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Electronic Supporting Information

Regioselectivity of the Pauson-Khand Reaction in Single-Walled Carbon Nanotubes

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The PKR in SWCNTs with acetylene

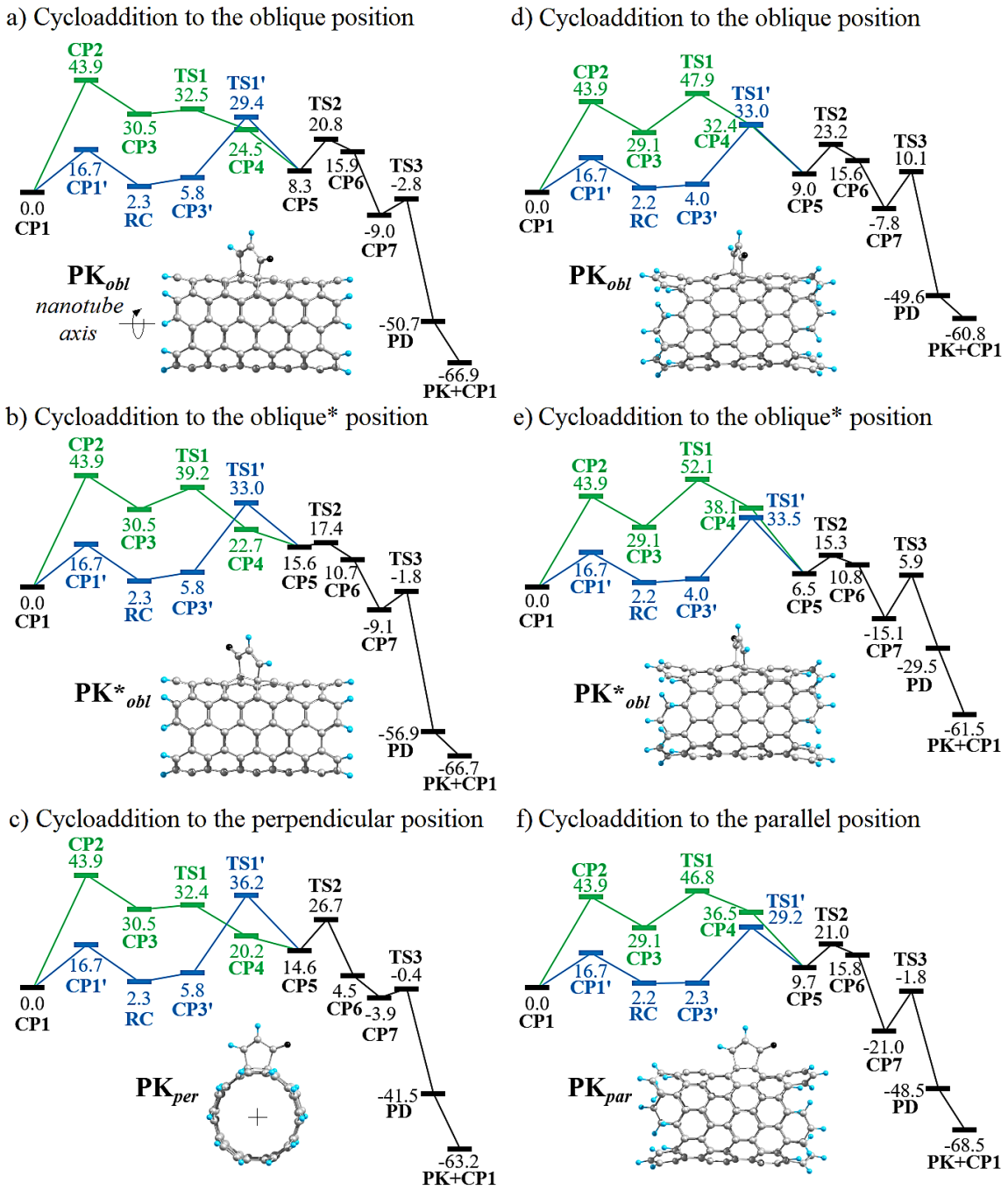


Figure S1. Gibbs energy profiles in kcal/mol for the Pauson-Khand reaction with acetylene in (5,5)-SWCNT (subsections a, b, and c) and (9,0)-SWCNT (subsections d, e, and f). Blue and green lines respectively correspond to the alternative and generally-accepted pathways. The alternative pathway converges to the generally-accepted mechanism (black lines).

The PKR in (5,5)-SWCNT is briefly discussed first. This cycloaddition can occur at the oblique and perpendicular positions relative to the nanotube axis. The distinction in the reaction pathways is given by the nanotube insertion. Because of symmetry arguments, only one **PK** adduct at the perpendicular position is possible, $\mathbf{PK}_{per}$; however, the formation of **PK** at the oblique position can be done via two pathways, $\mathbf{PK}_{obl}$ and $\mathbf{PK^*}_{obl}$.

In general, according to profiles schematized in Fig. S1, the determinant states are **CP1**, **CP2** and **TS1'**; wherein **CP1** is the turnover-frequency determining intermediate (TDI) in any case, yet the turnover-frequency determining transition state (TDTS) is **CP2** in the Magnus mechanism describing an energy barrier of 43.9 kcal/mol. On the other hand, **TS1'** is the TDTS for the alternative pathway with a more effective energy barrier of 29.4 kcal/mol via $\mathbf{TS1'}_{obl}$. Our results suggest that the PKR in (5,5)-SWCNT with acetylene can be difficult to proceed in laboratory in view of that an energy barrier of at least 29.4 kcal/mol, via $\mathbf{TS1'}_{obl}$, must be overcome.

In the case of the PKR in (9,0)-SWCNT, the cycloaddition can occur at the parallel and oblique positions with respect to the nanotube axis. Only one pathway leading to **PK** is possible at the parallel position, $\mathbf{PK}_{par}$, but two pathways can be distinguished at the oblique position, $\mathbf{PK}_{obl}$ and $\mathbf{PK^*}_{obl}$. In general, Fig. S1 shows that the TDTS is **TS1'** in the alternative pathway and the energy barrier via $\mathbf{TS1'}_{par}$ is at least 3.8 kcal/mol lower than the ones in the oblique pathways. The TDTS is still **CP2** in the Magnus mechanism with the same energy barrier of 43.9 kcal/mol. Besides, since $\mathbf{PK}_{par}$ is the most stable adduct, it is concluded that the parallel pathway is the most kinetically and thermodynamically favored reaction mechanism. As a final remark, it should be noticed that the energy barrier of 29.2 kcal/mol via $\mathbf{TS1'}_{par}$ in (9,0)-SWCNT is identical to the one via $\mathbf{TS1'}_{obl}$ in (5,5)-SWCNT, 29.4 kcal/mol; therefore, both armchair and zig-zag SWCNTs may be not thermally functionalized to form cyclopentenones with acetylene under laboratory conditions.

Table S1. Energy barriers and Gibbs energy changes in kcal/mol through different pathways for every step related to the Pauson-Khand reaction in (9,0)-SWCNT with 2-heptyne.

Step	$\Delta G^{\ddagger}$	Pathway	ΔG	Pathway
Nanotube Coordination	40.63	from **CP1** to **CP2**	24.43	from **CP1** to **CP3**$_{me}$
	15.83	from **CP1** to **CP1'**$_{me}$	-5.43	from **CP1** to **RC**$_{me}$
	16.05	from **CP1** to **CP1'**$_{bu}$	-6.70	from **CP1** to **RC**$_{bu}$
Nanotube Insertion	23.56	from **CP3**$_{me}$ to **TS1**$_{me,par}$	17.34	from **CP3**$_{me}$ to CP4$_{me,par}$
	27.24	from **RC**$_{me}$ to **TS1'**$_{me,par}$	13.12	from **RC**$_{me}$ to **CP5**$_{me,par}$
	33.99	from **RC**$_{me}$ to **TS1'**$_{me,obl}$	23.74	from **RC**$_{me}$ to **CP5**$_{me,obl}$
	38.79	from **RC**$_{me}$ to **TS1'***$_{me,obl}$	20.20	from **RC**$_{me}$ to **CP5***$_{me,obl}$
	29.40	from **RC**$_{bu}$ to **TS1'**$_{bu,par}$	20.21	from **RC**$_{bu}$ to **CP5**$_{bu,par}$
	39.51	from **RC**$_{bu}$ to **TS1'**$_{bu,obl}$	25.34	from **RC**$_{bu}$ to **CP5**$_{bu,obl}$
	46.24	from **RC**$_{bu}$ to **TS1'***$_{bu,obl}$	28.19	from **RC**$_{bu}$ to **CP5***$_{bu,obl}$
CO Insertion	1.95	from **CP5**$_{me,par}$ to **TS2**$_{me,par}$	-17.23	from **CP5**$_{me,par}$ to **CP6**$_{me,par}$
	1.63	from **CP5**$_{bu,par}$ to **TS2**$_{bu,par}$	-24.44	from **CP5**$_{bu,par}$ to **CP6**$_{bu,par}$
Reductive Elimination	8.99	from **CP7**$_{me,par}$ to **TS3**$_{me,par}$	-36.44	from **CP7**$_{me,par}$ to **PD**$_{me,par}$
	11.99	from **CP7**$_{bu,par}$ to **PD**$_{bu,par}$	-45.11	from **CP7**$_{bu,par}$ to **PD**$_{bu,par}$

Table S2. The ASM at the TDTS of the PKR in SWCNTs. The fragment *f*1 stands for the nanotube and *f*2 for the **CP1** fragment. All electronic energies in kcal/mol.

Structure		$\Delta E^{\ddagger}$ $(f1)_{strain}$	$\Delta E^{\ddagger}$ $(f2)_{strain}$	$\Delta E^{\ddagger}_{strain}$	$\Delta E^{\ddagger}_{int}$	$\Delta E^{\ddagger}$
acetylene and (5,5)-SWCNT	**TS1'$_{obl}$**	22.7	60.2	82.9	-69.6	13.3
	TS1'*$_{obl}$	23.5	63.2	86.7	-71.8	14.9
	TS1'$_{per}$	23.7	68.4	92.1	-71.5	20.6
acetylene and (9,0)-SWCNT	**TS1'$_{par}$**	23.7	59.3	83.0	-71.1	11.9
	TS1'$_{obl}$	19.5	57.1	76.6	-58.8	17.8
	TS1'*$_{obl}$	19.8	57.5	77.3	-60.8	16.5

In the case of (5,5)-SWCNT, the deformation in the nanotube [$\Delta E^{\ddagger}(f1)_{strain}$] is similar for the three reaction pathways (~23 kcal/mol), then the main contribution to the total strain is given by the deformation of **CP1** [$\Delta E^{\ddagger}(f2)_{strain}$], bringing about a larger deformation through the perpendicular pathway (68.4 kcal/mol). Given that $\Delta E^{\ddagger}_{int}$ results in -70 ± 2 kcal/mol for all the cases, we conclude that the strain is the main factor influencing the PKR in (5,5)-SWCNT with acetylene. Then the pathway with the lowest strain is the kinetically favored, that is **TS1'$_{obl}$** ($\Delta E^{\ddagger}_{strain}$ = 82.9 kcal/mol). In the case of (9,0)-SWCNT, $\Delta E^{\ddagger}(f1)_{strain}$ in the parallel cycloaddition is higher by ca. 4 kcal/mol than the ones in the oblique pathway, these latter with $\Delta E^{\ddagger}(f1)_{strain} \approx$ 20 kcal/mol. Besides, $\Delta E^{\ddagger}(f2)_{strain}$ in the parallel cycloaddition is also higher by ca. 2 kcal/mol than the ones in the oblique pathway, these latter with $\Delta E^{\ddagger}(f2)_{strain} \approx$ 57 kcal/mol. Therefore, the energy barrier via **TS1'$_{par}$** involves more distortion for the reactants, but it results in the lowest activation energy which is attributed to a significantly lower $\Delta E^{\ddagger}_{int}$ (-71.1 kcal/mol). Consequently, it is concluded that the interaction energy between **CP1** and the nanotube at the TDTS is the main factor controlling the course of the PKR in (9,0)-SWCNT with acetylene. This more favorable interaction energy in **TS1'$_{par}$** comes from better orbital interactions and, particularly, from a better $HOMO_{nanotube}$-$LUMO_{\mathbf{CP1}}$ interaction because of a more stabilized LUMO in the **CP1** fragment of the parallel attack, as reported in the following two tables.

Table S3. Absolute HOMO and LUMO energies in kcal/mol for fragments (*f*1 nanotube and *f*2 **CP1**) isolated from the corresponding **TS1'**. The HOMO and LUMO energies resulting in the entire **TS1'** complex are also reported. Calculations as obtained via O3LYP(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP (TZP for cobalt) including ZORA, FCA, and COSMO:N-methyl-2-pyrrolidone.

Structure		*H*(*f*1)	*L*(*f*1)	*HOMO*	*LUMO*	*H*(*f*2)	*L*(*f*2)
acetylene and (5,5)-SWCNT	**TS1'**$_{obl}$	-120.03	-92.54	-117.80	-91.60	-143.49	-101.42
	TS1'*$_{obl}$	-119.99	-91.92	-119.16	-93.24	-144.29	-104.10
	TS1'$_{per}$	-119.48	-93.65	-119.11	-93.93	-142.72	-105.73
optimized (5,5)-SWCNT		-119.80	-92.04	-	-	-	-
acetylene and (9,0)-SWCNT	**TS1'**$_{par}$	-126.54	-87.03	-124.90	-90.84	-141.06	-102.00
	TS1'$_{obl}$	-126.56	-86.50	-123.01	-90.56	-138.94	-95.91
	TS1'*$_{obl}$	-126.70	-85.88	-121.53	-89.43	-138.80	-91.11
optimized (9,0)-SWCNT		-126.56	-85.97	-	-	-	-
optimized **CP1**		-	-	-	-	-146.62	-82.74

Table S4. Energy decomposition analysis in kcal/mol for **TS1'**. Calculations as obtained via O3LYP(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP (TZP for cobalt) including ZORA, FCA, and COSMO:N-methyl-2-pyrrolidone.

Structure		*Pauli repulsion*	*interactions*				*Kinetic*	*Exchange Correlation*
			Electrostatic	*Orbital*	*Steric*	*Coulomb*		
acetylene and (5,5)-SWCNT	**TS1'**$_{obl}$	132307.02	-29923.20	-136340.03	102383.82	680.40	29112.55	-33826.06
	TS1'*$_{obl}$	132244.68	-29898.99	-136299.19	102345.69	685.63	29070.44	-33810.68
	TS1'$_{per}$	132258.26	-29909.60	-136296.73	102348.66	706.92	29075.98	-33821.47
acetylene and (9,0)-SWCNT	**TS1'**$_{par}$	130307.61	-29338.36	-134807.72	100969.25	-45.81	29141.20	-33595.53
	TS1'$_{obl}$	130316.02	-29342.23	-134806.97	100973.79	-29.77	29131.32	-33592.54
	TS1'*$_{obl}$	130300.49	-29340.38	-134794.82	100960.11	-6.07	29103.56	-33591.87

Materials and instrumentation

All chemicals were reagent-grade, purchased from commercial sources and used as received, unless otherwise specified. HiPco SWCNTs were purchased from NanoIntegris (www.nanointegris.com), purified grade with an individual diameter between 0.8 and 1.2 nm and individual length between 100 and 1000 nm. (6,5) enriched SWCNTs were produced by SourthWest Nano Technologies Inc. (www.swentnano.com), using the CoMoCAT® method, and purchased from Sigma Aldrich (www.sigmaaldrich.com). The denoted as (6,5)-SWCNTs presents a 0.7-0.9 nm diameter, 1 µm average length, mostly semiconducting and 95% purity.

Samples sonication was carried out by using an Elmasonic P 300 H sonicator bath (37 kHz).

Thermogravimetric analyses (TGA) were performed using a TGA/DSC Linea Excellent instrument by Mettler-Toledo, collected under a flow of nitrogen (90 mL/min). The sample (~0.5 mg) was introduced inside a platinum crucible and equilibrated at 40 ºC followed by a 10° C/min ramp between 40º C and 1000° C. The weight changes were recorded as a function of temperature.

Raman spectroscopy analyses were performed on an inVia Raman microscope (Renishaw) at room temperature, equipped with laser at 785 nm, on solid samples deposited onto a glass coverslip. The laser spot was focused on the sample surface using a long working distance 50X objective. Reported spectra are average of at least five measurements performed in different areas of the sample and normalized to the G-Band. The intensity ratio ID/IG was obtained by taking peak intensities without baseline corrections.

The XPS data signals were taken in increments of 0.07 eV with dwell times of 40 ms. The binding energy scale of the instrument was calibrated with respect to Au4f7/2 (84.0 eV) and Cu2p3/2 (932.6 eV) emissions. Charge effects on the samples were corrected by taking the C1s line of adventitious carbon at binding energy (BE) of 284.8 eV which gives an accuracy of ~0.1 eV. High resolution spectra envelopes were obtained by curve fitting synthetic peak components using the software “XPS peak”. The raw data were used with no preliminary smoothing. Symmetric Gaussian-Lorentzian (90%G-10%L) lines were used to approximate the line shapes of the fitting components. Atomic ratios were computed from experimental intensity ratios and normalized by atomic sensitivity factors.

Fluorescence excitation-emission maps were recorded on a HORIBA Jobin Yvon Nanolog 4 Spectrofluorometer equipped with a multichannel InGaAs detector. The pristine and the functionalized HiPco SWCNTs were prepared with 2% wt. SDBS in distillated water. The concentration of the prepared solutions was adjusted to be the same.

