.510630000	8	-2.951138000	1.247761000	-1.967787000
8	-0.471576000	1.952241000	1.145276000	8	-2.753295000	2.800539000	-0.253001000
6	-1.966201000	-1.862672000	1.113407000	6	-3.904318000	-1.141865000	-0.472093000
8	-2.951619000	-2.448851000	1.314001000	8	-3.825620000	-1.925146000	-1.327160000
8	-0.947531000	-1.314931000	1.011400000	8	-4.031786000	-0.360118000	0.376092000
6	-1.616494000	-0.210283000	-1.730620000	6	0.149130000	0.234321000	-0.769630000
8	-1.736452000	0.898079000	-1.144952000	8	-0.403560000	1.351534000	-0.651871000
8	-0.678501000	-0.643282000	-2.424009000	8	1.344541000	-0.057953000	-0.512663000
6	-3.337828000	1.789641000	0.610866000	6	-0.732726000	1.572720000	2.013699000
8	-3.500427000	0.766665000	1.145338000	8	-1.250838000	0.530715000	2.023533000
8	-3.297461000	2.871621000	0.187517000	8	-0.249063000	2.624426000	2.100546000
				6	2.882475000	-1.726811000	-1.671507000
				8	3.738572000	-0.946560000	-1.760030000
				8	2.114670000	-2.603787000	-1.665723000
$H_2NCOO^-(CO_2)_8$				$H_2NCOO^-(CO_2)_9$			
7	-0.809071000	0.740897000	0.152408000	7	0.737165000	0.869634000	-0.024329000
1	-0.505238000	1.120602000	1.041458000	1	0.344787000	1.555479000	-0.658237000
1	-1.702581000	0.268897000	0.213967000	1	1.683912000	0.602405000	-0.267885000
6	-2.695782000	2.790428000	-0.237348000	6	2.003856000	3.188124000	1.046637000
8	-2.391449000	3.129867000	-1.305041000	8	1.747258000	3.085497000	2.173612000
8	-3.062625000	2.507994000	0.830472000	8	2.301204000	3.354773000	-0.066537000
6	0.192011000	-0.088171000	-0.454493000	6	-0.123372000	-0.261016000	0.138924000
8	-0.220883000	-0.934396000	-1.281226000	8	0.432482000	-1.341170000	0.459837000
8	1.372834000	0.151351000	-0.112645000	8	-1.345644000	-0.038765000	-0.018985000
6	-2.566405000	-0.908024000	-2.347335000	6	2.972553000	-1.914479000	0.725190000
8	-3.113347000	-0.628417000	-1.354437000	8	3.309009000	-1.103993000	-0.042048000
8	-2.163203000	-1.194207000	-3.396601000	8	2.761197000	-2.756165000	1.496092000
6	3.870604000	0.826650000	-0.111042000	6	-3.928880000	0.246790000	0.378466000
8	3.715775000	1.752182000	-0.795377000	8	-3.794670000	0.837078000	1.369395000
8	4.127108000	-0.069611000	0.583883000	8	-4.160063000	-0.326828000	-0.605872000
6	2.259879000	-2.189321000	-1.210670000	6	-1.951332000	-2.681040000	-0.038032000
8	1.829877000	-2.857604000	-0.361004000	8	-1.594820000	-2.831183000	-1.135542000
8	2.783097000	-1.626518000	-2.083855000	8	-2.390412000	-2.641329000	1.037991000
6	-2.401570000	-0.336295000	2.793838000	6	2.019104000	1.509995000	-2.898999000
8	-1.447291000	-0.074404000	3.402017000	8	0.984268000	1.910344000	-3.243254000

8	-3.373510000	-0.587665000	2.210217000
6	1.748844000	-0.083331000	2.572968000
8	1.707148000	-1.242779000	2.555036000
8	1.801882000	1.074415000	2.685889000
6	0.890440000	2.868990000	-1.079249000
8	0.908798000	3.343826000	-0.016330000
8	0.867818000	2.470723000	-2.168370000
6	-1.190201000	-2.951590000	0.113750000
8	-1.066531000	-2.394318000	1.127261000
8	-1.372447000	-3.589415000	-0.840490000

8	3.066883000	1.131456000	-2.571799000
6	-2.070425000	0.963632000	-2.438093000
8	-1.896377000	-0.038858000	-2.996027000
8	-2.269834000	2.005753000	-1.958676000
6	-1.166503000	2.083917000	1.929616000
8	-1.312296000	2.928793000	1.142978000
8	-1.024797000	1.298746000	2.772445000
6	1.219073000	-2.260413000	-2.014102000
8	0.959826000	-1.246937000	-2.520305000
8	1.525186000	-3.297368000	-1.587719000
6	0.925108000	-0.953756000	3.174796000
8	0.086084000	-1.681065000	3.509899000
8	1.792523000	-0.220758000	2.918267000

