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Guanidine as a strong CO_2 adsorbent: A DFT study on cooperative CO_2 adsorption

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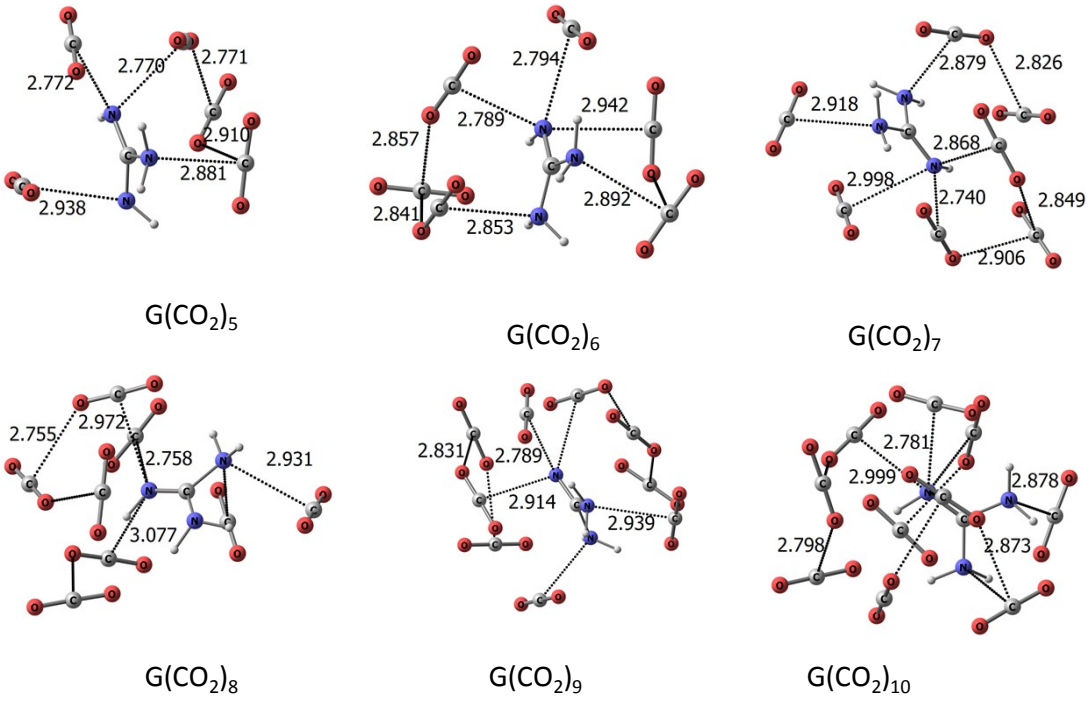
Supporting Information

Table of Contents

Sl. No.	Title	Page No.
1	**Fig. S1** Optimized geometries of $G(CO_2)_n$ complexes at M06-2X/6-311++G** level.	S3
2	**Fig. S2** Correlation between ΔE (kcal/mol) and number of CO_2 molecules (n) of $G(CO_2)_n$ complexes at M06-2X/6-311++G** level.	S3
3	**Fig.S3** Optimized geometries (side view with bowl depth) of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level for n= 4 to 10.	S4
4	**Table S1** O…HN and H…OC hydrogen bond angle (°) of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level.	S4
5	**Fig. S4** Correlation between ΔE (kcal/mol) and number of CO_2 molecules (n) of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level.	S5
6	**Table S2**. ZPE and BSSE corrected $\Delta E_{/CO2}$ and $\Delta G_{/CO2}$ (kcal/mol) of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level.	S5
7	**Table S3**. Average δ values of C nucleus of the CO_2 molecules in $(G\text{-}CO_2)_n$ complexes at M062X/6-311++G** level.	S6
8	**Fig. S5** QTAIM plots of $G(CO_2)_n$ complexes for n=5-10 at M06-2X/6-311++G**	S7
9	**Fig.S6** Correlation between $\Sigma\rho_b$ and ΔE for $G(CO_2)_n$ clusters.	S8

10	**Table S4.** Total values of QTAIM parameters (a.u.) of the non-covalent interactions in $G(CO_2)_n$ clusters.	S8
11	**Table S5.** Average values of QTAIM parameters (a.u.) of the non-covalent interactions in $G(CO_2)_n$ clusters.	S9
12	**Table S6.** Total values of QTAIM parameters (a.u.) of the O…HN non-covalent interactions in $(G\text{-}CO_2)_n$ clusters.	S9
13	**Table S7.** Average values of QTAIM parameters (a.u.) of the O…HN non-covalent interactions in $(G\text{-}CO_2)_n$ clusters.	S10
14	**Table S8.** Total values of QTAIM parameters (a.u.) of N-C covalent interactions in $(G\text{-}CO_2)_n$ clusters.	S10
15	**Table S9.** Average values of QTAIM parameters of the N-C covalent interactions in $(G\text{-}CO_2)_n$ clusters.	S11
16	**Table. S10** ΣV_n^N and ΣV_n^H for the $(G\text{-}CO_2)_n$ clusters in a. u. and the corresponding $\Delta\Sigma V_n^N$ and $\Delta\Sigma V_n^G$ in kcal/mol at M062X/6-311++G** level of theory.	S12
17	**Fig.S7** Correlation between ΣV_n (a.u.) and ΔE (kcal/mol).	S12
18	**Fig.S8 (a)** Variation of $\Sigma\Delta V_n^N$ (a.u.) with ΔE (kcal/mol) and **(b)** $\Sigma\Delta V_n^H$ with ΔE (kcal/mol).	S13
19	**Table S11.** BSSE and ZPE corrected ΔE (kcal/mol) for $(G\text{-}CO_2)_n$ complexes using different methods with dispersion correction in conjunction with basis set 6-311++G**	S13
20	**Table S12**. BSSE and ZPE corrected $\Delta E_{/CO2}$ (kcal/mol) for $(G\text{-}CO_2)_n$ complexes using different methods with dispersion correction in conjunction with basis set 6-311++G**.	S14
21	**Table S13** BSSE and ZPE corrected $\Delta G_{/G\text{-}CO2}$ (kcal/mol) for $(G\text{-}CO_2)_n$ complexes using different methods with dispersion correction in conjunction with basis set 6-311++G**.	S14
22	Cartesian coordinates of optimized geometry of higher energy linear structures of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level. Atomic number followed by X, Y, Z coordinates in Å.	S15
23	Cartesian coordinates of optimized geometry of cyclic structures of $(G\text{-}CO_2)_n$ clusters at M06-2X/6-311++G** level. Atomic number followed by X, Y, Z coordinates in Å.	S21
24	Cartesian coordinates of optimized geometry of cyclic structures of $G(CO_2)_n$ clusters at M06-2X/6-311++G** level. Atomic number followed by X, Y, Z coordinates in Å.	S29
25	References	S32

Structure and energetics



$G(CO_2)_5$ $G(CO_2)_6$ $G(CO_2)_7$

$G(CO_2)_8$ $G(CO_2)_9$ $G(CO_2)_{10}$

Fig. S1 Optimized geometries of $G(CO_2)_n$ complexes at M06-2X/6-311++G** level.

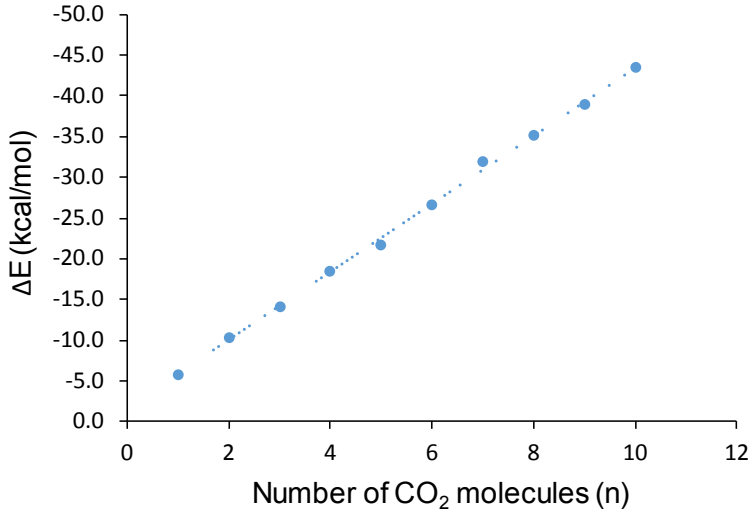


Fig. S2 Correlation between ΔE (kcal/mol) and number of CO_2 molecules (n) of $G(CO_2)_n$ complexes at M06-2X/6-311++G** level.

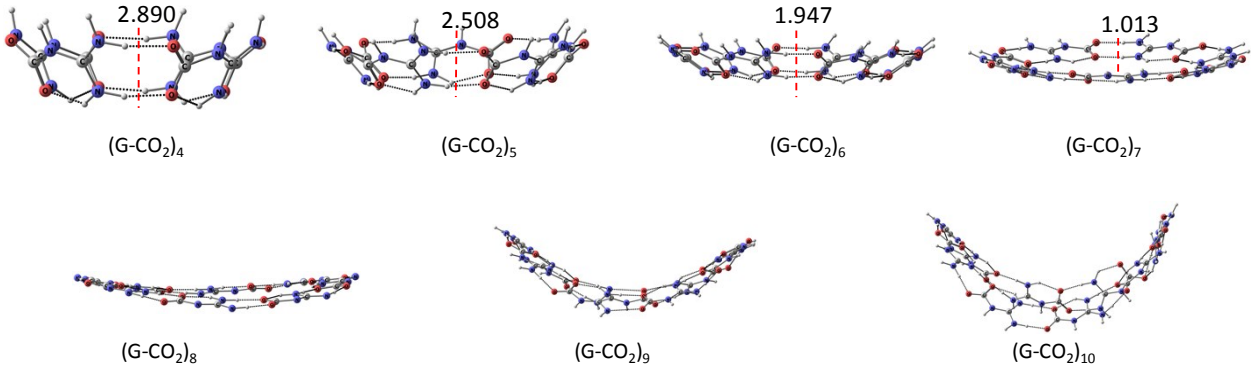


Fig.S3 Optimized geometries (side view with bowl depth) of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level for n= 4 to 10.

Table S1. O…NH and H…OC hydrogen bond angle (°) of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level.

System	O…HN	H…OC
$(G\text{-}CO_2)_2$	145.2	112.6
$(G\text{-}CO_2)_3$	153.4	113.9

$(G\text{-}CO_2)_4$	162.4	114.6
$(G\text{-}CO_2)_5$	168.4	116.1
$(G\text{-}CO_2)_6$	172.8	116.9
$(G\text{-}CO_2)_7$	176.7	117.2
$(G\text{-}CO_2)_8$	178.5	115.7
$(G\text{-}CO_2)_9$	176.7	114.7
$(G\text{-}CO_2)_{10}$	173.2	114.0

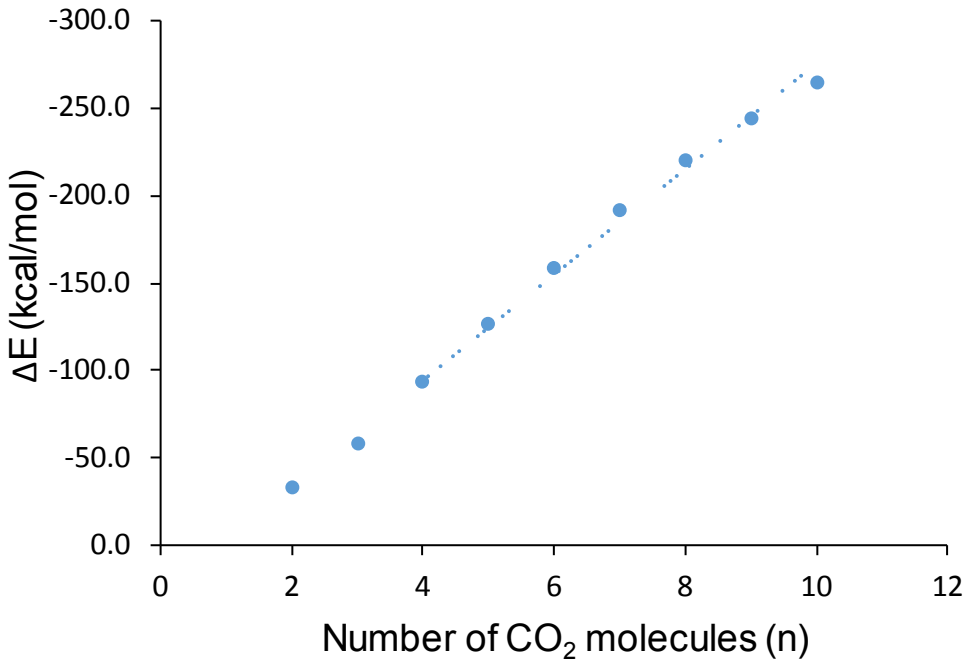


Fig. S4 Correlation between ΔE (kcal/mol) and number of CO_2 molecules (n) of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level.

Table S2. ZPE and BSSE corrected $\Delta E_{/CO2}$ and $\Delta G_{/CO2}$ (kcal/mol) of $(G\text{-}CO_2)_n$ complexes at M06-2X/6-311++G** level.

n	$\Delta E_{/CO2}$ (kcal/mol)	$\Delta G_{/CO2}$ (kcal/mol)
1	-5.7	2.3
2	-16.4	-0.5
3	-19.4	-1.0
4	-23.4	-4.1
5	-25.3	-5.7
6	-26.5	-6.6
7	-27.4	-7.7
8	-27.5	-7.8
9	-27.2	-7.1
10	-26.5	-6.3

NMR analysis

The formation of the G-CO_2 zwitterion is verified using the NMR analysis of the (G-CO_2)$_n$ clusters at the same level of DFT. NMR calculations are carried out for the (G-CO_2)$_n$ complexes and the reference compound TMS to obtain the magnetic shielding value (σ) of the C nucleus. Nuclear magnetic resonance (NMR) analysis has been carried out using the Gauge-Independent Atomic Orbital (GIAO) method[1] at M06-2X/6-311++G** level. The calculated magnetic shielding value (σ) is converted into a chemical shift (δ) by calculating the magnetic shielding of the reference compound,[2] trimethyl silane (TMS) using eq. 2,

$$\delta_{nucl} = \sigma_{ref} - \sigma_{nucl} \qquad \text{(S1)}$$

where δ_{nucl} is the chemical shift of the nucleus under study (here C of CO_2), σ_{ref} is the calculated shielding of TMS, and σ_{nucl} is the calculated shielding of the C.

Table S3. Average δ values of C nucleus of the CO_2 molecules in (G-CO_2)$_n$ complexes at M062X/6-311++G** level.

