Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information: *Ab initio* Screening of Pt-based Transition-metal Nanoalloys Using Descriptors Derived from the Adsorption and Activation of CO_2

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Contents

S1 Introduction

The present electronic supplementary information reports the following additional information to the manuscript:

1. Additional technical details, Section S2, convergence tests, S3, and further details about the calculated properties, Section S4.

2. Short discussion of the unary nanoclusters, Section S5.

3. Complete set of adsorption configurations and complementary data for the adsorption of CO_2 on several Pt_{55} clusters, Section S6, and for the CO_2/Pt_nTM_{55-n} systems, $n = 0, 13, 42$, Section S7.

4. Complementary analyses for the adsorbed systems, Section S8.

5. Cartesian atomic coordinates for the lowest energy configurations in the chemisorption and physisorption states, Section S9.

S2 Additional Technical Details: PAW Projectors

Table S1 lists the PAW projectors employed in this study, which were obtained from the VASP library, as well as the sizes for the cubic simulation boxes and cutoff energies employed (`ENCUT`) for all systems. To comply with the cutoff requirements of all elements and for consistency, we employed a cutoff energy of 489 eV for all calculations. To further improve the consistency between our calculations and keep the interactions among periodic images negligible, we employed cubic boxes with different sides, depending on the elements present (26 Å for systems containing Ag, 25 Å for Ru and Rh and 24 Å for all other TM), to result in similar distances between periodic images for all systems (at least 12 Å).

Table S1: Technical details on the PAW projectors: chemical specie, selected PAW projector, number of valence electrons, Z_{val}, recommended maximum cutoff energy for the plane-wave basis set within the `POTCAR` files, `ENMAX`, cutoff energy employed for all isolated and adsorbed systems, `ENCUT`, and size of the cubic boxes employed for the simulations.

Element	PAW projector `TITEL` in `POTCAR`	Z_{val}	`ENMAX` (eV)	`ENCUT` (eV)	box size (Å)
Fe	Fe_GW 31Mar2010	8	321	489	24
Co	Co_GW 31Mar2010	9	323	489	24
Ni	Ni_GW 31Mar2010	10	357	489	24
Cu	Cu_GW 19May2006	11	417	489	24
Ru	Ru_sv_GW 05Dec2013	16	348	489	25
Rh	Rh_GW 06Mar2008	9	247	489	25
Pd	Pd_GW 06Mar2008	10	251	489	24
Ag	Ag_GW 06Mar2008	11	250	489	26
Os	Os_sv_GW 23Mar2010	16	320	489	25
Ir	Ir_sv_GW 23Mar2010	17	320	489	24
Pt	Pt_GW 10Mar2009	10	249	489	24
Au	Au_GW 23Mar2010	11	248	489	24
C	C_GW_new 19Mar2012	4	414	489	–
O	O_GW 19Mar2012	6	434	489	–

S3 Computational Convergence Tests

Table S2 shows convergence tests using tight convergence criteria for the atomic forces and total electronic energy. For this test, all atomic positions of the selected CO_2/Pt_{55} systems were further optimized until the average forces across all 58 atoms of the system were much lower, by at least one order of magnitude, up to the limit of 0.001 eV/Å, employing an electronic convergence criteria of 10^{-7} eV. Those structural re-optimizations were stopped at the values shown in Table S2, which are significantly lower than the results obtained with the 0.05 eV/Å employed in the main study. The results in Table S2 show that the type of adsorption mode (physisorption or chemisorption) does not present any change. The physisorption configurations show very subtle structural changes, due to CO_2 rotations keeping the orientation almost constant with respect to the particle. The chemisorption structures presented the same adsorption site and very subtle differences in the geometric properties. As expected, the total energy shows small variations of at most 21 meV, due to the further relaxation; moreover, this caused a small change of the total magnetic moment, only for one case, which can be attributed to the slight relaxation of the cluster. Therefore, the results within 0.05 eV/Å and 10^{-5} eV are sufficient to accurately describe the adsorption mode and adsorption properties

of the systems.

Table S2: Converge test for the electronic energy and atomic forces convergence criteria performed for CO_2/Pt_{55} using two types of clusters, namely, distorted reduced-core (DRC) and close-packed wheel-type (WHE) presenting CO_2 chemisorption (C) or physisorption (P). The properties are: forces on the atoms averaged for CO_2 and Pt_{55} in the adsorbed system, $F_{av}^{CO_2}$ and $F_{av}^{Pt_{55}}$, respectively; convergence criteria for the total electronic energy, EDIFF; total electronic energy, E_{tot}, total magnetic moment, m_{tot}; O-C bond lengths, d_{O_1-C} and d_{O_2-C}; OCO angle, α_{OCO}; and shortest C-Pt, O1-Pt, and O2-Pt distances, d_{C-Pt}, d_{O_1-Pt}, and d_{O_2-Pt}, respectively.

	$F_{av}^{CO_2}$ eV/Å	$F_{av}^{Pt_{55}}$ eV/Å	EDIFF eV	E_{tot} eV	m_{tot} μ_B	$d_{O1\text{-}C}$ Å	$d_{O2\text{-}C}$ Å	α_{OCO} °	d_{C-Pt} Å	$d_{O1\text{-}Pt}$ Å	$d_{O2\text{-}Pt}$ Å
WHE^C	0.039	0.015	10^{-5}	-326.1747335	4	1.21	1.30	131.76	2.05	2.85	2.10
WHE^C	0.001	0.001	10^{-7}	-326.1859932	4	1.21	1.30	132.10	2.05	2.84	2.10
WHE^P	0.035	0.023	10^{-5}	-326.0604773	4	1.17	1.17	179.78	3.34	3.40	3.33
WHE^P	0.006	0.001	10^{-7}	-326.0757257	4	1.17	1.17	179.85	3.47	3.25	3.34
DRC^C	0.037	0.017	10^{-5}	-326.3909128	0	1.21	1.29	132.92	2.05	2.80	2.09
DRC^C	0.003	0.001	10^{-7}	-326.4114279	2	1.21	1.29	133.13	2.05	2.79	2.09
DRC^P	0.040	0.016	10^{-5}	-326.3957976	0	1.18	1.17	179.26	3.41	3.02	3.32
DRC^P	0.010	0.001	10^{-7}	-326.4108894	0	1.18	1.17	179.17	3.49	3.04	3.51

S4 Definitions - Energetic, Structural, and Electronic Properties

S4.1 Binding Energy

We calculated the binding energy, E_b, per atom of the binary nanoclusters using the following equation,

$$E_b = \frac{1}{55}\left(E_{tot}^{Pt_nTM_{55-n}} - nE_{tot}^{Pt} - (55-n)E_{tot}^{TM}\right), \quad (1)$$

where $E_{tot}^{Pt_nTM_{55-n}}$ is the total energy of the 55-atom nanoalloy, E_{tot}^{Pt} and E_{tot}^{TM} are the free atom total energies of the Pt and TM atoms, respectively. The possible values for n is this work are 13 and 42. For the unary nanoclusters, $E_b = \frac{1}{55}(E_{tot}^{TM_{55}} - 55E_{tot}^{TM})$, where $E_{tot}^{TM_{55}}$ is the total energy of the unary nanocluster.

S4.2 Excess Energy

To obtain the relative stability of the binary nanoclusters, we calculated the excess energy, E_{exc}, per atom using the following equation,

$$E_{exc} = \frac{1}{55}\left(E_{tot}^{\mathrm{Pt}_n\mathrm{TM}_{55-n}} - \frac{n}{55}E_{tot}^{\mathrm{Pt}_{55}} - \frac{55-n}{55}E_{tot}^{\mathrm{TM}_{55}}\right), \tag{2}$$

where, $E_{tot}^{\mathrm{Pt}_{55}}$ and $E_{tot}^{\mathrm{TM}_{55}}$ are the total energies of the lowest energy Pt_{55} and TM_{55} configurations. Additional technical details are discussed elsewhere, e.g., Piotrowski, M. J. *et al.*, J. Phys. Chem. C, **2016**, 120, 28844–28856; Mendes, P. C. D. *et al.*, J. Phys. Chem. C, **2019**, 124, 1158–1164.

S4.3 Adsorption and Interacting Energies

To characterize the adsorption mechanism of CO_2 on the unary and binary nanoclusters, we calculated the adsorption energy, E_{ad}, using the following equation,

$$E_{ad} = E_{tot}^{\mathrm{CO_2/Sub}} - E_{tot}^{\mathrm{CO_2}} - E_{tot}^{\mathrm{Sub}}\ , \tag{3}$$

where $E_{tot}^{\mathrm{CO_2/Sub}}$ is the total energy of the adsorbed system, while $E_{tot}^{\mathrm{CO_2}}$ and E_{tot}^{Sub} are the total energies of the isolated molecule and substrate, respectively. To calculate E_{ad}, all terms of the equation correspond to optimized structures. Differently, the interaction energy, E_{int}, was calculated from the energies of the isolated systems calculated for the fixed atomic positions (in the adsorption configurations) and simulation box. Thus,

$$E_{int} = E_{ad} - \Delta E_{tot}^{\mathrm{Mol}} - \Delta E_{tot}^{\mathrm{Sub}}\ , \tag{4}$$

where $\Delta E_{tot}^{\mathrm{Mol}}$ and $\Delta E_{tot}^{\mathrm{Sub}}$ are deformation energies that indicate the energy difference, for the isolated systems, between the most stable optimized configuration and the deformed geometry considering the adsorption positions for the isolated systems.

S4.4 Effective Bader Charges

The effective Bader charges were calculated as $Q_{eff} = Z_{val} - Q_{\mathrm{Bader}}$, in which Z_{val} is the valence charge shown in Table S1 and Q_{Bader} is the Bader charge (Henkelman, G. *et al.*, *Comput. Mater. Sci.* **2006**, 36,

354–360).

To calculate the Bader charges, it is necessary to partition the real space based on the electron density. This is done considering low-density regions as interfaces to define volumes around each atom that approximately contain its respective charge. to obtain accurate results, it is necessary to use a fine FFT-mesh, which can be done increasing the NGXF, NGYF and NGZF flags in the VASP software from the recommended values, for a single-point calculation for previously optimized atomic configurations to avoid prohibitive computational costs. To obtain our results, we considered the NGX(YZ)F recommended by VASP (which is mainly based on the size of the box and cutoff energy for the plane-wave basis set) and multiplied each by a factor of 3, thus, obtaining sufficiently converged results to study the trends for CO_2 adsorption. Furthermore, we employed the all-electron charge, i.e., the summed core and valence charges. For further details, we direct the reader to the literature cited in the main article (Henkelman, G. *et al.*, *Comput. Mater. Sci.* **2006**, 36, 354–360).

S5 Unary and Binary 55-atom Nanoclusters

The optimized configurations for the the isolated unary Pt_{55}, TM_{55} nanoclusters, and for the Pt_nTM_{55-n} nanoalloys, with $n = 13, 42$ are shown in Figure S1, while some of their properties are shown in Table S3. As explained in the main article, the structures for all nanoclusters were the putative global minimum configuration, except for Pt_{55}, which was studied in all morphologies assumed by the PtTM nanoalloys to obtain further insights into the effect of alloying with the TM component on the adsorption.

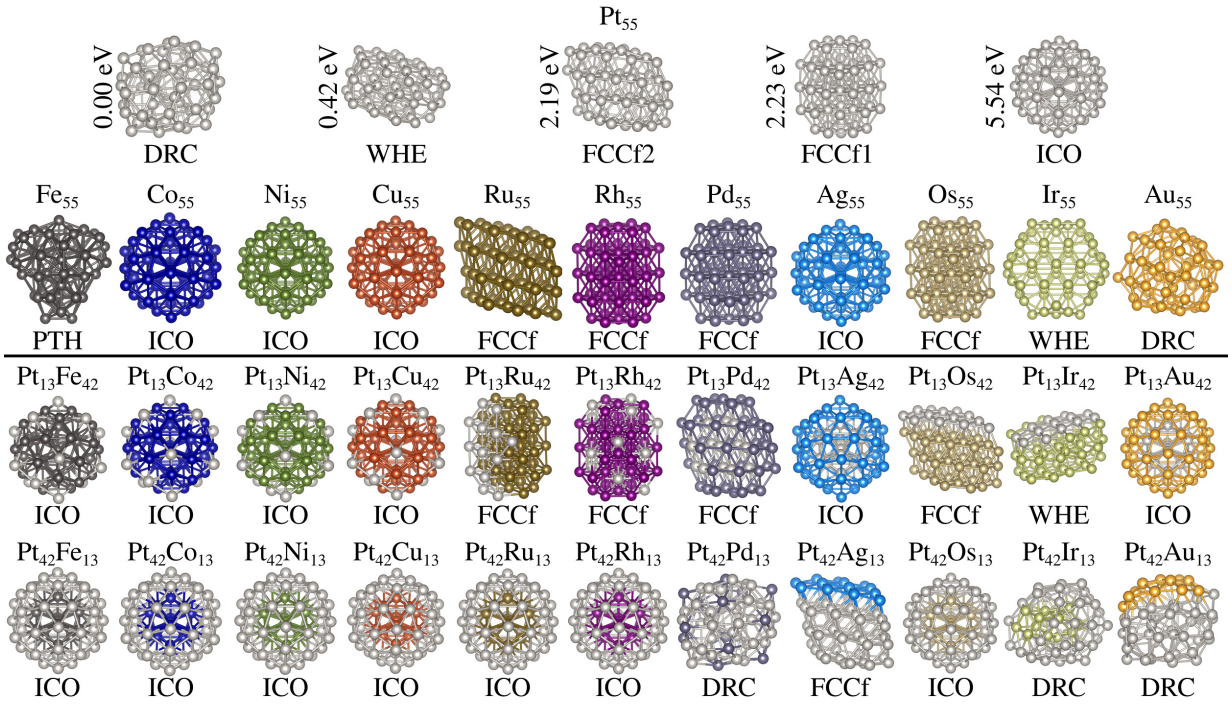

Figure S1: Optimized atomic configurations of isolated Pt_{55}, TM_{55} nanoclusters and Pt_nTM_{55-n} nanoalloys for $n = 13, 42$. The structures were named as distorted reduced-core (DRC), face-centered cubic fragments (two slightly different types, FCCf1 and FCCf2), polytetrahedron (PTH), hexagonal close-packed wheel-type (WHE) and icosahedron (ICO). For Pt_{55}, the total relative energy with respect to the lowest energy configuration (DRC) is indicated. Corresponding properties are available in Tables S3 and S4.

Table S3: Unary and binary nanoclusters properties: excess energy per atom, E_{exc}, binding energy per atom, E_b, total magnetic moment, m_{tot}, average effective coordination numer, ECN_{av}, (in number of nearest neighbors), average weighted bond lengths, d_{av}, and chemical order parameter, σ.

System	E_{exc} (eV)	E_b (eV)	m_{tot} (μ_B)	ECN_{av}	d_{av} (Å)	σ
Fe_{55}	-	−3.97	154	8.24	2.49	1.00
Co_{55}	-	−4.13	105	8.37	2.43	1.00
Ni_{55}	-	−3.97	40	8.39	2.43	1.00
Cu_{55}	-	−3.06	3	8.39	2.50	1.00
Ru_{55}	-	−5.64	6	7.60	2.57	1.00
Rh_{55}	-	−4.79	29	7.96	2.62	1.00
Pd_{55}	-	−3.17	22	7.93	2.70	1.00
Ag_{55}	-	−2.27	3	8.42	2.88	1.00
Os_{55}	-	−6.80	2	7.85	2.61	1.00
Ir_{55}	-	−6.19	1	6.28	2.58	1.00
Pt_{55}	-	−4.83	0	6.83	2.66	1.00
Au_{55}	-	−2.84	1	6.44	2.78	1.00
$Pt_{13}Fe_{42}$	−0.22	−4.39	124	8.17	2.53	0.38
$Pt_{13}Co_{42}$	−0.17	−4.46	88	8.37	2.48	0.35
$Pt_{13}Ni_{42}$	−0.13	−4.31	40	8.45	2.49	0.35
$Pt_{13}Cu_{42}$	−0.13	−3.61	2	8.46	2.54	0.35
$Pt_{13}Ru_{42}$	−0.05	−5.50	10	7.89	2.61	0.65
$Pt_{13}Rh_{42}$	−0.02	−4.82	20	7.93	2.63	0.20
$Pt_{13}Pd_{42}$	−0.03	−3.59	10	7.88	2.71	0.30
$Pt_{13}Ag_{42}$	−0.09	−2.96	0	8.42	2.85	0.38
$Pt_{13}Os_{42}$	−0.07	−6.41	2	7.70	2.63	0.68
$Pt_{13}Ir_{42}$	0.00	−5.87	4	6.26	2.59	0.57
$Pt_{13}Au_{42}$	−0.03	−3.34	2	8.44	2.84	0.38
$Pt_{42}Fe_{13}$	−0.28	−4.91	38	8.38	2.63	0.38
$Pt_{42}Co_{13}$	−0.22	−4.89	35	8.30	2.62	0.38
$Pt_{42}Ni_{13}$	−0.16	−4.79	22	8.29	2.62	0.38
$Pt_{42}Cu_{13}$	−0.14	−4.56	9	8.38	2.63	0.38
$Pt_{42}Ru_{13}$	−0.21	−5.24	6	8.39	2.69	0.38
$Pt_{42}Rh_{13}$	−0.07	−4.89	19	8.38	2.69	0.38
$Pt_{42}Pd_{13}$	−0.01	−4.45	2	6.94	2.67	0.21
$Pt_{42}Ag_{13}$	0.02	−4.20	1	7.49	2.73	0.68
$Pt_{42}Os_{13}$	−0.30	−5.60	4	8.39	2.70	0.38
$Pt_{42}Ir_{13}$	−0.08	−5.23	1	6.81	2.65	0.39
$Pt_{42}Au_{13}$	0.02	−4.34	1	6.83	2.70	0.60

Table S4: Unary Pt_{55} nanoclusters: characterization of different atomic configurations for Pt_{55} named as distorted reduced-core (DRC), face-centered cubic fragments (two slightly different types, FCCf1 and FCCf2), hexagonal close-packed wheel-type (WHE) and icosahedron (ICO). Total energy relative to the lowest energy configuration, ΔE_{tot}, binding energy per atom, E_b, total magnetic moment, m_{tot}, average effective coordination numer, ECN_{av} (in number of nearest neighbors) and average bond length, d_{av}.

System	Structure	ΔE_{tot} (eV)	E_b (eV)	m_{tot} (μ_B)	ECN_{av}	d_{av} (Å)
Pt_{55}	ICO	5.54	–4.73	12	8.35	2.73
Pt_{55}	FCCf1	2.23	–4.79	2	7.59	2.69
Pt_{55}	FCCf2	2.19	–4.79	4	7.33	2.68
Pt_{55}	WHE	0.42	–4.82	8	6.31	2.64
Pt_{55}	DRC	0.00	–4.83	0	6.83	2.66

S6 CO_2 Adsorption on Pt_{55}

Figure S2 shows the complete set of adsorption configurations for CO_2 adsorbed on the lowest energy unary platinum cluster, which is a low symmetry configuration with reduced number of atoms in the core region (distorted reduced-core, DRC), while the corresponding data is in Table S5. Furthermore, as shown in the main article, we studied the adsorption of CO_2 on Pt_{55} clusters of different types of structures; the adsorption configurations are shown in Figures S2 - S6 and corresponding data can be found in Tables S5 - S9.

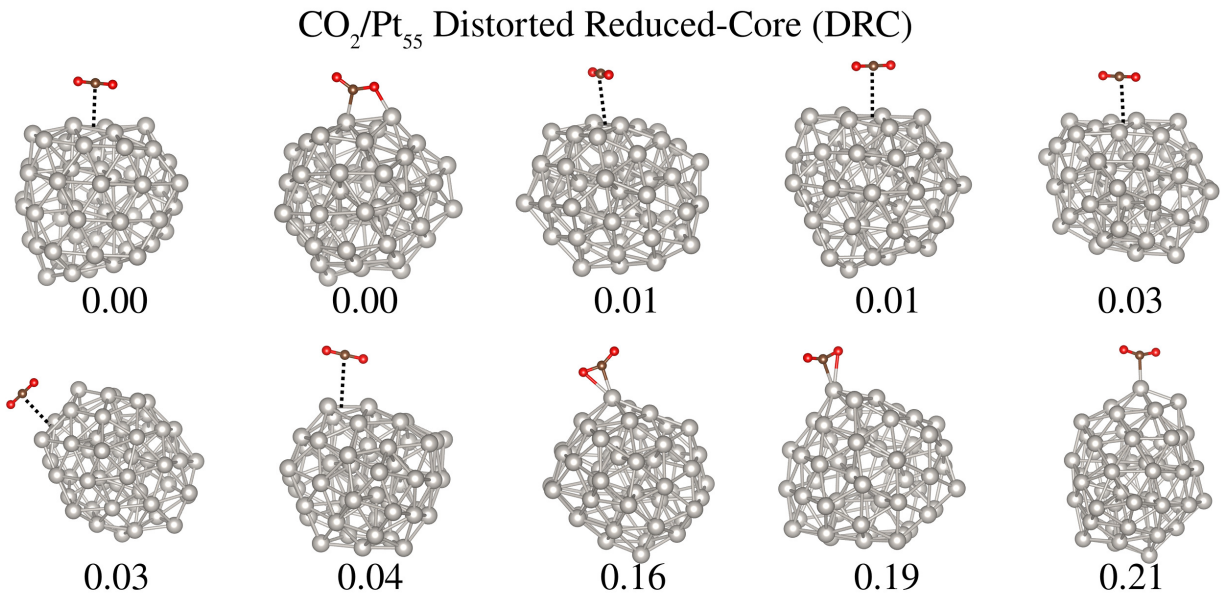

Figure S2: Optimized adsorption configurations for CO_2 interacting with the most stable Pt_{55} cluster, i.e., of the distorted reduced-core (DRC) structure. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S5.

Table S5: Adsorption properties for all configurations of CO_2 interacting with the most stable Pt_{55} cluster, i.e., of the distorted reduced-core (DRC) structure. Total energy relative to the lowest energy configuratio, ΔE_{tot}, adsorption energy, E_{ad}, total magnetic moment, m_{tot}, shortest distances between the C and TM atoms, d_{C-TM}, O and TM atoms, $d_{O1\text{-}TM}$ and $d_{O2\text{-}TM}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O−C bond lengths ($d_{O1\text{-}C}$ and $d_{O2\text{-}C}$) and OCO angle (Δ_{OCO}).

CO_2/Pt_{55} Distorted Reduced-core (DRC)											
ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{C\text{-}TM}$ (Å)	$d_{O1\text{-}TM}$ (Å)	$d_{O2\text{-}TM}$ (Å)	$d_{O1\text{-}C}$ (Å)	$d_{O2\text{-}C}$ (Å)	α_{OCO} (deg)	$\Delta_{O1\text{-}C}$ (%)	$\Delta_{O2\text{-}C}$ (%)	Δ_{OCO} (%)
0.21	−0.02	0	2.20	2.81	2.69	1.20	1.21	152.40	2.63	3.42	−15.31
0.19	−0.05	0	2.16	2.43	2.96	1.23	1.20	152.13	4.65	1.94	−15.45
0.16	−0.08	2	2.14	2.95	2.42	1.20	1.23	150.81	1.97	4.95	−16.19
0.04	−0.19	0	3.38	3.45	2.96	1.17	1.18	179.01	−0.09	0.24	−0.52
0.03	−0.21	0	3.35	3.18	3.12	1.17	1.17	179.55	0.04	0.09	−0.22
0.03	−0.21	2	3.42	3.47	3.56	1.17	1.17	178.83	−0.01	0.14	−0.62
0.01	−0.22	0	3.28	3.33	3.21	1.17	1.17	179.05	0.01	0.09	−0.50
0.01	−0.23	2	3.37	3.16	3.16	1.17	1.17	179.31	0.05	0.01	−0.35
0.00	−0.23	0	2.05	2.80	2.09	1.21	1.29	132.92	2.96	9.95	−26.13
0.00	−0.24	0	3.41	3.02	3.32	1.18	1.17	179.26	0.23	−0.12	−0.38

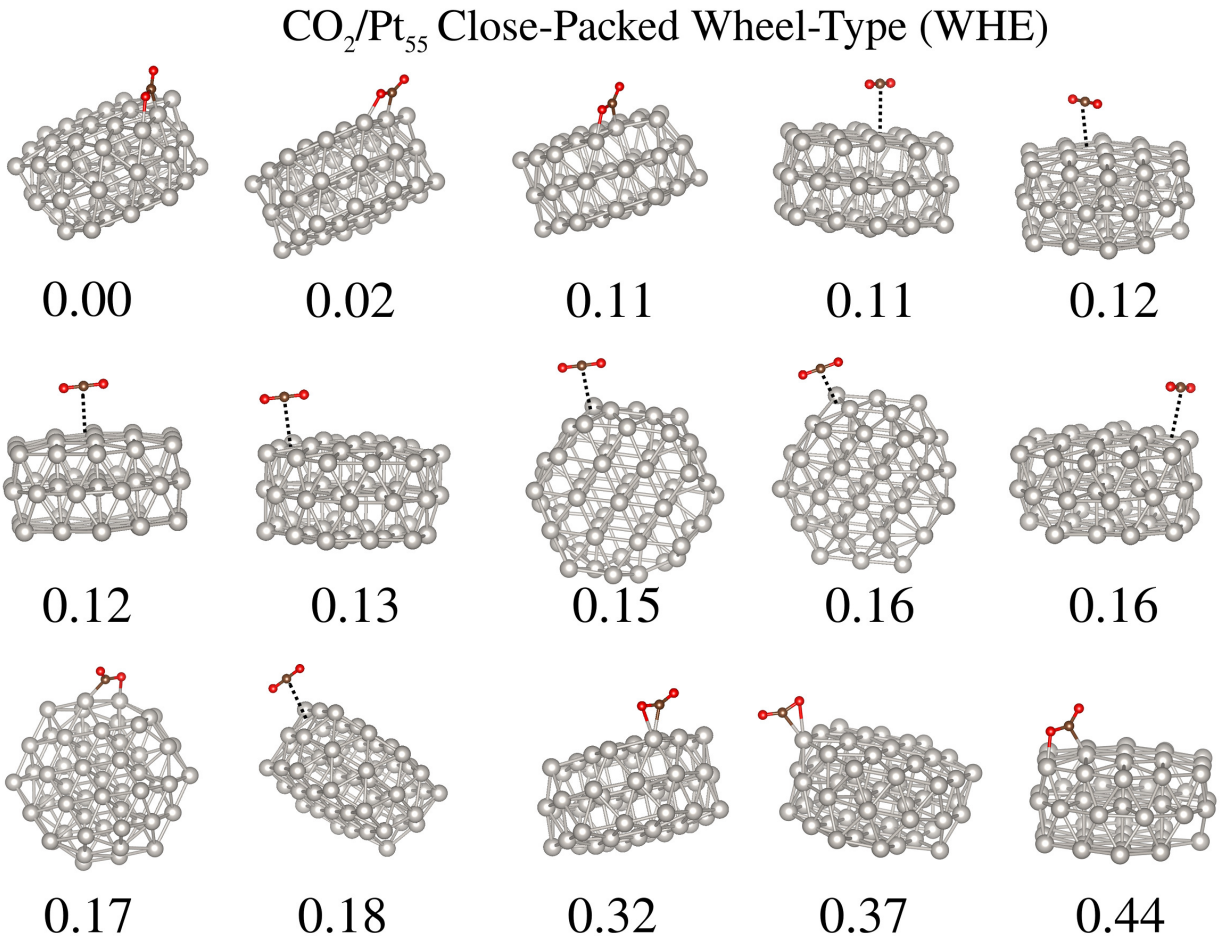

Figure S3: Optimized adsorption configurations for CO_2 interacting with Pt_{55} of the hexagonal close-packed wheel-type (WHE) structure. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S6.

Table S6: Adsorption properties for all configurations of CO_2 adsorbed on Pt_{55} of the hexagonal close-packed wheel-type (WHE) structure. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy, E_{ad}, total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O−C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

CO_2/Pt_{55} Hexagonal Close-packed Wheel-type (WHE)											
ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
0.44	0.00	6	2.12	2.81	2.11	1.20	1.28	135.57	2.71	9.01	−24.66
0.37	−0.06	6	2.14	2.41	2.95	1.23	1.20	151.70	4.86	1.97	−15.69
0.32	−0.11	4	2.10	3.03	2.28	1.20	1.25	147.35	2.18	6.35	−18.11
0.18	−0.26	4	3.27	3.49	3.48	1.17	1.17	178.73	−0.01	0.10	−0.67
0.17	−0.27	6	2.04	2.79	2.10	1.21	1.29	131.92	3.48	10.38	−26.69
0.16	−0.28	4	3.46	3.07	3.62	1.17	1.17	179.44	0.13	−0.11	−0.28
0.16	−0.28	4	3.27	3.19	3.68	1.18	1.17	179.19	0.18	−0.02	−0.42
0.15	−0.29	4	3.26	3.74	2.99	1.17	1.18	179.24	−0.16	0.24	−0.39
0.13	−0.30	4	3.43	3.16	3.26	1.17	1.17	179.73	0.07	0.02	−0.17
0.12	−0.32	4	3.41	3.46	3.26	1.17	1.17	179.64	0.00	0.06	−0.17
0.12	−0.32	4	3.43	3.46	3.31	1.17	1.17	179.73	0.04	0.04	−0.12
0.11	−0.32	4	3.34	3.40	3.33	1.17	1.17	179.78	0.03	0.07	−0.09
0.11	−0.32	6	2.08	2.09	2.82	1.28	1.21	133.89	9.02	3.33	−25.59
0.02	−0.42	6	2.04	2.83	2.09	1.21	1.30	132.40	3.03	10.55	−26.42
0.00	−0.44	4	2.05	2.85	2.10	1.21	1.30	131.76	3.16	10.57	−26.78

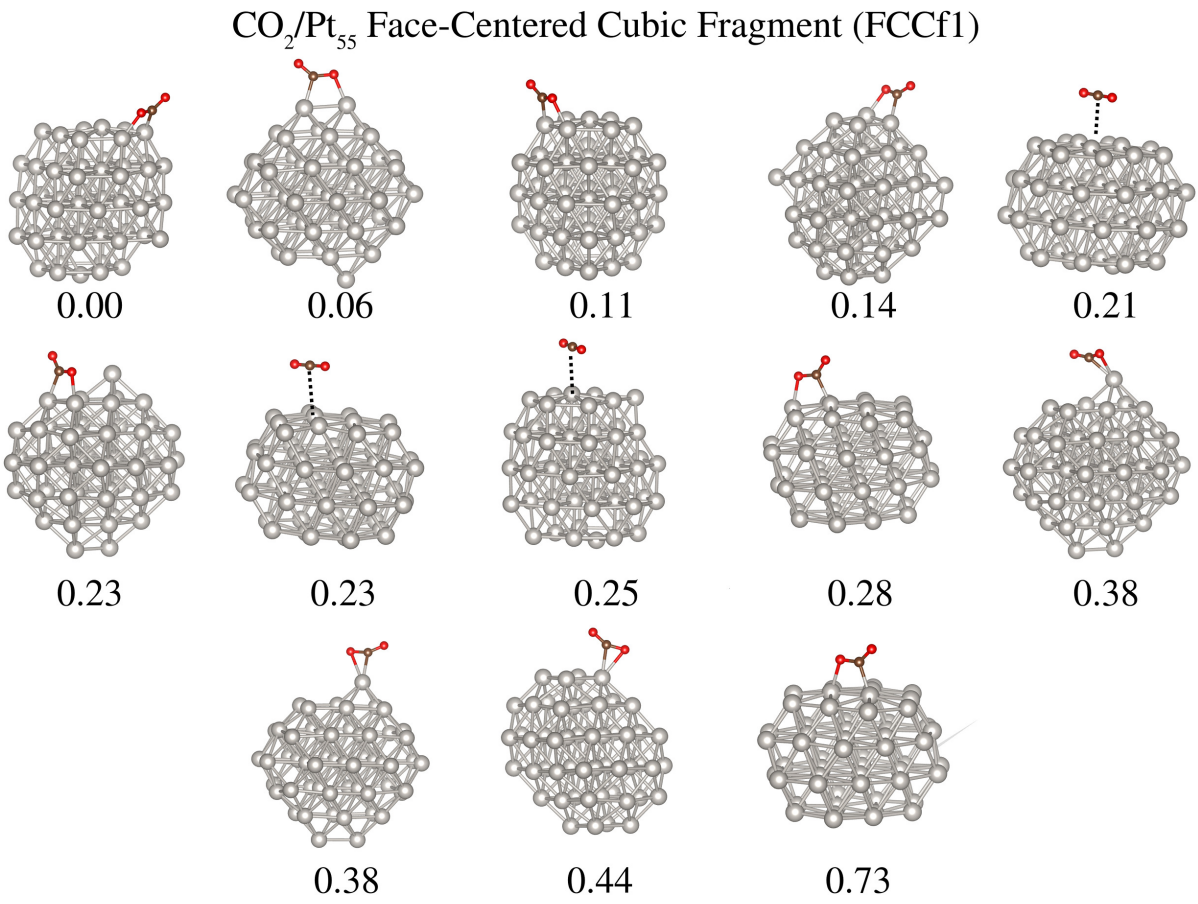

Figure S4: Optimized adsorption configurations for CO_2 interacting with Pt_{55} of the face-centered cubic fragment (FCCf1) morphology. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S7.

Table S7: Adsorption properties for all configurations of CO_2 adsorbed on Pt_{55} of the face-centered cubic fragment (FCCf1) morphology. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

CO_2/Pt_{55} Face-centered Cubic Fragment (FCCf1)											
ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
0.73	0.28	4	2.07	2.81	2.13	1.21	1.28	133.55	2.94	9.42	−25.78
0.44	−0.01	4	2.18	2.35	3.04	1.23	1.19	151.95	4.80	1.65	−15.55
0.38	−0.08	2	2.13	2.92	2.41	1.20	1.23	152.85	2.02	4.72	−15.06
0.38	−0.08	2	2.12	2.26	3.03	1.24	1.19	150.16	5.83	1.78	−16.55
0.28	−0.18	2	2.07	2.84	2.11	1.20	1.29	132.71	2.71	10.29	−26.25
0.25	−0.20	2	3.12	3.40	3.31	1.17	1.17	177.52	0.12	0.08	−1.35
0.23	−0.22	2	3.18	3.37	3.44	1.17	1.17	178.41	0.00	0.14	−0.85
0.23	−0.23	2	2.03	2.07	2.81	1.30	1.21	130.47	10.92	3.38	−27.49
0.21	−0.24	2	3.30	3.36	3.28	1.17	1.17	178.87	0.10	0.01	−0.60
0.14	−0.31	2	2.04	2.70	2.10	1.21	1.28	136.02	3.39	8.75	−24.41
0.11	−0.34	2	2.03	2.68	2.11	1.22	1.28	135.57	3.71	8.80	−24.66
0.06	−0.39	4	2.04	2.10	2.78	1.29	1.21	134.56	9.61	3.23	−25.22
0.00	−0.45	2	2.05	2.81	2.06	1.21	1.30	131.50	3.30	10.95	−26.92

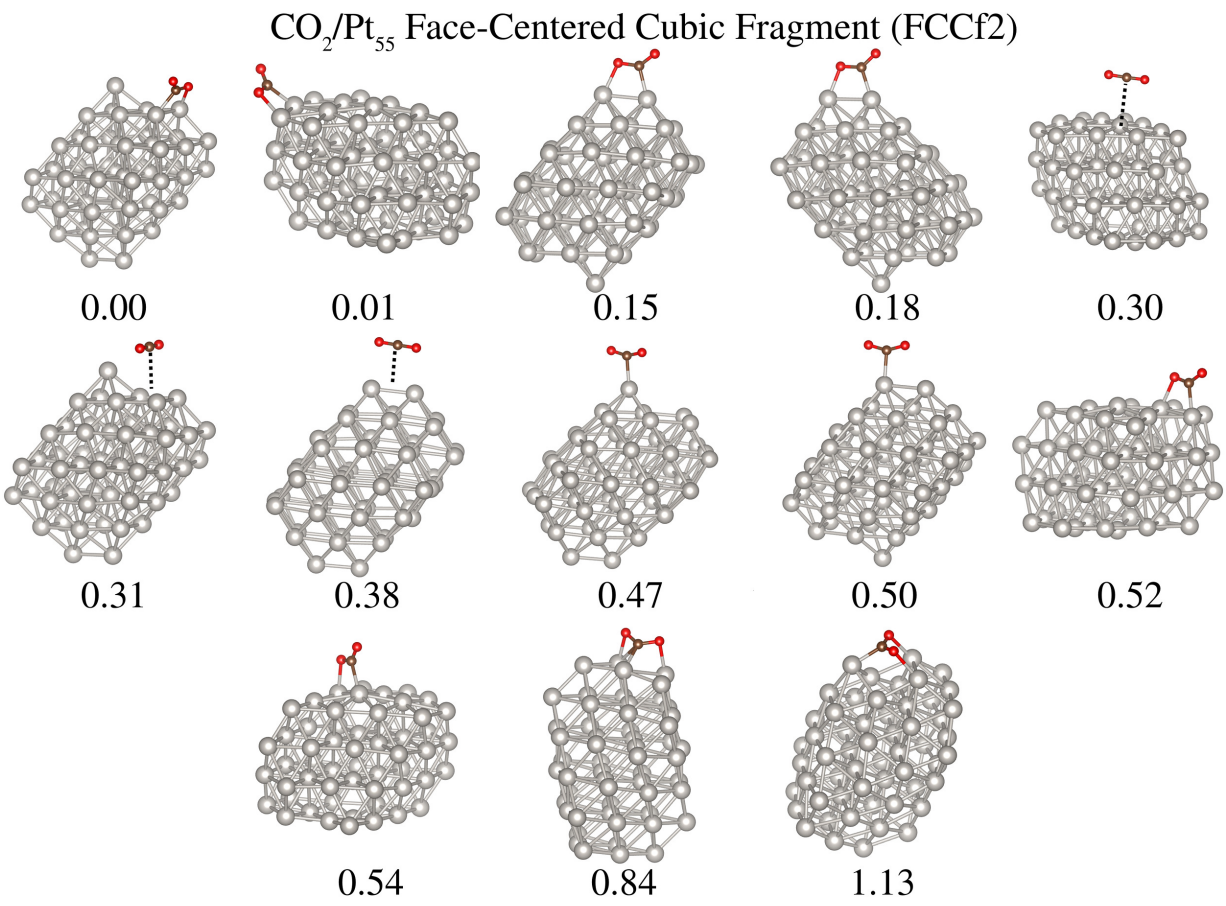

Figure S5: Optimized adsorption configurations for CO_2 interacting with Pt_{55} of the face-centered cubic fragment (FCCf2) morphology. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S8.

Table S8: Adsorption properties for all configurations of CO_2 adsorbed on Pt_{55} of the face-centered cubic fragment (FCCf2) morphology. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{C\text{-}TM}$), O and TM atoms ($d_{O1\text{-}TM}$ and $d_{O2\text{-}TM}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{O1\text{-}C}$ and $d_{O2\text{-}C}$) and OCO angle (Δ_{OCO}).

CO_2/Pt_{55} Face-centered Cubic Fragment (FCCf2)											
ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{C\text{-}TM}$ (Å)	$d_{O1\text{-}TM}$ (Å)	$d_{O2\text{-}TM}$ (Å)	$d_{O1\text{-}C}$ (Å)	$d_{O2\text{-}C}$ (Å)	α_{OCO} (deg)	$\Delta_{O1\text{-}C}$ (%)	$\Delta_{O2\text{-}C}$ (%)	Δ_{OCO} (%)
1.13	0.60	2	2.03	2.22	2.20	1.27	1.27	126.56	8.31	8.53	−29.67
0.84	0.31	2	2.05	2.16	2.16	1.28	1.28	123.90	9.45	9.42	−31.14
0.54	0.02	4	2.07	2.17	2.82	1.29	1.21	132.68	10.03	2.96	−26.27
0.52	0.00	4	2.05	2.20	2.71	1.28	1.22	134.45	8.93	3.87	−25.28
0.50	−0.03	4	2.16	2.78	2.69	1.22	1.21	149.83	3.78	3.31	−16.74
0.47	−0.06	4	2.18	2.71	2.72	1.21	1.21	154.01	2.94	3.03	−14.41
0.38	−0.15	4	3.34	3.11	3.11	1.17	1.17	179.42	0.06	0.07	−0.29
0.31	−0.22	4	3.24	3.39	3.40	1.17	1.17	178.78	0.10	0.09	−0.65
0.30	−0.23	4	3.18	3.38	3.43	1.17	1.17	178.10	0.08	0.10	−1.02
0.18	−0.35	4	2.04	2.79	2.10	1.21	1.29	134.35	3.15	9.70	−25.34
0.15	−0.37	2	2.05	2.14	2.78	1.28	1.21	135.54	9.14	3.23	−24.67
0.01	−0.52	2	2.01	2.04	2.82	1.31	1.21	129.90	11.95	3.25	−27.81
0.00	−0.53	2	2.02	2.09	2.72	1.29	1.22	132.98	9.93	3.74	−26.10

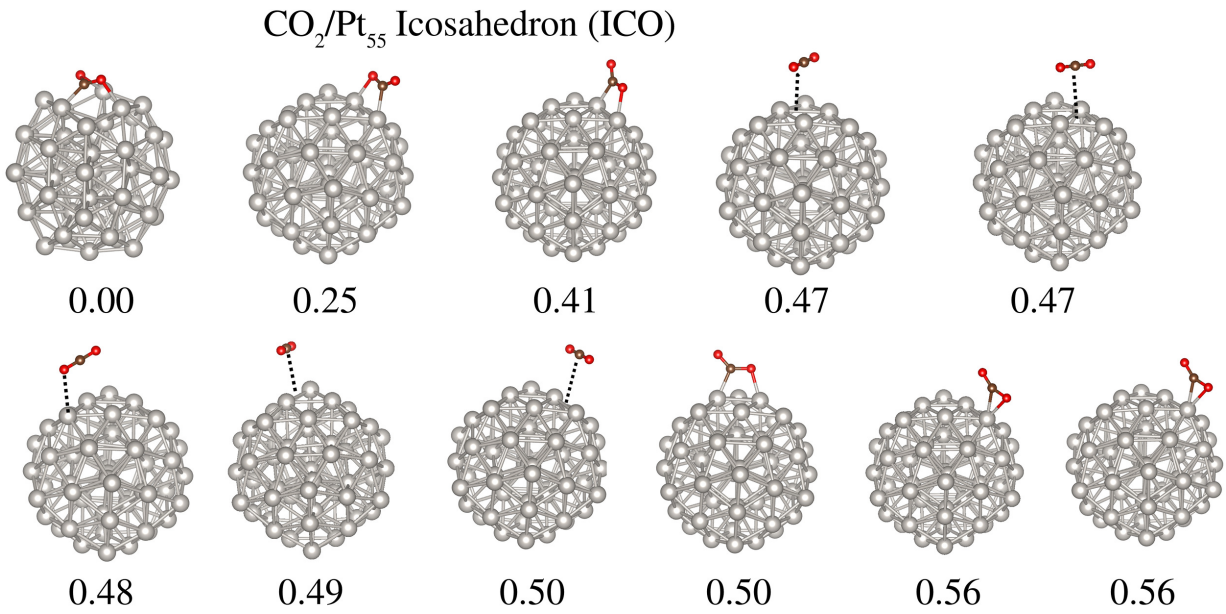

Figure S6: Optimized adsorption configurations for CO_2 interacting with Pt_{55} of the icosahedron (ICO) morphology. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S9.

Table S9: Adsorption properties for all configurations of CO_2 adsorbed on Pt_{55} of the icosahedron (ICO) morphology. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

CO_2/Pt_{55} Icosahedron (ICO)											
ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
0.56	−0.38	12.00	2.18	2.26	3.09	1.23	1.19	152.08	5.27	1.43	−15.49
0.56	−0.38	12.00	2.19	3.10	2.24	1.19	1.23	152.49	1.22	5.25	−15.26
0.50	−0.44	8.00	2.08	2.81	2.10	1.21	1.29	132.09	3.16	10.33	−26.59
0.50	−0.44	12.00	3.23	3.21	3.52	1.17	1.17	178.93	0.16	0.00	−0.56
0.49	−0.46	12.00	3.30	3.25	2.96	1.17	1.18	179.23	−0.11	0.29	−0.40
0.48	−0.46	12.00	3.53	3.00	4.01	1.18	1.17	179.30	0.28	−0.20	−0.36
0.47	−0.47	12.00	3.34	3.45	3.10	1.17	1.18	179.26	−0.09	0.22	−0.38
0.47	−0.47	12.00	3.38	3.44	3.38	1.17	1.17	179.19	−0.03	0.05	−0.42
0.41	−0.53	12.00	2.05	2.09	2.78	1.29	1.21	131.34	10.40	3.19	−27.01
0.25	−0.69	8.00	2.06	2.13	2.68	1.27	1.22	136.33	8.22	3.77	−24.24
0.00	−0.94	6.00	2.03	2.34	2.14	1.28	1.28	124.37	9.28	9.37	−30.89

S7 CO_2 Adsorption on Unary TM and Binary PtTM Nanoclusters

The complete set of optimized adsorption structures evaluated for the adsorption of CO_2 on unary TM_{55} clusters and Pt-based nanoalloys are shown in Figures S7 to S22.

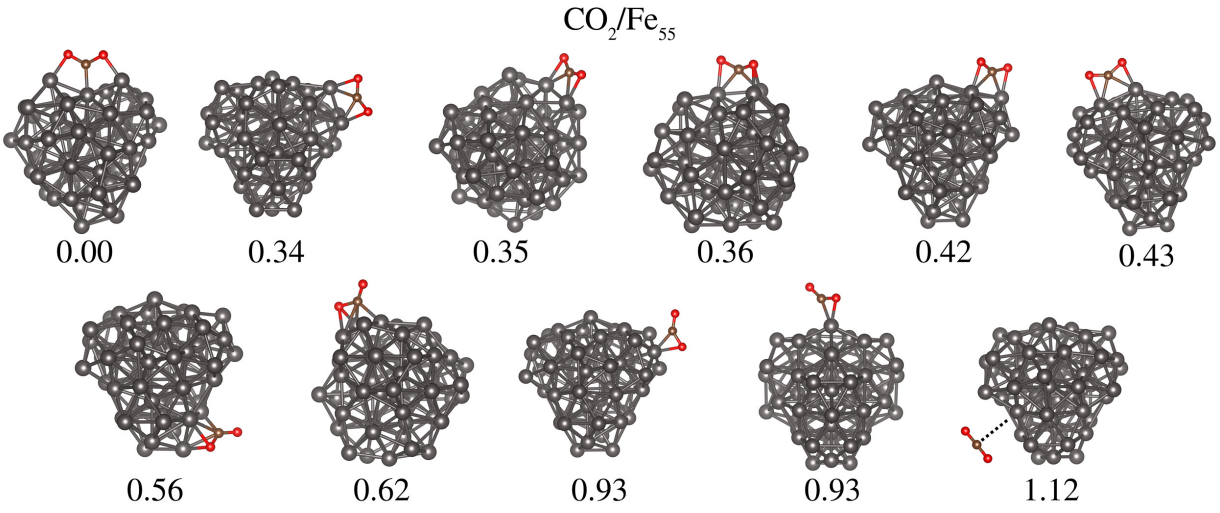

Figure S7: Optimized adsorption configurations for CO_2 interacting with the unary Fe_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S10.

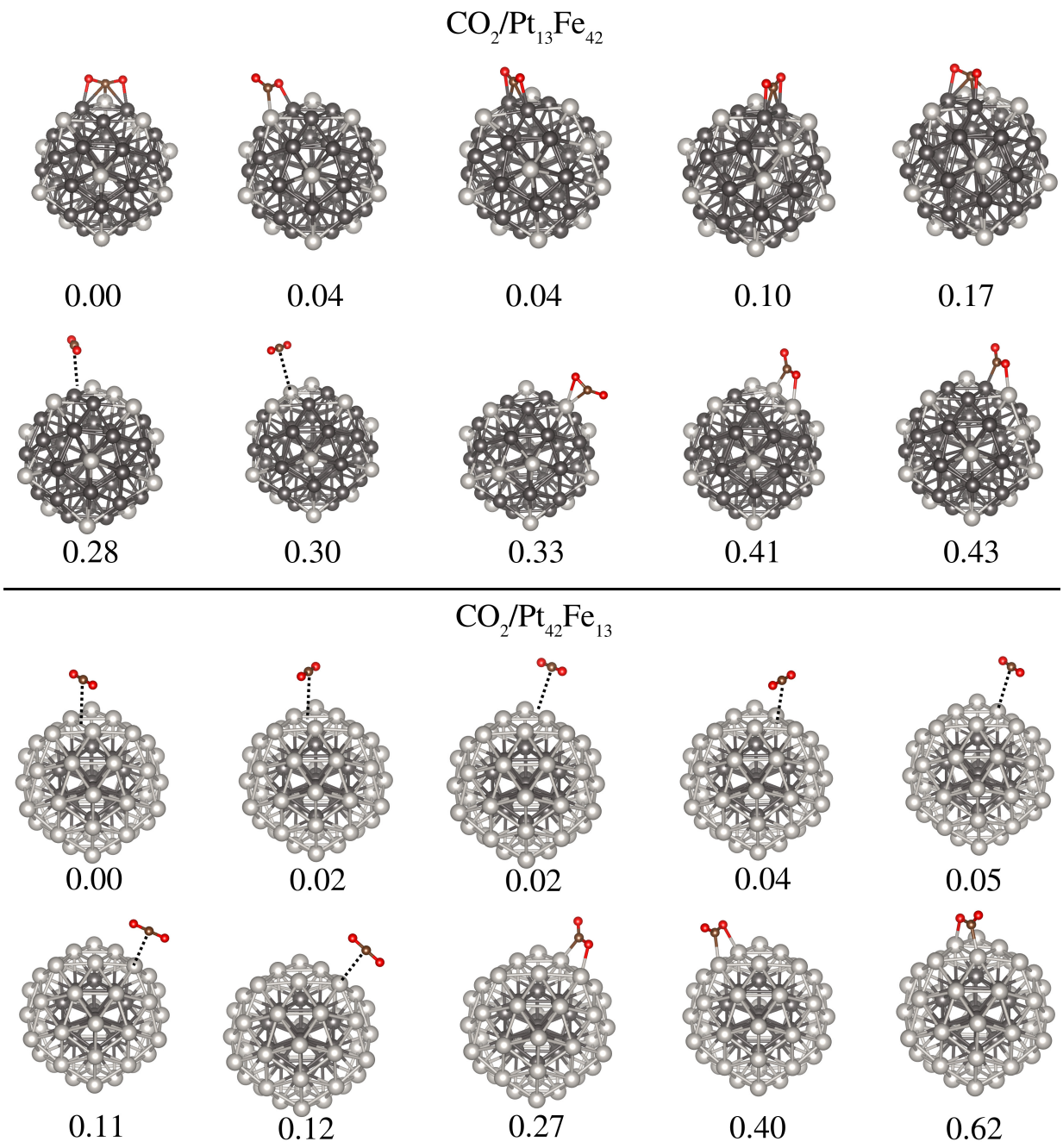

Figure S8: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Fe_{42}$ and $Pt_{42}Fe_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S10.

Table S10: Adsorption properties for all configurations of CO_2 adsorbed on Fe_{55}, $Pt_{13}Fe_{42}$ and $Pt_{42}Fe_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Fe_{55}											
1.12	−0.23	154	3.56	3.04	3.00	1.17	1.17	178.36	0.02	0.11	−0.88
0.93	−0.41	154	1.94	1.93	3.05	1.29	1.21	139.06	9.59	3.09	−22.72
0.93	−0.41	152	1.93	1.99	3.03	1.28	1.21	139.48	9.21	3.41	−22.48
0.62	−0.72	154	1.97	2.02	2.65	1.35	1.23	127.45	14.69	4.88	−29.17
0.56	−0.78	154	1.96	2.62	2.03	1.23	1.33	129.22	4.60	13.68	−28.19
0.43	−0.91	152	2.03	2.14	2.03	1.25	1.26	136.84	6.45	7.39	−23.95
0.42	−0.92	152	2.05	2.11	2.04	1.25	1.26	135.28	6.91	7.66	−24.82
0.36	−0.98	152	1.99	2.13	2.02	1.26	1.31	129.60	7.22	12.02	−27.98
0.35	−0.99	152	1.98	2.04	2.11	1.26	1.25	137.20	7.42	6.73	−23.75
0.34	−1.00	154	1.99	2.04	2.07	1.26	1.26	137.36	7.24	7.02	−23.66
0.00	−1.34	152	1.96	2.02	1.99	1.29	1.29	123.01	9.61	10.06	−31.64
CO_2/$Pt_{13}Fe_{42}$											
0.43	0.00	122	1.99	2.76	2.10	1.22	1.30	130.53	4.03	10.94	−27.46
0.41	−0.02	122	2.08	2.73	2.16	1.22	1.28	133.14	3.91	9.11	−26.01
0.33	−0.10	124	2.13	3.02	2.37	1.20	1.24	147.13	2.51	5.85	−18.24
0.30	−0.14	124	3.37	3.75	3.40	1.17	1.17	178.89	0.04	0.09	−0.59
0.28	−0.15	124	3.36	3.09	3.54	1.17	1.17	179.19	0.18	−0.06	−0.42
0.17	−0.26	124	2.11	2.07	2.06	1.28	1.28	127.69	8.88	8.90	−29.04
0.10	−0.34	124	2.09	2.13	2.15	1.24	1.24	139.21	6.15	6.05	−22.64
0.04	−0.39	124	2.09	2.12	2.10	1.25	1.25	137.83	6.26	6.51	−23.40
0.04	−0.39	122	2.06	2.75	1.97	1.22	1.29	133.37	3.92	9.60	−25.88
0.00	−0.43	124	2.05	2.06	2.04	1.28	1.28	128.67	8.71	8.81	−28.50
CO_2/$Pt_{42}Fe_{13}$											
0.62	0.40	36	2.09	2.13	2.82	1.29	1.21	132.47	9.83	2.99	−26.38
0.40	0.18	38	2.14	2.29	2.71	1.25	1.21	140.47	6.45	3.35	−21.93
0.27	0.05	38	2.06	2.77	2.14	1.21	1.28	135.22	2.98	9.00	−24.85
0.12	−0.10	38	3.12	3.36	3.32	1.17	1.17	179.28	0.10	0.13	−0.37
0.11	−0.11	38	3.10	3.51	3.13	1.17	1.18	178.99	−0.04	0.28	−0.53
0.05	−0.17	38	3.24	3.55	3.35	1.17	1.17	179.11	0.04	0.08	−0.46
0.04	−0.18	38	3.38	3.34	3.36	1.17	1.17	179.26	0.06	0.03	−0.38
0.02	−0.20	38	3.38	3.15	3.16	1.17	1.17	179.60	−0.01	0.12	−0.19
0.02	−0.21	38	3.42	3.50	3.52	1.17	1.17	179.18	0.03	0.04	−0.42
0.00	−0.22	38	3.42	3.24	3.19	1.17	1.17	179.25	0.01	0.07	−0.39

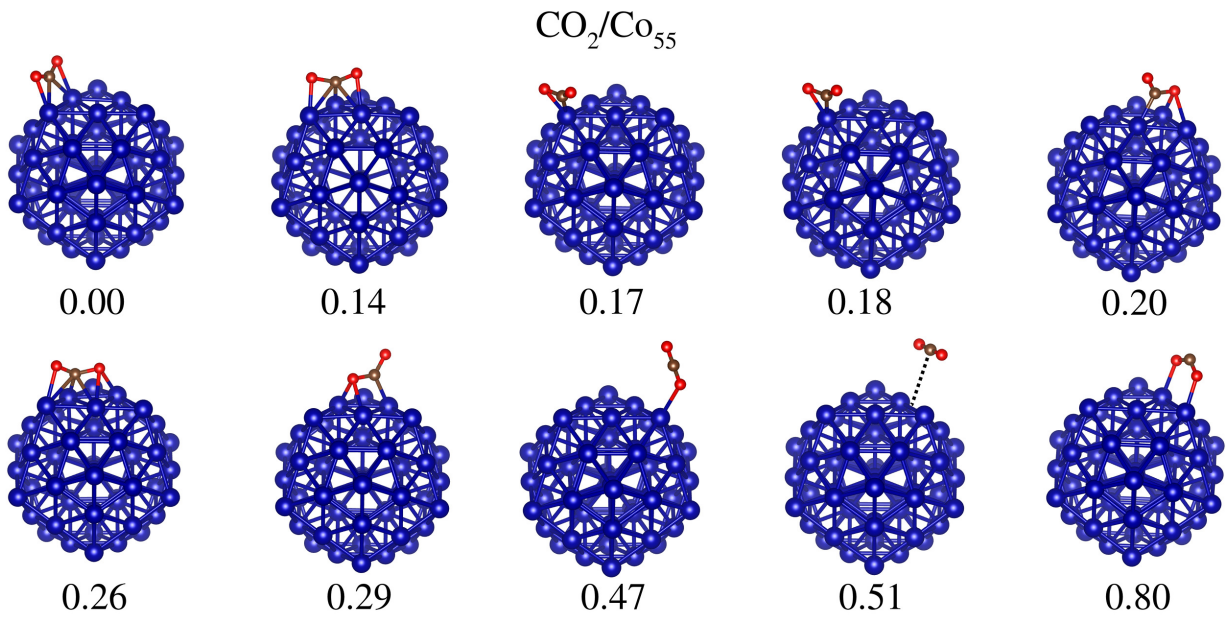

Figure S9: Optimized adsorption configurations for CO_2 interacting with the unary Co_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S11.

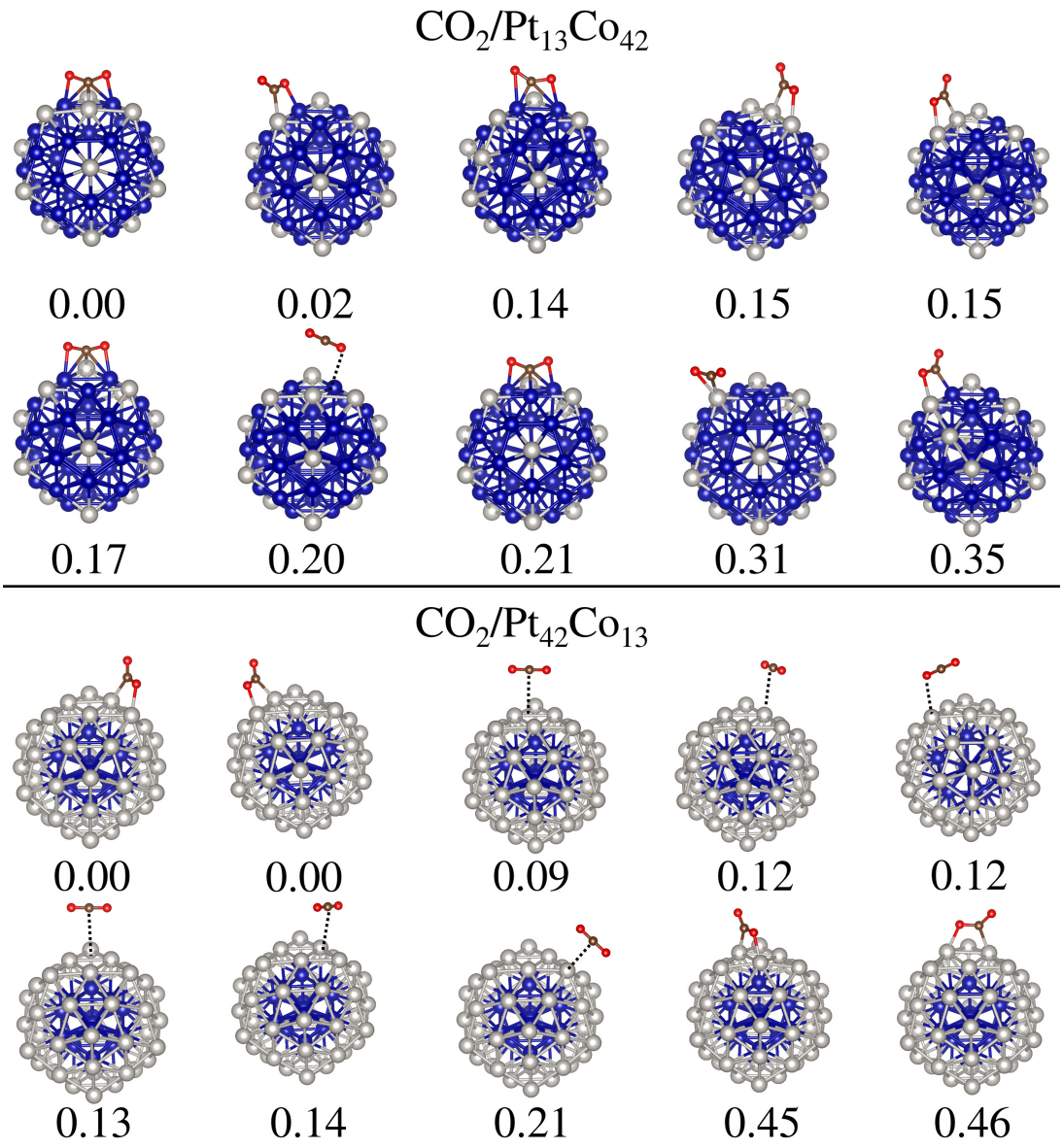

Figure S10: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Co_{42}$ and $Pt_{42}Co_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S11.

Table S11: Adsorption properties for all configurations of CO_2 adsorbed on Co_{55}, $Pt_{13}Co_{42}$ and $Pt_{42}Co_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Co_{55}											
0.80	0.15	103	2.78	1.96	2.07	1.25	1.23	134.15	6.29	5.19	−25.45
0.51	−0.14	105	3.35	3.10	3.21	1.17	1.17	178.99	0.01	0.14	−0.53
0.47	−0.18	105	3.23	4.29	2.27	1.17	1.18	179.97	−0.50	0.61	0.01
0.29	−0.36	103	1.92	2.08	2.73	1.34	1.22	127.79	14.35	3.81	−28.98
0.26	−0.39	103	1.91	2.15	2.15	1.28	1.31	125.89	8.99	12.10	−30.04
0.20	−0.45	103	1.93	2.72	2.03	1.22	1.33	128.88	3.68	13.72	−28.38
0.18	−0.47	103	1.94	1.94	3.01	1.27	1.20	143.54	8.11	2.47	−20.23
0.17	−0.48	103	1.93	1.94	2.99	1.27	1.20	143.71	8.13	2.46	−20.14
0.14	−0.51	103	1.97	2.08	1.94	1.28	1.30	126.51	8.77	11.04	−29.69
0.00	−0.65	103	1.94	2.16	2.04	1.24	1.26	138.93	5.78	7.03	−22.79
CO_2/$Pt_{13}Co_{42}$											
0.35	−0.06	84	1.95	2.73	2.13	1.22	1.29	132.40	3.84	10.17	−26.42
0.31	−0.10	88	2.14	2.31	3.06	1.24	1.20	147.48	6.08	2.25	−18.04
0.21	−0.20	84	1.95	2.01	2.04	1.29	1.28	125.30	9.80	9.43	−30.37
0.20	−0.21	86	3.16	3.90	2.59	1.17	1.18	178.83	−0.37	0.53	−0.62
0.17	−0.24	86	2.09	2.07	2.07	1.27	1.27	129.35	8.41	8.27	−28.11
0.15	−0.26	84	2.07	2.15	2.85	1.29	1.21	131.89	10.29	3.39	−26.70
0.15	−0.26	86	2.08	2.85	2.14	1.21	1.29	131.73	3.38	10.35	−26.79
0.14	−0.27	86	1.94	2.42	2.05	1.23	1.27	137.66	4.59	7.92	−23.50
0.02	−0.39	88	2.08	2.75	1.99	1.22	1.28	134.00	3.97	9.10	−25.53
0.00	−0.41	84	2.07	2.05	2.05	1.28	1.28	126.34	8.91	8.87	−29.79
CO_2/$Pt_{42}Co_{13}$											
0.46	0.13	33	2.07	2.10	2.82	1.29	1.21	132.17	10.08	2.97	−26.55
0.45	−0.12	33	2.07	2.82	2.10	1.21	1.29	132.30	3.02	10.10	−26.47
0.21	−0.11	35	3.02	3.27	3.24	1.17	1.17	178.26	0.13	0.16	−0.93
0.14	−0.19	35	3.22	3.18	3.68	1.17	1.17	178.97	0.16	−0.05	−0.54
0.13	−0.19	35	3.34	3.39	3.48	1.17	1.17	179.22	0.05	0.09	−0.40
0.12	−0.21	35	3.36	2.93	3.68	1.18	1.17	179.35	0.28	−0.25	−0.33
0.12	−0.21	35	3.33	3.29	3.09	1.17	1.17	179.27	−0.10	0.17	−0.38
0.09	−0.23	35	3.43	3.32	3.27	1.17	1.17	179.23	−0.01	0.05	−0.40
0.00	−0.33	33	2.04	2.83	2.07	1.21	1.30	131.65	2.75	10.98	−26.84
0.00	−0.33	33	2.04	2.82	2.06	1.21	1.30	131.80	2.79	10.93	−26.76

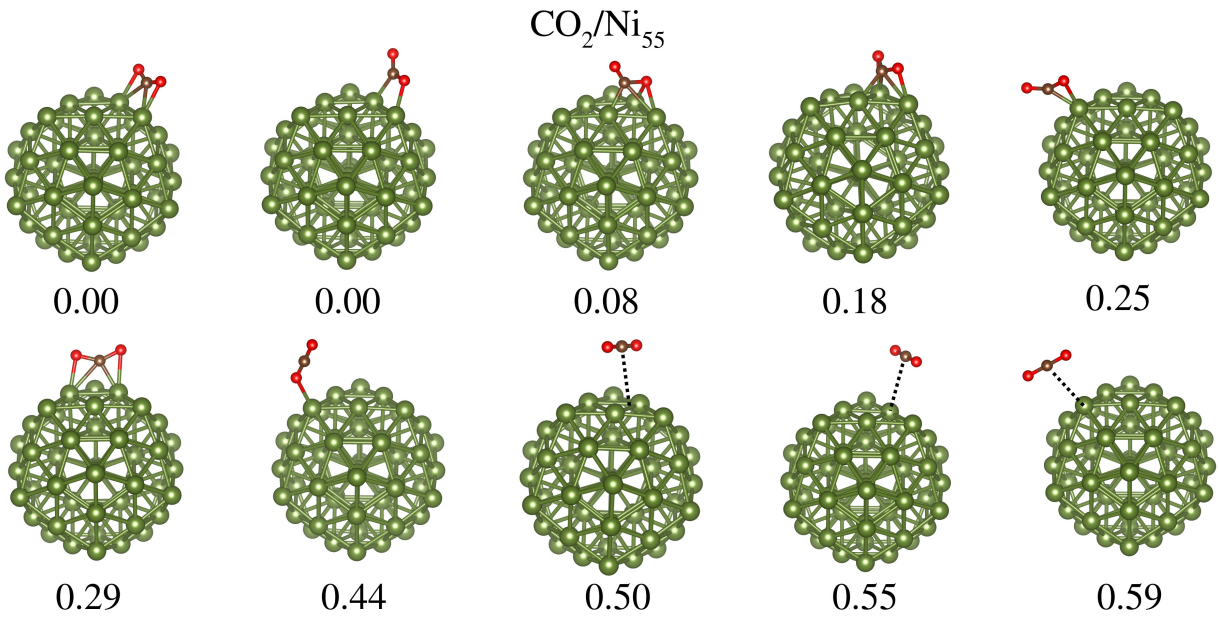

Figure S11: Optimized adsorption configurations for CO_2 interacting with the unary Ni_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S12.