$H_2NCOO^-(CO_2)_{10}$

7	-1.326146000	-0.016406000	0.221171000
1	-1.763322000	-0.877271000	-0.083997000
1	-1.767510000	0.813039000	-0.154656000
6	-0.286714000	3.369552000	0.718311000
8	0.594428000	3.939013000	0.219935000
8	-1.218389000	2.917560000	1.250230000
6	0.093504000	-0.042527000	0.031963000
8	0.655837000	1.073456000	-0.075011000
8	0.613203000	-1.183656000	0.035133000
6	2.670950000	2.431130000	-1.310291000
8	2.053836000	2.503557000	-2.292083000
8	3.358207000	2.422938000	-0.374195000
6	1.012426000	-3.565770000	1.167030000
8	1.460592000	-3.108855000	2.136342000
8	0.565039000	-4.109587000	0.242172000
6	3.070715000	-1.415954000	-0.914251000
8	3.024630000	-0.452540000	-1.561464000
8	3.229875000	-2.405257000	-0.322771000
6	-0.218863000	-2.483723000	-2.203981000
8	0.871715000	-2.665328000	-2.553894000
8	-1.346539000	-2.353328000	-1.942591000
6	-0.659395000	-1.191165000	2.816185000
8	-1.393032000	-2.062062000	2.575340000
8	0.062944000	-0.336373000	3.121174000
6	-0.605602000	1.442759000	-2.584992000
8	-1.087751000	2.435922000	-2.219135000
8	-0.170741000	0.452083000	-3.006506000
6	2.455639000	1.113668000	2.045977000
8	3.006732000	0.142809000	1.727412000
8	1.959492000	2.091004000	2.435516000
6	-3.459453000	0.990319000	1.988961000
8	-2.982066000	0.790703000	3.026984000
8	-3.998475000	1.202427000	0.979654000
8	-4.353823000	-1.458036000	-1.091247000
8	-3.442582000	0.180493000	-2.461607000
6	-3.888405000	-0.641033000	-1.772356000

$H_2NCOO^-(CO_2)_{11}$

7	-0.664185000	-0.799148000	0.586325000
1	-0.571739000	-1.795171000	0.432866000
1	-1.568627000	-0.431555000	0.319814000
6	-1.689870000	2.642157000	0.790836000
8	-1.485805000	3.482892000	0.015593000
8	-1.994051000	1.870451000	1.607041000
6	0.445428000	-0.043560000	0.091086000
8	0.216518000	1.160584000	-0.179744000
8	1.532415000	-0.665548000	0.020897000
6	0.789305000	3.266504000	-1.863648000
8	0.091831000	2.833049000	-2.685516000
8	1.496356000	3.782236000	-1.100504000
6	3.532258000	-2.158642000	1.036691000
8	3.796276000	-1.383935000	1.860619000
8	3.328631000	-2.993713000	0.254377000
6	3.440904000	0.451253000	-1.496877000
8	2.707299000	1.082405000	-2.139078000
8	4.263735000	-0.145248000	-0.930827000
6	-4.615386000	0.289613000	-0.360678000
8	-4.488909000	-0.817767000	-0.687628000
8	-4.770185000	1.393445000	-0.038711000
6	1.365891000	-2.527565000	-1.936661000
8	2.271591000	-2.087525000	-2.512086000
8	0.448284000	-3.042884000	-1.437597000
6	1.123595000	-0.971075000	2.962592000
8	1.015938000	-2.128387000	2.905144000
8	1.242112000	0.176253000	3.086359000
6	-1.266784000	0.334300000	-2.405954000
8	-2.229489000	0.829692000	-1.976443000
8	-0.354358000	-0.199915000	-2.882209000
6	1.979912000	2.552849000	1.478294000
8	2.937263000	2.047388000	1.059504000
8	1.073226000	3.107415000	1.951359000
6	-2.531583000	-0.687322000	2.957733000
8	-1.735453000	-0.580941000	3.794394000
8	-3.375093000	-0.811035000	2.166439000
8	-2.560908000	-3.393322000	-0.247058000
8	-2.585057000	-2.641542000	-2.444153000
6	-2.564947000	-3.010450000	-1.343136000