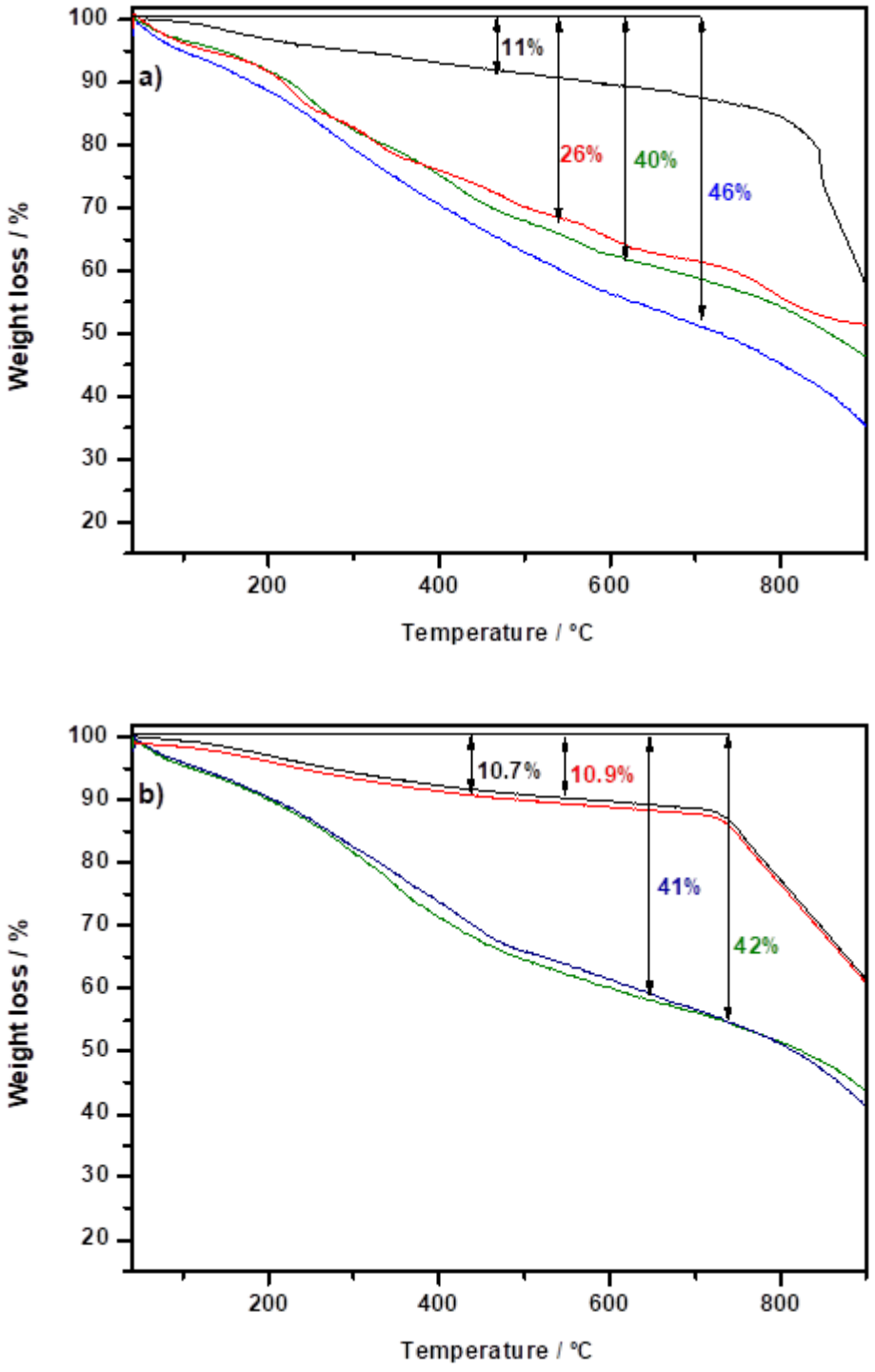


Figure S2. TGA profile of a) *pristine* HiPco SWCNT (—) and PK-funtionalizated derivatives with alkyne **1a** (—), **1b** (—), and **1c** (—); b) *pristine* (6,5) enriched SWCNT (—) and PK-funtionalizated derivatives with alkyne **1a** (—), **1b** (—), and **1c** (—). Heating rate: 10ºC/ min, atmosphere: Ar.

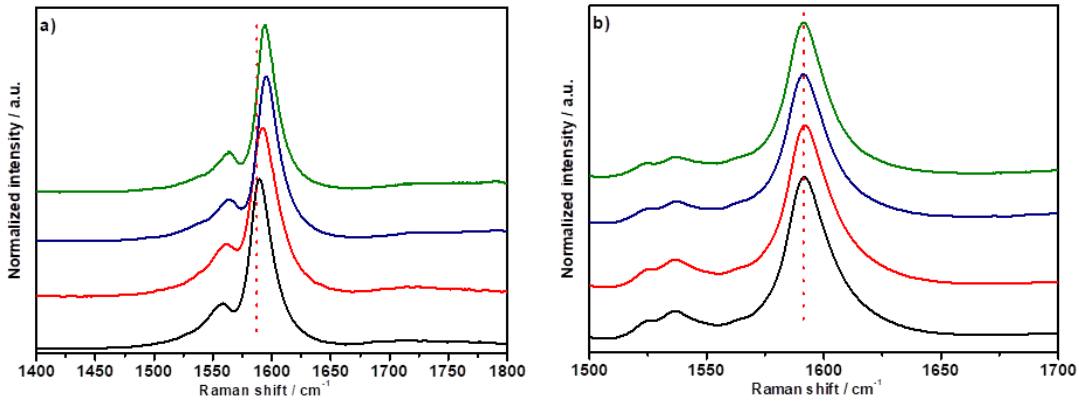


Figure S3. Comparison of G-band of a) *pristine* HiPco SWCNT (—) and PK-funtionalizated derivatives with alkyne **1a** (—), **1b** (—), and **1c** (—); b) *pristine* (6,5) SWCNT (—) and PK-funtionalizated derivatives with alkyne **1a** (—), **1b** (—), and **1c** (—).

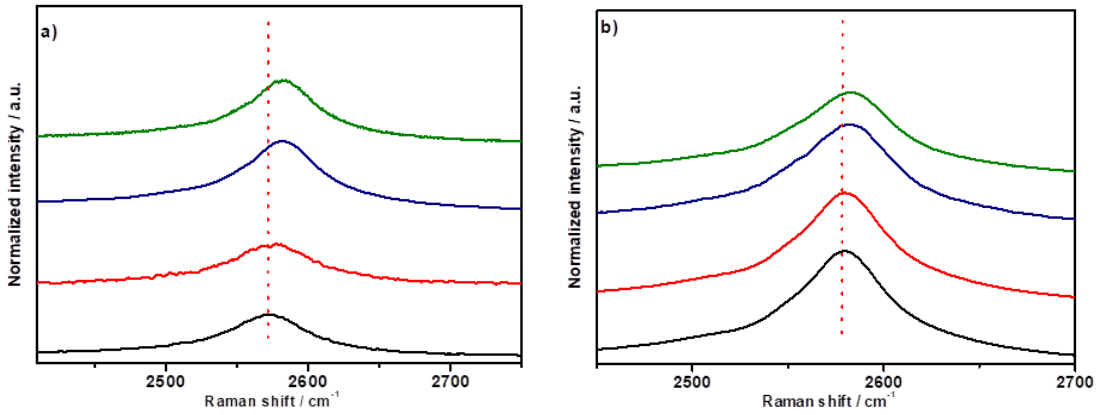


Figure S4. Comparison of 2D-band of a) *pristine* HiPco SWCNT (—) and PK-funtionalizated derivatives with alkyne **1a** (—), **1b** (—), and **1c** (—); b) *pristine* (6,5) SWCNT (—) and PK-funtionalizated derivatives with alkyne **1a** (—), **1b** (—), and **1c** (—).

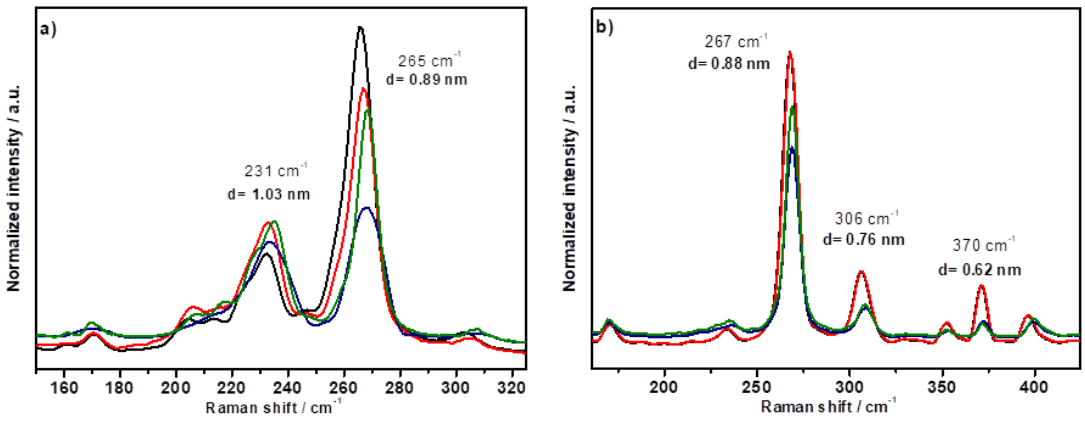


Figure S5. RBMs in Raman spectra for a) *pristine* HiPco SWCNT (—) and PK-funtionalizated derivatives with alkyne **1a** (—), **1b** (—), and **1c** (—); b) *pristine* (6,5) SWCNT (—) and PK-funtionalizated derivatives with alkyne **1a** (—), **1b** (—), and **1c** (—), taken with E_{exc}=1.58 eV(λ_{exc}=785 nm).

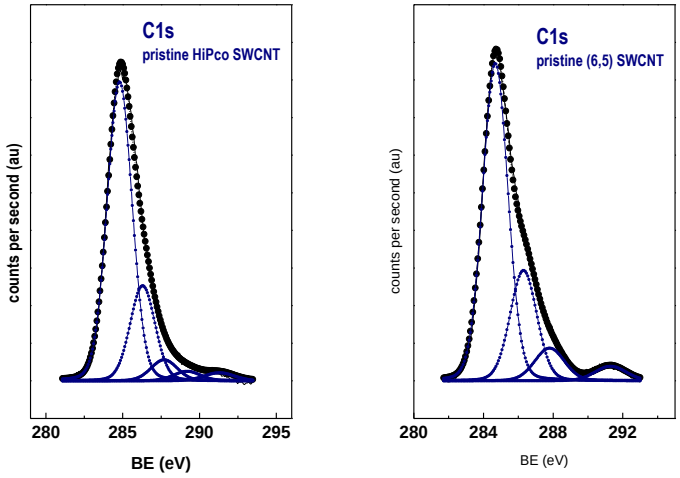


Figure S6. C1s core-level spectra of starting *pristine* HiPco and (6,5) enriched SWCNT.

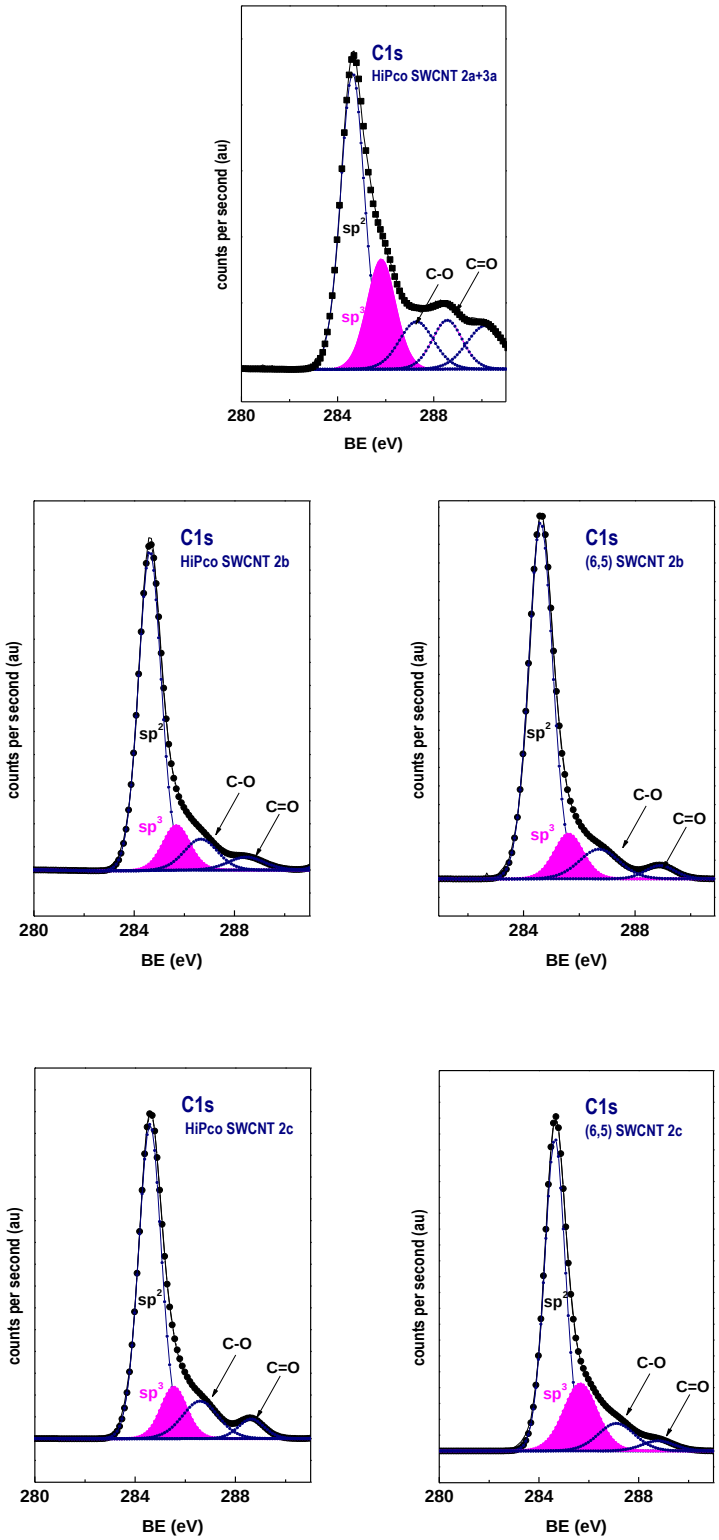


Figure S7. C1s core-level spectra of PK-funtionalized SWCNT. The magenta line correspond to sp^3 carbon atoms after reaction.

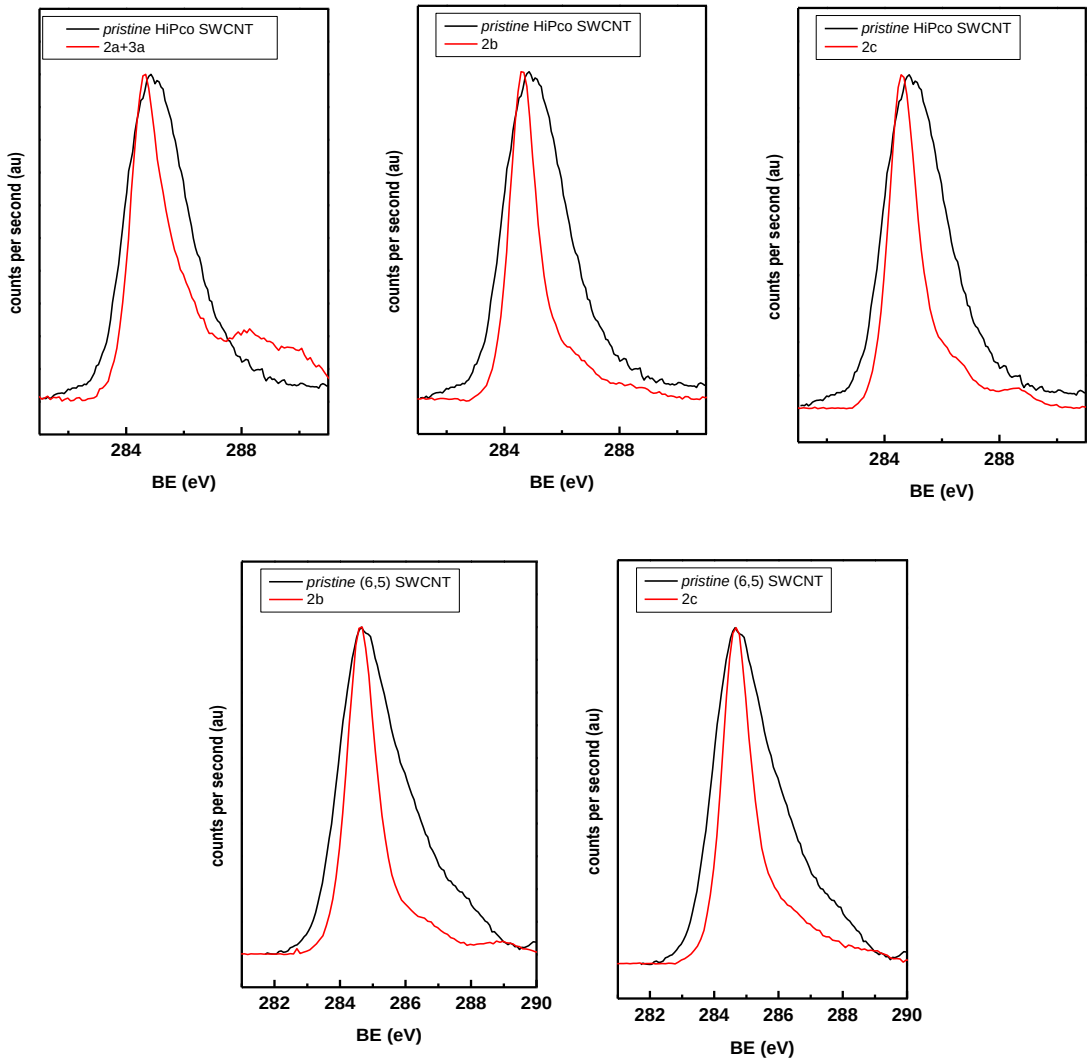


Figure S8. XPS C1s core-level spectra of *pristine* SWCNT compared to PK-functionalized SWCNT.

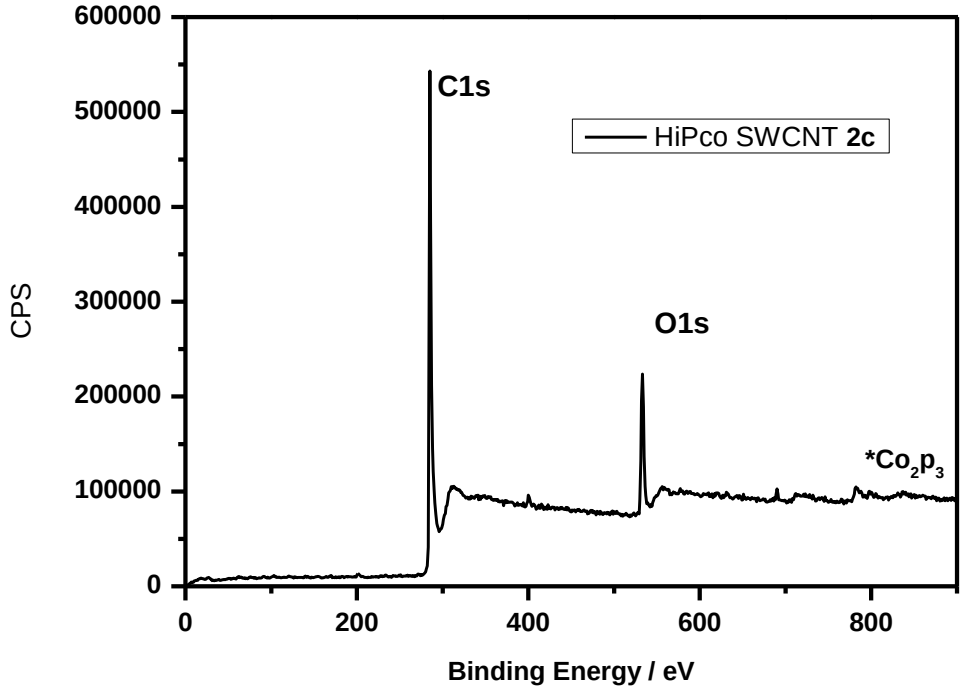


Figure S9. XPS analysis of HiPco SWCNT **2c** hybrid.