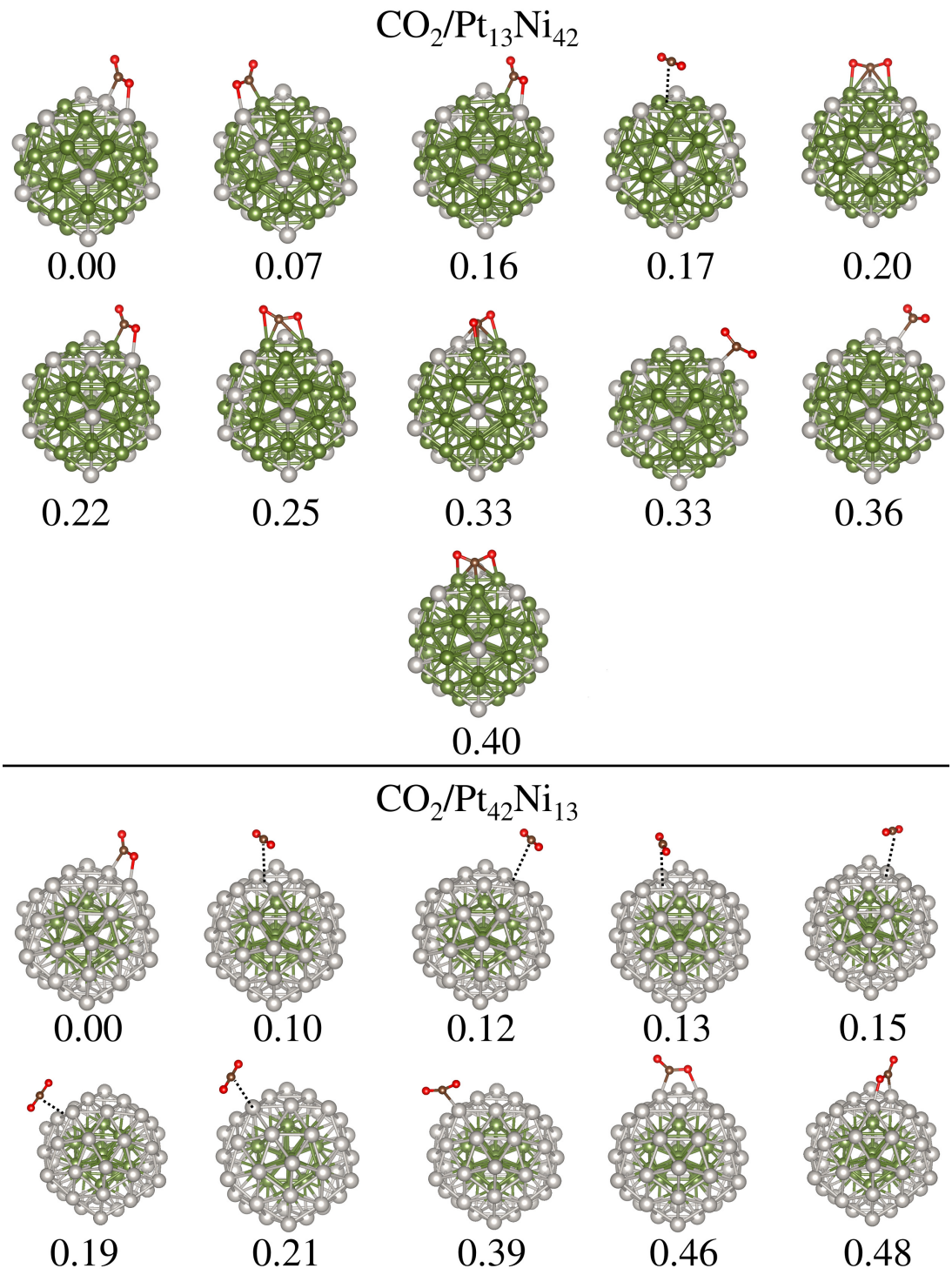

Figure S12: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Ni_{42}$ and $Pt_{42}Ni_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S12.

Table S12: Adsorption properties for all configurations of CO_2 adsorbed on Ni_{55}, $Pt_{13}Ni_{42}$ and $Pt_{42}Ni_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Ni_{55}											
0.59	−0.09	40	3.04	3.10	3.43	1.18	1.17	179.39	0.23	−0.02	−0.31
0.55	−0.13	40	3.09	3.29	3.21	1.17	1.17	178.68	0.07	0.07	−0.70
0.50	−0.19	40	3.34	2.97	3.33	1.18	1.17	178.80	0.19	−0.05	−0.64
0.44	−0.24	40	3.13	4.19	2.17	1.17	1.18	179.61	−0.49	0.61	−0.18
0.29	−0.40	40	1.92	2.04	2.22	1.25	1.23	140.11	6.70	5.13	−22.14
0.25	−0.44	38	1.93	1.96	2.95	1.25	1.20	148.24	6.59	2.04	−17.62
0.18	−0.51	38	1.98	2.03	1.95	1.27	1.29	130.30	7.92	9.62	−27.59
0.08	−0.61	40	1.88	2.71	2.00	1.21	1.34	129.03	3.15	14.53	−28.29
0.00	−0.69	38	1.90	2.67	1.89	1.21	1.29	133.72	3.44	10.34	−25.69
0.00	−0.69	38	1.88	2.04	2.10	1.24	1.24	141.71	5.86	5.93	−21.25
CO_2/$Pt_{13}Ni_{42}$											
0.40	0.05	40	2.00	2.05	2.24	1.27	1.26	131.44	8.39	7.44	−26.95
0.36	0.00	40	2.14	2.78	2.79	1.23	1.23	143.03	4.47	4.46	−20.52
0.33	−0.03	40	2.17	2.89	2.57	1.20	1.22	150.48	2.70	4.26	−16.38
0.33	−0.03	40	2.11	2.12	2.11	1.26	1.27	130.67	7.81	7.91	−27.38
0.25	−0.11	40	1.94	2.02	2.46	1.26	1.22	139.17	7.41	3.92	−22.66
0.22	−0.14	40	1.91	2.17	2.64	1.28	1.21	135.34	9.03	3.56	−24.79
0.20	−0.15	40	2.09	2.11	2.07	1.26	1.26	133.13	7.32	7.84	−26.01
0.17	−0.18	40	3.32	3.10	3.10	1.17	1.17	179.01	0.11	0.08	−0.52
0.16	−0.19	40	1.91	2.15	2.66	1.28	1.21	134.18	9.53	3.55	−25.43
0.07	−0.28	40	1.90	2.66	2.15	1.22	1.28	134.62	3.66	9.42	−25.19
0.00	−0.35	40	2.05	2.84	2.13	1.21	1.30	131.58	3.28	10.68	−26.88
CO_2/$Pt_{42}Ni_{13}$											
0.48	0.13	20	2.07	2.83	2.09	1.21	1.30	131.53	2.84	10.50	−26.90
0.46	0.10	20	2.07	2.10	2.83	1.29	1.21	131.90	10.12	2.91	−26.70
0.39	0.04	22	2.22	2.57	2.90	1.20	1.21	155.25	1.92	3.45	−13.72
0.21	−0.15	22	3.18	3.28	3.42	1.17	1.17	178.99	0.10	0.08	−0.53
0.19	−0.17	22	3.18	3.62	3.15	1.17	1.18	179.11	−0.09	0.26	−0.46
0.15	−0.21	22	3.19	3.52	3.29	1.17	1.17	178.87	−0.03	0.13	−0.59
0.13	−0.23	22	3.45	3.37	3.41	1.17	1.17	179.17	0.04	0.01	−0.43
0.12	−0.24	22	3.45	3.17	3.31	1.17	1.17	179.56	0.14	0.00	−0.21
0.10	−0.25	22	3.46	3.24	3.23	1.17	1.17	179.26	0.03	0.03	−0.38
0.00	−0.36	20	2.05	2.83	2.07	1.21	1.30	132.24	2.79	10.53	−26.51

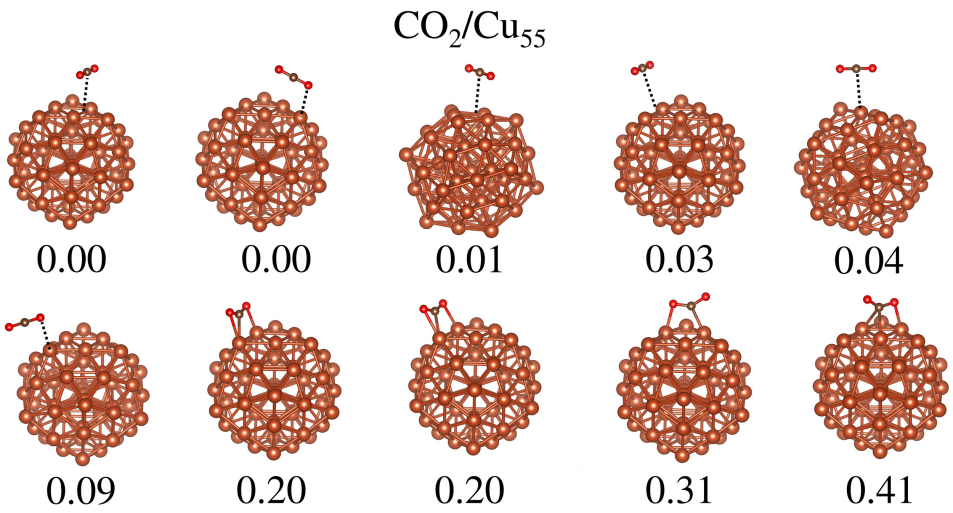

Figure S13: Optimized adsorption configurations for CO_2 interacting with the unary Cu_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S13.

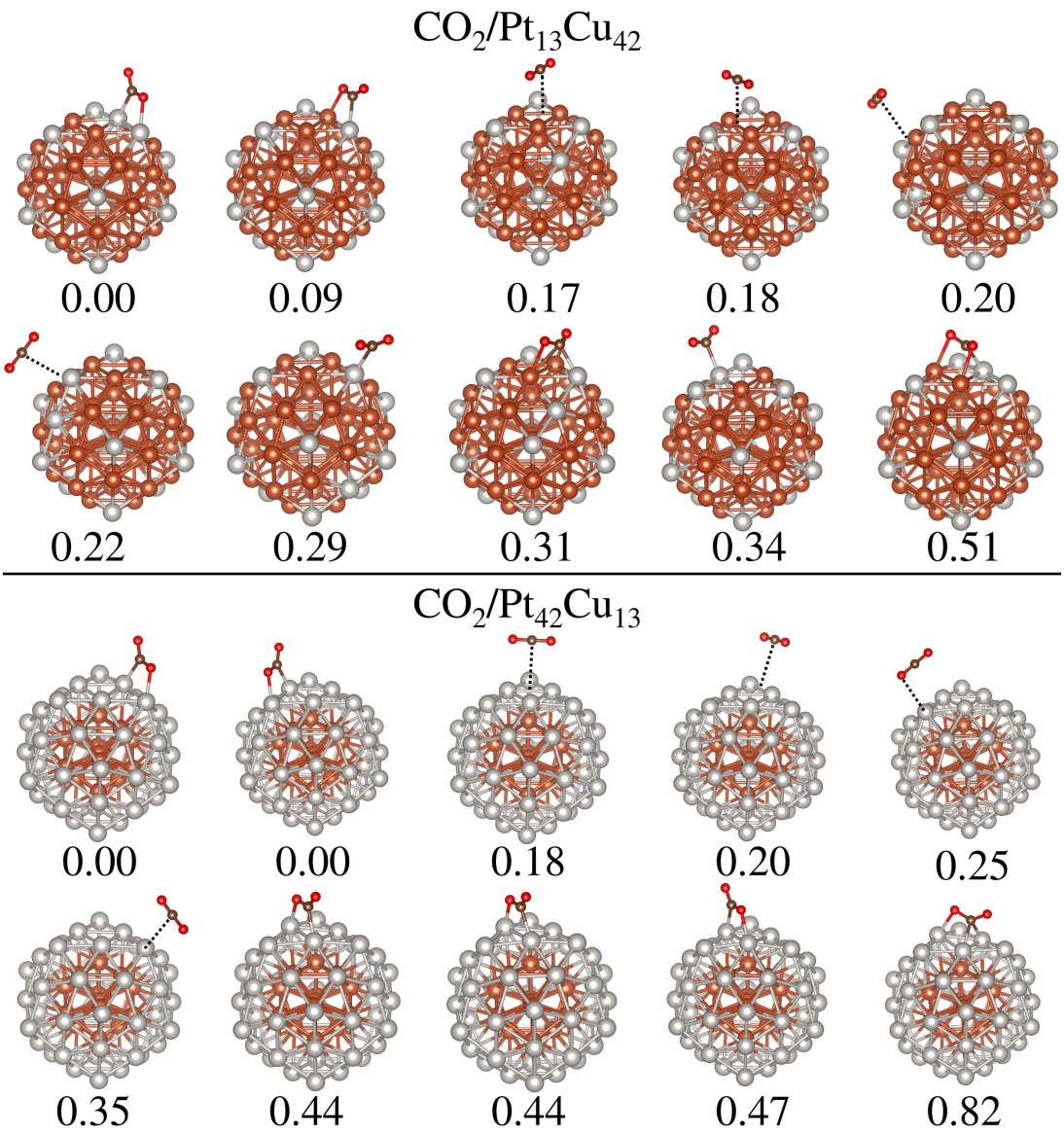

Figure S14: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Cu_{42}$ and $Pt_{42}Cu_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S13.

Table S13: Adsorption properties for all configurations of CO_2 adsorbed on Cu_{55}, $Pt_{13}Cu_{42}$ and $Pt_{42}Cu_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Cu_{55}											
0.41	0.25	1	2.31	2.85	2.08	1.22	1.26	136.68	3.98	7.29	−24.04
0.31	0.15	1	2.10	2.10	2.58	1.25	1.21	140.07	6.38	3.44	−22.16
0.20	0.04	1	2.06	2.16	2.37	1.23	1.22	145.11	4.71	3.69	−19.36
0.20	0.03	1	2.06	2.34	2.18	1.22	1.23	145.43	3.78	4.54	−19.18
0.09	−0.07	3	2.99	3.50	2.91	1.17	1.18	179.49	−0.11	0.28	−0.25
0.04	−0.12	3	3.14	3.31	3.42	1.17	1.17	179.03	0.06	0.06	−0.51
0.03	−0.13	3	3.26	3.54	3.34	1.17	1.17	179.23	0.06	0.08	−0.40
0.01	−0.15	3	3.48	3.10	3.53	1.17	1.17	179.06	0.08	0.04	−0.49
0.00	−0.16	3	3.15	2.65	3.57	1.18	1.17	179.41	0.40	−0.27	−0.29
0.00	−0.16	3	3.38	3.23	3.12	1.17	1.17	179.08	0.02	0.08	−0.48
$CO_2/Pt_{13}Cu_{42}$											
0.51	0.15	2	2.08	2.27	2.34	1.26	1.25	133.69	7.02	6.20	−25.70
0.34	−0.02	2	2.12	2.77	2.77	1.23	1.23	142.83	4.58	4.57	−20.62
0.31	−0.05	2	2.06	2.27	2.23	1.24	1.26	135.84	5.77	7.07	−24.51
0.29	−0.07	2	2.16	2.73	2.72	1.21	1.21	152.09	3.17	3.21	−15.48
0.22	−0.14	2	3.23	3.23	3.61	1.17	1.17	178.68	0.17	−0.05	−0.70
0.20	−0.16	2	3.16	3.41	3.35	1.17	1.17	179.69	0.04	0.10	−0.14
0.18	−0.18	2	3.28	3.16	3.01	1.17	1.17	179.43	0.01	0.12	−0.28
0.17	−0.19	2	3.47	3.22	3.24	1.17	1.17	179.83	0.07	0.03	−0.06
0.09	−0.27	2	2.07	2.67	2.05	1.22	1.26	138.00	4.09	7.31	−23.31
0.00	−0.36	2	2.06	2.82	2.11	1.21	1.29	132.30	3.23	10.04	−26.47
$CO_2/Pt_{42}Cu_{13}$											
0.82	0.43	5	2.12	2.22	2.51	1.28	1.26	131.72	9.48	7.38	−26.80
0.47	0.08	5	2.06	2.10	2.82	1.29	1.21	132.14	10.07	2.96	−26.57
0.44	0.05	7	2.06	2.82	2.10	1.21	1.29	132.08	2.93	10.13	−26.60
0.44	0.05	7	2.06	2.10	2.82	1.29	1.21	132.15	10.19	2.94	−26.56
0.35	−0.04	5	3.06	3.32	3.27	1.17	1.17	178.40	0.13	0.16	−0.86
0.25	−0.14	9	3.36	3.98	3.07	1.17	1.18	179.74	−0.21	0.26	−0.11
0.20	−0.19	9	3.49	3.18	3.46	1.18	1.17	179.97	0.19	−0.10	0.02
0.18	−0.21	9	3.55	3.31	3.29	1.17	1.17	179.31	0.01	−0.03	−0.35
0.00	−0.39	7	2.04	2.83	2.06	1.21	1.30	131.50	2.77	10.89	−26.92
0.00	−0.39	7	2.04	2.82	2.07	1.21	1.30	132.29	2.74	10.70	−26.48

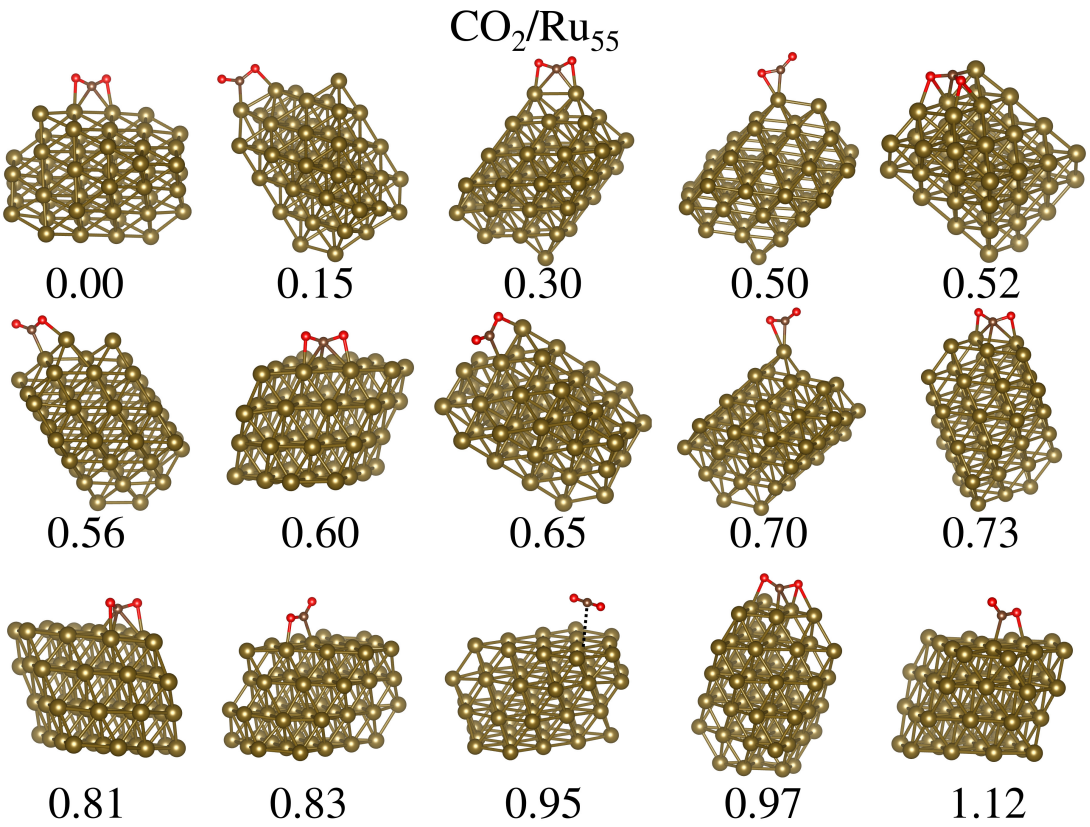

Figure S15: Optimized adsorption configurations for CO_2 interacting with the unary Ru_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S14.

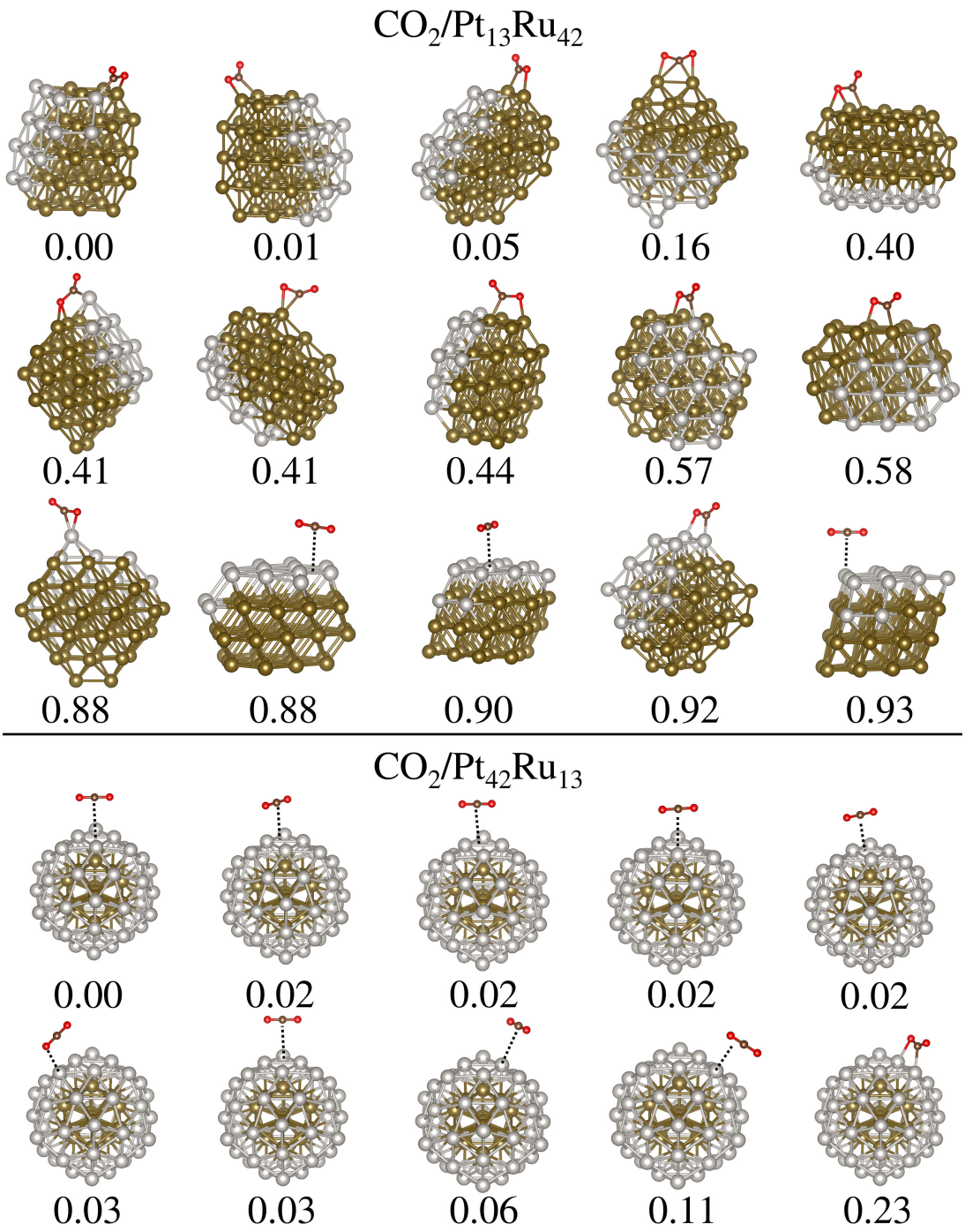

Figure S16: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Ru_{42}$ and $Pt_{42}Ru_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S14.

Table S14: Adsorption properties for all configurations of CO_2 adsorbed on Ru_{55}, $Pt_{13}Ru_{42}$ and $Pt_{42}Ru_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Ru_{55}											
1.12	−0.03	6	2.13	2.86	2.12	1.22	1.30	129.24	4.15	10.75	−28.18
0.97	−0.18	6	2.06	2.33	2.38	1.32	1.27	124.09	12.64	8.41	−31.04
0.95	−0.20	6	3.43	3.46	3.43	1.17	1.18	178.60	−0.09	0.25	−0.75
0.83	−0.32	4	2.11	2.79	2.12	1.22	1.30	130.84	4.04	10.51	−27.29
0.81	−0.34	4	2.10	2.18	2.17	1.29	1.29	123.50	10.30	10.33	−31.37
0.73	−0.41	6	2.11	2.15	2.15	1.30	1.30	122.37	10.96	10.93	−31.99
0.70	−0.45	4	2.13	2.38	3.03	1.25	1.21	145.80	6.53	2.89	−18.97
0.65	−0.50	6	2.11	2.87	2.05	1.22	1.31	130.12	3.80	11.57	−27.69
0.60	−0.54	6	2.13	2.12	2.16	1.30	1.30	123.34	10.53	10.45	−31.46
0.56	−0.59	4	2.09	2.05	2.95	1.33	1.22	128.32	13.11	3.71	−28.69
0.52	−0.63	6	2.07	2.18	2.19	1.32	1.31	119.72	12.78	11.81	−33.47
0.50	−0.65	6	2.05	3.10	2.12	1.21	1.28	141.73	2.78	8.85	−21.24
0.30	−0.85	4	2.07	2.14	2.24	1.26	1.25	135.80	7.68	6.62	−24.53
0.15	−1.00	6	2.00	2.60	2.08	1.23	1.29	133.68	4.99	10.21	−25.71
0.00	−1.15	6	2.19	2.19	2.20	1.25	1.26	133.98	6.98	7.01	−25.54
CO_2/$Pt_{13}Ru_{42}$											
0.93	−0.25	4	3.50	3.74	3.33	1.17	1.17	178.86	0.04	0.08	−0.60
0.92	−0.25	4	2.07	2.76	2.16	1.22	1.28	134.25	3.72	8.88	−25.39
0.90	−0.28	4	3.25	3.35	3.54	1.17	1.17	178.66	0.06	0.05	−0.71
0.88	−0.29	4	3.47	3.50	3.07	1.17	1.18	178.68	−0.09	0.21	−0.70
0.88	−0.30	4	2.08	3.00	2.27	1.20	1.25	147.78	2.13	6.62	−17.87
0.58	−0.59	4	2.04	2.68	2.15	1.23	1.29	132.00	4.72	10.10	−26.64
0.57	−0.61	4	2.05	2.85	2.10	1.21	1.32	128.52	3.58	12.29	−28.58
0.44	−0.73	4	2.07	2.03	2.83	1.33	1.21	128.87	13.16	3.57	−28.38
0.41	−0.76	4	2.05	3.13	2.07	1.20	1.29	139.32	2.48	10.30	−22.58
0.41	−0.77	4	2.03	2.85	2.12	1.21	1.35	126.25	3.24	15.09	−29.84
0.40	−0.78	4	2.07	2.94	2.14	1.21	1.38	125.13	2.98	17.36	−30.46
0.16	−1.01	4	2.03	2.12	2.29	1.27	1.25	136.72	7.89	6.33	−24.02
0.05	−1.13	6	2.02	2.60	2.07	1.23	1.29	134.58	4.61	9.95	−25.21
0.01	−1.16	4	2.05	2.74	2.04	1.22	1.31	130.98	4.24	11.84	−27.21
0.00	−1.18	4	2.02	2.77	2.00	1.22	1.32	129.10	3.62	12.21	−28.26
CO_2/$Pt_{42}Ru_{13}$											
0.23	−0.02	6	2.09	2.31	2.60	1.25	1.22	140.33	6.32	4.14	−22.01
0.11	−0.14	6	3.18	3.70	3.06	1.17	1.18	179.56	−0.15	0.31	−0.21
0.06	−0.19	6	3.18	3.42	3.37	1.17	1.17	178.99	0.07	0.04	−0.53
0.03	−0.21	6	3.41	3.38	3.38	1.17	1.17	179.08	0.00	0.04	−0.48
0.03	−0.21	6	3.08	3.82	2.69	1.17	1.18	179.07	−0.42	0.64	−0.49
0.02	−0.22	6	3.56	3.39	3.45	1.17	1.17	178.92	−0.03	0.10	−0.57
0.02	−0.22	6	3.37	3.53	3.51	1.17	1.17	178.98	−0.01	0.05	−0.54
0.02	−0.22	6	3.31	3.14	3.39	1.17	1.17	179.09	0.13	−0.07	−0.47
0.02	−0.22	6	3.40	3.52	3.53	1.17	1.17	179.11	−0.01	0.04	−0.46
0.00	−0.24	6	3.46	3.31	3.22	1.17	1.17	179.58	−0.01	0.04	−0.20

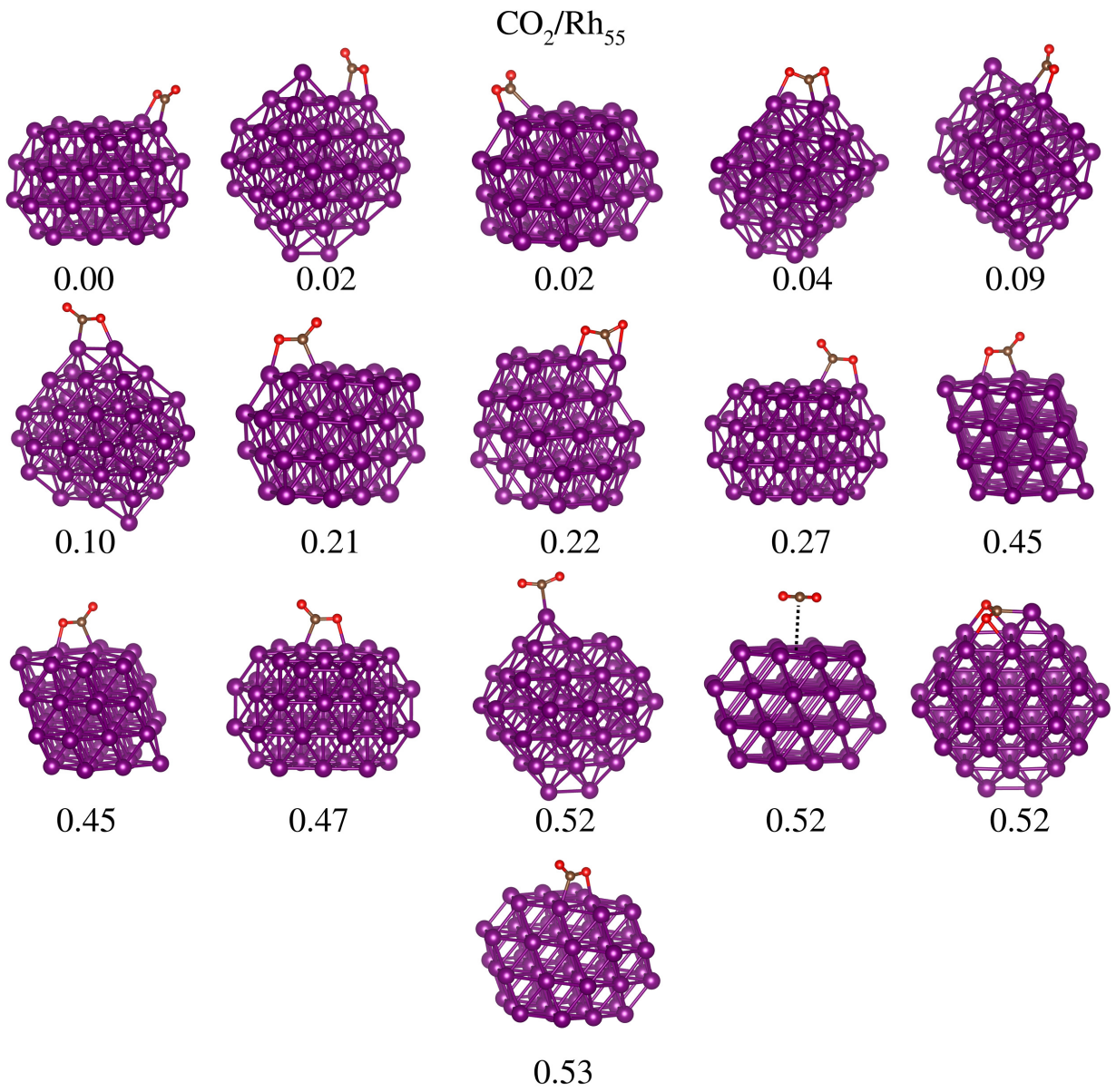

Figure S17: Optimized adsorption configurations for CO_2 interacting with the unary Rh_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S15.

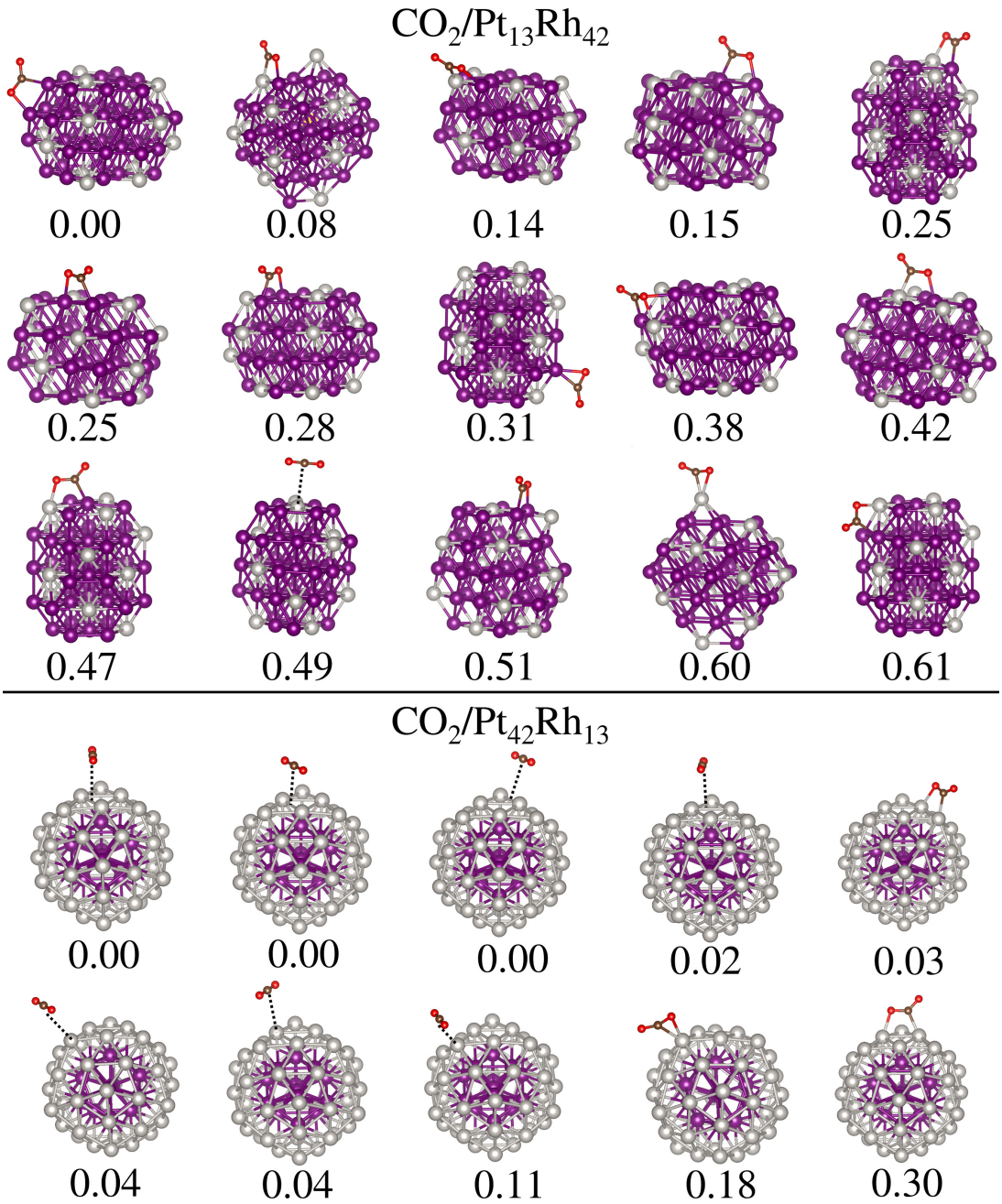

Figure S18: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Rh_{42}$ and $Pt_{42}Rh_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S15.

Table S15: Adsorption properties for all configurations of CO_2 adsorbed on Rh_{55}, $Pt_{13}Rh_{42}$ and $Pt_{42}Rh_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Rh_{55}											
0.53	−0.20	27	2.06	2.75	2.12	1.22	1.28	133.67	3.98	9.29	−25.71
0.52	−0.21	29	2.02	2.21	2.21	1.29	1.30	122.32	10.31	10.81	−32.02
0.52	−0.22	29	3.54	3.38	3.26	1.17	1.17	178.95	−0.01	0.08	−0.55
0.52	−0.22	31	2.08	2.62	2.68	1.22	1.21	151.94	3.71	3.47	−15.56
0.47	−0.26	29	2.06	2.83	2.09	1.22	1.29	131.31	3.72	10.10	−27.02
0.45	−0.28	29	2.06	2.07	2.80	1.29	1.22	130.82	10.32	3.76	−27.30
0.45	−0.29	29	2.06	2.06	2.79	1.29	1.22	130.85	10.32	3.76	−27.28
0.27	−0.46	31	2.05	2.05	2.81	1.30	1.21	130.92	10.93	3.47	−27.24
0.22	−0.52	33	1.99	2.17	2.42	1.26	1.23	138.54	7.14	5.12	−23.01
0.21	−0.52	29	2.05	2.81	2.05	1.21	1.30	130.71	3.47	11.10	−27.36
0.10	−0.64	29	2.03	2.07	2.73	1.29	1.22	134.88	9.61	3.76	−25.04
0.09	−0.64	31	2.05	2.04	2.83	1.30	1.22	130.86	10.45	3.80	−27.28
0.04	−0.70	27	2.02	2.17	2.17	1.28	1.28	127.52	8.82	8.87	−29.13
0.02	−0.71	29	2.03	2.75	2.03	1.22	1.30	132.39	3.77	10.49	−26.43
0.02	−0.71	31	2.03	2.75	2.06	1.22	1.29	132.90	3.94	10.17	−26.14
0.00	−0.73	29	2.02	2.67	2.06	1.22	1.28	134.44	4.05	9.56	−25.29
CO_2/$Pt_{13}Rh_{42}$											
0.61	−0.09	18	2.04	2.08	2.83	1.31	1.21	129.96	11.44	3.29	−27.78
0.60	−0.09	20	2.13	2.92	2.45	1.20	1.23	150.52	2.42	4.91	−16.35
0.51	−0.18	18	2.06	2.14	2.66	1.27	1.22	136.80	8.40	3.86	−23.97
0.49	−0.20	20	3.28	3.55	3.44	1.17	1.17	178.23	0.07	0.01	−0.95
0.47	−0.22	18	2.04	2.08	2.79	1.30	1.21	130.42	11.22	3.43	−27.52
0.42	−0.27	20	2.08	2.86	2.09	1.21	1.29	131.35	3.41	10.00	−27.01
0.38	−0.31	18	2.08	2.24	2.81	1.35	1.22	126.85	14.71	3.95	−29.51
0.31	−0.38	18	2.07	2.15	3.05	1.25	1.20	147.07	6.80	2.12	−18.27
0.28	−0.41	18	2.01	2.57	2.15	1.23	1.27	136.60	4.49	8.37	−24.09
0.25	−0.44	18	2.00	2.11	2.58	1.27	1.22	136.55	8.40	4.34	−24.12
0.25	−0.44	20	1.99	2.59	2.15	1.22	1.27	137.26	4.12	8.54	−23.72
0.15	−0.54	18	2.06	2.81	2.05	1.21	1.30	131.58	3.32	10.85	−26.88
0.14	−0.55	20	2.06	2.78	2.08	1.21	1.28	134.09	3.53	9.46	−25.48
0.08	−0.61	18	2.06	2.05	2.83	1.29	1.21	131.88	10.32	3.51	−26.71
0.00	−0.69	18	2.02	2.64	2.08	1.22	1.28	136.05	4.05	9.02	−24.39
CO_2/$Pt_{42}Rh_{13}$											
0.30	0.04	21	2.08	2.12	2.81	1.29	1.21	131.70	10.32	3.07	−26.81
0.18	−0.08	19	2.25	3.12	2.32	1.19	1.22	155.28	1.06	4.31	−13.70
0.11	−0.16	19	3.11	3.57	3.07	1.17	1.18	179.28	−0.10	0.32	−0.37
0.04	−0.22	19	3.19	3.47	3.36	1.17	1.17	178.85	0.06	0.11	−0.61
0.04	−0.22	19	4.02	3.29	2.87	1.17	1.18	179.71	−0.34	0.42	−0.13
0.03	−0.24	19	2.07	2.16	2.68	1.27	1.22	136.56	8.05	3.72	−24.11
0.02	−0.24	19	3.38	3.53	3.62	1.17	1.17	179.10	0.11	0.01	−0.47
0.00	−0.26	19	3.35	3.13	3.09	1.17	1.17	179.55	−0.03	0.16	−0.22
0.00	−0.26	19	3.37	3.21	3.18	1.17	1.17	179.21	0.03	0.05	−0.41
0.00	−0.27	19	3.47	3.40	3.41	1.17	1.17	179.17	0.02	0.01	−0.43

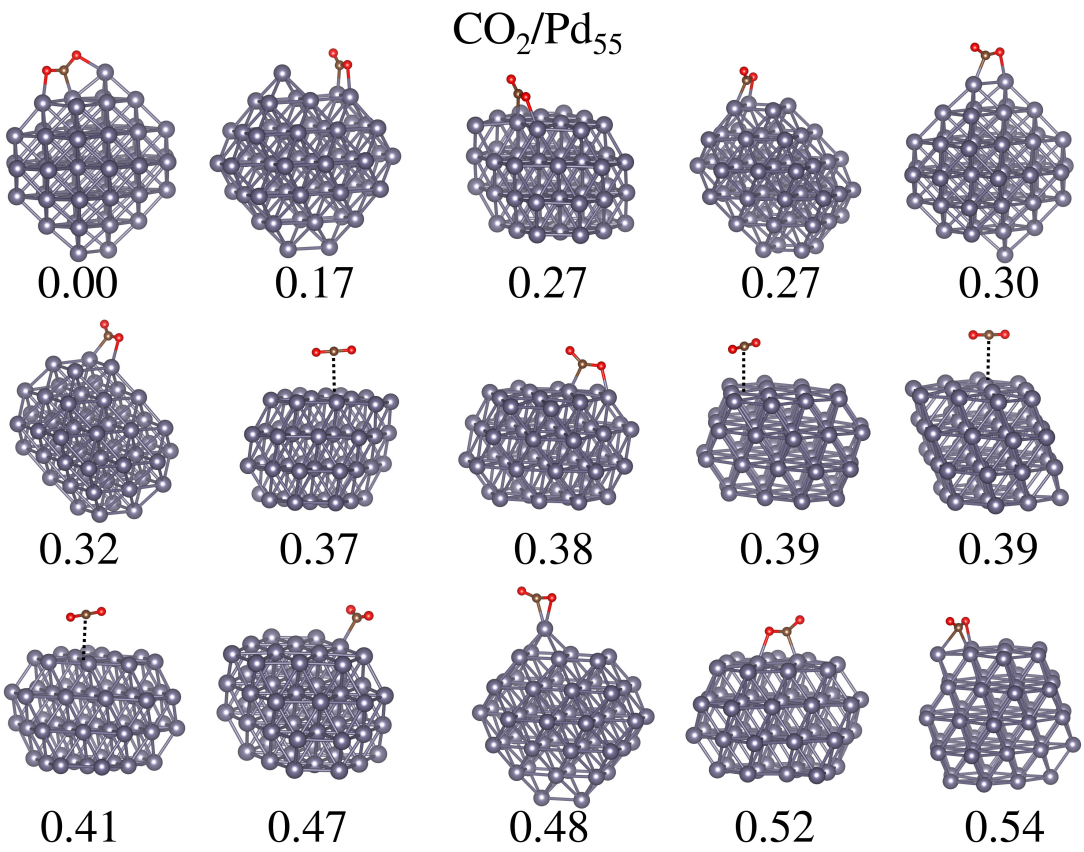

Figure S19: Optimized adsorption configurations for CO_2 interacting with the unary Pd_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S16.

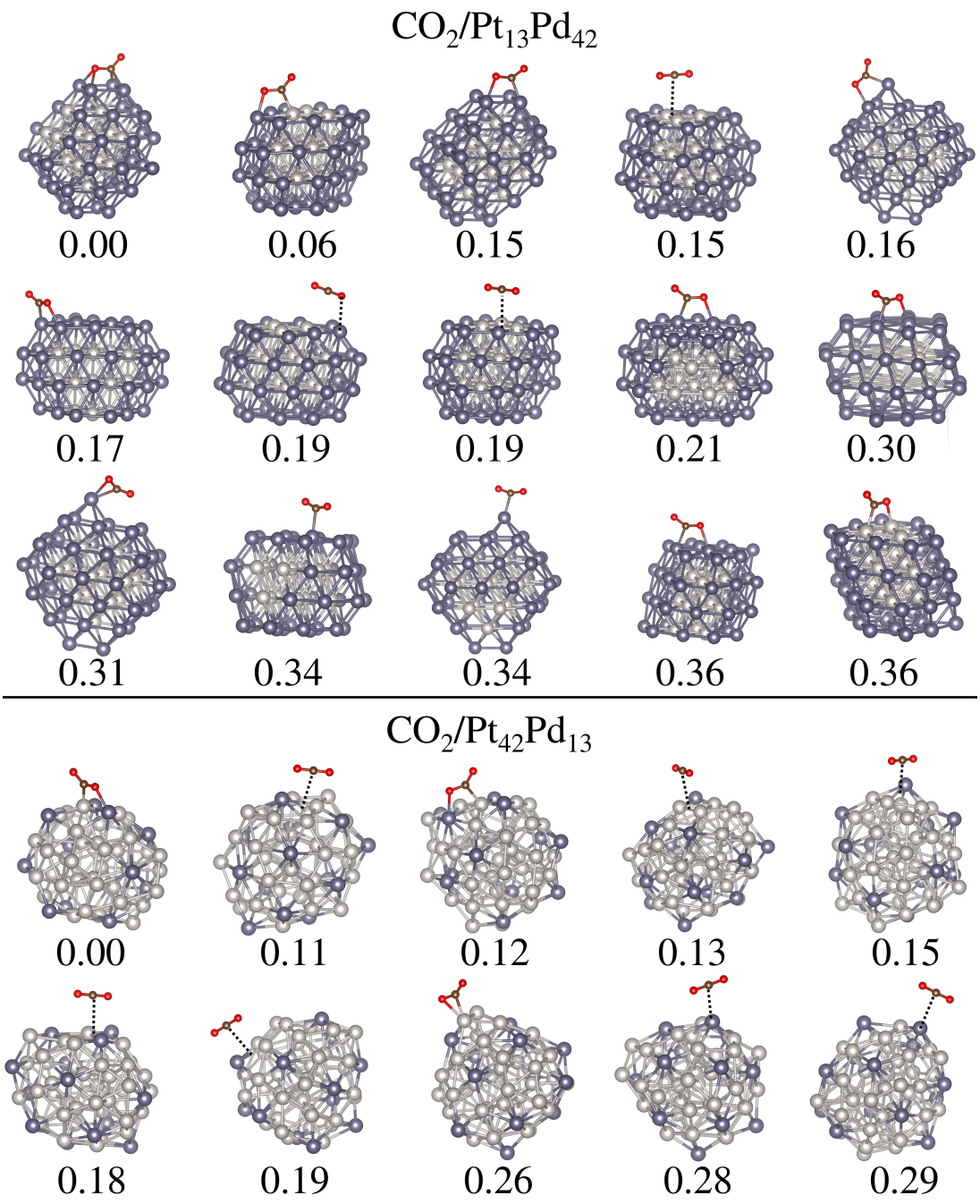

Figure S20: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Pd_{42}$ and $Pt_{42}Pd_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S16.

Table S16: Adsorption properties for all configurations of CO_2 adsorbed on Pd_{55}, $Pt_{13}Pd_{42}$ and $Pt_{42}Pd_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Pd_{55}											
0.54	−0.07	22	2.13	2.22	2.70	1.26	1.22	138.85	7.19	4.14	−22.83
0.52	−0.08	22	2.08	2.72	2.23	1.21	1.25	139.64	3.37	6.71	−22.40
0.48	−0.13	20	2.13	2.91	2.36	1.19	1.22	154.68	1.83	4.06	−14.04
0.47	−0.14	22	2.08	2.70	2.69	1.22	1.22	146.57	4.10	4.10	−18.55
0.41	−0.19	22	3.23	3.33	3.55	1.17	1.17	178.85	0.17	0.02	−0.61
0.39	−0.21	22	3.21	3.40	3.47	1.17	1.17	178.63	0.03	0.12	−0.73
0.39	−0.22	22	3.23	3.20	3.24	1.18	1.17	178.63	0.21	0.01	−0.73
0.38	−0.23	22	2.07	2.13	2.74	1.26	1.21	137.73	7.81	3.06	−23.46
0.37	−0.24	22	3.39	3.27	3.07	1.17	1.17	179.00	−0.03	0.10	−0.52
0.32	−0.29	22	2.03	2.59	2.18	1.22	1.25	141.84	3.70	6.30	−21.18
0.30	−0.31	22	2.03	2.20	2.57	1.24	1.22	142.60	6.11	3.69	−20.75
0.27	−0.34	18	2.02	2.67	2.16	1.22	1.26	137.49	3.91	7.72	−23.59
0.27	−0.34	22	2.06	2.15	2.75	1.26	1.21	138.53	7.28	3.29	−23.01
0.17	−0.43	20	2.01	2.62	2.13	1.22	1.26	139.48	3.69	7.04	−22.48
0.00	−0.61	18	2.01	2.13	2.15	1.25	1.26	130.54	6.99	7.15	−27.45
$CO_2/Pt_{13}Pd_{42}$											
0.36	−0.04	10	2.06	2.83	2.12	1.21	1.29	130.83	3.37	10.27	−27.29
0.36	−0.04	4	2.07	2.64	2.24	1.21	1.25	140.82	3.58	6.38	−21.74
0.34	−0.07	6	2.15	2.78	2.55	1.20	1.21	156.44	2.21	3.10	−13.06
0.34	−0.07	10	2.18	2.74	2.78	1.21	1.22	149.33	3.03	3.65	−17.01
0.31	−0.09	8	2.12	2.85	2.34	1.20	1.22	149.82	2.72	4.30	−16.74
0.30	−0.10	4	2.06	2.21	2.62	1.25	1.21	140.46	6.59	3.56	−21.94
0.21	−0.19	6	2.06	2.73	2.17	1.21	1.26	138.33	3.40	7.34	−23.13
0.19	−0.21	6	3.36	3.47	3.44	1.17	1.17	178.88	0.08	−0.04	−0.59
0.19	−0.22	6	3.28	2.81	3.40	1.18	1.17	178.62	0.45	−0.23	−0.74
0.17	−0.23	6	2.04	2.55	2.20	1.22	1.24	142.26	3.74	5.99	−20.94
0.16	−0.24	6	2.03	2.20	2.53	1.25	1.22	141.20	6.18	3.95	−21.53
0.15	−0.25	6	3.37	3.46	3.37	1.17	1.17	178.40	0.08	−0.01	−0.86
0.15	−0.25	8	2.02	2.64	2.19	1.22	1.26	138.88	3.87	7.28	−22.82
0.06	−0.35	8	2.05	2.83	2.08	1.21	1.29	131.76	3.24	10.19	−26.78
0.00	−0.40	4	2.13	2.21	2.79	1.33	1.23	127.69	13.67	4.94	−29.04
$CO_2/Pt_{42}Pd_{13}$											
0.29	−0.10	0	2.96	3.30	3.09	1.17	1.18	178.16	0.11	0.30	−0.99
0.28	−0.11	2	2.96	3.36	3.03	1.17	1.18	178.30	0.02	0.28	−0.91
0.26	−0.13	0	2.10	2.31	2.99	1.25	1.19	148.71	6.21	1.88	−17.35
0.19	−0.20	2	3.36	3.03	3.16	1.17	1.17	179.57	0.14	−0.04	−0.21
0.18	−0.21	0	3.39	3.60	3.39	1.17	1.18	178.89	−0.10	0.23	−0.59
0.15	−0.24	2	3.16	3.41	2.65	1.17	1.18	179.12	−0.30	0.49	−0.46
0.13	−0.26	2	3.45	3.20	3.22	1.17	1.17	178.97	0.04	−0.02	−0.54
0.12	−0.27	0	2.07	2.14	2.80	1.27	1.21	134.91	8.39	3.54	−25.03
0.11	−0.28	0	3.45	2.90	3.59	1.18	1.17	178.59	0.25	−0.18	−0.75
0.00	−0.39	0	2.07	2.78	2.12	1.21	1.27	135.48	3.36	8.25	−24.71

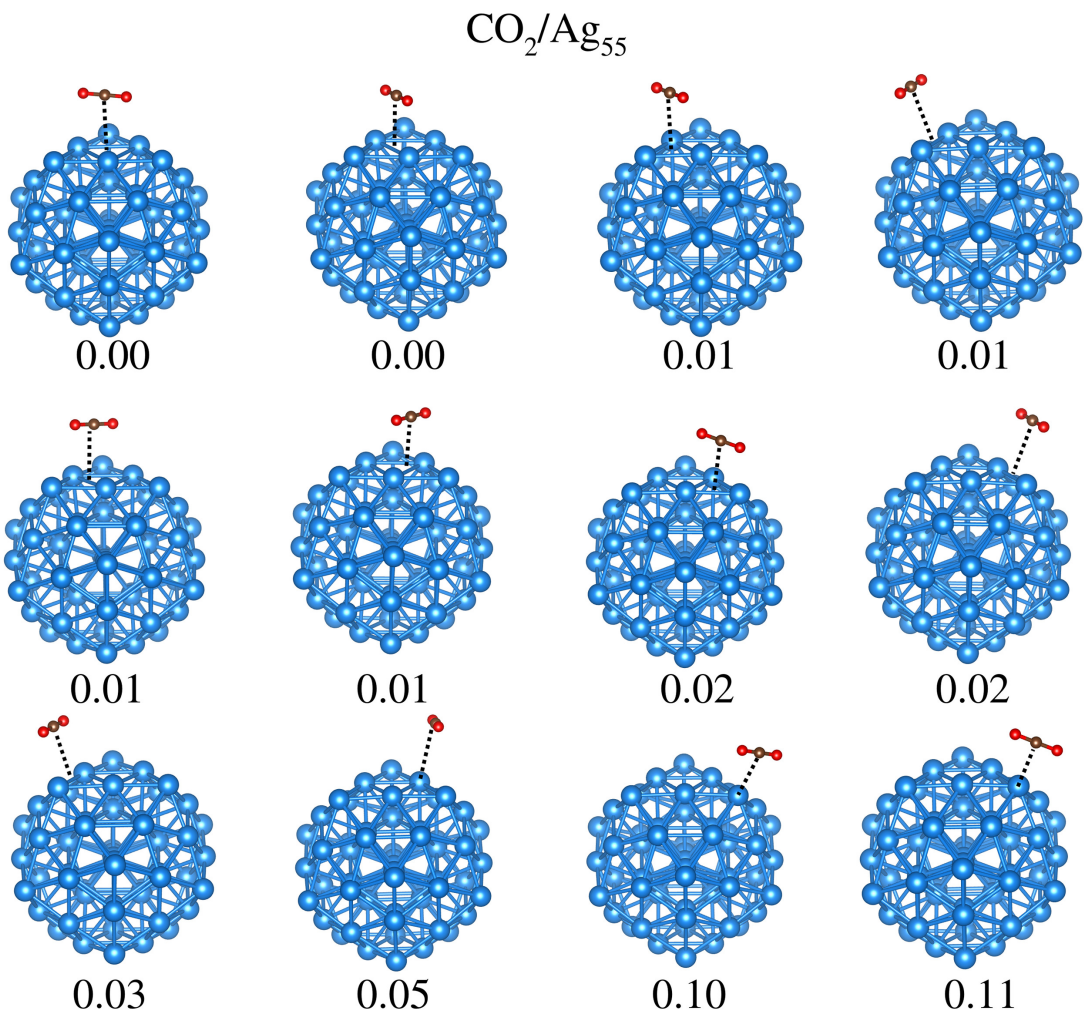

Figure S21: Optimized adsorption configurations for CO_2 interacting with the unary Ag_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S17.

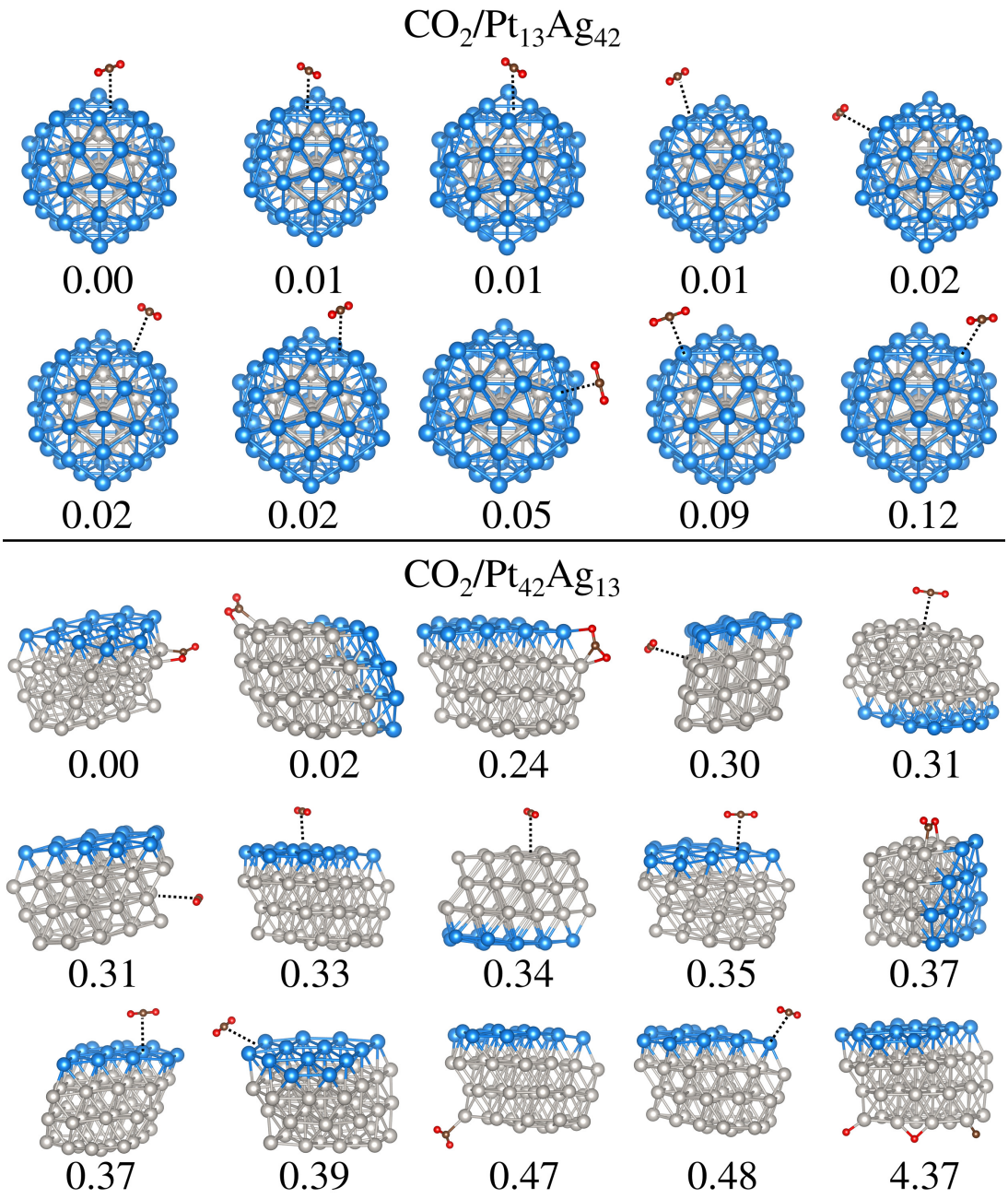

Figure S22: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Ag_{42}$ and $Pt_{42}Ag_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S17.

Table S17: Adsorption properties for all configurations of CO_2 adsorbed on Ag_{55}, $Pt_{13}Ag_{42}$ and $Pt_{42}Ag_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Ag_{55}											
0.11	−0.08	3	3.01	3.35	3.13	1.17	1.18	179.24	0.01	0.20	−0.39
0.10	−0.10	3	3.22	3.27	3.59	1.17	1.17	179.65	0.16	−0.01	−0.16
0.05	−0.15	3	3.33	3.48	3.60	1.17	1.17	179.52	0.03	0.03	−0.24
0.03	−0.17	1	3.27	3.10	3.06	1.17	1.17	179.79	0.01	0.11	−0.09
0.02	−0.17	3	3.28	3.11	3.18	1.17	1.17	179.75	0.03	0.05	−0.11
0.02	−0.17	3	3.40	3.40	3.17	1.17	1.17	179.58	−0.02	0.17	−0.20
0.01	−0.18	1	3.39	3.22	3.18	1.17	1.17	179.72	0.06	0.06	−0.12
0.01	−0.19	1	3.55	3.58	3.24	1.17	1.17	179.85	−0.04	0.06	−0.05
0.01	−0.19	3	3.44	3.17	3.17	1.17	1.17	179.78	−0.01	0.04	−0.09
0.01	−0.19	3	3.55	3.30	3.33	1.17	1.17	179.64	0.03	0.09	−0.17
0.00	−0.19	1	3.37	3.18	3.18	1.17	1.17	179.84	0.04	0.04	−0.06
0.00	−0.20	1	3.50	3.25	3.20	1.17	1.17	179.56	0.03	0.04	−0.21
CO_2/$Pt_{13}Ag_{42}$											
0.12	−0.07	0	3.04	3.26	3.27	1.17	1.17	179.15	0.13	0.13	−0.44
0.09	−0.10	2	3.16	3.54	3.19	1.17	1.18	179.59	−0.01	0.18	−0.19
0.05	−0.14	0	3.28	3.54	3.44	1.17	1.17	179.71	0.01	0.06	−0.13
0.02	−0.17	0	3.46	3.35	3.35	1.17	1.17	179.63	0.05	0.02	−0.17
0.02	−0.17	2	3.25	3.07	3.13	1.17	1.17	179.83	0.07	0.05	−0.06
0.02	−0.17	0	3.35	3.03	3.14	1.17	1.17	179.90	0.09	0.07	−0.02
0.01	−0.19	2	3.35	3.21	3.09	1.17	1.17	179.87	−0.05	0.15	−0.04
0.01	−0.19	0	3.54	3.45	3.43	1.17	1.17	179.87	0.05	0.04	−0.04
0.01	−0.19	0	3.28	3.14	3.09	1.17	1.17	179.68	0.03	0.09	−0.14
0.00	−0.19	0	3.48	3.20	3.18	1.17	1.17	179.98	0.05	0.05	0.02
CO_2/$Pt_{42}Ag_{13}$											
4.37	3.83	1	1.71	1.76	1.94	10.08	4.81	169.60	759.56	310.26	−5.75
0.48	−0.06	1	2.99	3.16	3.27	1.17	1.17	179.84	0.12	0.06	−0.06
0.47	−0.07	1	2.16	2.62	2.79	1.21	1.21	153.00	3.51	2.81	−14.97
0.39	−0.15	1	3.32	3.00	3.03	1.17	1.17	179.61	0.11	0.05	−0.19
0.37	−0.17	1	3.16	3.41	3.33	1.17	1.17	179.87	0.08	0.08	−0.04
0.37	−0.17	1	2.04	2.28	2.67	1.27	1.22	135.10	8.38	4.41	−24.92
0.35	−0.19	1	3.43	3.37	3.41	1.17	1.17	179.80	0.05	0.06	−0.08
0.34	−0.20	1	3.45	3.66	3.47	1.17	1.17	178.55	0.11	-0.03	−0.77
0.33	−0.21	1	3.35	3.30	3.28	1.17	1.17	179.67	0.03	0.07	−0.15
0.31	−0.23	1	3.24	3.46	3.45	1.17	1.17	178.70	0.04	0.05	−0.69
0.31	−0.23	1	3.17	3.37	3.43	1.17	1.17	177.48	0.04	0.17	−1.37
0.30	−0.24	1	3.29	3.45	3.56	1.17	1.17	178.04	0.14	0.06	−1.06
0.24	−0.30	1	2.04	2.49	2.35	1.23	1.24	141.77	4.79	6.14	−21.21
0.02	−0.52	1	2.01	2.05	2.85	1.32	1.21	129.07	12.39	3.35	−28.27
0.00	−0.54	1	2.04	2.12	2.72	1.28	1.22	133.77	9.22	3.97	−25.66

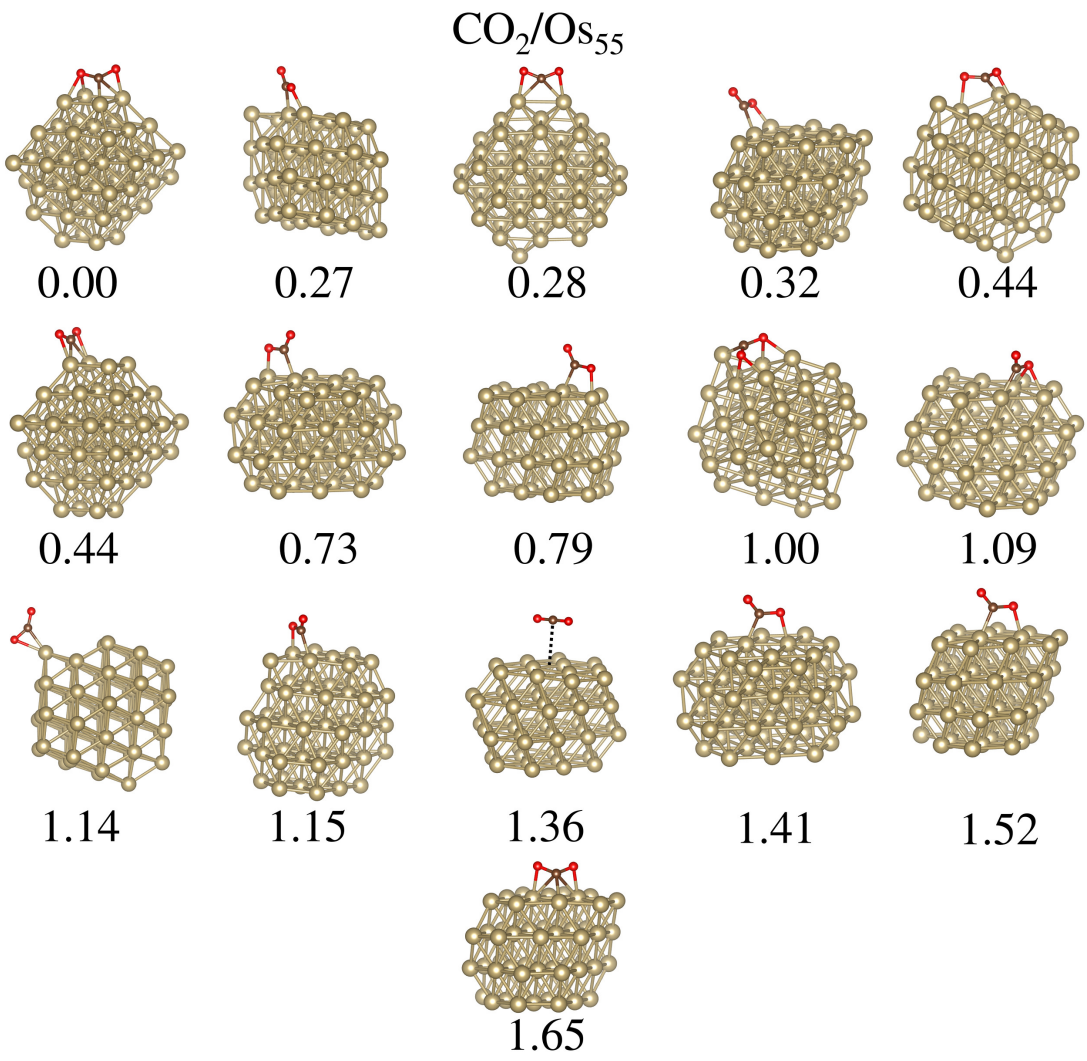

Figure S23: Optimized adsorption configurations for CO_2 interacting with the unary Os_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S18.