System	δ (ppm)
CO_2	139
G(CO_2)	140

$(G\text{-}CO_2)_2$	164
$(G\text{-}CO_2)_3$	168
$(G\text{-}CO_2)_4$	168
$(G\text{-}CO_2)_5$	169
$(G\text{-}CO_2)_6$	169
$(G\text{-}CO_2)_7$	169
$(G\text{-}CO_2)_8$	170
$(G\text{-}CO_2)_9$	170
$(G\text{-}CO_2)_{10}$	170

From theses δ values are calculated using the equation S1. The δ value observed for the CO_2 is 139 ppm. The values observed for the G-CO_2 is 140 ppm which is comparable to that of CO_2. From the complex $(G\text{-}CO_2)_2$ onwards the δ value is found to have a large jump to 160 ppm and it slightly increases to 164 ppm for $(G\text{-}CO_2)_3$ and beyond this δ value remains almost same 168 -170 ppm towards the larger clusters. This higher δ values shows the transformation of the C nuclei of CO_2 to the anionic nature in the zwitterion, G-CO_2 with partial negative charge on CO_2 and a partial positive charge on the imine unit. This δ value is in the range that is observed for the carbamate group, which again shows the formation of carbamate through the N-C covalent interaction.[3-6] The constant nature of the δ value beyond *n*=5 again shows that the nature of the electronic environment around the C nucleus remains same in higher clusters. This was also visible in the ΔE value of the $(G\text{-}CO_2)_n$ clusters, which showed a constant value of $\Delta E_{/G\text{-}CO2}$ for the higher clusters

QTAIM analysis

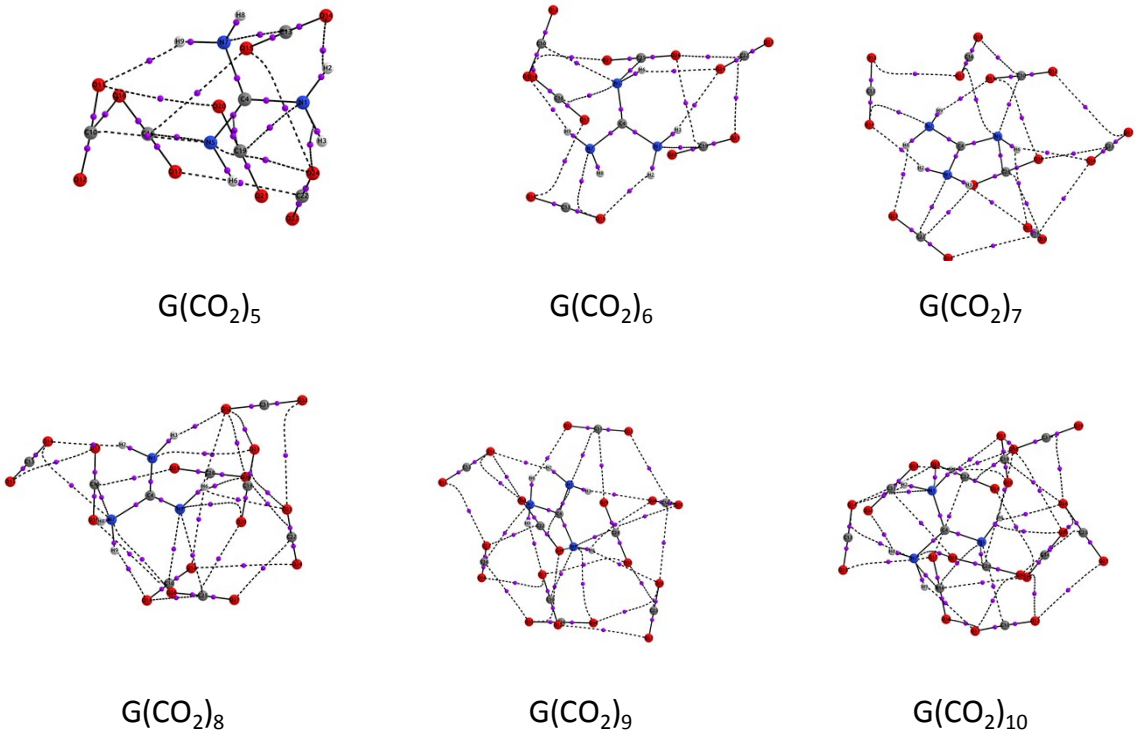


Fig. S5 QTAIM plots of $G(CO_2)_n$ complexes for n=5-10 at M06-2X/6-311++G**

In the $G(CO_2)_n$ clusters as well, Koch-Popelier criterion on ρ_b is valid for all the G…CO_2 non-covalent interactions and the sign of $\nabla^2\rho$ is positive(**Table S3**). The increased cooperativity in the large clusters is marked with very higher $\Sigma\rho_b$ resulting from the CO_2…CO_2 interactions. As observed in the case of the $(G\text{-}CO_2)_n$ clusters, here also $\Sigma\rho_b$ is in good linear correlation with ΔE, having a correlation coefficient of R = 0.9878 a. u.

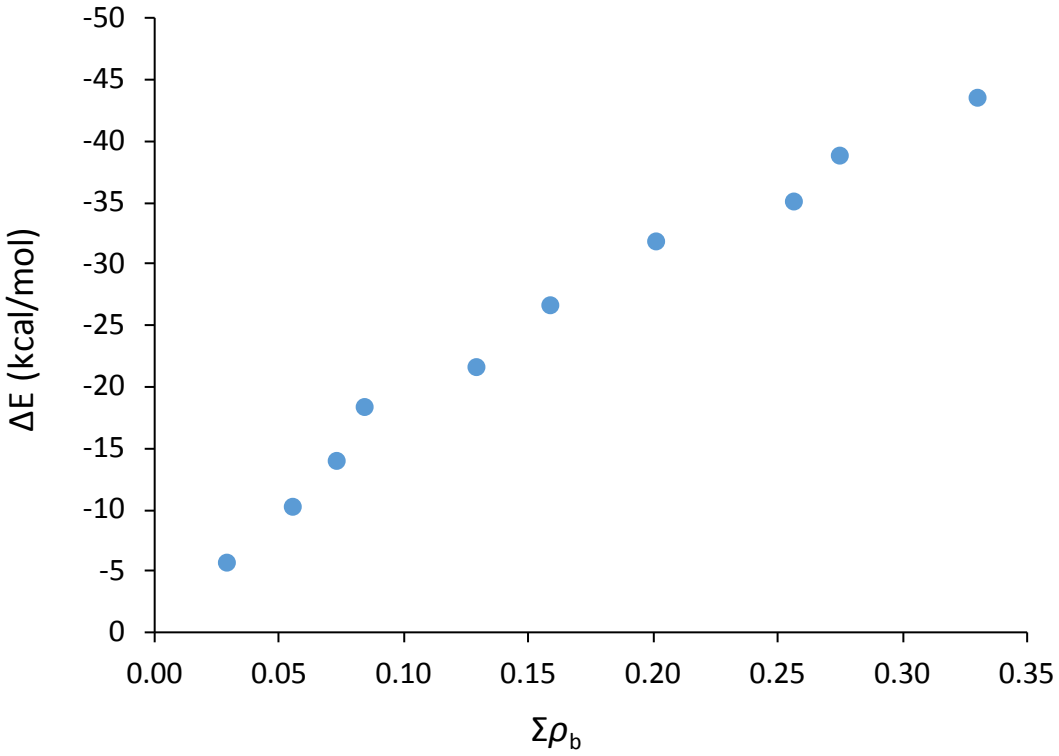


Fig.S6 Correlation between $\Sigma\rho_b$ and ΔE for $G(CO_2)_n$ clusters.

Table S4. Total values of QTAIM parameters (a.u.) of the non-covalent interactions in $G(CO_2)_n$ clusters.

n	Σρ	$\Sigma\nabla^2\rho$	$\Sigma\lambda_1$	$\Sigma\lambda_2$	$\Sigma\lambda_3$
1	0.0287	0.1075	-0.0270	-0.0204	0.1549
2	0.0546	0.2148	-0.0439	-0.0260	0.2847
3	0.0723	0.2800	-0.0547	-0.0294	0.3641
4	0.0833	0.3330	-0.0656	-0.0327	0.4314
5	0.1283	0.4987	-0.1026	-0.0569	0.6583
6	0.1586	0.6208	-0.1394	-0.0819	0.8421
7	0.2004	0.7917	-0.1705	-0.0963	1.0585
8	0.2556	1.0258	-0.2086	-0.1141	1.3484
9	0.2746	1.1129	-0.2338	-0.1288	1.4755
10	0.3298	1.3333	-0.2801	-0.1489	1.7622

Table S5. Average values of QTAIM parameters (a.u.) of the non-covalent interactions in $G(CO_2)_n$ clusters.

n	$\rho_{b.avg}$	$\nabla^2\rho_{.avg}$	$\lambda_{1.avg}$	$\lambda_{2.avg}$	$\lambda_{3.avg}$
1	0.0143	0.0537	-0.0135	-0.0102	0.0774
2	0.0109	0.0430	-0.0088	-0.0052	0.0569
3	0.0103	0.0400	-0.0078	-0.0042	0.0520
4	0.0104	0.0416	-0.0082	-0.0041	0.0539
5	0.0092	0.0356	-0.0073	-0.0041	0.0470
6	0.0092	0.0356	-0.0073	-0.0041	0.0470
7	0.0106	0.0414	-0.0093	-0.0055	0.0561
8	0.0100	0.0396	-0.0085	-0.0048	0.0529
9	0.0095	0.0380	-0.0077	-0.0042	0.0499
10	0.0095	0.0384	-0.0081	-0.0044	0.0509

Table S6. Total values of QTAIM parameters (a.u.) of the O…HN non-covalent interactions in $(G\text{-}CO_2)_n$ clusters.

System	$\Sigma\rho$	$\Sigma\nabla^2\rho$	$\Sigma\lambda_1$	$\Sigma\lambda_2$	$\Sigma\lambda_3$
$G(CO_2)$	0.0287	0.1075	-0.0270	-0.0204	0.1549
$(G\text{-}CO_2)_2$	0.1840	0.6904	-0.2582	-0.2444	1.1930
$(G\text{-}CO_2)_3$	0.2459	0.9208	-0.3449	-0.3198	1.5856
$(G\text{-}CO_2)_4$	0.4128	1.5099	-0.6204	-0.5854	2.7157
$(G\text{-}CO_2)_5$	0.5436	1.9398	-0.8388	-0.7990	3.5776
$(G\text{-}CO_2)_6$	0.6705	2.3568	-1.0490	-1.0049	4.4106
$(G\text{-}CO_2)_7$	0.7931	2.7601	-1.2501	-1.2026	5.2128
$(G\text{-}CO_2)_8$	0.7255	2.4471	-1.1626	-1.1196	4.7293
$(G\text{-}CO_2)_9$	1.0112	3.4369	-1.6048	-1.5464	6.5881
$(G\text{-}CO_2)_{10}$	1.0883	3.7676	-1.6940	-1.6323	7.0940

Table S7. Average values of QTAIM parameters (a.u.) of the O…HN non-covalent interactions in $(G\text{-}CO_2)_n$ clusters.

System	$\rho_{b.avg}$	$\nabla^2\rho_{.avg}$	$\lambda_{1.avg}$	$\lambda_{2.avg}$	$\lambda_{3.avg}$
$G(CO_2)$	0.0143	0.0537	-0.0135	-0.0102	0.0774
$(G\text{-}CO_2)_2$	0.0307	0.1151	-0.0430	-0.0407	0.1988
$(G\text{-}CO_2)_3$	0.0273	0.1023	-0.0383	-0.0355	0.1762
$(G\text{-}CO_2)_4$	0.0344	0.1258	-0.0517	-0.0488	0.2263
$(G\text{-}CO_2)_5$	0.0362	0.1293	-0.0559	-0.0533	0.2385
$(G\text{-}CO_2)_6$	0.0372	0.1309	-0.0583	-0.0558	0.2450
$(G\text{-}CO_2)_7$	0.0378	0.1314	-0.0595	-0.0573	0.2482
$(G\text{-}CO_2)_8$	0.0302	0.1020	-0.0484	-0.0467	0.1971
$(G\text{-}CO_2)_9$	0.0375	0.1273	-0.0594	-0.0573	0.2440
$(G\text{-}CO_2)_{10}$	0.0363	0.1256	-0.0565	-0.0544	0.2365

Table S8. Total values of QTAIM parameters (a.u.) of N-C covalent interactions in $(G\text{-}CO_2)_n$ clusters.

System	$\Sigma\rho$	$\Sigma\nabla^2\rho$
$G\text{-}CO_2$	0.0165	0.0599
$(G\text{-}C)_2$	0.4871	-1.1598
$(G\text{-}C)_3$	0.7544	-1.8788
$(G\text{-}C)_4$	1.0251	-2.6175
$(G\text{-}C)_5$	1.2970	-3.3574
$(G\text{-}C)_6$	1.5669	-4.0825
$(G\text{-}C)_7$	1.8347	-4.7956
$(G\text{-}C)_8$	2.1045	-5.5167
$(G\text{-}C)_9$	2.3670	-6.2036
$(G\text{-}C)_{10}$	2.6189	-6.8315

Table S9. Average values of QTAIM parameters of the N-C covalent interactions in (G-CO_2)$_n$ clusters.

System	$\rho_{b.avg}$	$\nabla^2\rho_{b.avg}$
G(CO_2)	0.0165	0.0599
(G-CO_2)$_2$	0.2436	-0.5799
(G-CO_2)$_3$	0.2515	-0.6263
(G-CO_2)$_4$	0.2563	-0.6544
(G-CO_2)$_5$	0.2594	-0.6715
(G-CO_2)$_6$	0.2611	-0.6804
(G-CO_2)$_7$	0.2621	-0.6851
(G-CO_2)$_8$	0.2631	-0.6896
(G-CO_2)$_9$	0.2630	-0.6893
(G-CO_2)$_{10}$	0.2619	-0.6831

MESP analysis

The sum of potential at the sp^2 N atom (ΣV_n^N) and all the H atoms (ΣV_n^H) of every G is computed for (G-CO_2)$_n$ clusters (**Table S9**). From the V_n values of single G molecule the predicted values for potential at the sp^2 N atom (ΣV_n^{N*}) and all the H atoms (ΣV_n^{H*}) are generated, using which the difference in V_n ($\Delta\Sigma V_n^N$ and $\Delta\Sigma V_n^G$) is calculated (**Table S9**). The value of $\Delta\Sigma V_n^N$ and $\Delta\Sigma V_n^H$ increases steadily with increasing value of *n*. Larger the clusters larger is the delocalisation of the potential from the sp^2 N centres to the CO_2 molecules. This clearly shows the impact of the cooperativity from the neighbouring G-CO_2 units in the dispersing the negative potential and thereby to stabilise the larger clusters.