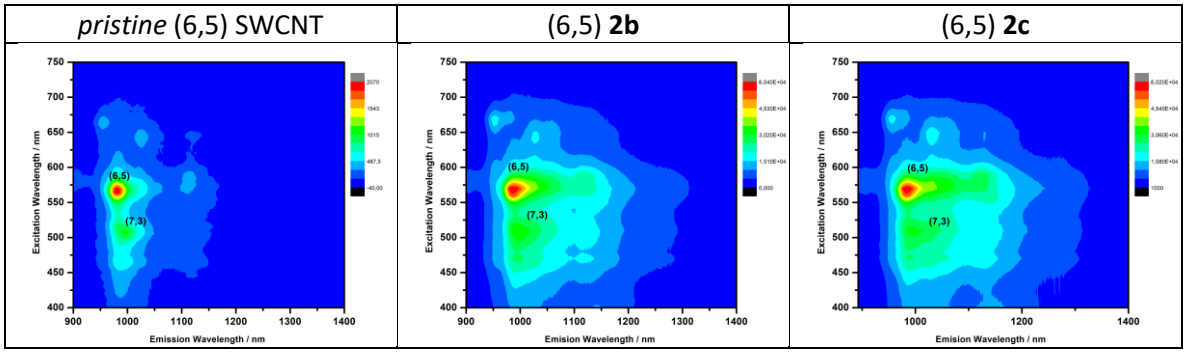


Figure S10. 3D photoluminescence maps for (6,5) SWCNT in D_2O at room temperature.

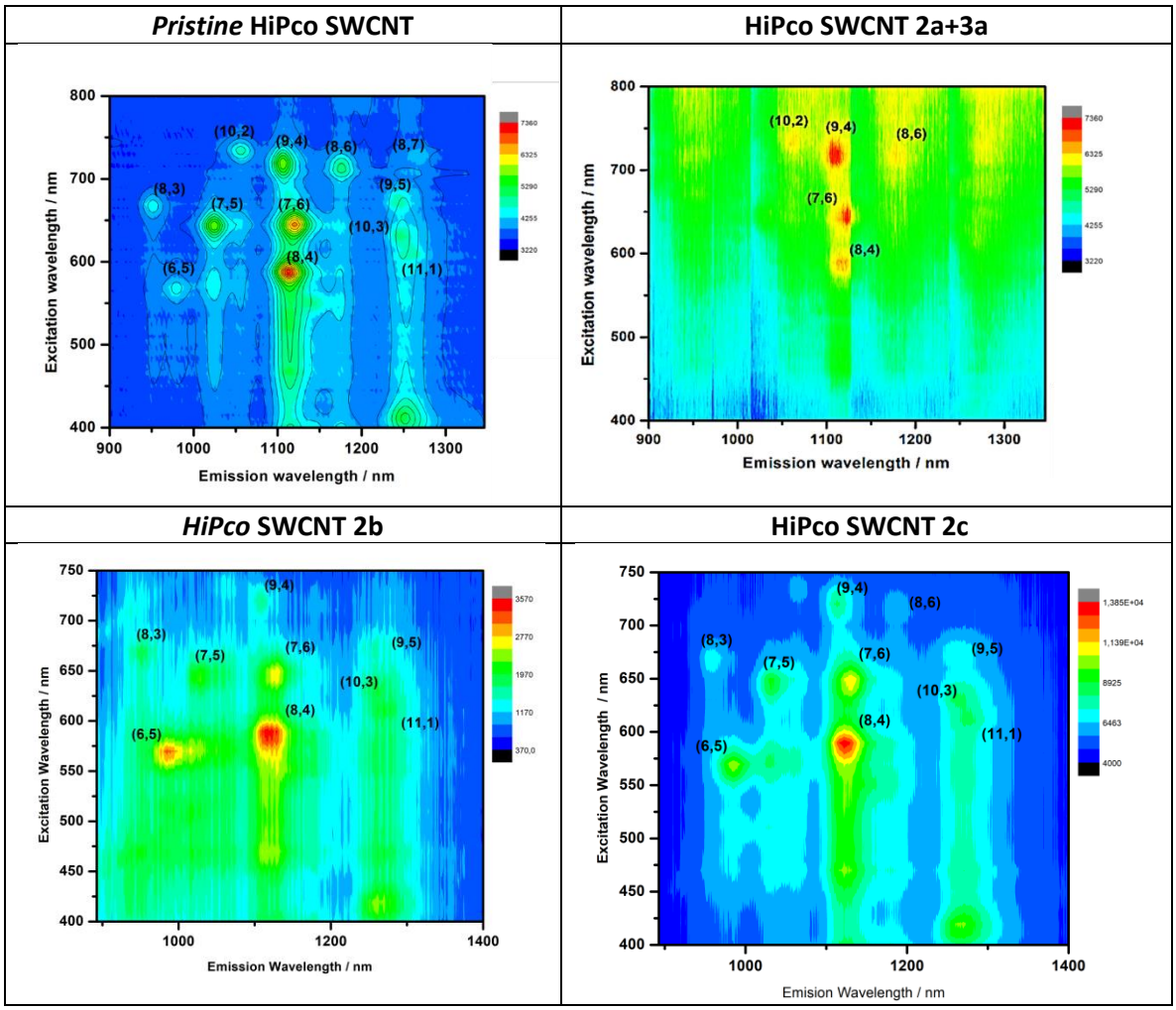


Figure S11. 3D photoluminescence maps for Hipco SWCNT and PK-derivatives in D_2O at room temperature.

Benchmarking DFT Methods for the Pauson-Khand Reaction

Experimental Reference:

D. R. Hartline, M. Zeller, C. Uyeda, "Well-Defined Models for the Elusive Dinuclear Intermediates of the Pauson–Khand Reaction" *Angew. Chem. Int. Ed.* **2016**, 55, 6084-6087.

Uyeda et al. reported a direct experimental investigation of the dinuclear metallacycle-forming step of a Pauson–Khand reaction. Their findings capitalize on well-defined d^9–d^9 dinickel complexes supported by a naphthyridine–diamine (NDI) pincer ligand as functional surrogates of $Co_2(CO)_8$. Figure S12 illustrates the mechanism they formulated:

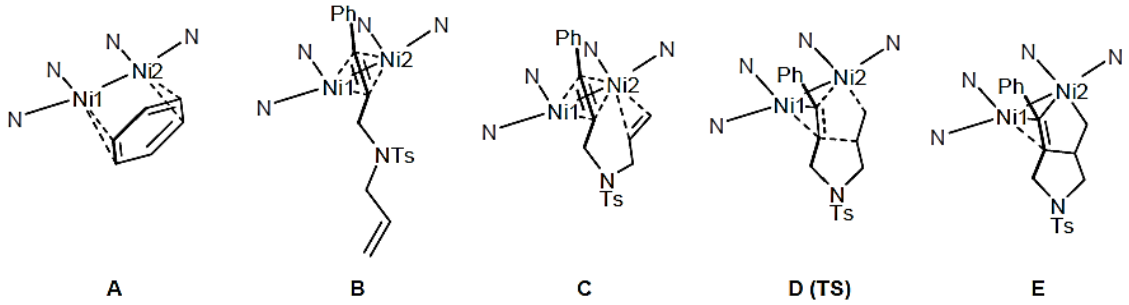


Figure S12. The Pauson–Khand reaction mediated by [NDI]Ni_2 complexes. Ts=p-toluenesulfonyl.

The formation of the intermediate C is an exergonic process; besides, C is directly detectable by ^{1}H NMR spectroscopy and decays with a half-life of 53 min at 30 °C, corresponding to an activation free energy of 22.7 kcal/mol. This energy barrier given by C and D(TS) was evaluated by means of several DFT methods including relativistic corrections within the zeroth-order regular approximation (ZORA) and the frozen-core approximation (FCA); the results are summarized as follows:

Table S5. Comparison of activation energies as calculated via several DFT methods.

Method	Energy Barrier [a] (kcal/mol)	
	$\Delta E^{\ddagger}$	$\Delta G^{\ddagger}$
BP86(D_3-BJ)/DZP [b]	17.9	15.6
BP86(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP	18.2	15.9
PBE(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP	19.8	17.6
PBE0(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP	21.7	19.4
B3LYP(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP	18.9	16.6
O3LYP(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP	**22.4**	**20.1**
Experimental [c]	-	22.7

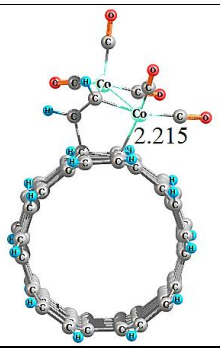
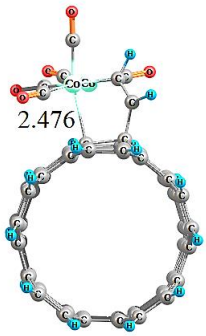
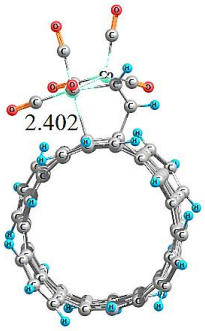
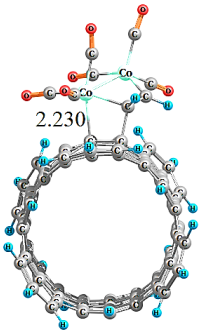
[a] Energy barrier is the difference between C and D(TS), see Figure S12.
[b] All the BP86(D_3-BJ)/DZP includes TZP basis set for cobalt.
[c] Estimations by the authors of the reference, Uyeda et al.

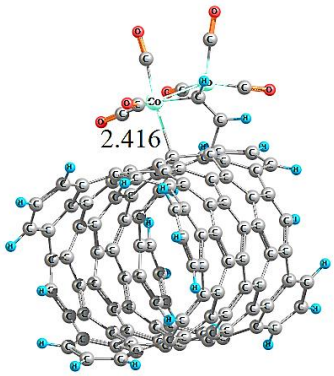
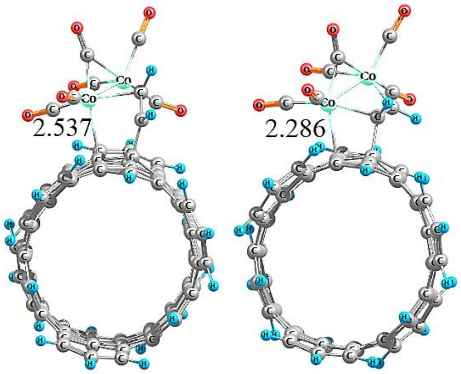
Conclusion: Since the energy corrected with the hybrid functional O3LYP approaches better to the experimental evidence, it is concluded that the performance of this method is suitable to determine Pauson-Khand energy profiles.

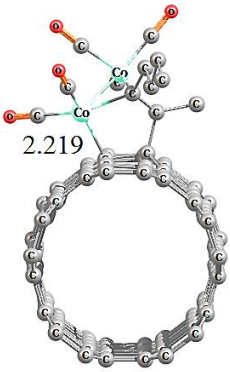
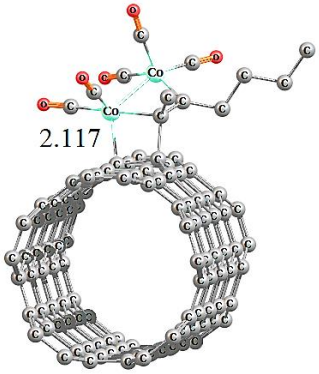
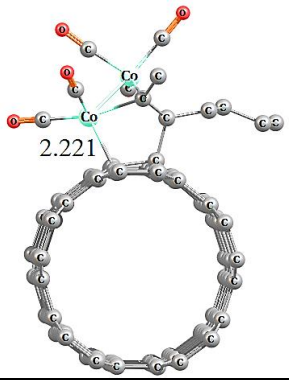
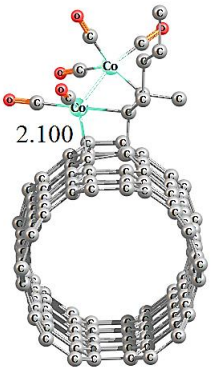
Stationary Points

In some cases, more than one structure representing a single stationary point were optimized. In this section, a brief discussion is provided to point out difficulties and schematize the criteria adopted to select the most suitable structure for the purposes of the current work. Energetic comparisons are given as the difference in absolute Gibbs energy calculated via O3LYP(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP (TZP for cobalt) including ZORA, FCA, and COSMO:N-methyl-2-pyrrolidone. In some cases, hydrogen atoms are hidden and the closest distance between cobalt and a carbon atom from the nanotube is usually depicted.

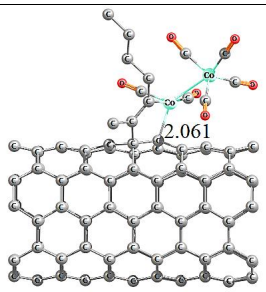
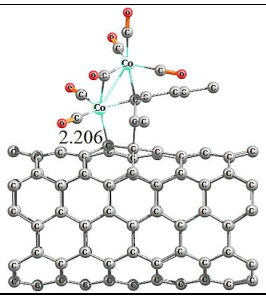
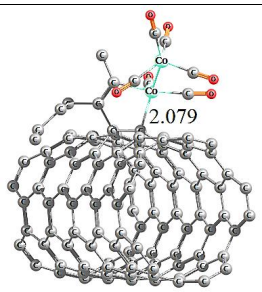
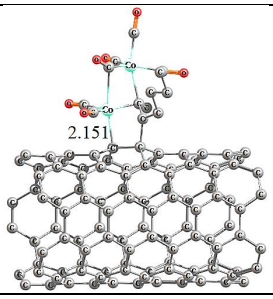
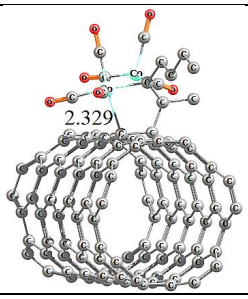
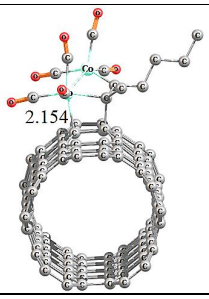
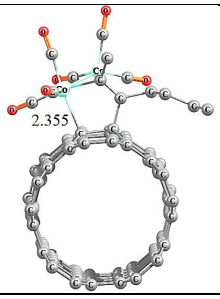
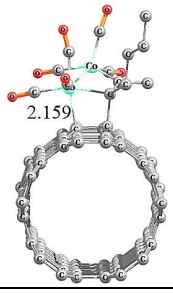
First case. The importance of the cobaltacycle.

Selected	**Discarded**
	
CP4$_{per}$ with (5,5)-SWCNT and acetylene. A stressed cobaltacycle results in a structure energetically destabilized. Observe that the selected structure shows a "more-open" cobaltacycle, that is a less stressed structure. As a result, the energy of the selected structure is 18.2 kcal/mol lower than the energy of the discarded one.	
	
CP5$_{obl}$ with (9,0)-SWCNT and acetylene. In this case, the discarded structure not only shows a more stressed cobaltacycle but also acetylene is highly distorted. Therefore, this results in a destabilization by 23.0 kcal/mol as compared to the selected one.	

	
CP5*$_{obl}$ with (9,0)-SWCNT and acetylene. Both previous criteria also apply in this case. The selected structure is more stable by at least 15 kcal/mol.	

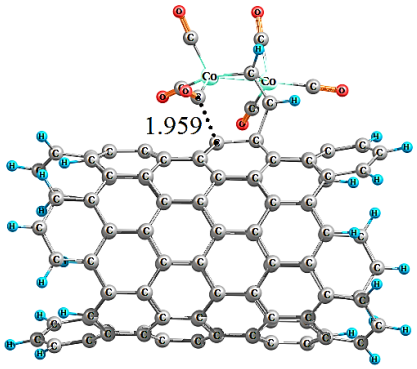
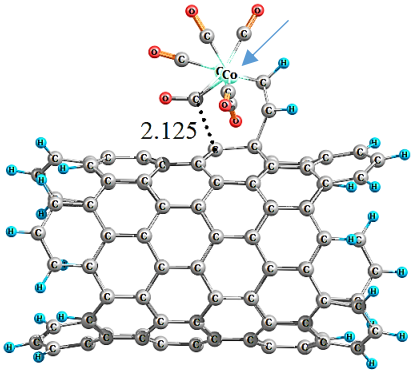
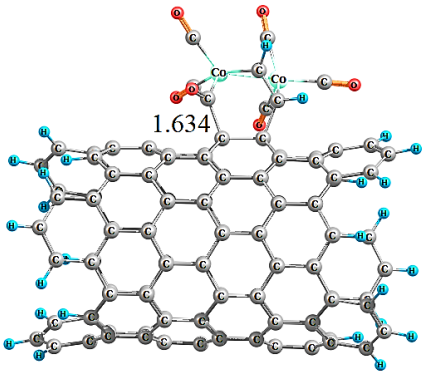
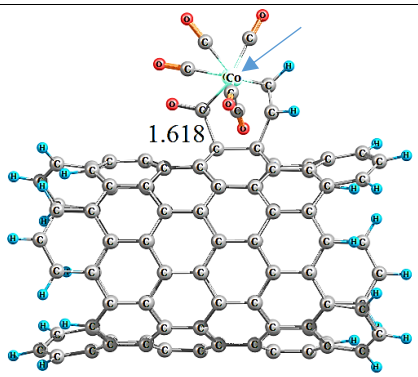
For the following structures, a stressed cobaltacycle is also discarded.	
Selected	**Discarded**
	
CP4$_{me,per}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 42 kcal/mol.	
	
CP4$_{bu,per}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 37 kcal/mol.	

For the following structures, a stressed cobaltacycle is also discarded.

Selected	Discarded
	
CP5*$_{me,obl}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 6 kcal/mol.	
	
CP5*$_{bu,obl}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 17 kcal/mol.	
	
CP5$_{me,per}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 29 kcal/mol.	
	
CP5$_{bu,per}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 20 kcal/mol.	

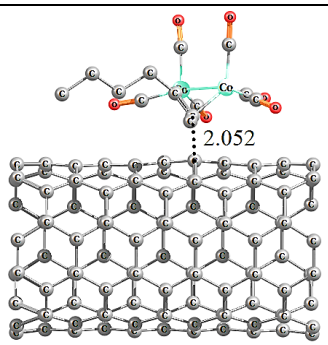
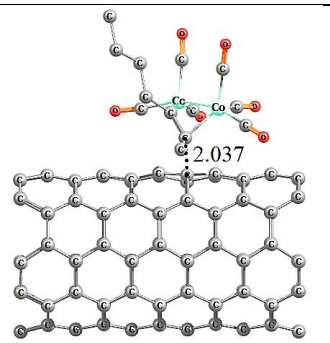
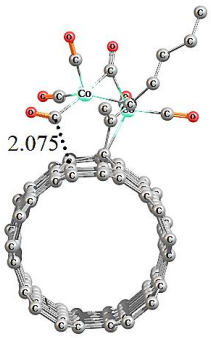
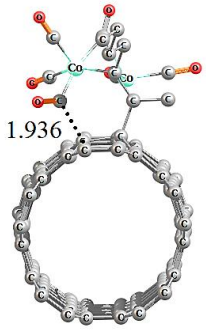
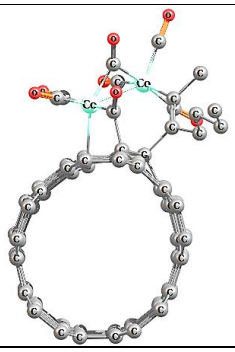
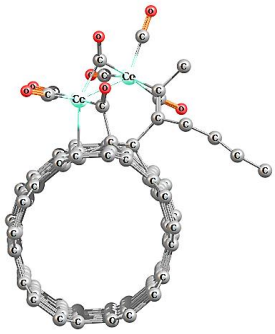
Second case. The importance of the localization of the cobaltacycle.