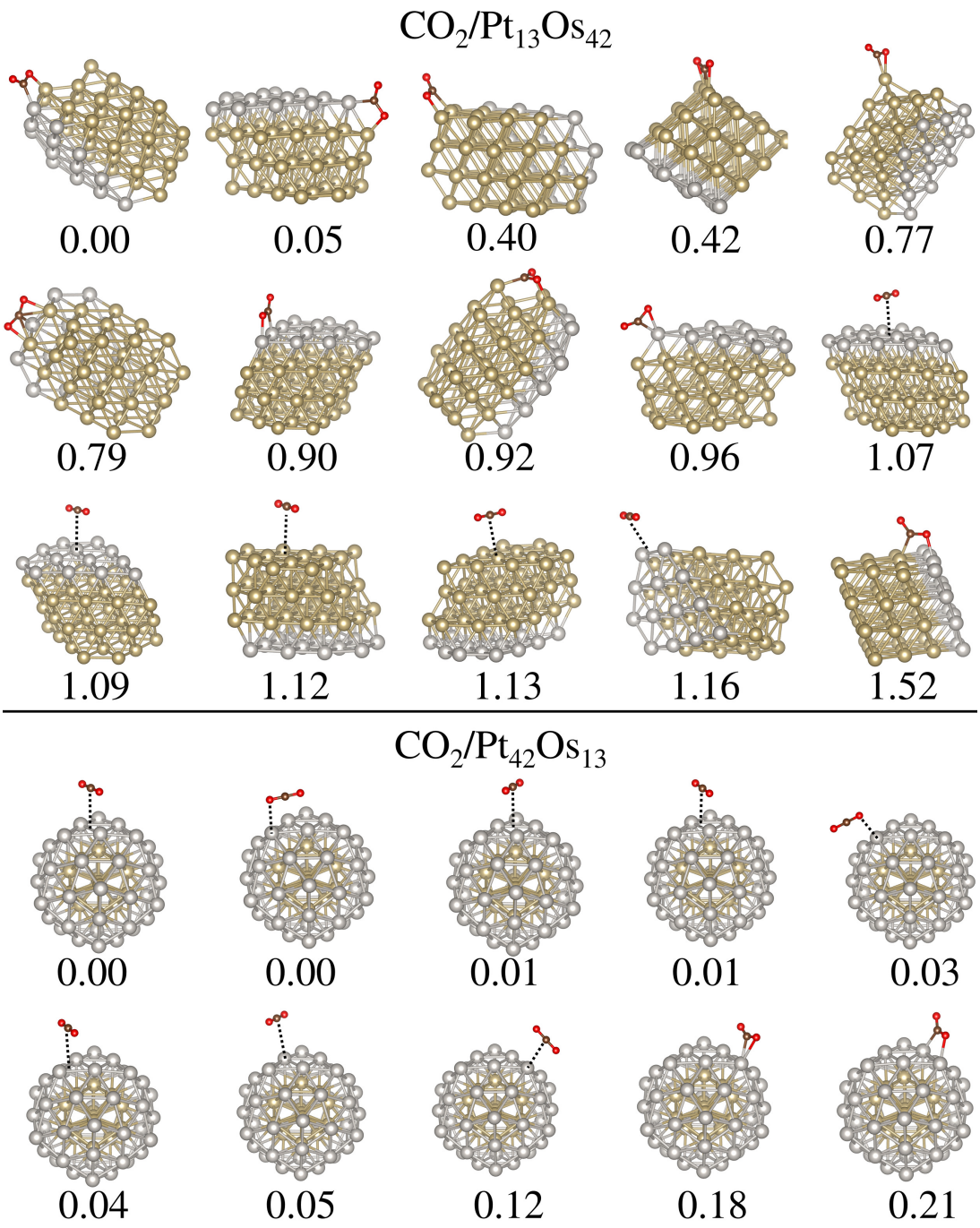

Figure S24: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Os_{42}$ and $Pt_{42}Os_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S18.

Table S18: Adsorption properties for all configurations of CO_2 adsorbed on Os_{55}, $Pt_{13}Os_{42}$ and $Pt_{42}Os_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Os_{55}											
1.65	0.09	0	2.10	2.13	2.16	1.32	1.30	119.16	12.54	1.20	−3.78
1.52	−0.04	2	2.13	2.10	2.90	1.32	1.22	127.28	12.22	3.85	−29.27
1.41	−0.15	2	2.13	2.93	2.09	1.21	1.33	126.59	3.56	13.00	−29.65
1.36	−0.20	2	3.73	3.60	3.44	1.17	1.17	179.31	-0.03	0.01	−0.35
1.15	−0.41	0	2.12	2.08	2.93	1.33	1.22	127.55	13.78	3.80	−29.12
1.14	−0.42	2	2.16	2.39	3.10	1.26	1.21	143.15	7.70	2.85	−20.44
1.09	−0.46	2	2.08	2.98	2.23	1.21	1.40	122.60	3.15	19.56	−31.86
1.00	−0.56	0	2.13	2.24	2.24	1.33	1.34	116.75	13.57	14.25	−35.12
0.79	−0.77	2	2.12	2.01	2.96	1.37	1.21	124.44	16.60	3.16	−30.84
0.73	−0.83	2	2.12	2.97	2.01	1.21	1.37	124.52	3.01	16.64	−30.80
0.44	−1.11	2	2.15	2.18	2.19	1.26	1.26	135.51	7.21	7.59	−24.69
0.44	−1.12	2	2.02	2.25	2.08	1.30	1.33	122.01	10.99	13.21	−32.20
0.32	−1.24	0	2.10	3.02	1.93	1.21	1.41	121.38	2.80	20.18	−32.55
0.28	−1.28	2	2.20	2.15	2.16	1.27	1.26	133.65	7.87	7.74	−25.72
0.27	−1.29	0	2.09	1.97	2.95	1.37	1.21	123.19	16.64	3.50	−31.54
0.00	−1.56	0	2.05	2.08	2.19	1.32	1.35	117.62	12.67	15.20	−34.64
$CO_2/Pt_{13}Os_{42}$											
1.52	0.20	2	2.14	2.11	2.91	1.31	1.22	128.60	11.43	3.85	−28.53
1.16	−0.16	2	3.44	3.29	3.31	1.17	1.17	178.91	0.08	0.04	−0.58
1.13	−0.19	2	3.52	3.52	3.70	1.17	1.17	179.01	−0.02	0.03	−0.52
1.12	−0.20	2	3.75	3.53	3.60	1.17	1.17	179.09	0.10	−0.08	−0.47
1.09	−0.23	2	3.30	3.65	3.38	1.17	1.17	178.52	−0.04	0.08	−0.79
1.07	−0.25	2	3.40	3.50	3.43	1.17	1.17	178.76	0.06	0.07	−0.66
0.96	−0.36	2	2.08	3.05	2.23	1.20	1.26	145.14	2.62	7.10	−19.34
0.92	−0.39	2	2.07	2.03	2.02	1.35	1.35	111.75	14.81	14.84	−37.89
0.90	−0.42	2	2.08	2.93	2.09	1.21	1.31	129.99	3.12	11.75	−27.76
0.79	−0.53	2	2.07	2.10	2.10	1.30	1.30	121.55	11.21	11.14	−32.45
0.77	−0.55	2	2.12	2.31	3.11	1.27	1.21	141.69	8.60	2.88	−21.26
0.42	−0.90	2	2.13	2.20	2.21	1.26	1.27	133.73	7.74	7.87	−25.68
0.40	−0.92	2	2.12	1.97	3.05	1.40	1.21	123.45	19.02	2.76	−31.40
0.05	−1.27	2	2.04	2.79	2.00	1.21	1.34	127.15	3.53	14.06	−29.34
0.00	−1.32	2	2.02	2.83	2.00	1.21	1.34	126.74	3.35	13.96	−29.57
$CO_2/Pt_{42}Os_{13}$											
0.21	−0.03	4	2.07	2.78	2.16	1.21	1.28	134.59	3.14	9.07	−25.20
0.18	−0.05	4	2.11	2.58	2.46	1.22	1.23	145.87	4.02	4.67	−18.94
0.12	−0.11	4	3.09	3.13	3.49	1.18	1.17	179.31	0.27	−0.01	−0.35
0.05	−0.19	4	3.23	3.52	3.37	1.17	1.17	179.10	0.04	0.09	−0.47
0.04	−0.19	4	3.44	3.54	3.58	1.17	1.17	179.21	0.04	0.08	−0.41
0.03	−0.20	4	3.16	4.00	2.59	1.17	1.18	179.49	−0.46	0.66	−0.25
0.01	−0.22	4	3.35	3.51	3.19	1.17	1.17	179.11	−0.07	0.11	−0.46
0.01	−0.22	4	3.42	3.49	3.51	1.17	1.17	178.96	0.04	0.03	−0.55
0.00	−0.23	4	3.38	3.32	3.00	1.17	1.18	179.42	−0.18	0.28	−0.29
0.00	−0.23	4	3.49	3.21	3.21	1.17	1.17	179.23	0.03	0.07	−0.39

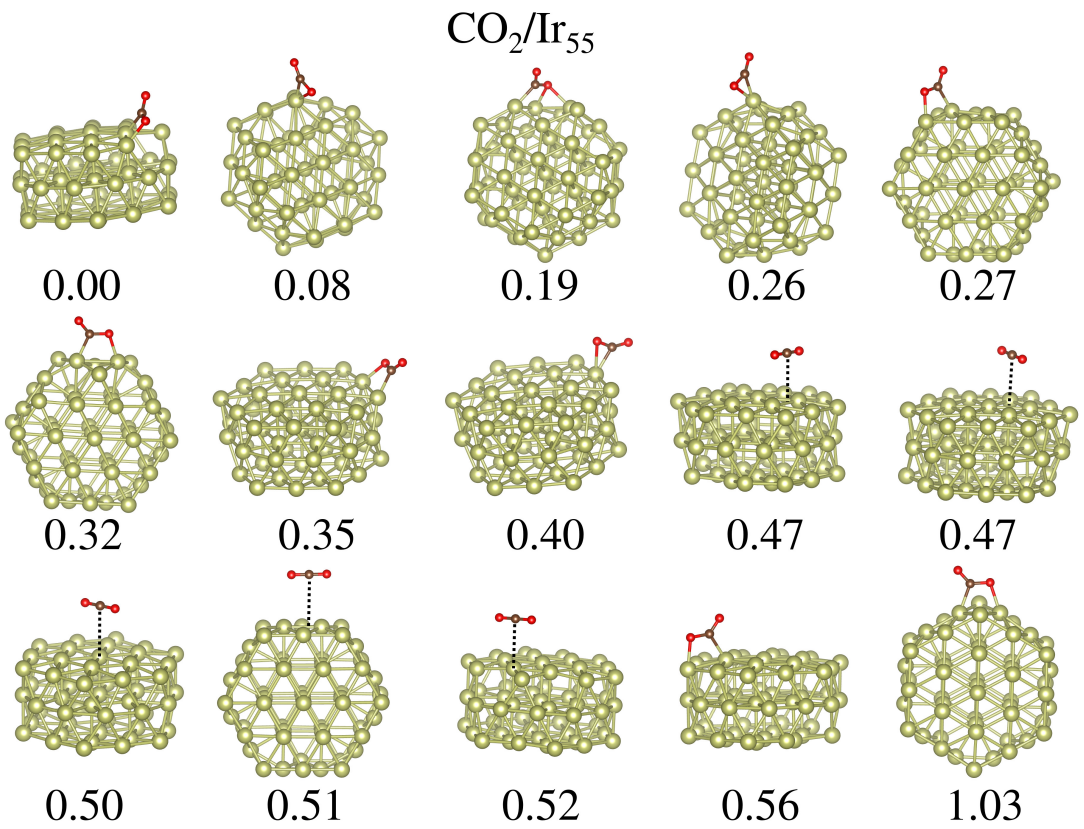

Figure S25: Optimized adsorption configurations for CO_2 interacting with the unary Ir_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S19.

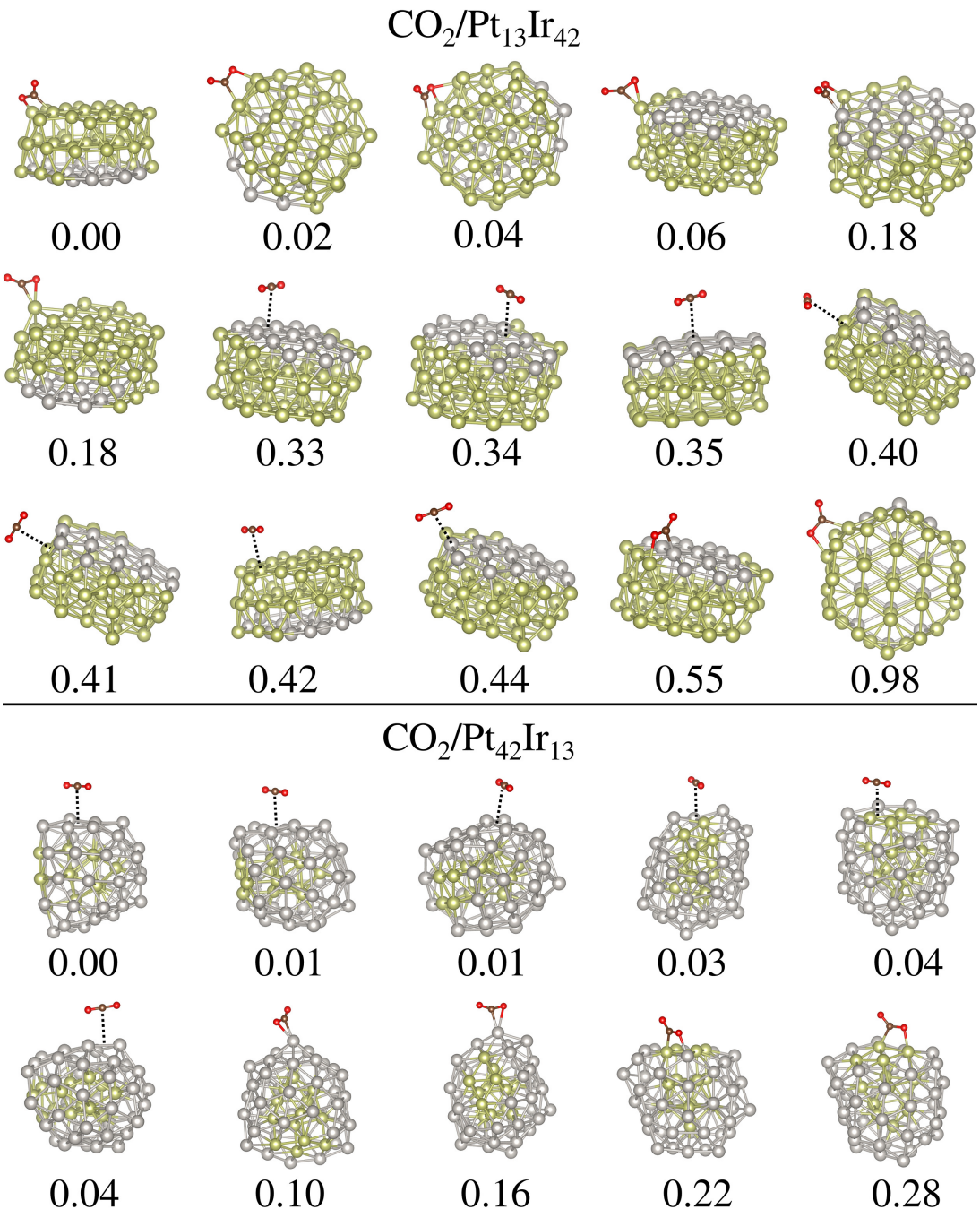

Figure S26: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Ir_{42}$ and $Pt_{42}Ir_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S19.

Table S19: Adsorption properties for all configurations of CO_2 adsorbed on Ir_{55}, $Pt_{13}Ir_{42}$ and $Pt_{42}Ir_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Ir_{55}											
1.03	0.34	3	2.08	2.13	2.87	1.32	1.21	129.37	12.25	3.22	−28.11
0.56	−0.13	3	2.11	2.81	2.08	1.21	1.30	132.31	3.16	10.81	−26.47
0.52	−0.17	1	3.42	3.67	3.56	1.17	1.17	179.73	0.02	0.02	−0.12
0.51	−0.18	3	3.61	3.55	3.54	1.17	1.17	179.49	0.04	0.05	−0.25
0.50	−0.19	1	3.42	3.60	3.63	1.17	1.17	179.67	0.00	0.03	−0.15
0.47	−0.22	3	3.64	3.37	3.53	1.17	1.17	179.57	0.06	-0.03	−0.21
0.47	−0.22	1	3.50	3.30	3.27	1.17	1.17	179.45	0.03	0.07	−0.27
0.40	−0.29	3	2.08	2.32	3.00	1.26	1.20	145.04	7.11	2.47	−19.40
0.35	−0.34	3	2.04	2.03	2.86	1.33	1.21	128.30	13.11	3.57	−28.70
0.32	−0.38	3	2.04	2.05	2.83	1.32	1.22	128.34	12.49	3.85	−28.68
0.27	−0.43	3	2.07	2.02	2.85	1.32	1.21	128.74	12.94	3.21	−28.45
0.26	−0.44	3	2.06	2.24	3.02	1.26	1.20	144.89	7.78	2.39	−19.48
0.19	−0.50	1	2.05	2.93	2.10	1.21	1.42	120.83	2.89	20.69	−32.85
0.08	−0.61	3	2.03	2.19	3.02	1.27	1.20	143.32	8.70	2.36	−20.35
0.00	−0.69	3	2.06	2.00	2.88	1.33	1.22	127.37	13.02	3.64	−29.22
CO_2/$Pt_{13}Ir_{42}$											
0.98	0.39	4	2.07	2.13	2.85	1.31	1.21	129.82	12.04	3.30	−27.86
0.55	−0.04	4	2.16	2.84	2.12	1.20	1.28	136.58	2.46	8.91	−24.10
0.44	−0.15	4	3.09	3.21	3.44	1.18	1.17	177.59	0.27	0.03	−1.31
0.42	−0.17	4	3.42	3.7	3.53	1.17	1.17	179.86	−0.01	0.03	−0.05
0.41	−0.18	0	3.48	3.52	3.25	1.17	1.17	179.38	−0.05	0.12	−0.31
0.40	−0.19	2	3.51	3.40	3.40	1.17	1.17	179.48	0.08	−0.01	−0.26
0.35	−0.24	2	3.3	3.43	3.59	1.17	1.17	179.30	0.07	0.01	−0.36
0.34	−0.26	4	3.46	3.39	3.42	1.17	1.17	179.30	0.01	0.00	−0.36
0.33	−0.27	4	3.47	3.23	3.24	1.17	1.17	179.69	0.03	0.03	−0.14
0.18	−0.41	2	2.05	2.21	3.03	1.27	1.20	143.88	8.44	2.27	−20.04
0.18	−0.41	2	2.05	2.83	2.04	1.21	1.31	130.49	2.92	11.84	−27.49
0.06	−0.53	4	2.05	2.22	3.02	1.27	1.20	144.55	8.07	2.26	−19.67
0.04	−0.55	2	2.03	2.92	2.09	1.21	1.41	121.11	3.06	20.55	−32.70
0.02	−0.57	2	2.05	2.05	2.85	1.32	1.22	128.07	12.45	3.68	−28.83
0.00	−0.59	4	2.06	2.00	2.88	1.33	1.21	127.35	13.19	3.54	−29.23
CO_2/$Pt_{42}Ir_{13}$											
0.28	0.01	1	2.08	2.77	2.07	1.21	1.29	132.51	3.42	10.12	−26.36
0.22	−0.04	1	2.10	2.08	2.84	1.29	1.21	131.82	10.14	3.26	−26.74
0.16	−0.11	1	2.16	2.96	2.45	1.20	1.23	150.98	2.05	4.70	−16.10
0.10	−0.17	1	2.13	3.04	2.28	1.19	1.24	149.19	1.75	6.02	−17.09
0.04	−0.23	1	3.33	3.40	2.94	1.17	1.18	179.42	−0.13	0.23	−0.29
0.04	−0.23	1	3.52	3.31	3.29	1.17	1.17	179.82	0.06	0.04	−0.07
0.03	−0.23	1	3.48	3.52	3.26	1.17	1.17	179.08	0.01	0.18	−0.48
0.01	−0.26	1	3.41	3.23	3.29	1.17	1.17	179.31	0.05	−0.03	−0.35
0.01	−0.26	1	3.42	3.44	3.46	1.17	1.17	178.89	0.01	0.12	−0.58
0.00	−0.27	1	3.49	3.17	3.35	1.17	1.17	178.90	0.07	−0.04	−0.58

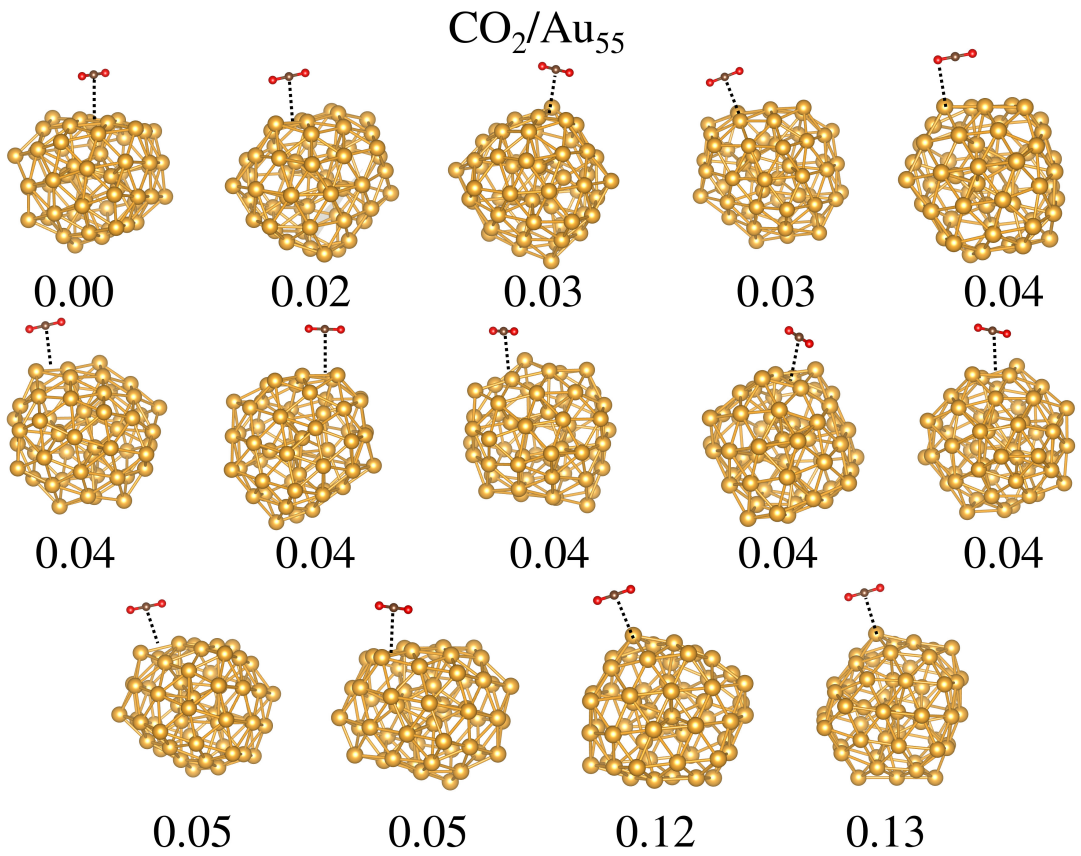

Figure S27: Optimized adsorption configurations for CO_2 interacting with the unary Au_{55} nanocluster. The energy relative to the lowest energy configuration, in eV, is shown below each structure. Dotted lines represent distances higher than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S20.

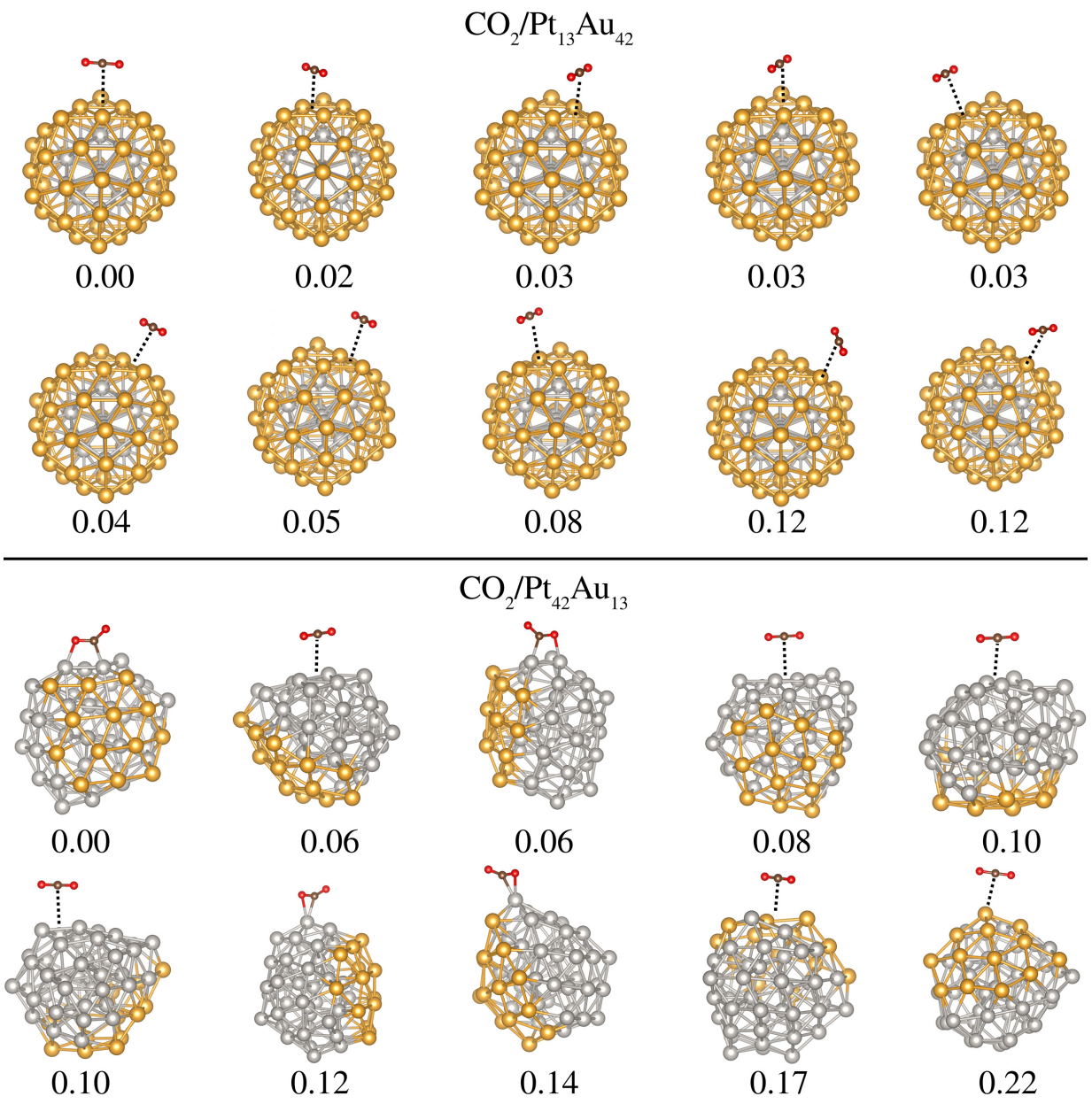

Figure S28: Optimized adsorption configurations for CO_2 interacting with $Pt_{13}Au_{42}$ and $Pt_{42}Au_{13}$ nanoalloys. The energy relative to the lowest energy configuration, in eV, is shown below the structure for each type of substrate. Dotted lines indicate distances greater than 2.5 Å between CO_2 and the substrate. Corresponding properties are available in Table S20.

Table S20: Adsorption properties for all configurations of CO_2 adsorbed on Au_{55}, $Pt_{13}Au_{42}$ and $Pt_{42}Au_{13}$. Total energy relative to the lowest energy configuration (ΔE_{tot}), adsorption energy (E_{ad}), total magnetic moment (m_{tot}), shortest distances between the C and TM atoms ($d_{\text{C-TM}}$), O and TM atoms ($d_{\text{O1-TM}}$ and $d_{\text{O2-TM}}$), OCO angle (α_{OCO}) and percentual variations, with respect to gas-phase CO_2, of the O – C bond lengths ($d_{\text{O1-C}}$ and $d_{\text{O2-C}}$) and OCO angle (Δ_{OCO}).

ΔE_{tot} (eV)	E_{ad} (eV)	m_{tot} (μ_B)	$d_{\text{C-TM}}$ (Å)	$d_{\text{O1-TM}}$ (Å)	$d_{\text{O2-TM}}$ (Å)	$d_{\text{O1-C}}$ (Å)	$d_{\text{O2-C}}$ (Å)	α_{OCO} (deg)	$\Delta_{\text{O1-C}}$ (%)	$\Delta_{\text{O2-C}}$ (%)	Δ_{OCO} (%)
CO_2/Au_{55}											
0.13	−0.08	1.00	3.03	3.26	3.26	1.17	1.17	178.82	0.12	0.10	−0.63
0.12	−0.08	1.00	3.07	3.22	3.37	1.17	1.17	178.95	0.13	0.04	−0.55
0.05	−0.16	1.00	3.47	3.80	3.51	1.17	1.17	179.79	−0.01	0.07	−0.09
0.05	−0.16	1.00	3.31	3.12	3.16	1.17	1.17	179.95	0.00	0.05	0.00
0.04	−0.16	1.00	3.50	3.52	3.36	1.17	1.17	179.64	−0.02	0.11	−0.17
0.04	−0.17	1.00	3.48	3.30	3.49	1.17	1.17	179.58	0.02	0.05	−0.20
0.04	−0.17	1.00	3.43	3.52	3.36	1.17	1.17	179.47	−0.05	0.09	−0.26
0.04	−0.17	1.00	3.46	3.34	3.55	1.17	1.17	179.89	0.14	-0.06	−0.03
0.04	−0.17	1.00	3.48	3.26	3.47	1.17	1.17	179.74	0.11	-0.07	−0.11
0.04	−0.17	1.00	3.43	3.16	3.83	1.18	1.17	179.90	0.20	-0.14	−0.02
0.03	−0.18	1.00	3.42	3.53	3.66	1.17	1.17	179.56	0.05	0.00	−0.21
0.03	−0.18	1.00	3.51	3.38	3.64	1.17	1.17	179.59	0.03	-0.05	−0.20
0.02	−0.19	1.00	3.40	3.32	3.40	1.17	1.17	179.70	0.08	-0.09	−0.13
0.00	−0.21	1.00	3.52	3.67	3.63	1.17	1.17	179.64	0.02	-0.02	−0.17
CO_2/$Pt_{13}Au_{42}$											
0.12	−0.11	2.00	3.10	3.33	3.31	1.17	1.17	179.09	0.10	0.11	−0.47
0.12	−0.12	2.00	3.08	3.46	3.14	1.17	1.18	179.06	−0.02	0.23	−0.49
0.08	−0.16	2.00	3.19	3.43	3.37	1.17	1.17	179.39	0.03	0.05	−0.31
0.05	−0.19	2.00	3.29	3.11	3.23	1.17	1.17	179.80	0.10	0.00	−0.08
0.04	−0.20	2.00	3.26	3.20	3.13	1.17	1.17	179.65	0.01	0.13	−0.16
0.03	−0.20	2.00	3.42	3.09	3.22	1.17	1.17	179.93	0.06	0.01	0.00
0.03	−0.20	2.00	3.48	3.31	3.32	1.17	1.17	179.74	0.02	0.05	−0.11
0.03	−0.20	2.00	3.41	3.31	3.31	1.17	1.17	179.49	0.03	0.05	−0.25
0.02	−0.22	2.00	3.31	3.21	3.13	1.17	1.17	179.65	0.00	0.07	−0.16
0.00	−0.23	2.00	3.48	3.20	3.19	1.17	1.17	179.81	0.03	0.06	−0.07
CO_2/$Pt_{42}Au_{13}$											
0.22	−0.09	3.00	3.14	3.24	3.47	1.17	1.17	179.10	0.13	0.02	−0.47
0.17	−0.15	1.00	3.31	3.21	3.26	1.17	1.17	179.65	0.03	0.04	−0.16
0.14	−0.17	1.01	2.09	2.32	2.97	1.24	1.20	149.38	5.98	1.97	−16.99
0.12	−0.19	1.00	2.11	3.01	2.29	1.19	1.24	148.82	1.87	6.07	−17.30
0.10	−0.21	1.00	3.39	3.27	3.02	1.17	1.17	179.51	−0.05	0.13	−0.24
0.10	−0.21	3.01	3.37	3.50	3.45	1.17	1.17	178.35	0.00	0.17	−0.89
0.08	−0.23	1.01	3.32	3.56	3.24	1.17	1.17	179.18	0.02	0.08	−0.42
0.06	−0.25	1.00	2.05	2.18	2.73	1.27	1.22	135.58	8.67	3.74	−24.65
0.06	−0.25	1.00	3.34	3.16	3.16	1.17	1.17	178.97	0.08	0.02	−0.54
0.00	−0.31	3.00	2.05	2.08	2.84	1.29	1.21	132.48	10.19	3.06	−26.38

S8 Complementary Analyses of the Adsorption Properties of the Most Stable Adsorption Configurations

Here we show the data for the adsorption properties of the lowest energy adsorption configurations considering bent (Table S21) and linear (Table S22) CO_2 for each substrate, which are shown in the main article as graphical plots. For the different Pt_{55} clusters, we show the data for adsorption energies, interaction energies and deformation energies, separately, in Table S23. Figure S29 shows some adsorption properties versus the adsorption energy plotted for the several adsorption structures simultaneously.

In the main article, various trends of the adsorption properties were investigated versus the type of metal for each composition. The main article shows graphs of the properties versus the type of metal for the most stable chemisorption and physisorption structures. Here, we also show, in Figure S30, a plot of this type, but considering the most stable adsorption configuration (physisorption and chemisorption) for each substrate. Figure S31 shows the electron density difference isosurfaces for the lowest energy adsorption structures with the charge of adsorbed CO_2 indicated. Figure S32 shows the interaction and adsorption energies versus the center of *d*-states; the results suggest grouping of data points, but do not allow the determination of strong correlations.

Table S21: Adsorption properties for carbon dioxide chemisorbed (bent) on the unary and PtTM substrates. Adsorption energy, E_{ad}, total effective charge of the adsorbed molecule (Q_{Mol}), interaction energy (E_{int}), deformation energies for the molecule and substrate (ΔE^{Mol} and ΔE^{Sub}), percent variation with respect to gas phase CO_2 for the CO bond lengths (Δd_{O1C} and Δd_{O2C}) and the OCO angle ($\Delta \alpha_{\mathrm{OCO}}$), and shortest distance between one atom of the CO_2 molecule and one atom of the substrate ($d_{\mathrm{Mol\text{-}TM}}$).

System	E_{ad} (eV)	Q_{Mol} (e)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	Δd_{O1C} (%)	Δd_{O2C} (%)	$\Delta \alpha_{\mathrm{OCO}}$ (%)	$d_{\mathrm{Mol\text{-}TM}}$ Å
CO_2/Fe_{55}	−1.34	−0.99	−4.73	2.98	0.41	9.61	10.06	−31.64	1.96
$CO_2/Pt_{13}Fe_{42}$	−0.43	−0.79	−3.12	2.42	0.27	8.71	8.81	−28.50	2.04
$CO_2/Pt_{42}Fe_{13}$	0.05	−0.37	−1.86	1.75	0.16	2.98	9.00	−24.85	2.06
CO_2/Co_{55}	−0.65	−0.68	−2.23	1.51	0.07	5.78	7.03	−22.79	1.94
$CO_2/Pt_{13}Co_{42}$	−0.41	−0.76	−3.24	2.60	0.23	8.91	8.87	−29.79	2.05
$CO_2/Pt_{42}Co_{13}$	−0.33	−0.38	−2.55	2.09	0.13	2.79	10.93	−26.76	2.04
CO_2/Ni_{55}	−0.69	−0.55	−2.08	1.31	0.08	5.86	5.93	−21.25	1.88
$CO_2/Pt_{13}Ni_{42}$	−0.35	−0.46	−2.53	2.10	0.08	3.28	10.68	−26.88	2.05
$CO_2/Pt_{42}Ni_{13}$	−0.36	−0.37	−2.47	2.04	0.08	2.79	10.53	−26.51	2.05
CO_2/Cu_{55}	0.03	−0.45	−1.00	0.98	0.05	3.78	4.54	−19.18	2.06
$CO_2/Pt_{13}Cu_{42}$	−0.36	−0.44	−2.47	2.01	0.10	3.23	10.04	−26.47	2.06
$CO_2/Pt_{42}Cu_{13}$	−0.39	−0.37	−2.55	2.04	0.11	2.74	10.70	−26.48	2.04
CO_2/Ru_{55}	−1.15	−0.72	−3.14	1.86	0.13	6.98	7.01	−25.54	2.19
$CO_2/Pt_{13}Ru_{42}$	−1.18	−0.55	−3.63	2.39	0.07	3.62	12.21	−28.26	2.00
$CO_2/Pt_{42}Ru_{13}$	−0.02	−0.36	−1.42	1.33	0.07	6.32	4.14	−22.01	2.09
CO_2/Rh_{55}	−0.73	−0.52	−2.68	1.86	0.08	4.05	9.56	−25.29	2.02
$CO_2/Pt_{13}Rh_{42}$	−0.69	−0.50	−2.48	1.73	0.07	4.05	9.02	−24.39	2.02
$CO_2/Pt_{42}Rh_{13}$	−0.24	−0.37	−1.91	1.63	0.05	8.05	3.72	−24.11	2.07
CO_2/Pd_{55}	−0.61	−0.50	−2.83	2.10	0.12	6.99	7.15	−27.45	2.01
$CO_2/Pt_{13}Pd_{42}$	−0.40	−0.63	−3.14	2.64	0.10	13.67	4.94	−29.04	2.13
$CO_2/Pt_{42}Pd_{13}$	−0.39	−0.40	−2.21	1.70	0.12	3.36	8.25	−24.71	2.07
CO_2/Ag_{55}	-	-	-	-	-	-	-	-	-
$CO_2/Pt_{13}Ag_{42}$	-	-	-	-	-	-	-	-	-
$CO_2/Pt_{42}Ag_{13}$	−0.54	−0.45	−2.51	1.88	0.10	9.22	3.97	−25.66	2.04
CO_2/Os_{55}	−1.56	−1.05	−5.79	3.99	0.24	12.67	15.20	−34.64	2.05
$CO_2/Pt_{13}Os_{42}$	−1.32	−0.58	−4.00	2.68	0.00	3.35	13.96	−29.57	2.00
$CO_2/Pt_{42}Os_{13}$	−0.05	−0.32	−1.08	0.97	0.06	4.02	4.67	−18.94	2.11
CO_2/Ir_{55}	−0.69	−0.59	−3.47	2.57	0.21	13.02	3.64	−29.22	2.00
$CO_2/Pt_{13}Ir_{42}$	−0.59	−0.60	−3.39	2.59	0.22	13.19	3.54	−29.23	2.00
$CO_2/Pt_{42}Ir_{13}$	−0.17	−0.26	−1.03	0.83	0.03	1.75	6.02	−17.09	2.13
CO_2/Pt_{55}	−0.23	−0.38	−2.38	1.96	0.19	2.96	9.95	−26.13	2.05
CO_2/Au_{55}	-	-	-	-	-	-	-	-	-
$CO_2/Pt_{13}Au_{42}$	-	-	-	-	-	-	-	-	-
$CO_2/Pt_{42}Au_{13}$	−0.31	−0.39	−2.53	2.00	0.22	10.19	3.06	−26.38	2.05

Table S22: Adsorption properties for carbon dioxide physisorbed (linear) on the unary and PtTM substrates. Adsorption energy, E_{ad}, total effective charge of the adsorbed molecule (Q_{Mol}), interaction energy (E_{int}), deformation energies for the molecule and substrate (ΔE^{Mol} and ΔE^{Sub}), percent variation with respect to gas phase CO_2 of the CO bond lengths (Δd_{O1C} and Δd_{O2C}) and OCO angle ($\Delta \alpha_{\mathrm{OCO}}$), and shortest distance between one atom of the CO_2 molecule and one atom of the substrate ($d_{\mathrm{Mol\text{-}TM}}$).

System	E_{ad} (eV)	Q_{Mol} (e)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)	Δd_{O1C} (%)	Δd_{O2C} (%)	$\Delta \alpha_{\mathrm{OCO}}$ (%)	$d_{\mathrm{Mol\text{-}TM}}$ Å
CO_2/Fe_{55}	−0.23	−0.07	−0.23	0.01	0.00	0.02	0.11	−0.88	3.00
$CO_2/Pt_{13}Fe_{42}$	−0.15	−0.05	−0.15	0.00	0.00	0.18	−0.06	−0.42	3.09
$CO_2/Pt_{42}Fe_{13}$	−0.22	−0.03	−0.23	0.00	0.00	0.01	0.07	−0.39	3.19
CO_2/Co_{55}	−0.18	−0.02	−0.19	0.01	0.00	−0.50	0.61	0.01	2.27
$CO_2/Pt_{13}Co_{42}$	−0.21	−0.04	−0.22	0.01	0.01	−0.37	0.53	−0.62	2.59
$CO_2/Pt_{42}Co_{13}$	−0.23	−0.03	−0.23	0.00	−0.01	−0.01	0.05	−0.40	3.27
CO_2/Ni_{55}	−0.24	−0.02	−0.25	0.01	−0.01	−0.49	0.61	−0.18	2.17
$CO_2/Pt_{13}Ni_{42}$	−0.18	−0.05	−0.19	0.00	0.00	0.11	0.08	−0.52	3.10
$CO_2/Pt_{42}Ni_{13}$	−0.25	−0.03	−0.22	0.00	−0.04	0.03	0.03	−0.38	3.23
CO_2/Cu_{55}	−0.16	−0.05	−0.17	0.00	0.00	0.02	0.08	−0.48	3.12
$CO_2/Pt_{13}Cu_{42}$	−0.19	−0.04	−0.19	0.00	0.00	0.07	0.03	−0.06	3.22
$CO_2/Pt_{42}Cu_{13}$	−0.21	−0.03	−0.22	0.00	0.01	0.01	−0.03	−0.35	3.29
CO_2/Ru_{55}	−0.20	−0.07	−0.20	0.00	0.00	−0.09	0.25	−0.75	3.43
$CO_2/Pt_{13}Ru_{42}$	−0.29	−0.04	−0.24	0.00	−0.05	−0.09	0.21	−0.70	3.07
$CO_2/Pt_{42}Ru_{13}$	−0.24	−0.03	−0.23	0.00	−0.01	−0.01	0.04	−0.20	3.22
CO_2/Rh_{55}	−0.22	−0.05	−0.22	0.00	0.00	−0.01	0.08	−0.55	3.26
$CO_2/Pt_{13}Rh_{42}$	−0.20	−0.05	−0.20	0.00	0.00	0.07	0.01	−0.95	3.28
$CO_2/Pt_{42}Rh_{13}$	−0.27	−0.03	−0.22	0.00	−0.04	0.02	0.01	−0.43	3.40
CO_2/Pd_{55}	−0.24	−0.04	−0.24	0.00	0.00	−0.03	0.10	−0.52	3.07
$CO_2/Pt_{13}Pd_{42}$	−0.25	−0.04	−0.26	0.00	0.01	0.08	−0.01	−0.86	3.37
$CO_2/Pt_{42}Pd_{13}$	−0.28	−0.03	−0.28	0.01	−0.01	0.25	−0.18	−0.75	2.90
CO_2/Ag_{55}	−0.20	−0.05	−0.19	0.00	−0.01	0.03	0.04	−0.21	3.20
$CO_2/Pt_{13}Ag_{42}$	−0.19	−0.05	−0.19	0.00	0.00	0.05	0.05	0.02	3.18
$CO_2/Pt_{42}Ag_{13}$	−0.24	−0.05	−0.24	0.00	−0.01	0.14	0.06	−1.06	3.29
CO_2/Os_{55}	−0.20	−0.05	−0.20	0.00	0.00	−0.03	0.01	−0.35	3.44
$CO_2/Pt_{13}Os_{42}$	−0.25	−0.04	−0.25	0.00	0.00	0.06	0.07	−0.66	3.40
$CO_2/Pt_{42}Os_{13}$	−0.23	−0.03	−0.23	0.00	0.00	0.03	0.07	−0.39	3.21
CO_2/Ir_{55}	−0.22	−0.03	−0.22	0.00	0.00	0.03	0.07	−0.27	3.27
$CO_2/Pt_{13}Ir_{42}$	−0.27	−0.03	−0.27	0.00	0.00	0.03	0.03	−0.14	3.23
$CO_2/Pt_{42}Ir_{13}$	−0.27	−0.03	−0.25	0.00	−0.02	0.07	−0.04	−0.58	3.17
CO_2/Pt_{55}	−0.24	−0.03	−0.25	0.00	0.01	0.23	−0.12	−0.38	3.02
CO_2/Au_{55}	−0.21	−0.03	−0.20	0.00	−0.01	0.02	−0.02	−0.17	3.52
$CO_2/Pt_{13}Au_{42}$	−0.23	−0.03	−0.21	0.00	−0.03	0.03	0.06	−0.07	3.19
$CO_2/Pt_{42}Au_{13}$	−0.25	−0.03	−0.25	0.00	0.00	0.08	0.02	−0.54	3.16

Table S23: Energetic analysis for the adsorption of CO_2 on Pt_{55} clusters of different morphologies, namely, restructured icosahedron (distorted ICO), icosahedron (ICO), hexagonal close-packed wheel-type (WHE), face-centered cubic fragments (two slightly different types, FCCf1 and FCCf2), and distorted reduced-core (DRC). Linear and bent CO_2, according to the OCO angle, correspond to the physisorbed and chemisorbed modes of CO_2, respectively. The energetic properties, in eV, are: adsorption energy, E_{ad}, interaction energy, E_{int}, deformation energies for the molecule, ΔE^{Mol}, and cluster, ΔE^{Sub}.

Mode	Substrate	E_{ad} (eV)	E_{int} (eV)	ΔE^{Mol} (eV)	ΔE^{Sub} (eV)
bent CO_2	Pt_{55} distorted ICO	−0.94	−3.44	2.81	−0.31
bent CO_2	Pt_{55} ICO	−0.69	−2.20	1.65	−0.14
linear CO_2	Pt_{55} ICO	−0.47	−0.23	0.00	−0.24
bent CO_2	Pt_{55} WHE	−0.44	−2.56	2.08	0.04
linear CO_2	Pt_{55} WHE	−0.32	−0.26	0.00	−0.06
bent CO_2	Pt_{55} FCCf1	−0.45	−2.67	2.13	0.09
linear CO_2	Pt_{55} FCCf1	−0.24	−0.25	0.00	0.00
bent CO_2	Pt_{55} FCCf2	−0.53	−2.59	1.97	0.10
linear CO_2	Pt_{55} FCCf2	−0.23	−0.24	0.01	0.00
bent CO_2	Pt_{55} DRC	−0.23	−2.38	1.96	0.19
linear CO_2	Pt_{55} DRC	−0.24	−0.25	0.00	0.01

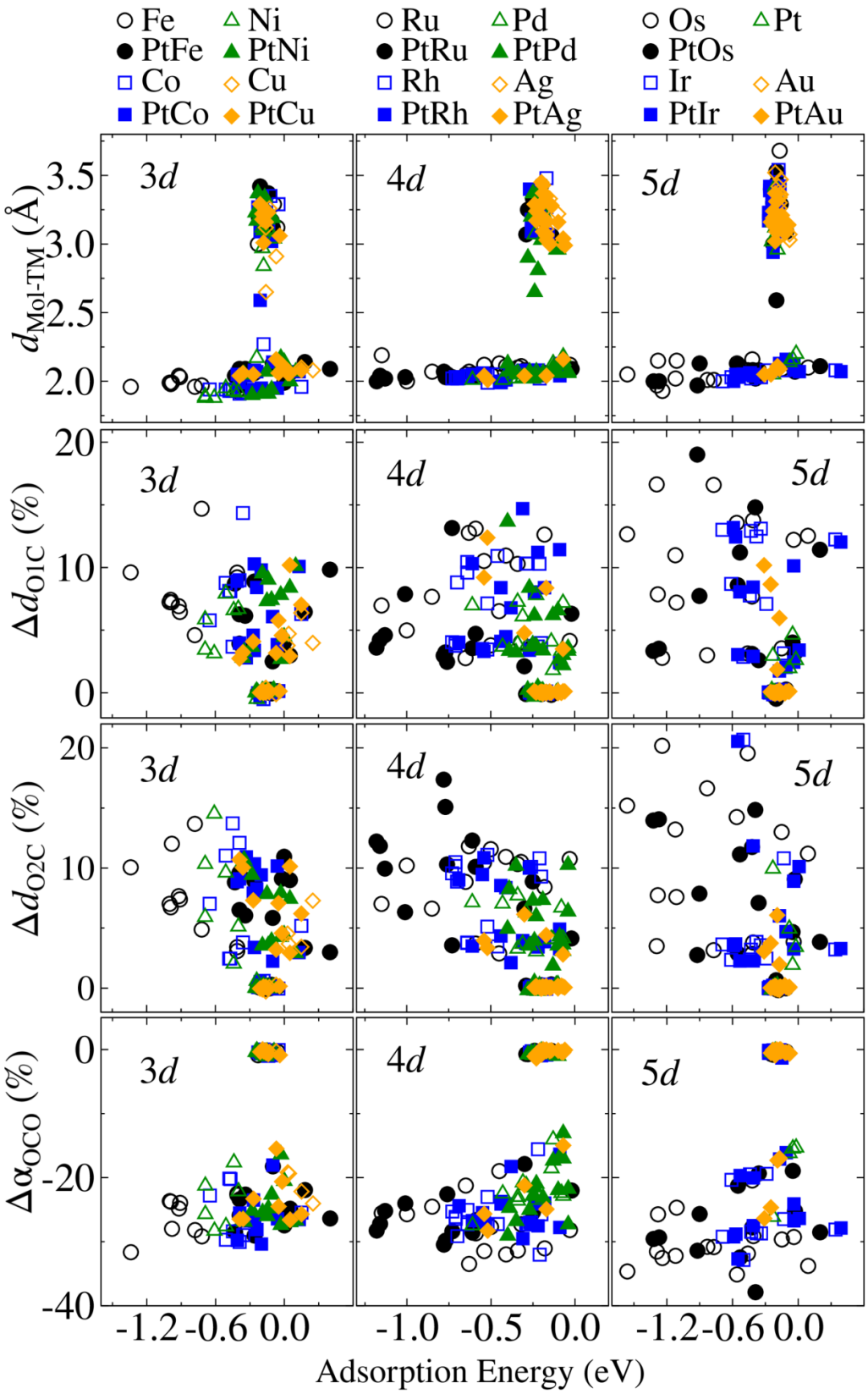

Figure S29: Geometric properties versus the adsorption energy for CO_2 adsorbed on the unary clusters and PtTM nanoalloys. Distance from the atom of the CO_2 molecule closer to the metal, $d_{\text{Mol-TM}}$ (Å), and percent variations after adsorption, with respect to gas-phase CO_2, of the O–C bond lengths, Δd_{O1C} and Δd_{O1C} (%) and OCO angle, $\Delta\alpha_{\text{OCO}}$ (%).

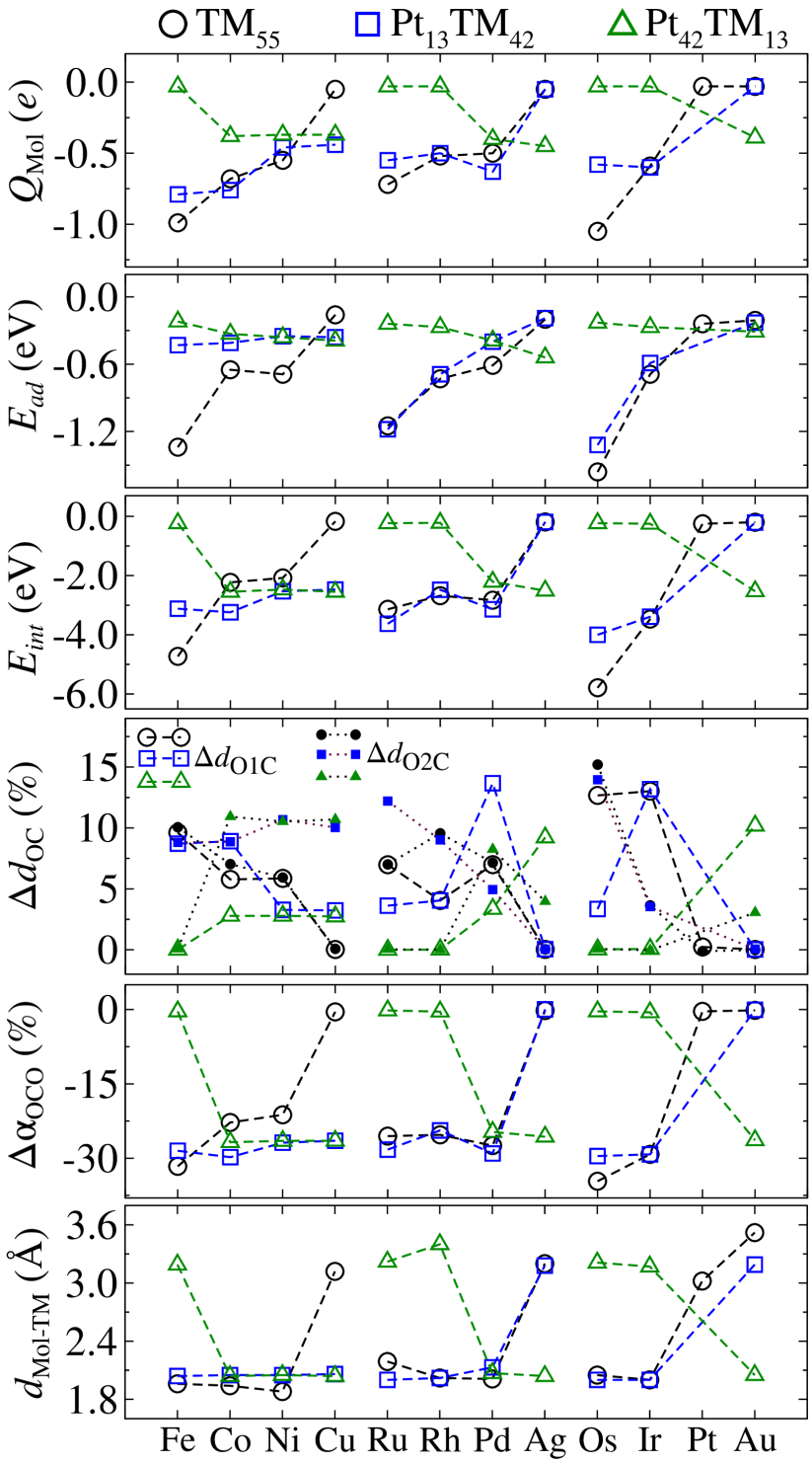

Figure S30: Adsorption properties of the most stable configurations for the adsorption (chemisorption or physisorption) of CO_2 on the unary clusters and PtTM nanoalloys. From the top: effective Bader charge on CO_2, Q_{Mol} (e), adsorption energy, E_{ad} (eV), interaction energy, E_{int} (eV), percent variations, with respect to gas-phase CO_2, of the bond lengths, Δd_{O1C} and Δd_{O2C}, and OCO angle, $\Delta\alpha_{\mathrm{OCO}}$, and shortest distance between an atom of the CO_2 molecule and a TM atom, $d_{\mathrm{Mol\text{-}TM}}$ (Å).

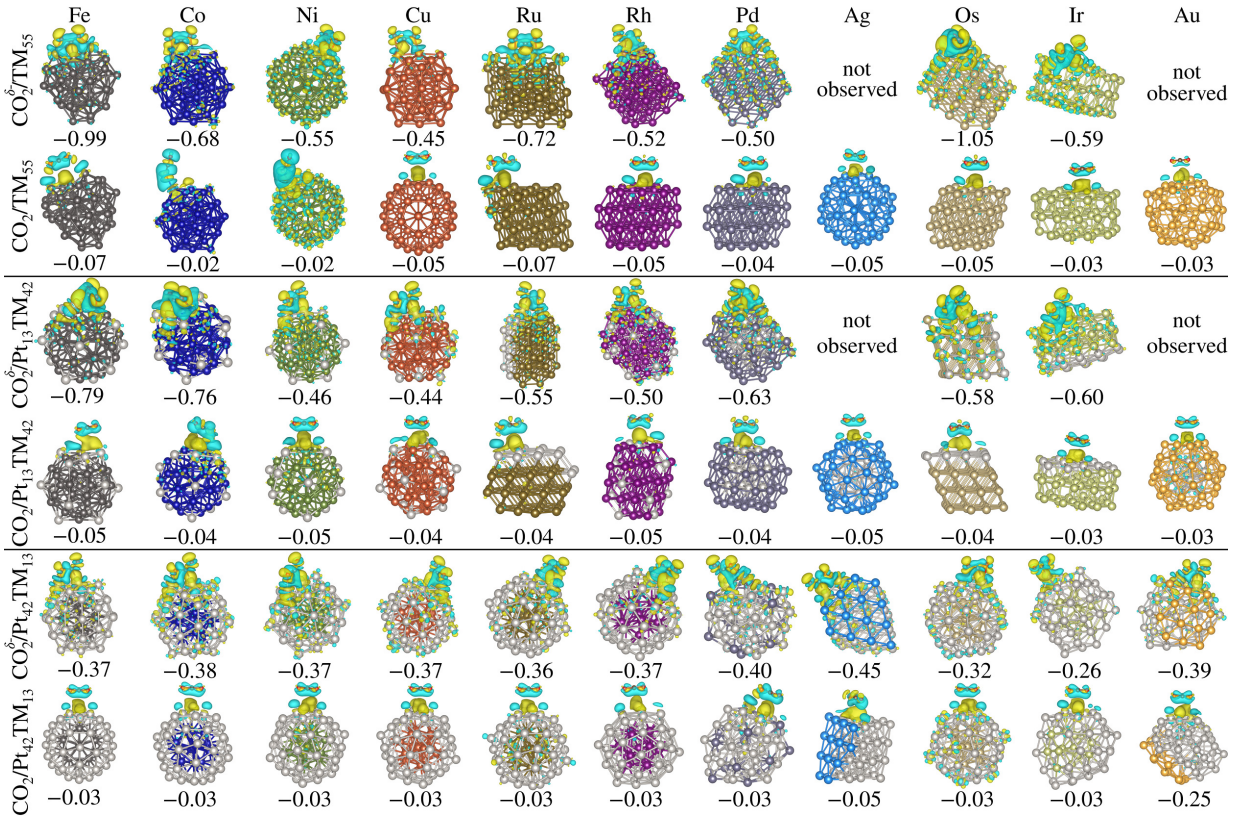

Figure S31: Electron density difference for the most stable adsorption structures of CO_2 ($CO_2{}^{\delta-}$ represents the bent molecule) adsorbed on the unary clusters and Pt_nTM_{55-n} nanoalloys for $n = \{13, 42\}$. The isosurface levels are of $1.5 \times 10^{-3}\, e\, a_0{}^{-3}$ and $3 \times 10^{-4}\, e\, a_0{}^{-3}$ for bent and linear CO_2, respectively (factor of 5); yellow and blue regions represent, respectively, accumulation and depletion of charge. The numbers below the configurations correspond to the total effective Bader charge of the adsorbed molecule (e).

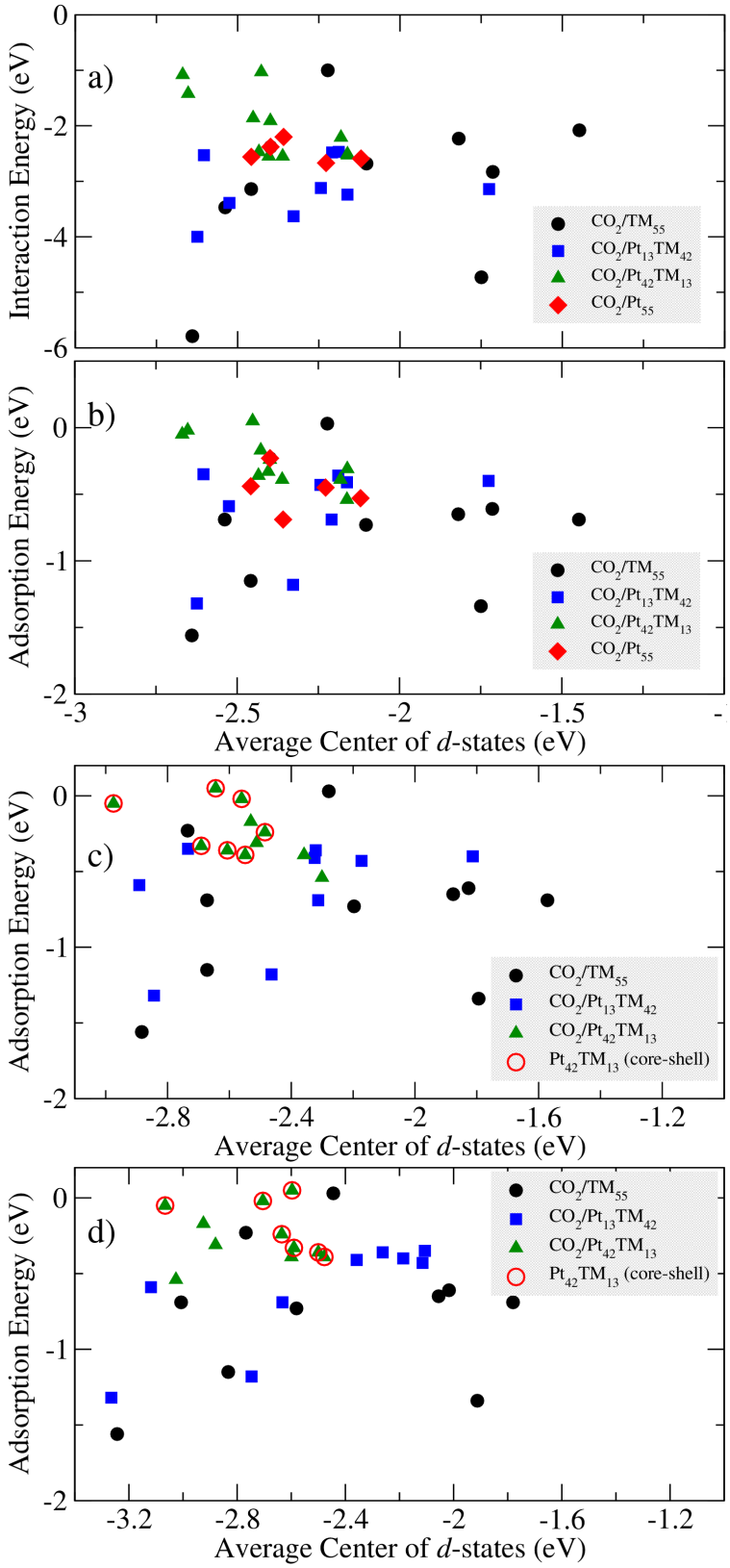

Figure S32: Graphs of the interaction energy and adsorption energy versus the center of occupied *d*-states, ε_d. The ε_d was calculated for a) and b) the transition-metal atoms of the cluster isolated and frozen in the adsorption configuration, c) the atoms closer to the adsorbate for the optimized isolated cluster, and d) all atoms of the isolated and optimized cluster.