Table. S10 ΣV_n^N and ΣV_n^H for the (G-CO_2)$_n$ clusters in a. u. and the corresponding $\Delta\Sigma V_n^N$ and $\Delta\Sigma V_n^G$ in kcal/mol at M062X/6-311++G** level of theory.

n	ΣV_n^N	ΣV_n^H	$\Delta\Sigma V_n^N$	$\Delta\Sigma V_n^H$
1	-5.1270	-18.4349	4.6	0.0
2	-9.9697	-36.7205	113.9	0.5
3	-14.9997	-55.0329	199.2	0.7
4	-20.0674	-73.3505	282.9	0.9
5	-25.1727	-91.7001	346.1	1.0

6	-30.2776	-110.0520	408.0	1.1
7	-35.3824	-128.4068	468.9	1.2
8	-40.4506	-146.7577	531.6	1.4
9	-45.5132	-165.1013	597.9	1.6
10	-50.5605	-183.4453	664.7	1.8
11	-55.5868	-201.7823	736.0	2.0

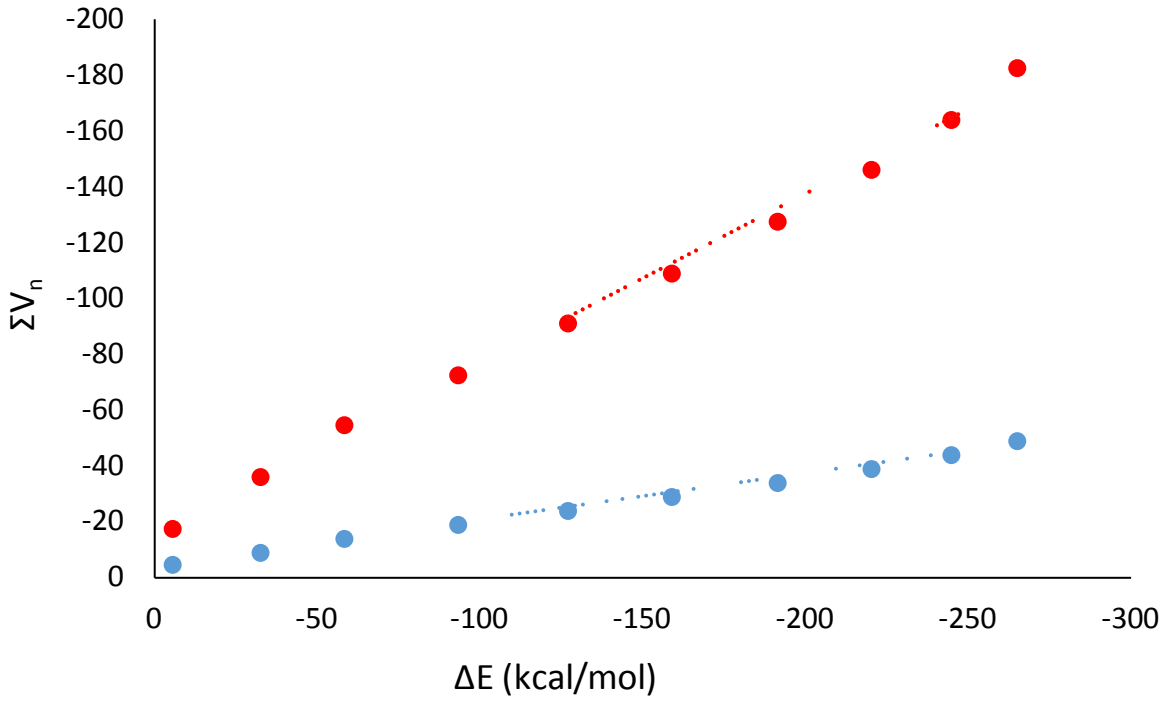
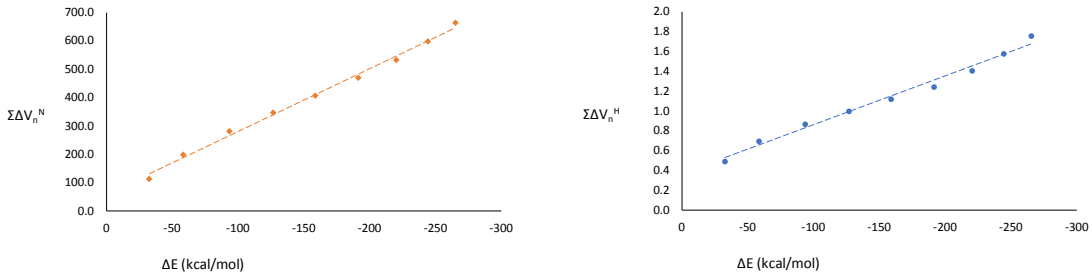


Fig.S7 Correlation between ΣV_n (a.u.) and ΔE (kcal/mol).

Fig. S7 gives the variation of ΣV_n^N and ΣV_n^H with ΔE. Both are giving good linear correlations with correlation coefficient of 0.998 in both the cases. These strong linear correlations suggest that the total interaction energy is directly proportional to the ability of the systems to undergo electron delocalization. Larger the *n* values larger will be the delocalization and resulting cooperative interactions leading to the formation more stable clusters.



a **b**

Fig.S8 (a) Variation of $\Sigma\Delta V_n^N$ (a.u.) with ΔE (kcal/mol) and **(b)** $\Sigma\Delta V_n^H$ with ΔE (kcal/mol).

Benchmark Study

Table S11. BSSE and ZPE corrected ΔE (kcal/mol) for $(G\text{-}CO_2)_n$ complexes using different methods with dispersion correction in conjunction with basis set 6-311++G**.

System	B3LYP	B3LYP-D3	M06-2X	M06-2X-D3	BP86-D3	wB97XD
$G(CO_2)$	-3.1	-5.3	-5.7	-3.5	-4.9	-4.7
$(G\text{-}CO_2)_2$	-19.8	-28.9	-32.8	-33.4	-34.1	-32.1
$(G\text{-}CO_2)_3$	-35.8	-54.3	-58.3	-60.1	-62.5	-58.3
$(G\text{-}CO_2)_4$	-67.2	-89.2	-93.4	-95.7	-99.0	-94.9
$(G\text{-}CO_2)_5$	-94.3	-120.9	-126.6	-129.1	-132.7	-128.4
$(G\text{-}CO_2)_6$	-120.2	-151.6	-158.8	-161.5	-165.4	-160.7
$(G\text{-}CO_2)_7$	-145.5	-182.1	-191.5	-193.9	-197.5	-192.7
$(G\text{-}CO_2)_8$	-168.8	-209.6	-219.9	-223.8	-226.4	-222.3
$(G\text{-}CO_2)_9$	-186.3	-232.7	-244.4	-248.2	-252.1	-246.6

Table S12. BSSE and ZPE corrected $\Delta E_{/CO2}$ (kcal/mol) for $(G\text{-}CO_2)_n$ complexes using different methods with dispersion correction in conjunction with basis set 6-311++G**.

System	B3LYP	B3LYP-D3	M06-2X	M06-2X-D3	BP86-D3	wB97XD
$G(CO_2)$	-3.1	-5.3	-5.7	-3.5	-4.9	-4.7
$(G\text{-}CO_2)_2$	-9.9	-14.4	-16.4	-16.7	-17.1	-16.1
$(G\text{-}CO_2)_3$	-11.9	-18.1	-19.4	-20.0	-20.8	-19.4
$(G\text{-}CO_2)_4$	-16.8	-22.3	-23.4	-23.9	-24.8	-23.7
$(G\text{-}CO_2)_5$	-18.9	-24.2	-25.3	-25.8	-26.5	-25.7
$(G\text{-}CO_2)_6$	-20.0	-25.3	-26.5	-26.9	-27.6	-26.8
$(G\text{-}CO_2)_7$	-20.8	-26.0	-27.4	-27.7	-28.2	-27.5
$(G\text{-}CO_2)_8$	-21.1	-26.2	-27.5	-28.0	-28.3	-27.8
$(G\text{-}CO_2)_9$	-20.7	-25.9	-27.2	-27.6	-28.0	-27.4

Table S13. BSSE and ZPE corrected $\Delta G_{/G\text{-}CO2}$ (kcal/mol) for $(G\text{-}CO_2)_n$ complexes using different methods with dispersion correction in conjunction with basis set 6-311++G**.

System	B3LYP	B3LYP-D3	M06-2X	M06-2X-D3	BP86-D3	wB97XD
$G(CO_2)$	4.4	2.4	2.3	4.4	2.8	3.0
$(G\text{-}CO_2)_2$	5.9	1.4	-0.5	-0.8	-1.1	-0.2
$(G\text{-}CO_2)_3$	6.6	0.4	-1.0	-1.6	-2.2	-0.9
$(G\text{-}CO_2)_4$	2.7	-2.8	-4.1	-4.8	-5.2	-4.2
$(G\text{-}CO_2)_5$	1.1	-4.3	-5.7	-6.2	-6.6	-5.8
$(G\text{-}CO_2)_6$	0.1	-5.2	-6.6	-7.1	-7.5	-6.7
$(G\text{-}CO_2)_7$	-0.7	-6.0	-7.7	-8.0	-8.3	-7.5
$(G\text{-}CO_2)_8$	-1.2	-6.3	-7.8	-8.7	-8.3	-7.9
$(G\text{-}CO_2)_9$	-0.4	-5.6	-7.1	-7.5	-7.7	-7.1

Cartesian coordinates of higher energy linear structures of $(G\text{-}CO_2)_n$ complexes.

$(G\text{-}CO_2)_2$	$(G\text{-}CO_2)_3$

SCF E = -787.885496131 a.u.

7	-5.584768000	-0.548899000	-0.167237000
1	-6.407220000	0.030705000	-0.134516000
1	-5.707507000	-1.529737000	0.023441000
6	-4.359622000	0.008194000	-0.089616000
7	-3.297665000	-0.765877000	0.107794000
1	-3.424820000	-1.760842000	0.233907000
7	-4.217925000	1.318655000	-0.217802000
1	-4.991481000	1.900525000	-0.490842000
1	-3.243807000	1.649108000	-0.214727000
6	-1.856936000	-0.347123000	0.122228000
8	-1.668695000	0.868927000	-0.038710000
8	-1.110169000	-1.292313000	0.295020000
7	1.223780000	1.358771000	0.360045000
1	0.237320000	1.151485000	0.215053000
1	1.500237000	2.320450000	0.256925000
6	2.156074000	0.405414000	0.125078000
7	3.439185000	0.742506000	0.033885000
1	3.695372000	1.712425000	0.146508000
7	1.781914000	-0.857435000	0.008024000
1	0.808179000	-1.119232000	0.125025000
1	2.556636000	-1.518142000	-0.110482000
6	4.652822000	-0.190065000	-0.140029000
8	5.685444000	0.449108000	-0.145222000
8	4.344847000	-1.379387000	-0.239740000

SCF E = -1181.85419552 a.u.

7	8.525385000	-1.334875000	-0.080005000
1	9.440238000	-0.927734000	-0.182795000
1	8.448989000	-2.333630000	-0.179986000
6	7.425912000	-0.560187000	-0.074596000
7	6.223531000	-1.132434000	-0.107867000
1	6.155899000	-2.139490000	-0.166406000
7	7.539602000	0.757372000	-0.030649000
1	8.435352000	1.201298000	0.080472000
1	6.652896000	1.272456000	0.018982000
6	4.898205000	-0.457425000	-0.041560000
8	4.940123000	0.781829000	0.036698000
8	3.973259000	-1.251653000	-0.077886000
7	2.213741000	1.791968000	-0.036423000
1	3.157469000	1.403285000	-0.002421000
1	2.111376000	2.789837000	0.030548000
6	1.126011000	1.009835000	0.033161000
7	-0.085108000	1.588127000	0.078846000
1	-0.144849000	2.595602000	0.051904000
7	1.250053000	-0.302163000	0.047114000
1	2.172690000	-0.732211000	0.002834000
1	0.374350000	-0.825188000	0.077785000
6	-1.404267000	0.931125000	0.121177000
8	-2.328460000	1.735437000	0.141468000
8	-1.387119000	-0.312309000	0.131416000
7	-4.097324000	-1.295113000	0.452882000
1	-3.157654000	-0.908091000	0.339811000
1	-4.184295000	-2.294913000	0.386733000
6	-5.182226000	-0.547685000	0.151044000
7	-6.378381000	-1.129716000	0.057242000
1	-6.447743000	-2.120414000	0.236660000
7	-5.050363000	0.755099000	-0.022778000
1	-4.132618000	1.192810000	0.037198000
1	-5.925482000	1.248754000	-0.216462000
6	-7.732470000	-0.469543000	-0.213232000
8	-7.662277000	0.748118000	-0.397386000
8	-8.626969000	-1.294789000	-0.194228000

$(G\text{-}CO_2)_4$

SCF E = -1575.82716903 a.u.

7	-5.259490000	2.464564000	-0.021587000
1	-6.236599000	2.158190000	-0.041855000
1	-5.057037000	3.445933000	-0.104858000
6	-4.263757000	1.572852000	-0.036657000
7	-2.993289000	2.016409000	-0.086755000
1	-2.828494000	3.012296000	-0.110698000
7	-4.524743000	0.280595000	0.003111000
1	-5.484016000	-0.063259000	0.052833000
1	-3.710116000	-0.332169000	0.004422000
6	-1.760248000	1.228973000	-0.088168000

$(G\text{-}CO_2)_5$

SCF E = -1969.80087853 a.u.