For the following structures, a structure with the Co-Co bond of the catalyst localized between the linking CO and the alkyne is discarded due to it causes an energetic destabilization, even though this may be small as shown in the second case.

Selected	**Discarded**
	
TS2$_{par}$ with (9,0)-SWCNT and acetylene. The selected structure is more stable by 7 kcal/mol.	
	
CP6$_{par}$ with (9,0)-SWCNT and acetylene. The selected structure is more stable by 2 kcal/mol.	

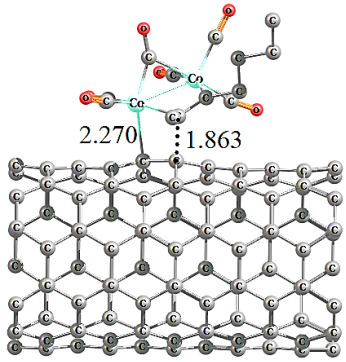
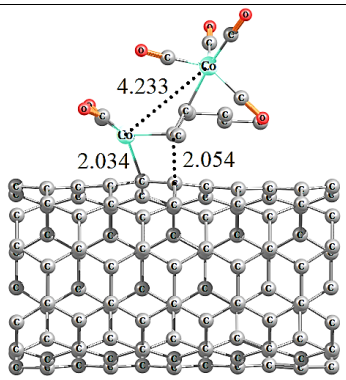
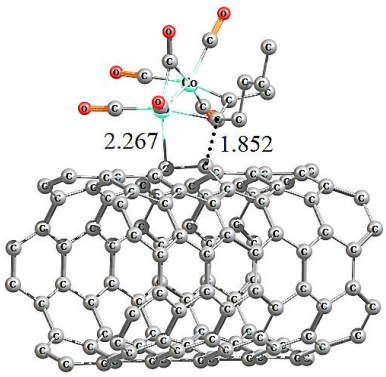
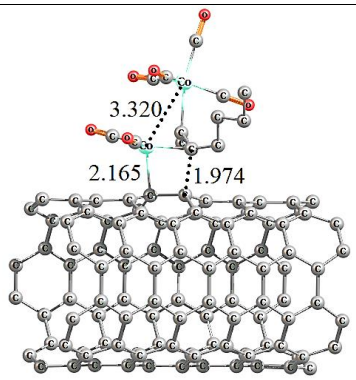
Third case. The importance of the orientation of the alkyne.

For the following structures, it is suggested that the orientation of the alkyne has no significant impact in terms of energetic stabilization; structures with different orientation of the alkyne are expected to differ by less than 3 kcal/mol.

Selected	**Discarded**
	
TS1'$_{me,obl}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 3 kcal/mol.	
	
TS2$_{me,per}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 3 kcal/mol.	
	
CP7*$_{bu,obl}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 2 kcal/mol.	

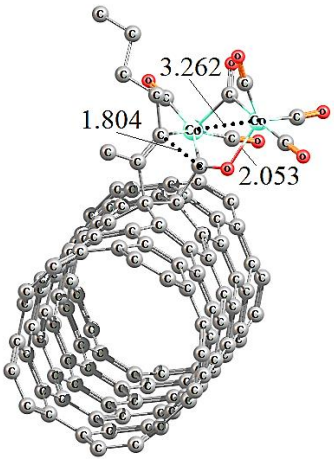
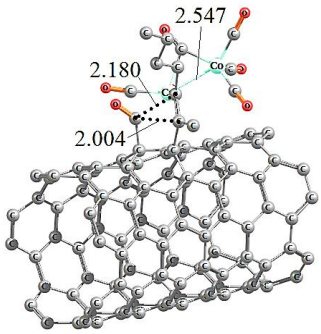
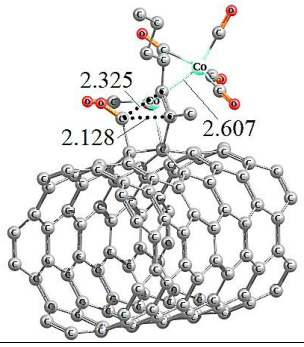
Fourth case. Separated cobalt atoms.

For the following structures, it is not clear whether the broken bond between the cobalt atoms results in a more stable structure. In the first case, the rupture of the Co-Co bond leads to a stabilization by 4 kcal/mol, but in the second one a destabilization by 15 kcal/mol is observed when compared to the energy of the selected structure. Nonetheless, most of the structures optimized for the current work show the cobalt atoms covalently linked; therefore, structures with separated cobalt atoms are discarded to keep consistency.

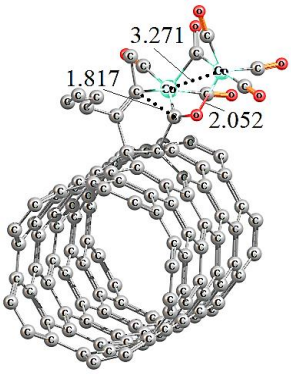
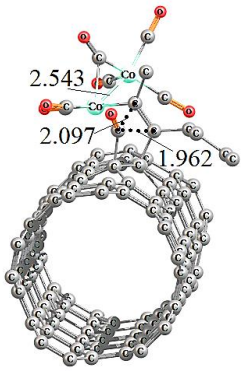
Selected	**Discarded**
	
TS1'*$_{me,obl}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is <u>less</u> stable by 4 kcal/mol.	
	
TS1'*$_{bu,obl}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 15 kcal/mol.	

*Fifth case. The **TS3** structure.*

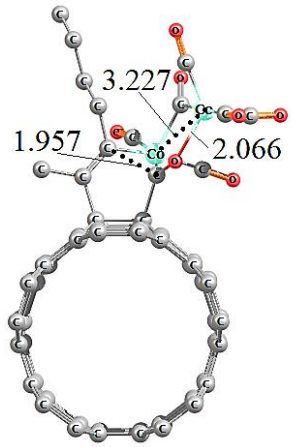
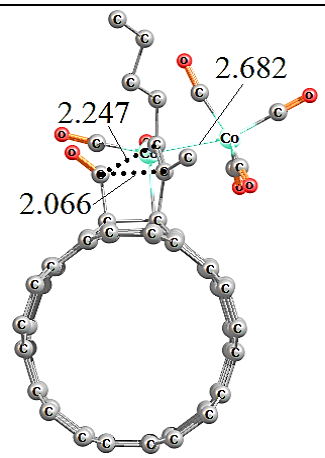
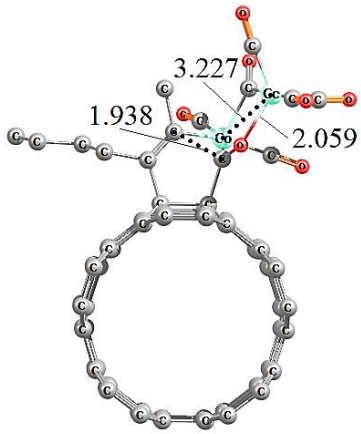
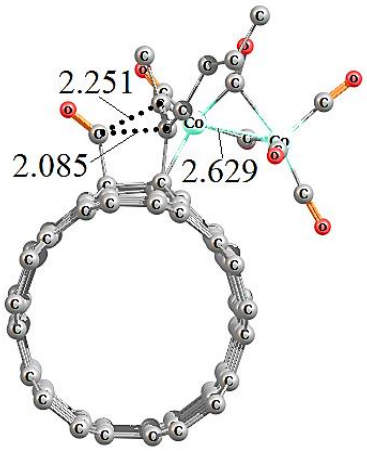
For the following structures, the selected structure is stabilized as compared to the discarded one, although it shows separated cobalt atoms and an apparent oxygen-cobalt covalent bond. On the other hand, the discarded structure suggests the formation of a 4-membered ring instead of a cyclopentenone; moreover, the linking CO appears to be more separated from the cobalt atom thus causing energetic destabilization. Therefore, the selected structure is more suitable for the purposes of the current work.

Selected	**Discarded**
	 

TS3*$_{me,obl}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 2 (discarded top) and 7 (discarded bottom) kcal/mol.

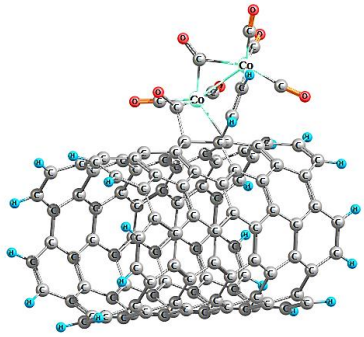
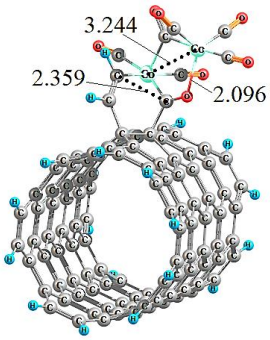
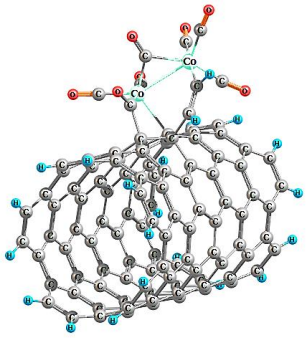
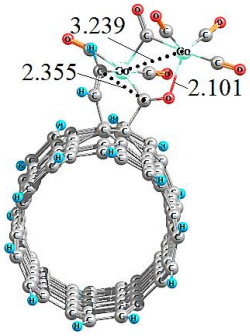
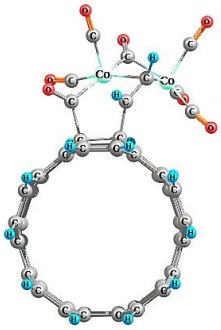
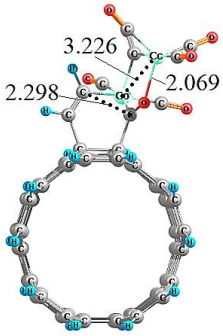
	

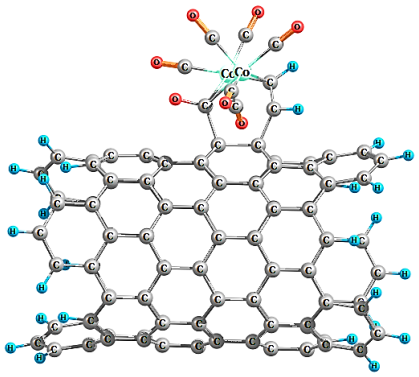
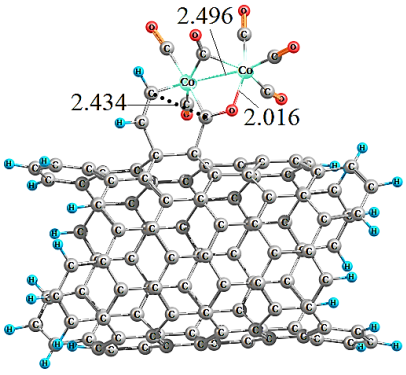
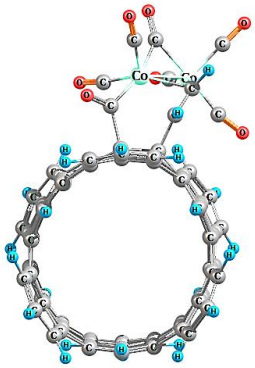
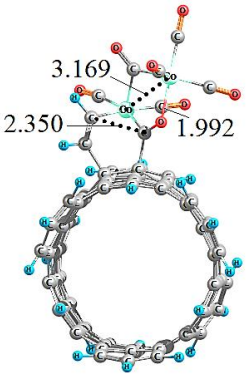
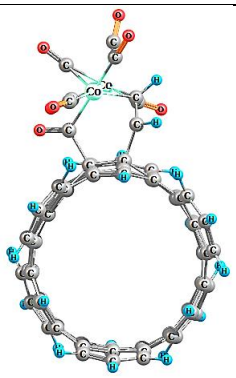
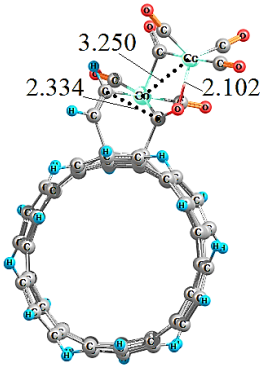
TS3*$_{bu,obl}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is <u>less</u> stable by 3 kcal/mol. Despite the selected structure is not more stable than the discarded one, it should be kept in mind that this latter does not correspond, unambiguously, to the formation of a cyclopentenone.

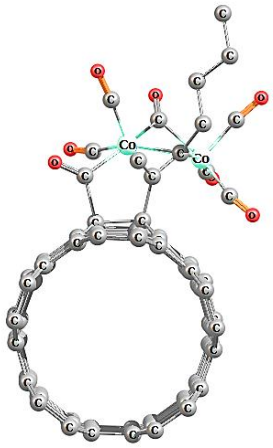
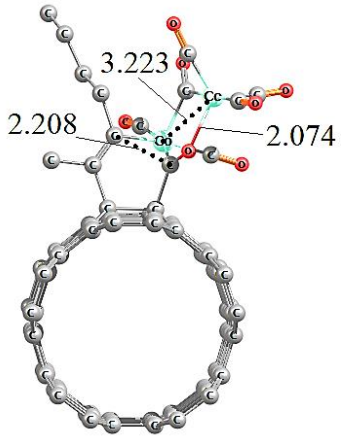
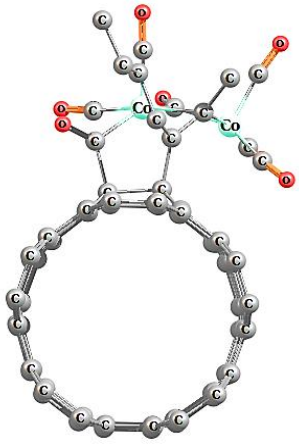
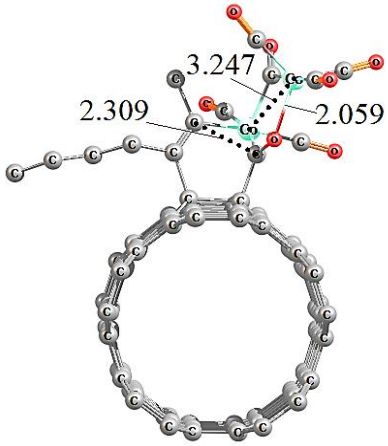
Selected	Discarded
	
TS3*$_{me,per}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 26 kcal/mol.	
	
TS3*$_{bu,per}$ with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 23 kcal/mol.	

*Sixth case. The **CP7** structure.*

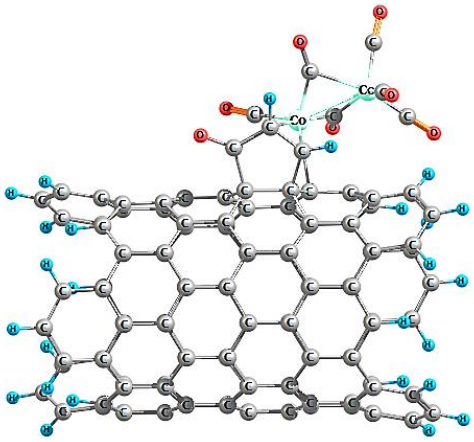
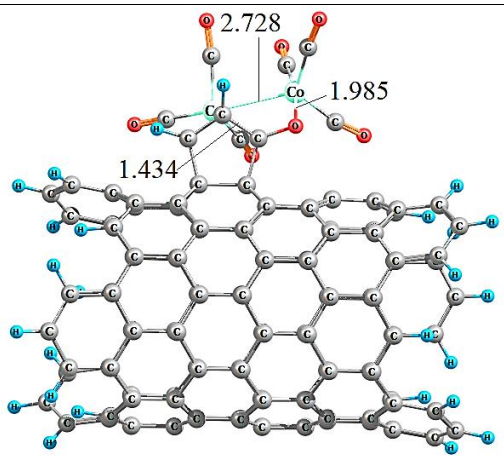
For the following structures, the discarded structure resembles **TS3** since it shows separated cobalt atoms and an apparent oxygen-cobalt covalent bond; however, vibrational-frequencies calculations demonstrate that both structures are local minima. Besides, the discarded structure is destabilized as compared to the selected one. Therefore, the selected structure is more suitable for the purposes of the current work.

Selected	**Discarded**
	
CP7$_{obl}$ with (5,5)-SWCNT and acetylene. The selected structure is more stable by 7 kcal/mol.	
	
CP7*$_{obl}$ with (5,5)-SWCNT and acetylene. The selected structure is more stable by 7 kcal/mol.	
	
CP7$_{per}$ with (5,5)-SWCNT and acetylene. The selected structure is more stable by 6 kcal/mol.	

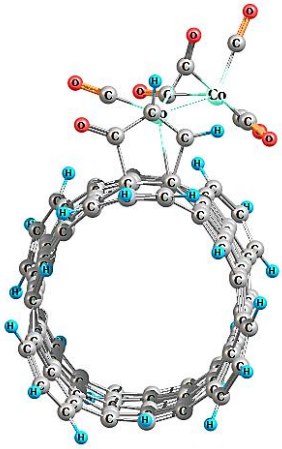
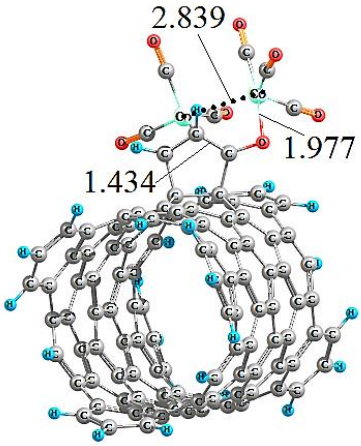
Selected	Discarded
	
CP7*par* with (9,0)-SWCNT and acetylene. The selected structure is more stable by 14 kcal/mol.	
	
CP7*obl* with (9,0)-SWCNT and acetylene. The selected structure is more stable by 17 kcal/mol.	
	
CP7*$_{obl}$ with (9,0)-SWCNT and acetylene. The selected structure is more stable by 19 kcal/mol.	

Selected	Discarded
	
CP7*me,per* with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 7 kcal/mol.	
	
CP7*bu,per* with (5,5)-SWCNT and 2-heptyne. The selected structure is more stable by 5 kcal/mol.	

Like the structures for **CP7**, the discarded structure in the case of the stationary point **PD** is also destabilized as compared to the selected one, and it also shows separated cobalt atoms and an apparent oxygen-cobalt covalent bond. Therefore, the selected structure is more suitable for the purposes of the current work.