S9 Cartesian Atomic Coordinates for the Lowest Energy Adsorption Structures

In this section we provide the cartesian atomic coordinates for the most stable adsorption configurations.

S9.1 CO_2/Pt_{55} distorted reduced-core (linear OCO angle)

C 1.4465788705336406 -0.1759373702177854 -6.9646501205998907

O 0.6267787284205096 -1.0148350426478501 -7.0421425621969673

O 2.2683346862608627 0.6564470088102762 -6.9014012058406520

Pt -2.4464334493835995 -2.5537710289184661 -3.8796358891289535

Pt 1.6585795106230814 -3.7760747425528907 -0.5641327607671847

Pt -0.8975731041201039 -4.1302293849772882 0.1102408632263168

Pt -1.1405806889865866 -0.2886288111708691 -1.9366050498544722

Pt -2.7371136076560845 1.8547425173809551 -2.4633052271945988

Pt -0.5293556832080543 1.4985022080228483 -4.0158028479058645

Pt -2.5396679405774716 0.0162066374883666 -4.5060850271559767

Pt -4.4023434014950702 0.1792815366473743 2.0883644534866126

Pt 0.5960668672205448 -0.8899318881580552 1.9474549254125244

Pt 0.8805980247484398 1.2802866242798763 -1.1963684550036322

Pt 2.4605124212870955 0.2675190029680091 0.5382296887318945

Pt 0.9458850414344467 -3.6322163106529919 2.0131373047194718

Pt -3.7046295831825482 -0.8003945148576727 -2.3198432261209194

Pt -2.4516178737186944 -2.6184495150041576 4.8951493584570800

Pt -4.0298588966026916 -2.3293194847226326 2.7707128086993493

Pt 4.7212568680737927 0.5512665866160510 -0.5962352033552363

Pt 2.4995245409948366 3.8473742998878961 1.2556993421174014

Pt 4.1369164833493146 -0.5756374030778780 -2.8889425243802971

Pt -1.8347895128278517 1.0498001339766196 0.1086389233988823

Pt -4.1997414740541057 2.7379934179276590 1.5317743991100508

Pt -2.8777429518355273 -3.2692582247229440 -1.4932931684010007

Pt 0.5417269076787560 4.2973244212553317 2.9396756995799680

Pt -0.1816134701646364 -1.2542536853549258 -4.1431529808851684

Pt 4.3652277019215706 -0.9882793808004252 1.6826519165821741

Pt 3.5735464547569258 1.9609225137387407 -2.4770176510414905

Pt 4.4145424400883755 3.2090002095510135 -0.3320307782962514

Pt -0.5256050720889877 3.4120395611994656 -2.1020448922895851

Pt 0.3348661434883981 1.6792088571964234 1.3682539637046962

Pt -1.7969477486594216 0.0057210572405701 2.3790387832141522

Pt 3.7144263031844948 0.3114335824489008 3.8831943953002432

Pt 3.4709609133025685 -3.4380475236297139 1.3134469646027749

Pt -4.1748226267981625 -1.6193939879496877 0.1647907077216667

Pt -1.4015827337025877 -0.1632776346226138 4.8983875214974475

Pt -3.0381260248942024 1.8079888027729327 3.8116427364430332

Pt -1.4989281597889581 -1.5376468556156098 0.3533562710055365

Pt 2.0330116047088875 -2.1190445608320454 -2.9101635108183888

Pt -4.3249834910103662 0.9357830704767497 -0.4402575224003082

Pt 1.8217262084494259 0.4101289431109781 -3.6230219944347559

Pt 4.1710095671817422 1.7447260970050096 1.7827588241831163

Pt -3.4623792146387391 -4.0346128585856755 0.8911312093231385

Pt 2.5736403472460223 -2.0222031362494919 3.3597886967543364

Pt -1.5872774975210342 -3.2855714814582138 2.5220706816684131

Pt 0.0872462841641150 -2.4153499766648716 4.2602288291010595

Pt 1.9742854862134271 3.6888957795465993 -1.2787746468874768

Pt -0.0275809100477494 4.1204090582485584 0.4027321750228406

Pt -2.4693325931095007 3.4590464511762509 -0.3560057056760288

Pt 1.1775525467099934 -0.0042894490296320 4.4100598979727437

Pt -1.8920092096081349 3.5974278099684076 2.2645819299578007

Pt 1.5388218519028902 3.0301443320342063 -3.7792027325950008

Pt -0.4198030469047803 2.0944714441465786 3.9966998152666418

Pt -0.2937472753026283 -3.1981040082401799 -2.2810797909303200

Pt 3.7757012535786112 -2.0058501664860016 -0.7911798773230472

Pt 0.9713316081617035 -1.3397739393880517 -0.7146469978357834

Pt 2.1250194524928441 2.2919845132045067 3.4150844824564364

Pt -4.0194878762890500 -0.5156941117385373 4.6380447806014518

S9.2 CO_2/Pt_{55} distorted reduced-core (bent OCO angle)

C 2.6978875805830329 4.9752038835979935 -2.8459001610920525

O 3.2069622650866343 5.9623010429181260 -2.3719021290294191

O 2.4900470434996551 4.5906808463913755 -4.0591313150344455

Pt -2.4808510414911931 -2.8027118809968585 -4.1092041927532943

Pt 1.5478403880980076 -4.0700133643817686 -0.7673886542324075

Pt -1.0085694502180591 -4.3993607612552470 -0.1128321232580520

Pt -1.1964582389013227 -0.5595422120510515 -2.1408959474664351

Pt -2.7473835323723579 1.5793566862525126 -2.6916113944731941

Pt -0.5117913079665730 1.1935403061061172 -4.1833514295832810

Pt -2.5702233896589446 -0.2387485140291356 -4.7571760062550208

Pt -4.4813022510452365 -0.0681671349509122 1.8476843108415630

Pt 0.5020013749380989 -1.1748683431549984 1.7261038974161786

Pt 0.9028756987464852 0.9475701653025131 -1.4861611214756858

Pt 2.4124731922102525 -0.0639393077268556 0.3604068384450370

Pt 0.8065985916658753 -3.9382949575550961 1.8099897754302068

Pt -3.7716620507090228 -1.0538609349883330 -2.5717092541520157

Pt -2.6059440088064987 -2.9120190179317036 4.6690173679602047

Pt -4.1380116423679505 -2.5887610933007914 2.5142601969023999

Pt 4.7017442295472422 0.2111910061366261 -0.7253761965021328

Pt 2.4128814264648666 3.4769479631137297 1.0838200674153258

Pt 4.0904159794679824 -0.8989458447184356 -3.0470291983402835

Pt -1.9123253308431221 0.7945060294645815 -0.1163517573412529

Pt -4.2633999067326451 2.4918690566124613 1.2716755148190122

Pt -2.9761764727237070 -3.5189058994101416 -1.7349060215888878

Pt 0.4583887655263224 3.9697289612091562 2.7440389074657090

Pt -0.2059479243368554 -1.5338378298189717 -4.3443972170829550

Pt 4.2775439812048957 -1.3409359591719709 1.5263953469432836

Pt 3.4121452141766930 1.5898293200986651 -2.5034050151058005

Pt 4.3981256764029402 2.8628691764089491 -0.4254461938507605

Pt -0.5336800616264654 3.1162544927412328 -2.3020312893165884

Pt 0.3031419910417872 1.3907068894573833 1.0698063512540512

Pt -1.8705731077065348 -0.2450702531423824 2.1505056351385003

Pt 3.6048310088820372 -0.0444004623107240 3.7503085241717167

Pt 3.3459568202129191 -3.7787183569987364 1.1305411416237197

Pt -4.2582880720091092 -1.8576020900800490 -0.0867427097674993

Pt -1.5323960308274895 -0.4803254432159610 4.6641464051655142

Pt -3.1577328972432896 1.5474453682694940 3.5762071861990772

Pt -1.5954178297264872 -1.8015385157712671 0.1395288085580348

Pt 1.9924574208059453 -2.4386522629588776 -3.1054985943381106

Pt -4.3925618443765719 0.6953999765212279 -0.6998627825936377

Pt 1.8198445490774799 0.0967493073767110 -3.9273596968993201

Pt 4.0941481304314875 1.3938991558764553 1.6682280591418273

Pt -3.5946631369586752 -4.2935027234249503 0.6384083823943774

Pt 2.4480354291884829 -2.3498554500014053 3.1630989263191993

Pt -1.7263755942890786 -3.5909498124811905 2.3015453178203189

Pt -0.0559199528667691 -2.7208084963311792 4.0369431027287899

Pt 2.0170409406836987 3.5930804721143743 -1.4865632190090248

Pt -0.0737199512583804 3.8522158376448439 0.1802775223489241

Pt -2.5073224436651076 3.2123867399352846 -0.5977329072821809

Pt 1.0501083790754187 -0.3238644368576106 4.2018789429086549

Pt -1.9578253287667640 3.3111645701347983 2.0223772992955351

Pt 1.5277173644127842 2.7395694236596433 -4.0512605582278791

Pt -0.5274691898623172 1.7624583739439423 3.7383044873740938

Pt -0.3678236082491602 -3.4751362892601976 -2.5005729445684310

Pt 3.7019124490272048 -2.3301544566184096 -0.9567649712259174

Pt 0.9093993216203609 -1.6336718388028444 -0.9343863942087369

Pt 2.0378380415133632 1.9642027324193523 3.2633417250004793

Pt -4.1485476559862642 -0.7939638400094952 4.3941113549729689

CO_2/Pt_{55} hexagonal close-packed wheel-type (linear OCO angle)

C 0.5043759984036347 0.3388998873206310 5.5686674264914329

O 1.2956315589439054 1.2050454309206462 5.5527924460162366

O -0.2862275400295646 -0.5282651882189046 5.5889410938164668

Pt 4.5911017949988064 -2.7702898997844088 -2.3914901961847184

Pt 4.6154083398880843 -0.1291667490334374 -2.4277894912444955

Pt 4.5765620263528284 2.4648228547564903 -2.4314216164215656

Pt -4.4617345473019832 -2.7742992388644669 -2.4556363017262273

Pt -4.5243598274689827 -0.1636791727141345 -2.4617707630322228

Pt -4.4485454891209848 2.4383233128154007 -2.4833253565747304

Pt -2.2291305591358466 -4.0975332495520647 -2.4483473021718565

Pt -2.2071104897179001 -1.4679713284075377 -2.9167991368431574

Pt -2.2040304207650365 1.1413222887994225 -2.8967126737030133

Pt -2.2413016804301424 3.8102002232821981 -2.4867200202180095

Pt 0.0619400348207531 -2.7868679035995161 -2.9023458787880623

Pt 0.0757650819379865 -5.3883944562142450 -2.4056284400306263

Pt 0.0598552625008935 2.4537195738866018 -2.8899378475493309

Pt 0.0462893595915526 5.0437103232559242 -2.4711508454164663

Pt 2.3357785564166518 -4.0832016965055207 -2.4287749596782104

Pt 2.3435308146469467 -1.4637812412780293 -2.8951439689143958

Pt 2.3257270728341410 1.1599369367327628 -2.9040907300113448

Pt 2.3429150357100657 3.8170150708358825 -2.4450111502222969

Pt 3.6559466753975975 -3.7086089023542890 -0.1032874197636309

Pt 4.9536507907338017 -1.5073670927946290 -0.1058701272934774

Pt 4.9618241532413343 1.1513123450209941 -0.1473837582940698

Pt -4.8908059257918932 -1.4697293552149373 -0.2007217872023537

Pt -4.9048653471701336 1.1752086753625604 -0.1929467528690472

Pt -3.5607073589554190 3.4535664938707269 -0.1968272588864926

Pt -3.5222079395358836 -3.7673807324838648 -0.1700466480488005

Pt -2.2438008381263082 -1.4691032043477976 -0.3038080928726208

Pt -2.2629639885969208 1.1638734294885735 -0.2838241888843092

Pt -1.2844550145175460 4.7722289634268122 -0.1908127937482194

Pt 0.0519721409242313 -2.8096688892398909 -0.2989567471101049

Pt -1.2112561488081541 -5.0826977131043289 -0.1244134961116474

Pt 0.0578012953384322 2.5090375342276747 -0.2779597406663674

Pt 1.3608938502465502 4.8061200702766289 -0.1768538196671097

Pt 1.3443764356631573 -5.0505863904542476 -0.1102606480210993

Pt 2.3558885659162794 -1.4729949658040373 -0.2922585709151653

Pt 2.3344371402008743 1.1836140462827427 -0.2906594451617126

Pt 3.6476050612493172 3.4787743278346017 -0.1789174132801223

Pt 4.6332984180267758 -0.1955042103797824 2.0872708086427343

Pt 4.5694375606695026 2.4983111547516144 2.0957941940106881

Pt -4.5076232059951131 -2.7634383120821315 2.0723523570245446

Pt -4.5576415394026011 -0.1674861767736465 2.0684885562521584

Pt -4.4419549237924656 2.4220414130674497 2.1179355466259677

Pt -2.1999363165963448 -4.1612094571205560 2.0685359263191634

Pt -2.1816947454976408 -1.5214934212396576 2.3012643311785110

Pt -2.2037283075760428 1.0968301110253658 2.3365129394169948

Pt -2.2458435758183839 3.7973170842895119 2.0741849485862272

Pt 0.0769606673210104 -2.8380495895015976 2.2679272989755992

Pt 0.0742233424132282 2.4176722285586889 2.3398531225675168

Pt 0.0391788597566512 5.0186218740456070 2.1290844483149017

Pt 2.3411885573308213 -4.1164801238630186 2.0860665457479426

Pt 2.3549089132443939 -1.5168297302469875 2.2750288238379994

Pt 2.3335060180769265 1.0981076934011160 2.3122770083501409

Pt 2.3434704892716089 3.8311018383263882 2.0861654766060509

Pt 0.0435351413338514 -0.1646468739310263 2.2979860422160332

Pt 0.0501713061622906 -0.1504489689804965 -0.3430273971418876

Pt 0.0627694105864103 -0.1595609517738231 -2.9961605563283458

CO_2/Pt_{55} hexagonal close-packed wheel-type (bent OCO angle)

C -2.7922118020829108 3.7721574784907070 -3.9220942932416056

O -2.1707468512974786 4.3460006987607311 -4.7871744559033580

O -3.9716308723963718 3.2328877969412253 -3.9190382158009642

Pt 4.7985361730070055 -3.0163962857810867 -1.7490766725583018

Pt 4.8383360369732662 -0.3726278924245163 -1.8369030023826916

Pt 4.8185028398698675 2.2245942549930038 -1.8586595753254016

Pt -4.2387161304310643 -2.9724800988631661 -1.9559980335077902

Pt -4.3058248002887707 -0.3627873010449945 -2.0141315281921761

Pt -4.2647787712564282 2.2667144156625230 -2.0774162460768446

Pt -2.0200408548814228 -4.3199648099655565 -1.9046620112995043

Pt -1.9735417641745880 -1.6968937594544313 -2.3852370023568215

Pt -1.9560179605412036 0.9001920794421705 -2.3980445316030812

Pt -1.9991892748564326 3.6009065410489867 -2.0367488271107073

Pt 0.2914820185323648 -3.0125596787181181 -2.3242045714143940

Pt 0.2812214974036454 -5.6105281019217390 -1.8001895964619574

Pt 0.3161377072434753 2.2205215669658656 -2.3914663811363193

Pt 0.3109654745654589 4.8502663585958139 -2.0095481876590773

Pt 2.5403614056294344 -4.3120813209898152 -1.8068921605528476

Pt 2.5682905650996024 -1.6988933383762428 -2.3053935617406234

Pt 2.5692024095294639 0.9239910472101227 -2.3257455779132910

Pt 2.5813353352817505 3.5902432789700778 -1.9263298694174160

Pt 3.8231491955706756 -3.9188662666293355 0.5353795560218224

Pt 5.1193886998955618 -1.7162630479753054 0.5197832781110396

Pt 5.1600787142738538 0.9384104803655633 0.4400971574854921

Pt -4.6938131689973526 -1.6059560448066306 0.2703294436652552

Pt -4.6652894543961017 1.0329814033474995 0.1719756190702963

Pt -3.3487924973036809 3.3359879072358427 0.2629640014569283

Pt -3.3426991508875035 -3.9424349205370164 0.3474104510780870

Pt -2.0589047816300892 -1.6568143045456820 0.2201493671194445

Pt -2.0514302403049283 1.0142647517935159 0.1996074706066191

Pt -1.0904832189503382 4.6443048353976852 0.2555828631128289

Pt 0.2183065960587629 -2.9979952221803665 0.2765084586355552

Pt -1.0606138416011839 -5.2782717086670257 0.4482854864550678

Pt 0.2315850638073483 2.3240669981958795 0.2227150241089088

Pt 1.5503631278525609 4.5953739554232538 0.3114262822703015

Pt 1.4970883227242697 -5.2352943403844545 0.5098151712906420

Pt 2.5275434338093343 -1.6821078181807467 0.3042629575386739

Pt 2.5334609448430547 0.9808379937557674 0.2793216541470038

Pt 3.8446342354859122 3.2625366123594577 0.3653370484788702

Pt 4.7666774215860501 -0.3793455105292287 2.6873875787488011

Pt 4.7314088628219961 2.3107757764295083 2.6741511144288070

Pt -4.3749645292951671 -2.8907815545458768 2.5377598469288412

Pt -4.3925609080747110 -0.2963623726790756 2.5470620448198433

Pt -4.2710596740370503 2.2848638560158476 2.5134687740191568

Pt -2.0639981435013373 -4.3155214003283948 2.6189636277751616

Pt -2.0474059445018313 -1.6691452590005460 2.8306218397337597

Pt -2.0560004562497309 0.9582991601716901 2.8229187601954795

Pt -2.0384732293584880 3.6482701135632376 2.5343463992273518

Pt 0.2014253381883697 -2.9915552577473190 2.8441141657737061

Pt 0.2280934340815537 2.2611577830981902 2.8479647714206653

Pt 0.2511622074553670 4.8786169255757361 2.6220083413600772

Pt 2.4601095646901885 -4.2826482492373739 2.7107644954310919

Pt 2.4788308326575890 -1.6858542641256558 2.8748425006288683

Pt 2.4807077100110253 0.9256686563062402 2.8820300530819063

Pt 2.5084235230435037 3.6456290801967692 2.6035192548783010

Pt 0.1849453793240339 -0.3204601844674964 2.8703443547024241

Pt 0.2366051138753176 -0.3375658994175110 0.2143050753803568

Pt 0.3008291361045071 -0.3920655927882051 -2.4425699875322548

S9.3 CO_2/Pt_{55} compact bulk fragment type 1 (linear OCO angle)

C -4.4144053063621245 -2.7521156245480372 -3.7323150171177488

O -4.0624350119808481 -3.8440853111307378 -3.4829886857779151

O -4.7815752700144936 -1.6698849305598518 -3.9963210108013012

Pt 0.2393538304380094 0.2250724033007325 2.5244539784462310

Pt 1.7168476668851804 0.2294597093377899 0.2577282291277053

Pt -2.3968138989803185 -1.8962743489170701 4.0980230268147118

Pt -3.8869987500060619 -1.8854770362306137 1.8215728335457226

Pt 0.2372903294156119 2.3812874449107708 0.9401637537712728

Pt 2.8830165748738317 -1.8891073250301857 4.0961885921593462

Pt -1.3086530348132142 2.4357316203911532 3.2825689850124418

Pt 3.2676538375375532 -2.0140030455647375 -0.5582400737207733

Pt -1.1686477436430556 0.2541348592018881 4.8141488937404961

Pt 1.5766576026881829 -1.9195151899244809 1.8545293077499634

Pt 3.1998248608048661 2.4797000830860716 1.0832296227962954

Pt 1.6482564711925844 0.2585390233797328 4.8129545793331250

Pt -2.4375527546899098 -4.0555882683327384 1.1914350420163922

Pt 4.4842428532705538 0.2624975540178600 0.2646956478847782

Pt 0.2348932746022028 2.4614406239649016 -4.0477026474214561

Pt 2.9248815100180501 -4.0458891536392789 1.1919744318220127

Pt -2.7632493465355958 0.1111605698069635 -2.1256008607024146

Pt 1.6576973132885593 0.2094432696907857 -4.2903654519556387

Pt -1.0884248353243704 -1.9259644311040034 1.8558666549591665

Pt -1.3617213419793197 -1.9958624991148344 -2.7416246619208149

Pt -1.1763146302856606 0.2058715078897972 -4.2882084344677871

Pt -2.8205508179323759 0.3459550533376696 2.6620950779498536

Pt 0.2466394139716312 0.2307407952860150 -2.0167533236151094

Pt -2.4278620861632030 2.3385775891392573 -3.5768139252985183

Pt 0.2449203420579718 -4.5112773632387144 1.1641493331822532

Pt 4.3771646995822913 2.3805079400188935 -1.3125661828554771

Pt 0.2453751607838024 -1.8981787149782405 -4.8687146265983721

Pt 3.2996862151747850 0.3554155807955476 2.6611738549372230

Pt -1.0989946379339584 2.3684891187026107 -1.3350768985278860

Pt 2.8966603948467311 2.3493022080460939 -3.5791928171639285

Pt 1.7802271221416124 2.4396248165537573 3.2819537975773923

Pt -3.9093535576635565 2.3678973426375878 -1.3099360975759125

Pt 1.5646922922524906 4.5208041462472828 1.6869174523722863

Pt 4.3723259885099948 -1.8737293231569943 1.8201832642229154

Pt 1.8870116802827477 -2.0051708893250941 -2.7606884951210677

Pt -1.1012324966753360 4.5172081423541126 1.6865258793814435

Pt -1.2306847398033041 0.2266362433614894 0.2603387436728795

Pt 0.2486094085298198 -4.0371103710650589 -3.2639425251409584

Pt 0.2307474022218790 4.9522205096795604 -0.6028656454900985

Pt -2.7276756837100811 2.4702235301051703 1.0834709910308573

Pt 1.5775014439321620 2.3714326195468844 -1.3338368926965638

Pt -2.4240329912372376 4.5053183419731466 -0.6243550963695930

Pt 0.2489112208895188 -1.9279141533059050 -0.4127542427021568

Pt 3.2607950212774037 0.1132191341714172 -2.1429511461521109

Pt 2.8885818800013841 4.5176343171808400 -0.6251986281983799

Pt 1.6590069227641377 -4.0979987061063659 -1.0686794394570305

Pt 1.5464790114936227 -4.0963969754087861 3.4686446121648871

Pt -1.0705585362687922 4.5273933681269298 -2.9106870867455203

Pt -2.7713461650350899 -2.0193464963680023 -0.5511056058449333

Pt -1.0578977635015550 -4.0998823088027647 3.4678309968464038

Pt 1.5317545347381119 4.5309323260995873 -2.9099427604688799

Pt -4.0066667807189225 0.2492440384237719 0.2685376405010114

Pt 0.2442582287098842 -2.0110702184347309 4.5652223284782529

Pt 0.2362549028451761 2.3809611289273525 5.3708051419558096

Pt -1.1645712307639622 -4.1022342754062029 -1.0679544135447794

S9.4 CO_2/Pt_{55} compact bulk fragment type 1 (bent OCO angle)

C -0.4395847596145316 -5.5836890608422545 4.1655546049488512

O -1.2250461331469933 -6.3491891067262687 4.6801842358610690

O 0.8614565862946574 -5.5607927829160735 4.1552740790896783

Pt 0.0335563065164527 0.3634975803545731 2.0614093968866238

Pt 1.4741895763100579 0.4048940983045509 -0.1994055962259425

Pt -2.6014516550614872 -1.7659703279463599 3.6577330106712869

Pt -4.1244550285367474 -1.7309700722705006 1.3970099320998801

Pt 0.0105110914561953 2.5407265299075252 0.5015349700453977

Pt 2.6955081110367121 -1.6947662915462043 3.6610716518343991

Pt -1.5414355616338615 2.5835483252038722 2.8404455248214897

Pt 3.0421213490722709 -1.8170228911078083 -1.0000175409639209

Pt -1.3765562191415701 0.4012631237316501 4.3595806656638585

Pt 1.3507006747983659 -1.8142100694869103 1.4521115564435649

Pt 2.9611412780710658 2.6494766170738178 0.6261603051625282

Pt 1.4327641646023443 0.4335699537777026 4.3657746154322874

Pt -2.6400274158608643 -3.8946873255539289 0.7866294046070128

Pt 4.2679244110097825 0.4458910103697972 -0.1928107293309975

Pt 0.0051055666860226 2.6449965439384213 -4.4964816592585910

Pt 2.7338054362455826 -3.8774457018711557 0.7104340439073797

Pt -3.0059688041152950 0.2686013667911978 -2.5751007164370336

Pt 1.4141169552691344 0.3919011773509508 -4.7443055755675596

Pt -1.3322588357092688 -1.7593623500475430 1.4141810594897515

Pt -1.6261471018371805 -1.8423298528092562 -3.1816365383799181

Pt -1.3843645232494119 0.3808610299293181 -4.7191866619278633

Pt -3.0435008711517804 0.4956455624214097 2.2202749442101726

Pt 0.0198375633236903 0.4033383806648764 -2.4505350662307515

Pt -2.6659666733066030 2.5066083237460992 -4.0133623944600112

Pt 0.0183229433849542 -4.3541854059978329 0.7099046735412133

Pt 4.1357695556285270 2.5692976861829813 -1.7707790617358694

Pt 0.0097692483224808 -1.7348967135185418 -5.2932674481777378

Pt 3.0703106081336480 0.5271669585714226 2.1971476988225578

Pt -1.3277230479573707 2.5506791196700016 -1.7746351179156989

Pt 2.6728437663618023 2.5329419630553058 -4.0428327314737986

Pt 1.5613969294711310 2.6140029245201797 2.8346337556532650

Pt -4.1244511911895234 2.5248044478671501 -1.7456810218185930

Pt 1.3317098818463466 4.6978439385245521 1.2430382432993698

Pt 4.1608993990297165 -1.6861063284545679 1.3695408505043338

Pt 1.6455784217281981 -1.8205219116345528 -3.2019811868936494

Pt -1.3223703878846416 4.6728297359726723 1.2555535870663381

Pt -1.4734500513923661 0.4089625801951248 -0.1995499908551026

Pt 0.0045991588683588 -3.8708518844659645 -3.6898881979090086

Pt 0.0014233461263636 5.1345903486765900 -1.0262328333274575

Pt -2.9581978632564430 2.6276726033375208 0.6508038024361631

Pt 1.3442189480743916 2.5731786062017692 -1.7938937246359683

Pt -2.6634979812100057 4.6765832323304828 -1.0479110943977887

Pt 0.0195159643784827 -1.7488176766726482 -0.8274208484503220

Pt 3.0199593441783308 0.2999470017263511 -2.5805521467169279

Pt 2.6661176180176471 4.7054944066440401 -1.0711023517967910

Pt 1.4326277005416794 -3.9104106723882657 -1.5161570126886041

Pt 1.3582822399587289 -3.9192956074049059 3.0084867378568743

Pt -1.3015609179346517 4.6899938402273635 -3.3299917262586427

Pt -3.0269288504103948 -1.8508819317824272 -0.9869208821811513

Pt -1.2464709516960668 -4.0305026512911040 3.1013847260122298

Pt 1.2992403798945751 4.7133366332590558 -3.3485884644362298

Pt -4.2494310718853523 0.4010835574534487 -0.1652611144333336

Pt 0.0325828340819237 -1.8411267144338435 4.1353485187655279

Pt 0.0097282051624848 2.5462868387993884 4.9144378477907429

Pt -1.3967896666997004 -3.9234827156122494 -1.4901550080385850

S9.5 CO_2/Pt_{55} compact bulk fragment type 2 (linear OCO angle)

C -6.4383877364500446 0.1130294577290857 0.1726352500215128

O -6.5241911732573659 -0.4095098714719213 -0.8749539234236284

O -6.3914528891878533 0.6367543427492731 1.2223530415633310

Pt 1.3973580197062594 1.3365383954168519 0.9015769621585775

Pt -2.9464091012343934 -2.6629891876842509 0.0317987080118249

Pt 1.1066730317608275 -2.7753982089017422 3.3515419958587906

Pt -3.0627802201836376 1.3927958900670585 2.2131957421809276

Pt 1.4815919157634285 -0.0220955955211998 -1.4179154533335843

Pt 1.2913411819657252 0.0535263561552178 3.2475086323012907

Pt 1.3043615545245837 4.0116052386958305 0.8572525335368336

Pt 1.6516832271303175 3.0491896606859985 -1.6291443113121331

Pt 3.4019219509436951 3.9889186252957929 2.4138694100719715

Pt 1.4151577960898427 -1.3040963163522108 0.9446492298035437

Pt 1.6961076276665574 -3.0985027764763791 -1.5326921481295197

Pt -1.0559754441801621 1.5522246142740179 3.9114598098179774

Pt -3.0445029443344120 -1.3830475763078856 2.2564683160822168

Pt 3.6802002613071423 1.3749092198751558 -2.0380478843921099

Pt -3.1025643265621090 0.0410715090455679 4.4567265530100819

Pt 1.3585192822645347 -3.9792911370340933 0.9857692848163623

Pt 3.6997942622572166 -1.4082346520013751 -1.9936144045172024

Pt 3.8246301469401933 -1.2296949590419068 2.5168553349525156

Pt -0.7921339289313805 0.0118118054715291 1.6021349225938910

Pt -3.1290149087173011 1.2304213213734065 -2.3231994019145872

Pt 3.4536851425063766 -3.8770269171548142 2.5430838090935723

Pt -1.0287863512711288 3.0805886991376594 1.7146215949692141

Pt -3.1036799966672417 -1.3643671778828701 -2.2820089971815167

Pt 1.0687359244120840 2.8805785092638647 3.2600587271527304

Pt -0.9888718385566184 -3.0573430068804930 1.8152454558948530

Pt -0.6211276742488101 -0.0612092314223844 -3.0620655497971359

Pt 3.8078015534693961 1.3465276481174751 2.4741656023951344

Pt 4.1108433792729180 0.0223028391892387 0.2262096949926246

Pt 3.7834823614942383 -0.0500781120502537 -4.2253491723756191

Pt -2.7738724854263621 -0.1010470967002572 -4.6288485639715482

Pt 3.6029293809463834 2.6486280155066035 0.1763670094837359

Pt -0.4687689072208050 2.8371282516111060 -3.1564252812783979

Pt -2.6544094700676188 2.4994800862063746 -4.6118955175120124

Pt 3.6377424618934064 -2.6093306997753727 0.2620662453500428

Pt -2.7811582169743927 3.8774251944549158 -2.3292822295253965

Pt -2.6178667848100323 -2.6984407633117184 -4.5311795176492993

Pt -0.7195573327401474 1.2996317750714155 -0.7717772673047666

Pt -0.4270864325218406 -2.9601112588429848 -3.0638069256848897

Pt -0.4815937212066457 1.2903468316638020 -5.3766743878279364

Pt -0.6872878525785309 3.9692816071115118 -0.7562198816109028

Pt -2.7259735000399905 -4.0054513937310672 -2.2056952913868559

Pt -0.4623510504563653 -1.4828554231634012 -5.3317641329212702

Pt -0.6994807419814810 -1.3523129362784421 -0.7282738809890749

Pt 1.6800663191104102 1.5423402587436434 -3.7825652464893369

Pt 1.6706321046679653 -0.0905173932516582 -5.8711017449550269

Pt -0.6327221465041815 -4.0176933314897836 -0.6280634308515293

Pt 1.7035563171345967 -1.6581625741110699 -3.7323163229589649

Pt 3.3821355469218686 0.0946362230639214 4.8149647491222396

Pt -3.2716906970449910 -0.0328887998841935 -0.0316095361205409

Pt -1.0369986283385879 -1.4586038928085607 3.9597340937351775

Pt 3.2102267734193530 2.6729984790660302 4.7169595877850075

Pt -2.9818817094709180 2.6015710668333183 -0.0517850035781532

Pt 0.9845251716562622 1.3920304412344231 5.5388321846762807

Pt 3.2446854115456345 -2.4879559534905544 4.8015497797822349

Pt 1.0021901043941241 -1.2100361200872431 5.5786211477784420

S9.6 CO_2/Pt_{55} compact bulk fragment type 2 (bent OCO angle)

C 0.6038751139683858 -0.3925684462333175 7.1283866255921922

O 0.5628748401904979 0.8937203438726603 7.2070526138236666

O 0.5886792557239819 -1.2756472688192664 7.9651665718326310

Pt 1.0147345793224640 1.3412543742920742 0.4772011103760204

Pt -3.3052824297091496 -2.6309263407157264 -0.3713036334050601

Pt 0.7664955307008126 -2.6719216563162096 2.9612570060722687

Pt -3.4640219907634253 1.4133774168499020 1.8100514739099047

Pt 1.0844950203951611 -0.0080253589357147 -1.8438001444331711

Pt 0.8921457466899363 0.0705406002160151 2.8523045649375760

Pt 0.9333942617712094 4.0331610170854386 0.4796043086780939

Pt 1.2864104682598723 3.0779983033588874 -2.0210754160382685

Pt 3.0154428411957830 3.9749171600428381 2.0352607430491467

Pt 1.0359466742253383 -1.2872603769383166 0.5129225156872765

Pt 1.3293662250791365 -3.0950895546121480 -1.9261260313955724

Pt -1.4763263494952752 1.5414566127080660 3.5176214428457424

Pt -3.4096500625347335 -1.3632243165562519 1.8433206266317859

Pt 3.2927011413805469 1.3906811728083854 -2.4481121863501620

Pt -3.5178203140826478 0.0502354093708163 4.0490891429963840

Pt 0.9850052272250900 -3.9681407567331934 0.5731346399621167

Pt 3.3238126466644604 -1.3915281256952843 -2.4076034129510653

Pt 3.4449512043928991 -1.2171044189554576 2.0919946210543863

Pt -1.1887733043805961 0.0388955220333013 1.1718965827166636

Pt -3.5494620215961006 1.2476657542108891 -2.6997624440098669

Pt 3.0512888959419837 -3.8421489418501249 2.1472014360598415

Pt -1.3800161840141203 3.0779189721830189 1.3225155738471859

Pt -3.5441388205233308 -1.3434314003705905 -2.6735785936790997

Pt 0.7098164788722063 2.7815131238037774 2.8918554504071743

Pt -1.3191550150766385 -2.9956159473101014 1.4124794936526639

Pt -1.0219629665636840 -0.0345393952308760 -3.4867832043822080

Pt 3.4057354990187876 1.3591192612072851 2.0559757252744308

Pt 3.7260721410839017 0.0414164979743765 -0.2040589788677680

Pt 3.4039665735841340 -0.0259517074782439 -4.6335628941854399

Pt -3.1925912094554127 -0.0805091657988227 -5.0104907206037339

Pt 3.2305984033644246 2.6683281832406660 -0.2291357098077871

Pt -0.8395655175085195 2.8939894258449144 -3.5367835170107735

Pt -3.0352549957704880 2.5036496541895010 -4.9881044927239966

Pt 3.2813063266446449 -2.5867475192827474 -0.1488831466030458

Pt -3.1544187002980979 3.8961866265599401 -2.7149693786982674

Pt -2.9952660682510568 -2.6570100458508801 -4.9102100912165607

Pt -1.1183961584772990 1.3167153663363360 -1.1977474837629298

Pt -0.7978383406752889 -2.9802200465420050 -3.4641107674604203

Pt -0.8616804960978199 1.3281478211897595 -5.7568026771721783

Pt -1.0621878264052902 3.9863148327907192 -1.1305611098590234

Pt -3.1164960587101009 -3.9870596249423791 -2.6000267421354817

Pt -0.8386399753906821 -1.4812610003493167 -5.7073623574177539

Pt -1.0930891975517532 -1.3231146658852173 -1.1649771317637878

Pt 1.3017942796939868 1.5888184142091115 -4.1817245909009895

Pt 1.2616928097400932 -0.0661689688494052 -6.2463218706035253

Pt -1.0193114222913180 -3.9971397487439475 -1.0227043172772845

Pt 1.3357254313536289 -1.6684842061218796 -4.1202783575712516

Pt 3.0184088158127289 0.0863905094873677 4.3715954382818207

Pt -3.7596509491302412 -0.0146975395030731 -0.4229919800175547

Pt -1.4056962072644636 -1.3967528569517638 3.5732395485356943

Pt 2.8368609661436133 2.6554317253472934 4.3552039239769478

Pt -3.3540491779084500 2.6091170548158242 -0.4437553167072714

Pt 0.5093907958474095 1.5293791049548571 5.2206623503324501

Pt 2.9118538976643138 -2.4829837345070462 4.4363641453591924

Pt 0.6758996679745528 -1.1310671249047155 5.2503510231180464

S9.7 CO_2/Pt_{55} icosahedron (linear OCO angle)

C 0.0070823352471486 6.7220383837367734 2.4691554637966484

O 1.1793897845058448 6.7343550827661041 2.4894216804945537

O -1.1662018593346497 6.7248731397257746 2.4554574770417905

Pt 0.0021546189609171 -0.3657529250024826 -0.1311878092287552

Pt -0.1056833993500944 1.0845722758270147 2.0048046380904911

Pt -0.0876600798026700 0.8994473845731803 -2.3846220221390264

Pt 0.0958858775185750 -1.6276065019009427 2.1219170424518663

Pt 0.1031561132239672 -1.8147020312716973 -2.2728688548381988

Pt 1.1958732716877973 1.9439138518180292 -0.2077737909456671

Pt -1.5292436023612543 1.7420683838821378 -0.2388797636819179

Pt 1.5252196509854228 -2.4781791494777132 -0.0347871608575984

Pt -1.1957473208194278 -2.6759329778955618 -0.0513995491053988

Pt 2.2152416798242278 -0.1560895000340951 1.2222756225988713

Pt 2.1924704005180029 -0.2585731274162790 -1.4917361610432809

Pt -2.1875152602424253 -0.4757606027577634 1.2266475978841247

Pt -2.2118416668655234 -0.5808623474865020 -1.4909837567174988

Pt -4.3451599476635723 -0.3408490595642379 -2.8207442222761823

Pt 0.0224470838642715 2.3167243692610646 4.2137654391785864

Pt 0.0117965571213884 2.3305687171722904 -4.4739582250320185

Pt -0.0127264124976697 -3.0682611781451894 4.2016635679489651

Pt -0.0212168285006921 -3.0514872207067438 -4.4829589736512174

Pt 2.7035912649222462 3.9683711380962898 -0.1312474202394535

Pt -2.6683746960941912 3.9933102238649787 -0.1341139535161998

Pt 2.6640053545534430 -4.7288241728943916 -0.1375519603304833

Pt -2.7110337866227328 -4.6949649900466621 -0.1435588135138927

Pt 4.3482308588452891 -0.3883594994199133 2.5506907008310091

Pt 4.3544244689292295 -0.3910408839783134 -2.8147361541844389

Pt -4.3493225609030803 -0.3435707305947004 2.5448273446062459

Pt -0.0027441885867249 4.2522003277451610 -0.1272521802617396

Pt -0.0066078360049789 -4.9881017352737675 -0.1585639200952022

Pt -4.5786520738678478 -0.3160937249261883 -0.1391758945815761

Pt 4.5844912601001022 -0.4229361262836523 -0.1311031173488674

Pt -0.0046888650752167 -0.3693463812137633 -4.7195797776484989

Pt -0.0012988683761207 -0.3659159336239476 4.4541307401379298

Pt 1.3699665435837556 -4.1055332922931917 2.1406999247171279

Pt -1.4552171390472717 -4.0688420579510574 2.1727991805856299

Pt 1.4009594366472848 -4.1056620743715051 -2.4262119875939230

Pt -1.4586682402551192 -4.0545220644903459 -2.4356245403251751

Pt 3.6929967490928961 -2.6831038894494506 -1.5764677420084925

Pt 3.7349380320168928 -2.6899435936135210 1.3106987451070577

Pt -3.7487044241393503 -2.6698887667906388 -1.5543768063617356

Pt -3.7353732662418730 -2.6411997387883450 1.2561226094818854

Pt 1.4532970770023672 3.3324703070677599 -2.4447339425048376

Pt 1.4565930925737911 3.3236133521506290 2.1657302041397810

Pt -1.3757640850588766 3.3701745382217729 -2.4151131197917031

Pt -1.3993851856320800 3.3701954458864924 2.1543484055597335

Pt -2.3051397962203870 1.0866431050380574 -3.8246440931868384

Pt 2.2971062027443896 1.0401321849776433 -3.8424274904649951

Pt -2.2905485713642681 -1.7603161680668138 -3.8656700136243969

Pt 2.2861106384300136 -1.7886073534236293 -3.8400191411141207

Pt -3.6903302563794531 1.9475061576065422 1.3093216228981022

Pt -3.7453670244645556 1.9542335939182567 -1.5722779584524331

Pt -2.2983835561833343 -1.7818543217196905 3.5696275498497791

Pt 2.3063802879579844 -1.8150500926864379 3.5642719085993906

Pt 2.2899010498370815 1.0268467833794621 3.5956433701805337

Pt -2.2842850310053011 1.0512064271831041 3.5736041247565962

Pt 3.7326993322336763 1.9116117253673752 -1.5294695415172224

Pt 3.7464768060327449 1.9406573142932424 1.2781948972462813

S9.8 CO_2/Pt_{55} distorted icosahedron (bent OCO angle)

C -3.1448406256547661 -3.2704725359695912 -2.6653625201388333

O -2.6002201257655746 -4.3851108072453089 -2.3432091672622342

O -3.2249908738599200 -2.8237822173016065 -3.8651590539852609

Pt 0.1780813092348955 -0.0094241309675482 0.0313480586738011

Pt 0.5680983924311581 1.4886347415681411 2.3570399004045974

Pt 0.4620934217002416 1.1568591502175154 -2.2017679736637348

Pt 0.2510102410710923 -1.3327769311608606 2.1637439831252943

Pt -0.9363259796801012 -1.6934742603832931 -2.1520652414233563

Pt 1.6369471770722284 2.1639913172698710 -0.0575271343757893

Pt -0.9555197507393066 2.4282047999509695 0.2790844886547317

Pt 0.7687727672274430 -2.5478996114981127 -0.4647500878634097

Pt -1.6464384315376968 -1.8878543121427829 0.3164663864622292

Pt 2.4525906327160540 -0.0471191386453065 1.1801204830653125

Pt 2.2537531644042974 -0.5903949156830646 -1.3706252681842133

Pt -1.8070352487761407 0.3800997558603718 1.7193401347318964

Pt -1.9666386716769899 0.4655393205015297 -1.2090327209238565

Pt -4.1327668421572499 0.2131807730463888 -2.4643279114829877

Pt 0.1476266035521897 2.8789820836913611 4.5204584703536907

Pt 0.1637862584707908 2.9829616500237170 -4.0346380320006547

Pt 0.0934045224457603 -2.4058368939656729 4.5052141505716685

Pt 0.3833375780462246 -2.2673499545479912 -4.2360786616203105

Pt 2.7928131475901856 4.5210952925377361 0.2816612318552518

Pt -2.4797752019621400 4.5792902887150353 0.2438783196499859

Pt 2.7900813435644323 -3.9470325295037911 0.1483202882729893

Pt -2.6714251031764289 -4.1909444541483447 0.3900981433333539

Pt 4.4012469272634078 0.2513430046334928 2.8791463354444655

Pt 4.4309459537302498 0.2998084482783188 -2.3927478016194801

Pt -4.1741422558245569 0.3254624638714849 2.8780974906708359

Pt 0.1782480624016264 4.8185544253792392 0.2837992875024804

Pt -0.0334518657112680 -4.6910015504412845 0.5724360242209305

Pt -4.3036047147114251 0.2553354198337547 0.2055188811784061

Pt 4.8227529325044172 0.3407770717006968 0.2417152522606132

Pt 0.0308328025030911 0.3213509600206261 -4.5504009734195607

Pt 0.1181244487653993 0.2345552724512936 4.6967616232417244

Pt 1.5646199253848423 -3.5020474108438657 2.4657683225059799

Pt -1.4104950818933399 -3.4416500876738008 2.5777065332090645

Pt 2.2171390354435041 -3.2589833849762995 -2.5140728793612439

Pt -0.2654068596533966 -4.1989047600326215 -2.3703366976713216

Pt 4.2741145134706553 -2.0772337692667042 -1.0055106628046284

Pt 3.8229430524247028 -2.1138835957950848 1.7016246926839294

Pt -3.8487041861556670 -2.1648824810754919 -1.1196758759253280

Pt -3.7517245646118735 -2.0101917203120214 1.7570957523721782

Pt 1.5387205116352221 3.9689919598808112 -1.9802255025461906

Pt 1.5683955785431671 3.9115111599697903 2.5283663663838727

Pt -1.2135253700372146 3.8694461528540351 -1.9703410531990004

Pt -1.2075328545696038 3.9130720329686017 2.4994829783886896

Pt -2.1326614044816687 1.7263362214684939 -3.5043154600497779

Pt 2.5670885398750856 1.8781305293683779 -3.4842186156504535

Pt -2.3166269104255943 -0.9079554158118850 -4.1507294573176017

Pt 2.4838265846338081 -0.8241652050268062 -3.8714378499746456

Pt -3.4689408365536321 2.5265988907817727 1.5758114826914900

Pt -3.5274496998993290 2.5698284869268999 -1.1909874248369692

Pt -2.1752610425120484 -1.1425755330237461 3.8907013208670751

Pt 2.3685387050019293 -1.1664082741888546 3.8394173025923353

Pt 2.4918260397163414 1.6629741314488011 4.0236602215650175

Pt -2.1297064267731334 1.7114246295185696 3.9001016282496828

Pt 3.9025792576576364 2.5446279550322091 -1.1372292227973466

Pt 3.8008714983179908 2.5103874918618372 1.6527877149146162

CO_2/Pt_{55} icosahedron (bent OCO angle)

C -5.5295560465996676 -1.4300092251927750 -2.8149870687799803

O -5.3172068557489176 -2.5590159198210931 -2.2752467103164120

O -6.4000320129956734 -0.9346349666285152 -3.5063605054891331

Pt 0.2884990868960652 0.0737065639996055 0.1522696628912002

Pt 0.4184545380806836 1.3090952653112857 2.4229268987600703

Pt 0.3955313949790077 1.5160897646922880 -1.9969687246261438

Pt 0.1613966190372106 -1.3870961118301379 2.2776248121093614

Pt 0.1967911031411215 -1.1968085314034467 -2.0831917808315472

Pt 1.8194952653611800 2.1845184417173100 0.2311753471124485

Pt -0.8826344602756482 2.4003014046806208 0.2216012763812537

Pt 1.4878318821832144 -2.2214293883858578 0.0939386080749634

Pt -1.2980743000214261 -2.0158929792280245 0.0074184371895756

Pt 2.5198554771363266 -0.1404737401259235 1.5186948692746993

Pt 2.4991728680775633 -0.0333909171827556 -1.1856624771211672

Pt -1.8813828231459286 0.2328114417886187 1.5163904760836919

Pt -1.9361557362207051 0.3005750461939545 -1.2194945801114523

Pt -4.0928410120280070 0.0144088525260917 -2.5306430303705598

Pt 0.3211453068084590 2.7886395647976943 4.4874806055715224

Pt 0.3249406585493916 2.7976551108872729 -4.1955590159081906

Pt 0.3465891415875788 -2.5919181450184898 4.5008812143707653

Pt 0.3351219044267903 -2.5983433307706076 -4.1837158566434285

Pt 2.9738450844265891 4.4414408106359184 0.1390974033448718

Pt -2.3773387627986633 4.4401958244872377 0.1471117500147364

Pt 3.0265700634275436 -4.2266425554342852 0.1693615679359848

Pt -2.3248701906431872 -4.3054017612695024 0.1940929380067678

Pt 4.6633388909811764 0.1308201658250778 2.8232601218159479

Pt 4.6597754653458709 0.1044060712385721 -2.5291783952286933

Pt -4.0162693139362151 0.0914722011668789 2.8692742484623635

Pt 0.3119458680069104 4.7145747655884360 0.1223172698291313

Pt 0.3334128392106361 -4.5262575030888783 0.1933641540404941

Pt -4.2735764086205634 0.0597872909096038 0.1994891745129453

Pt 4.9063488277877632 0.1527941258268563 0.1450381507695849

Pt 0.3195669561218625 0.1110452891405840 -4.4292952777380856

Pt 0.3158589986218780 0.0863828145756800 4.7615437640664728

Pt 1.8139851941946805 -3.5728484684022690 2.4747583690310444

Pt -1.0700855071411315 -3.6610867789748256 2.4622669867034208

Pt 1.7633576464746863 -3.5940486533139659 -2.1412368688991164

Pt -1.0419604787213199 -3.6710849353973978 -2.1258170556945570

Pt 4.0481182546562593 -2.1967173918734564 -1.2600561238590187

Pt 4.0922313033162849 -2.1983027220490290 1.5506677979552057

Pt -3.4598132822815284 -2.2986310556440395 -1.2667753442563709

Pt -3.3593571747540008 -2.2232639109755952 1.6455247916923090

Pt 1.7159672018797867 3.8231124279775419 -2.1345241472841563

Pt 1.6864973295684225 3.8112360242374925 2.4141930327597665

Pt -1.1407558763373284 3.7907447502505476 -2.1607999905799238

Pt -1.1235088425117734 3.7810383899368509 2.4579605030421394

Pt -1.9731695831224343 1.4991164036650282 -3.5615612947542763

Pt 2.5980783040503450 1.4958063275490330 -3.5442435939541665

Pt -1.9674508354435716 -1.3310797428588510 -3.5781248087473481

Pt 2.6065384921227288 -1.3167083957978394 -3.5477891934055803

Pt -3.4146465034814391 2.3846894007888886 1.5455370902017682

Pt -3.4285066567073805 2.4079015788702987 -1.2730064526084552

Pt -1.9554802075239621 -1.3070773109111864 3.8836349435724715

Pt 2.6062223491770160 -1.2769318725099235 3.8895082817355640

Pt 2.6318947350513451 1.5526573538285644 3.8492844901908967

Pt -1.9597986313863061 1.5156784299770123 3.8839405704751586

Pt 3.9989336345867139 2.3920146627700780 -1.2887324527847008

Pt 4.0371588171736921 2.4103797482477467 1.5813411420138674

S9.9 CO_2/Fe_{55}, $CO_2/Pt_{13}Fe_{42}$ and $CO_2/Pt_{42}Fe_{13}$

S9.10 CO_2/Fe_{55} (linear OCO angle)

C -4.4611071411802747 -4.1714501879404882 -2.3129596273004163

O -5.2069457657595049 -3.7891480476172972 -1.4921918794120428

O -3.7379537809466803 -4.5758758561142354 -3.1448134312780178

Fe 0.2422278909508546 0.2276469198462884 4.3289516761462270

Fe 0.2428799356746478 -3.9074441691873036 2.2695149242993908

Fe 1.3949931623508811 -1.9012403475070925 3.2000585048954315

Fe -0.9096445793917467 -1.9006252089506481 3.1994054909974308

Fe 2.5782824006841270 0.2288847469249417 3.4603892438549160

Fe 3.8199639107283017 -1.9553058769872140 2.8794464120459144

Fe 3.8213218151055153 2.4116116830948378 2.8789122384506483

Fe 2.3535415377354636 -3.3344853775745107 1.3094815705548637

Fe 4.5397748490826348 0.2293411120429679 1.8247498382206047

Fe 1.3961181475955402 2.3560966119486442 3.2000842750943983

Fe -2.0933602655070156 0.2291863083079905 3.4631458190942217

Fe -3.3369979681961133 -1.9573160220941843 2.8757028599153136

Fe 4.4791604992098843 -1.8118880014897250 0.4898270605652053

Fe 2.4197035008498085 -0.9220927638843271 1.2530156572490005

Fe -0.9084380660777227 2.3572469127621312 3.1998352645270378

Fe 0.2420797961694299 0.2273182156848733 1.9550302055540705

Fe -1.8631427753645400 -3.3346618138789146 1.3077552320452979

Fe 0.2440208509367348 -1.8854440096119709 0.8056498473038198

Fe 2.4198001704790113 1.3783552850523049 1.2523720750660434

Fe -3.3332890768591557 2.4112213770153494 2.8786660138675044

Fe 0.2385670236836632 -3.8753131605539308 -0.3960813362097265

Fe -1.9360184795796527 -0.9196953992239166 1.2573302998198006

Fe 4.4809950533648699 2.2697232514133758 0.4890833785849784

Fe 0.2430504781836054 4.3624881481161104 2.2725396949903676

Fe 2.3524823528022627 3.7904853568315837 1.3087330516487503

Fe 2.4152320947493684 -2.2269637767842876 -0.7768482640633136

Fe -4.0557404367850420 0.2230766507139620 1.8241393526945426

Fe 3.7010497811903984 0.2287803284868723 -0.7373975449258774

Fe -1.9342432729346632 1.3775409605960252 1.2524197071583005

Fe 0.2436317632920901 2.3420798052347664 0.8073736743498259

Fe -3.9870026185839165 -1.8257885490110737 0.4753441165015521

Fe 1.4052767018669514 0.2269773070019262 -0.6222377411901698

Fe -1.8653435555767213 3.7914859190352472 1.3085967400445728

Fe -1.9071045657556609 -2.2119255054428293 -0.7668446123895967

Fe 2.4138841615842002 2.6805564827217343 -0.7763397637575631

Fe -0.9167921277884825 0.2289462953504472 -0.6185768525816657

Fe 0.2519430097818707 -1.7185509136054669 -1.6179452863282604

Fe 1.4479495134687252 -3.4924189531910357 -2.6617915701714248

Fe -3.9924366724744007 2.2647406653766331 0.4903946496297324

Fe 0.2435076632604525 4.3307266479662898 -0.3935305235256311

Fe -3.2118321339510643 0.2263814866046182 -0.7375944472603360

Fe -0.9860057756263614 -3.4827203568929774 -2.6560664560148757

Fe 2.3619865626143492 -1.0096620319451772 -2.8176396080236090

Fe -1.9262852917740694 2.6816204929174261 -0.7757241248323803

Fe 0.2444021433040118 2.1736513222032916 -1.6134077800479547

Fe 2.3590212913143493 1.4656789717047807 -2.8170407053124729

Fe 0.2441325452514040 0.2282027180705541 -2.8724669035094612

Fe -1.8677088499025678 -1.0058871767891193 -2.8124540700631515

Fe 0.2451223658846451 -1.8409106184756019 -4.1063574448168021

Fe 1.4542774619253209 3.9450952930019931 -2.6587719485044632

Fe -1.8710859097307746 1.4656813132762507 -2.8152313597960257

Fe -0.9654270496191670 3.9439607312817242 -2.6584975555394044

Fe 1.5015087503907982 0.2281863078752847 -4.8781979418076444

Fe 0.2446381640241237 2.2961805468752199 -4.1058605817197522

Fe -1.0126211901249973 0.2276579494168892 -4.8750795147877275

S9.11 CO_2/Fe_{55} (bent OCO angle)

C -3.4108664804955220 3.4258829796420205 -1.5471679370579252

O -4.5969750539168635 3.3415176447091799 -1.0586191486433154

O -3.0976436210981655 4.2431826500653731 -2.4959595569500022

Fe 0.1787555239609420 -0.1955674745774534 4.2644313144929606

Fe 0.1901727623729626 -4.3450146622876940 2.1967282766535070

Fe 1.3525778632489267 -2.3137883807038886 3.1568535519724930

Fe -0.9569047781043620 -2.2971489282211444 3.1656240326497938

Fe 2.5578189715563893 -0.1914720154775491 3.4083748961845424

Fe 3.7999184243387925 -2.3672054001656520 2.8640301601957456

Fe 3.8153043656213059 1.9556248626045001 2.8294196701774008

Fe 2.3052996446008658 -3.7589521274816384 1.2961184916207993

Fe 4.5105570857772008 -0.2328598285400148 1.7732149048761940

Fe 1.3740654985821186 1.9449544174924069 3.1274150700580212

Fe -2.1382681937314567 -0.1380578768995040 3.3897329749383220

Fe -3.4010162648992646 -2.3018381518056366 2.8847064003405660

Fe 4.4431284487572436 -2.3154409250457633 0.4739942740821122

Fe 2.3819051095636263 -1.3521696730863155 1.2228818517023134

Fe -0.9410185597946734 1.9457871116813337 3.1224011627408559

Fe 0.1938974512935561 -0.1823802823303957 1.8911580508656816

Fe -1.9128156052568306 -3.7516610609281997 1.3257019820694140

Fe 0.1932744311871444 -2.3027936967982825 0.7788656740014741

Fe 2.3964675624005674 0.9488132603001098 1.2007851761543009

Fe -3.4252358385292547 1.9730947401265908 2.8361983851035979

Fe 0.2264528870043430 -4.2910927600173032 -0.4008427218617771

Fe -1.9798686861284507 -1.3219582043320965 1.2358811811001609

Fe 4.4794201317591886 1.8097055054722597 0.4370864773130239

Fe 0.2598432740730577 3.9703104946358119 2.2591912258083782

Fe 2.3414834712671349 3.3416705150670643 1.2411293420851897

Fe 2.3826303000062401 -2.6432657212488380 -0.7943555872191286

Fe -4.1104372629609278 -0.2006012199894283 1.7568394865231645

Fe 3.6724749073875147 -0.2428388582624273 -0.7552134200208858

Fe -2.0579949096951102 1.0088336642039710 1.1713365414269241

Fe 0.1939759822099978 1.8998731696606042 0.7538742654654051

Fe -4.0245805574382105 -2.3740733815211108 0.5182744228230167

Fe 1.3541275911844366 -0.2046251166320126 -0.6611027314832725

Fe -1.8136747826781834 3.4011666605916648 1.2818386443860954

Fe -1.9790828605973827 -2.6532076550459482 -0.7780681051249576

Fe 2.4158019531460626 2.2141015848444408 -0.8273031488181875

Fe -0.9564666228286205 -0.1839450885932337 -0.6368605386664867

Fe 0.1989983740066901 -2.1497361519556097 -1.6315163388396552

Fe 1.4402108846970583 -3.9205988211184604 -2.6560062682626211

Fe -4.1518939009207747 1.9924605379957052 0.3755782904504222

Fe 0.3171076003902016 3.8869765876104037 -0.3713100934454576

Fe -3.2622797964095058 -0.3546165735962692 -0.7460579293876417

Fe -0.9911394007416208 -3.9293816438630600 -2.6462299113787577

Fe 2.3143576765923344 -1.4500672647087427 -2.8542219517349587

Fe -1.9585714765611426 2.3092518345449049 -0.8494192959310378

Fe 0.2275413180178694 1.7923708801780105 -1.6840547610679077

Fe 2.3285987963689765 1.0240933779994084 -2.8667460530656865

Fe 0.2034702786047120 -0.2030829060342203 -2.8693557522738602

Fe -1.9058274654872411 -1.4745973192380486 -2.8532659789710171

Fe 0.2131168650801909 -2.2869915426538441 -4.1076690746323665

Fe 1.3598556226569558 3.5144592992797650 -2.7140584488063433

Fe -1.9163851927264295 0.9608105094911679 -2.8178854253267720

Fe -1.2069685320029775 3.6444648845719048 -2.6857792743974600

Fe 1.4462966620069926 -0.2195771628903387 -4.8981215114399914

Fe 0.1776611822456982 1.8416911554029980 -4.1428707090967345

Fe -1.0506530589643264 -0.2404904521214739 -4.8896045043576626

S9.12 $CO_2/Pt_{13}Fe_{42}$ (linear OCO angle)

C -4.4222445821402570 -2.0892006625928250 -5.0398049960823661

O -3.7208351900982897 -2.9816208747283053 -4.7363528258593552

O -5.1194427121059967 -1.2025350931184577 -5.3584592167686305

Pt -4.0000901159595852 0.2144043511958229 -2.3127684600933827

Pt 0.2566683985927887 2.7585839001452506 4.4767556214863076

Pt 0.2310757782957096 2.7100435848999158 -3.9592287697585697

Pt 0.3389168164434458 -2.4285716855507058 4.5437031237791254

Pt 0.1521208300362072 -2.5094887349252950 -3.9117732916516652

Pt 2.8499109025806990 4.3396126625181877 0.2488322344147725

Pt -2.3570807581994724 4.3398123405756124 0.2718131243497635

Pt 2.8723937422708254 -4.0927398357760687 0.2812287209045954

Pt -2.2654137459940098 -4.1737327713675310 0.4124675304509816

Pt 4.5200422646442719 0.1557748208638456 2.7893608357403612

Pt 4.4139204239960836 0.0776176089195248 -2.4190929619284138

Pt -3.9410784372248027 0.0772895694530062 2.9173932273837360

Pt -3.3219195865605271 -2.0917222026897182 -1.0062310484924317

Fe 0.2304781439403406 0.1098744771646969 0.2749461119974000

Fe 0.3148073220062966 1.1518579041483774 2.4577946333696343

Fe -0.0015367765175910 1.5284116487935935 -1.6648231082925349

Fe 0.3817242919051840 -1.3625959643122110 2.1837291129653358

Fe 0.0946178510734551 -1.0501983629248846 -1.7904127717827449

Fe 1.4895414616142324 2.1478723266932471 0.4041237644471461

Fe -1.0254773470309357 2.1372813639286576 0.5456313260960955

Fe 1.6300578604085960 -1.8341881603662455 0.0462495661638667

Fe -0.9956147423560801 -1.9829302361577541 0.1861813357375131

Fe 2.3474547777676746 0.1391383982455141 1.3943760579161453

Fe 2.1723274999546889 0.3350510431526745 -1.1575257643925194

Fe -1.7626460258599896 -0.0471391191165773 1.5615339027168915

Fe -1.9125476943836224 0.1097716209883315 -0.8660816977967324

Fe 0.2371728753063780 4.1921657335332885 0.1651433927210413

Fe 0.2912282063062393 -3.9359240991196547 0.4751113520332456

Fe -3.9732618988409008 0.0557752130672517 0.3293279940524523

Fe 4.3510038772612463 0.0531569379906200 0.1719383242389825

Fe 0.2737890456502952 0.1061037301970684 -3.8024897449040158

Fe 0.3164488040509677 0.1548403464151573 4.5164201648754245

Fe 1.6405464317111564 -3.2763638788313827 2.4264285624095820

Fe -1.0272264564141389 -3.2196665790969767 2.4658136045389063

Fe 1.3774856767803085 -3.3093601348696957 -1.7369166880427105

Fe -1.1202669542179124 -3.2872432566755005 -1.7956540874929601

Fe 3.6497985240598418 -1.9835191339893148 -1.0544939479257696

Fe 3.5364762284146063 -1.9389773385801801 1.5681366290774561

Fe -3.0731349758632720 -1.9999200796391141 1.6071474885905872

Fe 1.5849931110310147 3.3209640826512441 -1.8065106250942875

Fe 1.4528773569956537 3.5085080076431998 2.3063280503177643

Fe -1.0625069369923901 3.5642864002142263 -1.8444847772825443

Fe -1.0245583391211743 3.5407182023089598 2.3676358176571113

Fe -1.8389515296221892 1.3631316385415186 -3.1314262146886720

Fe 2.3083453736386628 1.3963304721425776 -3.1866830300453466

Fe -1.8989679314564414 -1.1683646704892874 -3.0187096515407625

Fe 2.2363615030813748 -1.2988632773323958 -2.9450932331739339

Fe -3.1624967017323669 2.1289373011128472 1.4691391993267484

Fe -2.9621532693496166 2.2083042905750272 -1.0708021858712875

Fe -1.6900564419031683 -1.0481730758161445 3.6650848794120710

Fe 2.3047294740860473 -0.9938194407690835 3.5961068606027875

Fe 2.3827472921265964 1.5079428377964474 3.5319024435187107

Fe -1.8271419794017640 1.4911941316945836 3.4840437087371776

Fe 3.6363605993824462 2.1737130886743081 -1.0162760889520033

Fe 3.6302283839331593 2.2083886325907187 1.4902664858839219

S9.13 $CO_2/Pt_{13}Fe_{42}$ (bent OCO angle)