7	2.374032000	1.053327000	-0.120085000
1	3.309352000	0.626094000	-0.078221000
1	2.305410000	2.054644000	-0.062560000
6	1.260754000	0.313484000	-0.077439000
7	0.067891000	0.945501000	-0.058655000
1	0.056201000	1.954322000	-0.087425000
7	1.333492000	-1.000301000	-0.063017000
1	2.248446000	-1.463600000	-0.072821000
1	0.444874000	-1.495346000	-0.044536000
6	-1.265776000	0.357963000	-0.032298000

8	-1.899367000	-0.008602000	-0.046781000
8	-0.749448000	1.924576000	-0.132070000
7	0.629094000	-1.287899000	-0.231862000
1	-0.272138000	-0.799370000	-0.165346000
1	0.627758000	-2.291594000	-0.175461000
6	1.791874000	-0.629268000	-0.133427000
7	2.935842000	-1.338938000	-0.105559000
1	2.882439000	-2.344830000	-0.168260000
7	1.808181000	0.686240000	-0.078303000
1	0.929948000	1.211758000	-0.097820000
1	2.731336000	1.113780000	-0.024388000
6	4.313932000	-0.839035000	-0.028803000
8	5.145084000	-1.742660000	-0.028458000
8	4.442269000	0.397222000	0.025808000
7	7.219094000	1.060433000	0.436041000
1	6.245029000	0.783163000	0.285513000
1	7.423464000	2.043852000	0.386933000
6	8.224369000	0.193552000	0.188163000
7	9.484061000	0.634767000	0.165944000
1	9.655770000	1.608969000	0.365328000
7	7.953648000	-1.084758000	-0.003505000
1	6.987367000	-1.410378000	-0.014825000
1	8.774600000	-1.674430000	-0.159595000
6	10.764552000	-0.172818000	-0.034781000
8	10.569042000	-1.373361000	-0.242304000
8	11.746606000	0.542858000	0.049411000
7	-11.334728000	-1.536398000	0.094610000
1	-11.734550000	-2.459799000	0.065557000
1	-11.956908000	-0.756746000	-0.040302000
6	-10.001874000	-1.362906000	0.086182000
7	-9.506489000	-0.128503000	-0.015443000
1	-10.141645000	0.652845000	-0.104579000
7	-9.193070000	-2.404374000	0.183328000
1	-9.550513000	-3.334154000	0.324239000
1	-8.191007000	-2.185080000	0.209089000
6	-8.077789000	0.272569000	0.012636000
8	-7.267578000	-0.659911000	0.129563000
8	-7.932585000	1.482696000	-0.087286000
$(G\text{-}CO_2)_6$			

8	-1.321199000	-0.886614000	-0.015991000
8	-2.161642000	1.201253000	-0.029209000
7	-3.992969000	-1.781548000	0.147424000
1	-3.025906000	-1.434468000	0.087622000
1	-4.144543000	-2.774902000	0.120093000
6	-5.041691000	-0.954476000	0.058547000
7	-6.282522000	-1.481547000	0.054722000
1	-6.381394000	-2.483013000	0.130549000
7	-4.857791000	0.347347000	-0.012779000
1	-3.907736000	0.732910000	-0.018773000
1	-5.704728000	0.910383000	-0.062031000
6	-7.567305000	-0.779887000	-0.009147000
8	-8.528172000	-1.545041000	0.016024000
8	-7.509197000	0.461443000	-0.079870000
7	-10.147280000	1.549802000	-0.417442000
1	-9.223842000	1.122206000	-0.296907000
1	-10.193602000	2.552725000	-0.360112000
6	-11.267657000	0.850107000	-0.138609000
7	-12.441622000	1.484021000	-0.078608000
1	-12.463458000	2.473687000	-0.274201000
7	-11.195297000	-0.455587000	0.044683000
1	-10.290726000	-0.927572000	0.035779000
1	-12.092533000	-0.909551000	0.230080000
6	-13.824742000	0.889799000	0.168868000
8	-13.816191000	-0.327217000	0.372803000
8	-14.684000000	1.752375000	0.117425000
7	14.296531000	2.058514000	0.075603000
1	14.642631000	3.003606000	0.055203000
1	14.963854000	1.316170000	-0.054051000
6	12.976595000	1.807365000	0.075590000
7	12.554017000	0.545475000	-0.021894000
1	13.233954000	-0.197212000	-0.111731000
7	12.108454000	2.799566000	0.175786000
1	12.411145000	3.749700000	0.309175000
1	11.121121000	2.523100000	0.204354000
6	11.153137000	0.060786000	0.012410000
8	10.287788000	0.942643000	0.129190000
8	11.079704000	-1.156571000	-0.083090000
7	8.483950000	-2.304415000	-0.010079000
1	9.440177000	-1.936134000	-0.032630000
1	8.344109000	-3.297534000	-0.082570000
6	7.434246000	-1.478392000	-0.014625000
7	6.193684000	-2.003686000	-0.054094000
1	6.094721000	-3.008169000	-0.081873000
7	7.612019000	-0.172193000	0.023819000
1	8.548103000	0.232631000	0.066505000
1	6.761518000	0.388507000	0.031728000
6	4.914526000	-1.300784000	-0.047783000
8	4.968695000	-0.056233000	-0.004797000
8	3.949741000	-2.060901000	-0.087661000
$(G\text{-}CO_2)_7$			

SCF E = -2363.77541743 a.u.			
7	5.475330000	1.070099000	-0.040671000
1	6.409616000	0.636947000	-0.023851000
1	5.412290000	2.071210000	0.025981000
6	4.358842000	0.335804000	-0.030677000
7	3.168535000	0.975095000	-0.000168000
1	3.163932000	1.984367000	0.007183000
7	4.423850000	-0.977935000	-0.056094000
1	5.337125000	-1.446044000	-0.075547000
1	3.533669000	-1.469474000	-0.056719000
6	1.834119000	0.397440000	0.000994000
8	1.767359000	-0.847054000	-0.021471000
8	0.941514000	1.245328000	0.025207000
7	-0.889658000	-1.740021000	0.062971000
1	0.082445000	-1.396683000	0.033651000
1	-1.048197000	-2.731644000	0.015864000
6	-1.929929000	-0.902574000	0.020945000
7	-3.176918000	-1.423859000	0.000813000
1	-3.279146000	-2.427513000	0.028648000
7	-1.738041000	0.399089000	0.006961000
1	-0.783228000	0.778676000	0.015283000
1	-2.577362000	0.972755000	-0.013884000
6	-4.449901000	-0.719791000	-0.026883000
8	-5.420210000	-1.477594000	-0.030675000
8	-4.395002000	0.525418000	-0.043499000
7	-6.960635000	1.663162000	-0.210637000
1	-6.029238000	1.226690000	-0.150441000
1	-7.018664000	2.666168000	-0.176766000
6	-8.081178000	0.938256000	-0.110895000
7	-9.267359000	1.580201000	-0.099301000
1	-9.271319000	2.586279000	-0.177500000
7	-8.019700000	-0.374786000	-0.037885000
1	-7.109036000	-0.847592000	-0.035607000
1	-8.914777000	-0.856165000	0.020263000
6	-10.611185000	1.004501000	-0.019378000
8	-10.671569000	-0.236580000	0.055112000
8	-11.495888000	1.857414000	-0.036882000
7	17.403024000	1.986427000	0.089370000
1	17.758143000	2.928371000	0.082790000
1	18.064335000	1.239089000	-0.042455000
6	16.081126000	1.747221000	0.085631000
7	15.647480000	0.489886000	-0.023948000
1	16.321028000	-0.257891000	-0.119648000
7	15.221576000	2.746050000	0.193666000
1	15.532407000	3.692616000	0.333642000
1	14.231762000	2.478517000	0.216947000
6	14.242921000	0.017498000	0.001383000
8	13.384336000	0.905309000	0.124152000
8	14.158851000	-1.198329000	-0.106153000
7	11.558107000	-2.327023000	-0.056759000
1	12.517310000	-1.965323000	-0.072155000
1	11.411002000	-3.318304000	-0.139491000

SCF E = -2757.75070394 a. u.			
7	-8.408807000	1.005059000	-0.399152000
1	-9.360504000	0.645405000	-0.236381000
1	-8.305489000	1.943584000	-0.744359000
6	-7.329542000	0.231083000	-0.254794000
7	-6.116584000	0.760901000	-0.530327000
1	-6.068584000	1.723805000	-0.829000000
7	-7.450524000	-1.014739000	0.150055000
1	-8.379812000	-1.398524000	0.358322000
1	-6.585157000	-1.539515000	0.247318000
6	-4.812487000	0.128865000	-0.428676000
8	-4.797412000	-1.059810000	-0.053008000
8	-3.886217000	0.879804000	-0.737509000
7	-2.202055000	-2.105695000	-0.022263000
1	-3.155165000	-1.709782000	-0.042302000
1	-2.085823000	-3.054747000	0.288658000
6	-1.125243000	-1.342373000	-0.226733000
7	0.097909000	-1.907057000	-0.101661000
1	0.152921000	-2.886481000	0.135520000
7	-1.257887000	-0.074426000	-0.550672000
1	-2.195381000	0.338963000	-0.639798000
1	-0.394814000	0.440310000	-0.703472000
6	1.398864000	-1.289329000	-0.285053000
8	2.335928000	-2.068139000	-0.102699000
8	1.403059000	-0.081173000	-0.594332000
7	3.991466000	0.953195000	-0.733713000
1	3.039377000	0.556589000	-0.683208000
1	4.094215000	1.928349000	-0.955319000
6	5.077748000	0.186672000	-0.608124000
7	6.293227000	0.765341000	-0.734913000
1	6.336827000	1.757892000	-0.912418000
7	4.961224000	-1.101121000	-0.363506000
1	4.029471000	-1.523001000	-0.260136000
1	5.832071000	-1.616783000	-0.266555000
6	7.604431000	0.150018000	-0.610378000
8	7.624913000	-1.074194000	-0.375234000
8	8.528673000	0.949829000	-0.760434000
7	-20.254325000	2.614424000	-0.078752000
1	-20.568239000	3.534708000	-0.339401000
1	-20.935319000	1.983109000	0.309715000
6	-18.947928000	2.302207000	-0.085793000
7	-18.561672000	1.108568000	0.369532000
1	-19.257401000	0.467674000	0.726169000
7	-18.057106000	3.165985000	-0.542297000
1	-18.336293000	4.048298000	-0.936968000
1	-17.084430000	2.840880000	-0.543712000
6	-17.185176000	0.561074000	0.402483000
8	-16.300709000	1.315421000	-0.032509000
8	-17.145505000	-0.571182000	0.864590000
7	-14.612642000	-1.835687000	0.990709000
1	-15.550345000	-1.422025000	0.958421000

6	10.514736000	-1.493890000	-0.039366000
7	9.269942000	-2.010461000	-0.079772000
1	9.164561000	-3.013680000	-0.124511000
7	10.701733000	-0.189872000	0.020622000
1	11.641138000	0.207967000	0.061948000
1	9.855912000	0.377088000	0.041960000
6	7.996542000	-1.300530000	-0.055224000
8	8.057440000	-0.056930000	0.007397000
8	7.025952000	-2.053578000	-0.101797000
7	-13.392102000	-1.065834000	0.443770000
1	-12.434219000	-0.729361000	0.302361000
1	-13.536019000	-2.059944000	0.396222000
6	-14.446015000	-0.262538000	0.187683000
7	-15.676978000	-0.780668000	0.159818000
1	-15.789223000	-1.762180000	0.365309000
7	-14.252617000	1.029233000	-0.006102000
1	-13.306497000	1.411702000	-0.019897000
1	-15.106058000	1.567322000	-0.171422000
6	-17.002027000	-0.056429000	-0.051349000
8	-16.882213000	1.153050000	-0.265458000
8	-17.939441000	-0.830864000	0.032577000
1	-14.503133000	-2.762875000	1.364214000
6	-13.538129000	-1.115667000	0.659408000
7	-12.318038000	-1.678419000	0.775208000
1	-12.254718000	-2.629575000	1.108150000
7	-13.671196000	0.121244000	0.222105000
1	-14.592174000	0.551458000	0.125177000
1	-12.805567000	0.599699000	-0.020745000
6	-11.020784000	-1.093611000	0.459809000
8	-11.030462000	0.078199000	0.034160000
8	-10.083742000	-1.862408000	0.666314000
7	10.268488000	-2.028567000	-0.305779000
1	9.308275000	-1.654975000	-0.341078000
1	10.387154000	-3.002235000	-0.085349000
6	11.333071000	-1.217406000	-0.270768000
7	12.554300000	-1.763656000	-0.089994000
1	12.623563000	-2.765955000	0.002332000
7	11.185656000	0.080906000	-0.423152000
1	10.248408000	0.477375000	-0.558221000
1	12.042471000	0.630333000	-0.406573000
6	13.850034000	-1.086923000	-0.044987000
8	13.829465000	0.147143000	-0.182063000
8	14.788705000	-1.867041000	0.127012000
7	17.340522000	-0.613495000	0.167146000
1	16.420267000	-1.068141000	0.134696000
1	18.132438000	-1.194448000	0.383135000
6	17.428755000	0.703155000	0.445589000
7	18.617046000	1.240023000	0.737139000
1	19.429826000	0.642292000	0.722040000
7	16.342281000	1.453953000	0.406136000
1	15.434916000	1.045346000	0.179837000
1	16.504836000	2.446226000	0.592320000
6	18.952359000	2.701530000	1.007961000
8	17.972249000	3.451832000	0.990719000
8	20.148114000	2.847196000	1.194542000

$(G\text{-}CO_2)_8$

SCF E = -3151.72598607 a.u.

7	-5.755295000	-0.349533000	0.075222000
1	-6.673794000	-0.822736000	0.095225000
1	-5.733898000	0.651387000	-0.016131000
6	-4.611655000	-1.037858000	0.064630000
7	-3.448052000	-0.350442000	-0.011319000
1	-3.487871000	0.657130000	-0.052212000
7	-4.621858000	-2.351433000	0.131888000
1	-5.516740000	-2.856192000	0.186716000
1	-3.713775000	-2.807372000	0.127879000
6	-2.093684000	-0.868202000	-0.024964000
8	-1.967936000	-2.107473000	0.034183000
8	-1.237527000	0.016049000	-0.095540000
7	0.708331000	-2.891008000	-0.062786000
1	-0.279434000	-2.589343000	-0.029026000

$(G\text{-}CO_2)_9$

SCF E = -3545.70135987 a.u.