Selected	**Discarded**
	

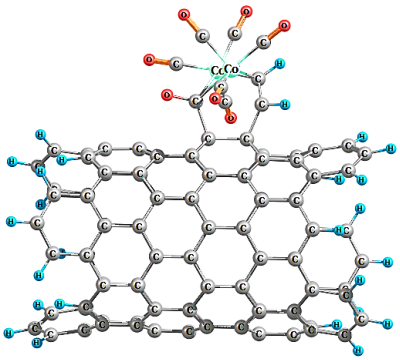
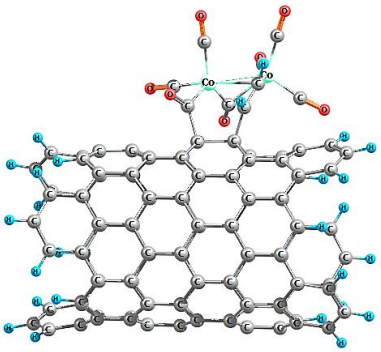
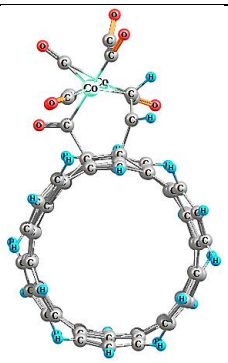
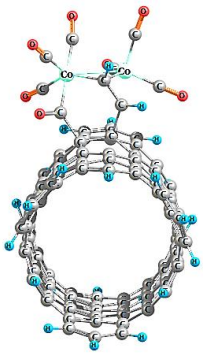
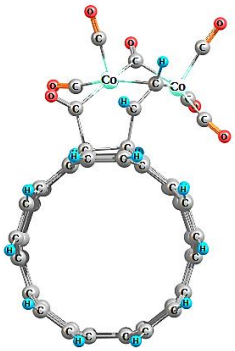
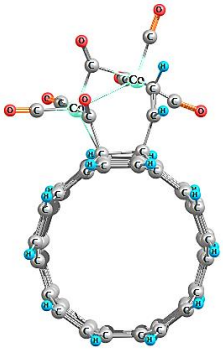
PD$_{par}$ with (9,0)-SWCNT and acetylene. The selected structure is more stable by 3 kcal/mol.

PD$_{obl}$ with (9,0)-SWCNT and acetylene. The selected structure is more stable by 23 kcal/mol.

Seventh case. Others.

For the following structures, it is not completely clear what factor or feature is affecting the electronic energy of the structure. Therefore, in these cases the criterium adopted is only based on terms of energetic stabilization so that the selected structure is the one more stable.

Selected	**Discarded**
	
CP7$_{par}$ with (9,0)-SWCNT and acetylene. The selected structure is more stable by 16 kcal/mol.	
	
CP7*$_{obl}$ with (9,0)-SWCNT and acetylene. The selected structure is more stable by 21 kcal/mol.	
	
CP7$_{per}$ with (5,5)-SWCNT and acetylene. The selected structure is more stable by 6 kcal/mol.	

Summary

Several difficulties to represent a stationary point of the Pauson-Khand reaction under study were described in seven cases. It is explained that the selection of a structure is not only based on terms of energetic stabilization, but consistency is also another factor to consider. That is to say, in the first case it is demonstrated that a stressed cobaltacycle leads to a strong energetic destabilization, then structures showing this characteristic must be discarded. The second and third cases suggest that the localization of the catalyst and the alkyne orientation can have no significant impact in the electronic energy as compared to a stressed cobaltacycle. The separated cobalt atoms described in the fourth case can lead to either an energetic stabilization or destabilization. However, structures shown covalently linked cobalt atoms are selected to keep consistency with all the structures optimized in the current work. One of the most difficult structures to optimize was **TS3**, which is described in the current work as the closing-ring step for the formation of a cyclopentenone; even though it shows separated cobalt atoms and an apparent oxygen-cobalt covalent bond. Other attempts to optimize **TS3** resulted in a structure resembling the formation of a 4-membered ring instead of a cyclopentenone. In some cases, those structures slightly differ in terms of electronic energy, but in other cases a strong energetic destabilization is observed for the discarded structure. In addition, the discarded structure, which is related to the formation of a 4-membered ring, cannot be unambiguously assigned to the formation of a cyclopentenone so that consistency is not achieved. **CP7** also represents another structure difficult to optimize. Some **CP7** structures show the same structural characteristics as **TS3**, even though these are indeed confirmed as local minima according to vibrational-frequency calculations. Moreover, these **CP7** structures resembling **TS3** are discarded because these are energetically destabilized. Finally, in some cases the selection of structures was only based on energy terms since no clear trends could be identified. Overall, the selection of structures to represent a stationary point must be done not only in terms of electronic energy, but also structural consistency related to the reaction pathway under study has to be considered.

Table S6. Absolute electronic and Gibbs energies for every structure under study as calculated in the gas phase at the BP86-(D_3-BJ)/DZP (TZP for cobalt) including ZORA and FCA; negative vibrational frequencies are included. Moreover, it is also reported the absolute electronic and Gibbs energies as calculated via O3LYP(D_3-BJ)/TZP//BP86(D_3-BJ)/DZP (TZP for cobalt) including ZORA, FCA, and COSMO:N-methyl-2-pyrrolidone. Red-colored labels stand for discarded structures according to the previous structural analysis.

Structures with (5,5)-SWCNT and acetylene					
Structure	BP86-(D_3-BJ)/DZP			O3LYP-(D_3-BJ)/TZP // BP86-(D_3-BJ)/DZP	
	E_{elec} (kcal / mol)	G (kcal / mol)	Neg Freq (cm^{-1})	E_{elec} (kcal / mol)	G (kcal / mol)
$Co(CO)_4$-$Co(CO)_4$	-3254.83	-3245.39		-4141.47	-4132.03
CO	-338.95	-347.94		-418.16	-427.15
H-C≡C-H	-520.67	-516.07		-628.87	-624.27
CP1	-3087.02	-3067.81		-3902.55	-3883.34
CP1'	-3066.93	-3047.49		-3886.06	-3866.62
CP2	-2707.88	-2692.69		-3427.47	-3412.28
CP2'	-2687.74	-2672.00		-3413.72	-3397.98
(5,5)-SWCNT	-24252.55	-23739.38		-30351.68	-29838.51
RC	-27346.63	-26799.41		-34266.82	-33719.60
CP3	-26979.51	-26436.61		-33807.10	-33264.20
CP3'	-27346.07	-26796.97		-34265.13	-33716.03
TS1 ***oblique***	-26979.43	-26433.17	-120	-33808.44	-33262.18
TS1* ***oblique***	-26976.10	-26433.21	-332	-33798.36	-33255.47
TS1 ***perpendicular***	-26979.29	-26434.82	-345	-33806.81	-33262.34
TS1' ***oblique***	-27323.34	-26774.82	-389	-34240.93	-33692.41
TS1'* ***oblique***	-27323.31	-26772.93	-384	-34239.27	-33688.89
TS1' ***perpendicular***	-27316.21	-26768.23	-346	-34233.64	-33685.66
CP4 ***oblique***	-26989.64	-26441.83		-33818.02	-33270.21
CP4* ***oblique***	-26990.75	-26442.99		-33819.76	-33272.00
CP4 ***perpendicular***	-26972.04	-26423.38		-33804.96	-33256.30
CP4 ***perpendicular***	-26990.98	-26443.18		-33822.34	-33274.54
CP5 ***oblique***	-27339.66	-26789.31		-34263.90	-33713.55
CP5* ***oblique***	-27335.33	-26783.78		-34257.76	-33706.21

CP5 ***perpendicular***	-27339.26	-26789.92		-34256.61	-33707.27
TS2 ***oblique***	-27327.12	-26777.16	-279	-34250.99	-33701.03
TS2* ***oblique***	-27327.75	-26776.91	-277	-34255.28	-33704.44
TS2 ***perpendicular***	-27321.67	-26771.99	-214	-34244.87	-33695.19
CP6 ***oblique***	-27328.32	-26777.44		-34256.82	-33705.94
CP6* ***oblique***	-27329.94	-26779.49		-34261.58	-33711.13
CP6 ***perpendicular***	-27329.83	-26777.98		-34269.19	-33717.34
CP7 ***oblique***	-27687.69	-27131.77		-34713.96	-34158.04
CP7' ***oblique***	-27681.16	-27125.98		-34706.43	-34151.25
CP7* ***oblique***	-27689.42	-27132.17		-34715.38	-34158.13
CP7'* ***oblique***	-27679.86	-27124.72		-34705.99	-34150.85
CP7 ***perpendicular***	-27680.54	-27124.55		-34708.89	-34152.90
CP7 ***perpendicular***	-27674.92	-27119.95		-34701.5	-34146.53
CP7' ***perpendicular***	-27673.60	-27118.54		-34701.88	-34146.82
TS3 ***oblique***	-27673.77	-27119.70	-214	-34705.84	-34151.77
TS3* ***oblique***	-27673.67	-27118.68	-212	-34705.77	-34150.78
TS3 ***perpendicular***	-27670.97	-27116.69	-251	-34703.72	-34149.44
PD ***oblique***	-27718.39	-27161.51		-34756.59	-34199.71
PD* ***oblique***	-27722.53	-27166.76		-34761.71	-34205.94
PD ***perpendicular***	-27715.52	-27157.86		-34748.12	-34190.46
PK ***oblique***	-25165.94	-24629.16		-31493.60	-30956.82
PK* ***oblique***	-25164.35	-24627.63		-31493.37	-30956.65
PK ***perpendicular***	-25161.01	-24624.55		-31489.56	-30953.10

Structures with (9,0)-SWCNT and acetylene					
Structure	BP86-(D_3-BJ)/DZP			O3LYP-(D_3-BJ)/TZP // BP86-(D_3-BJ)/DZP	
	E_{elec} (kcal / mol)	G (kcal / mol)	Neg Freq (cm^{-1})	E_{elec} (kcal / mol)	G (kcal / mol)
(9,0)-SWCNT	-24202.31	-23670.46		-30223.28	-29691.43
RC	-27299.87	-26735.61		-34136.80	-33572.54
CP3	-26936.67	-26373.47		-33681.74	-33118.54
CP3' ***parallel***	-27299.50	-26733.31		-34138.64	-33572.45
CP3' ***oblique***	-27300.54	-26732.53		-34138.81	-33570.80
TS1 ***parallel***	-26920.82	-26358.40	-223	-33663.22	-33100.80
TS1 ***oblique***	-26910.41	-26350.60	-294	-33659.51	-33099.70
TS1* ***oblique***	-26913.76	-26350.52	-311	-33658.77	-33095.53
TS1' ***parallel***	-27275.30	-26706.96	-385	-34113.88	-33545.54
TS1' ***oblique***	-27270.42	-26704.2	-383	-34107.95	-33541.73
TS1'* ***oblique***	-27271.75	-26703.71	-409	-34109.34	-33541.30
CP4 ***parallel***	-26931.68	-26365.79		-33677.03	-33111.14
CP4 ***oblique***	-26923.02	-26358.95		-33679.26	-33115.19
CP4* ***oblique***	-26924.93	-26358.23		-33676.20	-33109.50
CP5 ***parallel***	-27295.68	-26725.52		-34135.24	-33565.08
CP5 ***oblique***	-27293.69	-26723.38		-34136.1	-33565.79
CP5 ***oblique***	-27272.31	-26705.18		-34109.93	-33542.80
CP5* ***oblique***	-27294.04	-26725.33		-34136.96	-33568.25
CP5* ***oblique***	-27283.99	-26715.89		-34121.10	-33553.00
CP5* ***oblique***	-27272.48	-26703.68		-34111.93	-33543.13
TS2 ***parallel***	-27279.05	-26709.46	-280	-34123.34	-33553.75
TS2 ***parallel***	-27272.13	-26702.84	-217	-34116.39	-33547.10
TS2 ***oblique***	-27269.15	-26699.62	-253	-34121.07	-33551.54
TS2* ***oblique***	-27280.24	-26712.73	-305	-34126.95	-33559.44
CP6 ***parallel***	-27281.30	-26710.49		-34129.78	-33558.97
CP6 ***parallel***	-27277.60	-26706.52		-34127.81	-33556.73
CP6 ***oblique***	-27273.05	-26701.99		-34130.24	-33559.18

CP6* ***oblique***	-27282.06	-26712.23		-34133.79	-33563.96
CP7 ***parallel***	-27638.35	-27063.05		-34582.55	-34007.25
CP7 ***parallel***	-27647.31	-27072.46		-34597.80	-34022.95
CP7' ***parallel***	-27629.01	-27054.96		-34582.64	-34008.59
CP7 ***oblique***	-27629.57	-27055.68		-34583.57	-34009.68
CP7' ***oblique***	-27616.31	-27044.14		-34564.78	-33992.61
CP7* ***oblique***	-27641.19	-27066.21		-34591.99	-34017.01
CP7* ***oblique***	-27625.50	-27051.18		-34570.32	-33996.00
CP7'* ***oblique***	-27623.64	-27050.48		-34571.11	-33997.95
TS3 ***parallel***	-27625.14	-27050.77	-348	-34578.04	-34003.67
TS3 ***oblique***	-27613.11	-27040.16	-257	-34564.74	-33991.79
TS3* ***oblique***	-27615.57	-27043.68	-273	-34567.91	-33996.02
PD ***parallel***	-27670.86	-27094.32		-34626.92	-34050.38
PD' ***parallel***	-27664.13	-27088.23		-34623.66	-34047.76
PD ***oblique***	-27669.49	-27093.90		-34627.15	-34051.56
PD' ***oblique***	-27645.69	-27072.73		-34601.93	-34028.97
PD* ***oblique***	-27649.92	-27074.32		-34606.99	-34031.39
PK ***parallel***	-25113.89	-24558.62		-31366.66	-30811.39
PK ***oblique***	-25107.15	-24552.29		-31358.48	-30803.62
PK* ***oblique***	-25108.35	-24553.64		-31359.05	-30804.34

Structures with (5,5)-SWCNT and 2-heptyne					
Structure	BP86-(D_3-BJ)/DZP			O3LYP-(D_3-BJ)/TZP // BP86-(D_3-BJ)/DZP	
	E_{elec} (kcal / mol)	G (kcal / mol)	Neg Freq (cm^{-1})	E_{elec} (kcal / mol)	G (kcal / mol)
CH_3-$(CH_2)_3$-C≡C-CH_3	-2413.26	-2330.72		-2908.80	-2826.26
CP1	-4987.03	-4885.42		-6187.87	-6086.26
CP1' ***me***	-4964.98	-4865.06		-6170.35	-6070.43
CP1' ***bu***	-4963.98	-4865.03		-6169.16	-6070.21
CP2	-4608.61	-4513.65		-5713.44	-5618.48
CP2' ***me***	-4585.40	-4489.01		-5697.08	-5600.69
CP2' ***bu***	-4585.64	-4489.49		-5695.91	-5599.76
RC ***me***	-29250.54	-28620.46		-36557.11	-35927.03
RC ***bu***	-29247.21	-28620.18		-36552.57	-35925.54
CP3 ***me***	-28886.06	-28260.52		-36096.90	-35471.36
CP3 ***bu***	-28881.02	-28257.11		-36091.60	-35467.69
TS1 ***me , oblique***	-28870.12	-28242.05	-477	-36079.81	-35451.74
TS1 ***bu , oblique***	-28874.16	-28248.36	-495	-36082.22	-35456.42
TS1* ***me , oblique***	-28867.98	-28241.23	-411	-36075.63	-35448.88
TS1* ***bu , oblique***	-28868.05	-28242.24	-527	-36077.60	-35451.79
TS1 ***me , perpendicular***	-28851.11	-28224.96	-468	-36058.23	-35432.08
TS1 ***bu , perpendicular***	-28861.77	-28236.50	-323	-36073.23	-35447.96
TS1' ***me , oblique***	-29239.15	-28608.53	-368	-36535.08	-35904.46
TS1' ***me , oblique***	-29232.43	-28602.75	-391	-36530.79	-35901.11
TS1' ***bu , oblique***	-29234.69	-28603.84	-295	-36529.14	-35898.29
TS1'* ***me , oblique***	-29224.96	-28593.35	-334	-36525.20	-35893.59
TS1'* ***me , oblique***	-29226.49	-28596.03	-292	-36528.49	-35898.03
TS1'* ***bu , oblique***	-29226.54	-28594.63	-282	-36529.29	-35897.38
TS1'* ***bu , oblique***	-29210.74	-28580.70	-512	-36512.29	-35882.25
TS1' ***me , perpendicular***	-29215.20	-28584.45	-377	-36519.09	-35888.34
TS1' ***bu , perpendicular***	-29217.47	-28585.97	-285	-36521.99	-35890.49
CP4 ***me , oblique***	-28885.23	-28256.19		-36102.37	-35473.33

CP4 *bu , oblique*	-28889.88	-28260.75		-36104.13	-35475.00
CP4* *me , oblique*	-28883.60	-28255.52		-36098.10	-35470.02
CP4* *bu , oblique*	-28886.00	-28257.45		-36102.46	-35473.91
CP4 *me , perpendicular*	-28895.35	-28265.46		-36109.35	-35479.46
CP4 *me , perpendicular*	-28854.73	-28226.73		-36065.80	-35437.80
CP4 *bu , perpendicular*	-28893.18	-28264.17		-36107.83	-35478.82
CP4 *bu , perpendicular*	-28855.82	-28230.30		-36067.81	-35442.29
CP5 *me , oblique*	-29254.98	-28621.13		-36558.05	-35924.20
CP5 *bu , oblique*	-29251.51	-28617.53		-36556.32	-35922.34
CP5* *me , oblique*	-29238.48	-28608.86		-36547.92	-35918.30
CP5* *me , oblique*	-29230.18	-28598.57		-36543.47	-35911.86
CP5* *bu , oblique*	-29241.11	-28610.48		-36548.28	-35917.65
CP5* *bu , oblique*	-29220.40	-28588.27		-36532.60	-35900.47
CP5 *me , perpendicular*	-29250.64	-28618.16		-36554.10	-35921.62
CP5 *me , perpendicular*	-29216.60	-28586.65		-36522.99	-35893.04
CP5 *bu , perpendicular*	-29246.27	-28611.70		-36550.55	-35915.98
CP5 *bu , perpendicular*	-29218.37	-28588.57		-36525.51	-35895.71
TS2 *me , oblique*	-29220.79	-28590.93	-312	-36534.19	-35904.33
TS2 *bu , oblique*	-29222.69	-28592.26	-317	-36533.68	-35903.25
TS2* *me , oblique*	-29221.62	-28592.21	-310	-36531.53	-35902.12
TS2* *bu , oblique*	-29226.34	-28594.73	-312	-36536.34	-35904.73
TS2 *me , perpendicular*	-29219.85	-28585.00	-248	-36534.11	-35899.26
TS2 *me , perpendicular*	-29214.29	-28582.16	-157	-36533.89	-35901.76
TS2 *bu , perpendicular*	-29219.29	-28586.36	-254	-36535.86	-35902.93
CP6 *me , oblique*	-29222.81	-28591.42		-36537.77	-35906.38
CP6 *bu , oblique*	-29225.53	-28592.59		-36541.61	-35908.67
CP6* *me , oblique*	-29223.98	-28592.52		-36538.76	-35907.30
CP6* *bu , oblique*	-29227.41	-28594.18		-36544.39	-35911.16
CP6 *me , perpendicular*	-29219.74	-28586.32		-36546.05	-35912.63
CP6 *bu , perpendicular*	-29217.17	-28582.98		-36545.44	-35911.25
CP7 *me , oblique*	-29574.08	-28936.34		-36988.46	-36350.72
CP7 *bu , oblique*	-29578.97	-28941.36		-36993.74	-36356.13