C -3.4323264951315497 -0.0029908736936383 -4.3647084436614003

O -3.2902103984482345 -1.1919704166883789 -4.8027549354124703

O -3.1623594423729973 1.0993847340342993 -4.9483194085902555

Pt -3.9904211171646384 0.0934891415757027 -2.3984173807218001

Pt 0.1862863914428762 2.5978543477922416 4.4985363168366375

Pt 0.2542323104999821 2.6756444116783826 -3.9712728736464156

Pt 0.2913761372514294 -2.5689171739717955 4.5060249575386537

Pt 0.1929874188882703 -2.6807226472222747 -3.9586461135504605

Pt 2.7532531978547059 4.2551457389353438 0.2737902479796946

Pt -2.4259057681875476 4.2091394176561607 0.2728330262599448

Pt 2.8370590650836860 -4.1731189599303509 0.2413693240989475

Pt -2.3324395311611568 -4.3025379232634204 0.4130000963150398

Pt 4.4260412054235854 0.0628595270382531 2.8261182996366658

Pt 4.3708694963461721 0.0384528335558821 -2.3570603340308862

Pt -3.9917403127611486 -0.0253798261579389 2.9409324641359413

Pt -3.3948789061099305 -2.1984924667537729 -1.0047445177423251

Fe 0.1305411050578211 -0.0131081418095564 0.2193801101421072

Fe 0.2424551887528902 1.0382772179674711 2.3997330874664229

Fe -0.1133453403310245 1.2917446391213230 -1.7977268810298339

Fe 0.3250063246115599 -1.4645008493646059 2.1544628385005682

Fe 0.0253354957564599 -1.2303629029068950 -1.8392499746781530

Fe 1.2381444405876127 2.1373171766311505 0.3474678761154567

Fe -1.2079272378962873 1.9523069584019361 0.3821551673024795

Fe 1.4932661315196132 -1.9750140500679794 0.0301522196831697

Fe -1.1022059920838743 -2.0944960529659382 0.1949621260767396

Fe 2.2884450344172791 0.1050941700858324 1.3193114047158803

Fe 2.0641640873176472 0.2040542640002801 -1.1674552202886490

Fe -1.8465416327173294 -0.1470025618277736 1.5009122201207772

Fe -1.9521156953612095 -0.0896553023231816 -1.0163149191445404

Fe 0.1646061053088736 4.1990224471666409 0.2748084444543376

Fe 0.2284679692818789 -4.0619833918678232 0.4555428833539371

Fe -3.9910884265898545 -0.0773371749036821 0.3803062639193087

Fe 4.3493382771492728 0.0317380471393177 0.2200984574031529

Fe 0.1645935798527693 -0.0062284345599752 -3.8298962398020135

Fe 0.2642690163910783 0.0158867217352046 4.4781762955054845

Fe 1.5907503407628596 -3.3902490342134892 2.3812304016430739

Fe -1.0695101871479373 -3.3566655428393726 2.4433176336706497

Fe 1.3754150570611277 -3.4081772122940701 -1.7905616357161582

Fe -1.1521503252206351 -3.4025603279022341 -1.7843741183426554

Fe 3.5660025901423129 -1.9897695452748656 -0.9896587329180546

Fe 3.4416694062517159 -1.9992228189770009 1.5632845682019463

Fe -3.1474831251572866 -2.1323301704351105 1.6161169096487944

Fe 1.5130863532247201 3.2145407983503618 -1.7819650818200534

Fe 1.4899682679055184 3.3541544104068737 2.3927708331559989

Fe -0.9808889324305703 3.4429157662020384 -1.7726042414457739

Fe -0.9703900728745580 3.3260026157578797 2.2895789049527666

Fe -1.9296781683758368 1.5104584838751269 -3.3755501080010211

Fe 2.2419581070353676 1.2949983531797238 -3.1589748072923571

Fe -1.9630815852107748 -1.5124773149141482 -3.2549506350697763

Fe 2.1970009047172869 -1.3558949826549731 -2.9699303600898448

Fe -3.2219460598127068 2.0299429046879180 1.4991291525881509

Fe -3.0103554967723465 2.0768611907404577 -1.1554195353856871

Fe -1.7428004426932766 -1.1756977591418347 3.6271120432818433

Fe 2.2463934179593705 -1.1129079123463721 3.5685053725882137

Fe 2.3080249746386654 1.3490226985062992 3.6145626568667533

Fe -1.8589128906664847 1.3404469206183749 3.4979916352035989

Fe 3.5106506130983508 2.0484999892988722 -0.8984043497192404

Fe 3.5090455710864363 2.1445158451331019 1.5652866087366872

S9.14 $CO_2/Pt_{42}Fe_{13}$ (linear OCO angle)

C -3.4575832995183391 3.9609458074336081 -4.5852714391997846

O -3.0856978558555270 4.9248163279256287 -4.0298654270011376

O -3.8366305536433356 3.0053456851224989 -5.1515343983583115

Fe 0.1847053489516335 -0.2088613290243875 0.2425317458661307

Fe 0.1918247576679782 1.0565234016668037 2.3379127013624470

Fe 0.2015013552689964 1.0792568567303920 -1.8499899000292941

Fe 0.1886323603247946 -1.4965157006209933 2.3172318879574427

Fe 0.1973485890705722 -1.5212257414568087 -1.8314856341817509

Fe 1.4926717527552831 1.8676934058766039 0.2667398839742767

Fe -1.1050780532600819 1.8823674548032554 0.2635706543170708

Fe 1.4660720417177679 -2.2897396055881516 0.2621908992647719

Fe -1.0894809578422184 -2.2987018182956942 0.2593042607686109

Fe 2.2557577192779248 -0.2276253119347201 1.5401959217508714

Fe 2.2845730815345111 -0.2301235244916496 -1.0224818458853142

Fe -1.8889308962291094 -0.2264817457302049 1.5461651563004781

Fe -1.9096791905120925 -0.2279084608483211 -1.0405820233040912

Pt -4.0136931335991424 -0.2117570124716779 -2.3556332725710791

Pt 0.1826959296256692 2.3796572948430028 4.4488075518364756

Pt 0.2012046239615377 2.3829818190510381 -3.9553041288734376

Pt 0.1779953009980458 -2.8076845168156255 4.4427094174056814

Pt 0.1935098279626506 -2.8134587400168294 -3.9543135233053301

Pt 2.7920062314841938 3.9856092124804889 0.2550957386576731

Pt -2.4076949151476605 3.9932655694521828 0.2472460341767868

Pt 2.7760846569850091 -4.4138851215932222 0.2522916839039566

Pt -2.4119425627054913 -4.4103660417967978 0.2431358673103738

Pt 4.3798278337712588 -0.2199182366140762 2.8496100203723214

Pt 4.3954667405170937 -0.2202586364011699 -2.3393481331709203

Pt -4.0170212814124842 -0.2117593120446526 2.8379901637899736

Pt 0.1930679869206755 4.2030193945184227 0.2530074065072738

Pt 0.1813806657340886 -4.6350502703225471 0.2473714283394454

Pt -4.2306158478261384 -0.2112593332019360 0.2410221923817306

Pt 4.6083082852702990 -0.2200678087306459 0.2565856895343841

Pt 0.1995674912760914 -0.2159159128420432 -4.1680587801379811

Pt 0.1794332440034645 -0.2140857230025444 4.6696190649773479

Pt 1.5448080871899630 -3.7925645511662531 2.4601248343759541

Pt -1.1865089998642468 -3.7895727544554547 2.4551313960914602

Pt 1.5529724587504767 -3.7916380289501892 -1.9607367685553601

Pt -1.1770514692839815 -3.7891344764276913 -1.9646172608786769

Pt 3.7646161398389739 -2.4282143333095072 -1.1116428446348166

Pt 3.7588747684587909 -2.4281980091033231 1.6200455660593254

Pt -3.3876950029089401 -2.4205221108286801 -1.1240836287176381

Pt -3.3932346767227117 -2.4207701798635886 1.6074401406963799

Pt 1.5633287406985104 3.3559477456166422 -1.9557630793538006

Pt 1.5545049486752718 3.3591466954863498 2.4617722144188670

Pt -1.1640389815975021 3.3530147855688495 -1.9536192902668037

Pt -1.1784055454571374 3.3620852198118771 2.4570903211368251

Pt -2.0039253380278148 1.1416320994343052 -3.3179450262154702

Pt 2.4059954720070817 1.1477368480672108 -3.3197564273983917

Pt -2.0173018832444058 -1.5822473264777099 -3.3289822704337051

Pt 2.4032187129276301 -1.5832480467815011 -3.3220013185312012

Pt -3.3862189830091105 1.9983380276396248 1.6094148916890734

Pt -3.3810216435329630 1.9958244520126285 -1.1195878506109955

Pt -2.0310141107489099 -1.5786501625484299 3.8214143033939236

Pt 2.3900817113220447 -1.5825837789750605 3.8283852726868646

Pt 2.3926011864782448 1.1489021656918523 3.8287459234303287

Pt -2.0273378400614512 1.1531507727880359 3.8206544851337845

Pt 3.7687098682062543 1.9908065015465728 -1.1087410407148695

Pt 3.7644551023780077 1.9919261191642144 1.6207905924618538

S9.15 $CO_2/Pt_{42}Fe_{13}$ (bent OCO angle)

C -5.0475943792500244 -2.4120889965654491 -2.3905074265289921

O -5.4676033164682556 -3.5426238135944970 -2.3241892870085623

O -5.4066651747172427 -1.3446354560823821 -2.9955249026472819

Fe 0.3004803419585511 0.1349525183871501 0.1437910038430843

Fe 0.2767182462951125 1.4225808560276370 2.2211274766784399

Fe 0.2854902631526363 1.4112314119562936 -1.9330072591791412

Fe 0.2912527458306199 -1.1547731697584152 2.2326268716867625

Fe 0.2682226073112743 -1.1478228581049372 -1.9235944806380436

Fe 1.5731687690841567 2.2286776807670354 0.1354814223825782

Fe -0.9877218328833828 2.2037382160881980 0.1451435255922000

Fe 1.5880160511633217 -1.9573681516406254 0.1402073544414266

Fe -0.9258375993989554 -1.9249699924001604 0.1758630229529592

Fe 2.3746160712375679 0.1243641522630152 1.4368050136173212

Fe 2.3726426016396061 0.1325721346599404 -1.1592358244077863

Fe -1.7867162447415255 0.1228519682631563 1.3994443172861661

Fe -1.8153425005518629 0.1038646980205040 -1.1473502677209124

Pt -3.9999938485435007 0.1987464462660291 -2.5271014658116266

Pt 0.2875246205161103 2.7251327619422896 4.3453086778954626

Pt 0.2906964314225119 2.7328791842599300 -4.0624581383063925

Pt 0.2907204345712259 -2.4674696342887077 4.3510716129902631

Pt 0.2874140101225379 -2.4559204929714435 -4.0504910569385659

Pt 2.8915141600829730 4.3325356234225350 0.1442576095000687

Pt -2.3107898182689355 4.3394486720583654 0.1387723090369990

Pt 2.8949283137315285 -4.0779948768494441 0.1396084103347741

Pt -2.2888897996434161 -4.0480767689925647 0.1415219074876326

Pt 4.4966939493320375 0.1319823947362024 2.7412668329949783

Pt 4.4952173685574612 0.1278893379832542 -2.4570574852747127

Pt -3.9029706591859452 0.1308259369752942 2.7274691481557083

Pt 0.2900657209431645 4.5401298201253466 0.1372589287136971

Pt 0.2956227638107979 -4.2848543413650129 0.1393206220834724

Pt -4.1332735191419223 0.1451441274876977 0.1352047106240368

Pt 4.7071227833368114 0.1330879361738837 0.1416423147742058

Pt 0.2936955990500407 0.1375424584762228 -4.2879327982660689

Pt 0.2889067478182591 0.1295717532251544 4.5540441573690620

Pt 1.6614254968173046 -3.4344175737548173 2.3502422210949101

Pt -1.0761234558967261 -3.4378086854613623 2.3533732486450516

Pt 1.6521827892810541 -3.4412090496248999 -2.0691707692722874

Pt -1.0799325192708928 -3.4266035607895033 -2.0623018340071626

Pt 3.8610212195369882 -2.0770053386340250 -1.2221951042191703

Pt 3.8733433870232381 -2.0772340947368053 1.5067170041085820

Pt -3.3511194437036509 -2.1061361994287835 -1.2536888886473809

Pt -3.2822516796854537 -2.0724131407711499 1.4901053014574996

Pt 1.6528600714341510 3.7028517080294230 -2.0652779779714008

Pt 1.6590001758965927 3.6994869201193565 2.3530614953862248

Pt -1.0772233080855753 3.7150880873726995 -2.0740890329845181

Pt -1.0837149284290253 3.6940473951530586 2.3482959070176390

Pt -1.9105865368907105 1.4912086474727653 -3.4049993910753971

Pt 2.4926880695022677 1.4886145111040381 -3.4321201304694275

Pt -1.9137403493694998 -1.2092938697307354 -3.4295659363017270

Pt 2.4958158996716757 -1.2302272219893766 -3.4330114334628599

Pt -3.2900844829787332 2.3476883252992979 1.5093392534862780

Pt -3.2453156558876697 2.3038620889162940 -1.2211893221876275

Pt -1.9211373790742798 -1.2329821638195704 3.7100115923721555

Pt 2.5047838950167711 -1.2313887729905357 3.7215076623765633

Pt 2.4998787168996359 1.4966198544131337 3.7150286747799646

Pt -1.9229251535462724 1.4959173711624947 3.7126806427571744

Pt 3.8668145432746805 2.3363278580541835 -1.2206901383438469

Pt 3.8670087202907921 2.3338553676833205 1.5091500977475443

S9.16 CO_2/Co_{55} (linear OCO angle)

C -6.4079749211928974 1.2489985425562671 -3.4893346834275838

O -7.2141565406259573 2.0886779387353713 -3.5716177337507840

O -5.5932466901301616 0.3995108681819216 -3.4063356248946373

Co 0.3474344998460151 -0.0678710606047425 0.1895494638981581

Co 0.3776922742568232 1.1688112723549724 2.2015377170603245

Co 0.4214894499028530 1.1755804982302911 -1.8138969799792650

Co 0.2798392235665733 -1.3129995500218674 2.1976199231079314

Co 0.3248464648854475 -1.3065422947740879 -1.8197631628858342

Co 1.6677605695161768 1.8912651949549739 0.2064970472970153

Co -0.8087840504898568 1.9867927647696499 0.1829562881914959

Co 1.5125612478865911 -2.1268222729575785 0.1990593681383017

Co -0.9670152325973261 -2.0272231040957904 0.1757486502350907

Co 2.3430349007622446 -0.1480636653565612 1.4527027529599947

Co 2.3710246422090986 -0.1443818824766880 -1.0310821826964722

Co -1.6670756320277675 0.0082298135596200 1.4119804964632769

Co -1.6450230750348496 0.0128742850006012 -1.0725708547422097

Co -3.6234794121994689 0.0958238277768156 -2.3204593863305099

Co 0.4044526811039866 2.3862231714785795 4.1800036476421543

Co 0.4835167579620308 2.3980647540184123 -3.7883585412340746

Co 0.2131216903029110 -2.5352228342323602 4.1696308801991933

Co 0.2930401066581450 -2.5206991534201886 -3.7972844890279212

Co 2.9660749792707399 3.8185639651351884 0.2235303314292278

Co -1.9589604191347014 4.0061248273769809 0.1713654525115573

Co 2.6556062300473666 -4.1451830972875019 0.2087788047307702

Co -2.2671760055828809 -3.9507886803503189 0.1541858368544502

Co 4.3032637769990583 -0.2267138758524962 2.6930157888882476

Co 4.3562660882537321 -0.2200685581886820 -2.2301798834692881

Co -3.6579826959150825 0.0823314461514342 2.6080270722104468

Co 0.5083082384904652 3.9489545047196191 0.1981644495728569

Co 0.1927953914905221 -4.0845051102493652 0.1834873152021479

Co -3.6629108087489648 0.0898708772161181 0.1475236923151857

Co 4.3635274488360345 -0.2243398114105123 0.2322704793901607

Co 0.3916755305409279 -0.0607118898572449 -3.8265112704783433

Co 0.3079133115663693 -0.0758158034426743 4.2091657565780700

Co 1.4433636591785834 -3.3697951476153611 2.2068563587768044

Co -1.0385600619003661 -3.2722910122466771 2.1796183896434500

Co 1.4844402524202680 -3.3634930795580824 -1.8122386414819309

Co -0.9960527324148688 -3.2626227620125632 -1.8366312341795061

Co 3.5333454397314794 -2.2003549085062946 -1.0212523532335029

Co 3.5057224790437553 -2.2038916500498984 1.4625848272733433

Co -2.9630954900686284 -1.9441570663472942 -1.0894814681110616

Co -2.9892940064763032 -1.9508437979008872 1.3926721368379105

Co 1.7390053953306932 3.1353392667606834 -1.7992687059539789

Co 1.6960192794526341 3.1297771714115794 2.2176160782124765

Co -0.7455298080007821 3.2335762798311944 -1.8266985733758196

Co -0.7863408353521349 3.2258306423317804 2.1938901176201546

Co -1.5772653761349744 1.2550596094830644 -3.0758451042452655

Co 2.4394566223585903 1.0995158754462608 -3.0383929580462055

Co -1.6730649380629146 -1.2224047372009783 -3.0813675648075729

Co 2.3424518202068914 -1.3823296884371599 -3.0426788549077179

Co -2.8334817920128330 2.0639796526591669 1.4026748778095883

Co -2.8061692755760710 2.0665867413661041 -1.0803286982432332

Co -1.7409570241288677 -1.2368361060785895 3.4164468114345490

Co 2.2748198253458263 -1.3917001929882635 3.4590913798611296

Co 2.3712202511595200 1.0888131261832401 3.4644560951929537

Co -1.6438357814928608 1.2470683285322599 3.4225471841271591

Co 3.6895611767688141 1.8152136626550750 -1.0138551930847313

Co 3.6627808999503477 1.8112138846434844 1.4701786709218658

S9.17 CO_2/Co_{55} (bent OCO angle)

C -2.1078131837598932 4.9203940941096151 -1.5072178015593583

O -1.6982907399226943 5.0076587265331893 -2.6750421189856635

O -2.7715040009683389 5.5968372233517423 -0.6839541021429713

Co 0.1166157958253665 -0.2794511256303124 0.0910573739228955

Co 0.1551826647271707 0.9454165611776205 2.1020967979019112

Co 0.1783340435990258 0.9821104909942066 -1.9184217349497796

Co 0.0508803638978771 -1.5286714048871870 2.0937797615542788

Co 0.0832846461823179 -1.5061839687399177 -1.9208882410213732

Co 1.4506360495662478 1.6663440567381889 0.1050646603065264

Co -1.0216641732949179 1.7633568030724023 0.0635128308967197

Co 1.2712859174566833 -2.3320975381720066 0.0917616261318770

Co -1.2043828884897789 -2.2352094232498585 0.0763228475411202

Co 2.1115569983667206 -0.3693305271925250 1.3495049991289862

Co 2.1273082737469626 -0.3570776069491749 -1.1369830935491638

Co -1.8952362491831853 -0.2080767768757666 1.3152483148638963

Co -1.8758462985566848 -0.2032488897313388 -1.1707454042981507

Co -3.8442031947976791 -0.1172150635358050 -2.4072300146272561

Co 0.1889191014441979 2.1606356778184344 4.0854464655743161

Co 0.2793009644636998 2.1645563938478825 -3.9167739409847684

Co -0.0166286119593803 -2.7561652908370489 4.0674556031575868

Co 0.0427918798384891 -2.7231074112233946 -3.9008770607004593

Co 2.7570427155434820 3.5909532372260919 0.1259654356020033

Co -2.1693070690280050 3.8071118777773716 0.0780350166207207

Co 2.4056110949310656 -4.3519813873612092 0.1011004800788112

Co -2.5088318221353973 -4.1584094158576663 0.0583609903292555

Co 4.0773399820336751 -0.4533780980491670 2.5861649712086283

Co 4.1150716972131942 -0.4327505743962724 -2.3387956557686280

Co -3.8826685485578705 -0.1266029496736493 2.5212977001040340

Co 0.3215736739924863 3.7150138421648018 0.1182858928254814

Co -0.0519513758125928 -4.2932420164602076 0.0789249059796636

Co -3.8888785756172273 -0.1133356095684014 0.0560269650585408

Co 4.1295999727913095 -0.4516620602571094 0.1236916870629213

Co 0.1505355766386694 -0.2671157628286301 -3.9237639184850721

Co 0.0861930095513422 -0.2960497529788660 4.1057884720513247

Co 1.2090100111815967 -3.5878742823409047 2.0960306031928777

Co -1.2684924758713625 -3.4893026480244123 2.0770829006338909

Co 1.2364498504995649 -3.5661094678742726 -1.9214074016379232

Co -1.2378958370074753 -3.4719220292390700 -1.9356264049280405

Co 3.2882382468172477 -2.4130351650945068 -1.1350676671710431

Co 3.2701922363582816 -2.4241296334937941 1.3531998884817051

Co -3.2009157061566289 -2.1557330239199528 -1.1836311414703804

Co -3.2197389966207095 -2.1566444096860033 1.3037512809510448

Co 1.5120107270806726 2.9157940513823570 -1.8987993508535546

Co 1.4749378851940036 2.9021255954225991 2.1168402055044986

Co -0.9801706425631455 3.0948199166119901 -1.9873557629915730

Co -1.0107328223036540 2.9976890827422400 2.1056962770932106

Co -1.8066646392623160 1.0543423330937491 -3.1699093625426329

Co 2.1992371238691359 0.8832176911736828 -3.1387270291588489

Co -1.9155080911610232 -1.4296937866506871 -3.1815029146673446

Co 2.1011423472024346 -1.5966509146664647 -3.1501993384004301

Co -3.0456500054653373 1.8539541683956715 1.3240686128141865

Co -3.0369638387651539 1.8313756152065865 -1.1728388749351968

Co -1.9663653023258072 -1.4509568378564799 3.3170092919323988

Co 2.0498180573261933 -1.6217450350369580 3.3509332679623531

Co 2.1449501791155492 0.8612845999969670 3.3634555663449195

Co -1.8658161324961751 1.0364976139882511 3.3234040599581416

Co 3.4632061186897753 1.5926574341279975 -1.1186281708858026

Co 3.4438640169379906 1.5800128013853811 1.3680207539446876

S9.18 $CO_2/Pt_{13}Co_{42}$ (linear OCO angle)

C -3.6847777468939440 -3.0670490549413763 -4.5308185187974424

O -3.9723682039322301 -4.1495366351170668 -4.1975451374815300

O -3.3990755525274650 -1.9809425864648236 -4.8900470826009652

Pt -3.9777280145699900 0.4277756331689518 -2.2407437432528909

Pt 0.2976233229550583 2.6451305805975793 4.4096903686658848

Pt 0.1978481130548622 2.7708008194071341 -3.8318648109110076

Pt 0.2148644891015937 -2.4309453387125610 4.3299495943356998

Pt 0.0881675887197491 -2.3234885190666978 -3.9100367505919427

Pt 2.8093931794421025 4.2314815945547286 0.2867997875214576

Pt -2.2505983310504987 4.3543251385671811 0.3864502181053528

Pt 2.6701366061650496 -4.0101448335817507 0.1198405669448994

Pt -2.3662748768769446 -3.9683211067428181 0.2652114325634973

Pt 4.3583216788440531 0.0096329100617186 2.7008163714377917

Pt 4.2647856556655066 0.0838337097491667 -2.3839855446796698

Pt -3.8774808161627585 0.2268227307202823 2.8621645124060584

Pt -3.3075255086108650 -1.8547942767153880 -1.0435604130447111

Co 0.1894812020150510 0.1608406035565831 0.2425920125177750

Co 0.2522739759893995 1.3701651798688119 2.2760295455267729

Co 0.1863521270965818 1.4527619121051445 -1.7430710786950869

Co 0.2074574440109889 -1.1207684405566698 2.2341906405010312

Co 0.1098256734930579 -1.0501631885051466 -1.7871336781342184

Co 1.4877914458336445 2.1397786469068945 0.2514144343415503

Co -1.0018585356438459 2.2062194026326680 0.3003854751216681

Co 1.3948288929886596 -1.8769612243767368 0.1925970631258695

Co -1.0886841876715889 -1.8285886034229484 0.2459302472175495

Co 2.2209926309616583 0.1015591452093568 1.4557289327779404

Co 2.1787541193216886 0.1371247398496210 -1.0362963041655679

Co -1.8019425353045155 0.1764952502284517 1.5164785236122866

Co -1.8354579164692877 0.2423528811180423 -0.9782806008126124

Co 0.2879792861822284 4.2023258761250437 0.3167592687373850

Co 0.1385097018785671 -3.9051989109527319 0.2121650510125339

Co -3.8469164783173180 0.3348583793832652 0.3107607925965179

Co 4.2396614081146682 0.1313943498599016 0.1680402864573263

Co 0.1238421559647345 0.2365648890892110 -3.8007136576314076

Co 0.3001765466296543 0.1006883266997350 4.2984945223356590

Co 1.4308921033771631 -3.1785874775468392 2.2069986210881001

Co -1.0843118786722579 -3.1405516465087575 2.2705758565036516

Co 1.3413815219692451 -3.1098041808645678 -1.8526352401267059

Co -1.0993539439728577 -3.0997239809938111 -1.7793234274650271

Co 3.4141489526937110 -1.9119718014229412 -1.0880860410695026

Co 3.4438411109708160 -1.9487046163426753 1.3961690702747318

Co -3.0592211347869980 -1.8536696782072144 1.5939199120542198

Co 1.5322080638419531 3.4369435314062469 -1.7653868007266031

Co 1.5962942632739836 3.3391705003578829 2.3238299581548021

Co -1.0007549406379057 3.5323664524216727 -1.7011587873622287

Co -0.9425879185746361 3.4364226960488922 2.3495893855816408

Co -1.8555839093664888 1.5575419362852014 -2.9962755627556903

Co 2.2173767959737085 1.4601254075466810 -3.0267805062301467

Co -1.8974813856312360 -0.8942286673849434 -3.0857156697970631

Co 2.1294159226150051 -1.0714886837292581 -3.0938200984704083

Co -3.0151607435400982 2.2472058168510212 1.5919953160002938

Co -3.0405466610994085 2.3341699629014543 -0.9232741887753027

Co -1.8039638097112929 -1.1119996821668017 3.5330749879054983

Co 2.2481781147016320 -1.1590993120841886 3.4942725647870847

Co 2.3132538448120541 1.3316809186374852 3.5062392412481311

Co -1.7453883823849006 1.3922488581306305 3.5889897902123757

Co 3.5131344053836675 2.1355039174091837 -1.0250415275452416

Co 3.5558510683678386 2.1004197489528909 1.4734508194499285

S9.19 $CO_2/Pt_{13}Co_{42}$ (bent OCO angle)

C -3.0465090266302015 -2.9721108816150958 -2.8670983916494408

O -2.5614437234750769 -4.1510449807077530 -2.7867697028126401

O -3.2601023520127912 -2.3132614565765279 -3.9397462064547910

Pt -4.0257675829440238 0.3550844954669958 -2.3206603733481672

Pt 0.2078668374141870 2.7409502279586477 4.2703091083599904

Pt 0.1373096971592985 2.6896685215807552 -3.9743930021453964

Pt 0.2095589416596653 -2.3297841931980670 4.3299347204342187

Pt 0.1648514614887402 -2.3979172410495848 -3.9489096508962604

Pt 2.7245760415965918 4.2640319717924049 0.1160676985165963

Pt -2.3545496767177498 4.3186547402751208 0.1865259476911177

Pt 2.7031348326935216 -3.9629604403835983 0.1698374010412152

Pt -2.3432768905220884 -4.0079621155510390 0.4017605627106007

Pt 4.3005038209820867 0.1758027174459459 2.6606442726908992

Pt 4.2296183700363947 0.1142136992281723 -2.4388623343395381

Pt -3.9328422019872393 0.1994788657790411 2.7496215215766795

Pt -3.3183126537227965 -1.9558498272471649 -1.0847633834121582

Co 0.1444321194112375 0.1546547059709826 0.1575635890014922

Co 0.1769565292427587 1.4163796198277498 2.1635047306187514

Co 0.1327698312060078 1.4045218245228159 -1.8531100393053550

Co 0.1780154315695626 -1.0660570506587999 2.1929709320572299

Co 0.0553595015720588 -1.1278995767436879 -1.8450421001455113

Co 1.4050668552555834 2.1656134812397441 0.1342791166087607

Co -1.0767971486813055 2.1900278789102559 0.1638096593113799

Co 1.3906120488217484 -1.8583504067644878 0.1796078152476724

Co -1.0826445288564175 -1.8653370659155268 0.1912449927631399

Co 2.1775362667448093 0.1622764712171818 1.3811540136374076

Co 2.1365867540200556 0.1380437123943341 -1.1034956636705631

Co -1.8384684554461730 0.1795622814110504 1.4236705016724129

Co -1.8691191467011778 0.1732608271950641 -1.0798049239904146

Co 0.1838042863579830 4.2178542178129410 0.1515996167671090

Co 0.1744361367679375 -3.9098088006115304 0.2597324351157311

Co -3.8861747152389627 0.2884552758849838 0.2154143312242920

Co 4.1925795481943595 0.1507782332083127 0.1144382796520148

Co 0.1107006798702513 0.1472343828747841 -3.8776122633298571

Co 0.2013977728210419 0.2031154226805813 4.2197446802982856

Co 1.4773601616811760 -3.0904930048000678 2.2423522739144430

Co -1.0631304785866407 -3.0847467328982829 2.2916241741531365

Co 1.3757013453820122 -3.1319626074563884 -1.8341863403789405

Co -0.9968370015680649 -3.3291580390910567 -1.7532299947546250

Co 3.4244316608457410 -1.8800742246225479 -1.0805648155205092

Co 3.4530425503045166 -1.8651929435527574 1.3928163573826366

Co -3.0583590640785703 -1.8593550874373943 1.5538971627708036

Co 1.4119477936380775 3.4271710526861612 -1.9022134741399470

Co 1.4447649824974578 3.4431914688689731 2.1561515872365473

Co -1.0604104032970669 3.4916269445617432 -1.8588777594095434

Co -1.0524981523831345 3.4630714173136981 2.1883085149857577

Co -1.9016471839172597 1.4729694820108523 -3.0983400162445407

Co 2.1550295286822205 1.4112625944642321 -3.1303166431044844

Co -1.9250874603479931 -0.9227277209463990 -3.2551733195844492

Co 2.1198558851780716 -1.1217506366644454 -3.1128475241152302

Co -3.0807638485403119 2.2387765895098810 1.4778333303722291

Co -3.1211363002802957 2.2537620650659265 -1.0375135560506039

Co -1.8255627692174246 -1.0205837852672073 3.5087108748153439

Co 2.2167197309823763 -1.0551612279359699 3.4356848087713927

Co 2.2187097664176321 1.4339106554447756 3.4068978963815169

Co -1.8340311506961031 1.4554188347806292 3.4653478899311492

Co 3.4203758030800913 2.1542800625770142 -1.1330015942456755

Co 3.4598589422736126 2.1844453057336168 1.3634722753366844

S9.20 $CO_2/Pt_{42}Co_{13}$ (linear OCO angle)

C -3.4543511786611250 3.8864545897151395 -4.6658335760621794

O -3.2199725411470750 4.8212373833540765 -3.9976210360148934

O -3.6952643706743382 2.9606671926604902 -5.3452987602888422

Co 0.1874154587883552 -0.2104137955120634 0.2543496072403308

Co 0.1853962097098270 1.0266212363861171 2.2565833419692445

Co 0.2171904518895669 1.0279707945660561 -1.7413547282798647

Co 0.1938559817490935 -1.4535786122911631 2.2463211685249633

Co 0.1885746587829090 -1.4366793644784022 -1.7538188323125135

Co 1.4386864140977333 1.7828256562398461 0.2587732424547239

Co -1.0508036290899530 1.7850011170313287 0.2701229906746482

Co 1.4005887926789089 -2.2219475867691214 0.2408277140788093

Co -1.0626459586888111 -2.2040763620843373 0.2369874123082982

Co 2.1804177322625486 -0.2072169860080432 1.4994269077491142

Co 2.1926326232600983 -0.2162400996250852 -0.9799625490725767

Co -1.8110724354076819 -0.2134170357042244 1.4989461837566718

Co -1.8193711804713868 -0.2013585566967865 -0.9671694586372532

Pt -4.0296089025582118 -0.1908764738881789 -2.3545093267323183

Pt 0.1864863254630478 2.3836093647615604 4.4766885629833437

Pt 0.2140981229295978 2.4062651596470577 -3.9552511648556536

Pt 0.1765214396723812 -2.8347134999752397 4.4625047536967193

Pt 0.1881216092524046 -2.8035590865955937 -3.9702448491024502

Pt 2.8122486906416659 3.9943827034417669 0.2749673139316484

Pt -2.4075480184589404 4.0137210246330524 0.2684764628135938

Pt 2.7751279708860208 -4.4406310248380896 0.2353662149651616

Pt -2.4386233645682127 -4.4147870836822305 0.2295758147443991

Pt 4.4032061468234369 -0.2273882951524630 2.8652600242985344

Pt 4.4078387954277218 -0.2183286220158653 -2.3452161000317653

Pt -4.0259844839235592 -0.2129221047146032 2.8623672718590671

Pt 0.2084130686510395 4.1550778942308471 0.2820395165478548

Pt 0.1645101568602632 -4.5861135254727055 0.2239035422055848

Pt -4.1949426894529749 -0.2081035009481084 0.2591128697383271

Pt 4.5582228882009455 -0.2160206314857379 0.2565796447732728

Pt 0.2105310008657185 -0.2025142072799461 -4.1165959796011675

Pt 0.1755606051159616 -0.2198937808282448 4.6213833252431549

Pt 1.5152960564917535 -3.7597191703468207 2.4194929704339940

Pt -1.1856295570744682 -3.7448525586956594 2.4180084988760551

Pt 1.5220401853735435 -3.7361141456555762 -1.9464291465916923

Pt -1.1827400857721841 -3.7584060232438565 -1.9626199989980813

Pt 3.7099072679888812 -2.4035032019831801 -1.1087006835544089

Pt 3.7031917169837589 -2.4002076159069423 1.5866702713408434

Pt -3.3492586193741323 -2.3764141922858864 -1.1049408458022101

Pt -3.3826191049261363 -2.4047535823475004 1.6011024388560293

Pt 1.5710963568694181 3.3220678482151049 -1.9174318951153375

Pt 1.5572774337823796 3.3357525586971750 2.4697364604268901

Pt -1.1300547872885602 3.3175436470836219 -1.9040074831367577

Pt -1.1533452879977830 3.3132928455897428 2.4487320308801404

Pt -1.9665507350281601 1.1346780935630718 -3.2604979086093313

Pt 2.3953485770211769 1.1370559816839358 -3.2713486657591972

Pt -1.9979480455355347 -1.5567893955776129 -3.2868542249731427

Pt 2.3954330761602174 -1.5700843595713014 -3.3140613994202028

Pt -3.3460886931407456 1.9784368249092192 1.6239548811285354

Pt -3.3443987696324102 1.9818220374258224 -1.0794852374394144

Pt -1.9972784621564081 -1.5641320024548204 3.7724527773767931

Pt 2.3613285255753143 -1.5702742163411163 3.7872470941859242

Pt 2.3756264944064922 1.1341284828932483 3.8013039613140704

Pt -2.0144961780550341 1.1442457489041036 3.8222404457457446

Pt 3.7662539986772332 1.9829361010223516 -1.0943466680609704

Pt 3.7221522457444145 1.9602364138017705 1.6120948013297407

S9.21 $CO_2/Pt_{42}Co_{13}$ (bent OCO angle)

C -5.0647853729097285 -2.3907103224969029 -2.3151283222914620

O -5.5483312465558470 -3.4950206141460041 -2.3259341808886229

O -5.4357444085860784 -1.2761557331601632 -2.8743463224593380

Co 0.2799224015957123 0.1304651398445544 0.1286277918816414

Co 0.2996734455218686 1.3519690012756020 2.1475493199089297

Co 0.3083535740478034 1.3709152440049210 -1.8543529327859551

Co 0.3175120570633814 -1.0938792712273193 2.1602054578638890

Co 0.2955495117537970 -1.1139336770739556 -1.8578354679061451

Co 1.5450529153206949 2.1112927036746796 0.1541718478845877

Co -0.9281731762249033 2.1341307611712632 0.1449365007405823

Co 1.5641088685308526 -1.8636012124927144 0.1427969632036974

Co -0.9010935133126781 -1.9175335893664285 0.1807497497072182

Co 2.2946902362990933 0.1199499215992243 1.3790203255454716

Co 2.3024895563320245 0.1171847231058424 -1.0871715042552821

Co -1.7042805397488356 0.1198907061876901 1.3820464369841665

Co -1.7056549083261432 0.0765508100845797 -1.0712144747629000

Pt -4.0185027544426042 0.1834172812097347 -2.5385949526103064

Pt 0.2846595858400268 2.7305083157458419 4.3429915548138203

Pt 0.3020788676194739 2.7567485888369450 -4.0897370073667476

Pt 0.2823447451311525 -2.4662712311032018 4.3281714482327951

Pt 0.2939816819188997 -2.4577367417484219 -4.0810605781752249

Pt 2.9052750060146044 4.3479081553637462 0.1386667421101522

Pt -2.3081541544531534 4.3727572997876765 0.1385510778245789

Pt 2.8764861276940810 -4.0703748837153109 0.1313220073535839

Pt -2.3162443291260919 -4.0451091288438485 0.1180242796473325

Pt 4.4899230070607903 0.1350580646289845 2.7273543500263098

Pt 4.4976114438474308 0.1289285639898503 -2.4700619737059326

Pt -3.9194911234910927 0.1439601812266812 2.7361651910163265

Pt 0.3048845803413985 4.4882752990935524 0.1460123710961230

Pt 0.2774419790476462 -4.2554590949314948 0.1157885239032806

Pt -4.0733375040702136 0.1475857434231071 0.1329780002689334

Pt 4.6689591116445008 0.1321682533331658 0.1234820459026591

Pt 0.2995856667702120 0.1432147272907948 -4.2321855234326007

Pt 0.2838522172044931 0.1287177972162216 4.5273131534264648

Pt 1.6339263935200954 -3.4175663807303036 2.3207682673029244

Pt -1.0883367297146185 -3.4102473698896394 2.3230604299929944

Pt 1.6248947787870636 -3.3992529291550526 -2.0536009089044618

Pt -1.0767926246338808 -3.4022132971567278 -2.0684000127555318

Pt 3.8425000239068936 -2.0706450636759670 -1.2270508865775756

Pt 3.8425973726923957 -2.0613947618352406 1.4851888965406412

Pt -3.3449638159797539 -2.0987910054787187 -1.2622082029031207

Pt -3.2714697093403595 -2.0504523821449188 1.4741177734019293

Pt 1.6531167384205441 3.6540126326349562 -2.0371184505176330

Pt 1.6553852619229641 3.6862274471482981 2.3419253532686466

Pt -1.0409318185875387 3.6801895515888670 -2.0438498483895233

Pt -1.0598507566721311 3.6524856361950016 2.3235529593573916

Pt -1.8751557061821424 1.4670982419471261 -3.3444884119606590

Pt 2.4756934982767467 1.4698032920208763 -3.3959061039195553

Pt -1.8892644301045793 -1.1987101411145942 -3.3978548237376436

Pt 2.4865399105938470 -1.2248189979420820 -3.4235406371771364

Pt -3.2376771887682070 2.3292288723986947 1.4890899830425259

Pt -3.1957901377616684 2.2844725048180625 -1.2043163396216428

Pt -1.9056033383375963 -1.2199519895167887 3.6567353780152279

Pt 2.4833444207754196 -1.2210036262498447 3.6863660096817159

Pt 2.4709671958175692 1.4904604509768864 3.6787364286647262

Pt -1.9127788729178148 1.4918092148526190 3.6912895746829570

Pt 3.8585959292158822 2.3265780176979791 -1.2222048461741504

Pt 3.8204100497182925 2.3168703008216149 1.4804065199849270

S9.22 CO_2/Ni_{55} (linear OCO angle)

C -6.3396205451680041 1.1733004969025629 -3.2370245939624285

O -7.1148599319413401 2.0417881077785891 -3.3194389279928620

O -5.5601857726929600 0.2908488783483839 -3.1588243679194408

Ni 0.3475201559260550 -0.0648147582252702 0.1781368727133252

Ni 0.3734688967349923 1.1088004642999154 2.1800439017309516

Ni 0.2983455789748252 1.2077869316808778 -1.7907367043126470

Ni 0.4009310023510939 -1.3572098272381892 2.1129382193755122

Ni 0.3255616480147662 -1.2258621370240546 -1.8565589139851422

Ni 1.5547641458519945 1.9396860322762404 0.1938714266374035

Ni -0.8957376169952576 1.9119815550347985 0.2240600252425839

Ni 1.5959070467385579 -2.0407491058036547 0.0824733354176150

Ni -0.8531877996427117 -2.0730720936452540 0.1165999115750306

Ni 2.3709161947476054 -0.0830918763061747 1.3639327067604639

Ni 2.3104202330077803 -0.0055741922382858 -1.0913858499584570

Ni -1.6242950795887734 -0.1301293783420022 1.4061217496853893

Ni -1.6719679330376178 -0.0551300505312068 -1.0474385169191904

Ni -3.6440130833554609 -0.0227049151575479 -2.1938066537811070

Ni 0.3664310016397753 2.2627964826311535 4.1899121169056803

Ni 0.2604524058243344 2.4700825418885524 -3.6686121705290615

Ni 0.4247459231782344 -2.6035742117656193 4.0532905650724347

Ni 0.3201869968292210 -2.3764788539777291 -3.8010941702708356

Ni 2.7183204855795196 3.8927506552677418 0.2595514050663851

Ni -2.1279915154723299 3.8383364595996694 0.3299986631414999

Ni 2.8130838470119985 -3.9555239523480106 0.0455529904334064

Ni -2.0289529954065064 -4.0225589290442345 0.1122571162630869

Ni 4.3095086557412108 -0.0873024194329312 2.5599706128237907

Ni 4.2267256164299347 0.0514023496671810 -2.2956168415477647

Ni -3.5575926347803439 -0.1782133655560231 2.6840393960865159

Ni 0.2943052717506167 4.0028225919816967 0.2954071268600924

Ni 0.3950008917161098 -4.1349987420427867 0.0812985825457925

Ni -3.7046278560984658 -0.1122778370591239 0.2513888217296937

Ni 4.4075986460688856 -0.0118349178674010 0.1305913080705416

Ni 0.2687623226476820 0.0527911477865778 -3.8997705338799102

Ni 0.4109536412813272 -0.1752507391870361 4.2110634225288353

Ni 1.6624656796678496 -3.3802632444620917 2.1030157741298678

Ni -0.8305403408142245 -3.4123790991486098 2.1329251292655007

Ni 1.5985836261744395 -3.2932702908363654 -1.9476447432969273

Ni -0.9017424409285657 -3.3137593925561868 -1.9205756307469712

Ni 3.6436693792459631 -2.0155633336395455 -1.1564471159244796

Ni 3.6694194902874906 -2.0927831203759650 1.3483698418970473

Ni -2.9309499725487549 -2.0976250447014957 -1.0760483797977798

Ni -2.8843024501959911 -2.1618228826793340 1.4232864444630950

Ni 1.5203678169756354 3.3042294352247685 -1.7682509821770622

Ni 1.5820911410326643 3.1675921046745232 2.2744228856062980

Ni -0.9791947718551453 3.2679624262986167 -1.7394000089034900

Ni -0.9025723744795155 3.1361143437937189 2.3040194854698051

Ni -1.7504745717037520 1.2751572954599171 -3.0409868804495348

Ni 2.3163057743837050 1.3234299983810871 -3.0919863931362981

Ni -1.7229054588853221 -1.2547325164898959 -3.1064162595327671

Ni 2.3393972073432834 -1.2032024580690193 -3.1545774839957792

Ni -2.9280245970658876 1.8765128077605970 1.5253667432614730

Ni -2.9740991760827513 1.9703155283494702 -0.9622553591583685

Ni -1.6072810502806587 -1.4298658350152147 3.4287018747916180

Ni 2.4316788274890953 -1.3863653464648253 3.3949590913623711

Ni 2.3951471839441969 1.1186478665765316 3.4502295816587356

Ni -1.6276046766857228 1.0626956318150436 3.4872260295696913

Ni 3.5898455958654893 2.0442939852535416 -1.0560893205905060

Ni 3.6198423152497283 1.9658587484993264 1.4459636446272672

S9.23 CO_2/Ni_{55} (bent OCO angle)

C 4.0890486423985211 0.5302066162859945 -3.7908505206828758

O 3.4309173120032090 1.2400773819320661 -4.5684247601490044

O 5.2012676752197722 -0.0095006853118756 -3.6679907983987978

Ni -0.2126285553336801 -0.0294430529330575 0.2025616356427674

Ni -0.2187994810282029 1.2532587566768625 2.1645828211806166

Ni -0.0447967785685660 1.1314916220191995 -1.8240089138419175

Ni -0.3244226073367661 -1.2069781778566353 2.2247880627152870

Ni -0.2148513507654501 -1.3144933218554244 -1.7435346770715021

Ni 1.0949149672822276 1.9055785383487065 0.2085809328435667

Ni -1.3445322632616767 2.0142453186433338 0.1018592143500502

Ni 0.9308233358432253 -2.0741741957304551 0.3043989905942709

Ni -1.5258086619464246 -1.9684003377244641 0.2134272726107896

Ni 1.7359499965329197 -0.0871167558802578 1.5069025257451483

Ni 1.8154148995633930 -0.1387766846722210 -0.9723192771052341

Ni -2.2502365989382405 0.0986291068913082 1.3580367870369889

Ni -2.1522841652948941 0.0273136705175043 -1.1012403826958799

Ni -4.0693982199925420 0.0671980020190938 -2.3348698815601883

Ni -0.2624958487822547 2.4958417912174893 4.0871257578600888

Ni -0.0233955750041270 2.2978920462011843 -3.7670839778700071

Ni -0.5009908304867247 -2.3351361432537328 4.2009223025025131

Ni -0.2256401747180413 -2.5739871744432712 -3.6345234750408157

Ni 2.3545694049687835 3.7905790645509976 0.2174756015451903

Ni -2.4767407408206026 3.9930162042278958 0.0396495535027629

Ni 1.9981489935091161 -4.0743068999565617 0.4296767101038691

Ni -2.8307509252410998 -3.8533939194910065 0.2404917087777342

Ni 3.5916247253532392 -0.1331644410907556 2.8110745031307398

Ni 3.8149661284849063 -0.2689371040122078 -2.1148650269633014

Ni -4.2243857828837728 0.2128712703142687 2.4796284733520344

Ni -0.0601858119700777 4.0326399752912847 0.1159316816656103

Ni -0.4196939938232217 -4.0920693931119123 0.3374613882971932

Ni -4.2737707616326910 0.1527549347455076 0.0619043428606231

Ni 3.8074196492237800 -0.2288871009326792 0.3912444343225298

Ni -0.1441234351531461 -0.1457708972392221 -3.8399979396974939

Ni -0.3777675345211283 0.0808566660548868 4.2606551691676637

Ni 0.7967930154082533 -3.3123647991961800 2.3945457809452484

Ni -1.6985296085717965 -3.1884766221676468 2.2779933417558511

Ni 0.9256189487164387 -3.4504700544997551 -1.6588935609242526

Ni -1.5675725579338045 -3.3223295509655966 -1.7566471165887616

Ni 2.9924920694257278 -2.2459449820940556 -0.8231242003690659

Ni 2.8995611728515902 -2.1879525223414724 1.6916467505730151

Ni -3.5435641939193907 -1.9534190043912874 -1.0926160087929009

Ni -3.6312950229866701 -1.8734762613832598 1.3881484312234893

Ni 1.2070705549578171 3.1607617326248967 -1.8390972969602852

Ni 1.0937001959301023 3.2503691224846136 2.2231959867147011

Ni -1.2837726382202439 3.2419944582711580 -1.9354314573461753

Ni -1.3964057584905378 3.3469207399921519 2.1165594585838687

Ni -2.1032523014972977 1.2278919305870455 -3.1549673147157375

Ni 1.9796996877272821 1.0851596000995374 -3.1375932617328037

Ni -2.2185500104494089 -1.2854970878531533 -3.1031523271602386

Ni 1.8154029347076308 -1.5153564201417262 -2.9160186203461120

Ni -3.4549183602102271 2.1741003171238606 1.2848829949292135

Ni -3.3770272367794600 2.1048899215312789 -1.2008128961053532

Ni -2.4200578146843270 -1.0939401865479981 3.4320260868685213

Ni 1.6149840549546519 -1.2869642363333893 3.6193188649616475

Ni 1.7300872001396044 1.2209793295523765 3.5551622053706855

Ni -2.3051423864788152 1.4025267428546748 3.3748874077098843

Ni 3.1671644956950704 1.8177593254807969 -0.9103228270029154

Ni 3.0901479268280498 1.8929238268712807 1.5716393396774644

S9.24 $CO_2/Pt_{13}Ni_{42}$ (linear OCO angle)

C -3.2411244433218900 3.8488456547446792 -4.2556281328129906

O -2.8635102808177755 4.8002009877304541 -3.6804137238267991

O -3.6294046804623057 2.9097240396964055 -4.8429808699343084

Pt -3.9219062336152457 -0.1176116049330615 -2.3273658378312128

Pt 0.1756444138048026 2.3082924571692556 4.3052087849224785

Pt 0.1991664412276238 2.3148318397300147 -3.8463627084269056

Pt 0.1858808763465594 -2.7232832443098585 4.3173501938612704

Pt 0.1900163236126074 -2.7234184223689728 -3.8483722537016440

Pt 2.7032845254035265 3.8762144436974375 0.2345378679814943

Pt -2.3383066621836703 3.8786949578103553 0.2390197342527492

Pt 2.7115192805834956 -4.2838544217261916 0.2377891117624885

Pt -2.2965898127648514 -4.3657506877660648 0.2889805266998700

Pt 4.2605819790837502 -0.2068650913757825 2.7574232116003214

Pt 4.2538468134333813 -0.2099075526503892 -2.2844916076490485

Pt -3.8954732987491290 -0.2025045336118708 2.7627593092838172

Pt -3.2390108800168131 -2.3243057363586872 -1.0726496879848089

Ni 0.1639408903329370 -0.2164908596073992 0.2257057724958394

Ni 0.1824493102894916 1.0063585965838855 2.1963436709073205

Ni 0.1610044094526467 1.0135259318453360 -1.7370284790478543

Ni 0.1792031709102893 -1.4376300981149446 2.1968000071879903

Ni 0.1380701911369103 -1.4447100799996044 -1.7371676452562888

Ni 1.3914300696633606 1.7599062330260646 0.2304883070959046

Ni -1.0408397601085375 1.7641963696721272 0.2271108138003531

Ni 1.3882081987552231 -2.1853356430741386 0.2356830684792569

Ni -1.0401449927655899 -2.2017827195232518 0.2426048557761087

Ni 2.1437515670588394 -0.2109167893266090 1.4455574480625373

Ni 2.1417212640734413 -0.2083423497923306 -0.9835213723583037

Ni -1.8140564442211118 -0.2242008175788758 1.4301121956769176

Ni -1.8072389694462294 -0.1964845228747722 -0.9960806365559270

Ni 0.1848254034469457 3.8778576173303754 0.2325829397730229

Ni 0.1967973337803560 -4.3101111876381104 0.2451081854356519

Ni -3.9264557401594593 -0.1837708534551274 0.2361005500490912

Ni 4.2482712452792697 -0.2021975996448790 0.2355971052951951

Ni 0.1787004024079360 -0.2037663115440140 -3.8416351689565307

Ni 0.1888004372392547 -0.2094943980651095 4.3037969456272611

Ni 1.4443213372303387 -3.5112650607163833 2.2772234999970262

Ni -1.0682272714125332 -3.5294267997080078 2.2905212798720855

Ni 1.4370404165455892 -3.5108644610862005 -1.8002070293525581

Ni -1.0647253175434890 -3.5449285540353022 -1.8103271056932968

Ni 3.4811058821246790 -2.2439475853089026 -1.0152151587149731

Ni 3.4795940219490302 -2.2436889004995266 1.5002350633035775

Ni -3.1249746989191425 -2.2696680361051169 1.5216477465225928

Ni 1.4457881191843893 3.0952015661540639 -1.8002225704534176

Ni 1.4421495903554971 3.0853071389514333 2.2680677730259129

Ni -1.0708191473127200 3.0981993131207344 -1.8047098394773258

Ni -1.0737799870391718 3.0967390028303048 2.2648255775790620

Ni -1.8558225203113152 1.0670692586080617 -3.0834615120796691

Ni 2.2266905653772215 1.0596192563952083 -3.0566859445096206

Ni -1.8682953856715954 -1.4572792165354973 -3.1013682694865885

Ni 2.2168992748042808 -1.4672290220522943 -3.0564742443662158

Ni -3.1241731770717158 1.8336354200589038 1.4876254041389840

Ni -3.1230458148127247 1.8531784094997721 -1.0277383483753884

Ni -1.8573339230169821 -1.4763632613269029 3.5235427686015708

Ni 2.2254613629523248 -1.4690720268879773 3.5298960288454593

Ni 2.2195247469474446 1.0537637717687249 3.5224461807844385

Ni -1.8578957895925785 1.0525189343665313 3.5209268856716145

Ni 3.4766545468835814 1.8290168803067401 -1.0174680235864706

Ni 3.4808108196595513 1.8335703685052800 1.4939573560688846

S9.25 $CO_2/Pt_{13}Ni_{42}$ (bent OCO angle)

C -5.0643024337821432 -2.2638698019425547 -2.0012497918323424

O -5.6473222248654684 -3.3068714404528219 -1.8025585021636641

O -5.4073371843919338 -1.1960682334247073 -2.6549213244023404

Pt -3.8314874659036944 0.2203335356199913 -2.4586727050423880

Pt 0.2913178214611143 2.6525336988899380 4.1926915110430860

Pt 0.3067157801212355 2.6510581762217935 -3.9552113788364922

Pt 0.2961100997379756 -2.3939175665545793 4.2094653735267862

Pt 0.2956755147925135 -2.3898840821008154 -3.9670155991578300

Pt 2.8219179921218078 4.2125209640988110 0.1169340212779354

Pt -2.2158138735293020 4.2195268093493006 0.1205786323751220

Pt 2.8235257304194157 -3.9526484867273837 0.1044691444102000

Pt -2.1756631610416592 -4.0189256640941071 0.1730741132279857

Pt 4.3764239913314222 0.1380105932911963 2.6282909698660273

Pt 4.3740503270349098 0.1267448543513591 -2.4113036236659413

Pt -3.7724386777856607 0.1349017607929445 2.6461601170560085

Pt -3.1876589992069269 -2.0140223705505402 -1.2028396312558958

Ni 0.2849781293158225 0.0985000997218785 0.1240534148705404

Ni 0.2889654341802846 1.3256760563875238 2.0939316892204838

Ni 0.2930024234786524 1.3425847560046880 -1.8443948215437562

Ni 0.2940698573618724 -1.1079634879733378 2.0970006595015844

Ni 0.2711266384711919 -1.1097053550563094 -1.8490645901297349

Ni 1.5095942922067118 2.0861108239401647 0.1231009711315457

Ni -0.9253917400297926 2.0868390125946039 0.1179906163356275

Ni 1.5175248506868566 -1.8566768742472772 0.1253560631532141

Ni -0.9147095486653793 -1.8855770017565872 0.1388761800098511

Ni 2.2671385671002540 0.1122039951362367 1.3368265244751150

Ni 2.2591918595251785 0.1181577448518364 -1.1010468936584517

Ni -1.6899520903709508 0.1076910280400691 1.3243298000477448

Ni -1.6767951744221243 0.1500529904631602 -1.1283030924623152

Ni 0.3050842970622572 4.1967901771287135 0.1180916544931961

Ni 0.3132016111036549 -3.9735282403041161 0.1165854279532706

Ni -3.7757159611360196 0.1862900923633523 0.1293321676129125

Ni 4.3741199149130310 0.1186636483790961 0.1117750622381795

Ni 0.2883748312622466 0.1345752406529678 -3.9474402151944092

Ni 0.2992582460200584 0.1299321046934240 4.2064712276541281

Ni 1.5693568283418242 -3.1800658106925859 2.1668790824944111

Ni -0.9522240248360874 -3.1965395793631082 2.1866208674093937

Ni 1.5502892808942270 -3.1841446092829742 -1.9303249121314743

Ni -0.9535170744120915 -3.2077293752107785 -1.9270142290123833

Ni 3.5953581940431105 -1.9095688829336053 -1.1471805414415723

Ni 3.5974187987457693 -1.9149877708712812 1.3813893848365548

Ni -3.0001259339040791 -1.9375531704020543 1.4131562448742450

Ni 1.5608172262738875 3.4185999827310827 -1.9116738593646183

Ni 1.5559835174203129 3.4154702520230362 2.1510733476159514

Ni -0.9592486206198629 3.4350192427572734 -1.9185287308002554

Ni -0.9656320899623474 3.4212190329681702 2.1511732139045474

Ni -1.7677671896596749 1.4221967732285938 -3.1642736908854614

Ni 2.3371878637717325 1.3822723364990683 -3.1791938385209511

Ni -1.7412223017418651 -1.1041396483050521 -3.2252189331493453

Ni 2.3287154979391911 -1.1346040771915360 -3.1790485610509451

Ni -2.9981543778361397 2.1838152880701802 1.3735156963123571

Ni -2.9896015848636344 2.1946530928006744 -1.1823079411710478

Ni -1.7399100399307408 -1.1436598965771034 3.4298763598217059

Ni 2.3395184560220033 -1.1352845576922410 3.4200910280308916

Ni 2.3281527660004135 1.3791015179064952 3.4118645336651792

Ni -1.7403208937175194 1.3871488776906207 3.4113420758080499

Ni 3.5872227055320476 2.1586632213558437 -1.1381946791769384

Ni 3.5909233219221148 2.1700782027033636 1.3746149097967357

S9.26 $CO_2/Pt_{42}Ni_{13}$ (linear OCO angle)

C -6.3671219431116306 0.2673790575489609 -2.7594697390330420

O -6.6307951245370411 1.2051975699017043 -2.1057816970339296

O -6.1168926988606973 -0.6692654145675480 -3.4201056690565430

Ni -1.3301320535900576 -1.5425317772572245 -0.4984013145218353

Ni 2.5785698827611929 -0.4936312192319082 -0.5080284397174226

Ni 0.6187551909177406 -1.1036052271150913 -1.9235259843620456

Ni -0.5813005731163549 -1.3594769480178359 1.8685380905601685

Ni 1.2793628358560127 1.3374644871456132 -1.5512727840250216

Ni 0.0877017530467548 1.0741874839810135 2.2363989957032580

Ni 0.3555313346449883 -0.0174103773622253 0.1628129985196198

Ni 1.0296397769979819 -2.2893080434694206 0.1854824438326388

Ni 1.7708324536344353 -0.6943953168304503 1.9251873499800161

Ni -0.3308623962682517 2.2581643466869381 0.1262289371764089

Ni 2.0384507804182670 1.5032564853829145 0.8085624747808053

Ni -1.0730873690097606 0.6549012852973860 -1.6025366948376047

Ni -1.8779680782780499 0.4567362887936121 0.8125384023742648

Pt 4.9689312427012844 -1.1830051729149036 -1.1612792021491261

Pt -1.2018021918898079 -2.8184752974167009 -2.8418442892512523

Pt 1.6959528401931721 0.2446142379873046 -3.9695345900657006

Pt 2.3824182847417461 2.7027683583246538 -3.4561588567874679

Pt 0.9167476468470143 -2.2334780719855520 -4.2433594990635175

Pt -3.5762877016253025 1.3569083787676826 -1.0365519164535362

Pt -3.2112687176297712 -3.1838320104044979 -1.2041731696667524

Pt -0.9228494150145997 -0.3943533555831319 -4.0066172625676089

Pt -2.5677876291118817 -3.0753538391615352 1.3213791776027837

Pt -0.8281711450308452 4.7949041827242418 0.0659730761753680

Pt -4.2859049836358576 1.1554865103332215 1.4582640787631160

Pt -0.1064478962475217 -3.9203023024157351 2.0604697008047790

Pt -0.8907142242216696 -4.1405624605221867 -0.5081552990937650

Pt 0.7983463206430327 3.8999753484376369 -1.7700411228454127

Pt -3.0520952563334074 -0.8934463643253568 -2.4248224997510661

Pt -3.1307783583018374 -0.8195408222947606 2.7040511313306217

Pt 3.8241323010846875 0.7927133060001493 -2.4134218885333816

Pt -1.0035793594851281 -0.2748407326415790 4.2748158572178045

Pt 4.3008943600170007 -1.3900826720400554 1.3430834182010305

Pt 3.8927374081620316 3.1524852261767387 1.4975798837634129

Pt -1.6882396083170921 -2.7267806624022168 3.7457300589244449

Pt -0.5663270657274228 3.6479686960416147 2.3910987757150739

Pt 3.0498235577164294 -1.7756584189359972 -2.8065092150262885

Pt 4.6104732706002816 1.0317822039760356 0.1683289525640587

Pt 1.6221616927649798 0.3659605145464072 4.3278146786586777

Pt 2.5299542899615428 -3.2955951678985156 2.0802313864403157

Pt -3.9183827913432339 -1.0616354636413574 0.1295179841996410

Pt -0.1688942182438442 2.1737453995309539 -3.6100177556126294

Pt 1.2518710512483189 -3.6629941273423978 -2.0930304244005846

Pt 3.7602556235472218 0.8660761693341869 2.7322137182223338

Pt 3.3763611699670735 -3.1412219015073739 -0.4925128142205712

Pt -0.2270820581260384 2.1994642391602137 4.5290784722679014

Pt 1.8901535608595612 2.7885275932074385 3.1375845187540126

Pt -2.3582966946753228 1.7476105188253619 3.0959308800946896

Pt -2.6842972886324024 3.1175691795499518 0.7918381636768006

Pt 1.5141193050748711 -4.8146258455900082 0.2261502843180249

Pt 3.2529144631908151 3.0416504036131555 -1.0284072655290399

Pt -2.6697080128249553 1.4700258299056175 -3.4845668563750998

Pt -1.8281887158862578 3.2628894448492098 -1.7811574714529852

Pt 1.5724097405640727 4.1066472032400601 0.8004537808748611

Pt 0.8652161907805810 -2.2081540626919662 3.9225152635686529

Pt 3.3605452401329527 -1.4934968737024514 3.7714307863676311

S9.27 $CO_2/Pt_{42}Ni_{13}$ (bent OCO angle)

C -4.6813565937710058 -0.6721996754706765 -3.7436354805601599

O -5.4957063222392213 -1.5457913886218211 -3.9084051883936333

O -4.5179471894325198 0.4842805783765957 -4.3061877975612113

Ni -1.3642795876473586 -1.6345567101470475 -0.3295279028534336

Ni 2.5234007196632171 -0.3933884212529176 -0.3806148156824510

Ni 0.4710187687210835 -1.0372223692440155 -1.8722430903081779

Ni -0.6486608733413780 -1.2582179541841654 1.9819765416478781

Ni 1.1718745213514175 1.3210789570016559 -1.5275479902839351

Ni 0.0298314758943205 1.0848458134113923 2.3194806747565355

Ni 0.2542285941222561 0.0109475656042168 0.2222579245407327

Ni 0.9877630053394076 -2.2361279584654552 0.1966630481467710

Ni 1.7213814005914139 -0.6744878556944431 1.9375846637018430

Ni -0.4170491759660765 2.2883569014753684 0.2201037046973439

Ni 1.8869698969442754 1.6304676625829482 0.8248326470730926

Ni -1.1920822659435424 0.7369797278295238 -1.5150116462793406

Ni -1.9900327994731666 0.4620069590598740 0.7865655886642510

Pt 4.8998238989727065 -1.0965946097311192 -1.1583323332149291

Pt -1.2891466414274846 -2.8301553828576536 -2.7074703156898750

Pt 1.5580688349119289 0.2694289774577003 -3.9476847729974427

Pt 2.2231998351059654 2.7329098317646316 -3.4569384555918106

Pt 0.8007232065334188 -2.2205810083362385 -4.1339516304178208

Pt -3.7338900658849536 1.3503628138360517 -0.9372664921298616

Pt -3.2571745376865224 -3.1982596980099958 -1.0320110083820122

Pt -1.0561435694774066 -0.4119530449363474 -3.9255603808795136

Pt -2.5993141867361378 -3.0512004163941784 1.4779496049804131

Pt -0.9656393079499571 4.8321036655260245 0.0843705369611899

Pt -4.3179078858958713 1.1627421834930198 1.5887447866344067

Pt -0.0897124334227654 -3.8211631073480623 2.1849041401691167

Pt -0.9239991673814233 -4.1565189610209421 -0.3764617147180013

Pt 0.6381001741866109 3.8914006686758809 -1.7398311151637778

Pt -3.2226257215773573 -0.9451154836886111 -2.3331496316600493

Pt -3.1278535691091336 -0.7741940800674125 2.8408650984482868

Pt 3.6894257871783736 0.8343984244758895 -2.4126564004948445

Pt -1.0206072279075138 -0.1801105157822718 4.4198921495914369

Pt 4.2944372289864008 -1.2839331188815677 1.3595436839634161

Pt 3.8070182421229481 3.2681839102892871 1.4741891358802697

Pt -1.6672083885002338 -2.6515080225643581 3.8812041099930887

Pt -0.6658421471549906 3.7204954421822292 2.4315196886841024

Pt 2.9266240082598158 -1.7214198773727201 -2.7393187171181435

Pt 4.5530826935910076 1.1305010098068682 0.1473774942748775

Pt 1.6006789136996740 0.5058845415114963 4.3844902888105288

Pt 2.5348752994645891 -3.1676621347412786 2.1591479944520913

Pt -4.0016676501732684 -1.0693963805549138 0.2778199230009636

Pt -0.3542761316771627 2.1380135197997339 -3.5468460933973507

Pt 1.1912108802909258 -3.6535649184486756 -1.9893801441851977

Pt 3.6556911229358415 0.9749759022386801 2.6929533214607879

Pt 3.3345501411239389 -3.0636089775924420 -0.4359588249235476

Pt -0.2546943952932571 2.3134116301370495 4.5845268551114300

Pt 1.8239522039279410 2.9010625321514283 3.1488602312426570

Pt -2.3876354998885394 1.8035176264758415 3.1903935600765472

Pt -2.7729132087458805 3.1277008518668028 0.8625623666733818

Pt 1.5058906806116865 -4.7419339231250985 0.3549168685020180

Pt 3.1111296843402498 3.0826591633231786 -1.0258560335371225

Pt -2.8925739085636821 1.4612978616439574 -3.4651302913738640

Pt -1.9820634107808908 3.2083196729961703 -1.7320667170323585

Pt 1.4526474597289716 4.1817235225738836 0.8084509174583417

Pt 0.8751469188380611 -2.0722787833846033 4.0129291155605449

Pt 3.3672582656102690 -1.3469131396483476 3.8219683196715248

S9.28 CO_2/Cu_{55} (linear OCO angle)