7	-2.912105000	-1.547241000	-0.421332000
1	-3.784908000	-2.079928000	-0.263524000
1	-2.975864000	-0.553588000	-0.560611000
6	-1.712745000	-2.121216000	-0.307552000
7	-0.612094000	-1.348293000	-0.467180000
1	-0.740273000	-0.369856000	-0.678522000
7	-1.608870000	-3.407586000	-0.054089000
1	-2.457386000	-3.976847000	0.074249000
1	-0.664666000	-3.776845000	0.010835000
6	0.781353000	-1.739479000	-0.402779000
8	1.015676000	-2.939838000	-0.157948000
8	1.558515000	-0.803339000	-0.604301000
7	3.745807000	-3.492103000	-0.130327000
1	2.734575000	-3.277009000	-0.146480000

1	0.912404000	-3.873115000	0.004471000	1	4.033008000	-4.427570000	0.100310000
6	1.709029000	-2.007724000	-0.086104000	6	4.665459000	-2.534536000	-0.269102000
7	2.980186000	-2.473627000	-0.082848000	7	5.972146000	-2.878025000	-0.177272000
1	3.125513000	-3.472190000	-0.069154000	1	6.203353000	-3.847916000	-0.021483000
7	1.459167000	-0.716777000	-0.117265000	7	4.304683000	-1.290646000	-0.497494000
1	0.486277000	-0.380379000	-0.113418000	1	3.305727000	-1.045644000	-0.551614000
1	2.270270000	-0.105025000	-0.142000000	1	5.059186000	-0.617691000	-0.598773000
6	4.217186000	-1.716668000	-0.115861000	6	7.138697000	-2.026104000	-0.303242000
8	5.223353000	-2.428354000	-0.108270000	8	8.202680000	-2.637111000	-0.184006000
8	4.110217000	-0.474277000	-0.146394000	8	6.925790000	-0.814577000	-0.510358000
7	6.587248000	0.799865000	-0.095108000	7	9.282976000	0.637768000	-0.807266000
1	5.674991000	0.315003000	-0.112196000	1	8.415333000	0.086774000	-0.698533000
1	6.596839000	1.804110000	-0.141082000	1	9.205409000	1.631697000	-0.937225000
6	7.738069000	0.126404000	-0.168992000	6	10.485706000	0.092049000	-0.609701000
7	8.893489000	0.827866000	-0.214048000	7	11.576097000	0.888176000	-0.692774000
1	8.845346000	1.835292000	-0.177932000	1	11.442474000	1.864031000	-0.912734000
7	7.741284000	-1.189303000	-0.189556000	7	10.601243000	-1.192771000	-0.350567000
1	6.853091000	-1.707039000	-0.160030000	1	9.760505000	-1.781341000	-0.278627000
1	8.655240000	-1.632117000	-0.233969000	1	11.548471000	-1.537791000	-0.220137000
6	10.255213000	0.323847000	-0.274176000	6	12.973702000	0.526350000	-0.529914000
8	10.390095000	-0.915366000	-0.300837000	8	13.213251000	-0.668982000	-0.268114000
8	11.100690000	1.219280000	-0.291579000	8	13.739709000	1.479543000	-0.677893000
7	-17.649266000	0.034036000	0.201341000	7	-14.750487000	-2.076993000	0.483230000
1	-18.082879000	0.959008000	0.135368000	1	-15.265117000	-1.190698000	0.373684000
1	-18.246360000	-0.759839000	0.356734000	1	-15.259102000	-2.889113000	0.787551000
6	-16.322315000	-0.128966000	0.153917000	6	-13.421329000	-2.135005000	0.364162000
7	-15.821968000	-1.375285000	0.281534000	7	-12.807183000	-3.320912000	0.582626000
1	-16.463953000	-2.144506000	0.405453000	1	-13.375840000	-4.120619000	0.818507000
7	-15.527988000	0.906533000	-0.016101000	7	-12.732645000	-1.063881000	0.035998000
1	-15.920788000	1.844422000	-0.116047000	1	-13.215502000	-0.170883000	-0.121861000
1	-14.530789000	0.704121000	-0.050934000	1	-11.726766000	-1.185619000	-0.047824000
6	-14.424947000	-1.789192000	0.249127000	6	-11.391790000	-3.627102000	0.497051000
8	-13.584149000	-0.886972000	0.088966000	8	-10.633966000	-2.688061000	0.193314000
8	-14.281797000	-3.005169000	0.389300000	8	-11.136964000	-4.809746000	0.745675000
7	-11.673999000	-3.966418000	0.320601000	7	-8.480824000	-5.549428000	0.598463000
1	-12.653120000	-3.638826000	0.343763000	1	-9.483834000	-5.296383000	0.651017000
1	-11.485041000	-4.946299000	0.443311000	1	-8.204698000	-6.492114000	0.813038000
6	-10.664664000	-3.097106000	0.257672000	6	-7.550564000	-4.615024000	0.402006000
7	-9.397680000	-3.570293000	0.292639000	7	-6.247545000	-4.984409000	0.416107000
1	-9.259585000	-4.567874000	0.360783000	1	-6.027236000	-5.957716000	0.566942000
7	-10.901054000	-1.805210000	0.157987000	7	-7.896115000	-3.362108000	0.191819000
1	-11.862934000	-1.448090000	0.128029000	1	-8.886764000	-3.086506000	0.182266000
1	-10.081395000	-1.206127000	0.102924000	1	-7.132893000	-2.708783000	0.038760000
6	-8.154870000	-2.824853000	0.221195000	6	-5.074789000	-4.158777000	0.212155000
8	-8.252467000	-1.584828000	0.122743000	8	-5.273978000	-2.943885000	0.007499000
8	-7.154401000	-3.541903000	0.269946000	8	-4.017479000	-4.789852000	0.271884000
7	13.102823000	-1.615768000	-0.514113000	7	15.980265000	-1.121332000	-0.114916000
1	12.114501000	-1.331908000	-0.437463000	1	14.968888000	-0.929715000	-0.178260000
1	13.315959000	-2.597788000	-0.487697000	1	16.270015000	-2.049706000	0.139505000
6	14.098444000	-0.727084000	-0.412331000	6	16.882540000	-0.132720000	-0.117844000
7	15.370334000	-1.180352000	-0.417079000	7	18.181060000	-0.444385000	0.082234000
1	15.526427000	-2.172635000	-0.511479000	1	18.427435000	-1.413688000	0.214998000
7	13.836207000	0.558872000	-0.321788000	7	16.506536000	1.110957000	-0.323854000

1	12.862063000	0.882916000	-0.310591000
1	14.644916000	1.174651000	-0.267170000
6	16.607207000	-0.403549000	-0.348399000
8	16.477422000	0.828473000	-0.261652000
8	17.616343000	-1.110366000	-0.388630000
7	20.051372000	0.356055000	-0.366426000
1	19.171666000	-0.173447000	-0.387732000
1	20.906269000	-0.172430000	-0.334528000
6	20.067070000	1.614240000	0.118365000
7	21.234984000	2.209498000	0.377460000
1	22.085156000	1.701532000	0.184421000
7	18.927550000	2.254148000	0.312686000
1	18.035599000	1.802870000	0.106785000
1	19.031679000	3.215758000	0.644284000
6	21.483515000	3.635431000	0.853357000
8	20.452249000	4.282317000	1.057791000
8	22.677716000	3.863290000	0.942976000
7	-20.134710000	6.577502000	-0.364721000
1	-21.085271000	6.907238000	-0.397250000
1	-19.403747000	7.245671000	-0.545315000
6	-19.860775000	5.267691000	-0.251125000
7	-18.592733000	4.858933000	-0.319865000
1	-17.862026000	5.540485000	-0.474191000
7	-20.837261000	4.394140000	-0.069924000
1	-21.792128000	4.690636000	0.041229000
1	-20.543255000	3.418047000	0.039777000
6	-18.080885000	3.475929000	-0.171253000
8	-18.945742000	2.604285000	0.023836000
8	-16.864671000	3.416887000	-0.267942000

1	15.513282000	1.328390000	-0.467386000
1	17.250909000	1.805048000	-0.331612000
6	19.335237000	0.452883000	0.093626000
8	19.096664000	1.657156000	-0.093448000
8	20.397433000	-0.140425000	0.292539000
7	22.688165000	1.537423000	0.224726000
1	21.860781000	0.928775000	0.234565000
1	23.572316000	1.115050000	0.450844000
6	22.549602000	2.862506000	0.432969000
7	23.630483000	3.611888000	0.669150000
1	24.534411000	3.163557000	0.665485000
7	21.348586000	3.410638000	0.380197000
1	20.523200000	2.839240000	0.195823000
1	21.338351000	4.424709000	0.510902000
6	23.710889000	5.121706000	0.855319000
8	22.615493000	5.689833000	0.821549000
8	24.865801000	5.481654000	1.006365000
7	-17.765741000	4.125460000	-0.483050000
1	-18.739407000	4.427460000	-0.388727000
1	-17.076147000	4.815758000	-0.725993000
6	-17.389017000	2.866445000	-0.234771000
7	-16.084541000	2.548521000	-0.359358000
1	-15.435729000	3.268301000	-0.643007000
7	-18.276598000	1.960620000	0.119171000
1	-19.260555000	2.216485000	0.219018000
1	-17.915065000	1.024299000	0.289269000
6	-15.447434000	1.255192000	-0.144746000
8	-16.195192000	0.320490000	0.202039000
8	-14.233997000	1.279261000	-0.343152000
7	-24.567820000	5.697024000	0.230800000
1	-25.033243000	6.587841000	0.173956000
1	-25.111459000	4.906696000	0.536035000
6	-23.237089000	5.601602000	0.076170000
7	-22.642041000	4.422810000	0.267541000
1	-23.201312000	3.626553000	0.542050000
7	-22.526657000	6.663310000	-0.265973000
1	-22.965903000	7.545916000	-0.466473000
1	-21.522393000	6.501607000	-0.394659000
6	-21.204824000	4.100385000	0.102894000
8	-20.480457000	5.051685000	-0.237657000
8	-20.960809000	2.926081000	0.334511000

Cartesian coordinates of cyclic structures of $(G\text{-}CO_2)_n$ complexes.

$(G\text{-}CO_2)_2$

SCF E = -787.915203086 a.u.

7	2.318321000	-2.036369000	0.205439000
1	2.992737000	-2.663081000	0.608451000
1	1.403706000	-2.382587000	-0.090175000
6	2.536563000	-0.716214000	0.172689000
7	1.642476000	0.043842000	-0.456434000
1	0.861527000	-0.492033000	-0.844886000
7	3.624757000	-0.174058000	0.719073000
1	4.185451000	-0.706233000	1.362064000
1	3.628744000	0.850411000	0.724390000
6	1.472005000	1.505395000	-0.306934000
8	2.408601000	2.113756000	0.199692000
8	0.361673000	1.880602000	-0.726057000
7	-2.318300000	2.036348000	0.204775000
1	-2.992582000	2.663008000	0.608096000
1	-1.403498000	2.382467000	-0.090406000
6	-2.536597000	0.716208000	0.171888000
7	-1.642483000	-0.043830000	-0.457231000
1	-0.861456000	0.492039000	-0.845516000
7	-3.624852000	0.174029000	0.718121000
1	-4.185610000	0.706157000	1.361093000
1	-3.628873000	-0.850438000	0.723336000
6	-1.471977000	-1.505376000	-0.307627000
8	-2.408750000	-2.113789000	0.198605000
8	-0.361466000	-1.880511000	-0.726333000

$(G\text{-}CO_2)_3$

SCF E = -1181.89142049 a.u.

7	4.130557000	0.772942000	-0.471425000
1	4.912711000	0.878518000	-1.096567000
1	3.555791000	1.611934000	-0.293378000
6	3.580862000	-0.437715000	-0.330298000
7	2.532865000	-0.574501000	0.482755000
1	2.204710000	0.258868000	0.989785000
7	4.098502000	-1.506175000	-0.941791000
1	4.759842000	-1.382088000	-1.688990000
1	3.531645000	-2.354925000	-0.874147000
6	1.643980000	-1.721872000	0.584687000
8	1.876068000	-2.696259000	-0.159580000
8	0.727882000	-1.550514000	1.391916000
7	-0.950474000	-2.764046000	-0.904086000
1	-0.091876000	-3.062405000	-0.436018000
1	-0.837078000	-2.517049000	-1.873922000
6	-1.914763000	-2.150304000	-0.203412000
7	-2.910567000	-1.521224000	-0.863602000
1	-2.867261000	-1.535118000	-1.873290000
7	-1.906799000	-2.205266000	1.117519000
1	-0.981476000	-2.277083000	1.545746000
1	-2.628068000	-1.645904000	1.567124000
6	-3.585342000	-0.305945000	-0.353234000
8	-3.912110000	0.470176000	-1.250627000
8	-3.668876000	-0.208001000	0.880378000
7	-2.298965000	2.744613000	-0.609629000
1	-3.093075000	2.100334000	-0.696138000
1	-2.164078000	3.370339000	-1.387097000
6	-1.214799000	2.339658000	0.071936000
7	-0.023307000	2.919734000	-0.194041000
1	0.035128000	3.519323000	-1.004470000
7	-1.324256000	1.404666000	0.992290000
1	-2.229713000	0.972274000	1.180661000
1	-0.472350000	1.128159000	1.480194000
6	1.282759000	2.467768000	0.283164000
8	2.222537000	2.844179000	-0.422935000
8	1.276509000	1.751681000	1.296789000

$(G\text{-}CO_2)_4$

SCF E = -1575.88150241 a.u.

7	-1.284800000	-3.201277000	1.030928000
1	-2.133477000	-2.642972000	1.194899000
1	-0.417948000	-3.026482000	1.533415000
6	-1.168825000	-3.911003000	-0.070501000
7	0.027193000	-4.432111000	-0.437733000
1	0.068438000	-4.948566000	-1.304350000
7	-2.241748000	-4.158156000	-0.831780000
1	-3.101802000	-3.606660000	-0.692302000

$(G\text{-}CO_2)_5$

SCF E = -1969.86686571 a.u.