CP7* ***me , oblique***	-29576.94	-28937.78		-36991.38	-36352.22
CP7* ***bu , oblique***	-29579.42	-28941.07		-36995.01	-36356.66
CP7* ***bu , oblique***	-29577.25	-28940.90		-36990.53	-36354.18
CP7 ***me , perpendicular***	-29564.61	-28927.51		-36991.43	-36354.33
CP7' ***me , perpendicular***	-29566.93	-28929.43		-36984.87	-36347.37
CP7 ***bu , perpendicular***	-29561.31	-28925.21		-36990.99	-36354.89
CP7' ***bu , perpendicular***	-29568.21	-28933.42		-36984.86	-36350.07
TS3 ***me , oblique***	-29565.02	-28928.11	-208	-36984.48	-36347.57
TS3 ***bu , oblique***	-29564.02	-28929.11	-211	-36980.48	-36343.57
TS3* ***me , oblique***	-29562.99	-28925.95	-112	-36985.25	-36348.21
TS3* ***me , oblique***	-29568.49	-28932.53	-258	-36982.14	-36346.18
TS3* ***me , oblique***	-29566.29	-28931.25	-107	-36975.81	-36340.77
TS3* ***bu , oblique***	-29567.09	-28930.17	-157	-36989.73	-36352.81
TS3* ***bu , oblique***	-29577.26	-28942.65	-261	-36990.73	-36356.12
TS3 ***me , perpendicular***	-29566.97	-28931.80	-220	-36987.35	-36352.18
TS3 ***me , perpendicular***	-29551.86	-28916.83	-220	-36961.44	-36326.41
TS3 ***bu , perpendicular***	-29567.68	-28932.47	-246	-36986.20	-36350.99
TS3 ***bu , perpendicular***	-29552.01	-28916.44	-474	-36963.09	-36327.52
PD* ***me , oblique***	-29623.80	-28985.66		-37049.68	-36411.54
PD* ***bu , oblique***	-29624.95	-28987.18		-37052.31	-36414.54
PD ***me , perpendicular***	-29616.05	-28979.70		-37034.52	-36398.17
PD ***bu , perpendicular***	-29607.99	-28971.24		-37028.07	-36391.32
PK* ***me , oblique***	-27065.11	-26447.77		-33778.37	-33161.03
PK* ***bu , oblique***	-27065.59	-26449.36		-33780.40	-33164.17
PK ***me , perpendicular***	-27061.23	-26444.85		-33775.60	-33159.22
PK ***bu , perpendicular***	-27061.90	-26446.31		-33777.44	-33161.85

Structures with (9,0)-SWCNT and 2-heptyne					
Structure	BP86-(D_3-BJ)/DZP			O3LYP-(D_3-BJ)/TZP // BP86-(D_3-BJ)/DZP	
	E_{elec} (kcal / mol)	G (kcal / mol)	Neg Freq (cm^{-1})	E_{elec} (kcal / mol)	G (kcal / mol)
RC ***me , parallel***	-29204.16	-28556.81		-36430.47	-35783.12
RC ***bu , parallel***	-29208.23	-28559.33		-36433.29	-35784.39
CP3 ***me , parallel***	-28837.77	-28192.62		-35971.26	-35326.11
CP3 ***bu , parallel***	-28835.04	-28192.03		-35967.11	-35324.10
CP3' ***me , parallel***	-29197.31	-28548.05		-36420.06	-35770.80
CP3' ***bu , parallel***	-29199.42	-28553.03		-36420.78	-35774.39
TS1 ***me , parallel***	-28812.77	-28168.45	-177	-35946.87	-35302.55
TS1' ***me , parallel***	-29176.89	-28527.23	-412	-36405.54	-35755.88
TS1' ***bu , parallel***	-29178.84	-28529.04	-354	-36404.79	-35754.99
TS1' ***me , oblique***	-29172.54	-28524.84	-402	-36396.83	-35749.13
TS1' ***bu , oblique***	-29173.61	-28526.59	-325	-36391.90	-35744.88
TS1'* ***me , oblique***	-29171.10	-28522.31	-230	-36393.12	-35744.33
TS1'* ***bu , oblique***	-29165.13	-28516.54	-200	-36386.74	-35738.15
CP4 ***me , parallel***	-28822.23	-28174.85		-35956.15	-35308.77
CP4 ***bu , parallel***	-28823.66	-28176.90		-35957.18	-35310.42
CP4* ***me , oblique***	-28844.44	-28196.63		-35982.42	-35334.61
CP4* ***bu , oblique***	-28829.98	-28181.94		-35964.95	-35316.91
CP5 ***me , parallel***	-29185.27	-28534.93		-36420.34	-35770.00
CP5 ***bu , parallel***	-29186.09	-28535.76		-36414.51	-35764.18
CP5 ***me , oblique***	-29179.70	-28531.19		-36407.89	-35759.38
CP5 ***bu , oblique***	-29180.57	-28531.68		-36407.94	-35759.05
CP5* ***me , oblique***	-29181.10	-28530.40		-36413.62	-35762.92
CP5* ***bu , oblique***	-29174.66	-28523.24		-36407.62	-35756.20
TS2 ***me , parallel***	-29183.68	-28533.34	-151	-36418.39	-35768.05
TS2 ***bu , parallel***	-29182.39	-28530.78	-209	-36414.16	-35762.55
CP6 ***me , parallel***	-29192.91	-28540.97		-36439.17	-35787.23
CP6 ***bu , parallel***	-29193.73	-28541.98		-36440.37	-35788.62

CP7 ***me , parallel***	-29528.47	-28873.18		-36872.48	-36217.19
CP7 ***bu , parallel***	-29525.52	-28870.23		-36864.66	-36209.37
TS3 ***me , parallel***	-29521.54	-28868.28	-248	-36861.46	-36208.20
TS3 ***bu , parallel***	-29514.28	-28859.71	-319	-36851.95	-36197.38
PD ***me , parallel***	-29565.46	-28908.67		-36910.42	-36253.63
PD ***bu , parallel***	-29564.26	-28908.55		-36910.19	-36254.48
PK ***me , parallel***	-27007.78	-26371.19		-33647.72	-33011.13
PK ***bu , parallel***	-27001.99	-26367.69		-33644.51	-33010.21

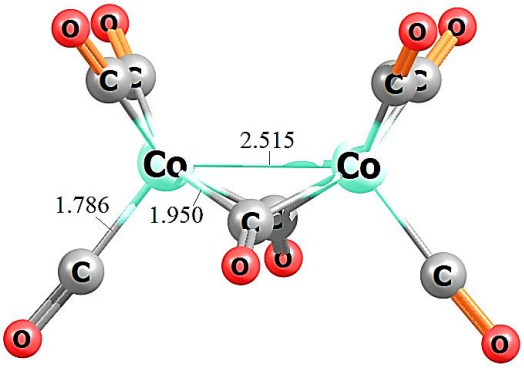
Structures with (6,5)- and (8,0)-SWCNT and 2-heptyne					
Structure	BP86-(D_3-BJ)/DZP			O3LYP-(D_3-BJ)/TZP // BP86-(D_3-BJ)/DZP	
	E_{elec} (kcal / mol)	G (kcal / mol)	Neg Freq (cm^{-1})	E_{elec} (kcal / mol)	G (kcal / mol)
(6,5)-SWCNT	-21578.53	-21105.01		-26941.83	-26468.31
RC ***me***	-26570.79	-25981.92		-33141.73	-32552.86
TS1' ***me , obliue***	-26554.28	-25963.03		-33130.74	-32539.49
CP5 ***me , oblique***	-26563.97	-25968.99		-33139.37	-32544.39
(8,0)-SWCNT	-21499.44	-21026.65		-26849.57	-26376.78
RC ***me***	-26497.99	-25908.29		-33051.69	-32461.99
TS1' ***me , parallel***	-26480.74	-25890.71		-33038.00	-32447.97
CP5 ***me , parallel***	-26483.27	-25889.31		-33044.13	-32450.17

Table S7. Cartesian coordinates and 3D image for every structure under study as calculated in the gas phase at the BP86-(D_3-BJ)/DZP (TZP for cobalt) including ZORA and FCA. Structures are listed as these are in **Table S6**.

$Co(CO)_4$-$Co(CO)_4$

18
Co2C8O8

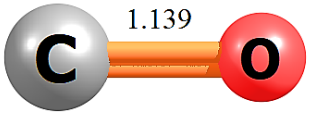
Co	-0.008818987	0.003420912	-1.257265947
O	1.488066186	-2.201248068	0.000000000
O	2.265436389	0.233162778	-3.100552165
C	0.845082908	-1.217517972	0.000000000
C	1.397535641	0.145735765	-2.348740739
Co	-0.008818987	0.003420912	1.257265947
C	0.578883915	1.372262293	0.000000000
C	-1.213079270	1.199968588	-1.855161712
C	-0.948173698	-1.413956865	-1.847786683
C	-1.213079270	1.199968588	1.855161712
C	-0.948173698	-1.413956865	1.847786683
C	1.397535641	0.145735765	2.348740739
O	1.006968301	2.466725531	0.000000000
O	-1.969620362	1.967219368	-2.261083866
O	-1.534256859	-2.321992389	-2.244998308
O	-1.969620362	1.967219368	2.261083866
O	-1.534256859	-2.321992389	2.244998308
O	2.265436389	0.233162778	3.100552165



CO

2
CO

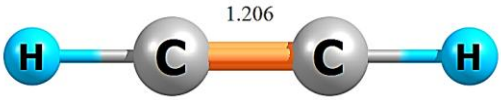
C	0.000000000	0.000000000	-0.650873000
O	0.000000000	0.000000000	0.488310000



H-C≡C-H

4
C2H2

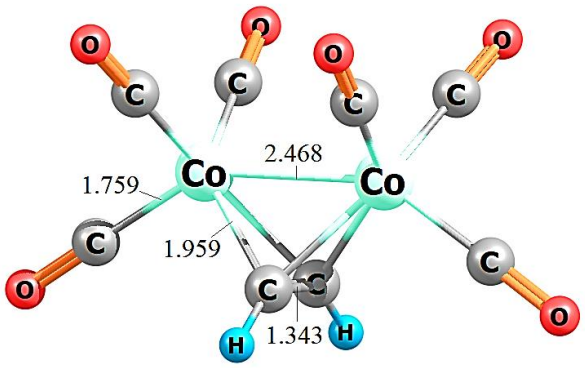
C	0.000000000	0.000000000	-0.603196000
C	0.000000000	0.000000000	0.603196000
H	0.000000000	0.000000000	1.673275000
H	0.000000000	0.000000000	-1.673275000



CP1

18
Co2C8H2O6

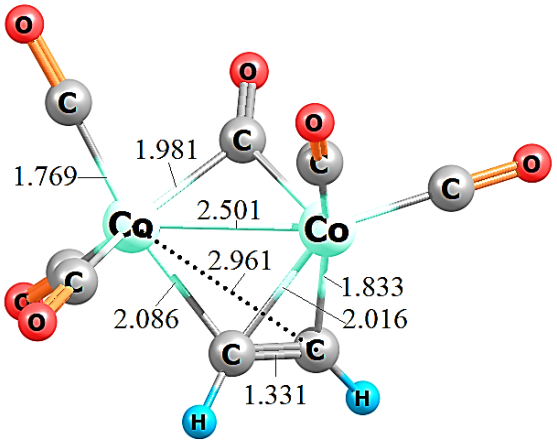
Co	-1.234216086	-0.004418032	0.155456367
Co	1.234028396	0.002737000	0.165616387
C	-1.507555922	1.447902091	-0.860919409
C	-2.726266831	-0.021467557	1.086546477
C	-1.490951605	-1.438081873	-0.890973006
C	1.498388160	1.446802724	-0.864443321
C	2.718907214	0.014536345	1.108031095
C	1.515741341	-1.438379063	-0.864654380
O	-3.696172108	-0.033879562	1.713695019
O	-1.674507126	2.395524132	-1.497190749
O	-1.643180940	-2.374788411	-1.546814574
O	1.657452947	2.387695255	-1.512632474
O	3.683932828	0.022751766	1.742831485
O	1.684904061	-2.379771076	-1.509465033
C	-0.007952447	0.658706699	1.531779101
C	-0.003110066	-0.684054199	1.520505883
H	-0.003458704	-1.559581998	2.162594730
H	-0.013110053	1.522274162	2.189877890



CP1’

18
Co2C8H2O6

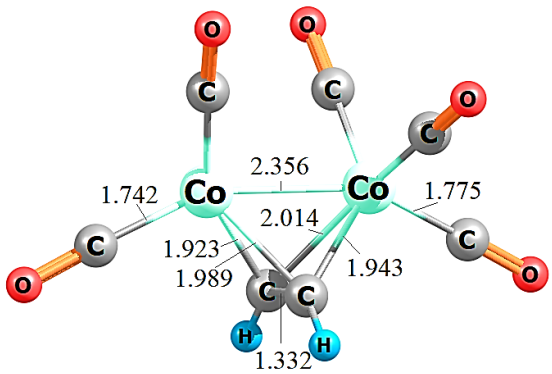
Co	1.378179307	-0.058564807	-0.356161500
Co	-1.100192990	0.097920881	-0.057409893
C	0.423538557	0.753009105	1.026194459
C	3.009157795	0.402061049	0.101734235
C	1.311569806	-1.779293559	0.180523622
C	-1.909453728	1.675028431	-0.320936625
C	-1.919173332	-1.198741144	-0.971109420
C	-1.773285851	-0.462265997	1.479650890
O	4.075315358	0.735239970	0.396667130
O	0.602856044	1.360369523	2.016381182
O	1.265293771	-2.888852217	0.493164958
O	-2.502454359	2.652733781	-0.470940111
O	-2.453532387	-2.008197758	-1.596539249
O	-2.248743630	-0.791983873	2.477943395
C	1.124633858	1.175801159	-1.687303269
C	0.032395113	0.420656569	-1.779307293
H	-0.469419847	0.078954208	-2.688584154
H	1.682904359	1.936416998	-2.226142007



CP2

16
Co2C7H2O5

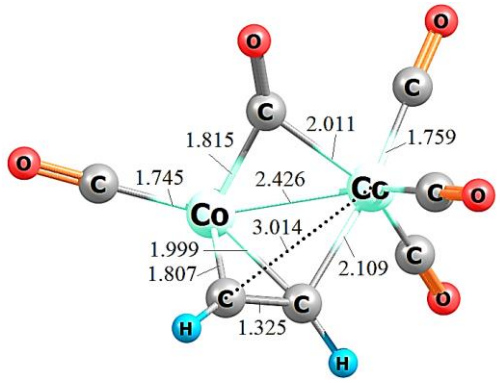
Co	1.215926128	0.308669924	-0.121523757
Co	-1.099662587	0.109516434	0.262072162
C	1.581380030	-1.334799235	-0.677345504
C	2.822054238	0.929921571	0.142905115
C	-1.256141134	-1.631045240	0.622657896
C	-2.631246372	0.751027943	0.890616627
C	-1.296754127	0.259622636	-1.501677477
O	3.882116423	1.341651167	0.370014512
O	1.796967688	-2.433830386	-0.968914472
O	-1.340384220	-2.755298773	0.869978236
O	-3.618657336	1.187341207	1.300783048
O	-1.396310113	0.341169526	-2.651134514
C	0.238142980	0.584776331	1.588098650
C	0.128873145	1.624920314	0.763845919
H	0.060728405	2.710758819	0.768521013
H	0.471300277	0.293822275	2.609153805



CP2’

16
Co2C7H2O5

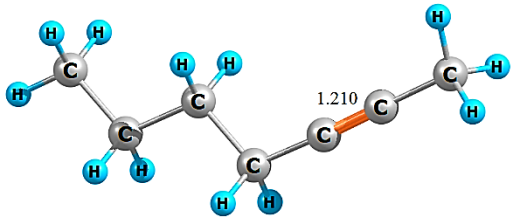
Co	1.413033692	0.393977712	-0.225323568
Co	-0.976793096	0.047629423	0.002768670
C	0.601095394	-1.193559316	0.114875454
C	3.080585636	-0.104446193	-0.348872934
C	-1.729888347	-0.147021545	1.610444924
C	-1.747953970	1.297421508	-1.027030454
C	-1.728354705	-1.295614376	-0.849333242
O	4.186681769	-0.451288076	-0.378427045
O	0.798894488	-2.322418807	0.397158292
O	-2.241492459	-0.270160107	2.637141716
O	-2.252803220	2.112016547	-1.671360255
O	-2.246675175	-2.174473013	-1.388841159
C	1.397801996	1.395035985	1.278522373
C	0.193990677	1.622812748	0.773882819
H	-0.399619844	2.536233632	0.866950036
H	2.090539801	1.679373148	2.066443972



CH_3-$(CH_2)_3$-C≡C-CH_3

19
C7H12

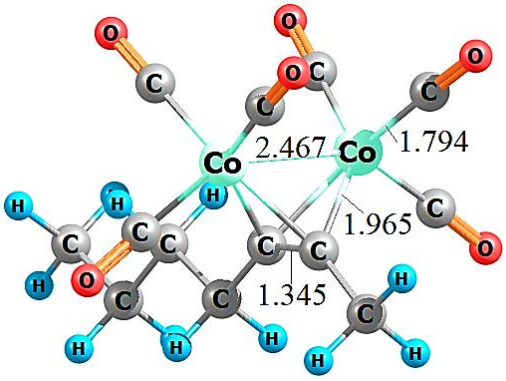
C	-2.465091360	0.029289535	0.000307333
C	-1.347135094	-0.434812890	0.003227489
C	-3.809149926	0.576082178	-0.003110842
H	-4.193501219	0.691394214	1.020772328
H	-3.832769018	1.564930336	-0.483862069
H	-4.502154287	-0.079226968	-0.550471252
C	0.015805651	-0.936902419	0.006082408
H	0.171839492	-1.586565431	-0.872709644
H	0.172208125	-1.575575037	0.892810593
C	1.064596598	0.184651530	-0.001269365
H	0.901546247	0.817288483	-0.890446208
H	0.901519239	0.828787884	0.879591097
C	2.490835161	-0.354234164	0.002043550
H	2.635724236	-0.993652916	0.890380734
H	2.635409622	-1.005326217	-0.877823441
C	3.534673525	0.759033419	-0.005493671
H	4.556821074	0.353481488	-0.002933105
H	3.423724116	1.393594592	-0.898422858
H	3.423954127	1.405406701	0.878953252