C -4.7309982658545966 4.5174105706203713 1.6195547037298383

O -4.9395045029274645 3.9944970008069713 2.6487939289300075

O -4.5333477138568998 5.0549291533527603 0.5949315729094056

Cu 0.2580355750460759 -0.2468227381208965 -0.0880094519446657

Cu 0.2527154477322389 -0.2462572309875089 2.3171466337777988

Cu 0.2525402188063868 -0.2463243408362803 4.6705336642604758

Cu 2.0219899200299913 -1.5449911570638040 3.4566995779420240

Cu 1.9932511674681128 -1.5150184429942317 0.9871664627850323

Cu 2.0048094714352080 1.0179513633597124 0.9821756940431414

Cu -0.3972456881926700 1.8048922493092603 0.9867629333180816

Cu -1.8991973140150276 -0.2441023839727439 0.9883958018001695

Cu -0.4154088147684273 -2.2951457774115616 0.9911275615717359

Cu 0.9105876163211767 -2.2972799366195309 -1.1637394239013843

Cu 2.4129015429709559 -0.2487593779088673 -1.1634078081427019

Cu 0.9316524535103373 1.8017026708106398 -1.1688449707488444

Cu -1.4793180816371045 1.0246997903444666 -1.1651109864465439

Cu -1.4920784529716979 -1.5100006905276462 -1.1587099505428937

Cu 0.2636050810587241 -0.2473272668173070 -2.4944128092238684

Cu 3.6938693862659013 -2.7546769681272272 2.0391529013716281

Cu 3.7151232646444603 2.2521397781255228 2.0352882600358471

Cu -1.0327561496598332 3.8078479028503676 2.0401042443983415

Cu -4.0070509106305696 -0.2359617581811893 2.0402790319235096

Cu -1.0711717498368512 -4.2991532670129677 2.0477010208907331

Cu 1.5537512612727047 -4.3018394367799706 -2.2157317046589724

Cu 4.5229641198882540 -0.2570108052895523 -2.2154304643941969

Cu 1.5893847221802548 3.8039300859154546 -2.2261699218387121

Cu -3.1766973266259422 2.2634686780722300 -2.2180800214609149

Cu -3.2001686585169589 -2.7426938104748038 -2.2112917763198339

Cu 0.2645649260125785 -0.2495368860241445 -4.8472383553599139

Cu 2.0292090795015545 1.0446176773207851 3.4529189645915781

Cu -0.4170801646704671 1.8443193995266836 3.4636456288252080

Cu -1.9371588763018803 -0.2620127840418138 3.4661604634101395

Cu -0.4472269240615969 -2.3294992374320023 3.4672363503494439

Cu 3.8133787053707513 -0.2537711399072566 2.0916723301173392

Cu 1.3436532059855286 -3.6295943395105033 2.1102919832733451

Cu 2.6912428476836361 -3.6280841251714255 -0.0811654874247351

Cu 4.2285057758885767 -1.5384287177517979 -0.0824005473103084

Cu 1.3718017749677889 3.1440121246004633 2.0893581515565161

Cu 4.2349938952092678 1.0559686818006029 -0.1032685410515141

Cu 2.7351574605596305 3.1212710725344506 -0.0977184563907740

Cu -2.5962409421074719 1.8408124675083839 2.1099230986980246

Cu 0.2904786703838614 3.9318388286978898 -0.0834833870318134

Cu -2.1692123131049650 3.1379371119118113 -0.1002636604040190

Cu -2.6289274828207292 -2.3307410204451449 2.1014896596479020

Cu -3.7112814210871372 1.0451224545597555 -0.0946606506449057

Cu -3.7215647393727815 -1.5497061874158351 -0.0715849941748074

Cu -2.2201593119621927 -3.6139683620000929 -0.0788215617335850

Cu 0.2268685875171988 -4.4254880939107002 -0.0944043745262006

Cu 3.1148376297854545 -2.3362317721908985 -2.2830318779026384

Cu -0.8556433194041527 -3.6371726042423225 -2.2653598090361498

Cu 0.9310120567680221 -2.3400403921755801 -3.6388901043421042

Cu 3.1465436412995835 1.8365949228271419 -2.2773397029077755

Cu 2.4544396091216889 -0.2359328303350015 -3.6419286878812982

Cu -0.8246408045637575 3.1357168527069899 -2.2901761441386070

Cu 0.9663320236416800 1.8337986146111700 -3.6457849587367064

Cu -3.2997697290234393 -0.2375700968962622 -2.2691257199319153

Cu -1.5025664239018692 1.0527483192484468 -3.6343540739290829

Cu -1.5137850564510995 -1.5370837928454637 -3.6285702396748802

S9.29 CO_2/Cu_{55} (bent OCO angle)

C -0.4775311672811408 5.6483232291924397 1.6000165822773031

O -1.0147733633670537 6.0535091611120011 2.6143619078380311

O 0.1511045846426687 5.9633183629503010 0.5956210604319383

Cu 0.0217738073420196 -0.3143636539567211 -0.0854075927859411

Cu 0.0657461871103369 -0.3495192028347019 2.3184172572749162

Cu 0.1071232729234498 -0.3867232248952092 4.6780294541969738

Cu 1.8079697381452364 -1.7261021172780060 3.4337551335504459

Cu 1.7337864423897189 -1.6632226824476701 0.9488936138902206

Cu 1.8280564337958980 0.8698126554151572 0.9732146920184734

Cu -0.5554174693880877 1.7556344038364928 1.0238882636737119

Cu -2.1203600414569888 -0.2521716702505074 1.0107290641016109

Cu -0.7023812197307943 -2.3471597485111060 0.9787482075481651

Cu 0.6043375770930811 -2.3648451866297959 -1.2004632943556428

Cu 2.1629134780729391 -0.3772658418596989 -1.1876823618498518

Cu 0.7380034218194896 1.7329749271760280 -1.1364237293010999

Cu -1.6888274243257211 1.0244927642741546 -1.1263632216110293

Cu -1.7775119035123321 -1.5110560074716686 -1.1501035411019414

Cu -0.0174337445818064 -0.2807229256724809 -2.4921294915618546

Cu 3.4064064499024811 -2.9831214609383236 1.9631224594428434

Cu 3.5961968137439770 2.0256380910400908 2.0179384500896731

Cu -1.1174388560678477 3.7638419207123039 2.1382993892349305

Cu -4.2187528173753872 -0.1954741669782748 2.0902772886365710

Cu -1.4113535321349655 -4.3391287299632522 2.0208376978179672

Cu 1.1760036112950205 -4.3725707387116044 -2.2922471833842337

Cu 4.2619235527436148 -0.4478425092187904 -2.2690527950004480

Cu 1.4673654574454007 3.6885097569301539 -2.2171955804261074

Cu -3.3660214709907432 2.3339440650392449 -2.1418747961022291

Cu -3.5364238819112170 -2.6833199843266611 -2.1922580434359134

Cu -0.0591641619322995 -0.2606195921227396 -4.8499820614439955

Cu 1.9196769943355907 0.8184439309229078 3.4643827818192650

Cu -0.5617084299740877 1.7363522979197201 3.4992154375170230

Cu -2.1114203190330709 -0.2973926779305912 3.4737700815811081

Cu -0.6812141779195694 -2.4284123428844309 3.4458035480766940

Cu 3.5978412048857580 -0.4842687962455471 2.0395022387913855

Cu 1.0351503071016781 -3.7515057867075283 2.0765681730745200

Cu 2.3768307100189690 -3.7708042254696492 -0.1701079149121368

Cu 3.9613772341705316 -1.7479932077546918 -0.1598652473065838

Cu 1.2889648147931370 2.9310941322540858 2.1743544369314236

Cu 4.0626442079316734 0.8018181278192146 -0.1215063479641001

Cu 2.6420872100000015 2.9334252012275162 -0.1050259273188201

Cu -2.7378419095156783 1.8461069468477209 2.1847570070725624

Cu 0.1891772681167412 3.8880314735213206 -0.0608128690969918

Cu -2.3443482723129687 3.1064157454316588 -0.0033798152797429

Cu -2.8873822918581578 -2.3307699768568595 2.1247989477934652

Cu -3.9232695676300278 1.0908282604210031 -0.0208605345897011

Cu -4.0066179093622605 -1.4636277881766118 -0.0509486664311678

Cu -2.5769611129505829 -3.5940599243472802 -0.0806819322658042

Cu -0.1127240879528681 -4.4550601795455718 -0.1280826382964049

Cu 2.7945473087122581 -2.4829840383455375 -2.3394084116628164

Cu -1.2257837755784049 -3.6163287456421953 -2.3210111377987914

Cu 0.5828523066660455 -2.3819985887285524 -3.6675018774657246

Cu 2.9295350924463763 1.6876219275865738 -2.3180301388543967

Cu 2.1543308732601094 -0.3378569787082625 -3.6497787872571621

Cu -0.9888078187246928 3.1013066082192013 -2.2570479350526398

Cu 0.7330203775733298 1.7861086515279085 -3.6287024318608587

Cu -3.5468490919496940 -0.1722048542860675 -2.2188253079755214

Cu -1.7703840868186358 1.0678570172921100 -3.6122272573258556

Cu -1.8580428328404519 -1.4849121029727170 -3.6343143036057199

S9.30 $CO_2/Pt_{13}Cu_{42}$ (linear OCO angle)

C -2.5338343612563055 0.0118658200563997 -6.2240158771568392

O -2.4943778980843199 -1.1610918792443903 -6.2390457551780081

O -2.5714545736233347 1.1844189371698375 -6.2118815192127368

Pt -4.0001145789727826 0.0375699438095579 -2.2796299589053000

Pt 0.1230812612237891 2.5567737648043476 4.4845984894340747

Pt 0.1618101733254569 2.5391986764538661 -3.8083739851233407

Pt 0.1076124622346517 -2.5470853620850491 4.4805853581877875

Pt 0.1949197746057647 -2.5512900934225318 -3.8202796654830493

Pt 2.6831967068145488 4.1360316627422336 0.3320686879451885

Pt -2.4284618915745941 4.1249679093382481 0.3427121797810813

Pt 2.6883057253578997 -4.1351268700687349 0.3283812988205881

Pt -2.4101946916969510 -4.1871132338916777 0.3759704978926708

Pt 4.2464437904681658 -0.0087383749174050 2.9175086678776161

Pt 4.2923427848596249 0.0117529643628814 -2.2103136626525011

Pt -4.0034428346037032 0.0149973405253137 2.9232112682466775

Pt -3.2748862653569120 -2.1163142752271611 -0.9753482484866378

Cu 0.1383588839254857 0.0004990983575224 0.3379969758225290

Cu 0.1230269801129030 1.2499904787195140 2.3588276142713882

Cu 0.1464474155812539 1.2495520107002187 -1.6806296798530180

Cu 0.1260318198563793 -1.2507022317854448 2.3567613950832929

Cu 0.1420894216119295 -1.2592793248429610 -1.6848337142649221

Cu 1.3849973134440290 2.0233479741031584 0.3463812189337610

Cu -1.1163880272544147 2.0224949195263999 0.3295648178257019

Cu 1.3869240265807734 -2.0257122979482904 0.3442166520270274

Cu -1.0935435212075133 -2.0331099543774176 0.3466172719087970

Cu 2.1562116342257607 0.0024528799843642 1.5869191303379981

Cu 2.1655337395050527 -0.0028618305007699 -0.9079671250117816

Cu -1.9009149271379988 -0.0042372522971787 1.5788710451594854

Cu -1.8765714203609571 0.0189409521307010 -0.9165525580449252

Cu 0.1274900543724724 4.2006038240733030 0.3340484875021739

Cu 0.1378562803713821 -4.2081116811099388 0.3344468536453960

Cu -4.0713436270216530 0.0180206309282969 0.3353788968089724

Cu 4.3251771591011625 -0.0008802396610809 0.3556527630434792

Cu 0.1952678732847744 -0.0062810069292960 -3.8351381549248256

Cu 0.1251081700467853 0.0064319949929688 4.5227527460857706

Cu 1.4153253142520652 -3.4036940454790798 2.4315961786902314

Cu -1.1589308747156137 -3.3901911603357338 2.4318002512329304

Cu 1.4437886436997054 -3.3829247777061333 -1.7552053027084948

Cu -1.1294638441647804 -3.4116301183279436 -1.7672809509174652

Cu 3.5455070155539872 -2.0828598330236314 -0.9287675022180242

Cu 3.5256848281682167 -2.1070673722992872 1.6448931543097007

Cu -3.2667280097617244 -2.0943524934028357 1.6482349882414358

Cu 1.4159620193806244 3.3918011708521068 -1.7467060689874874

Cu 1.4230477639369015 3.3836873851658611 2.4321021880945448

Cu -1.1626851514081251 3.3916595930614744 -1.7640396044395708

Cu -1.1511586596722341 3.3932460390044614 2.4252619202577979

Cu -1.9362359454458977 1.3012760476626555 -3.0393312008750453

Cu 2.2575746856406020 1.3017505586450075 -3.0364093365872993

Cu -1.9273599802686674 -1.3025020246263053 -3.0714269345616945

Cu 2.2686321743671014 -1.2984161227279059 -3.0410064334531643

Cu -3.2554509664401365 2.0882428560812869 1.6263569263306135

Cu -3.2677819191296287 2.0962466661699146 -0.9624919867926796

Cu -1.9659203702841455 -1.2740755376123956 3.7291291567837463

Cu 2.2116467374470030 -1.3108096262392215 3.7124084626738778

Cu 2.2165787334891043 1.3025019637688924 3.7213350238174527

Cu -1.9670148966461272 1.3061928871328419 3.7282185221117574

Cu 3.5331757537824098 2.0882065092129452 -0.9263340917548231

Cu 3.5291021154607591 2.1017355605532257 1.6482002284080881

S9.31 $CO_2/Pt_{13}Cu_{42}$ (bent OCO angle)

C -5.1170010909363413 -2.1877187265181646 -2.0924272072851244

O -5.6952229324635830 -3.2352928602592423 -1.9077021091125625

O -5.4387859719072598 -1.1210090490424647 -2.7438235946867482

Pt -3.8830989061741756 0.2825898648236752 -2.5048742196969225

Pt 0.3052005479057728 2.6427034472557787 4.2767391700490052

Pt 0.3141855030203637 2.6754699503598993 -4.0250208385243136

Pt 0.2739174998182574 -2.4504022700542367 4.2556670353168107

Pt 0.3036166291856061 -2.4126921028552561 -4.0337020198349451

Pt 2.8680423906862562 4.2281596463905755 0.1332649905710093

Pt -2.2464660787373218 4.2737621961323082 0.1442387929091003

Pt 2.8357148987644281 -4.0320324525600340 0.1061504442418451

Pt -2.2787151170494666 -4.0069491995490489 0.1130052795907673

Pt 4.4287013152748589 0.0909687314591925 2.6793635934163267

Pt 4.4344263176510417 0.0817675422763853 -2.4288807750582033

Pt -3.8367632193535068 0.1654718628325056 2.6950089995613689

Pt -3.2570244297792068 -1.9866942398923277 -1.2359291173027809

Cu 0.2902949916396946 0.1090533002326679 0.1223476044753321

Cu 0.3017807948004977 1.3516326415739752 2.1472244662631899

Cu 0.3093269384744927 1.3725952317735541 -1.8983454722558544

Cu 0.2899673457173919 -1.1458759016513933 2.1456001042925146

Cu 0.2751891168855071 -1.1388566885874449 -1.8990694986062429

Cu 1.5581562561419715 2.1253071451883092 0.1315515297825277

Cu -0.9395282723613928 2.1499470203181406 0.1326424935178330

Cu 1.5368359404177903 -1.9180395240897652 0.1214311657790340

Cu -0.9607494605613663 -1.9080847936420144 0.1234973445669981

Cu 2.3175198305540552 0.0924022754412177 1.3782073725687494

Cu 2.3151912764244060 0.1031247108438849 -1.1210528309156955

Cu -1.7337208133048168 0.1104945105104221 1.3656634980414748

Cu -1.7304341908560086 0.1537521239061595 -1.1401349307140491

Cu 0.3234652665178390 4.3062971300895230 0.1392263290897203

Cu 0.2749304978648310 -4.0862160450499294 0.1073650509270237

Cu -3.8792560604783648 0.2028318580151667 0.1314008878895892

Cu 4.4762472102936117 0.1052892217033104 0.1321232832457473

Cu 0.3090265221065533 0.1331704290200464 -4.0706315694308612

Cu 0.3072043311049106 0.0887597467691621 4.3131279287565283

Cu 1.5609918153093365 -3.2908315638441112 2.2048498166863761

Cu -1.0264975010972957 -3.2839655988397172 2.2158601268863953

Cu 1.5618078743849524 -3.2866214175233135 -1.9748041708585418

Cu -1.0087414463178788 -3.2817310855560531 -1.9971498774205272

Cu 3.6788405216808031 -1.9972464861011665 -1.1577419849388888

Cu 3.6743689952530203 -2.0118140707328354 1.4331766403097377

Cu -3.1196205978557727 -1.9684865170008794 1.4418404501297553

Cu 1.6160977355267048 3.5002930910136656 -1.9632897588551130

Cu 1.6094247754220370 3.4886939374569503 2.2300151145318634

Cu -0.9359667235209695 3.5488460896849072 -1.9521436958145890

Cu -0.9673956777208638 3.5019247165130847 2.2252666878792886

Cu -1.7856980404212695 1.4837643468403630 -3.2447249598198975

Cu 2.3991375386453515 1.4041976072499156 -3.2501264156933440

Cu -1.7867243415480298 -1.1177891794174530 -3.2842032235079688

Cu 2.3852148770048109 -1.1879578573081591 -3.2537429232148773

Cu -3.0736213606435121 2.2434785097385395 1.4326237710105318

Cu -3.0368246966238561 2.2765927207566148 -1.2022782073300831

Cu -1.8142324192654917 -1.1956036331628144 3.5019264045443195

Cu 2.3929200169793448 -1.2202462959465801 3.5162505248508187

Cu 2.3966099709619084 1.3865196468640186 3.5040830758677246

Cu -1.7818041033089798 1.3999116382424392 3.5143226466741697

Cu 3.6998478090615676 2.1927583314788559 -1.1632493273172488

Cu 3.7096901008067564 2.1996263364291901 1.4299861039719013

S9.32 $CO_2/Pt_{42}Cu_{13}$ (linear OCO angle)

C -6.4360442211532352 0.1201971605689057 -2.7831432076705718

O -6.7194841119130899 1.0367253549013060 -2.1082038430868288

O -6.1650228552345467 -0.7945333432477508 -3.4647746919798323

Cu -1.3622513922694885 -1.5376022145538031 -0.4938427148927915

Cu 2.5809152872943946 -0.5647685286751145 -0.4778993594112984

Cu 0.6276917228464356 -1.0775549569612999 -1.9631715288161602

Cu -0.6249630708969622 -1.3210387274424289 1.8940558629094038

Cu 1.3261542590380664 1.3064481823797658 -1.5886437954720383

Cu 0.0699747929579360 1.0617739980750629 2.2674296310933140

Cu 0.3493282705065539 -0.0072604068329218 0.1522832586950957

Cu 0.9163176261951964 -2.3261762326639230 0.1865936683973008

Cu 1.7995825414388928 -0.7180667072836020 1.9036717670632579

Cu -0.2180079405567348 2.3116794794634439 0.1184712659651423

Cu 2.0603259774481515 1.5228072740834235 0.7999139675930516

Cu -1.0965868978298943 0.7041347739537780 -1.5969691145073956

Cu -1.8827601914092646 0.5492935583878162 0.7835411653396869

Pt 5.0141662401008844 -1.1822910393222614 -1.1748428304872385

Pt -1.1796556641459599 -2.8162761379458603 -2.8301986922149696

Pt 1.7168471281472328 0.2615755670837581 -4.0236296057826282

Pt 2.4105530456480277 2.7262865861484160 -3.4644773816918328

Pt 0.9241900395615961 -2.2301701252214778 -4.2746548932368471

Pt -3.6059034264025449 1.3569016687146067 -1.0423111883296010

Pt -3.2079012859650842 -3.2120831978303590 -1.2178619873013568

Pt -0.9081449212981205 -0.3776901619738268 -4.0060203242777481

Pt -2.5532356656088382 -3.0754698329198904 1.3142808529586563

Pt -0.8374017507790921 4.8314126597339380 0.0547885056987360

Pt -4.3132531059979851 1.1707114593152042 1.4788565214901594

Pt -0.1035914791631978 -3.9326816719226327 2.0782398851702104

Pt -0.8683308294250072 -4.1580539753782633 -0.5073065537542498

Pt 0.8073824586038807 3.9228740528640431 -1.7752570087405304

Pt -3.0487534695920786 -0.8920483073660439 -2.4289717389472494

Pt -3.1113012636331145 -0.8120798368131272 2.6951170717555537

Pt 3.8116858340614543 0.7989060391232286 -2.3932892869985154

Pt -1.0114885242707903 -0.2737584858456198 4.3234855648173340

Pt 4.3171960499616784 -1.3693879693161108 1.3498071801854983

Pt 3.9112317167176665 3.1980766822735012 1.5195536502977771

Pt -1.7090720750978949 -2.7374506925597535 3.7676094707813381

Pt -0.5662196121902134 3.6675248354202274 2.4015982448500135

Pt 3.0398659121431750 -1.7629284683923221 -2.8035948007905138

Pt 4.6163467994212688 1.0481241374541230 0.1738417178870359

Pt 1.6147436368305677 0.3655848658737700 4.3089544676716205

Pt 2.5179054887121586 -3.2574654542956898 2.0813790986412344

Pt -3.9230406012133230 -1.0633079467434083 0.1286037875308623

Pt -0.1513007993582516 2.1851936680086572 -3.6243499222970006

Pt 1.2699313041536753 -3.6820649868277799 -2.0997699146015738

Pt 3.7630660969856500 0.8772420608026532 2.7364003165033455

Pt 3.3673866335183593 -3.1154639230750272 -0.4962530229041264

Pt -0.2198272975057982 2.2191144282460700 4.5777367425113873

Pt 1.8836973148316440 2.7976791163954013 3.1285205046307847

Pt -2.3392644378883993 1.7530011955869040 3.1093708225390588

Pt -2.6684547151598021 3.1085302024175236 0.8024552815786952

Pt 1.5417767736294845 -4.8441531185553410 0.2479116019165057

Pt 3.2535742347302570 3.0624747741817275 -1.0110561897145129

Pt -2.6910519876181684 1.4823086424820271 -3.5055566086166743

Pt -1.8133155998218697 3.2450302922546976 -1.7766703822929970

Pt 1.5722735097064113 4.1439763317262210 0.8091185550907150

Pt 0.8556772233802281 -2.1981797945839494 3.9290766822083856

Pt 3.3958412748278226 -1.4955828033706109 3.8100534750459176

S9.33 $CO_2/Pt_{42}Cu_{13}$ (bent OCO angle)

C -4.7288294506703474 -0.6429599485387314 -3.7509687895465307

O -5.5689602439883084 -1.4909957524023039 -3.9157786196364706

O -4.5414577673798613 0.5191790422689930 -4.2986302936658438

Cu -1.4198879054100852 -1.5662291238715209 -0.3680924902100148

Cu 2.5090724736397543 -0.4975147238776074 -0.4412100483757541

Cu 0.5293061601983378 -1.0712677273353730 -1.8764922582063681

Cu -0.6497783992088126 -1.2681720062901771 1.9952242689733533

Cu 1.1926118692870671 1.3243219824159738 -1.5559742599432349

Cu 0.0109933851733364 1.1330025221364863 2.3254268900930208

Cu 0.2672041175084528 0.0286060811064122 0.2180510103412638

Cu 0.8903159091608512 -2.2732117723594332 0.2896632958987339

Cu 1.7695622428284783 -0.6244547579155082 1.9550004955389886

Cu -0.3510120141429910 2.3338859110022039 0.1511185988950182

Cu 1.9564799115038132 1.5951457798914888 0.8200038655821834

Cu -1.2540875229286690 0.6560071131928620 -1.5232887246585447

Cu -1.9558857576725450 0.5510789678485750 0.8791246398402420

Pt 4.9236838109915766 -1.0777187654003839 -1.1552386266346639

Pt -1.2877640650633384 -2.8421263054694119 -2.6980855860392987

Pt 1.5571877758309367 0.2541646337463126 -3.9509228318274223

Pt 2.2249428151743653 2.7513750961184646 -3.4849556556383403

Pt 0.8094392887515949 -2.2496309801719203 -4.1672731495439086

Pt -3.7248719395400438 1.3215897753945596 -0.9423025175813954

Pt -3.2547997314952215 -3.2551200087596275 -1.0303824244965982

Pt -1.0515781671949056 -0.4324484245066493 -3.9145400402456767

Pt -2.5609846215711900 -3.0798826986314225 1.4891331101428715

Pt -1.0037016734013782 4.8604544730875725 0.0902401491685873

Pt -4.3801842918494645 1.1371512767969101 1.5821905553897659

Pt -0.0617791722318617 -3.8592169962545935 2.2022942873007745

Pt -0.8921205291226335 -4.1718622745870597 -0.3619018711541716

Pt 0.6174311184717527 3.9373377996619734 -1.7681987348993387

Pt -3.2657022360058945 -0.9943576368790623 -2.3729829499997246

Pt -3.1242620992230488 -0.7912479578643357 2.8287046966446709

Pt 3.6900660339511817 0.8417602506350725 -2.4192301807235195

Pt -1.0151574006265114 -0.1866497539790792 4.4090172058980839

Pt 4.3207659308082897 -1.2658650821406923 1.3818606575645918

Pt 3.8006899867757666 3.3063402527812507 1.4761024838318137

Pt -1.6607626738786592 -2.6764609621690116 3.9126023673191863

Pt -0.6918044999878954 3.7101354471528962 2.4360208759788247

Pt 2.9697062115351156 -1.7330664676986398 -2.7794658912184795

Pt 4.5229591567071141 1.1507002062366931 0.1577127925028571

Pt 1.6051745207163468 0.5087787577344596 4.3936602914773566

Pt 2.5578463605619768 -3.1536101686318840 2.1528132943245994

Pt -3.9578436910170747 -1.0985263110797376 0.2613407476645592

Pt -0.3532869460600660 2.1303252256095959 -3.5245335055456133

Pt 1.2098911943331516 -3.6184255436646051 -1.9752006912473528

Pt 3.6822457990212976 1.0039556806674304 2.7235951175709490

Pt 3.3494383343847480 -3.0335207451896675 -0.4264846134920158

Pt -0.2754523716014971 2.3154264720290705 4.6031999672373916

Pt 1.8158286913803008 2.9150568507774945 3.1510482038959511

Pt -2.4314636836369625 1.7967632562664138 3.2043833691421915

Pt -2.7855672866714936 3.0928495285450532 0.8583712391197221

Pt 1.5517143283222423 -4.7708877245926686 0.3495013078573147

Pt 3.0844043879034566 3.0939618163091067 -1.0375621963452994

Pt -2.8944778763374877 1.4588560934659363 -3.4807321190859524

Pt -1.9816715676895309 3.2078652982544735 -1.7302657624954110

Pt 1.4202463424761373 4.1872159843475050 0.8068651276632196

Pt 0.8875270410243705 -2.0621454235408585 4.0023623042049676

Pt 3.3984003871859714 -1.3357155316792646 3.8440616153938949

S9.34 CO_2/Ru_{55} (linear OCO angle)

C 6.0023887936555829 1.8675099376021975 3.1842593383548921

O 6.1747942096202655 1.0922524748217100 2.3226672809004039

O 5.8578086758607482 2.6492890615821394 4.0504290773815876

Ru 0.7191351252428950 1.3400044451663580 0.6748593651754847

Ru -3.4953038649803592 -2.7470211433323724 -0.2170374509844303

Ru 0.7256690178735147 -2.7085398152505036 3.0257488715316421

Ru -3.6499039282739343 1.1815235090351164 2.0343218061420649

Ru 0.9244965049536090 -0.1109273518751718 -1.5421849382345916

Ru 0.6396355572917233 -0.0478439411326736 3.0510984808899027

Ru 0.6613893102091483 3.8131724312142272 0.7218339795046330

Ru 0.7474120342167488 2.4838722304382341 -1.5823680292414817

Ru 2.7089176047882493 3.8418422334056936 2.2617940645537744

Ru 0.7498846726949225 -1.4960575134677676 0.7186980546746052

Ru 0.7909643856057079 -2.7090726435938284 -1.5033977110494363

Ru -1.6482482732630199 1.2026546440081731 3.6551432280164668

Ru -3.6254713063512858 -1.3769007700393787 2.0732312384658118

Ru 2.9192547476455442 1.1810831950441314 -2.2184386617411507

Ru -3.6505073500261278 -0.0665432653976327 4.2543345905727898

Ru 0.7372940694379880 -3.9678068415852410 0.8365259884624060

Ru 2.9412743167624544 -1.3872154073965179 -2.1794102722458071

Ru 2.7607413085065589 -1.4195304732551139 2.3793029910861163

Ru -1.6240951794471217 -0.0889965128838171 1.4119659265672411

Ru -3.4496040453585786 1.2367288512246040 -2.5062231019849217

Ru 2.7909397091787302 -3.9094113136148567 2.3735832615396748

Ru -1.5037620525663487 2.4993757423908867 1.3796805018732403

Ru -3.4254171988443329 -1.5629334556255634 -2.4605254055638563

Ru 0.6695321767284378 2.6179716922873584 2.9474106153086326

Ru -1.4513033412348610 -2.6725452347320422 1.4619691393767513

Ru -1.2997264388020735 -0.1582208962742070 -3.2111442574908939

Ru 2.7229445086474455 1.3489640498025601 2.3376436993240159

Ru 2.8381009710879646 -0.0657618046255736 0.1159996877432295

Ru 3.0435893880904286 -0.1375311129372824 -4.3982115628273410

Ru -3.3494612791560296 -0.1973700478350037 -4.6200055138293328

Ru 2.8055966715478249 2.5437029012566708 0.0862103193532587

Ru -1.3842124598206165 2.5091717980691164 -3.1493670864105368

Ru -3.2877790601821832 2.2797408884876731 -4.8246744097840404

Ru 2.8569969435631113 -2.6760766841266759 0.1626910857931962

Ru -3.4540680616737984 3.7307092539858404 -2.5207021866631538

Ru -3.2478923190498610 -2.6779099892364311 -4.7439007489593443

Ru -1.4501172057565848 1.3089210952611354 -0.8577807894362016

Ru -1.3400246376480962 -2.8237010794565744 -3.0638954344999241

Ru -1.1219744227195907 1.1609633219105364 -5.3127621129515239

Ru -1.4337445156825170 3.7783808705480713 -0.9469718633204999

Ru -3.3897337513688397 -4.0555505088862569 -2.3938686857284224

Ru -1.0997533289328398 -1.5410079523023967 -5.2686410600031257

Ru -1.4238178481693620 -1.5510148744066796 -0.8129843458523295

Ru 0.9603305019491081 1.0988861227848601 -3.8349292169238267

Ru 0.8540688176617599 -0.1841388727148718 -6.0245313169592407

Ru -1.3654634904330720 -4.0215872155190446 -0.8234980076049997

Ru 0.9815622298462944 -1.3926433772573177 -3.7958246578485508

Ru 2.6383084534550654 -0.0074807630260648 4.5064186400123729

Ru -3.5392197149695939 -0.1288356766827802 -0.2638919954929148

Ru -1.6235162212968279 -1.3172102196552726 3.6948296060331791

Ru 2.4831221217242958 2.4579705157222835 4.6445832245859142

Ru -3.5418062335856870 2.4885871772985690 -0.3009539296257297

Ru 0.3002901778436538 1.2765688804275239 5.1318593599910658

Ru 2.5397490701471099 -2.4683877691311240 4.7100190538034505

Ru 0.3297354537566548 -1.3140727965196375 5.1690122762398101

S9.35 CO_2/Ru_{55} (bent OCO angle)

C -4.4046595510067919 -2.7052260753660429 1.5004036251496031

O -4.8612335618165270 -2.3540793751982338 2.6151746905073447

O -4.7268426056655510 -3.5839596274650689 0.6642188016627872

Ru 1.3173289820137886 1.5937872867640013 0.7569680802346614

Ru -2.9811972318049293 -2.5421730424158651 -0.1759954086308012

Ru 1.2879058249120341 -2.4491332411357614 3.1109375964403285

Ru -3.0481004324546386 1.4613719322492813 2.1169840202273593

Ru 1.5068361844455402 0.1440319595446748 -1.4545696062948186

Ru 1.2115772947413290 0.2130044554994664 3.1325463635387392

Ru 1.2573857845041314 4.0685279680589446 0.7965503241805379

Ru 1.3328938790600799 2.7332362201901779 -1.5009924009993334

Ru 3.3071818813647633 4.0989406700700588 2.3370252071644964

Ru 1.3126356771460463 -1.2501662394531010 0.8087485389283513

Ru 1.3639647047729582 -2.4641955801502213 -1.4065679367472481

Ru -1.0423446886432119 1.4780629454412919 3.7386607781874592

Ru -3.0968556854865290 -1.1073959998090488 2.2361770949000839

Ru 3.5034107932399898 1.4229680592461191 -2.1282764898997373

Ru -3.0449527273790986 0.2516865356634317 4.3572301523291319

Ru 1.3104085184041525 -3.7159399915026170 0.9288354572630927

Ru 3.5193066879827355 -1.1450297374445828 -2.0848477661317353

Ru 3.3338859973330952 -1.1662342843293283 2.4656489013361882

Ru -1.0295444170407972 0.1745121474550892 1.4982526796794473

Ru -2.8726090852692030 1.4947560902927264 -2.4141893041863525

Ru 3.3598663163974010 -3.6548062519847901 2.4790664989385660

Ru -0.9161667912974979 2.7670287336337451 1.4619899591904308

Ru -2.8467025193959623 -1.2973973782337245 -2.3785433497577655

Ru 1.2616294969299371 2.8775430749348549 3.0248091258873968

Ru -0.8719735052636256 -2.4137564253556976 1.5502155999634657

Ru -0.7248674221853068 0.0999502300630372 -3.1169207056409007

Ru 3.3189532657308236 1.6139914394545156 2.4205107630133962

Ru 3.4234285906683937 0.1814978310057868 0.2047768954386810

Ru 3.6238359681955723 0.1050318385627946 -4.3088582637997517

Ru -2.7668526124678814 0.0673430772303951 -4.5350430450430350

Ru 3.3964334936912124 2.7907906718900288 0.1606198927419768

Ru -0.7993961067113663 2.7692874616046752 -3.0565905874581953

Ru -2.6990588595327454 2.5466682784412917 -4.7319127223726269

Ru 3.4266497347709350 -2.4282719424926626 0.2579889840979828

Ru -2.8665037165549707 3.9916248520503159 -2.4404580139558916

Ru -2.6588942524532442 -2.4125013870252032 -4.6638734117131255

Ru -0.8768766723073161 1.5613136484256473 -0.7615595770650616

Ru -0.7547749557335580 -2.5478024363870890 -2.9803660320779066

Ru -0.5359072101795336 1.4200461892005944 -5.2208404821018508

Ru -0.8456893383680019 4.0349017328707886 -0.8612543747899757

Ru -2.7875658909994847 -3.8077484823647003 -2.3395708652553568

Ru -0.5187642800789559 -1.2653437762621533 -5.1863553880509441

Ru -0.8532199888519630 -1.2826321521321205 -0.7202420589993639

Ru 1.5468345673106934 1.3512629070277593 -3.7486396680408749

Ru 1.4424837302735563 0.0659815435059418 -5.9369482923179833

Ru -0.7818739836067311 -3.7563118912387972 -0.7447047234160329

Ru 1.5611703517063293 -1.1430790074086006 -3.7027109106230958

Ru 3.2294886138796506 0.2569550044256996 4.5855432630917194

Ru -2.9569666739775142 0.1300426592419445 -0.1719596911664443

Ru -1.0347188180246014 -1.0440718745610722 3.7855260141465994

Ru 3.0834631526956766 2.7248314549621377 4.7148973131573522

Ru -2.9569500830923876 2.7525020231618322 -0.2131739256975116

Ru 0.9044106790433194 1.5413744166140309 5.2148132396980911

Ru 3.1096674081229412 -2.2016542348552681 4.7998981722744816

Ru 0.9090260883128399 -1.0459449042113289 5.2609469688639674

S9.36 $CO_2/Pt_{13}Ru_{42}$ (linear OCO angle)

C -3.9336804066392421 4.3135118453847392 3.1925448873750581

O -4.3454430089304967 3.3350678208033933 3.6888571973639470

O -3.5392391397861851 5.3091558292045136 2.7082689956558368

Pt 0.4447277147033966 1.9841258331063494 5.1710879828494134

Pt -1.0485709676995831 -0.1255902702561389 4.5973309202282300

Pt -0.9687999692233970 -4.5072360276266723 3.0225528598424796

Pt -1.1106972010528822 2.1836117426458315 3.0320948290008296

Pt -0.9862167312183509 4.2650329053836211 1.3593486931778349

Pt -2.3475525215158859 -2.2587757464460747 3.7757394703498273

Pt -2.4068930980504306 -4.5267819960514224 0.6475154262389023

Pt -2.3771885688176981 4.1896843001792954 -0.9504259356203874

Pt -2.5110990297211337 -0.0340683041506045 2.2989576272486474

Pt -2.4870737171042796 2.0800617668668240 0.7464194221515743

Pt -3.7552647035566351 -2.2750695096483047 1.4056712324609908

Pt -3.8264039069095732 -0.1553053129111653 -0.1459134737116189

Pt -3.7888862537269059 1.9861791372670285 -1.6945956825923885

Ru 0.1389265721417258 -2.3794115452655209 -0.8341636836969827

Ru 0.2705539679970640 2.0134159083559604 0.6551290544951057

Ru 0.1854649610206509 -4.4747430318421006 -3.7258859335493235

Ru 0.2489509632772195 -0.1142809210394157 2.1638426361510130

Ru 0.1304233622758359 -0.1884657695829922 -2.4330656619273707

Ru 0.2657665076011171 4.1136524293697336 -0.9643965576027272

Ru 0.2157185051020831 -4.4088832855518083 0.6780768872876360

Ru 0.1855763440302581 -2.2575749174383888 -5.3349448155110855

Ru 0.1644507109397590 1.9337416396085034 -3.9109039384296511

Ru 0.2474664411318382 -2.2760049934065179 3.6942154617382967

Ru 1.5651567471334280 3.9884702676404107 -3.1786506872177061

Ru 1.5002628374802456 -0.2230615055179868 -4.5701199277106603

Ru 1.5291670640563719 -0.1234974800246107 -0.0819868465939470

Ru -1.0498477841752369 -0.1991626159551801 -0.1157491681185134

Ru -1.1098203316989381 -2.2780085587197365 1.4465470743544802

Ru 1.6141243488139583 4.1336545437605663 1.2358689890834147

Ru 1.4688211712456321 1.9891424371647299 -1.6294722913553787

Ru -1.0839294867005662 -4.3979199028008189 -1.6046997253877717

Ru 1.5821366647360806 1.9901154939687149 2.8256688402187908

Ru 1.5083132326472597 -4.3851725203942884 -1.5403333268338719

Ru 1.5056023391059741 -2.2851613788650096 1.4531604459944489

Ru 1.6078601365090344 -0.2041654616488353 4.3433719208809762

Ru -1.1101901695928202 -0.2313254664212632 -4.5762242145302849

Ru 1.4341403302428473 -2.3721771365102020 -3.1560219074411271

Ru -0.9946180232301013 4.0643987362938852 -3.2110715762754110

Ru -1.1225317547369580 1.9491545056399757 -1.7134734752927998

Ru 1.6735215705792172 -4.3213440895207524 2.9479059396077658

Ru -1.1011316164643876 -2.3709986586492939 -3.1471697227261579

Ru 2.7777659430440496 1.9071249013063103 -3.8767516905864068

Ru 2.8261547715069142 4.0113644316995281 -0.9917258907269203

Ru 2.7671986344320998 -4.3905951320485155 0.7713757457309608

Ru -2.3495704902095769 1.9385871777467822 -3.9031915813796960

Ru 2.8286486330174361 -2.2727482511733301 3.6327131845784746

Ru 2.8153775076674572 1.9983785196953858 0.6345256043179078

Ru 2.8041750551497184 -0.2484558908974659 -2.3659475813969393

Ru -2.4152414103189388 -2.3258972602906560 -0.8725122055559656

Ru 2.8164955932249960 -2.2870314605342847 -0.8370099146357627

Ru 2.8330387012215268 -0.1337080566694143 2.1414825147879859

Ru -2.4280966347563355 -0.1782386387605822 -2.3963794589088443

Ru 4.0719498271151346 1.9526124081064062 -1.7266103592825504

Ru 4.0715447808223200 -0.1504928060518151 -0.1699558526576176

Ru 4.0985049858638849 -2.2688906785273146 1.3890792440850381

S9.37 $CO_2/Pt_{13}Ru_{42}$ (bent OCO angle)

C -0.1675696285425106 -5.4749007612901472 4.0957988724093761

O -0.8894255983433105 -6.2473555366236670 4.6951985485422041

O 1.1470793740639611 -5.4309981283765847 4.0528345380819033

Pt 0.1886107369488658 2.4842992182749741 5.1257091164055444

Pt -1.2602938774160717 0.3610926848187366 4.5402482730978830

Pt -1.1208934299580893 -4.0598991884291387 3.0142681811565293

Pt -1.3729737382393499 2.6940603945324932 2.9806881601290387

Pt -1.2705867333621974 4.7827439721898655 1.3129082668382472

Pt -2.5134176738926235 -1.7941684992209497 3.6911515539477384

Pt -2.5598136338093247 -3.9946390103983376 0.6144789671096299

Pt -2.6503020300726461 4.7086970149855407 -0.9946525449240492

Pt -2.7317597210251710 0.4615026144214577 2.2467851061631321

Pt -2.7428088607976160 2.5806095339391044 0.6943823584301260

Pt -3.9496323057336111 -1.7691552214532948 1.3353821750197890

Pt -4.0479643063441069 0.3518141273111228 -0.2213444570918740

Pt -4.0345105702648905 2.5052446549571696 -1.7595799361168483

Ru -0.0647646810611665 -1.8197484954903533 -0.9085215237074648

Ru 0.0202753067416404 2.5597830243483113 0.6152332288685584

Ru 0.0255447034817583 -3.9204068666652603 -3.7788465533077771

Ru 0.0364619106684142 0.4218408045159964 2.1041851034628771

Ru -0.0809209978423572 0.3808388564935398 -2.4989065308547915

Ru -0.0068444290021121 4.6659812932754257 -1.0142675157590515

Ru 0.0674969850264965 -3.8384542731693561 0.6226691139154470

Ru -0.0298618836833216 -1.6980620542413396 -5.4014430900852144

Ru -0.0741389817350143 2.5054707478013363 -3.9554284780340203

Ru 0.0956505749823670 -1.7602516123484016 3.6049873195327735

Ru 1.2873543413350450 4.5731107494864895 -3.2345948815603904

Ru 1.2708730022932377 0.3537649846304251 -4.6407416223942759

Ru 1.3109748384681124 0.4646878359869875 -0.1493809523748254

Ru -1.2598518863934789 0.3652111837596725 -0.1878925796641980

Ru -1.3015786132812541 -1.7282722256216023 1.3658603424768876

Ru 1.3472464758333913 4.7025296707237265 1.1841767143316471

Ru 1.2350333667065365 2.5614931889222978 -1.6780320374121225

Ru -1.2603726230009022 -3.8511488554201723 -1.6624235713739919

Ru 1.3219861916531821 2.5574317636708530 2.7904412212804903

Ru 1.3421037385035999 -3.8001673875646791 -1.6047000409548182

Ru 1.3302910709727749 -1.6970458069441421 1.3593953729530814

Ru 1.4001330874950950 0.3271491929480561 4.2816877608277322

Ru -1.3304621386364597 0.3183663930627632 -4.6405111674810291

Ru 1.2245372876866834 -1.7924044586125234 -3.2393104246536435

Ru -1.2698030302834480 4.6122845126921526 -3.2585869073787217

Ru -1.3798173371287943 2.4857073631586397 -1.7618538733312124

Ru 1.5762568871857257 -3.8412660504453688 2.9118033386252655

Ru -1.3079935430910268 -1.8261854358378129 -3.1989579592174882

Ru 2.5344507350250427 2.5023583156488280 -3.9277815610244322

Ru 2.5628801535790027 4.5960065141612576 -1.0308382981629924

Ru 2.5985287460676045 -3.8210307283424232 0.7082739162001304

Ru -2.5918430939298607 2.4768253064569699 -3.9585160085069764

Ru 2.6363649883646061 -1.7379570104210598 3.5352387343179470

Ru 2.5685652238290024 2.5753218611809787 0.6077683936795834

Ru 2.5740718580574358 0.3262528030511356 -2.4340816007291961

Ru -2.6126147587635180 -1.8002414856748474 -0.9366218663353995

Ru 2.6275346375532300 -1.7011873611431030 -0.8977344057678668

Ru 2.6131236419819928 0.4631447115827079 2.0843564649670272

Ru -2.6428026126890525 0.3432017217137981 -2.4731499985639367

Ru 3.8195472976476181 2.5534672927127406 -1.7827723451823350

Ru 3.8534350284666949 0.4551966211718714 -0.2373789465182854

Ru 3.9092105277041678 -1.6725444748528553 1.2929405356986443

S9.38 $CO_2/Pt_{42}Ru_{13}$ (linear OCO angle)

C -3.5246790358750375 4.0208071744171558 -4.6715536004303928

O -3.1679722748308756 4.9931759965508817 -4.1213984939352555

O -3.8840200218447904 3.0527633382982380 -5.2288051626530754

Ru 0.1923973780410217 -0.2198737477308464 0.2550730286439004

Ru 0.1895783800433772 1.0875312103662673 2.3670805275504572

Ru 0.1961109901275861 1.0841597337232400 -1.8549891409935162

Ru 0.1846336657116434 -1.5223349764818916 2.3635323938296002

Ru 0.1945678019837873 -1.5256246504677038 -1.8592694924403332

Ru 1.5012345852954148 1.8922171517918291 0.2561778040384674

Ru -1.1078915287362698 1.8923633633688415 0.2544397750659030

Ru 1.4922084504095836 -2.3313054780149098 0.2530228830973333

Ru -1.1180346574214060 -2.3312640737084487 0.2510585920724137

Ru 2.2993511785751943 -0.2192652525675675 1.5599577179532800

Ru 2.3053347545158904 -0.2201250457319769 -1.0501525770370206

Ru -1.9226500717149972 -0.2172862491298876 1.5572164487298026

Ru -1.9151235554057719 -0.2200083875082292 -1.0521004953443582

Pt -4.0948236352653584 -0.2180732197082856 -2.4006434088342501

Pt 0.1898753883010459 2.4420787680942122 4.5623402656070002

Pt 0.2073196643365901 2.4328832078492888 -4.0358904390490427

Pt 0.1766098122362794 -2.8723147845569494 4.5447850052668928

Pt 0.1976449602446958 -2.8835918366515321 -4.0526725100819601

Pt 2.8618924510115731 4.0870455097280445 0.2626979250526454

Pt -2.4523498458203608 4.0759371280466823 0.2571854127070691

Pt 2.8375975493752050 -4.5132914559144748 0.2540020578604438

Pt -2.4778396948169288 -4.5248229087910978 0.2499732604041174

Pt 4.4778609530745683 -0.2218447810647549 2.9112214132557508

Pt 4.5030501545943302 -0.2206594923915827 -2.4008427611182586

Pt -4.1176709824604067 -0.2143193396991970 2.9126464255728530

Pt 0.2047356931181451 4.2808140183428893 0.2606856926754100

Pt 0.1810204697226772 -4.7198692818191823 0.2530747943767500

Pt -4.3076931774381748 -0.2155373065722653 0.2544514350361896

Pt 4.6908392763412508 -0.2212515253310553 0.2564184297159397

Pt 0.2040301816816983 -0.2239333106592899 -4.2455920225307233

Pt 0.1839999468055866 -0.2169572621765025 4.7534091106111527

Pt 1.5704534415819524 -3.8613106373164663 2.5032968107866780

Pt -1.2124960886521305 -3.8586334167075562 2.4981094495462783

Pt 1.5804110755988434 -3.8605784490542292 -1.9991072805038739

Pt -1.1992636979571079 -3.8603026308193109 -1.9974637819671774

Pt 3.8325772688701591 -2.4683485352194268 -1.1346283359486602

Pt 3.8256401495964196 -2.4713847610599737 1.6473604954052052

Pt -3.4488458826165069 -2.4706129747370285 -1.1398487712563448

Pt -3.4553160059700536 -2.4646241776962605 1.6396150005464256

Pt 1.5956570183176491 3.4218192273122630 -1.9877153469010183

Pt 1.5855104309054970 3.4190109778921909 2.5090038340616534

Pt -1.1848646533478155 3.4227171898433451 -1.9914234767847243

Pt -1.1929720282638987 3.4230865008031865 2.5086264560654152

Pt -2.0445008014643373 1.1659725492944597 -3.3857400051326350

Pt 2.4540704074552346 1.1681455938750820 -3.3820271795204508

Pt -2.0510755647949672 -1.6131359982368463 -3.3898866053938361

Pt 2.4482016504496564 -1.6121202767597307 -3.3830693200168831

Pt -3.4467680850638103 2.0326371903056208 1.6456077424182611

Pt -3.4421305371531972 2.0334148272988473 -1.1357325736105688

Pt -2.0695859737664066 -1.6050824537141115 3.8906172563188144

Pt 2.4314653875824113 -1.6131523359440556 3.8958604486864132

Pt 2.4345187317509853 1.1697953289231495 3.8992387211279222

Pt -2.0610809451026322 1.1738551257413921 3.8928796698204473

Pt 3.8370845378749450 2.0293132077519327 -1.1292351819070325

Pt 3.8321649602523444 2.0312966943235877 1.6491216794844989

S9.39 $CO_2/Pt_{42}Ru_{13}$ (bent OCO angle)

C -5.5295592357259276 -1.4726828183649769 -2.6861634069546656

O -5.3475472367647265 -2.5978890331143236 -2.1805408741473618

O -6.3621544884431378 -0.8561506168177172 -3.3330967999551251

Ru 0.3082285268243372 0.0877989313112800 0.1456494051464655

Ru 0.3046907996344559 1.3994090827352526 2.2488685054525850

Ru 0.2907975210792789 1.3936384845617065 -1.9720361541747653

Ru 0.3147648285560143 -1.2118803384851811 2.2466910500328798

Ru 0.2989027144862498 -1.2162349946337896 -1.9696262289180186

Ru 1.6021402153604323 2.2064263539941638 0.1312443771091757

Ru -1.0049912176235956 2.1996932956724686 0.1399667294816679

Ru 1.6072557278219055 -2.0145018240574224 0.1430674915832778

Ru -1.0354948706167590 -2.0168263315267869 0.1214273562109361

Ru 2.4188578310817093 0.1054129860517219 1.4356553716657963

Ru 2.4066279995200399 0.0941832533144412 -1.1746562498661004

Ru -1.8018125017053179 0.0882418590422670 1.4539742708929617

Ru -1.8156497368643045 0.0808300064352471 -1.1570204390175962

Pt -4.0514490977110009 -0.0139538482243054 -2.4821594820649926

Pt 0.3252269973554943 2.7706091317053168 4.4454817716599635

Pt 0.2984558819267856 2.7384611229500582 -4.1539527451369107

Pt 0.3496836983675737 -2.5423455421525780 4.4499492561290426

Pt 0.3257718808646902 -2.5873336841216767 -4.1507907612878689

Pt 2.9601139774264715 4.4145328921246856 0.1245890028567690

Pt -2.3479651458382480 4.3812822203912933 0.1512202327987780

Pt 2.9911560665397472 -4.1832900802074287 0.1505427806837503

Pt -2.3093542099497038 -4.2680247334777244 0.2010255911670270

Pt 4.6069091809775591 0.1217114601456034 2.7788319544728863

Pt 4.6113430109260394 0.1062721052647172 -2.5275999666622293

Pt -3.9688349708761717 0.0851550936064918 2.8495620345791157

Pt 0.3019211534338438 4.5910690782788075 0.1327367293764939

Pt 0.3460872660483487 -4.4063702457680138 0.1647233623757530

Pt -4.1844919145077091 0.0905909327986084 0.2031989466424397

Pt 4.8108111204918105 0.1163946017946385 0.1264889622027602

Pt 0.3009204295232225 0.0796678225081690 -4.3544619915633058

Pt 0.3350572487017765 0.1153752724767939 4.6467446324360582

Pt 1.7357029366588543 -3.5306332719229543 2.4041522948672442

Pt -1.0383240339463242 -3.5447146769279771 2.4221617118276817

Pt 1.7188110773762098 -3.5475810308238023 -2.0971737426027524

Pt -1.0473755951262200 -3.5840546050495008 -2.0831262269011153

Pt 3.9622082865543926 -2.1372479748364741 -1.2525791021394159

Pt 3.9699676479834838 -2.1304259415354667 1.5253923054654352

Pt -3.3018688497190078 -2.2302027144456984 -1.1810927433881444

Pt -3.3024567314889333 -2.1810509289773332 1.5930387863056741

Pt 1.6818278120175953 3.7327131631225354 -2.1111080098742727

Pt 1.6991907820763716 3.7407805777264009 2.3758360069395814

Pt -1.1119677588993284 3.7133208960189807 -2.1134531893270845

Pt -1.0841760111956136 3.7286318406494732 2.4029335872602435

Pt -1.9692847638709812 1.4462529690465540 -3.4762966036379837

Pt 2.5492595771102864 1.4713208850248534 -3.5060832059589919

Pt -1.9208953006108744 -1.3216588514586549 -3.4933699395216000

Pt 2.5669780500814987 -1.2990139325931440 -3.4996147341115820

Pt -3.3270684990139348 2.3365690949030506 1.5545239670754953

Pt -3.3437165239949653 2.3035597569463873 -1.2381556833726535

Pt -1.9066333312512664 -1.2938625320025747 3.8083697120192923

Pt 2.5822746604045994 -1.2703301947497341 3.7810087304182574

Pt 2.5681298220158641 1.5095803684159046 3.7726070146732416

Pt -1.9185322551536312 1.4909503577435248 3.8050540978495762

Pt 3.9344112742400998 2.3525153754448045 -1.2577209306670154

Pt 3.9471182774306373 2.3653094740690372 1.5151611815932400

S9.40 CO_2/Rh_{55} (linear OCO angle)

C -4.4367125862910211 -2.0607109793601146 -4.0197005852132852

O -3.8708424922833626 -2.9798558960714430 -4.4783635996648403

O -5.0202854031806536 -1.1456444302012649 -3.5725164447903448

Rh 0.2523932034354895 0.2056126468961804 2.5498044954703056

Rh 1.5337993018486853 0.1835413929589107 0.2706505656750866

Rh -2.3345003328006837 -1.9170351647611275 4.0869103636930708

Rh -3.6721972850730662 -1.9194087111818414 1.8441454639216919

Rh 0.2382013418869880 2.3200587304861711 1.0205535264123287

Rh 2.8685880494501363 -1.8974377158963607 4.0649720702019350

Rh -1.0738909759563060 2.3946245239725408 3.3195729254774369

Rh 2.9382166405527776 -1.9624578918881588 -0.5188702484125765

Rh -1.0531690450825435 0.2128814028979796 4.8077216393097304

Rh 1.5802518953582598 -1.9323492930832187 1.7933577707967963

Rh 2.9138566751739239 2.3573253844417965 1.0740409133280580

Rh 1.5809992965138946 0.2216204980022450 4.7935970777120849

Rh -2.3414011310366818 -4.0804816408859415 1.0883876166617144

Rh 4.1746202840780215 0.2059141258476170 0.2585996577755204

Rh 0.2145918219218149 2.3338582051914663 -3.5692645177618090

Rh 2.8649629979817690 -4.0620934810576044 1.0666643459346059

Rh -2.4577859828533795 0.1168606999516734 -2.0067525212128214

Rh 1.5460223958975015 0.1857177799527431 -4.2442527456823180

Rh -1.0659985061770034 -1.9410487180589799 1.8053761962884460

Rh -1.1328211305608646 -2.0057614108065396 -2.7527572905420277

Rh -1.1010076979763603 0.1755825685279876 -4.2345294077235618

Rh -2.4255291756411408 0.2462875301415561 2.5904033284427661

Rh 0.2309921070225466 0.1675433551149795 -1.9912070126614980

Rh -2.3864412889000173 2.2798915822602237 -3.4875327967377339

Rh 0.2624659365618934 -4.1563060786962591 1.1075135126742428

Rh 4.1614371227266780 2.3399830416527707 -1.2576867047596896

Rh 0.2285815492389967 -1.8903083280044533 -4.9194453316758739

Rh 2.9318300735830065 0.2652302016826839 2.5643597861988794

Rh -1.1047158293819321 2.2940324320151384 -1.2292910118448777

Rh 2.8191728906795728 2.2999145662767031 -3.5088922248920942

Rh 1.5744969642289477 2.4046966429723367 3.3059846424017345

Rh -3.7089341276660543 2.3120911782268463 -1.2214170747578559

Rh 1.5515859662317038 4.4523094572138708 1.7516281859765079

Rh 4.1868094439369408 -1.8899679334704544 1.8103635555495845

Rh 1.6185974348246961 -1.9980396659350699 -2.7672133116998379

Rh -1.0839416268492958 4.4421252415211496 1.7659605803641421

Rh -1.0505728648589137 0.1751529497619779 0.2825354777163633

Rh 0.2418737876908586 -4.0921631941853551 -3.3325420968819888

Rh 0.2221547849405684 4.5214732570394105 -0.4966971476836648

Rh -2.4372774963556627 2.3379884446832753 1.0994435556014002

Rh 1.5577489654300263 2.3026532847671031 -1.2429916020028722

Rh -2.3890621427857601 4.4262597211590426 -0.5028310441563579

Rh 0.2467801893681934 -1.9603269935194902 -0.4668754609980155

Rh 2.9209340811306310 0.1336618921625064 -2.0293080939458346

Rh 2.8316828141534391 4.4469216970916907 -0.5296835235752009

Rh 1.5825649065691429 -4.0827698902336120 -1.1693736008255440

Rh 1.6021735432563116 -4.0428475159385302 3.3359461338580383

Rh -1.1058192342120985 4.4247316315256526 -2.7480880549538824

Rh -2.4453743780644763 -1.9830157375649751 -0.4953881450840061

Rh -1.0615823087380756 -4.0524481056187112 3.3472285294739574

Rh 1.5247665382800126 4.4337927296172417 -2.7621424978684286

Rh -3.6895525910592606 0.1767329460003712 0.2951226703422175

Rh 0.2662628498674444 -1.9390586685511801 4.1416732994026555

Rh 0.2615603783664858 2.2862739918091677 5.4702854108772225

Rh -1.0815605984027439 -4.0918082888523220 -1.1571891995296826

S9.41 CO_2/Rh_{55} (bent OCO angle)

C 4.4886307747705985 -2.0940468172316327 3.8323884174931622

O 4.7104070987960895 -2.1804539655702624 5.0292805995448022

O 5.2245245779965828 -2.0898116870364700 2.7790233945569143

Rh -0.2342391315620848 0.2030222224842576 2.1241589293869567

Rh 1.0210485046818998 0.1934452677582926 -0.1712521317524587

Rh -2.8482049979859241 -1.9124704317883612 3.6688024436659687

Rh -4.1778745537126554 -1.9328722336144366 1.4461877371229750

Rh -0.2667263790716565 2.3211919518502175 0.5864878421552281

Rh 2.4963378981107027 -1.9136811839368562 3.5649704816557404

Rh -1.5479448225726320 2.3900674493129261 2.9028712027119341

Rh 2.4379648501017499 -1.9510885251014087 -0.9323398242128330

Rh -1.5175177756490119 0.1911812220967690 4.3887896383464158

Rh 1.1066950897582042 -1.9052210441339212 1.3861149356585247

Rh 2.4134196835008410 2.3633874341804604 0.6164064364489822

Rh 1.1197417887524277 0.2038325823997866 4.3493251301758793

Rh -2.8554384845858465 -4.0696858814170414 0.6759213829890446

Rh 3.6722259062059521 0.2151524471010291 -0.2180763206045963

Rh -0.3128304063420448 2.3463261593681497 -4.0142379749821240

Rh 2.3510012518403585 -4.0472016268312219 0.6000700882416358

Rh -2.9854287592524713 0.1084850803979010 -2.4179093473077429

Rh 0.9978832025143727 0.1935702839338405 -4.6897785927654008

Rh -1.5707657410607188 -1.9240682414819588 1.3877686407554766

Rh -1.6766946260530422 -2.0079413514009556 -3.1739086440333053

Rh -1.6472302791774571 0.1840508612691238 -4.6501712285867720

Rh -2.9341667221319128 0.2371782554151480 2.1785915087961372

Rh -0.2949938864535970 0.1719629856564808 -2.4267612104526193

Rh -2.9177110860974835 2.2881042650777164 -3.8977186556087928

Rh -0.2304824060467045 -4.1278213059166804 0.6804974155600494

Rh 3.6339812108056719 2.3412317399804725 -1.7251873581364461

Rh -0.3259293470194256 -1.8997548882353399 -5.3478706080203304

Rh 2.4513623813577041 0.2753513064913521 2.1045128230260191

Rh -1.6213949351608012 2.2975155857851779 -1.6533517150780750

Rh 2.2998325111149427 2.2987758657493020 -3.9662976389529958

Rh 1.0983243229863784 2.3942864836307467 2.8701079782426775

Rh -4.2126182700903385 2.3203245484637693 -1.6358626909691563

Rh 1.0526082209966883 4.4459897012060949 1.3308532686166632

Rh 3.7835434339860825 -1.8747103232360629 1.3190735268026745

Rh 1.0764183639320204 -1.9826960861465082 -3.2275356145077239

Rh -1.5863410071224924 4.4355271691820617 1.3428123922776283

Rh -1.5559563670328278 0.1820970616469425 -0.1392694616371567

Rh -0.2907463548549747 -4.0846538799472656 -3.7603185255908200

Rh -0.2766035888877458 4.5284919925245957 -0.9171601033259843

Rh -2.9399290896695334 2.3291216535668116 0.6961487612399839

Rh 1.0364823617359700 2.3125866517945783 -1.6912519812149338

Rh -2.9065533613377141 4.4255430525900961 -0.9098204970920928

Rh -0.2555267037847462 -1.9530462539712701 -0.8907647569777107

Rh 2.3851065709178627 0.1313763510307170 -2.4798336613657468

Rh 2.3290126775614723 4.4568311450600460 -0.9683520533678244

Rh 1.0731210562045415 -4.0651134838867522 -1.6158591333513581

Rh 1.0768857549068325 -4.0445804274520727 2.8971687481996100

Rh -1.6219468998580386 4.4308057676504546 -3.1589067597413290

Rh -2.9510699259493549 -1.9750220778245520 -0.9047876620530612

Rh -1.5572195984276935 -4.0407666667100175 2.9323978437219922

Rh 0.9949249316056021 4.4425435214972069 -3.1925854132302844

Rh -4.2029978077108936 0.1867642360217375 -0.1153811471733742

Rh -0.2159934891884139 -1.9453958326817300 3.7210603544619603

Rh -0.2081465735499042 2.2648960895507488 5.0443166727194368

Rh -1.5842610477414074 -4.0889141761722216 -1.5635578824814342

S9.42 $CO_2/Pt_{13}Rh_{42}$ (linear OCO angle)

C 0.3634628089635943 -3.0203921769463236 6.7214167363153834

O 1.5320187404714474 -2.9122660058062633 6.7009529523906597

O -0.8018652565528968 -3.1420374185462285 6.7754478739363302

Pt -0.0258894379016045 -4.0487520581268530 -3.9845748883618075

Pt -0.0290483483440291 2.3569868443649389 4.9632339492396760

Pt -0.0210584825470256 -1.9387983995964140 3.6444485868278091

Pt 1.2713273141912289 4.5343500717942300 -3.3542212260373288

Pt 1.3458402662995865 0.2479828127059548 -4.8987503184126089

Pt 1.3204538821368244 4.5579379595502152 1.2248454013826464

Pt 2.6371010798743466 -4.0405689844300428 0.4655580877211301

Pt -2.6724057163193922 4.5336784095028557 -1.0280069861790913

Pt -2.6711228326727503 2.3137176501835945 -4.1406770095986420

Pt -2.7807653776022674 0.3159200277523478 2.0176657833546305

Pt -2.7940319549990318 -1.9640586348387612 -1.1247496812415432

Pt 2.7736509810119272 0.3293893263683235 2.0387895179478148

Pt 4.0014786533621738 2.3631719970203831 -1.8365103886107508

Rh -0.0123170643558596 -1.9069568042883289 -1.0590432849213731

Rh -0.0335284055774205 2.3770126633814033 0.4204083486964859

Rh -0.0035687835372217 0.2484079066900847 1.9570123823684926

Rh -0.0368038299929147 0.2238687571583882 -2.5729202078151876

Rh -0.0138420291945491 4.6150583864269237 -1.0616134194864841

Rh -0.0210741773188634 -4.1030086137875177 0.5133693825301132

Rh -0.0523042889664755 -1.8566959679243764 -5.5204311258800765

Rh -0.0160635118421038 2.4177261077997447 -4.1986300859333134

Rh -1.3469006345140584 0.2554827525200921 4.2323850823849130

Rh -1.3520587224245091 -4.0213720052448387 2.7525752815679017

Rh 1.2789930624422023 0.2550036814975427 -0.3252463337551077

Rh -1.3050619880628607 0.2471993261942613 -0.3163192998241577

Rh -1.3534759518664947 2.4215564008389925 2.7235273915135201

Rh -1.3434270073026440 -1.8950512993142152 1.2090857790854899

Rh 1.3077579383291993 2.3792127479277756 -1.8429388331104684

Rh -1.3276858900382655 4.5030476833040156 1.2110229665752263

Rh -1.3437725265318663 -4.0768704344401163 -1.7430723914996444

Rh 1.3120331041004523 2.4343507705986203 2.7301129078741888

Rh 1.3188812409782429 -4.0584138129564682 -1.7741361739079138

Rh 1.3168938462257618 -1.8706503506022152 1.2045454723741167

Rh 1.3057857872506244 0.2656887140496473 4.2413132818819586

Rh -1.3336258046211131 0.2153720679189010 -4.8320058212270203

Rh 1.3697348546157233 -1.9385947153651384 -3.3501248764889739

Rh -1.3167778201220055 4.4598012314188473 -3.3187772158745683

Rh -1.3637847561423606 2.3737689496512449 -1.8379780523289750

Rh 1.2987961352509851 -3.9951896701940659 2.7369258026677312

Rh -1.4227326126375446 -1.9418593918939742 -3.3542677065577280

Rh -2.6406508901203991 -1.8717202845605629 3.4810823719797495

Rh 2.5916353445960887 2.3461021608293526 -4.0872937013646800

Rh -2.6235815244506848 -4.0278204790231138 0.5188172249836314

Rh 2.5959741463325749 4.4937394037320555 -1.0608588077583851

Rh 2.5926269131062862 -1.8517632109913471 3.4872170645235738

Rh 2.6480185205506523 2.4284250292599285 0.4908186464641366

Rh 2.6505440945467869 0.1726545382756574 -2.6031438942449019

Rh -2.7051308002771166 2.4143091189390620 0.4986926991532308

Rh 2.6908744428058440 -1.9138729265887888 -1.1049759158648413

Rh -2.7123520332151982 0.1574241505387404 -2.6102460689606750

Rh -3.9710231795721413 -1.8764610281409522 1.2442466465065198

Rh -3.9691708445056202 0.2681204812212513 -0.3348058958447249

Rh 3.9290205027402831 0.2493327601977847 -0.3265257351147128

Rh 3.9401763989142142 -1.8422597864356516 1.2178382783395341

Rh -3.9761775749677648 2.3396335704294033 -1.8205105543809101

S9.43 $CO_2/Pt_{13}Rh_{42}$ (bent OCO angle)