7	-3.701244000	-2.235298000	0.896281000
1	-4.034998000	-1.269087000	1.029316000
1	-2.852684000	-2.587961000	1.330800000
6	-4.210189000	-2.984439000	-0.056502000
7	-3.652465000	-4.178882000	-0.376556000
1	-4.068773000	-4.711280000	-1.126263000
7	-5.308948000	-2.593152000	-0.709919000
1	-5.656045000	-1.625157000	-0.603083000

1	-2.103952000	-4.554294000	-1.746728000
6	1.338125000	-3.999501000	0.028182000
8	1.361375000	-3.358901000	1.095827000
8	2.260261000	-4.316761000	-0.727415000
7	3.201709000	-1.284739000	1.030745000
1	2.643425000	-2.133413000	1.194810000
1	3.027069000	-0.417905000	1.533320000
6	3.911302000	-1.168786000	-0.070771000
7	4.432347000	0.027247000	-0.437983000
1	4.948720000	0.068610000	-1.304644000
7	4.158330000	-2.241698000	-0.832108000
1	3.606772000	-3.101705000	-0.692589000
1	4.554360000	-2.103895000	-1.747101000
6	3.999646000	1.338059000	0.028142000
8	4.317062000	2.260384000	-0.727160000
8	3.358677000	1.360954000	1.095574000
7	1.284511000	3.201304000	1.030639000
1	2.133145000	2.642964000	1.194739000
1	0.417563000	3.026512000	1.532956000
6	1.168774000	3.911084000	-0.070781000
7	-0.027202000	4.432180000	-0.438076000
1	-0.068491000	4.948668000	-1.304672000
7	2.241815000	4.158250000	-0.831892000
1	3.101838000	3.606743000	-0.692282000
1	2.104171000	4.554414000	-1.746850000
6	-1.338027000	3.999449000	0.027963000
8	-1.360949000	3.358631000	1.095481000
8	-2.260333000	4.316860000	-0.727365000
7	-4.158392000	2.241792000	-0.831984000
1	-3.606812000	3.101782000	-0.692455000
1	-4.554617000	2.104122000	-1.746913000
6	-3.911228000	1.168771000	-0.070841000
7	-4.432407000	-0.027197000	-0.438065000
1	-4.948910000	-0.068486000	-1.304651000
7	-3.201367000	1.284525000	1.030524000
1	-2.643001000	2.133148000	1.194590000
1	-3.026574000	0.417584000	1.532857000
6	-3.999774000	-1.338041000	0.028018000
8	-3.359011000	-1.360987000	1.095568000
8	-4.317059000	-2.260328000	-0.727385000

1	-5.598143000	-3.101730000	-1.528453000
6	-2.347030000	-4.672165000	0.020876000
8	-1.779795000	-4.060006000	0.946129000
8	-1.963770000	-5.645373000	-0.635389000
7	0.983208000	-4.210669000	0.894354000
1	-0.038900000	-4.228930000	1.027870000
1	1.581647000	-3.513346000	1.329150000
6	1.537743000	-4.925804000	-0.059137000
7	2.845975000	-4.764693000	-0.379590000
1	3.223264000	-5.324766000	-1.129782000
7	0.825643000	-5.849129000	-0.713134000
1	-0.202076000	-5.879965000	-0.605803000
1	1.219465000	-6.280186000	-1.532484000
6	3.718903000	-3.676408000	0.019207000
8	4.763049000	-3.611939000	-0.636780000
8	3.311940000	-2.948900000	0.945279000
7	4.308157000	-0.367225000	0.896216000
1	4.009955000	-1.345097000	1.028796000
1	3.829148000	0.416854000	1.331023000
6	5.160497000	-0.059955000	-0.056232000
7	5.412017000	1.234302000	-0.375353000
1	6.061887000	1.420427000	-1.124932000
7	5.819193000	-1.022018000	-0.710355000
1	5.530648000	-2.009112000	-0.604613000
1	6.352591000	-0.779894000	-1.528351000
6	4.645930000	2.400674000	0.022493000
8	3.826985000	2.238413000	0.947434000
8	4.907995000	3.413602000	-0.633285000
7	2.770881000	5.217876000	-0.711376000
1	3.620462000	4.638644000	-0.604200000
1	2.706072000	5.798666000	-1.530371000
6	1.651792000	4.888827000	-0.058116000
7	0.498660000	5.527286000	-0.378859000
1	0.522880000	6.202149000	-1.129071000
7	1.680034000	3.984004000	0.895047000
1	2.517791000	3.398288000	1.028718000
1	0.785976000	3.771062000	1.329331000
6	-0.847500000	5.159472000	0.018817000
8	-0.946562000	4.331710000	0.944851000
8	-1.729697000	5.720857000	-0.637939000
7	-4.106996000	4.246809000	-0.712506000
1	-3.293187000	4.875540000	-0.606382000
1	-4.680451000	4.364742000	-1.530743000
6	-4.139893000	3.081291000	-0.058456000
7	-5.104231000	2.182111000	-0.377416000
1	-5.739705000	2.413482000	-1.126745000
7	-3.269764000	2.828836000	0.893982000
1	-2.453749000	3.444663000	1.026731000
1	-3.343316000	1.913057000	1.329005000
6	-5.170251000	0.788418000	0.021157000
8	-4.412322000	0.438747000	0.946244000
8	-5.977900000	0.122686000	-0.634022000

$(G\text{-}CO_2)_6$

SCF E = -2363.84963434 a.u.

7	2.462740000	4.570494000	0.692793000
1	3.237850000	3.897033000	0.793046000
1	1.521228000	4.388392000	1.029119000
6	2.612414000	5.648862000	-0.043426000
7	1.564183000	6.473472000	-0.294717000
1	1.723401000	7.285996000	-0.871679000
7	3.810132000	5.966778000	-0.541212000
1	4.600579000	5.301840000	-0.468050000
1	3.886622000	6.723469000	-1.199359000
6	0.167413000	6.247992000	0.011862000
8	-0.093547000	5.264472000	0.731440000
8	-0.593022000	7.077365000	-0.498366000
7	-2.727895000	4.418501000	0.692558000
1	-1.756867000	4.752627000	0.791971000
1	-3.041168000	3.512527000	1.029882000
6	-3.586821000	5.086749000	-0.044331000
7	-4.825296000	4.591421000	-0.294783000
1	-5.449185000	5.134946000	-0.872515000
7	-3.262904000	6.282223000	-0.543634000
1	-2.291724000	6.634071000	-0.470944000
1	-3.879960000	6.726347000	-1.202097000
6	-5.328693000	3.269470000	0.013187000
8	-4.607696000	2.552349000	0.733658000
8	-6.427128000	3.025242000	-0.496983000
7	3.262655000	-6.281838000	-0.543878000
1	2.291512000	-6.633760000	-0.471010000
1	3.879556000	-6.725769000	-1.202617000
6	3.586770000	-5.086597000	-0.044158000
7	4.825259000	-4.591301000	-0.294596000
1	5.449044000	-5.134708000	-0.872552000
7	2.728025000	-4.418536000	0.693117000
1	1.756905000	-4.752464000	0.792256000
1	3.041421000	-3.512686000	1.030660000
6	5.328730000	-3.269435000	0.013610000
8	4.607863000	-2.552479000	0.734373000
8	6.427075000	-3.025095000	-0.496705000
7	7.074262000	-0.315615000	-0.539663000
1	6.893138000	-1.332635000	-0.467772000
1	7.768401000	-0.003079000	-1.196987000
6	6.199803000	0.562394000	-0.041858000
7	6.389966000	1.882661000	-0.292161000
1	7.173365000	2.151485000	-0.868744000
7	5.190611000	0.152398000	0.693490000
1	4.995115000	-0.855651000	0.793505000
1	4.561932000	0.876532000	1.029834000
6	5.496069000	2.979322000	0.014610000
8	4.513604000	2.713138000	0.733704000
8	5.834181000	4.052853000	-0.494982000

$(G\text{-}CO_2)_7$

SCF E = -2757.83062274 a.u.

7	4.565280000	3.999654000	0.359911000
1	5.049542000	3.090622000	0.417498000
1	3.570625000	4.115349000	0.531150000
6	5.217501000	5.077664000	-0.014647000
7	4.579263000	6.267815000	-0.152193000
1	5.118866000	7.070234000	-0.440534000
7	6.528469000	5.025112000	-0.255298000
1	7.036568000	4.121324000	-0.228397000
1	7.001217000	5.833750000	-0.620810000
6	3.169199000	6.546012000	0.004531000
8	2.450158000	5.599348000	0.377975000
8	2.862620000	7.713655000	-0.261478000
7	-0.285104000	6.059226000	0.350081000
1	0.727358000	5.868458000	0.403037000
1	-0.996853000	5.355935000	0.525815000
6	-0.719702000	7.240321000	-0.029331000
7	-2.047986000	7.485435000	-0.164926000
1	-2.337737000	8.406833000	-0.456915000
7	0.140202000	8.229399000	-0.277219000
1	1.163487000	8.063060000	-0.246420000
1	-0.196213000	9.102821000	-0.644514000
6	-3.145893000	6.558886000	-0.002656000
8	-4.249654000	7.047762000	-0.268743000
8	-2.855200000	5.407648000	0.375303000
7	-4.922247000	3.558746000	0.357922000
1	-4.141300000	4.231033000	0.407989000
1	-4.816561000	2.564235000	0.536484000
6	-6.115945000	3.954389000	-0.024537000
7	-7.135547000	3.068404000	-0.159218000
1	-8.036759000	3.415772000	-0.451373000
7	-6.352860000	5.242859000	-0.275784000
1	-5.584265000	5.938620000	-0.247652000
1	-7.243432000	5.522557000	-0.649462000
6	-7.095331000	1.632668000	0.005910000
8	-6.014127000	1.143424000	0.385844000
8	-8.165186000	1.073512000	-0.260191000
7	3.442150000	-7.469135000	-0.304562000
1	2.449513000	-7.766448000	-0.262327000
1	4.127499000	-8.115996000	-0.654801000
6	3.791427000	-6.209451000	-0.040460000
7	5.095866000	-5.856316000	-0.169591000
1	5.753585000	-6.557043000	-0.477118000
7	2.889024000	-5.335118000	0.345713000
1	1.893637000	-5.601386000	0.396601000
1	3.227072000	-4.395078000	0.530360000
6	5.684683000	-4.546863000	0.000566000
8	4.925757000	-3.638517000	0.389791000
8	6.889983000	-4.507016000	-0.271179000

7	-5.190857000	-0.152451000	0.693850000
1	-4.995183000	0.855590000	0.793582000
1	-4.562409000	-0.876606000	1.030580000
6	-6.199643000	-0.562427000	-0.042071000
7	-6.389785000	-1.882702000	-0.292349000
1	-7.172930000	-2.151518000	-0.869282000
7	-7.073710000	0.315610000	-0.540501000
1	-6.892741000	1.332641000	-0.468377000
1	-7.767512000	0.003080000	-1.198184000
6	-5.496040000	-2.979374000	0.014824000
8	-4.513866000	-2.713197000	0.734315000
8	-5.833963000	-4.052908000	-0.494891000
7	-3.810348000	-5.967268000	-0.540390000
1	-4.600717000	-5.302205000	-0.467534000
1	-3.886938000	-6.724281000	-1.198156000
6	-2.612520000	-5.649013000	-0.043077000
7	-1.564277000	-6.473637000	-0.294267000
1	-1.723540000	-7.286387000	-0.870898000
7	-2.462732000	-4.570277000	0.692574000
1	-3.237937000	-3.896950000	0.793008000
1	-1.521161000	-4.387977000	1.028630000
6	-0.167477000	-6.247978000	0.012033000
8	0.093530000	-5.264138000	0.731155000
8	0.592928000	-7.077505000	-0.497988000

7	8.001020000	-1.968255000	-0.269979000
1	7.610877000	-2.928862000	-0.243580000
1	8.923958000	-1.832628000	-0.645188000
6	7.228558000	-0.911052000	-0.015027000
7	7.761395000	0.330131000	-0.150067000
1	8.722339000	0.409076000	-0.447641000
7	5.982851000	-1.074022000	0.371585000
1	5.572210000	-2.019019000	0.422511000
1	5.455533000	-0.224560000	0.551594000
6	7.101212000	1.605701000	0.015625000
8	5.916239000	1.576739000	0.399731000
8	7.820659000	2.574022000	-0.254423000
7	-5.851395000	-1.625049000	0.360344000
1	-5.891964000	-0.595546000	0.413195000
1	-5.006397000	-2.161465000	0.534741000
6	-6.906275000	-2.313049000	-0.015939000
7	-6.848388000	-3.662546000	-0.151091000
1	-7.682669000	-4.151364000	-0.439593000
7	-8.063593000	-1.696418000	-0.260596000
1	-8.128919000	-0.661728000	-0.234299000
1	-8.839136000	-2.219445000	-0.629330000
6	-5.699614000	-4.525387000	0.010301000
8	-4.641742000	-3.984088000	0.385405000
8	-5.929767000	-5.710835000	-0.253763000
7	-3.700768000	-7.359392000	-0.249680000
1	-4.550219000	-6.765055000	-0.225702000
1	-3.777834000	-8.297431000	-0.603376000
6	-2.495952000	-6.837194000	-0.015009000
7	-1.405530000	-7.634863000	-0.147282000
1	-1.544822000	-8.593852000	-0.428536000
7	-2.374251000	-5.579903000	0.348467000
1	-3.204599000	-4.970006000	0.402922000
1	-1.427131000	-5.251866000	0.514182000
6	-0.013832000	-7.273336000	0.003940000
8	0.224447000	-6.105250000	0.366587000
8	0.768033000	-8.195044000	-0.255345000

$(G\text{-}CO_2)_8$

SCF E = -3151.80828765 a.u.

7	-4.148454000	-5.653200000	0.357075000
1	-3.196464000	-6.045190000	0.359624000
1	-4.346024000	-4.668797000	0.203694000
6	-5.189558000	-6.432734000	0.560944000
7	-6.449419000	-5.929937000	0.557264000
1	-7.216023000	-6.565070000	0.721927000
7	-5.027567000	-7.735071000	0.785612000
1	-4.086408000	-8.176178000	0.718034000
1	-5.834926000	-8.327710000	0.875186000
6	-6.873811000	-4.566015000	0.346969000
8	-5.985105000	-3.718724000	0.145503000
8	-8.103755000	-4.429592000	0.397806000
7	-6.939586000	-1.072132000	-0.086521000

$(G\text{-}CO_2)_9$

SCF E = -3545.78206152 a.u.