CP1

33
Co2C13H12O6

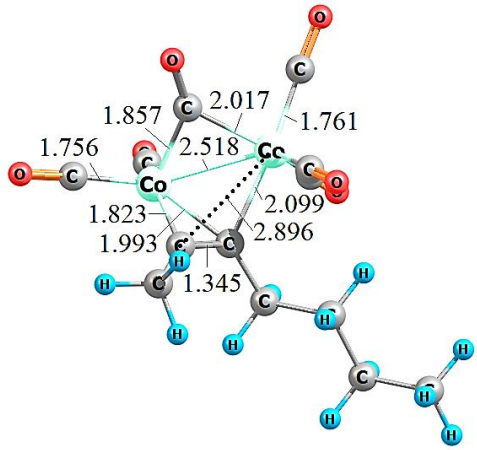
Co	-0.252470781	-1.381988865	-0.219777216
Co	-0.827852154	1.013179471	-0.084536392
C	-1.851780827	-2.035246151	-0.705349727
C	0.465681548	-2.762895531	0.588321064
C	0.760099562	-1.311214260	-1.697910765
C	-2.554622631	0.907715694	-0.559104308
C	-0.817715457	2.468106367	0.894881671
C	0.079168857	1.585802136	-1.521847514
O	0.952780263	-3.649485597	1.150903502
O	-2.898826874	-2.443266174	-0.970694192
O	1.422890148	-1.258758092	-2.642490397
O	-3.675510275	0.814312474	-0.820188912
O	-0.790950848	3.408197152	1.569693528
O	0.674288994	1.954374745	-2.440689687
C	-0.763476839	-0.323783668	1.354341561
C	0.483645534	-0.001916996	0.968065782
C	-1.613452842	-0.593564527	2.533629694
H	-1.213210940	-1.450258406	3.099888209
H	-1.622587721	0.283160072	3.201476818
H	-2.646858469	-0.820857097	2.242733789
C	1.848483869	0.296662665	1.460448654
H	2.190795560	-0.562721981	2.067395294
H	1.784235028	1.160105780	2.149063401
C	2.859901896	0.587520764	0.358559787
H	2.910662881	-0.280205065	-0.319359020
H	2.499246203	1.436802267	-0.244261130
C	4.251816375	0.897752762	0.898477579
H	4.193932852	1.765160152	1.579029065
H	4.605102511	0.046779348	1.506707269
C	5.252043455	1.184069417	-0.217310995
H	4.926155125	2.043705801	-0.822976034
H	6.250392225	1.410350293	0.183962905
H	5.344564622	0.318218027	-0.890893781



CP1'*me*

33
Co2C13H12O6

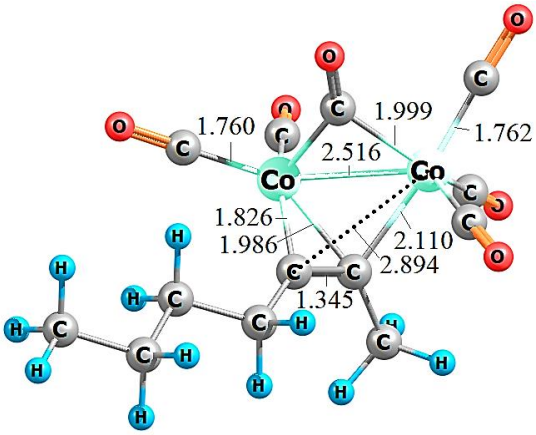
Co	1.445352483	-0.744368409	0.373766401
Co	-0.171809229	1.099445903	-0.196747050
C	1.754021401	0.750719141	-0.683307655
C	2.912316463	-1.631712116	-0.004049179
C	1.765434725	-0.123779595	2.037055177
C	-1.005433979	0.879300046	-1.756540235
C	-1.134331172	1.413796250	1.272681299
C	0.271942642	2.798612983	-0.333373029
O	3.836961926	-2.265683263	-0.291121693
O	2.563414096	1.255167046	-1.370814445
O	1.925368667	0.252493631	3.116620785
O	-1.589934022	0.770659094	-2.749004423
O	-1.788756974	1.628974459	2.201996609
O	0.524452845	3.918885261	-0.451354866
C	0.303150999	-1.720209632	-0.658258735
C	-0.515434599	-0.952191006	0.082815176
C	0.264273832	-2.823613248	-1.621276730
H	1.164368957	-3.450209241	-1.588680391
H	-0.633057963	-3.444778612	-1.460091131
H	0.177606346	-2.397973709	-2.636966893
C	-1.781290344	-1.409549921	0.759057620
H	-1.827507805	-1.016052091	1.786622760
H	-1.732191980	-2.509899745	0.847388054
C	-3.050463465	-1.026818652	-0.000764361
H	-3.126260454	0.071222956	-0.060545723
H	-2.975986116	-1.389084398	-1.041326922
C	-4.306988993	-1.587701766	0.656651801
H	-4.227081628	-2.686744436	0.721415013
H	-4.364387446	-1.216863134	1.694634891
C	-5.574936001	-1.204994176	-0.100271660
H	-5.541122749	-1.579229543	-1.135252139
H	-6.471641754	-1.620488967	0.381633906
H	-5.688914763	-0.110913110	-0.144138747



CP1'*bu*

33
Co2C13H12O6

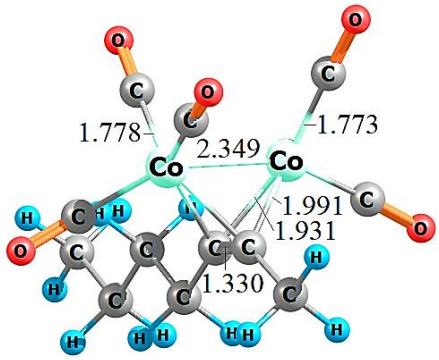
Co	-0.452559752	0.799219237	-0.687372711
Co	1.463434364	-0.510824007	0.284645005
C	0.326581187	0.970243323	0.997442100
C	-1.737859973	1.976818115	-0.445171906
C	0.644707920	1.726660119	-1.778977614
C	0.992953464	-1.890588017	1.312390835
C	2.594674972	-0.825267497	-1.064244191
C	2.738428082	0.214555469	1.261050233
O	-2.575707651	2.761164147	-0.297627077
O	0.208076277	1.555410662	2.011213322
O	1.355246997	2.274138198	-2.505813039
O	0.735251223	-2.815556378	1.957623275
O	3.338656348	-1.036881669	-1.923546893
O	3.580435367	0.646305549	1.922512204
C	-1.321023564	-0.789660194	-0.453891400
C	-0.123439440	-1.141295951	-0.954578215
C	0.155314392	-2.177187057	-2.005177565
H	-0.782952497	-2.471494102	-2.500629939
H	0.847142787	-1.801589690	-2.770488592
H	0.605987703	-3.073913830	-1.554429343
C	-2.603120569	-1.387966617	-0.065930628
H	-2.421010924	-1.972244452	0.858876619
H	-2.862002833	-2.146358164	-0.832683531
C	-3.756994195	-0.416231580	0.143487493
H	-3.473166848	0.307284803	0.925049777
H	-3.915334050	0.162352475	-0.781735448
C	-5.051411671	-1.116826505	0.542400013
H	-5.334490942	-1.838121629	-0.244183308
H	-4.877755752	-1.706917841	1.459226039
C	-6.192630188	-0.130727885	0.772866576
H	-5.939160659	0.579541337	1.574828735
H	-6.395282523	0.453593203	-0.137887144
H	-7.120019503	-0.647784254	1.057911013



CP2

31
Co2C12H12O5

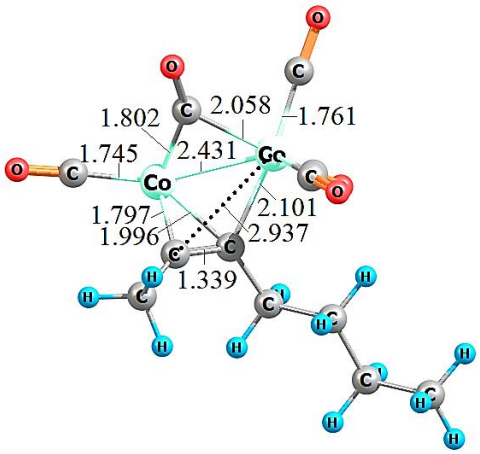
Co	-0.565625260	-1.217416556	0.154372626
Co	-0.465144594	1.127436333	0.057571873
C	-0.282307845	-2.828354211	-0.427266555
C	-2.041326778	-1.450323304	1.109201185
C	0.312734228	2.597021091	-0.546540783
C	-2.187688505	1.581209841	0.126838785
C	0.098592924	1.016516237	1.740171023
O	-0.097865034	-3.885625468	-0.873978554
O	-3.053047638	-1.569751480	1.660267864
O	0.856041840	3.533492952	-0.955853019
O	-3.311839745	1.849916111	0.130459334
O	0.457712361	0.924461942	2.837803252
C	0.662651292	-0.208276420	-0.942253771
C	-0.547278554	-0.080656645	-1.480483059
C	2.116969414	-0.319823128	-1.204684290
H	2.427413180	0.526674300	-1.844846394
H	2.290495580	-1.242012326	-1.790502742
C	2.954311351	-0.345957279	0.071044724
H	2.756801825	0.576715840	0.642198333
H	2.614089983	-1.184210328	0.704950668
C	4.448661291	-0.473737680	-0.201926876
H	4.640118345	-1.405921265	-0.761437457
H	4.767482705	0.354874351	-0.858467867
C	5.278002355	-0.461044148	1.078757674
H	4.992654141	-1.294323386	1.739239206
H	6.352419356	-0.552331964	0.863401878
H	5.122134530	0.475418732	1.636240256
C	-1.339701847	-0.174484853	-2.718313422
H	-1.095911446	0.682100951	-3.369173989
H	-1.093962371	-1.100359471	-3.262078279
H	-2.416270219	-0.152229915	-2.509633133



CP2'*me*

31
Co2C12H12O5

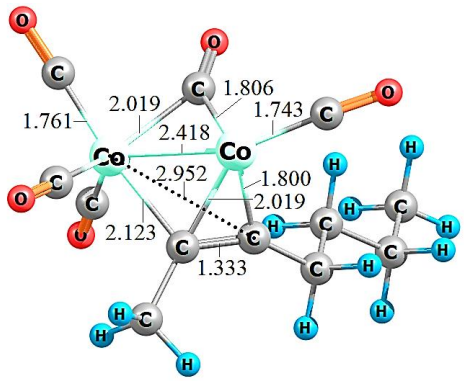
Co	1.624629386	-0.667265037	0.547463720
Co	-0.053925384	1.066939670	0.257710383
C	1.945913607	0.935935880	-0.208875225
C	3.201925450	-1.403298118	0.420004138
C	-0.854656834	1.175659715	-1.326671827
C	-1.082715256	1.031729069	1.715658228
C	0.359199238	2.765478596	0.473572072
O	4.225515529	-1.927683566	0.256058730
O	2.704793030	1.589165267	-0.834708516
O	-1.392697658	1.254838332	-2.347381920
O	-1.769817592	1.041761827	2.647139968
O	0.591325395	3.889385737	0.603052499
C	0.632189721	-1.666833468	-0.567672891
C	-0.298525375	-1.017062791	0.142906195
C	-1.608974455	-1.629021141	0.587452131
H	-1.779075040	-1.422959535	1.655941390
H	-1.516837562	-2.725677847	0.491314951
C	-2.813704555	-1.159152735	-0.225868256
H	-2.955655761	-0.076332537	-0.078413460
H	-2.605536594	-1.302807713	-1.300543568
C	-4.093524488	-1.894855941	0.157947018
H	-3.949705849	-2.979912995	0.014318684
H	-4.286830603	-1.744778707	1.234272294
C	-5.294752723	-1.421246602	-0.654855575
H	-5.471338306	-0.345593045	-0.501059348
H	-5.126108527	-1.581258521	-1.731094881
H	-6.210412323	-1.959695612	-0.370920377
C	0.838653961	-2.675496208	-1.608340073
H	-0.043663581	-3.334864445	-1.675300085
H	0.937367940	-2.168428720	-2.583282785
H	1.740245688	-3.277472707	-1.438246460



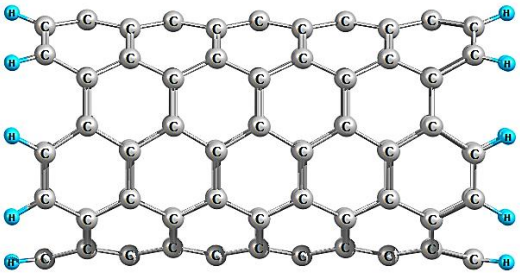
CP2'*bu*

31
Co2C12H12O5

Co	-0.276373068	-0.989055186	0.994034038
Co	1.392096422	0.244183863	-0.247354560
C	0.047970955	-1.167093064	-0.773544308
C	-1.549671486	-2.164155959	1.186804351
C	0.925719823	1.695256015	-1.163731261
C	2.717795251	0.392512036	0.945379620
C	2.395138672	-0.558999517	-1.451293552
O	-2.472416848	-2.866440482	1.267096650
O	-0.359462683	-1.637977444	-1.778794825
O	0.621583907	2.650632946	-1.740934373
O	3.584121602	0.476066920	1.707824431
O	3.064602803	-1.050498961	-2.253963689
C	-1.179314595	0.558707831	1.168731472
C	0.082436604	0.981049719	1.252396998
C	-2.592769666	0.936869721	1.099891576
H	-2.707316920	1.998572789	1.385935986
H	-3.196212389	0.322117694	1.787114261
C	-3.100344754	0.735766835	-0.342870121
H	-2.483536405	1.343090797	-1.026997468
H	-2.942706531	-0.317000384	-0.627088756
C	-4.573183884	1.099077521	-0.491360124
H	-5.166739477	0.495000322	0.216546423
H	-4.721337147	2.155206938	-0.207289877
C	-5.072872379	0.867799434	-1.914097650
H	-4.504776070	1.478051158	-2.632789859
H	-4.952707081	-0.187596974	-2.202778099
H	-6.136475243	1.128444072	-2.011966742
C	0.592468426	2.123031992	2.092290982
H	1.410564204	1.798213882	2.749879584
H	0.978413326	2.933958059	1.458720919
H	-0.217894711	2.523564478	2.719752721



(5,5)-SWCNT



130
C110H20

H	-7.061489960	-3.738624123	0.006544307
H	-7.061487372	-1.161544370	-3.552765253
H	-7.061543909	-3.100011973	-2.088470502
H	-7.061647891	1.028080824	-3.593456811
H	-7.061837668	3.019947572	-2.202656457
H	-7.061916657	3.027959708	2.191562979
H	-7.061953547	3.735424043	-0.132514148
H	-7.062116823	1.279627431	3.510605751
H	-7.061887507	-1.149288921	3.556492970
H	-7.061655596	-2.945156076	2.302628496
C	-6.116034421	-3.033299032	1.770978466
C	-6.115964724	-2.621568124	-2.336673878
C	-6.115950893	-3.479635430	0.479288846
C	-4.916469092	-3.436622125	-0.297922522
C	-6.115952155	-1.531052491	-3.160300929
C	-4.916455299	-0.778655510	-3.359776405
C	-4.916444001	-3.019348202	-1.667636121
C	-6.116131005	1.412142658	-3.215171453
C	-4.916551129	0.652967540	-3.386466635
C	-6.116380164	3.494349855	0.349544926
C	-6.116240607	2.532601153	-2.432744792
C	-4.916804728	2.954939704	-1.778754565
C	-6.116376440	3.096230663	1.656869052
C	-4.916913467	2.604590452	2.260434592
C	-4.916844311	3.422782823	-0.425485032
C	-6.116487409	0.746722956	3.430491811
C	-4.916959332	1.461832372	3.123158960
C	-6.116359501	-0.619641439	3.456176436
C	-4.916772508	-1.345618930	3.175676367
C	-4.916621109	-2.519655538	2.355987332
C	-3.692793370	-2.924985728	1.767200025
C	-3.692653184	-2.584539866	-2.235124485
C	-3.692732067	-3.391876475	0.415617059
C	-2.458936505	-3.395471374	-0.296445063
C	-3.692654664	-1.443391723	-3.096880039
C	-2.458927388	-0.767178092	-3.320421124
C	-2.458880858	-2.984451340	-1.645953924
C	-3.692835695	1.327168936	-3.148452189
C	-2.459030001	0.643294357	-3.346639692
C	-3.693102908	3.404728394	0.289242101
C	-3.692962195	2.499553173	-2.329694222
C	-2.459257822	2.921212628	-1.755736567
C	-3.693129997	2.988003588	1.657136201
C	-2.459397223	2.572352644	2.235409083
C	-2.459298777	3.381953372	-0.422395905
C	-3.693169393	0.776597160	3.326927635
C	-2.459410457	1.446534160	3.085488868
C	-3.693056701	-0.653143614	3.353679920
C	-2.459220319	-1.331512910	3.137347927
C	-2.459080605	-2.488103783	2.329626056
C	-1.225315396	-2.929617511	1.762380030
C	-1.225150169	-2.581235769	-2.241176968
C	-1.225243254	-3.392638727	0.422487500
C	0.000179709	-3.415825553	-0.293845515
C	-1.225151756	-1.449929604	-3.095517263
C	0.000215206	-0.775726937	-3.338922715
C	0.000237557	-2.999820949	-1.659396025
C	-1.225332216	1.334107655	-3.147259527
C	0.000132287	0.651548846	-3.365477125
C	-1.225606420	3.405694783	0.296172839
C	-1.225455037	2.496324798	-2.335537581
C	-0.000103422	2.936324427	-1.769669782
C	-1.225633066	2.992645041	1.652262339
C	-0.000243143	2.590429970	2.245517930
C	-0.000168606	3.402444463	-0.420419995
C	-1.225642072	0.770592440	3.330245806
C	-0.000234540	1.451230989	3.105767073
C	-1.225545668	-0.646808650	3.356682996
C	-0.000082750	-1.335222883	3.157598312
C	0.000039181	-2.505555695	2.340237008
C	1.225461270	-2.929455669	1.762368598
C	1.225654593	-2.581030791	-2.241041083
C	1.225553652	-3.392528461	0.422505429
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RC

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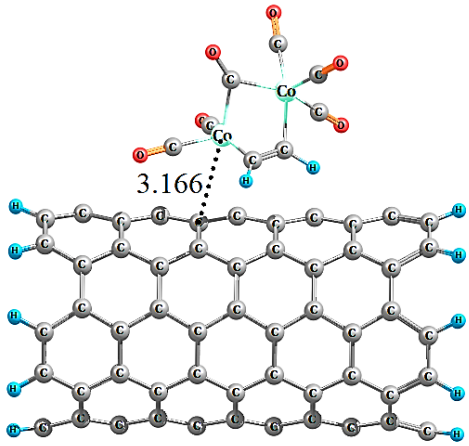

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CP3

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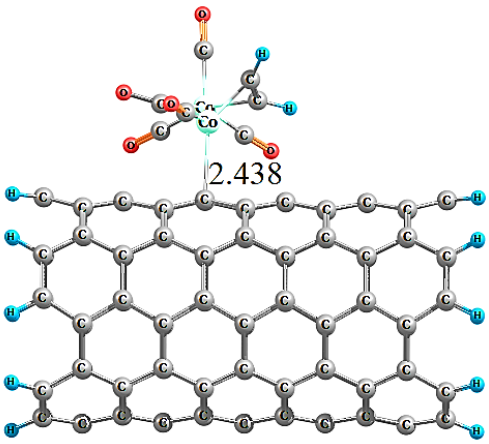