C -2.8451979988885454 -5.5280616862799326 2.0010103997480013

O -3.6853629509569070 -6.1656900296377097 1.3871408277271509

O -2.2403171688234989 -5.6421446988073436 3.1216682028265188

Pt 0.1278097001201720 -3.9204563199122617 -3.7076486211003350

Pt 0.1768806947942661 2.5559962732396122 5.1896445308496295

Pt 0.1961142999115520 -1.7782652341713376 3.9005156160010483

Pt 1.4074320708689729 4.6660842905847835 -3.1476671455928753

Pt 1.5000098274099269 0.3665059956282926 -4.6723783306149400

Pt 1.5062186654009055 4.7425416122739659 1.4290342065565393

Pt 2.8550697459046517 -3.8700524178674240 0.7169907617468271

Pt -2.5154453273344441 4.6632924324677818 -0.7916314264642513

Pt -2.5213583801870074 2.4358031105534184 -3.8861274209542054

Pt -2.5841881460861158 0.4664929287273619 2.2882387341118049

Pt -2.6310905006414993 -1.8332458774347455 -0.8370358291847405

Pt 2.9650472599153193 0.5111330642978570 2.2529027442426961

Pt 4.1580221463670943 2.5230565055548340 -1.6427005204260607

Rh 0.1552588671723401 -1.7616354324994572 -0.7935173266345633

Rh 0.1345624727665731 2.5263085121429456 0.6540189849149027

Rh 0.2042311573931957 0.4069135542707033 2.2074586211924703

Rh 0.1203436854346632 0.3610960723058428 -2.3287684999374618

Rh 0.1419007488799787 4.7583198701876563 -0.8313426175083186

Rh 0.2032040412054162 -3.9526921242452482 0.7927993372914385

Rh 0.0778447215457426 -1.7372767550355035 -5.2597911245413353

Rh 0.1355919137110564 2.5287904811454891 -3.9604161520579830

Rh -1.1043927361276036 0.4298231149820849 4.4906441590458641

Rh -1.1171660698073422 -3.8910996637092952 3.1144889745193356

Rh 1.4479076334455758 0.4048618611151202 -0.0920347266872155

Rh -1.1388990854444909 0.3820582169489286 -0.0588636076602038

Rh -1.1580838138535738 2.5844734782814642 2.9646848499808387

Rh -1.1533304168415768 -1.7692689772044621 1.4922691123896739

Rh 1.4584219817902460 2.5205105745012459 -1.6155948257637724

Rh -1.1469410552495525 4.6584429889808581 1.4423889716833527

Rh -1.1640055149961990 -3.9491247644185474 -1.4413755212902395

Rh 1.5032863626483022 2.6280009871200618 2.9424410591651373

Rh 1.4788272319878875 -3.9137230268200249 -1.4984864793528068

Rh 1.5151347469619334 -1.7129002101073638 1.4493293873227922

Rh 1.5400916151105042 0.4775469594184331 4.4759367035845097

Rh -1.1827493096514949 0.3436142096481367 -4.5932282245366221

Rh 1.5209416044087689 -1.8083453232159137 -3.1043031205834350

Rh -1.1718176579434934 4.5955649132974798 -3.0830251218739115

Rh -1.2091563899532716 2.5044909027506739 -1.5934743857273508

Rh 1.5463813504942534 -3.8103597578566557 3.0079403724125537

Rh -1.2591995540913690 -1.8151916342595205 -3.0756921863842881

Rh -2.4066106856882614 -1.6743987366046360 3.7743248398102414

Rh 2.7386752844444731 2.4760985908835509 -3.8732515886973524

Rh -2.4079978511446685 -3.9090141553428479 0.8838812041414176

Rh 2.7598025873182062 4.6515690866259325 -0.8763706389680662

Rh 2.8129212950541111 -1.6489835861879119 3.7149598489902314

Rh 2.8075311072702096 2.5963085006880786 0.6962355016068646

Rh 2.8055513006243631 0.3110407844417808 -2.3816858490524955

Rh -2.5159855574115562 2.5557709689913235 0.7563617185204898

Rh 2.8658591803940352 -1.7640553670823329 -0.8744483153807884

Rh -2.5502351465361692 0.2920647697276776 -2.3583643998941697

Rh -3.7923129126804751 -1.6986454205890831 1.5311410178391600

Rh -3.7874346951957922 0.3977332851509265 -0.0638373159579684

Rh 4.0990552678336298 0.4179954548835920 -0.1177301047621541

Rh 4.1446255727749852 -1.6594996732064646 1.4346649427030700

Rh -3.8212772158284021 2.4738265206781285 -1.5523242033346489

S9.44 $CO_2/Pt_{42}Rh_{13}$ (linear OCO angle)

C -2.1248813815132346 -0.1360237816766545 -6.8247860748036882

O -2.6958953178468210 -1.1430579751758112 -6.6347706089741694

O -1.5594950785535930 0.8708304852868732 -7.0308085535883169

Rh 0.1202097927194316 0.0082472800031720 0.3464498121642671

Rh 0.1274260656606223 1.3102532597887835 2.5015369708821114

Rh 0.1154344700196634 1.3403123080003587 -1.7878270743991656

Rh 0.1282597047475363 -1.3277164948304847 2.4807066404127185

Rh 0.1194992690459788 -1.2901874488279634 -1.8100905842845385

Rh 1.4292592456993307 2.1439440418923748 0.3407324341074289

Rh -1.1973777791794280 2.1400299339426736 0.3508448373254778

Rh 1.4394788875551603 -2.1231846687046043 0.3086129396495932

Rh -1.1911808680636757 -2.1283544457581307 0.3187450709187931

Rh 2.2641628219660572 -0.0012916895800256 1.6509401531586858

Rh 2.2505721883223400 0.0193597060997820 -0.9893409588045334

Rh -2.0155323649378851 -0.0026122799445209 1.6778111429890683

Rh -2.0104119890289835 0.0096283598365150 -0.9782669752321984

Pt -4.2019251364484829 0.0240432829339372 -2.2472261086111147

Pt 0.1338525178524656 2.6221136382725287 4.6857443101460250

Pt 0.0902735019714977 2.7068676273005505 -3.9024070843430163

Pt 0.1313253282565523 -2.6680718938911734 4.6481837400141135

Pt 0.0911525065303380 -2.6347460670311866 -3.9361692105745454

Pt 2.7648103737805974 4.3057824313785176 0.4077987519562640

Pt -2.5369114566708837 4.3028591025288128 0.4297433306312929

Pt 2.7665170840179925 -4.2882869149596843 0.3509153008572622

Pt -2.5381656111074866 -4.2891023169643345 0.3709806781253869

Pt 4.4125133106034200 -0.0100131335550106 3.0154930772525059

Pt 4.4129283298423090 0.0280865320405345 -2.2913740673638698

Pt -4.1605509438668049 -0.0121710148471525 3.0489728854984457

Pt 0.1122483908807574 4.5406090984235465 0.4322626244836723

Pt 0.1125030734426889 -4.5236038700147265 0.3741342096803344

Pt -4.4015897218831608 0.0047019942752759 0.4042951584721863

Pt 4.6376818954756072 0.0088974213655181 0.3660363557988731

Pt 0.1015538468120673 0.0375029665123579 -4.1678642275278373

Pt 0.1293337316284875 -0.0244836184487522 4.8991098439291605

Pt 1.5173340792761456 -3.6561118158062635 2.6093846925205630

Pt -1.2741853551466806 -3.6526189974616110 2.6218707280830387

Pt 1.5044382941598524 -3.6464883924002724 -1.9016726477294668

Pt -1.2971815178702735 -3.6435384505984727 -1.8892491782718381

Pt 3.7821145794180371 -2.2487196307098403 -1.0385052735341107

Pt 3.7778513677077776 -2.2645745376967521 1.7551380132357650

Pt -3.5644509235858619 -2.2503851551558611 -1.0007121907704510

Pt -3.5286714010695959 -2.2642461135931948 1.7855922465670242

Pt 1.5044760695594221 3.6913281829788218 -1.8552023967555433

Pt 1.5177957920252485 3.6419485728514207 2.6604819469140359

Pt -1.2960765088662747 3.6889597265535410 -1.8402539404180109

Pt -1.2706967361726571 3.6357275657394204 2.6718051754136569

Pt -2.1774643149046833 1.4379601889260862 -3.2616715353869101

Pt 2.3735258485211945 1.4407790445947155 -3.2939673251595560

Pt -2.1771869865704860 -1.3707719429989511 -3.2818725458823788

Pt 2.3752059948490927 -1.3737322844316295 -3.3137118945706181

Pt -3.5292811905229722 2.2587586869624214 1.8183107813710484

Pt -3.5617265706269516 2.2809465768943924 -0.9693234262836838

Pt -2.1265302630311140 -1.4095188747707559 4.0336049239831357

Pt 2.3820974832628776 -1.4085558739189334 4.0132733708204160

Pt 2.3840129821979286 1.3741369906234908 4.0332585464929540

Pt -2.1259595366674229 1.3717175826893369 4.0552637939549658

Pt 3.7791681323607142 2.2849726122145904 -1.0059234874165470

Pt 3.7743119939662155 2.2608644828424049 1.7849628828758366

S9.45 $CO_2/Pt_{42}Rh_{13}$ (bent OCO angle)

C -4.4500280996712318 -0.6343761162168250 -4.3990764382256540

O -3.5588111188912586 -1.3561207937051978 -4.9383772938773625

O -5.5649105753695967 -0.2433686138356174 -4.6890390146374044

Rh 0.2252492839722150 0.0302423234813946 0.2359947090173043

Rh 0.2395531396105435 1.3095183593634463 2.4025914018214025

Rh 0.2595595089980282 1.4010784897711186 -1.8619966951308873

Rh 0.1878798281582941 -1.3307196008622868 2.3513212957790772

Rh 0.1306857316463963 -1.2305002612275096 -1.9525563183200110

Rh 1.5938703051931626 2.1457075665647172 0.2819496839249320

Rh -1.0428472625937044 2.2032616178865210 0.2583889361055059

Rh 1.4973444274300365 -2.1213689721019913 0.1889038214548311

Rh -1.1331587137967889 -2.0793295321833463 0.2047403242820912

Rh 2.3607122384682766 -0.0252643137672505 1.5811327227470453

Rh 2.3626194901697652 -0.0130239170545411 -1.0628142265999474

Rh -1.9244909454478651 0.0611940910801777 1.5493964932758486

Rh -1.9183180565777167 0.1037225438019738 -1.0877174878286786

Pt -4.0187623335710345 0.1398855206452919 -2.5323021655448330

Pt 0.2448261724263492 2.6199099034961959 4.5879766618185531

Pt 0.3828723636760236 2.7876194719886955 -3.9934042196528763

Pt 0.1505767549366712 -2.6839627936090538 4.5066229162165330

Pt 0.3118733441782237 -2.5672460439690870 -4.0955379176380946

Pt 2.9783392267303310 4.2857401090924929 0.3644527531759790

Pt -2.3160922175811947 4.4088314721883046 0.3112263397044491

Pt 2.8312652122701731 -4.2964715501721011 0.2328686958570448

Pt -2.4803450374760727 -4.2197011741758184 0.1631983711410745

Pt 4.4990501779759358 -0.0770266049657932 2.9640101383206612

Pt 4.5787188457907275 0.0083317116398672 -2.3265434004297392

Pt -4.0799951565151922 0.0775959711076361 2.8797868350020495

Pt 0.3379076401526184 4.5677777510524686 0.3266167688858324

Pt 0.1720579996588425 -4.4830801143964676 0.2000748401920361

Pt -4.2848924659794445 0.1282021905330531 0.1916115185489820

Pt 4.7636969705171621 -0.0305510862428494 0.3217734078911855

Pt 0.3580490864978971 0.1294419212966834 -4.2822940242828249

Pt 0.1938967566003815 -0.0347034384887558 4.7747220197203299

Pt 1.5471427460494878 -3.6835141128891991 2.4788568476922377

Pt -1.2457177795182903 -3.6398697760140508 2.4521757900400765

Pt 1.6226333212465225 -3.5969730413735270 -2.0187560129361426

Pt -1.1665709947801970 -3.5870661923127845 -2.0788921092020320

Pt 3.9072405688283243 -2.2555336309152096 -1.0994195487056622

Pt 3.8337262955326494 -2.2994473949476868 1.6716559297510820

Pt -3.4491420016673713 -2.1447403730074113 -1.1981013458282141

Pt -3.4759454216834129 -2.1783247694787091 1.5816224851652885

Pt 1.7454530867687836 3.7271128054785225 -1.9208844498557329

Pt 1.6816024701710899 3.6253440204268381 2.5878329232808506

Pt -1.0414347905516428 3.7961552940876309 -1.9581265136990511

Pt -1.1025617336534452 3.6809833369364084 2.5582049649331284

Pt -1.9076469372640235 1.5916556021641082 -3.3933971859131962

Pt 2.5928583011864292 1.4657012545642505 -3.3261340632115246

Pt -1.9417180758255046 -1.2857450102271428 -3.5042751410332498

Pt 2.5456070170466916 -1.3354062013123857 -3.3676539843625477

Pt -3.3873405925198328 2.3551848986022894 1.6582388608216265

Pt -3.3379912010216839 2.3906501372238020 -1.1341824660326758

Pt -2.0766533966109222 -1.3831432079527273 3.8617034190728514

Pt 2.4294139840838502 -1.4480554389896283 3.9170961923622576

Pt 2.4867391915479988 1.3345965104988344 3.9661206167679435

Pt -2.0254266719037348 1.4150308570751784 3.9112702200709371

Pt 3.9559623442475074 2.2586449442172674 -1.0465275896546575

Pt 3.9218177487037709 2.2155134001297903 1.7438707077619748

S9.46 CO_2/Pd_{55} (linear OCO angle)

C -4.3666644352597475 -2.0366230871935271 -4.0904553468618658

O -3.8360415637478509 -2.9765257449364966 -4.5486298563943279

O -4.9144761708581681 -1.0996452595638089 -3.6429543417853392

Pd 0.2463840732645455 0.2102108891803796 2.6306440628789884

Pd 1.5987837002976510 0.1818663857542258 0.2772527541040073

Pd -2.4248624457690786 -1.9602206200832941 4.1999615349950448

Pd -3.7954822064639027 -1.9859375406243376 1.8682216516389472

Pd 0.2256218649524309 2.3805258320496789 1.0516012355695821

Pd 2.9452733208951205 -1.9345813221404717 4.1791938265297333

Pd -1.1728802387975525 2.4459317210188760 3.4062790593018306

Pd 3.0610462992060441 -2.0310588039880950 -0.5561959451907869

Pd -1.1356769097346033 0.2197671814244733 4.9683065543210798

Pd 1.6076959091385250 -1.9814166486937466 1.8500042104900041

Pd 3.0136465776343444 2.4164164566554054 1.1175985681826714

Pd 1.6395402473682692 0.2363110369393105 4.9612070327693489

Pd -2.4241314138373324 -4.1958270413698910 1.0739719305803470

Pd 4.3363338882360711 0.2046012555607795 0.2618694613197892

Pd 0.2152400978847054 2.3948571616278405 -3.7143057632433063

Pd 2.9477718626553093 -4.1719949060800632 1.0757770195492797

Pd -2.5775175782258737 0.1105427204270151 -2.0678772607616569

Pd 1.6257097977767971 0.1918457890083105 -4.3969851197606804

Pd -1.0957507920114056 -1.9956284890351550 1.8555601274659297

Pd -1.2176662566486423 -2.0560529568669170 -2.8222717244399487

Pd -1.1654290940847671 0.1762925963186573 -4.3814533075012374

Pd -2.5723917482996024 0.2540446726597607 2.6811790477203967

Pd 0.2356690436782545 0.1464226121578221 -2.0588866589717600

Pd -2.4805020877940764 2.3251142749926683 -3.6051991044580944

Pd 0.2663580808607247 -4.3247422376562268 1.0918134818303897

Pd 4.2756894100029985 2.3904197223803521 -1.2737145879765903

Pd 0.2318042691848499 -1.9434889815767860 -5.0518986936717294

Pd 3.0668904802596098 0.2724160656638133 2.6576516719993366

Pd -1.1436947657548329 2.3556650935857752 -1.2729396237273163

Pd 2.9127802284966409 2.3634627493738951 -3.6175281336023382

Pd 1.6533641641356249 2.4485331089366471 3.3993940831628553

Pd -3.8338949531799011 2.3563150794689931 -1.2519443295072270

Pd 1.5645201570773892 4.5802706720335928 1.8562465043963978

Pd 4.3084177262980896 -1.9478517396485961 1.8382742708593207

Pd 1.7152511550379623 -2.0516712777538078 -2.8471550576341578

Pd -1.1309559307995327 4.5797722837492838 1.8428537431206446

Pd -1.1243659160349599 0.1720838725250675 0.2948990905800455

Pd 0.2469977633738863 -4.1743268367435169 -3.4544249345244609

Pd 0.2092973379501002 4.6663414871719739 -0.5053805597623918

Pd -2.5607350479915683 2.4026260866936977 1.1395391703989295

Pd 1.5823707679556582 2.3616917760752778 -1.2808916611598937

Pd -2.4754653647007734 4.5561056078274280 -0.4910748771992514

Pd 0.2516250445621955 -2.0336386470827779 -0.4870294547485391

Pd 3.0498092963846064 0.1263540442712184 -2.1082663176591510

Pd 2.8897798919775255 4.5747278458931682 -0.4872090278118223

Pd 1.6575160408988703 -4.2371841015515654 -1.2281038702819755

Pd 1.6206738689038422 -4.1450547427241657 3.4182626986626712

Pd -1.1486068232519324 4.5352483811523596 -2.8244995182425559

Pd -2.5702004496863671 -2.0527258186652761 -0.5354685423144564

Pd -1.0877731513350577 -4.1508019470972881 3.4158169728850085

Pd 1.5574057407465789 4.5507598685621540 -2.8192639324242297

Pd -3.8650473328923445 0.1822494406523867 0.3104855747022882

Pd 0.2626246605079006 -1.9991832804852989 4.3071003676922555

Pd 0.2383419378536820 2.3625895547589235 5.6141391718990326

Pd -1.1400220282969338 -4.2462012949900947 -1.2230973279890593

S9.47 CO_2/Pd_{55} (bent OCO angle)

C 1.1710356461324944 4.0110774139034895 4.0292846215897153

O 1.4887803862149762 5.0306694339868283 3.3704860100739773

O 0.7999007377399675 3.8935221605476733 5.2241887481154468

Pd -0.0661144801928643 -0.0927257671217297 2.1741278926695142

Pd 1.2922255627081056 -0.1290685940965982 -0.1683693430769410

Pd -2.7339943604348140 -2.3710836796231285 3.7395301954835518

Pd -4.0786381713164355 -2.4080823058377363 1.4086590536336987

Pd -0.0906876613900018 2.0526703456708684 0.5769106971381420

Pd 2.6768501117827728 -2.1918621670391834 3.7469738234277803

Pd -1.5851478071191143 2.0642227981691206 2.9324891016582728

Pd 2.8040082680114389 -2.3271493137958861 -0.9738292980707698

Pd -1.4628840923547792 -0.1431670747495224 4.5131661922591384

Pd 1.3320528195553778 -2.2726754785818959 1.4075582059939304

Pd 2.6529453590065102 2.1805628679265125 0.6616963957132004

Pd 1.2974748941168364 -0.0727302089401383 4.5063599533827983

Pd -2.6478517160701487 -4.5883927874310508 0.6580826136195451

Pd 4.0135994171824043 -0.0498972986355287 -0.1295322210373989

Pd -0.1078388393108977 2.0165436604707874 -4.1954225111647911

Pd 2.7368663565207689 -4.4489582526830755 0.6704654232533599

Pd -2.8758734902032335 -0.3154129504959545 -2.5404598737241328

Pd 1.3373698380260080 -0.1780324246385068 -4.8389185326660584

Pd -1.3724738995670553 -2.3600448037104127 1.4000637907224116

Pd -1.4831512416599826 -2.4603199262206155 -3.2720399795295338

Pd -1.4480177599674033 -0.2277618682766270 -4.8427877196539821

Pd -2.8888200314625245 -0.1751522017659382 2.2007244647227435

Pd -0.0617244976605015 -0.2252166465697541 -2.5175488817083944

Pd -2.8070826630675012 1.9047657306841461 -4.0642976983256762

Pd 0.0564380776757987 -4.6590215311774994 0.6726161189111387

Pd 3.9275315889986184 2.0943365245985563 -1.7052589825603091

Pd -0.0137479918002178 -2.3437813419557458 -5.4731100028072373

Pd 2.7095442512706129 0.0421648054850807 2.2306939514673991

Pd -1.4542952214393527 1.9637462941012325 -1.7519960014377227

Pd 2.6021903315750730 2.0093306382120661 -4.0675620664983612

Pd 1.2387403770797669 2.3046938321972177 2.9749643063525721

Pd -4.1509940669095409 1.9117788610761417 -1.7238273887637321

Pd 1.2065231826584530 4.4686843992172012 1.3313978324923961

Pd 4.0352527134250638 -2.1948114727457466 1.4226589078568159

Pd 1.4695845947356729 -2.3911566718777881 -3.2649446389669872

Pd -1.4939606310228180 4.1690473502548819 1.3374139712756812

Pd -1.4239928129435673 -0.2059489383788303 -0.1723962464598273

Pd 0.0376110404633319 -4.5576950078942868 -3.8618839377688761

Pd -0.1298152976216040 4.2988034825097028 -0.9734431705118937

Pd -2.8945180418702923 1.9918317198992808 0.6470041924657183

Pd 1.2461247341389075 2.0106064589319659 -1.7563078865073434

Pd -2.8335693501434318 4.1442250660376381 -0.9961933513031515

Pd -0.0088645684013095 -2.3938194971549298 -0.9336354605449092

Pd 2.7693892825402222 -0.1910146440209977 -2.5413258956024651

Pd 2.5456828891468395 4.2813495033710911 -0.9999833762417328

Pd 1.4578387470802574 -4.5687259739058739 -1.6384504673229665

Pd 1.4044917749446362 -4.4293348453641546 3.0025655223218224

Pd -1.5013633384482010 4.1497851959735463 -3.3102549020515624

Pd -2.8291595049585969 -2.4657359015819194 -0.9891535057762862

Pd -1.3071273776232712 -4.5169752357417075 2.9897977619482377

Pd 1.1998508046808278 4.1847415536944528 -3.3084076844317738

Pd -4.1807593044671423 -0.2609372341030370 -0.1822472720786271

Pd -0.0295345783165336 -2.3191620831157391 3.8372084641333610

Pd -0.1960260975274796 1.9924093573743062 5.1637940401050706

Pd -1.3518748921411192 -4.6357153250622609 -1.6372939561940016

S9.48 $CO_2/Pt_{13}Pd_{42}$ (linear OCO angle)

C -4.3320146908773758 -2.7662233759124106 -3.7284106700803568

O -4.0049443120811237 -3.8691957955972534 -3.4951701852544295

O -4.6831149235560900 -1.6760067059804094 -3.9800293848420667

Pt 0.2457607844691411 2.4394605855526308 0.9922589686808819

Pt 0.2904332592952060 -1.9950689013665102 -0.4385345503680033

Pt 0.2725278463295729 0.2481557897263781 -2.0614309135213746

Pt 0.2623147335679575 0.2230109802545391 2.6052888902713454

Pt 1.5855947419423615 2.4280800770195485 -1.3386513901523702

Pt -1.0853536771576502 -1.9773881768139017 1.8901599148178019

Pt -1.1299858530588140 0.2319718959655769 0.2930808305218459

Pt 1.6803164218585114 0.2292570743568215 0.2581699605133557

Pt -1.1251604509070672 2.4333197994149343 -1.3167790790030363

Pt 1.6139236090121243 -1.9688697117549427 1.8623614598425038

Pt -1.2123079591248513 -1.9592086184216022 -2.7518908293845881

Pt -2.5979175809472643 -1.9829862483675651 -0.5092069236976887

Pt -2.6179651188561994 0.1595190138263066 -2.0482736960432986

Pd 0.2020751949938548 -4.0960522606555614 -3.4470108392299101

Pd 0.2575453907447846 -4.3917430797912100 1.0970818827075040

Pd 0.2038379441071686 4.8044959520990682 -0.5433693234301175

Pd 0.1787504568393744 -1.9204417477891518 -5.0124873761827304

Pd 0.2487818923055755 2.4040783537467654 5.5110647937720705

Pd 0.1911708700470413 2.4702618684529067 -3.8596907617017413

Pd 0.2613045479793624 -2.0125637584944354 4.4101225656172129

Pd 1.5415898048536738 4.6074997069533214 -2.8801385926373095

Pd -1.0849099835388978 -4.1525456816546704 3.4222512657898383

Pd 1.5553262788796618 4.6061740756975738 1.7849019329484277

Pd -1.1273842918204264 0.2540873805273066 4.9010323044425883

Pd -1.1214132475085810 4.5934657112305874 1.7945682794456588

Pd 1.5779675652217338 0.2317566964799161 -4.3928962647806378

Pd 1.6185917922557869 -4.1284404490290783 3.4219300973195956

Pd -1.1589794011948198 4.5917181037236690 -2.8736564921254066

Pd -1.1700871701947599 -4.1437065866411942 -1.1933518692135123

Pd -1.1963537134178794 2.4558536763851642 3.3220179368509779

Pd 1.6156504055418959 -4.1824523929027517 -1.2116029118638820

Pd 1.6432359261181262 0.2662450774766415 4.8834915974602966

Pd 1.6850236363143323 2.4690979086946978 3.3156017568427893

Pd -1.2062605818647449 0.2113667774678775 -4.3325098998454790

Pd 1.7275370311033102 -1.9847243708848659 -2.8135862290675240

Pd -2.4183604804711880 -1.9394413611418955 4.1742595019658113

Pd 2.8954028689994189 4.6019858460478833 -0.5834376617149787

Pd 2.8827745304096695 2.4106575503803338 -3.6432670604605688

Pd -2.4377198040286903 -4.1343274334300464 1.1079255949037121

Pd -2.5049784156304629 4.5665761957156565 -0.5506619721690694

Pd 2.9422794157549239 -4.1316911941363355 1.0956299227659880

Pd 2.9372107434299632 -1.9169431367530461 4.1433983431951962

Pd -2.4993799131667718 2.3689635760393815 -3.5812799248823568

Pd 3.0840745536693461 2.4698698775287307 1.0659887282494467

Pd -2.6106513621042780 2.4282658207329133 1.0874424899129214

Pd -2.6431472810898207 0.2848860973200135 2.6541016231304217

Pd 3.1171023455624081 0.1609448928706100 -2.1494725435595017

Pd 3.1267542687932952 -2.0065604116675484 -0.5704958540956796

Pd 3.1566968860054612 0.3210668434245781 2.6289637161832653

Pd 4.2896423998074109 2.4126429419909634 -1.3268245503210074

Pd -3.8156215994675673 -1.9463057024462724 1.8523241556522028

Pd -3.8829355847256029 2.3619930748298525 -1.2697091780345147

Pd 4.3045145411134635 -1.9164045079424046 1.8077433397473295

Pd -3.9523400732744598 0.1942491362035880 0.2790008418663402

Pd 4.4235747827394674 0.2583132514383290 0.2416642322458032

S9.49 $CO_2/Pt_{13}Pd_{42}$ (bent OCO angle)

C -3.3363267191945392 4.4524577154913842 -2.5689207315367875

O -4.0270040296701763 3.3796042918607534 -2.9555042686775104

O -3.6343992455035954 5.6361249931879662 -2.7263802358184042

Pt 0.1972732098066963 2.0429324866263330 0.9346279284454106

Pt 0.2722035499047813 -2.3916956319985041 -0.4867790732347471

Pt 0.2384559358222463 -0.1608642150108530 -2.1117558488686563

Pt 0.2351893172024873 -0.1689773882930086 2.5534010166452412

Pt 1.5174234885406850 2.0430676991855674 -1.3974027044506614

Pt -1.1044543373065274 -2.3703311465104417 1.8416171218230164

Pt -1.1657551868377134 -0.1765052897777937 0.2451365042634923

Pt 1.6493011404707711 -0.1605010903283299 0.2085071517267791

Pt -1.1901094014654838 1.9914392852516156 -1.3838189918722983

Pt 1.5960162021517721 -2.3506601089783232 1.8118536065847688

Pt -1.2390335350595116 -2.3899989324430160 -2.8036505736712098

Pt -2.6228833293457372 -2.4075736599277389 -0.5581063012544161

Pt -2.6810680523645294 -0.3018696811487465 -2.1201987790544909

Pd 0.2211348974928702 -4.5042917736903512 -3.4927563329633124

Pd 0.2500860382207602 -4.7832697401246378 1.0513815559762612

Pd 0.1227284653217307 4.4050599240120079 -0.5963138773310672

Pd 0.1448361389833604 -2.3212777837050500 -5.0632135556008455

Pd 0.2192218566693248 2.0375716009449536 5.4500306167653205

Pd 0.1489612289340137 2.0559081346363670 -3.9377813142396509

Pd 0.2569303424705723 -2.3798734082045390 4.3720073067557461

Pd 1.4484766125610180 4.2231716094534244 -2.9511174529758066

Pd -1.0813161770928936 -4.5225863350934503 3.3910684903549257

Pd 1.4844695508950767 4.2188158954864470 1.7252424062988942

Pd -1.1553472710653836 -0.1217765245707894 4.8522288722694693

Pd -1.1905938322689018 4.1803932661427270 1.7570446848660324

Pd 1.5531931127394933 -0.1767201204262216 -4.4481173231453850

Pd 1.6150147994815061 -4.4995487530436460 3.3753786665806929

Pd -1.2575056953684858 4.1803010919760091 -2.9444455050550276

Pd -1.1847475051341487 -4.5546674322599969 -1.2393011780445193

Pd -1.2412197953431374 2.0435322860409939 3.2716150772554715

Pd 1.6118332324240228 -4.5599516683868568 -1.2554608410764918

Pd 1.6160397863234095 -0.1015741309852418 4.8292977563978292

Pd 1.6600879102177462 2.0848422160786728 3.2597397987040444

Pd -1.2326199381024960 -0.1944396440207561 -4.3609484645564285

Pd 1.7195221992407486 -2.3682646437981423 -2.8681090871001396

Pd -2.4321825390222083 -2.3194608747830796 4.1215577961560603

Pd 2.8098613151925962 4.2241492805130143 -0.6569379816331229

Pd 2.8134918031990912 2.0381297544557504 -3.6864733388801132

Pd -2.4435991785261431 -4.5402711310071631 1.0791201721480737

Pd -2.5703848062143271 4.1638687332733895 -0.6024991820016425

Pd 2.9288604466711430 -4.5080631847674830 1.0411043183495772

Pd 2.9273693379509416 -2.2812171733425388 4.0957608407166068

Pd -2.5900543359269710 1.8727487666018623 -3.7018179893061380

Pd 3.0300586251298407 2.1005219379051421 1.0049207210906119

Pd -2.6706847435781311 2.0250773249528060 1.0322043516029189

Pd -2.6918411167060485 -0.1114523073667171 2.6059084356625033

Pd 3.0861810092986071 -0.2114980678395038 -2.1957644066814788

Pd 3.1152181256190490 -2.3723668080883642 -0.6153159065781915

Pd 3.1286581433402549 -0.0541827132995210 2.5690039657693444

Pd 4.2289360994061296 2.0499020833411747 -1.3873496364238123

Pd -3.8367407025105651 -2.3472907213112468 1.8083213950011614

Pd -4.0028273732272490 1.8637046652534968 -1.3399323108248447

Pd 4.2935756880471239 -2.2813042958203362 1.7620507581646225

Pd -3.9586052911263900 -0.2112326589532538 0.2163501135147760

Pd 4.4006945282314227 -0.1077660033662167 0.1896917629675383

S9.50 $CO_2/Pt_{42}Pd_{13}$ (linear OCO angle)

C 1.2008004720242449 0.2331288962519450 -7.0896292137041481

O 0.5387874060678622 -0.7385670411484838 -7.0981373385478044

O 1.8623240971019268 1.1988021651915222 -7.1098762179122996

Pd -0.1228568532622284 4.3255953514293273 0.3162396166221761

Pd -0.1428769469281946 -1.4053254306181115 -4.3612205803511177

Pd 0.1845143850000116 -2.5638616076381298 4.3626985304946864

Pd -0.3794141004176489 2.0783802666258402 4.2751266045014216

Pd -0.8671711760522091 -4.2144346304002944 0.1188491872802199

Pd 1.5013990463327389 2.9920381283979132 -3.8542382867507490

Pd -2.8468447743796874 1.9142758632428103 -2.6160419739415728

Pd 3.5637289626933955 -3.5582568277594633 1.3281947559696186

Pd 3.7979889416731192 0.2387439160289585 4.0023367700025609

Pd -4.0795796579398980 -0.4846787497391695 4.7097515959278837

Pd -4.2241171549757750 -1.5332005232746104 0.1936483276115848

Pd -4.2303258857393198 2.8694006269460934 1.6339747287650568

Pd 4.4073694637289025 3.2326045492014592 -0.3264565490126923

Pt -0.2978505605534857 -3.1852520914709630 -2.2750139480607503

Pt 0.4100136596081675 1.6909070087333029 1.5409039657941641

Pt -0.5426086439838887 1.3792911155586489 -4.0151965901051714

Pt -0.5741215639942315 3.2907415293423923 -2.1366162273340796

Pt 0.5593577778204751 4.2153079359338212 2.9460998590388252

Pt 0.6218888059674327 -0.9811194532613235 1.9600819250749588

Pt 0.8928030393280882 1.2953491116219114 -1.1178796159336144

Pt 0.9751776794161754 -3.6199951021308494 1.9730016119719187

Pt 0.9752877309056781 -1.3313151933928948 -0.6886844691599652

Pt -1.0958243130611247 -0.4092504460150334 -2.1076633690982591

Pt 1.1724461212406603 -0.1013738562712521 4.3784969758692416

Pt -1.4056076420583323 -0.2871788263170693 4.7770675797336182

Pt -1.4994700045232061 -1.5289142632961001 0.2776631180975155

Pt -1.5047987147133142 -3.1709762076596406 2.4881334468196563

Pt 1.6858721520203315 -3.7662030218901017 -0.5935033674256640

Pt -1.7115173496301856 0.1552396114018816 2.2660655201186222

Pt -1.5745847432281923 1.0759480365207368 -0.0994556588580966

Pt -1.7419770745877912 3.3744707463770287 2.2078934896668407

Pt 1.7751650078702508 0.2997611379951209 -3.6383379481856855

Pt 1.9007411190235761 3.7378456305331187 -1.3109037558135721

Pt 2.0435645868589498 -2.1828363878871309 -2.8712875791386621

Pt 2.1545540777743497 2.2056444764506593 3.4890755896078058

Pt -2.4830426787067923 -2.5804648124868170 -3.7735765968813704

Pt -2.4531992180235820 -2.6673878023815161 4.8532200666610255

Pt -2.5200904350986013 3.3930969101145698 -0.3806593127155036

Pt -2.5589829933673984 -0.0720970887799342 -4.5393821380113213

Pt 2.4633743155737227 0.2671118185978451 0.5909693640228160

Pt 2.3733179548285070 3.6060127157345225 1.2168991888116356

Pt 2.6208280194439162 -2.0620570375374059 3.3181994806024040

Pt -2.8779767981962232 -3.2217183321800822 -1.3836650076798118

Pt -2.9746282938646500 1.7880483515350736 3.8400545848000620

Pt -3.4352077544774895 -3.9979022065356582 0.9701177041968851

Pt 3.3447200383077771 1.8443690541247040 -2.2967218953906867

Pt -3.6885973510056003 -0.7102904423844499 -2.2666392712359800

Pt 3.7552445193814101 -2.0192389536287227 -0.7420084714102326

Pt -3.9473801602550500 -2.2272772643651551 2.7703625708546928

Pt 4.1126034644789744 -0.5753106146491888 -2.8542405927498882

Pt -4.1114889724200170 1.0640324110748016 -0.3704364870614938

Pt 4.1968209513287613 1.6888657266096290 1.8251085090699164

Pt -4.3192727388152976 0.2581396270316724 2.1245805153501882

Pt 4.3756716262425401 -1.0222403748217597 1.7014319771280821

Pt 4.7450491322174662 0.5055718713139999 -0.5387746979958912

S9.51 $CO_2/Pt_{42}Pd_{13}$ (bent OCO angle)

C 2.7501992913113247 4.9342220509573567 -2.8625442960315524

O 3.2753564142969145 5.8853946065011415 -2.3248125364751355

O 2.5745190274598695 4.5551495471186003 -4.0614334846864821

Pd -0.1447691410667107 4.0710203346938032 0.1319389250884967

Pd -0.1407836899364734 -1.6454311017930709 -4.5827508923923261

Pd 0.0014841350467581 -2.8187032868627857 4.0995563916536835

Pd -0.4941214285024194 1.8233852002854205 4.0579281567015961

Pd -0.9664423931566619 -4.4689965665721916 -0.1506827517553241

Pd 1.4673026840262542 2.7435013173969254 -4.0832614501893705

Pd -2.8258706834935339 1.6623847937378147 -2.7967094596661339

Pd 3.4278805990177030 -3.8450678162737906 1.1372747049746486

Pd 3.6587382630120997 -0.0426893147762335 3.8258766800767554

Pd -4.2198477538826724 -0.7398975455656440 4.4385190539951385

Pd -4.3819800399637705 -1.7636230546069658 -0.0671786413625771

Pd -4.2958067328414549 2.6398808820941029 1.3852295797870986

Pd 4.3762468965923125 2.8859572376321974 -0.5107499290222709

Pt -0.3431660676220594 -3.5052306391098687 -2.5708541979840791

Pt 0.2769579936145055 1.4578713473038356 1.2678913956396936

Pt -0.4297741248990568 1.0125999367276617 -3.9288677640993419

Pt -0.5999677154316745 3.1151620105266251 -2.3138413748500475

Pt 0.5026050303057319 3.9591290568007040 2.7543481724180165

Pt 0.4848646403286556 -1.2245328375781870 1.7155506635091791

Pt 0.7245613155103532 0.9782678012717991 -1.4209201406897232

Pt 0.8346739411112425 -3.8672811715837008 1.7369170674503871

Pt 0.8825818338573252 -1.5864149090218322 -0.9525458244074635

Pt -1.3320519985303980 -0.9779532651246619 -2.2254036423513610

Pt 1.0281212278799765 -0.3638121787905273 4.1542065372155594

Pt -1.5511709708263874 -0.5410721960591640 4.5354955701390338

Pt -1.6555341228213634 -1.8216634901879736 0.2163188053810113

Pt -1.6716739305044988 -3.5674837048909471 2.2647354990794359

Pt 1.5842379401641258 -4.0321713222480193 -0.8298555772815167

Pt -1.8268524026540034 -0.0313404248170250 2.0378087917483962

Pt -1.6789364611108015 0.7844407230123844 -0.3726968058092496

Pt -1.8127832460771531 3.1681243612562580 2.0087004586499142

Pt 1.8960212937022864 -0.0373943727398387 -4.0613906292796162

Pt 1.9354080516398982 3.5802363664875503 -1.5276472811906774

Pt 2.0107133943132904 -2.4565646048273355 -3.0871390587266432

Pt 2.0253648367105281 1.9047265272152665 3.2432399454148393

Pt -2.5433448101963823 -2.7933407451107279 -4.0451389870230283

Pt -2.6184565388031231 -2.9165947311434413 4.5987321702418100

Pt -2.5557627789194477 3.1371797760814020 -0.5763832453914098

Pt -2.4886163722459944 -0.2703376863086280 -4.7184101300804286

Pt 2.3323157319236270 0.0360941117470974 0.3655734173361317

Pt 2.3288246573756215 3.3387911855930992 1.0156459491732392

Pt 2.4638456712045063 -2.3316103681252991 3.1181477562086415

Pt -2.9531059369518378 -3.3953511557262925 -1.6415876880199494

Pt -3.0949405868924309 1.5703938015531584 3.6145419284809450

Pt -3.5657492602224998 -4.2492601341665628 0.6602942857874868

Pt 3.1814373954537558 1.4756359714620431 -2.4244641595782848

Pt -3.8884152044469253 -0.8975073747039513 -2.5602262881387108

Pt 3.6553279312560800 -2.3039201691804636 -0.9140130023917618

Pt -4.0762455278331595 -2.4794573095025094 2.4905004705396796

Pt 4.1265577896414802 -0.9033512496632443 -3.0142470646521065

Pt -4.2207673626794380 0.8336229726733777 -0.6030292288517490

Pt 4.1024090526150720 1.3986760288866196 1.6534474476336780

Pt -4.4235276540169215 0.0259825458176837 1.8782903160201312

Pt 4.2168594802003065 -1.3005247245763509 1.5151127678585916

Pt 4.6750484169576572 0.2007489568033105 -0.6930373758248859

S9.52 CO_2/Ag_{55} (linear OCO angle)

C 3.9865140207960121 4.3132202826318533 3.9618628110153695

O 4.8640426833088233 3.5598965684786155 3.7644731084789038

O 3.1039612668381364 5.0622689707105799 4.1530320384197408

Ag -0.2064148125875406 -0.2212409072715035 -0.2040773959475732

Ag -0.2216754940588407 1.2093297408128754 2.1445428378275140

Ag -0.2157059226289945 1.2233025705492837 -2.5627329676324724

Ag -0.2029357415578378 -1.6769878559968847 2.1475503102790059

Ag -0.1976891817141201 -1.6622465244759399 -2.5552036257724944

Ag 1.2428440111499615 2.1158326900539732 -0.2363093748177991

Ag -1.6542166546191381 2.1248058931464744 -0.2039545438169154

Ag 1.2406780096603305 -2.5704815762531403 -0.2060805404762409

Ag -1.6564560936336850 -2.5663629071064564 -0.1803652497851855

Ag 2.1363150867204825 -0.2148300104145927 1.2440977794611963

Ag 2.1443531260599960 -0.2315411515640254 -1.6613799596208689

Ag -2.5628301991662052 -0.2223663273063824 1.2423990626855057

Ag -2.5515604984122464 -0.2297144267593637 -1.6559846617350547

Ag -4.8684748004838907 -0.2444643887750623 -3.0896873250337333

Ag -0.2293858652613689 2.6336982529148303 4.4537725560876664

Ag -0.2364076653609903 2.6400145202865941 -4.9046281601663226

Ag -0.2044841457583776 -3.1245572867922355 4.4687928419567706

Ag -0.2043453069045297 -3.1033041256774156 -4.8674550862631163

Ag 2.6637204709744999 4.4238664497069919 -0.2450897903995106

Ag -3.0957457576670806 4.4377971309423430 -0.2103487952043694

Ag 2.6614453391606716 -4.9019262829910506 -0.2173709514637149

Ag -3.0876340020979964 -4.8856300278886406 -0.1860153296171647

Ag 4.4421240253359464 -0.2144346388642423 2.6715842980328555

Ag 4.4655920708910681 -0.2450770419853624 -3.1055733851179315

Ag -4.9016074499309381 -0.2363829971303625 2.6619913334076832

Ag -0.2132758257556708 4.5658056954637365 -0.3852212873516658

Ag -0.2148102588582212 -5.0132039269525590 -0.1113836292596366

Ag -5.0031660700028580 -0.1744172512253460 -0.2139592368763729

Ag 4.5885944922371946 -0.3321131181940381 -0.2212412803133363

Ag -0.1509720713436657 -0.2394414573844524 -5.0146592565791250

Ag -0.3158834201485225 -0.2433458331161972 4.6055581952197473

Ag 1.2896918185309005 -4.0967640929309184 2.1941140167030233

Ag -1.7137069775880562 -4.1059982027115014 2.2132156797443550

Ag 1.3366396260168971 -4.0528282931524977 -2.6290826444419100

Ag -1.6348858540185212 -4.0876799767954806 -2.5542415068119930

Ag 3.6746375616626796 -2.6332236036660071 -1.6816156232644681

Ag 3.6568567750436225 -2.6316866373282490 1.2678990876987724

Ag -4.1177722297104751 -2.5929918779241916 -1.5901122989127228

Ag -4.0596923911025531 -2.6524335635358174 1.3307154032499748

Ag 1.2909839139779946 3.6340228076925811 -2.6676313726869103

Ag 1.0946386353683832 3.6839743828504625 2.0848643555336315

Ag -1.7389200949997188 3.6180519133931663 -2.6388256218318209

Ag -1.8292081440282091 3.5679667166166542 2.2369167097306182

Ag -2.6345877393641226 1.2823393794594729 -4.0634935392615690

Ag 2.1670864779933896 1.2234594481327108 -4.1064290249216322

Ag -2.5607905122399193 -1.6259311984537439 -4.1346498537024390

Ag 2.1840139749793148 -1.6926377962489740 -4.1116272049229936

Ag -4.1278008145878573 2.1529682700194712 1.2386069334897825

Ag -4.0820598035895355 2.1612827236546366 -1.6947344201832062

Ag -2.6112603556917144 -1.7174104299227493 3.6577125798123227

Ag 2.2182617254652297 -1.7889724701787009 3.6309415905230904

Ag 2.1020854322703024 1.0880571055849619 3.7665743950214283

Ag -2.6291286220742167 1.2054234826394168 3.6974608641371818

Ag 3.6283686677334419 2.1971372232236841 -1.8068156837253915

Ag 3.7520415647723429 2.1081059880087212 1.0793018394015235

S9.53 CO_2/Ag_{55} (bent OCO angle)

Chemisorbed CO_2 was not observed for the optimized systems.

S9.54 $CO_2/Pt_{13}Ag_{42}$ (linear OCO angle)

C -3.5163182084691886 4.2051439801330082 -4.6611361006620742

O -3.3185592774802863 5.1241299132097744 -3.9588316512585005

O -3.7137230580576954 3.2859646610682711 -5.3632607937369565

Pt 0.1912106673299450 -0.2265235463255917 0.2509650481236462

Pt 0.1667280876689331 1.1756839779156079 2.5404741052047557

Pt 0.2254814624167719 1.1748181516142262 -2.0330753540801467

Pt 0.1538986254982920 -1.6250958105052016 2.5359960004730335

Pt 0.2147396217723337 -1.6358859049438141 -2.0327245387768427

Pt 1.6194643779231808 2.0456982858787338 0.2455244841562067

Pt -1.2348624412047389 2.0468189628723450 0.2599002945522947

Pt 1.6152337186040615 -2.5028278162011741 0.2351415089889099

Pt -1.2367474606613185 -2.5005339845852976 0.2665609537450692

Pt 2.4866352884554237 -0.2238617388373738 1.6432623118503451

Pt 2.6294756052333286 -0.2446291940870368 -1.2327396495336602

Pt -2.2450824061309875 -0.2188300581165370 1.7403138510320255

Pt -2.1012291351892731 -0.2217357792474059 -1.1434774010441822

Ag -4.4347489708765062 -0.2188171016364375 -2.5970367982263438

Ag 0.1601878196316945 2.6184492789261911 4.8846068490518393

Ag 0.2454241470780732 2.6160363271675884 -4.3701005479385540

Ag 0.1475629316474059 -3.0690339130022695 4.8744179649549686

Ag 0.2141152672861815 -3.0843280697912681 -4.3688931404257056

Ag 3.0675106703292383 4.3814368972827733 0.2510951262489888

Ag -2.6758245385230781 4.3892886385377912 0.2547900369168041

Ag 3.0555833835864981 -4.8481851966524392 0.2493369254809503

Ag -2.6862860552725349 -4.8405326826184902 0.2726720861360321

Ag 4.8187491329953280 -0.2346319031646582 3.1025119472286287

Ag 4.9547765984181904 -0.2507304891030704 -2.6546670205570990

Ag -4.5652439808612568 -0.2186316790097824 3.1708240329238637

Ag 0.1946025467941113 4.4657440775894841 0.2582332073361290

Ag 0.1868774920654917 -4.9267214867636602 0.2527057386769877

Ag -4.5646476463039427 -0.2143108548227537 0.2604024797408328

Ag 4.9523394910235687 -0.2367755867313059 0.2483571910620083

Ag 0.2324197209051996 -0.2366635920259212 -4.4512697669627723

Ag 0.1547782422988718 -0.2244432081753960 4.9638108137795527

Ag 1.6238114680504638 -4.0169030759187150 2.5967490041546304

Ag -1.2937518712263933 -4.0242560995213523 2.6147350848116346

Ag 1.6585202336817051 -4.0399635777703224 -2.1053082311321853

Ag -1.2635186166188175 -4.0272843548889945 -2.0879688783542614

Ag 4.0481474463623641 -2.6052687390607332 -1.2157084145914263

Ag 4.0037065586426550 -2.5801420264337755 1.6979208637206749

Ag -3.6241510661824821 -2.5682070772208760 -1.1861410591508310

Ag -3.6624722073048757 -2.5774755586224316 1.7218079329133797

Ag 1.6835397355387658 3.5627806046184718 -2.1003399813052415

Ag 1.6346293167591746 3.5674672945910006 2.6090404558938793

Ag -1.2299992145635905 3.5692827543078600 -2.0932715103851418

Ag -1.2828566302746267 3.5658525634676006 2.6075933615051552

Ag -2.1304400255666351 1.2104755297546061 -3.5496310206312032

Ag 2.6068200234528374 1.2089009232511150 -3.5663166272609610

Ag -2.1522171919540556 -1.6829822058882113 -3.5431038143831977

Ag 2.5925104341136063 -1.7032413037258278 -3.5674167448103917

Ag -3.6662938200555955 2.1365859663300073 1.7142166688039677

Ag -3.6229767063841392 2.1308693730616186 -1.2021217361609819

Ag -2.2204755356290145 -1.6760999809344845 4.0814784250375462

Ag 2.5187670814564189 -1.6714627327837492 4.0471376328095934

Ag 2.5342665883935176 1.2245166394010545 4.0546362307362624

Ag -2.2088113339933599 1.2331482574053552 4.0777818052926964

Ag 4.0468163057289654 2.1150391291330894 -1.2059556077992042

Ag 4.0119073076417928 2.1228841415987967 1.7054959658245592

S9.55 $CO_2/Pt_{13}Ag_{42}$ (bent OCO angle)

Chemisorbed CO_2 was not observed for the optimized systems.

S9.56 $CO_2/Pt_{42}Ag_{13}$ (linear OCO angle)

C 2.8774521761870178 -5.0748237023626555 -2.3966160931389044

O 3.2283479929003689 -4.4095535864240887 -3.2986865609327931

O 2.5546833044284996 -5.7666507689168558 -1.5053635293365573

Ag 2.5726454058559285 3.2551581341647875 5.2227633482553673

Ag 2.6963553769890103 -2.5004632087095366 5.2752656418677653

Ag 2.9633901068017248 0.3854299111932135 5.3789308939838065

Ag 2.7737116392899077 4.6630489460457527 2.7777060376678593

Ag 3.2478137625148920 1.8320074132235260 2.8560603934219451

Ag 3.3044333106911910 -1.0759325869831784 2.8844920838266801

Ag 2.9667676892640835 -3.9274990592582957 2.8507783320206492

Ag 3.2457043538300043 3.2694553136622537 0.3538144174603469

Ag 3.4674956726737478 0.3703625443550877 0.4143192732131825

Ag 3.3699085146048193 -2.5199869925440161 0.4190246932667788

Ag 3.4133648698972823 1.7748152497170562 -2.0187002551118391

Ag 3.4757890951601236 -1.0744099705750365 -1.9875020094328102

Ag 3.4166945808027385 0.3216927877584903 -4.4164404388133089

Pt 0.4060795979381198 1.6170565829408461 5.6409786841908307

Pt 0.4578248504661040 -0.9484596210526269 5.6660463376188197

Pt -0.9872731653460766 -1.1772785470331000 -5.1977685010309616

Pt -1.0593965660574882 1.5970177536219445 -5.2156522717770990

Pt -1.2270339304512834 0.2188437512359127 -2.9268046942554440

Pt 0.9456703561609466 0.3354848713257783 3.3986125015619355

Pt 0.7101370375040407 4.3284822821508202 0.9881135227561039

Pt 0.5660350193625913 3.1258041100550957 3.3649164593481653

Pt -0.8555835914537623 -2.6619388235578483 -2.9522630100695433

Pt -1.1137101118694226 -3.7381295478880205 -0.5635036913528438

Pt 0.6913230166773808 -2.4747721060715255 3.4190170363553127

Pt 0.8940812872339196 -3.6956815410750870 1.0637213576439644

Pt 1.0076775800140789 1.6486505714929889 1.0514970259544374

Pt -0.9987829341592264 3.1194964832881067 -2.9982171063114582

Pt 1.0416815197839420 -0.9944370175532048 1.0783557935898733

Pt 1.0776953216138880 3.1182067095850523 -1.3557428879251430

Pt -1.3062002262249834 4.2359826169120565 -0.6344730961304023

Pt -1.2634906266958963 -1.0500311102557642 -0.6158159073565767

Pt 1.1904705282885233 -2.4812901967208960 -1.2881990392330747

Pt -1.3084112900830533 1.5441067626539877 -0.6458933237005283

Pt -1.4329894072020279 -2.7485094501573810 1.8477887353730920

Pt -1.5645301297391316 3.2667406647079118 1.7890515440655270

Pt 1.0733235561606711 0.2608711151008893 -5.8343481372636763

Pt 0.9903425171625703 0.3172740596301095 -1.3087244442760708

Pt 1.1387924439969863 1.7505258336925436 -3.6240656641702791

Pt -1.4892232567506956 -1.2008280595471637 3.9842064544789775

Pt 1.2039230193368868 -1.1745003167066894 -3.5880803220457849

Pt -1.2767535510229073 0.2658820078432482 1.6871276291927733

Pt -1.5550707304622924 1.7668368132876346 3.9621884712798718

Pt -3.0868260049376408 -2.4233632568157777 -4.4222451235742257

Pt -3.2287186896189608 2.7289170240391250 -4.4632297667550862

Pt -3.3596009752872962 0.1479689198433096 -4.5446170985122691

Pt -3.1652129233252575 -3.7548080794129595 -2.1441211925798513

Pt -3.7657049267290383 -1.1333544486419331 -2.2244897624727429

Pt -3.8461954295100069 1.4470394075123409 -2.2530697700240423

Pt -3.3576409804987946 4.1011522340715167 -2.2173997038070246

Pt -3.4383612383067037 -2.4025779150522335 0.0869311994079202

Pt -3.5482685852261682 2.7712870098465823 0.0296914645302321

Pt -4.0092954399926297 0.1726390402832538 0.0242493889833954

Pt -3.5585838228157587 -1.1574104859715799 2.3129396007468213

Pt -3.6067516474038097 1.5698282583416394 2.2789144740630114

Pt -3.5600053224216714 0.2386252157045931 4.5345306052648962

S9.57 $CO_2/Pt_{42}Ag_{13}$ (bent OCO angle)

C 0.7316695006732640 -0.4001831724784319 7.0393146003890283

O 0.6189212455126795 0.8709286375232119 7.1512775185869852

O 0.7829526157806054 -1.3165146977050199 7.8422755428890225

Ag 2.9871776182257346 2.9860160957377322 4.5090991901661832

Ag 3.0431296983263554 -2.7264321380540131 4.6361802804269550

Ag 3.3349484396448457 0.1625727632359484 4.6090122205429918

Ag 3.0491720187755402 4.3738058726545361 2.0760895342124077

Ag 3.4843436525818579 1.5593848690093959 2.1116675991310165

Ag 3.4956013470718394 -1.3607457078400176 2.1761989601145517

Ag 3.1330286641081124 -4.1981728942026617 2.2320345345448560

Ag 3.4130284734829530 2.9751253189516818 -0.3683562103452085

Ag 3.5804578136225782 0.0418039076993562 -0.3057985552784144

Ag 3.4633691137464089 -2.8731732778648378 -0.2574763874731347

Ag 3.4628280814286381 1.4317164072975053 -2.7204761854870485

Ag 3.4936585228203239 -1.4484280125646662 -2.6736525384987218

Ag 3.3433155286520715 -0.0426084879110375 -5.0939580704251632

Pt 0.7029408922490780 1.5072006998881464 5.1258995001136789

Pt 0.8611080311728391 -1.1082365008617712 5.1347174361869223

Pt -1.0977364010970894 -1.4872934312752888 -5.6693509636074904

Pt -1.1345822884326295 1.3012680203136833 -5.7138985221543361

Pt -1.2173770918632216 -0.0619527474226287 -3.4012645933739507

Pt 1.1846090211559062 0.1098710964709835 2.7957149549266127

Pt 0.9099430979167672 4.0400099752475027 0.4292044734282292

Pt 0.8378478026649377 2.8262993412508561 2.8202020840558770

Pt -0.9079355997935840 -2.9493620582794855 -3.4185385300765319

Pt -1.0808334601312770 -3.9975764040368253 -1.0036240378913488

Pt 0.9304216466169647 -2.6467950175343362 2.8753466283712465

Pt 0.9891419917278571 -3.9868231263265641 0.5475193594931409

Pt 1.1719689582273374 1.3721488340820236 0.4325732602721681

Pt -0.9736634776225631 2.8218845134618098 -3.4933075738111867

Pt 1.1837160274814889 -1.2982057344971778 0.4677262760615655

Pt 1.1635327162495270 2.8023468730486756 -1.9502572597910326

Pt -1.1562469550444348 3.9799031833080636 -1.1287557451000254

Pt -1.1805617582832653 -1.3107668459443558 -1.0841358032582009

Pt 1.2168881581365618 -2.8354973490820936 -1.8668363506724204

Pt -1.2014128418797678 1.2838084764402380 -1.1215606541158978

Pt -1.2804488070771971 -2.9526109742950504 1.4037886641673898

Pt -1.3475907646346503 3.0448525375894460 1.3175218223178500

Pt 0.9437360819699973 -0.0765032793371072 -6.3982625549655587

Pt 1.0618954908885885 -0.0267282613201856 -1.9124594924369573

Pt 1.1218423602218597 1.4273716495305280 -4.2114725540363427

Pt -1.2331088170217186 -1.3621590988392305 3.5281334415407537

Pt 1.1664072982478284 -1.5473713095217809 -4.1818135426952239

Pt -1.1050090269325932 0.0420613112560442 1.2049734020834955

Pt -1.3074405337961676 1.5348965372293435 3.4873897225778094

Pt -3.1954122147660238 -2.6686573871007231 -4.8013699720410017

Pt -3.2511256978478098 2.4829408434423041 -4.8818766673320368

Pt -3.4117243682104132 -0.0970541211007580 -4.9108766440075708

Pt -3.1959477137409427 -3.9819223073366632 -2.5158240438402588

Pt -3.7644432690287011 -1.3555262806872170 -2.5822814663318114

Pt -3.7971720489154168 1.2367023241308452 -2.6183739818476659

Pt -3.2772554313444777 3.8771187508670675 -2.6261266460789190

Pt -3.3509986019423250 -2.6163037550208172 -0.2863552797602908

Pt -3.3994491366762762 2.5701628016095746 -0.3680214106157613

Pt -3.9023738435627702 -0.0288100634032851 -0.3315118385790579

Pt -3.3760437929729430 -1.3531216996939464 1.9260099836712847

Pt -3.4081685823656640 1.3942687420006421 1.8833667738739586

Pt -3.3095393843974206 0.0590657582608341 4.1346363117825788

S9.58 CO_2/Os_{55} (linear OCO angle)

C -4.5663588431835604 -2.1180281789646549 -4.1043297196417834

O -4.0045057528244330 -3.0596426671863974 -4.5196517694949510

O -5.1395239823537331 -1.1791881799459960 -3.6969945160732354

Os 0.2426157789696565 0.2437715936310413 2.6599637618980538

Os 1.6901643600426834 0.1974854681044457 0.2911719455815194

Os -2.3671871925579686 -1.9366047193929992 4.0990118228263199

Os -3.6685483310674121 -1.9418712336035215 1.8729377341516329

Os 0.2399007264936604 2.3987727879731349 0.9722641207111412

Os 2.8502576385181659 -1.9267094941129670 4.1129713707348330

Os -1.0488453821356720 2.4519102474946974 3.3091083796809273

Os 2.9340084286394168 -1.9766705091259731 -0.4387857697439966

Os -1.0706474863128763 0.2489798740207982 4.8002345454227182

Os 1.6647929440722846 -1.9407014751715870 1.8687246271263498

Os 2.9336956035761053 2.3596071691830636 1.0137678835284458

Os 1.5374195340169727 0.2526194631459327 4.8074729025956353

Os -2.3469363571462849 -4.0901475031158325 1.2010380868798931

Os 4.1935523119207394 0.2049601516571286 0.3120948186919710

Os 0.2569069198700308 2.2891773027803226 -3.5903594569545203

Os 2.8566149362972602 -4.0830684346589106 1.2181090726916000

Os -2.4252375111455677 0.1077645660231818 -2.0120289735404837

Os 1.5742996185730018 0.1289933067612730 -4.2142289759742910

Os -1.1693789153668148 -1.9466300563476102 1.8599035050829211

Os -1.0218849209378829 -2.0572388123365712 -2.7673040393613322

Os -1.0523866977885605 0.1311048095591560 -4.2241990603519719

Os -2.4273147239375796 0.2795363625503355 2.5789620985887298

Os 0.2506787429724234 0.1834977163144613 -2.0552924742500345

Os -2.3506041661802817 2.3480592091473866 -3.5369894425351855

Os 0.2542789318009409 -4.0928287221574164 1.1450501846776284

Os 4.1575449613132669 2.3613015403378226 -1.2799270390946615

Os 0.2646665398241483 -1.9275629496598514 -4.9405488362727930

Os 2.9118237304586563 0.2957340086791093 2.5909644404256884

Os -1.1514796620605345 2.3165421957769761 -1.3008675461951869

Os 2.8655997627187699 2.3488316331716486 -3.5198989921014867

Os 1.5217168219897710 2.4586156487177178 3.3232735470643395

Os -3.6550103847403097 2.3491906458644896 -1.3050352288730394

Os 1.5091519652482561 4.4734206494033195 1.7164420165958172

Os 4.1628309249222895 -1.9281740688599627 1.8948125981544572

Os 1.5481477446154686 -2.0522761542711496 -2.7630609889987090

Os -1.0308343244385738 4.4731656469926815 1.7080985844692886

Os -1.1954220182394177 0.1932986238949541 0.2850211036143437

Os 0.2718651395199551 -4.1718195242505374 -3.3024221440047605

Os 0.2449783930962841 4.4622240839343759 -0.5843524548064226

Os -2.4475142489626127 2.3498949857105478 1.0045353946881908

Os 1.6542688290379686 2.3191836320794930 -1.3010008661789174

Os -2.3639069532410413 4.4597146938304952 -0.6087249741826094

Os 0.2570161622632678 -2.0433630616321818 -0.4017157035973860

Os 2.9389789867394760 0.1099664085704821 -2.0000583155010165

Os 2.8551547568825630 4.4663027162233071 -0.5940695680384110

Os 1.5661861056269843 -4.0867439457749297 -1.1182032499087646

Os 1.6194155793740110 -4.0074074855321005 3.4044403159486394

Os -1.1464104891450448 4.4022890655210496 -2.7938224315469085

Os -2.4232323227403492 -1.9839429176696302 -0.4548346432377868

Os -1.1320133060669431 -4.0138480420061917 3.3968942297608629

Os 1.6470545404482972 4.4045729777230633 -2.7867173571002413

Os -3.6973293037763817 0.1937143102096239 0.2909307631772408

Os 0.2425355023823345 -1.9302189057228925 4.1447587725357664

Os 0.2318506591402309 2.3190459352022481 5.4669975032792051

Os -1.0474603050155022 -4.0885623886899047 -1.1345315930232780

S9.59 CO_2/Os_{55} (bent OCO angle)