7	-7.313304000	2.118324000	-1.141561000
1	-6.865525000	2.985740000	-0.815984000
1	-6.876242000	1.204146000	-1.072732000
6	-8.482291000	2.164178000	-1.745448000
7	-9.059465000	1.040419000	-2.237282000
1	-9.963799000	1.124101000	-2.676992000
7	-9.118874000	3.324910000	-1.899729000
1	-8.798857000	4.167035000	-1.376163000
1	-10.048918000	3.325411000	-2.283084000
6	-8.581255000	-0.320741000	-2.173038000
8	-7.476336000	-0.511208000	-1.634538000
8	-9.370636000	-1.131995000	-2.676296000
7	-6.834981000	-3.243932000	-1.257244000

1	-6.545950000	-2.019306000	0.000767000	1	-7.005323000	-2.240691000	-1.409568000
1	-6.368779000	-0.234556000	-0.149980000	1	-6.023310000	-3.602028000	-0.762713000
6	-8.241738000	-0.899552000	-0.174354000	6	-7.726957000	-4.134715000	-1.638194000
7	-8.773336000	0.339663000	-0.321277000	7	-7.548892000	-5.454583000	-1.381221000
1	-9.776568000	0.421953000	-0.391354000	1	-8.269187000	-6.097230000	-1.675102000
7	-9.068425000	-1.942187000	-0.127071000	7	-8.823068000	-3.760246000	-2.293531000
1	-8.709689000	-2.900678000	0.067239000	1	-9.025736000	-2.753735000	-2.472363000
1	-10.062122000	-1.788652000	-0.137571000	1	-9.518113000	-4.446398000	-2.532557000
6	-8.088592000	1.606412000	-0.428628000	6	-6.478621000	-6.093704000	-0.653034000
8	-8.862282000	2.563008000	-0.571148000	8	-6.652072000	-7.312109000	-0.510886000
8	-6.846162000	1.588418000	-0.366419000	8	-5.540230000	-5.372836000	-0.269008000
7	-5.652606000	4.146888000	-0.366963000	7	-3.360330000	-6.881615000	0.724684000
1	-6.044666000	3.195113000	-0.368605000	1	-4.111853000	-6.289644000	0.345555000
1	-4.668186000	4.344469000	-0.213705000	1	-2.399938000	-6.567834000	0.827628000
6	-6.432820000	5.188191000	-0.567303000	6	-3.638408000	-8.079416000	1.195077000
7	-5.930316000	6.448159000	-0.559900000	7	-2.680280000	-8.842544000	1.775815000
1	-6.564991000	7.215040000	-0.725147000	1	-2.941521000	-9.755653000	2.116666000
7	-7.734923000	5.026628000	-0.792993000	7	-4.878380000	-8.562819000	1.122525000
1	-8.175812000	4.085251000	-0.724795000	1	-5.586239000	-8.088874000	0.522712000
1	-8.327934000	5.834844000	-0.871391000	1	-5.051090000	-9.511878000	1.407731000
6	-4.566650000	6.872282000	-0.347441000	6	-1.280513000	-8.542303000	1.965559000
8	-3.719122000	5.983315000	-0.148269000	8	-0.874279000	-7.439793000	1.557373000
8	-4.430532000	8.102390000	-0.394306000	8	-0.662542000	-9.460872000	2.521232000
7	9.067240000	1.944733000	-0.141817000	7	9.388069000	0.202663000	-2.808440000
1	8.708941000	2.902673000	0.055612000	1	9.362280000	-0.811520000	-2.572210000
1	10.060995000	1.792116000	-0.158609000	1	10.221561000	0.574105000	-3.231714000
6	8.241288000	0.901186000	-0.181698000	6	8.511036000	1.040751000	-2.256863000
7	8.773208000	-0.337674000	-0.330461000	7	8.707216000	2.373778000	-2.409995000
1	9.776074000	-0.418987000	-0.406662000	1	9.534775000	2.678691000	-2.900274000
7	6.939614000	1.072735000	-0.085145000	7	7.471466000	0.580505000	-1.593234000
1	6.545700000	2.019851000	0.002309000	1	7.330258000	-0.433281000	-1.485582000
1	6.369157000	0.234525000	-0.143009000	1	6.838449000	1.275185000	-1.208070000
6	8.089371000	-1.605546000	-0.430194000	6	7.932806000	3.465094000	-1.866901000
8	6.847353000	-1.588906000	-0.359193000	8	6.896473000	3.172659000	-1.243800000
8	8.863581000	-2.561239000	-0.575923000	8	8.429357000	4.574755000	-2.104224000
7	7.738420000	-5.028123000	-0.771869000	7	7.365046000	6.636109000	-0.688816000
1	8.178308000	-4.085712000	-0.712712000	1	7.786777000	5.855949000	-1.235240000
1	8.331274000	-5.836257000	-0.852077000	1	7.837050000	7.523998000	-0.671712000
6	6.434706000	-5.188863000	-0.555544000	6	6.108842000	6.555100000	-0.253363000
7	5.932135000	-6.448829000	-0.548539000	7	5.543707000	7.658415000	0.296154000
1	6.568025000	-7.216127000	-0.707030000	1	6.103463000	8.495149000	0.365109000
7	5.653255000	-4.147038000	-0.362882000	7	5.439861000	5.424996000	-0.347591000
1	6.045462000	-3.195279000	-0.363321000	1	5.908244000	4.577285000	-0.695500000
1	4.668099000	-4.344367000	-0.214123000	1	4.494173000	5.428620000	0.022877000
6	4.567586000	-6.872846000	-0.341508000	6	4.228418000	7.803016000	0.874142000
8	3.718735000	-5.983765000	-0.148515000	8	3.471572000	6.817048000	0.820898000
8	4.432154000	-8.103122000	-0.386067000	8	4.032329000	8.928937000	1.351763000
7	-1.072868000	6.937512000	0.088692000	7	1.948512000	-7.235823000	1.514410000
1	-2.019929000	6.543909000	-0.000057000	1	0.919843000	-7.250696000	1.539405000
1	-0.235141000	6.366803000	0.150703000	1	2.483452000	-6.514908000	1.039144000
6	-0.900550000	8.239593000	0.178730000	6	2.642706000	-8.200078000	2.081712000
7	0.338513000	8.771203000	0.326857000	7	3.997785000	-8.209652000	2.026500000
1	0.420859000	9.774414000	0.397229000	1	4.485195000	-8.982327000	2.454990000

7	-1.943314000	9.066148000	0.132682000	7	2.028509000	-9.183570000	2.736858000
1	-2.901742000	8.707686000	-0.062469000	1	0.991734000	-9.279848000	2.697911000
1	-1.789883000	10.059831000	0.145270000	1	2.570399000	-9.953414000	3.090754000
6	1.605752000	8.086838000	0.431996000	6	4.877091000	-7.290656000	1.343051000
8	1.588393000	6.844439000	0.367710000	8	4.354793000	-6.303432000	0.794972000
8	2.561969000	8.860902000	0.574929000	8	6.067626000	-7.627996000	1.400971000
7	5.027180000	7.734825000	0.789792000	7	7.746526000	-6.227491000	-0.212706000
1	4.085595000	8.175529000	0.724782000	1	7.111640000	-6.788152000	0.393737000
1	5.835162000	8.326769000	0.878524000	1	8.685506000	-6.557058000	-0.359086000
6	5.188713000	6.432504000	0.564415000	6	7.449776000	-4.960613000	-0.500363000
7	6.448662000	5.929922000	0.558360000	7	8.395353000	-4.195645000	-1.099348000
1	7.215439000	6.565268000	0.721447000	1	9.289327000	-4.617037000	-1.302868000
7	4.147418000	5.652809000	0.362193000	7	6.259683000	-4.472891000	-0.219044000
1	3.195444000	6.044668000	0.365640000	1	5.530376000	-5.086674000	0.168746000
1	4.344969000	4.668549000	0.207832000	1	6.094670000	-3.505926000	-0.482371000
6	6.873147000	4.566454000	0.345350000	6	8.305460000	-2.816951000	-1.519159000
8	5.984388000	3.718830000	0.145481000	8	7.237760000	-2.220877000	-1.290340000
8	8.103251000	4.430622000	0.392563000	8	9.342607000	-2.408877000	-2.059519000
7	1.942462000	-9.066760000	0.128749000	7	-5.299705000	8.234771000	1.532855000
1	2.901646000	-8.708054000	-0.062239000	1	-4.386618000	8.525090000	1.942400000
1	1.789023000	-10.060453000	0.139923000	1	-6.106165000	8.816301000	1.683097000
6	0.899723000	-8.240199000	0.174262000	6	-5.450112000	7.033922000	0.978356000
7	-0.339617000	-8.771946000	0.319784000	7	-6.687734000	6.665817000	0.563373000
1	-0.422012000	-9.775177000	0.389778000	1	-7.440956000	7.328839000	0.669503000
7	1.072267000	-6.938001000	0.086120000	7	-4.418336000	6.228906000	0.832188000
1	2.019414000	-6.544418000	-0.001866000	1	-3.474822000	6.546376000	1.092619000
1	0.234475000	-6.367323000	0.147514000	1	-4.602875000	5.336373000	0.383899000
6	-1.606907000	-8.087662000	0.424314000	6	-7.086435000	5.455556000	-0.115476000
8	-1.589437000	-6.845163000	0.361114000	8	-6.215462000	4.583617000	-0.284951000
8	-2.563231000	-8.861849000	0.565686000	8	-8.282014000	5.456220000	-0.439973000
				7	1.617512000	9.332165000	2.532004000
				1	2.563557000	9.173182000	2.126108000
				1	1.434484000	10.211025000	2.985928000
				6	0.590004000	8.579769000	2.138549000
				7	-0.662507000	8.961477000	2.490377000
				1	-0.769680000	9.823829000	3.003295000
				7	0.793589000	7.483809000	1.438332000
				1	1.751358000	7.188823000	1.204015000
				1	-0.032688000	6.951450000	1.182640000
				6	-1.921782000	8.342120000	2.148959000
				8	-1.877023000	7.278961000	1.504710000
				8	-2.900242000	8.983090000	2.556576000

$(G\text{-}CO_2)_{10}$

SCF E = -3939.74930800 a.u.

7	8.444617000	-0.737202000	0.767401000
1	8.212740000	0.156160000	1.223429000
1	7.768147000	-1.291815000	0.250850000
6	9.695693000	-1.141965000	0.709017000
7	10.041148000	-2.249299000	0.006373000
1	11.017339000	-2.501406000	-0.035838000
7	10.655340000	-0.459721000	1.333887000

1	10.406494000	0.301435000	1.997458000
1	11.593032000	-0.823060000	1.344186000
6	9.192944000	-3.103593000	-0.792574000
8	7.971801000	-2.861846000	-0.775542000
8	9.816633000	-3.986631000	-1.394863000
7	6.455454000	-4.971760000	-1.830147000
1	6.972716000	-4.190328000	-1.402965000
1	5.478352000	-5.169752000	-1.634351000
6	7.016558000	-5.692316000	-2.777214000
7	6.316322000	-6.647445000	-3.437147000
1	6.780544000	-7.156487000	-4.174474000
7	8.289873000	-5.483537000	-3.117565000
1	8.895229000	-4.901089000	-2.506439000
1	8.730145000	-6.104800000	-3.774798000
6	4.930300000	-7.020836000	-3.264055000
8	4.554420000	-7.890294000	-4.059650000
8	4.301197000	-6.445457000	-2.356639000
7	1.899861000	-7.736405000	-1.699269000
1	2.786172000	-7.246113000	-1.882272000
1	1.393039000	-7.674395000	-0.819886000
6	1.298049000	-8.389278000	-2.670618000
7	0.076833000	-8.944042000	-2.481863000
1	-0.356375000	-9.427060000	-3.254591000
7	1.877118000	-8.502618000	-3.868058000
1	2.878142000	-8.253321000	-3.983732000
1	1.445290000	-9.081202000	-4.568382000
6	-0.733599000	-8.918322000	-1.278378000
8	-0.263911000	-8.377525000	-0.276952000
8	-1.837360000	-9.485269000	-1.435353000
7	-8.355366000	5.534830000	-2.933373000
1	-8.915356000	4.941582000	-2.286669000
1	-8.840728000	6.224329000	-3.482288000
6	-7.046881000	5.684220000	-2.721887000
7	-6.395166000	6.677539000	-3.373624000
1	-6.933602000	7.287453000	-3.970574000
7	-6.406041000	4.870164000	-1.909743000
1	-6.904370000	4.081096000	-1.476814000
1	-5.408875000	5.030553000	-1.802827000
6	-5.004687000	7.058726000	-3.276995000
8	-4.275620000	6.373637000	-2.538493000
8	-4.731952000	8.054064000	-3.962216000
7	-2.322791000	9.206845000	-3.512644000
1	-3.231498000	8.741382000	-3.723117000
1	-2.151058000	10.123162000	-3.889687000
6	-1.485450000	8.703371000	-2.608879000
7	-0.368198000	9.408273000	-2.302915000
1	-0.242870000	10.309859000	-2.738491000
7	-1.733172000	7.543493000	-2.035676000
1	-2.614619000	7.049613000	-2.226623000
1	-1.048957000	7.219302000	-1.358524000
6	0.639764000	9.112268000	-1.311714000
8	0.573503000	8.009455000	-0.740766000
8	1.458083000	10.031676000	-1.168027000

7	-3.857953000	-8.212803000	0.077866000
1	-3.304880000	-8.496279000	-0.732331000
1	-4.508807000	-7.433499000	0.097823000
6	-3.559460000	-8.771467000	1.231085000
7	-4.133270000	-8.366445000	2.383950000
1	-3.948749000	-8.900943000	3.220292000
7	-2.706509000	-9.805411000	1.263560000
1	-2.182674000	-9.953843000	0.397575000
1	-2.231197000	-10.002781000	2.129314000
6	-5.094548000	-7.299972000	2.572570000
8	-5.384186000	-6.622804000	1.569272000
8	-5.501995000	-7.210948000	3.736178000
7	-10.512634000	0.516819000	1.607999000
1	-10.234090000	-0.263342000	2.236520000
1	-11.398926000	0.965291000	1.766725000
6	-9.592496000	1.138053000	0.869286000
7	-9.931648000	2.295777000	0.251225000
1	-10.877409000	2.632034000	0.355251000
7	-8.387680000	0.624857000	0.736649000
1	-8.187250000	-0.308531000	1.121270000
1	-7.741206000	1.138552000	0.145105000
6	-9.129614000	3.108301000	-0.634227000
8	-7.941280000	2.774419000	-0.791799000
8	-9.756384000	4.058922000	-1.120682000
7	7.740632000	5.366551000	4.082828000
1	7.112145000	6.167068000	3.862349000
1	8.551273000	5.538122000	4.653223000
6	7.692865000	4.260992000	3.339917000
7	8.671188000	3.334990000	3.495673000
1	9.424554000	3.543618000	4.133798000
7	6.707354000	4.069366000	2.488167000
1	5.975064000	4.781789000	2.366956000
1	6.728873000	3.200577000	1.962092000
6	8.866791000	2.103385000	2.766094000
8	7.978287000	1.775294000	1.959140000
8	9.926467000	1.531528000	3.054668000
7	3.073547000	9.783021000	0.998233000
1	2.429756000	9.914639000	0.189644000
1	3.594107000	10.579190000	1.325989000
6	3.520558000	8.559484000	1.283847000
7	4.572730000	8.436081000	2.128555000
1	4.984286000	9.278893000	2.500774000
7	2.934996000	7.499617000	0.766248000
1	2.085235000	7.610682000	0.197926000
1	3.315956000	6.596657000	1.032694000
6	5.238312000	7.232802000	2.571646000
8	4.812786000	6.151151000	2.129735000
8	6.176760000	7.461200000	3.347370000
7	-6.843196000	-4.301018000	2.198418000
1	-6.952295000	-3.477894000	1.613115000
6	-7.607176000	-4.360486000	3.268459000
7	-8.473661000	-3.360849000	3.565163000
1	-9.066167000	-3.468454000	4.374973000

7	-7.551362000	-5.417259000	4.079620000
1	-6.794148000	-6.119345000	3.969052000
1	-8.081718000	-5.412251000	4.934166000
6	-8.763527000	-2.171311000	2.797183000
8	-8.061367000	-1.962684000	1.790640000
8	-9.694408000	-1.503210000	3.264755000
1	-6.267523000	-5.111672000	1.933005000

Cartesian coordinates structures of $G(CO_2)_n$ complexes.

$G(CO_2)$

SCF E = -393.937166624 a.u.

7	2.715356000	-0.558597000	0.167860000
1	3.426056000	-0.020952000	-0.307762000
1	2.845915000	-1.554107000	0.073324000
6	1.411936000	-0.113930000	-0.028680000
7	0.359959000	-0.835501000	-0.099493000
1	0.577996000	-1.827508000	-0.109878000
7	1.328931000	1.261789000	-0.141416000
1	1.954696000	1.781444000	0.456592000
1	0.374361000	1.595582000	-0.119054000
6	-2.171459000	0.059694000	0.029234000
8	-1.809249000	1.160604000	0.063150000
8	-2.622201000	-1.000964000	0.001200000

$G(CO_2)_2$

SCF E = -582.521554562 a.u.

7	2.617485000	-1.152526000	-0.416644000
1	3.279350000	-0.657774000	0.165441000
1	2.829795000	-1.062146000	-1.398903000
6	1.285161000	-0.936225000	-0.093271000
7	0.295601000	-0.882613000	-0.901470000
1	0.594619000	-0.935196000	-1.870846000
7	1.076885000	-0.744893000	1.262073000
1	1.698852000	-1.254894000	1.872387000
1	0.101064000	-0.825688000	1.521761000
6	-2.298318000	-0.574372000	-0.078495000
8	-2.024786000	-0.951436000	0.982978000
8	-2.648280000	-0.198189000	-1.110186000
6	0.319936000	1.916935000	0.095025000
8	1.375484000	2.089383000	-0.343253000
8	-0.736688000	1.779979000	0.540822000

$G(CO_2)_3$

SCF E = -771.104458776 a.u.

7	-2.142772000	-1.858719000	-0.015205000
1	-2.613080000	-2.549410000	0.552435000
1	-2.124841000	-2.094626000	-0.996600000
6	-0.948000000	-1.371660000	0.500136000
7	0.049828000	-0.952893000	-0.186383000
1	-0.066419000	-1.149097000	-1.177883000
7	-0.924191000	-1.330127000	1.876887000
1	-1.802411000	-1.094085000	2.316866000
1	-0.146519000	-0.790743000	2.233516000
6	0.791280000	1.615380000	0.694333000
8	0.652261000	1.336785000	1.807263000
8	0.935604000	1.949271000	-0.402783000
6	-2.060789000	1.050235000	-0.917120000
8	-2.057943000	0.605410000	-1.983099000

$G(CO_2)_4$

SCF E = -959.688469532 a.u.

7	0.056817000	-2.631926000	-0.602352000
1	0.652577000	-3.409339000	-0.353164000
1	-0.159304000	-2.604393000	-1.588157000
6	0.406067000	-1.411341000	-0.045919000
7	0.205096000	-0.258664000	-0.572985000
1	-0.123261000	-0.340609000	-1.532629000
7	1.008345000	-1.517012000	1.189623000
1	0.685965000	-2.285572000	1.760903000
1	1.029815000	-0.635975000	1.689451000
6	0.697527000	2.086910000	0.899841000
8	0.763159000	1.482580000	1.884732000
8	0.634169000	2.742251000	-0.047799000
6	3.148935000	-0.201879000	-0.537550000

8	-2.081241000	1.506026000	0.144835000
6	2.778739000	-0.650840000	-0.579690000
8	2.609871000	-1.129521000	-1.617035000
8	3.004678000	-0.166540000	0.445648000
8	3.190761000	-1.097355000	-1.266880000
8	3.141022000	0.695053000	0.190328000
6	-2.510806000	-1.318525000	0.463099000
8	-2.867169000	-1.136034000	-0.622394000
8	-2.171386000	-1.513032000	1.548612000
6	-1.941491000	1.623460000	-0.828805000
8	-2.161065000	1.650997000	0.307346000
8	-1.751864000	1.607710000	-1.966495000

$G(CO_2)_5$

SCF E = -1148.27053303 a.u.

7	-0.505846000	-2.188229000	-0.138576000
1	-0.027863000	-2.775495000	0.532888000
1	-0.165499000	-2.334612000	-1.078582000
6	-0.610321000	-0.853984000	0.225744000
7	-0.655857000	0.148445000	-0.570529000
1	-0.485034000	-0.130160000	-1.533408000
7	-0.685466000	-0.658278000	1.595276000
1	-1.211323000	-1.368862000	2.087742000
1	-0.998924000	0.277909000	1.824284000
6	-2.143245000	2.390112000	0.096690000
8	-2.540168000	1.851479000	1.041128000
8	-1.787342000	2.975842000	-0.831868000
6	2.153269000	-1.118415000	1.771477000
8	1.936177000	-2.251286000	1.854741000
8	2.411073000	0.003985000	1.692010000
6	1.143047000	2.094135000	0.236130000
8	1.828062000	1.868589000	-0.666888000
8	0.494987000	2.364506000	1.154292000
6	-3.289184000	-1.580918000	-0.858058000
8	-3.596146000	-1.511742000	0.253163000
8	-3.002546000	-1.654671000	-1.975227000
6	3.012782000	-0.422023000	-1.680289000
8	3.789347000	0.223598000	-2.232329000
8	2.244147000	-1.099774000	-1.137306000

$G(CO_2)_6$

SCF E = -1336.85622939 a.u.

7	0.152957000	-1.789420000	0.213915000
1	-0.493238000	-2.553929000	0.060388000
1	0.623799000	-1.834843000	1.107405000
6	-0.344255000	-0.538724000	-0.112110000
7	-0.086827000	0.566072000	0.486169000
1	0.464651000	0.405312000	1.325647000
7	-1.194572000	-0.554626000	-1.206379000
1	-0.900525000	-1.179112000	-1.946704000
1	-1.407476000	0.379150000	-1.539093000
6	-1.193067000	3.011726000	-0.290828000
8	-1.762648000	2.498299000	-1.159199000
8	-0.648208000	3.578739000	0.552189000
6	-3.464157000	-2.187430000	-0.466070000
8	-4.251813000	-1.357910000	-0.609622000
8	-2.702781000	-3.048922000	-0.327016000
6	-2.797626000	0.422648000	1.620103000
8	-2.630910000	-0.707460000	1.812786000
8	-2.992041000	1.545795000	1.448404000
6	2.475734000	-1.535424000	-1.422300000
8	1.815627000	-1.100360000	-2.266731000
8	3.162301000	-1.968822000	-0.601588000
6	3.546778000	-0.519777000	1.812064000
8	4.652942000	-0.311784000	1.573696000
8	2.437883000	-0.730418000	2.078113000
6	1.965369000	1.728396000	-1.003243000
8	2.725817000	1.101461000	-0.392742000
8	1.253734000	2.368975000	-1.644449000

$G(CO_2)_7$

SCF E = -1525.44219885 a.u.

7	-1.259570000	1.479062000	-1.069859000
1	-2.254633000	1.652146000	-1.141489000
1	-0.765874000	1.534208000	-1.949699000
6	-0.901958000	0.417640000	-0.260878000
7	0.091340000	-0.378155000	-0.425789000
1	0.536190000	-0.255308000	-1.331531000
7	-1.743997000	0.248521000	0.828541000
1	-2.046520000	1.115932000	1.256357000

$G(CO_2)_8$

SCF E = -1714.02532964 a.u.

7	-0.903868000	-2.059340000	-0.658058000
1	-1.800362000	-2.528170000	-0.688827000
1	-0.282326000	-2.442852000	0.042614000
6	-0.962970000	-0.680909000	-0.676274000
7	-0.089077000	0.119264000	-0.180271000
1	0.636921000	-0.405083000	0.302419000
7	-2.095128000	-0.172039000	-1.300301000
1	-2.366824000	-0.694211000	-2.124800000

1	-1.363545000	-0.405980000	1.503182000
6	0.713170000	-2.512006000	1.175738000
8	0.144725000	-2.035319000	2.066193000
8	1.302686000	-3.029523000	0.330750000
6	-4.477075000	-0.101495000	-0.130617000
8	-4.339855000	0.921317000	-0.655146000
8	-4.645852000	-1.116099000	0.390707000
6	-2.188623000	-2.268752000	-0.887847000
8	-2.589714000	-1.585637000	-1.731970000
8	-1.807862000	-2.966192000	-0.051938000
6	2.296671000	1.860327000	-1.350246000
8	3.007218000	1.880916000	-0.441483000
8	1.592728000	1.842429000	-2.268013000
6	-0.254868000	3.487876000	0.731801000
8	-1.176721000	3.322027000	1.409384000
8	0.668602000	3.684821000	0.067305000
6	3.522092000	-1.618389000	-0.906181000
8	2.861339000	-0.916289000	-1.549254000
8	4.203443000	-2.313683000	-0.291265000
6	1.822059000	0.442138000	1.709229000
8	1.073152000	1.285246000	1.964662000
8	2.592506000	-0.390392000	1.490935000

1	-1.991826000	0.815362000	-1.509296000
6	-0.294660000	2.867123000	-0.068471000
8	-0.891846000	2.885643000	-1.060263000
8	0.305566000	2.912187000	0.915803000
6	-4.565732000	-1.331813000	-0.232249000
8	-4.066957000	-2.349007000	-0.471881000
8	-5.091409000	-0.332098000	-0.001962000
6	-2.642688000	0.636696000	1.491807000
8	-2.712698000	-0.477624000	1.795301000
8	-2.594852000	1.749686000	1.190611000
6	1.883388000	-2.041085000	-1.855400000
8	1.672076000	-1.304011000	-2.717281000
8	2.102508000	-2.792801000	-1.004234000
6	3.192919000	1.006174000	-0.002637000
8	2.981713000	-0.122894000	-0.171286000
8	3.429797000	2.117536000	0.172228000
6	0.780634000	1.330998000	-2.751441000
8	-0.157725000	0.961332000	-3.312831000
8	1.730322000	1.727465000	-2.223683000
6	0.690451000	0.855972000	2.704243000
8	-0.397243000	0.950958000	3.074932000
8	1.790321000	0.740172000	2.363864000
6	2.465493000	-2.230249000	1.759736000
8	1.312039000	-2.108404000	1.716300000
8	3.605877000	-2.362853000	1.825934000

$G(CO_2)_9$

SCF E = -1902.60866667 a.u.

7	0.927049000	1.531542000	0.926435000
1	1.894742000	1.825425000	0.972592000
1	0.461229000	1.393700000	1.811762000
6	0.593578000	0.656061000	-0.088549000
7	-0.291746000	-0.273747000	-0.039521000
1	-0.661240000	-0.385785000	0.903181000
7	1.325458000	0.868475000	-1.248460000
1	1.485062000	1.848799000	-1.450194000
1	0.927784000	0.380510000	-2.043384000
6	-0.911467000	-1.794128000	-2.294420000
8	-0.629299000	-0.904038000	-2.981280000
8	-1.209461000	-2.707104000	-1.657502000
6	4.215317000	0.899540000	-0.713594000
8	3.946404000	1.590624000	0.175264000
8	4.507701000	0.227296000	-1.603606000
6	2.367102000	-1.796215000	-0.807031000
8	2.856361000	-1.478911000	0.193573000
8	1.901170000	-2.109671000	-1.813777000
6	-2.519863000	1.948378000	1.592544000
8	-3.314923000	2.218758000	0.801834000
8	-1.724238000	1.683993000	2.389915000
6	2.099519000	-0.782896000	2.731636000
8	3.110944000	-0.244997000	2.863932000

$G(CO_2)_{10}$

SCF E = -2091.19468783 a.u.

7	-0.478944000	1.576769000	-1.100177000
1	-1.307899000	1.994127000	-1.510574000
1	0.065602000	1.073721000	-1.790672000
6	-0.742215000	0.845679000	0.046658000
7	-0.171464000	-0.252130000	0.398224000
1	0.455184000	-0.582370000	-0.332233000
7	-1.710861000	1.415375000	0.855186000
1	-1.704175000	2.428846000	0.845757000
1	-1.693443000	1.042058000	1.797665000
6	-0.149566000	-1.101400000	3.046307000
8	-0.524374000	-0.062770000	3.398416000
8	0.236746000	-2.147313000	2.753654000
6	-4.215104000	1.524700000	-0.559814000
8	-3.608853000	1.939676000	-1.453695000
8	-4.848095000	1.130542000	0.320704000
6	-3.001308000	-1.268406000	0.825116000
8	-3.184457000	-1.249271000	-0.317251000
8	-2.843863000	-1.281361000	1.967894000
6	3.118649000	1.672703000	-0.897260000
8	3.569158000	1.952104000	0.127898000
8	2.676708000	1.388054000	-1.927093000
6	-1.666898000	-1.529766000	-2.570087000
8	-1.943067000	-0.453754000	-2.885114000

8	1.072084000	-1.304850000	2.623623000	8	-1.387298000	-2.611452000	-2.274361000
6	-3.538280000	-1.494777000	0.571564000	6	3.035103000	-1.660756000	0.785414000
8	-3.149003000	-0.666217000	1.281762000	8	2.854609000	-0.946679000	-0.112502000
8	-3.947556000	-2.318063000	-0.121532000	8	3.237280000	-2.370974000	1.665928000
6	-2.273442000	1.117572000	-1.661260000	6	1.665295000	1.377483000	2.162269000
8	-1.545881000	2.013479000	-1.739877000	8	1.085313000	2.332232000	1.866035000
8	-3.022016000	0.240334000	-1.604353000	8	2.258320000	0.436781000	2.475856000
6	-0.117716000	3.991203000	-0.227656000	6	0.490277000	4.135392000	-0.224059000
8	0.742719000	3.959186000	-0.999917000	8	-0.558936000	4.311082000	0.230490000
8	-0.975384000	4.055729000	0.541689000	8	1.541373000	4.001568000	-0.680901000
6	-0.286439000	-3.193938000	0.942932000	6	-0.218540000	-3.243829000	0.200540000
8	0.742215000	-3.506086000	0.519847000	8	-1.286773000	-3.446105000	0.584175000
8	-1.312180000	-2.905877000	1.387889000	8	0.854639000	-3.065741000	-0.195678000
				6	2.087121000	-1.294710000	-2.780497000
				8	1.014332000	-0.908366000	-2.567267000
				8	3.144330000	-1.683128000	-3.013448000

References

1. R. Ditchfield, *Mol. Phys.*, 1974, **27**, 789-807.
2. L. B. Casabianca, *Magn. Reson. Chem*, 2020.
3. Q. Yang, M. Bown, A. Ali, D. Winkler, G. Puxty and M. Attalla, *Energy Procedia*, 2009, **1**, 955-962.
4. J. Seravalli and S. W. Ragsdale, *Biochemistry*, 2008, **47**, 6770-6781.
5. T. M. Abbott, G. W. Buchanan, P. Kruus and K. C. Lee, *Canadian Journal of Chemistry*, 1982, **60**, 1000-1006.
6. C. Perinu, B. Arstad and K.-J. Jens, *Energy Procedia*, 2013, **37**, 7310-7317.