C 3.1599929775268816 -4.1567481334105780 2.9405567713108334

O 3.6549656967328144 -5.0336561059982374 2.0848444358162816

O 3.9844857162466436 -3.1845752283379456 3.3883514092138207

Os -0.1930221141436821 0.3539025409743414 2.2684380448519827

Os 1.2334221162226040 0.2967764958990156 -0.0705028723509619

Os -2.8368329409537711 -1.8266884960615757 3.7260050561182747

Os -4.0913151419553433 -1.8435141663470676 1.5170462889124843

Os -0.1883603080151790 2.5357853447800762 0.5911744557608808

Os 2.4166458659217067 -1.7095296166053062 3.8136903489900500

Os -1.5174948496656686 2.5541548118013493 2.9159797548190221

Os 2.5395792727592177 -1.8901052803887284 -0.7332567185010722

Os -1.5340167970142264 0.3652886743571483 4.4112802901740897

Os 1.2617285335809409 -1.8662522200783203 1.5531131783361398

Os 2.4794131306669183 2.4822031258574553 0.6643620587517015

Os 1.0499949557392636 0.4293401391194419 4.4415025534324819

Os -2.7826230194061612 -3.9666400434574998 0.8459879759565988

Os 3.7437683279315177 0.3334383876021175 -0.0858416596984361

Os -0.2158360327388369 2.3817748320935008 -3.9596607863223148

Os 2.4417812707526405 -4.0139120359745393 0.7443691127867349

Os -2.8972544101237734 0.2311268532505108 -2.3928917698738821

Os 1.1086618751723005 0.2081517526167954 -4.5989662402900011

Os -1.5947519999812148 -1.8172543422157093 1.4988116749180898

Os -1.4757205152421964 -1.9690004521534208 -3.1110243233085959

Os -1.5023173833289665 0.2016749421254883 -4.5918334096861502

Os -2.8714455876856508 0.3903987167594831 2.1826445255954776

Os -0.1799663634434072 0.2663544198568769 -2.4264346659362039

Os -2.8224028998008581 2.4249718343613038 -3.9272668231663181

Os -0.1344812721808868 -3.9856931149895489 0.8200541002234681

Os 3.6981596544036872 2.4539312401189930 -1.6873912146702401

Os -0.1941819905492697 -1.8535349350351469 -5.3150916804036585

Os 2.4684240591046898 0.3979476122882443 2.2127186927311322

Os -1.6123013143129032 2.4319848521375844 -1.7115015574906116

Os 2.4302420984933288 2.4177128821747642 -3.9091924427428686

Os 1.0526731447001776 2.5760073636881300 2.9269573627218928

Os -4.1129638841576170 2.4382914583638096 -1.6945923969282055

Os 1.1035688660055438 4.6116142558433806 1.2502564728905976

Os 3.7798408300722226 -1.7214923399235547 1.5409449399766397

Os 1.0918519969964731 -1.9582915011984356 -3.1392548397229141

Os -1.4728121802210286 4.6029368631032082 1.2798628043920197

Os -1.6375104787467070 0.3100722587644523 -0.0976591256448676

Os -0.1817579947867802 -4.0749763250502911 -3.6542523519762375

Os -0.2127722931413505 4.5663228978600570 -1.0179683114851605

Os -2.8899719686735441 2.4672830626346878 0.6451172354078873

Os 1.1895701087710204 2.3955625466227017 -1.6676235307918268

Os -2.8071768772185539 4.5652870210588317 -1.0046940940701226

Os -0.1674966005633554 -1.9314333459021968 -0.7592140494088943

Os 2.4769108383101308 0.1992700393419068 -2.3835565375301164

Os 2.4198345442709819 4.5538135103640611 -1.0263878957281185

Os 1.1202796978042269 -3.9763981771431220 -1.4930697249584717

Os 1.1309937611710392 -3.8977108581033280 3.0946001377786128

Os -1.5913223318018925 4.5028443648700103 -3.2066472182116761

Os -2.8549230486379589 -1.8556592565767547 -0.8316743420599385

Os -1.6116728166199028 -3.8826207796260634 3.0398401461085762

Os 1.2056163883338851 4.4688771826924691 -3.2092979068489718

Os -4.1436102541017821 0.3073237586324308 -0.0985412433791003

Os -0.1530753628509078 -1.8030709928389586 3.7983174200667871

Os -0.2708640686943102 2.4864368891954127 5.0737531287551674

Os -1.4901506269331737 -3.9901051837937205 -1.4652906436117923

S9.60 $CO_2/Pt_{13}Os_{42}$ (linear OCO angle)

C 6.1861268961226381 0.0174534944698201 1.4374682887857615

O 6.2085555626345972 1.1876375802240480 1.3517188546061343

O 6.1890331993552072 -1.1528844424683504 1.5259406605591963

Pt 2.3444788116916504 2.7411882654927235 4.8718046696252486

Pt 2.3678909225245683 -2.5623821954930803 4.9545458876032926

Pt 2.6489913239417326 0.0911374249651253 4.9047327216801797

Pt 2.6170032180118654 4.1025507725961852 2.4763429218729534

Pt 2.9083573247029126 1.3921165911067364 2.5133182908578044

Pt 2.9198006218758321 -1.2832900837322481 2.5556102180575824

Pt 2.6522400753791868 -3.9961098121242502 2.6038929300445153

Pt 2.9110063961046073 2.8377763473232442 0.1189000328591284

Pt 3.0040303656807854 0.0186364701609531 0.2332270603014131

Pt 2.9361199427286437 -2.8035794527709945 0.2073027656699334

Pt 3.0368967388515999 1.4160064405800965 -2.0996027441513387

Pt 3.0503498392094350 -1.4514621431968755 -2.0545994679898851

Pt 3.0730995491024822 -0.0545329887762803 -4.3935925532684417

Os 0.2364459142933156 1.2729223166925892 5.4125721855495383

Os 0.2471143723772640 -1.0952097514742032 5.4496852954614621

Os -1.0969327465727117 -1.4380958829631985 -5.2925649455476700

Os -1.1096311892581501 1.2639864856037342 -5.3349961174018272

Os -1.2649816658617608 -0.0538274301230724 -3.1663533460969373

Os 0.5328272620676039 0.0537699030496735 3.1115931184135577

Os 0.6295278836219337 3.9611340369296104 0.7766051990796380

Os 0.5114848184734017 2.7171468298630002 3.0758309941336957

Os -1.2813418975184641 -2.7363989123307131 -3.0350422001711763

Os -1.3535337978880311 -3.9504403901526666 -0.7377657745265753

Os 0.5347077970567915 -2.6093573330995894 3.1599924513513282

Os 0.6641466929503881 -3.9244217544133777 0.9008879993317920

Os 0.6623640747885051 1.4212206304625485 0.8183935620154148

Os -1.3058152426736991 2.6310927435539213 -3.1196476364740353

Os 0.6747815516889721 -1.3842400159297175 0.8624976414003416

Os 0.7921179556878355 2.6291805485670188 -1.5334766783358689

Os -1.3892744354029174 3.9169041814283894 -0.8615801763817132

Os -1.3672542393723142 -1.4507912921988397 -0.7559289333142460

Os 0.8157408467069144 -2.6648705930637351 -1.4501462291027256

Os -1.3796279661830690 1.4179508128315439 -0.8011245284535817

Os -1.4593053614311924 -2.6419517623729809 1.5973762340342890

Os -1.4830897367948148 2.6817273306216847 1.5134828198935768

Os 0.8604002146384188 -0.0884183794477978 -5.9830870704245500

Os 0.7304870330580782 -0.0167947656719470 -1.4226687858339615

Os 0.8765859290341937 1.2668147699989518 -3.7628358811497100

Os -1.6084856996190353 -1.2198504064945281 3.8311454632608788

Os 0.8886365570951271 -1.3724828850161364 -3.7211021141255385

Os -1.5026740918216397 0.0187375468532829 1.4671662516635953

Os -1.6200373216692510 1.3303676036520458 3.7910582063091995

Os -3.2676096792869003 -2.5551407426821782 -4.7328904371117444

Os -3.2904516229640270 2.3782703577734559 -4.8102365797949052

Os -3.4259567293780959 -0.0865753907859657 -4.6029719339174129

Os -3.4004565341865769 -3.9797645079037118 -2.3300605209380465

Os -3.4352368784682699 -1.4771855294738745 -2.4107864239209942

Os -3.4481193949309454 1.3725710652399543 -2.4554816471721677

Os -3.4360800379752279 3.8765261233536257 -2.4537112768077498

Os -3.5416571260806187 -2.6477486960037004 -0.1499990644888404

Os -3.5652260301654048 2.6132726397705350 -0.2325689441600142

Os -3.5897926761768306 -0.0183795312821822 -0.2361168847755201

Os -3.6412662162761813 -1.2753895794140890 2.1120290365324332

Os -3.6529184146294438 1.3120170958908151 2.0714952373512863

Os -3.7945929588709260 0.0514602418049725 4.2343218975320065

S9.61 $CO_2/Pt_{13}Os_{42}$ (bent OCO angle)

C 1.6428937088018685 3.3758467642272496 6.3003160964386833

O 2.1011225165568805 4.3051002610621438 6.9294270854357221

O 0.5574609250312560 2.6594293941698148 6.6085930923259522

Pt 2.5306217604381707 2.7786080225943306 4.5812012249621317

Pt 2.5508698374139773 -2.5578932622657038 4.7518272530181243

Pt 2.9182954416455194 0.0853688197940733 4.5471004731624278

Pt 2.9136205093700771 3.9581557772949774 2.0966132010456731

Pt 3.1906552546212557 1.3034025119491917 2.1886190524823559

Pt 3.2233520046027810 -1.3693265629859013 2.2638328403545587

Pt 3.0058437416733450 -4.0933720501891599 2.3881387572243993

Pt 3.1642358006550801 2.6648595471811083 -0.2588344538942260

Pt 3.2865332698308776 -0.1444744419467547 -0.0989029300564508

Pt 3.2282417291421370 -2.9412445845196262 -0.0577597274804181

Pt 3.2766334950511458 1.2076814061792447 -2.4527611145976529

Pt 3.3045409766972100 -1.6638682524831421 -2.3728125528860904

Pt 3.2977300569884993 -0.3043307920212906 -4.7191702613607687

Os 0.3980303309980203 1.2548981444967684 5.1923448307696107

Os 0.4471734566703360 -1.0540621273662347 5.2967181739837761

Os -0.8739760336230581 -1.7317654834800360 -5.5425253946597550

Os -0.9021731636962623 0.9416805963056269 -5.6437254622749915

Os -1.0329696138361650 -0.3231494502069226 -3.4428586884829429

Os 0.8251204095478418 -0.0812272691857773 2.8675886513567934

Os 0.8667022893792651 3.7692022895371928 0.3958169094627856

Os 0.8027492311953269 2.5989842587292999 2.6958002645443777

Os -1.0215834850432088 -2.9982707562945472 -3.2533239372074934

Os -1.0657165371484918 -4.1620954218299264 -0.9339803285587327

Os 0.8877389335220202 -2.7588860513411535 2.8602222847952676

Os 0.9598544380674593 -4.0831321461011605 0.6684868902284520

Os 0.9259699488100906 1.2164700056130151 0.5064276936849478

Os -1.0808187108777285 2.3672649790750313 -3.4373368695539099

Os 0.9542618424342151 -1.5139271379319423 0.6063687753320181

Os 1.0441326344814432 2.4136352413536675 -1.8618069924797271

Os -1.1585674901691374 3.6876910902952278 -1.2171481712455929

Os -1.0942258731569505 -1.6566812163563709 -1.0050791103553076

Os 1.1027931859710909 -2.8735858974862141 -1.6772839470428587

Os -1.1299019968536990 1.1849879232769918 -1.1111568547980137

Os -1.1543794864298680 -2.8039649270833640 1.3784541078773123

Os -1.2166448283553839 2.5031420135168845 1.1872668679802285

Os 1.0986827096212379 -0.3897484047354965 -6.2735354002508252

Os 1.0013494504497431 -0.2414679187321749 -1.7549513798689647

Os 1.0990594936979241 1.0017766602019358 -4.1046922031944728

Os -1.3129799241650082 -1.3436796886772244 3.5800746523549072

Os 1.1429938817344447 -1.6382366261335661 -4.0098261373296378

Os -1.2130958161478351 -0.1564188608240901 1.2082808980573605

Os -1.3606109007453289 1.2113204220941194 3.4736731777681062

Os -3.0154403070821063 -2.8834811696645875 -4.9244679607083635

Os -3.0672579564786524 2.0791585485155135 -5.1037780890891744

Os -3.1870921403382266 -0.3946074015874273 -4.8702375546983943

Os -3.1090894215563210 -4.2470760930088014 -2.5142611819555198

Os -3.1844672087890542 -1.7375016669854142 -2.6392986072860904

Os -3.2089246669866007 1.0899971454372155 -2.7383442864601495

Os -3.2127084710493796 3.6046983339322987 -2.7989699411804918

Os -3.2555175458012116 -2.8544775960684059 -0.3505434611975016

Os -3.3184451413613698 2.3761194690715550 -0.5426559294742299

Os -3.3295140019685472 -0.2374249276260348 -0.4949689657791483

Os -3.3488495115215673 -1.4599719842932795 1.8891973129714645

Os -3.4006781512479263 1.1237531271905321 1.7679257107770334

Os -3.4936348806714586 -0.0638825836832784 3.9766816170134236

S9.62 $CO_2/Pt_{42}Os_{13}$ (linear OCO angle)

C -3.4344877354106709 4.1419999745485203 -4.6017756059020840

O -3.0541217664596245 5.0987974038137915 -4.0393830977193819

O -3.8212341521082571 3.1940092177737820 -5.1754900506985981

Os 0.1882467122006823 -0.2268580547071027 0.2518039325295285

Os 0.1835389005620583 1.0977148327240636 2.3892438416752309

Os 0.1897741219382023 1.0954624886212174 -1.8885560496617804

Os 0.1814334004958093 -1.5480864633789178 2.3923113860762149

Os 0.1902319315823911 -1.5491963529243875 -1.8855303174842775

Os 1.5122815665994411 1.9125654039485955 0.2502003849562973

Os -1.1349773699289549 1.9154558191453972 0.2450707947846820

Os 1.5081558407910232 -2.3657364855765644 0.2572648946236428

Os -1.1379033798565945 -2.3639167701409174 0.2520982238866399

Os 2.3246486701212463 -0.2286517248339844 1.5764017354514988

Os 2.3286118127844069 -0.2276087280125246 -1.0666611153058425

Os -1.9567080932928052 -0.2242519235493020 1.5695043254147523

Os -1.9505102330990869 -0.2243778158256501 -1.0742781155488079

Pt -4.1272454774518605 -0.2390523275950581 -2.4348743880682786

Pt 0.1817836192526736 2.4477569983721130 4.5677372395026081

Pt 0.1978080501965604 2.4316131077081131 -4.0721846227120082

Pt 0.1785100915427970 -2.8859274644779780 4.5741894576245299

Pt 0.1930248742349125 -2.9001813061058872 -4.0653337547840982

Pt 2.8599109148891748 4.0949129672804219 0.2613417635645510

Pt -2.4727689488059670 4.1047360942865305 0.2548070567038119

Pt 2.8480796844858385 -4.5556009008790097 0.2472154633145119

Pt -2.4842466385553785 -4.5462674817901574 0.2407335135671119

Pt 4.5014329381727700 -0.2129883051653605 2.9373067078636650

Pt 4.5105438311028418 -0.2408587886234444 -2.4128837846840034

Pt -4.1371922545923399 -0.2101721599515723 2.9146353537946306

Pt 0.1943235124582834 4.3035066403249376 0.2526421615266584

Pt 0.1822724224393782 -4.7539145173797994 0.2518079511287653

Pt -4.3389134077561593 -0.2200807415454927 0.2401074380216967

Pt 4.7123940551424877 -0.2293643832429700 0.2609213104756004

Pt 0.1988437506139670 -0.2345514624813146 -4.2797134062184856

Pt 0.1777622643669960 -0.2194804255529322 4.7809733545807891

Pt 1.5802154354185614 -3.8862868043347549 2.5176160254254643

Pt -1.2212438449077514 -3.8840942055466292 2.5138394733843712

Pt 1.5854253726532683 -3.8935274610192865 -2.0112217730664605

Pt -1.2097717821242162 -3.8926377288353415 -2.0151099013360017

Pt 3.8498683510017262 -2.4951878709050974 -1.1370021371532901

Pt 3.8425057804864275 -2.4882175752038389 1.6570724697507389

Pt -3.4743290585901998 -2.4906976839793264 -1.1532175168826131

Pt -3.4808013399156756 -2.4833776247171984 1.6437920691741625

Pt 1.5979126513621906 3.4320887483495595 -2.0126708184925599

Pt 1.5856447341288635 3.4404062486425628 2.5185093409516908

Pt -1.1981443551323381 3.4340124349692132 -2.0109969141550921

Pt -1.2100269412358113 3.4433000237595457 2.5133335741611718

Pt -2.0656305762664329 1.1622473217708615 -3.4152809741471923

Pt 2.4611247889201553 1.1666545576225198 -3.4085508938948603

Pt -2.0700906862961190 -1.6343657624242065 -3.4161954468187292

Pt 2.4567057882236902 -1.6337918597314156 -3.4082372857859955

Pt -3.4765709049359295 2.0446198621227536 1.6381074000183511

Pt -3.4677754593473078 2.0377250239484135 -1.1561648278643899

Pt -2.0867565110262745 -1.6190137135740919 3.9100769906932311

Pt 2.4444688541625212 -1.6234313283087671 3.9172128176306797

Pt 2.4437065542602530 1.1789030826726326 3.9189733765249306

Pt -2.0824896864206766 1.1817798448654095 3.9107009269755046

Pt 3.8544606416214964 2.0323426204363275 -1.1420570297060484

Pt 3.8482886853033449 2.0391434846129979 1.6558170723331707

S9.63 $CO_2/Pt_{42}Os_{13}$ (bent OCO angle)

C -4.6822335844841065 -0.8616931698509216 -4.3297480491757980

O -3.9556310641247467 -1.5605683017345855 -5.0168993681573637

O -5.7968149301246097 -0.3603432433406411 -4.2140575604713417

Os 0.2631667894864699 0.0514473781630360 0.2481048027151337

Os 0.2365191355253106 1.3768951714137085 2.3760992736609405

Os 0.2551217832081578 1.3707280251188143 -1.8976921125498327

Os 0.2436118495481989 -1.2672941526022745 2.3791187821537401

Os 0.2334838143641229 -1.2669572000546940 -1.9031379181665711

Os 1.5679874014498203 2.1912627647385969 0.2414382230915377

Os -1.0807026045154478 2.1869199060501918 0.2331590356246180

Os 1.5781419292945005 -2.0828638389426306 0.2420884775415230

Os -1.0690825012024494 -2.0875471278026776 0.2396133454867347

Os 2.3850174768702397 0.0583539457200439 1.5712956827692790

Os 2.3932566487681788 0.0474494105329266 -1.0740200036476479

Os -1.8976258738387861 0.0523824808150137 1.5519448354784513

Os -1.8929532280790851 0.0453991461926068 -1.0949649171737144

Pt -4.0626508081995514 0.0053352663692219 -2.5063724895409436

Pt 0.2393428543152511 2.7267473173532619 4.5607857274055714

Pt 0.2957218459827561 2.7194546972822975 -4.0761146001933941

Pt 0.2457717688603213 -2.6100752874408633 4.5743082082281381

Pt 0.3305902120939188 -2.6418371080536711 -4.0660081219523594

Pt 2.9214159892164262 4.3819431096466053 0.2546146230930899

Pt -2.4079372752325785 4.3818157206189978 0.2270598345014127

Pt 2.9414559121817994 -4.2660081829831027 0.2883751213313010

Pt -2.3845302308495393 -4.2858745020261519 0.2535134908655243

Pt 4.5637400136457460 0.0636725076117090 2.9300747167820425

Pt 4.6032353013616563 0.0760453806696288 -2.3943437007077475

Pt -4.0699880415926417 0.0340606680936329 2.9135667672298178

Pt 0.2553491798543874 4.5808978476274440 0.2351584574403168

Pt 0.2795739273222171 -4.4788922838833765 0.2654033166483730

Pt -4.2619972835625735 0.0388668750549104 0.2161314588650002

Pt 4.7834096577878800 0.0661378297957178 0.2714729770362453

Pt 0.3077883835551256 0.0446731962024189 -4.2873835216454559

Pt 0.2438809366740998 0.0593969599164829 4.7694239112595529

Pt 1.6556786754748989 -3.5971796294079512 2.5308388037153393

Pt -1.1370729586643578 -3.6134824349927790 2.5191407568469755

Pt 1.6976766149298175 -3.6155666681080860 -1.9889276016190129

Pt -1.1021495568023607 -3.6385034715309930 -2.0105461252759707

Pt 3.9350946204258124 -2.2010666290471406 -1.1232400861201266

Pt 3.9168969214317495 -2.1975869738226876 1.6696017890093715

Pt -3.3889077309957423 -2.2363965250781574 -1.1433007112697193

Pt -3.4011845621688450 -2.2257602176415507 1.6430723717378513

Pt 1.6700184690954922 3.7200177808204145 -2.0124895342814710

Pt 1.6432289795578880 3.7171583354555642 2.5105311173128460

Pt -1.1270342474351367 3.7180432529052707 -2.0282122938489593

Pt -1.1615209644986513 3.7094862088355578 2.5013830320859647

Pt -1.9742786157407533 1.4606891781989790 -3.4267916518096979

Pt 2.5492954751716326 1.4536676051536275 -3.4017568691823943

Pt -1.9325369420939473 -1.3857270193912223 -3.4332715620020231

Pt 2.5670417067727507 -1.3455995826519322 -3.3918086119109141

Pt -3.4241240249155021 2.3040039720183785 1.6119549232914130

Pt -3.4004478564381198 2.2945767427515613 -1.1763694042855335

Pt -2.0141144817755627 -1.3530862205555243 3.9013829201459531

Pt 2.5065869268831489 -1.3290632907318438 3.9239926299797903

Pt 2.5077671468280927 1.4600562708404321 3.9151244783754051

Pt -2.0221675303146709 1.4565781834681908 3.8929969069714230

Pt 3.9237147507710000 2.3271858463858930 -1.1292037017575765

Pt 3.9071037989409017 2.3276240798543237 1.6638897180648939

S9.64 CO_2/Ir_{55} (linear OCO angle)

C -2.1495136804844734 -0.0129192809657797 -5.3908601162163734

O -2.0970608618881532 -1.1846406286879239 -5.4192488568025237

O -2.2010559612648319 1.1594614250209041 -5.3736546016278908

Ir 4.6444960723205089 -2.7569491004271454 -1.8763943579118314

Ir 4.6775140719422810 -0.1354828402466852 -1.9135035725016059

Ir 4.6672811688073734 2.4372719329437817 -1.8543771622416740

Ir -4.2852900679106982 -2.7631884846770953 -1.7617542879528652

Ir -4.3375499806065809 -0.1581077335442247 -1.8039544035433031

Ir -4.3353116923058179 2.4440094007748234 -1.7382494441313538

Ir -2.0577748577309642 -4.0470475207159806 -1.8423768245060279

Ir -2.0959149870267990 -1.4578328082181153 -2.1312668512625899

Ir -2.1159670127387007 1.1912413853614021 -2.1044961369168491

Ir -2.1005608411845000 3.7836863761688972 -1.8287817566545643

Ir 0.1731153477175486 -2.7499180418350546 -2.1418300916583974

Ir 0.2352983700694637 -5.3193079057538837 -1.8341560688866123

Ir 0.1668579888173478 2.4999482658505263 -2.1375149234791526

Ir 0.1709823482284122 5.0603757430669409 -1.7888870205290177

Ir 2.4143068935214944 -3.9918376330736498 -1.7547525837900830

Ir 2.4425599128034388 -1.4305415212670107 -2.1640709911905334

Ir 2.4391734395525027 1.1840338672061073 -2.1842345247031880

Ir 2.4320384189228412 3.7778270909876230 -1.8781975214108473

Ir 3.6878661102753418 -3.5863270236729479 0.4499004688898551

Ir 4.9291884746698722 -1.4402243018043412 0.2981233282281034

Ir 4.9485650094583775 1.0800022472666786 0.3244954521136331

Ir -4.5729833766907957 -1.4176142878332660 0.4137469136608495

Ir -4.5866171047427082 1.0785338753848412 0.4244013756384761

Ir -3.2787313862505063 3.3660271383923206 0.4098738207955363

Ir -3.2113446172483457 -3.6617920973490206 0.4121967008286275

Ir -2.0134799523312794 -1.4160562610682286 0.3790350303667506

Ir -2.0289246747798395 1.1420686634213810 0.3943155599175047

Ir -1.1189026936001327 4.6177742849820129 0.3836299335286825

Ir 0.2016786034255137 -2.6697131100780007 0.3643060057646711

Ir -1.0157355654967088 -4.8962991862910039 0.3590905416721799

Ir 0.1922187927261069 2.4289915539845461 0.3677156254682365

Ir 1.5130112577342376 4.6225109974811831 0.3573808025731295

Ir 1.4607948786994363 -4.8805156887526921 0.4722991202171511

Ir 2.3945919897247818 -1.3958778709021464 0.3440345834318134

Ir 2.4044867289577794 1.1494760375130655 0.3325328786317969

Ir 3.6728108287131369 3.3723367695676432 0.3275359557088053

Ir 4.6945983664158337 -0.2026241747608113 2.5255680811867234

Ir 4.6937403432365192 2.4088280325631235 2.4916793254962886

Ir -4.2089544440254150 -2.7606041235649856 2.5839639484962977

Ir -4.2917655959720173 -0.1686196634789683 2.6359639949268074

Ir -4.2746824078233496 2.4255770138222497 2.5873700844979814

Ir -1.9441521347306048 -4.0581976668402744 2.5974955915230171

Ir -2.0415301774374783 -1.4670295039586003 2.9100514811907199

Ir -2.0498514547302364 1.1619362397715998 2.9075508040405329

Ir -2.0445611447438172 3.7663498756207439 2.6219261394801943

Ir 0.2472872161858297 -2.7355966592904446 2.8571418377354560

Ir 0.2218896122399676 2.4804365529550969 2.8762450759121694

Ir 0.2237565763967697 5.0387399402423343 2.5371169214192757

Ir 2.4850554844704891 -4.0306035451374944 2.6098020431997866

Ir 2.4654734313488720 -1.4468822428381580 2.8405135676712177

Ir 2.4996660730474374 1.1734767565747530 2.8611622247476460

Ir 2.4857012992721335 3.7687088992722533 2.5647246570708293

Ir 0.2265961743742450 -0.1440894319502819 2.9266408191125683

Ir 0.1844853417538829 -0.1142871294060912 0.3720801826417969

Ir 0.1611300479149746 -0.1189028978065254 -2.1990487798678271

S9.65 CO_2/Ir_{55} (bent OCO angle)

C -0.1301672894721249 -3.9260928417197656 3.8778055339853621

O -1.1203691777272147 -4.7465567510796740 3.5559399349085643

O 0.5290785857641375 -3.9304077058774505 4.8989658609517726

Ir 4.5559454035878071 -2.5859428923114978 -2.3029495438759771

Ir 4.5943263577692948 0.0231762944745284 -2.3465667329685989

Ir 4.6099638871630377 2.5968763440907674 -2.3417830305155327

Ir -4.3918230902421351 -2.4958509897959500 -2.3422399698549761

Ir -4.4158661198178590 0.0844808812074411 -2.4127420722115165

Ir -4.3872225908428044 2.6788964497235890 -2.3785084786995068

Ir -2.1740746751576876 -3.8268400532554727 -2.3407167775301296

Ir -2.1648516051454014 -1.2406827832359639 -2.6681029071432985

Ir -2.1728325724045079 1.3846306574153473 -2.6924638507645753

Ir -2.1393148318856423 3.9839562369311166 -2.4284692129217227

Ir 0.0725004506309969 -2.5581059788265934 -2.5983589060082473

Ir 0.1422221738973623 -5.1219875264327746 -2.2260195104038090

Ir 0.1114997518204432 2.6870848778774947 -2.6958079207133459

Ir 0.1261833809740930 5.2581589378663436 -2.3883000087950812

Ir 2.3184123176963403 -3.8078948041162333 -2.1880098519862248

Ir 2.3516926863227279 -1.2708889180727898 -2.6279575173970819

Ir 2.3799606674188438 1.3513972609519349 -2.6847549999392655

Ir 2.3808671031317004 3.9590279341614441 -2.4241819535710594

Ir 3.5733504232399445 -3.3842833101122194 0.0041107594897802

Ir 4.8246191537067320 -1.2400423237525111 -0.1232673246699179

Ir 4.8497548320881405 1.2754879546643554 -0.1274363995043731

Ir -4.6943014030076009 -1.1479718022281944 -0.1792445065782556

Ir -4.6769998103021306 1.3580823121164707 -0.1934842712726033

Ir -3.3629243961632960 3.6241248551385929 -0.2109965356913666

Ir -3.3475904251225672 -3.4130408734123980 -0.1311305512447075

Ir -2.1283844272067509 -1.1719602004302694 -0.1562781750939256

Ir -2.1224320030187429 1.3813951055883320 -0.1769579496644074

Ir -1.1900190718651908 4.8574664423437559 -0.2213166038162946

Ir 0.0572653668909201 -2.4517011309645680 -0.0895793326245489

Ir -1.1820817311678875 -4.6522591693651689 -0.1104541299358673

Ir 0.0985436623230346 2.6432769444943824 -0.1875695941237350

Ir 1.4322939970089157 4.8309520468022447 -0.2186321240199672

Ir 1.3136342103937675 -4.6253959114988161 0.0830113235252758

Ir 2.2761678381051174 -1.1896354578375867 -0.1126299596592935

Ir 2.3016248461434166 1.3522416940802102 -0.1665047122841231

Ir 3.5811757294289559 3.5724733122227592 -0.1950746645249418

Ir 4.5852375153989504 0.0286723765269208 2.0815641859225584

Ir 4.5667164645617744 2.6541424122136830 2.0029306138163134

Ir -4.3737831970297156 -2.4652920441455413 2.0048175495237288

Ir -4.4287515746833561 0.1236846453469169 2.0353714473200482

Ir -4.3862144138352575 2.7141879879137649 1.9705078251278074

Ir -2.2269992897154371 -3.8228170506185206 2.1624570762358548

Ir -2.1874547902565564 -1.1938500055665024 2.3574842958580788

Ir -2.1844497814441799 1.4255131722912269 2.3323080431328815

Ir -2.1454524537375215 4.0284599573111697 2.0067318675200418

Ir 0.1123636878285789 -2.4435106988509974 2.4730753727025609

Ir 0.1068806721764736 2.7399740230407241 2.3187897018592718

Ir 0.1209669001246431 5.2926341050924366 1.9466728207849977

Ir 2.4434958945554359 -3.7463507219009200 2.1735394058390778

Ir 2.3079934135310789 -1.1791616853871993 2.3692135668710144

Ir 2.3819609833349902 1.4002202409704949 2.3490250468076752

Ir 2.3693521371683111 4.0175285110060237 2.0135802860351957

Ir 0.0809199723188862 0.1330313610943630 2.5483300135495011

Ir 0.0789793922630008 0.1058186410771878 -0.1422228898769440

Ir 0.0984108624837094 0.0714696547595526 -2.7355195618821497

S9.66 $CO_2/Pt_{13}Ir_{42}$ (linear OCO angle)

C -2.1535707010319527 -0.0229871713312673 -5.4459627181059505

O -2.0785848940977782 -1.1937789572266591 -5.4566881218634196

O -2.2310887439567377 1.1476033323195594 -5.4411401442931480

Pt 0.1720230983415522 -0.1299897731442886 -2.3513528017064451

Pt 0.1485099889693224 2.5344444375253095 -2.2346942747697063

Pt 0.1856213822871695 -2.7748682095649504 -2.2625221830971589

Pt -2.0786611374322082 -4.1668579048381780 -1.8974493861169779

Pt -2.1080342288899718 -1.4486612450569967 -2.2418037846593832

Pt -2.1303901230166851 1.2129402397252951 -2.2013681020624758

Pt 2.4539476179131796 3.8932689337166138 -1.9055878516172480

Pt 2.4626506015161480 -1.4537682351225831 -2.2865015296624924

Pt 2.4439618550024109 1.1981586758808829 -2.2988139903996205

Pt -4.3517148257823166 -2.7847766767240505 -1.7548634806968315

Pt -4.4483056527136373 -0.1152372035392644 -1.8313233301788308

Pt 4.7254300659767923 2.4814025106578295 -1.8472416171708210

Pt 4.7980455137110427 -0.1778814008615942 -1.9651108145703424

Ir 0.1832865984939273 -0.1135693016767585 0.3516699976331999

Ir 0.1877330911392791 2.4303514415350391 0.3805578594756756

Ir 0.1221476089146869 5.0955316677474585 -1.7202862376845309

Ir 0.2294761202896860 2.4510046399845478 2.8680366388316521

Ir 0.1969574135387566 -2.6631094121268384 0.3604800235102502

Ir 0.2376827872633502 -0.1633643853935499 2.9403031599763474

Ir 0.2344841674871498 5.0194454554419004 2.5812995676037969

Ir 0.2348433288462594 -2.7386604163472126 2.8132074098497086

Ir 0.3344718249107832 -5.3475456476412777 -1.7462947493301058

Ir -1.0169953103728522 -4.9019580127176816 0.3727899448358679

Ir -1.1229370401148910 4.6355625396459335 0.4500637049903076

Ir 1.4483761403679474 -4.8915582354547062 0.5852965341775654

Ir 1.4867040124391055 4.6537598213975571 0.3923957393691322

Ir -1.9636009760789948 -4.0680785161448370 2.6060107573758864

Ir -2.0197287272830895 -1.4124811212100588 0.3670002626989138

Ir -2.0268032433984402 1.1448835391458310 0.4063575793854777

Ir -2.0334241589103126 3.7476182999493495 2.6693519919372908

Ir -2.0327309396673705 -1.4659999800592571 2.8610150103661955

Ir -2.1184670134439543 3.8179024573466207 -1.7615693638383880

Ir -2.0297496631605227 1.1403733147623869 2.8951138217465577

Ir 2.3918707579317937 -1.3895069715078849 0.3379320119713154

Ir 2.4043936229103622 1.1540795297041526 0.3190413994673107

Ir 2.4272826760484234 -4.0023371378735622 -1.6240182902002398

Ir 2.4721776905876602 -1.4407274476292964 2.7894554841863681

Ir 2.4697368868070821 -4.0268088991950073 2.6913111309736091

Ir 2.4898161961385954 3.7675021476439521 2.5834960263190418

Ir 2.4914080815487232 1.1603992299048114 2.8101564875835039

Ir -3.2119609215315492 -3.6744678837601588 0.4410601487116384

Ir -3.2892028581485118 3.3782693825888646 0.4717440279842813

Ir 3.6731027354947461 3.3816014057945494 0.3658636320235123

Ir 3.7097887324928553 -3.5767831939630637 0.5716083973846496

Ir -4.2121648419124362 -2.7476222214745456 2.5636868264402133

Ir -4.2640570333647254 2.4093857654744988 2.6297889959924805

Ir -4.3376940615599793 2.5045944246573444 -1.6727972578024803

Ir -4.2979807395216199 -0.1706294257604813 2.6563843908463745

Ir 4.6313966926223440 -2.8567391177878361 -1.7842787730582788

Ir 4.6807897831679446 2.4152675388985076 2.4733809020365229

Ir 4.7133231509331113 -0.1915455812217444 2.5397652691402688

Ir -4.5812323309077172 -1.4081773936156987 0.4525404161636995

Ir -4.6017072676087221 1.1217983447571498 0.4588657606037594

Ir 4.9378068910359172 -1.4460571974184087 0.3153395630979712

Ir 4.9615403187788596 1.0693852011837526 0.3592979281945242

S9.67 $CO_2/Pt_{13}Ir_{42}$ (bent OCO angle)

C -0.1465660173270911 -3.8920163402357542 3.8792751222890591

O -1.1197667981557056 -4.7365855459012121 3.5596427609061023

O 0.4912782780932303 -3.8597333833475282 4.9121108221512975

Pt 0.0980069120800492 0.0651029034971469 -2.8652254558764496

Pt 0.0961776600755681 2.7202849723909210 -2.7926265310428309

Pt 0.1030025920736041 -2.5849937683586042 -2.7256780744304403

Pt -2.1845158196680878 -3.9417045879221444 -2.3900093066434045

Pt -2.1771348490199522 -1.2432268655045267 -2.7859560994258543

Pt -2.1936252670121452 1.4147253456574855 -2.7836599236530541

Pt 2.3976099783200229 4.0735605366855907 -2.4522489003769574

Pt 2.3889459840377012 -1.2726718079377637 -2.7490226572878096

Pt 2.3835896192295523 1.3750892975415123 -2.8109892008372461

Pt -4.4536534638939740 -2.5367193618902082 -2.3447303935113832

Pt -4.5296459552498698 0.1247498132453355 -2.4347670872320939

Pt 4.6639370227848049 2.6471120026817641 -2.3387781194681998

Pt 4.7173281640976432 -0.0033211467456482 -2.4009829648535006

Ir 0.0796679349732991 0.1095821583102996 -0.1599632969308611

Ir 0.1012779160608718 2.6498873388254092 -0.1732308783988601

Ir 0.0632187150021434 5.2882681961556317 -2.3131620333686516

Ir 0.1124510081704614 2.7113512614585131 2.3103033255078445

Ir 0.0470376555255682 -2.4471839886097566 -0.0850444271028192

Ir 0.0919854010599514 0.1166500571484548 2.4478949236458152

Ir 0.1413366815028067 5.2693788619350208 1.9991235776875826

Ir 0.1089834070527915 -2.4482607300513592 2.4295610504598844

Ir 0.2330622662633181 -5.1439721134662442 -2.1402254497965383

Ir -1.1697090426440868 -4.6815715667457596 -0.0742796848490896

Ir -1.1964276074178175 4.8650389537157261 -0.1403345692292936

Ir 1.2964064622472475 -4.6297161916326210 0.1869926688616670

Ir 1.4039232541130049 4.8699859649001809 -0.1804637041560091

Ir -2.2665828806712960 -3.8507123614876431 2.1783748693756118

Ir -2.1348451015605368 -1.1732884388018885 -0.1644394008635230

Ir -2.1251891727709915 1.3814262914285127 -0.1636568116776895

Ir -2.1432635816611829 4.0083382058040034 2.0760243781458025

Ir -2.1910724088039371 -1.1947119507311843 2.3162054061458330

Ir -2.1687382830282815 4.0258959308191526 -2.3596115431654314

Ir -2.1619462772297191 1.4064108423008541 2.3200239875098121

Ir 2.2719166254001464 -1.1910739975387319 -0.1233053436005584

Ir 2.3138815971299080 1.3545030332581973 -0.1883845884088892

Ir 2.3306606547247521 -3.8171808271381771 -2.0871752740603955

Ir 2.3245444432374582 -1.1879704852104034 2.3169904556020833

Ir 2.4526462494263792 -3.7505565939181285 2.2354090790287731

Ir 2.3832351214610443 4.0060436485318647 2.0408355705993864

Ir 2.3900433888905392 1.3962973918790915 2.2989502525282313

Ir -3.3292010769430616 -3.4229517602835440 -0.1175503388712484

Ir -3.3758239937131500 3.6166759464772698 -0.1415596784071211

Ir 3.5776577086571995 3.5694212178194933 -0.1646885192727816

Ir 3.5925812328234641 -3.3976877405693742 0.0848585693405029

Ir -4.3766620853780251 -2.4728067834346348 1.9687922923349688

Ir -4.3873420606154605 2.6912110934525426 2.0082051062299908

Ir -4.3909945098243695 2.7477436204344716 -2.3106850986465441

Ir -4.4253141349480005 0.1098414283839606 2.0579328482098487

Ir 4.5489340007157386 -2.6799139908266678 -2.2271259043478167

Ir 4.5755714772660427 2.6636270391498282 1.9761735069584163

Ir 4.5894978371367428 0.0341916449291784 2.0914791301555948

Ir -4.7068625516408451 -1.1435245526933784 -0.1496116746391442

Ir -4.7090275447803611 1.3820204517477270 -0.1554063895424167

Ir 4.8155337060767414 -1.2547110187379431 -0.1015347188531019

Ir 4.8779795282481464 1.2643524491556919 -0.0990456608461012

S9.68 $CO_2/Pt_{42}Ir_{13}$ (linear OCO angle)

C 1.1535239156808692 0.2290183739818295 -7.0855790203641922

O 0.2933688168544060 -0.5480776233694716 -7.2697329165231670

O 2.0200756247255218 1.0015532699758127 -6.9224733240581040

Ir 0.4897756111935610 1.7110004312963287 1.3713824446927714

Ir 0.6960103391366635 -0.8241125641941388 1.9866954183990269

Ir 0.8690619682088127 1.2153296212288245 -1.1894345506530957

Ir 1.0437402594509160 -1.3385748039533061 -0.6113357957007277

Ir -1.0148799145224383 -0.5661254553266674 -1.9016778192520369

Ir -1.3054724421229351 -1.4421438714461230 0.5166532012392342

Ir -1.5966543526008361 0.3520156167425538 2.3121398792603580

Ir -1.5072841116039117 1.0859590490972462 -0.1104257532558986

Ir 2.4753143070036150 0.3031510295516143 0.5920655127880690

Ir -3.4480808424773683 -0.8616348068353216 -2.2214690113403206

Ir -3.7692523614030473 -1.6321999001135490 0.1940264213293788

Ir -3.9847271922249052 0.8067504975586691 -0.3241066216236799

Ir -4.0395465175158156 0.0837626620879047 2.0940256926613685

Pt -0.0893683000393496 4.1442478523164086 0.4060284058021175

Pt -0.2009492889689314 -1.3099247219685966 -4.2327209323676191

Pt 0.0144204082080966 -2.3570677019750557 4.1682076606804381

Pt -0.3888256052418053 -3.2371723234731009 -2.3738067892358989

Pt -0.4082401894568241 2.0867260684251079 4.0413565052271361

Pt -0.5681993826236352 1.4629334763138724 -4.0378809510599973

Pt -0.5468669036075257 3.3425225410903012 -2.0923785851661636

Pt 0.5200825259739080 4.2734495656556861 2.9721091161122244

Pt -0.9545951148570045 -4.0335693901007668 0.0424002744012448

Pt 0.9115407890658359 -3.5954786981994209 1.9682741694073667

Pt 1.1900472377171654 -0.0073992081957942 4.4887607541314312

Pt -1.4490187198258311 -0.1865562868406671 4.8235051034588068

Pt -1.6498317196506096 -3.3419835475708473 2.4613579404321797

Pt 1.4965845281687122 3.0094197011667649 -3.7586173072362490

Pt 1.6029439519194359 -3.8065645560312751 -0.6297988222952877

Pt -1.8924652117223029 3.5641402058471927 2.2616160122356757

Pt 1.7645910314233029 0.3682508908286987 -3.6473916853301658

Pt 1.9362474701168240 3.7697814058360972 -1.2750884024136464

Pt 1.9543678167554472 -2.1571009686581180 -2.8988922294592081

Pt 2.1637625869402446 2.3001366904591487 3.5318727887454520

Pt -2.5375687106949854 -2.6325508998974714 -3.9907558914104078

Pt -2.4799208214325534 -2.6300840767839544 4.8819216369313434

Pt -2.5166676380110213 3.4044245496228500 -0.3473227071933802

Pt -2.5752001597055663 -0.0367492603434315 -4.5046943778211181

Pt 2.4087921938096977 3.6689835514300482 1.2595848729717176

Pt 2.5393889524907753 -1.9984279598091783 3.3300064521317214

Pt -2.7247574248620618 1.7707886283066365 -2.4530042527672231

Pt -2.9906002268723166 -3.4308679430633093 -1.6098802461244481

Pt -3.0560498046422242 1.8534578027316835 3.9119163286717065

Pt -3.5324475038061940 -4.0935568123515873 0.8279554472919630

Pt 3.4296242520758349 -3.4601781099814142 1.2997300751482730

Pt 3.3577300662442995 1.8464188382003934 -2.2707267220037020

Pt 3.7562572315622647 0.2893406228204497 3.9543275687321362

Pt 3.6576997652843279 -1.9597334912007200 -0.7472635569987858

Pt -4.0971438761642025 -2.3859920996329231 2.7598052225180467

Pt -4.0710218680244354 -0.5221525383999123 4.6101767961232794

Pt -4.2113566189945848 2.6257802163578647 1.5654189036312529

Pt 4.0821041423973830 -0.5858736600490290 -2.8717130906497461

Pt 4.2164036369572617 1.7158407263110371 1.8511933130333607

Pt 4.3925065025161745 -1.0124703246237781 1.7212062312457654

Pt 4.4005603116154619 3.1910003245180061 -0.2867476335011740

Pt 4.7704665801784065 0.5181393946298966 -0.5408011536294086

S9.69 $CO_2/Pt_{42}Ir_{13}$ (bent OCO angle)

C 6.3007289682161911 3.2333136765856936 -1.1321008068490503

O 7.2715421142684669 3.0307336552336666 -0.4682087333184638

O 5.8022682530084460 3.5803941299575839 -2.2171022951957702

Ir 0.2198570532958024 1.5469497787016535 1.0390298042474686

Ir 0.4097305699996301 -0.9833588282434182 1.6889685924076561

Ir 0.5873738599997418 1.0214911565151250 -1.5178321777619506

Ir 0.7372167173906961 -1.5213319183881162 -0.9041831395093437

Ir -1.3273886063933953 -0.7588524180231677 -2.1913204824016410

Ir -1.6113809425951013 -1.5799232827154754 0.2350699718346242

Ir -1.8648207453034920 0.2261021981898739 2.0160230689655951

Ir -1.7830989701799906 0.9369831748553792 -0.4257035295819568

Ir 2.1893091460251246 0.1181098619368055 0.2706317807573143

Ir -3.7675151828942899 -0.9935786957503567 -2.5047562771383318

Ir -4.0795895601253065 -1.7403335700941001 -0.0805166973418453

Ir -4.2661988285314898 0.6961057517850242 -0.6186120965429834

Ir -4.3076871506205556 -0.0074271919687239 1.8097410865126731

Pt -0.2951847766786477 3.9715541884670098 0.0514863124409738

Pt -0.5556617094565939 -1.4827662940667694 -4.5537799097531613

Pt -0.2874747897823060 -2.5100908361339394 3.8626549637479308

Pt -0.7727423013143293 -3.3993388530366766 -2.6840908483424548

Pt -0.6223530870044203 1.9411938494087484 3.7305358458421209

Pt -0.8767497800641986 1.3061366201657365 -4.4022363265435134

Pt -0.7983248021550742 3.1507508826751507 -2.4328076461532695

Pt 0.3345679598032729 4.1105921267976466 2.6301598698304116

Pt -1.3166491230819448 -4.1727550090547663 -0.2502253702974157

Pt 0.5717858991943741 -3.7730741376355348 1.6591563086903214

Pt 0.9449201290712439 -0.1814272811438599 4.1778839084031185

Pt -1.6966599035518863 -0.3154026196959454 4.5227719963252451

Pt -1.9798667797390002 -3.4764548861907945 2.1775002195949038

Pt 1.2205746833659192 2.8159406755376337 -4.1164564052336940

Pt 1.2338849868004533 -3.9983001215800287 -0.9507564528749816

Pt -2.0785596099085635 3.3954366298887959 1.9155730508388673

Pt 1.4225983222755560 0.1604305091060039 -3.9856153260643601

Pt 1.7156615628302887 3.6183820316856807 -1.6527233664615537

Pt 1.5836828980956950 -2.3576031455314514 -3.2083934818124944

Pt 1.9442973851486192 2.1040878512282348 3.1870063737159167

Pt -2.9160138824526354 -2.7789268166905452 -4.2785498380311084

Pt -2.7850827500758766 -2.7372385305188325 4.5968723801246805

Pt -2.7583975041817905 3.2688577596563788 -0.6759783212601013

Pt -2.9043279019591624 -0.1893093692591976 -4.8070627542753117

Pt 2.1893197406035418 3.3935414288748826 0.8666396857288886

Pt 2.2353722027996068 -2.2040735161201153 3.0127212731730180

Pt -2.9813477933155466 1.6098854945535446 -2.7559440789386804

Pt -3.3672022100498080 -3.5716089202002714 -1.8931305688939883

Pt -3.2748114406369315 1.7546568253639490 3.6221986667154815

Pt -3.8876371737099125 -4.1998432147897713 0.5618746701705378

Pt 3.0856459551881588 -3.6811094685589425 0.9746371189917525

Pt 3.0319970847499031 1.6120984553202589 -2.6064690673956732

Pt 3.5067176952400660 0.0706415109575569 3.6150665897888641

Pt 3.3215771774786584 -2.1966765721166213 -1.0832943002252027

Pt -4.4093303046661454 -2.4738151789669307 2.4881281889501508

Pt -4.3321255705081096 -0.6020081825445236 4.3284943512115293

Pt -4.4416992738024952 2.5309325447431914 1.2735810359139552

Pt 3.7295339686538926 -0.8222970195472681 -3.2175759921617177

Pt 3.9758136822833801 1.4973657249521124 1.4928191378481228

Pt 4.0797094197925494 -1.2404539269476573 1.3765464532513103

Pt 4.2364516480293481 2.9924109072095590 -0.6629468807152937

Pt 4.4637433711303736 0.2543004051609201 -0.9053995349481182

S9.70 CO_2/Au_{55} (linear OCO angle)

C -0.9522205650713116 -6.7258552203283353 -0.6313160245387339

O -1.7026667182445174 -6.5081963246277921 -1.5063632686096915

O -0.2023223529682867 -6.9504916237151422 0.2416853728468452

Au -1.0542903814110525 3.2823473571628523 3.6904644044530919

Au 1.6979983596781838 -0.0767168386505824 5.0291671984340089

Au 1.0679846845215288 2.5838357621803065 5.2419271710613957

Au -1.3584378493185683 4.8650830194501236 -0.5152940929907823

Au -1.1064132714652861 0.8802709571314427 5.0478731218152131

Au -0.5901280419685802 5.4444719267787276 2.0583248805968219

Au 1.8541717406629146 0.9401164365714780 0.8099065162181203

Au 1.6166151620690674 -2.5512927589473384 3.7918771575605348

Au 1.1126889593808245 -3.7555638698729683 1.3620322079966420

Au -3.9189882211970457 -2.4067980136959419 -0.3048321201942469

Au 3.0583485272445663 1.8128538889772965 3.5322002689709135

Au 4.6633694383431816 -1.2770523082092382 0.6553472257530897

Au -2.1074596838961370 3.3413728727340097 -2.7023230334246797

Au -1.2943509789097623 -0.1511802216670415 -1.7912336758657388

Au -4.2674828915079557 1.7145077026731188 -2.1162093146155456

Au -1.8474758082795195 0.5788382746306648 0.8157311920742234

Au -4.3058889285542010 -0.6211230293825321 1.8273456174194036

Au 0.5084638738925125 4.3169568194940746 -2.4396188590920591

Au -0.2102301658399175 2.1648532877529312 -0.7319693540136003

Au -0.1573322034832168 2.4834559090529225 -4.3896689726112879

Au -1.5038250716677468 -3.4275717680822697 0.4821039005217569

Au 3.7042599270385019 -3.3584640802308132 2.2203968699669758

Au 1.2802911428675654 4.5270221779306583 0.2481700688319844

Au 4.3633047516432768 1.1640102090010946 -0.6417556532629336

Au 2.0364751341239873 1.3380079204229325 -5.5643235815928112

Au -2.6168775539480724 -1.1363772100167424 3.8994465363106139

Au 0.2917344286085286 -1.2514329338977366 0.3049384590541989

Au -2.7498183254518982 3.7961723187170553 1.6414629504996092

Au 1.4158933858862812 0.1593837813337708 -1.8813492987926603

Au -0.9382831231002329 -3.2980793363942644 3.1669799634004168

Au -3.9677199205639337 4.1091001297017531 -0.8351502508834392

Au 1.5576712899146385 4.0125156777562330 2.9312618557192049

Au -0.1659566836878619 -0.1818347837874293 -5.1480497581430544

Au 3.5802708028381871 1.2777890684119082 -3.2675810963950784

Au 3.9650220675817169 -1.1917069494421366 -2.0194614481006905

Au 5.1854687770620416 1.0834607430599943 1.9596175560804505

Au 3.1881769810575897 -3.3103259053923462 -0.4411340925914262

Au 2.3903396726020181 -1.0514231219426968 -4.3281948835600819

Au -4.3844071777115277 1.8684185394881332 0.6843818592259028

Au 0.1770739934683436 -2.6957329026377397 -3.9662729942763555

Au -1.9739237392295892 -2.9148084533472693 -2.1772911341798746

Au 0.1214545879909194 0.0800092677694601 2.6778854435690995

Au 3.4974152150425790 3.1678731165778413 1.1447845635197582

Au 2.4371842026517938 3.6626179720270531 -4.2152033258811699

Au -3.5317682775777350 -3.1980423252969845 2.3062431505031524

Au -5.5784278469621258 -0.2298961874967625 -0.5918158273815470

Au -2.4708008855439965 0.9992909283420468 -4.1040075987100355

Au -3.9436289854501934 -0.9461922070263882 -2.6460210195914584

Au 3.0055194490201491 3.3908314002664448 -1.5577577212523990

Au -3.0878786005094274 1.5029444194662547 3.1690532259531663

Au 2.6825228898424718 -3.4476179491243566 -3.1050160798428017

Au -2.2993374640911406 -1.7540689517214034 -4.6533236245576539

Au 0.5804626777507269 -3.5084478387810942 -1.3530762639251235

Au -0.4455038893056984 -1.7901111638757954 5.4399512186651782

Au 3.6936634841324385 -0.8320076072714386 3.2450544118551932

S9.71 CO_2/Au_{55} (bent OCO angle)

Chemisorbed CO_2 was not observed for the optimized systems.

S9.72 $CO_2/Pt_{13}Au_{42}$ (linear OCO angle)

C -3.5145629801586011 4.2039824783065898 -4.6599124818532918

O -3.3023482982671819 5.1249484326058576 -3.9646740045060973

O -3.7293047090609903 3.2849771100231253 -5.3574180967948806

Pt 0.1913846846531086 -0.2269942953452438 0.2521634083965018

Pt 0.2185012251394349 1.1589668157030033 2.5049448910799175

Pt 0.2534861098109262 1.1934682738157347 -2.0638529249775814

Pt 0.1483859440119239 -1.6588321150150351 2.5643595421850680

Pt 0.1647108572596902 -1.5978098908678939 -2.0078691233000203

Pt 1.5818036133872422 2.1094986431470542 0.2482741869794171

Pt -1.2075811322339423 2.0281549982724147 0.2269512305544791

Pt 1.5716259274638738 -2.4930573816020845 0.2652707625934151

Pt -1.2119406608716563 -2.5573282135173399 0.2432344579126119

Pt 2.4528001630127161 -0.2347424923429165 1.6498876818169206

Pt 2.4646765664785502 -0.2261245773265577 -1.1223428444574408

Pt -2.0642677472106428 -0.2320952776316175 1.6571816785106550

Pt -2.0820312434569637 -0.2229324363076560 -1.1263231443119202

Au -4.3843195388307183 -0.2206280808082797 -2.5717656742446735

Au 0.2029642311793873 2.5849210585589324 4.8143311668481878

Au 0.2325317814762035 2.6390066155093228 -4.3794889198570459

Au 0.1613777461209737 -3.1022653966419957 4.8829630314048043

Au 0.1754264445608475 -3.0343748997490652 -4.3113419391858407

Au 3.0458609308520845 4.4139688695302501 0.2457004952331702

Au -2.6209384070898611 4.3509237221912391 0.2245722416622290

Au 2.9918832254292909 -4.8140100923341445 0.2724679279443868

Au -2.6717451578491964 -4.8642899339781165 0.2543796609263208

Au 4.7586506546534304 -0.2343800011207043 3.0923888278762632

Au 4.7773230366930690 -0.2198971808941091 -2.5551409178437314

Au -4.3824303028757878 -0.2392460114418010 3.0798858464415488

Au 0.1953630744286769 4.5269637348404510 0.2648478648567537

Au 0.1775082311128128 -4.9846727778213600 0.2656626309640319

Au -4.5394640993009983 -0.2186844036124738 0.2569834811979169

Au 4.9276894408545946 -0.2347817768266838 0.2667435092582736

Au 0.2124471872258837 -0.2122030044301946 -4.4944310704024026

Au 0.1696586773224586 -0.2476145507816883 4.9830689075339025

Au 1.6208149600778397 -4.0449053074034422 2.6318808400340936

Au -1.2902320529561813 -4.0701867307559665 2.6200569170914427

Au 1.6303407702933441 -4.0280250222040754 -2.0898668971490650

Au -1.2733731320404047 -4.0708501463843136 -2.1061188735216625

Au 4.0122554968303428 -2.5965713465529641 -1.1872516128546506

Au 4.0018533105920895 -2.5967760566855214 1.7169840775865557

Au -3.6245526791248803 -2.6011882042385830 -1.1951120292057118

Au -3.6142273218464585 -2.5945609309430564 1.6949883165368449

Au 1.6847304354810415 3.6192706859244614 -2.1242632746221428

Au 1.6717106345941781 3.6076292092855633 2.6161254910814096

Au -1.2014373605372697 3.5864901325994953 -2.1123321000796693

Au -1.2588545819411650 3.5686036232422662 2.5920587337451266

Au -2.1127255604503024 1.2125188454875575 -3.5520299290567099

Au 2.5910507276642054 1.2344971420700812 -3.5843282538591037

Au -2.1888729994808678 -1.6903146605359689 -3.5515473904395662

Au 2.5454859190454036 -1.6762356647607080 -3.5397687789301422

Au -3.6346164126682048 2.1320682548988446 1.6900350796740600

Au -3.6259851646331196 2.1477425108848802 -1.2310635928386466

Au -2.1963431612727380 -1.7064534978052963 4.0928579670078635

Au 2.5162382078117735 -1.6981082021092826 4.0739691275516394

Au 2.5600576285844081 1.2165861994824798 4.0787552565063558

Au -2.1635633375234811 1.2265397673813547 4.0585006406418405

Au 3.9946963152544122 2.1437274973101292 -1.1917848705575198

Au 3.9904238823253966 2.1356859397050556 1.6975528652155167

S9.73 $CO_2/Pt_{13}Au_{42}$ (bent OCO angle)

Chemisorbed CO_2 was not observed for the optimized systems.

S9.74 $CO_2/Pt_{42}Au_{13}$ (linear OCO angle)

C 3.4477238906240957 -5.0191834479317787 -2.9592568290112018

O 3.4410429130683675 -5.6025843278032834 -1.9407348878496926

O 3.4602904612405356 -4.4538833127157140 -3.9870200567312954

Au -0.2523035452094083 4.6657834944634136 0.1821661807480045

Au -0.7081920538226646 1.8298285236061116 -4.5967561813062270

Au -0.7556390776711558 3.7775729939749039 -2.4385321997624994

Au 0.5108802083257794 4.6721033029955494 2.9211975727646502

Au 1.4659664284243601 3.3679957661131614 -4.0664525411340344

Au -2.0602320955632920 4.0236941117850122 2.1636221869907031

Au 1.9197470538255808 4.2993660719864781 -1.4568900262371571

Au -2.8500597634051172 3.8422210008754143 -0.6382359258667530

Au -2.7315988109933458 0.0651106328027693 -4.9733394016154060

Au 2.5376746085535502 4.1526807067154250 1.1899021785713761

Au -3.0170284224134929 2.1234097721403846 -2.9401917887858398

Au -4.4676034726212306 3.0015765150824296 1.4219113002375836

Au -4.4148437779938652 1.1933021843238658 -0.7206548570988619

Pt -0.2586501082694360 -1.1374006323668053 -4.4804414221827225

Pt -0.0221736895278314 -2.1664687127854836 3.9722038860663158

Pt -0.4574402083579289 -2.8715291118071913 -2.4485275104898614

Pt -0.5093963786922769 2.3216566804310266 3.8085466347350794

Pt 0.3042195145716023 2.1624994334349865 1.2625334925613518

Pt 0.5100240640840997 -0.4840810816290639 1.7662939619675526

Pt -1.0069281742258862 -3.8887601508053282 -0.0984969941021891

Pt 0.7620858453130553 1.6501260607841737 -1.3619734526111646

Pt 0.8281000759784648 -3.4326760768948517 1.7927126235249238

Pt 0.8440736197094768 -0.9486744216124892 -0.8886092576477856

Pt -1.2026487314750589 0.0317865007615110 -2.3889403704335406

Pt 1.0954884482227316 0.2364231432343085 4.2163232605631125

Pt -1.4954187494939155 0.0191659273763156 4.5665005775033540

Pt -1.6023376891703875 -1.2231610980862706 0.1019945824223683

Pt -1.6972736944529092 -3.0895160461921853 2.2738628116121964

Pt 1.5088397261319895 -3.3901430889632720 -0.7773680022717332

Pt -1.9122817117065025 0.4200231766775204 2.0165494451300097

Pt -1.6895940747803671 1.4259442710127834 -0.3178226937710306

Pt 1.6202075860779364 0.6343745609593496 -3.8637763452498826

Pt 1.8911156651764653 -1.8686840248868621 -3.0631757339751013

Pt 2.1149423116064860 2.4840677342808442 3.3049026535404433

Pt -2.5285468848025823 -2.5055060405134948 -4.1028836682498406

Pt -2.5014469717062355 -2.4610354177396814 4.6961517848792953

Pt 2.3878100723435307 0.5986991970954387 0.3899771355929395

Pt 2.4303830665163448 -1.7822823301964730 3.0880849476059646

Pt -3.0449584228641968 -3.1425303912881613 -1.6968551111239834

Pt -3.1536597166382827 2.0146187333186814 3.6488653982297450

Pt -3.5829906826216935 -3.8885146146000618 0.7108300041904839

Pt 3.3513521426957325 -3.2229384123859037 1.1150126173994044

Pt 3.2012316204284788 2.1402574146178233 -2.3708007557561581

Pt -3.7180139247965607 -0.6857418894037026 -2.5497292046627082

Pt 3.6762653780978556 0.4317910320659586 3.7618175057994696

Pt 3.6700600081993877 -1.7678099386900905 -0.9746825474642186

Pt -4.1022458410133789 -2.1234217080102229 2.5380011937178937

Pt -4.0900337485898470 -0.3692695109850896 4.3861324693976433

Pt -4.2101123093873865 -1.4286734074763225 -0.0463879413751008

Pt 3.9302524195430411 -0.2561110929469732 -3.0257842778119448

Pt 4.1815670309084672 1.9151078299753126 1.7040149301689407

Pt -4.5248788943445097 0.3761360544705392 1.8782229316418497

Pt 4.2756639075600562 -0.7731290549559284 1.4556125049532092

Pt 4.4894622575476939 3.3781987365024775 -0.4533109323021122

Pt 4.7120613018355799 0.7281877798087157 -0.7063158556358157

S9.75 $CO_2/Pt_{42}Au_{13}$ (bent OCO angle)

C 1.8730492766121190 -0.0910010712286970 -5.8725522887454806

O 0.9785207823441544 -0.9795464174314406 -6.1562516844582111

O 2.6771976711602106 0.5034741562954341 -6.5515329940600351

Au -0.1502007945249639 4.4066901613655052 0.4512432525571159

Au -0.6856086495544398 1.4735151512672111 -4.0070805740183575

Au -0.7476977933300022 3.5846506091976895 -2.1439936462595095

Au 0.6498864847193664 4.4228883610526726 3.1538475744405479

Au 1.4583338692645622 3.1198012573148484 -3.8819858184023821

Au -1.9445734058897850 3.7866806803429371 2.4658939709448835

Au 1.9503251612222448 3.9700741761732647 -1.2808204896614366

Au -2.7775994688972228 3.6002253098830526 -0.2811771446582188

Au -2.8123364058366827 -0.0313358817882525 -4.7039857546148864

Au 2.6308840083432958 3.9229958004853449 1.3433986258780668

Au -3.0363957609495786 1.8801806014931666 -2.5712291584825553

Au -4.3744044679666318 2.7677305706732005 1.7830062330309553

Au -4.4371085706165774 0.9703594874289498 -0.3640540778609807

Pt -0.1721185161875036 -1.3939506867182496 -4.4698580694835135

Pt 0.1559111781042111 -2.4453626518616085 4.1323113371662759

Pt -0.3268039418851715 -3.1927797426934772 -2.3960465094643513

Pt -0.3627544484822289 2.0381698003816506 3.9893635213585719

Pt 0.3932594499718408 1.8609074439264255 1.3982521037437299

Pt 0.6486005771277688 -0.7909773793072246 1.8810816670761201

Pt -0.9093488709108586 -4.0705431556499230 0.0233157268676760

Pt 0.7434250332747299 1.3602094733474246 -1.3146908359887521

Pt 0.9593846313009982 -3.6508043909424446 1.8816095201243646

Pt 0.9007826959115226 -1.2319056279087013 -0.8494468637307686

Pt -1.3228559875129280 -0.5766401215640196 -2.1495106566078408

Pt 1.2579644574028706 -0.0418944176898899 4.3318173336506023

Pt -1.3183231737059069 -0.2754909454693157 4.7528513878769720

Pt -1.4948318102991900 -1.4678212536291388 0.3406703890381970

Pt -1.5528399326315077 -3.3423143050376600 2.4562740819836466

Pt 1.6192801000943282 -3.6912588067796710 -0.6876228027127378

Pt -1.7382359369270199 0.2273280476939404 2.2358574686870072

Pt -1.6569402949050920 1.1417277815540574 -0.1626538962758307

Pt 1.7828688951853335 0.3112674759345149 -3.8676210243909028

Pt 2.0221267671270606 -2.1964543233693794 -2.9589097759474110

Pt 2.2293757949757920 2.2142433597706512 3.4004172887497588

Pt -2.4525431377576270 -2.5710143125741398 -3.8768271124583360

Pt -2.3166883717588087 -2.7479821086407776 4.8860227290766689

Pt 2.4485677648899715 0.3363405108229652 0.4026807054881005

Pt 2.6029155751533608 -2.0627690436700492 3.2161835355263428

Pt -2.9588065810126567 -3.3043814786770804 -1.5085757159216118

Pt -3.0077871654587520 1.7533310985370010 3.9694771237005342

Pt -3.4504343403016380 -4.1047545343184426 0.8894896491422561

Pt 3.4758399116727903 -3.4827845586359034 1.1984706776359215

Pt 3.2327734098744090 1.8077215487421601 -2.2975611860554959

Pt -3.8881768471481850 -0.8620897110134349 -2.3101537202070257

Pt 3.8228399037214924 0.1846722070594433 3.8350282660404500

Pt 3.7565259960649913 -2.0376890907690308 -0.8913667967897854

Pt -3.9680239055344986 -2.3921637497472981 2.7809613338145804

Pt -3.9168982019490448 -0.6617529611786770 4.6697430248029699

Pt -4.1231503783024346 -1.6602067252268045 0.2227613839912732

Pt 4.0872726055293596 -0.5645506087076511 -2.9488933766084240

Pt 4.2441958637588693 1.6452917648915655 1.7419560063958088

Pt -4.3509400491893659 0.1359479849247514 2.2009376767550184

Pt 4.3490896155442860 -1.0228807795709836 1.5199546267674617

Pt 4.4652478153777784 3.0788042703014211 -0.4161679413262607

Pt 4.8379819136965851 0.4398717509381145 -0.6343083071207789