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C	-3.648526258	1.404940814	-3.280472957
C	-5.183952455	-2.042658143	-1.895438192
C	-4.222570209	0.098484804	-3.369730195
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C	-5.159529208	-1.888628204	2.115133123
C	-4.720968455	-0.876425597	3.025085383
C	-6.123404505	-1.155801299	-2.476865784
C	-7.444230313	-1.165764445	-1.930609429
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C	-5.626336060	-0.048729637	-3.239158687
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H	-7.498938987	1.009910552	-3.628874391
C	-3.798929251	4.180946526	0.572564127
C	-4.849961027	4.755085256	-0.207480496
H	-5.634607372	5.332715557	0.277545085
C	-4.059553588	3.533803104	-2.148048433
C	-4.976940953	4.439894730	-1.531972085
H	-5.859810830	4.773158729	-2.074268828
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C	-4.024879365	3.695364096	1.903460505
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H	-5.973782920	4.600799094	2.306627433
C	-6.438868177	-1.770515205	1.517344863
C	-7.392170409	-0.945865650	2.191103576
H	-8.443436547	-0.990245313	1.912456771
C	-5.578209010	0.216163643	3.305699390
C	-6.973039732	0.021252640	3.061791155
H	-7.699131145	0.727726538	3.459698960
H	1.882421912	6.036859190	-2.700025410
H	0.693581448	5.467948643	-0.108952800

CP3’

148
Co2C118H22O6

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C	-3.091815101	3.586336138	2.911281359
C	-3.629605289	6.350042663	-1.713169915
C	-2.017166669	4.198910283	-2.279046413
C	-4.531596830	3.623095464	-1.707648661
O	-2.981616358	3.669649606	4.058345509
O	-4.863106516	5.887488541	1.090086157
O	-3.885390454	7.395920472	-2.124159377
O	-1.192406469	4.055260645	-3.075424765
O	-5.311944446	2.867113124	-2.097699451
C	-1.642419817	4.663110505	1.138835141
C	-1.600734541	5.203837559	-0.065558900
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H	-7.000092098	-1.540210021	1.693623241
H	-7.176098884	-1.134208145	-0.696721528
H	-6.247261555	-2.959483306	3.209519413
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H	-3.576740846	-7.682031515	0.366110126
H	-4.124888766	-6.758051488	2.545884840
H	-3.739294449	-7.326133157	-1.796915786
H	-4.566084024	-5.780144191	-3.478709914
H	-5.611634718	-3.879025341	-3.778365959
C	-4.995928008	-3.046856831	-3.441986757
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C	-2.759072345	0.283810617	1.870773034
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C	-3.047191521	-1.776971080	3.138656730
C	-2.274286164	-0.615689072	2.839145891
C	-1.155079991	-5.154060560	2.055627810
C	-2.362756500	-3.015607739	3.339507087
C	-0.943193454	-3.026837661	3.226064987
C	-0.831152180	-5.700314506	0.774337014
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C	-0.328700712	-4.115766233	2.573878883
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C	-1.417717089	-1.962845229	-3.421314180
C	-0.682047996	-0.746294318	-3.289530984
C	-1.949487539	1.443498164	-0.134941611
C	-1.296053689	0.345310609	-2.626329411
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C	-1.861898115	1.237745803	1.279408178
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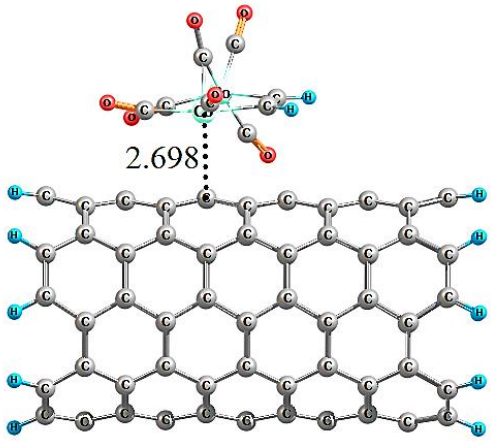

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C	1.258208377	0.605237943	3.222474118
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C	3.417487604	1.801037449	3.257316291
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C	5.434587286	-1.687150545	-1.843134376
C	4.948465244	-0.777231554	-2.833415939
C	6.137922588	-0.574641620	2.718211802
C	7.477311009	-0.504192425	2.222895630
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TS1*oblique*

146
Co2C117H22O5

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H	-7.518760368	1.459744650	-3.585422961
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C	-4.358714665	2.679487877	-3.205724361
C	-4.372255326	5.160113806	-0.548490977
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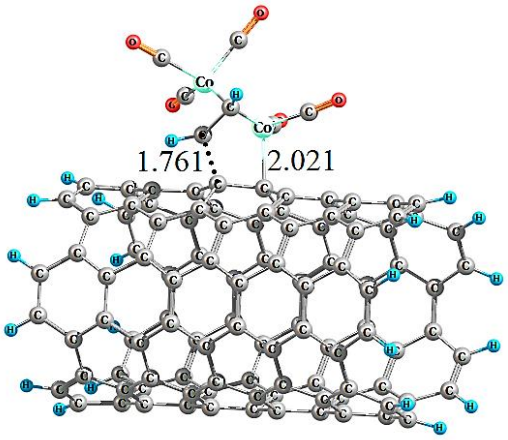

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C	5.269412878	-2.617925394	3.131949487
H	5.897689121	-3.410134637	3.534796814
C	4.767729841	-1.138019083	-2.350376780
C	6.072765275	-1.293507054	-1.777362078
H	6.842385284	-1.843054311	-2.315928558
C	5.246440103	-0.341406146	0.291330851
C	6.301521431	-0.916973782	-0.484524125
H	7.246945693	-1.177516555	-0.011770293
C	2.777912877	-4.646103885	-3.078919390
C	4.173762385	-4.610638029	-3.362181218
H	4.740258368	-5.538115477	-3.421107112
C	4.168156653	-2.193837169	-3.127965881
C	4.849096562	-3.417584990	-3.388834347
H	5.933939161	-3.429821896	-3.472876459
C	1.755483535	-6.385872138	0.427176922
C	2.766544643	-7.042545493	-0.339543169
H	3.463697371	-7.722361420	0.146931245
C	2.193162130	-5.659011448	-2.245258118
C	2.980503066	-6.686871818	-1.642821817
H	3.843678521	-7.091047141	-2.168589475
H	3.721178758	2.442427918	-2.024431177
H	2.472237264	5.017034650	-2.116190017

TS1*_oblique_

146
Co2C117H22O5

Co	-1.650133523	5.678147609	0.503841007
Co	0.564975880	4.780265472	-0.256481751
C	-1.161809743	7.304956024	-0.043549991
C	-2.907876446	6.035101198	1.682703543
C	0.214189470	4.887406608	-1.993379659
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O	-3.733995375	6.251488714	2.462660434
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C	-0.864970517	4.167910216	1.506281970
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H	-6.998952997	-1.164271804	3.565245149
H	-6.518931824	-5.187844587	1.826204765
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H	-6.428289873	-5.736748594	-0.301156615
H	-6.506631166	-4.812195282	-2.547997427
H	-6.705185416	-2.952558867	-3.697971182
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C	-6.367369602	1.605172813	-0.236938233
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C	-3.833035790	0.781620748	2.405592125
C	-2.669316373	1.395526492	1.872443232
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C	-3.230707351	-4.302159394	2.034501674
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C	-1.433001722	1.761363629	-1.449628793
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C	-0.141000967	1.519476451	-2.025567779
C	-1.369359275	1.045943692	2.381504926
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C	-0.713860720	-4.155687724	-1.927625259
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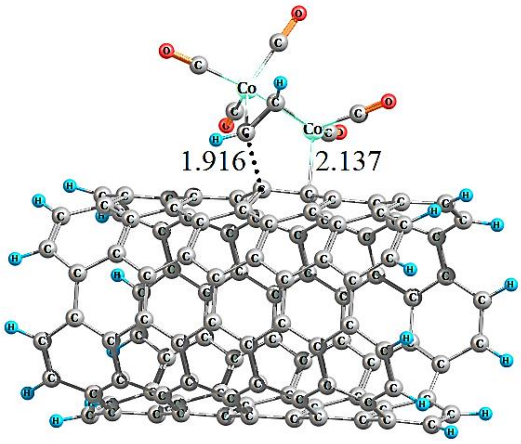
C	1.457770314	-1.493445027	-3.318129861



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C	2.234925698	1.961394576	1.892885565
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TS1*perpendicular*

146
Co2C117H22O5

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H	-5.156731512	4.596698693	3.716076032
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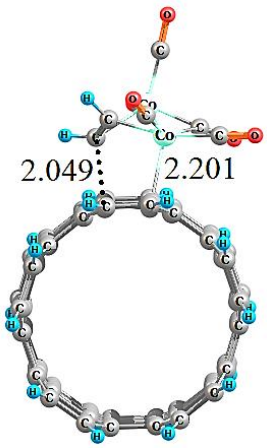

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H	6.855063828	-2.754911948	-3.752109387
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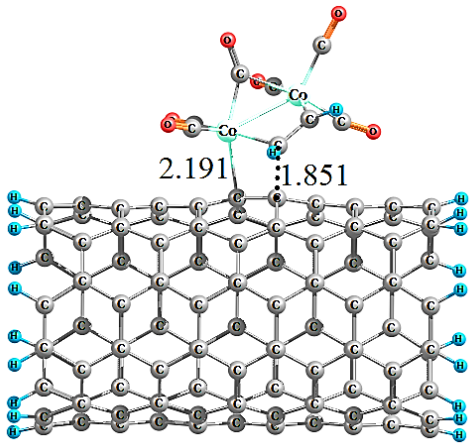
C	6.234425956	0.617377527	2.593992677
C	7.563029732	0.613812351	2.068128688
H	8.345503613	0.047466073	2.569776843
H	-2.166100018	-3.523386146	2.813413697
H	-4.759388479	-3.684543656	2.324337007

TS1'*oblique*

148
Co2C118H22O6

Co	1.712862743	-4.267113801	-0.508902530
Co	4.256956555	-4.243134853	0.346985255
C	2.888118614	-5.685545015	-0.587049393
C	0.699193273	-4.849232732	-1.848459833
C	5.629785603	-5.292934645	-0.100876246
C	5.095890032	-2.861320029	1.037873371
C	3.718989058	-4.865272757	1.946309968
O	0.063955401	-5.279511311	-2.709968110
O	3.041051154	-6.809867312	-0.874904426
O	6.553686185	-5.930271831	-0.367324330
O	5.841208732	-2.122345051	1.524884197
O	3.377334245	-5.256493899	2.976705447
C	2.874385484	-3.095548458	-1.756585963
C	4.153678005	-3.385733388	-1.379120419
C	0.888756743	-4.938680893	0.931184050
O	0.371015620	-5.405619074	1.848532790
H	5.812668219	3.650542025	-3.716278225
H	7.272153697	1.077672404	-0.560789052
H	6.742978417	1.931778195	-2.778300287
H	7.087747243	1.457546935	1.601724797
H	6.263883033	3.044813958	3.250652278
H	4.232590991	6.858476132	2.430404609
H	5.255638694	4.960596436	3.548552847
H	3.764264178	7.687158175	0.447939482
H	3.962522617	7.240459370	-1.932140413
H	4.706528668	5.780931167	-3.383770270
C	4.112517714	4.869260791	-3.361405823
C	5.991973180	1.366021533	-2.230173803
C	4.737801380	3.663907929	-3.546825156
C	4.032088423	2.441385487	-3.346060599
C	6.289863392	0.883644100	-0.988378106
C	5.265321623	0.286090607	-0.188158926
C	4.644091407	1.302039182	-2.713371608
C	6.042210449	1.420370708	1.901815591
C	5.130982779	0.569487985	1.205874676
C	4.215218981	4.894406175	3.235932767
C	5.578981132	2.311506592	2.829002907
C	4.182006518	2.392984136	3.114024440
C	3.639131430	5.963340894	2.607449060
C	2.337490299	5.843417847	2.029075560
C	3.520969776	3.647618874	3.318454444
C	3.010950054	7.072944763	-0.041941816
C	2.030204390	6.386086931	0.738555060
C	3.122692934	6.820729072	-1.381412666
C	2.257209913	5.874025166	-2.010144580
C	2.742940850	4.921509359	-2.968118754
C	1.963237026	3.762894227	-3.210738129
C	3.813550760	0.305785353	-2.156883577
C	2.619314700	2.504829051	-3.385102272
C	1.853247399	1.316641639	-3.206124075
C	4.145908924	-0.242906281	-0.870541191
C	3.122685979	-0.912166334	-0.145255525
C	2.445714013	0.205637176	-2.563171051
C	3.871897190	0.336890280	1.805044930
C	2.947966435	-0.570563657	1.192086865
C	2.111948162	3.690870569	3.182863139
C	3.391869106	1.265105350	2.775520660
C	2.002594667	1.257990952	3.081117754
C	1.507657743	4.810799652	2.530997127
C	0.180612660	4.664732737	2.032415565
C	1.354580503	2.489375550	3.295736847
C	0.912365880	5.861999098	0.042760683
C	-0.125151959	5.202486796	0.764885683
C	1.028975686	5.601176863	-1.358217121
C	0.094931139	4.704585605	-1.954226110
C	0.573618594	3.768754655	-2.895520806
C	-0.218902960	2.619787567	-3.181536601
C	1.611856571	-0.814333287	-2.042428358
C	0.438425752	1.369836644	-3.323641919
C	-0.311002893	0.179484987	-3.170281379
C	2.088223647	-1.647760918	-0.912871793
C	0.994726123	-2.240732907	-0.088562963
C	0.293051542	-0.926510985	-2.502157052
C	1.694885008	-0.845948653	1.848652412
C	0.797336454	-1.775718325	1.283573079
C	-0.069186122	2.541639633	3.213174986
C	1.218559257	0.099311029	2.790661338
C	-0.155169956	0.097226661	3.146407579
C	-0.669093654	3.650879047	2.568996264
C	-1.996788979	3.520854393	2.081535522
C	-0.814554935	1.344633264	3.357943156
C	-1.273056153	4.711177051	0.071281994
C	-2.306645292	4.064527127	0.799890056
C	-1.160090284	4.458028380	-1.320105212
C	-2.089280323	3.572088423	-1.929501349



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C	-1.723948367	0.223823874	-3.295896455
C	-2.482350144	-0.980003375	-3.165663017
C	-0.240336516	-2.555878404	-0.780415176
C	-1.314255090	-3.152149928	-0.042433189
C	-1.891524277	-2.087046679	-2.518832990
C	-0.454338373	-1.985930693	1.911809080
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C	-2.228616882	1.391305650	3.255024690
C	-0.935323020	-1.048038251	2.861594438
C	-2.324374566	-1.049949584	3.198925577
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C	-4.158222853	2.347265678	2.102577569
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C	-3.437397826	3.553683149	0.105172013
C	-4.466394041	2.883584833	0.834529290
C	-3.326343492	3.302898048	-1.284370493
C	-4.252241815	2.397068217	-1.888426258
C	-3.772819004	1.467056515	-2.835074744
C	-4.561385113	0.317708058	-3.126284180
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C	-2.451621322	-3.651344276	-0.729899223
C	-2.642071137	-3.153603866	1.988043827
C	-4.400583135	0.225917633	3.305872811
C	-3.115308008	-2.208726384	2.953490156
C	-5.006103518	1.336078980	2.638395300
C	-5.610658544	2.383738549	0.148043394
C	-5.500517133	2.134259086	-1.255652214
C	-5.149978172	-0.961923541	3.491984467
C	-6.573652580	-0.843005558	3.432197871
H	-7.203303484	-1.659423563	3.780695948
C	-6.337406802	1.213035363	2.166767289
C	-7.151081687	0.214056891	2.785771865
H	-8.228388051	0.217419295	2.630426380
C	-3.565182056	-4.060203129	1.404101982
C	-4.764305317	-4.322984060	2.140522063
H	-5.394161090	-5.168371217	1.869701300
C	-4.484789669	-2.217692000	3.314010852
C	-5.209993222	-3.427899101	3.070346182
H	-6.186689610	-3.576979507	3.526937169
C	-4.060545574	-3.252384995	-2.534931834
C	-4.855137911	-4.313337675	-1.991644710
H	-5.770245200	-4.618915754	-2.495530816
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H	-5.264055544	-5.533098320	-0.303554834
C	-5.951493225	0.332166053	-2.846185536
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H	-7.785487874	-0.792240709	-3.240617858
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C	-6.065953664	-2.027546060	-3.396273853
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H	-8.707452786	1.045707923	0.652232901
C	-6.435413171	1.267362685	-1.876632799
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H	-8.522340085	0.624889582	-1.733647452
H	2.607308357	-2.955390183	-2.810802663
H	5.022926402	-3.250234974	-2.034623666

TS1'*_oblique_*

148
Co2C118H22O6

Co	3.422303734	-3.428398205	0.512755431
Co	1.886790902	-5.540128282	-0.102267545
C	3.911914621	-5.183560727	0.716139611
C	4.536166784	-2.821191879	1.757095538
C	1.903612006	-7.213766295	0.516432695
C	0.299358251	-5.413788284	-0.845607080
C	2.710500269	-5.673004736	-1.694817654
O	5.303472951	-2.495519660	2.556129705
O	4.733159839	-5.961157357	1.016690217
O	1.849776955	-8.301638428	0.896504575
O	-0.715333753	-5.590235940	-1.372165336
O	3.236366944	-5.754104208	-2.718752842
C	1.812760266	-3.580986955	1.848606461
C	1.303174951	-4.820504919	1.584284131
C	4.312597252	-3.180255014	-1.016311432
O	4.902440273	-3.007460445	-1.991840517
H	6.329432114	2.869244764	-3.444810237
H	7.341607108	1.201732567	0.460959960
H	7.102541137	1.505192159	-1.936790766
H	6.900357832	2.062805199	2.452790831
H	5.882762814	3.985950392	3.534968580
H	4.023205975	7.424924924	1.502545099
H	4.868488809	5.889819879	3.182774040
H	3.817542184	7.735105568	-0.661484916
H	4.304494134	6.734176275	-2.820602876
H	5.203503186	4.990020623	-3.793137144
C	4.606298263	4.097850219	-3.613813542
C	6.283467414	1.060317861	-1.374798336
C	5.242004020	2.900419863	-3.415856927
C	4.507058270	1.753057689	-2.995148335
C	6.418968546	0.888544067	-0.024567421
C	5.301090843	0.474314829	0.762656039
C	5.019429393	0.841591699	-2.006774495
C	5.824317672	2.071366868	2.617685732
C	5.008281182	1.049542527	2.044526722
C	3.875720240	5.726458644	2.767773219
C	5.251459649	3.155418714	3.225017617
C	3.829622956	3.276156061	3.287082492
C	3.399203485	6.592393110	1.822367174
C	2.181016320	6.307259058	1.132108832
C	3.160899505	4.527763892	3.074250311
C	3.124162961	7.006187368	-1.077076126
C	2.045955632	6.510829492	-0.280973937
C	3.398531828	6.442218200	-2.292596366
C	2.609080287	5.353694260	-2.774511787
C	3.199774098	4.210819705	-3.411263409
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C	4.103166774	0.008689718	-1.328416075
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C	2.321165725	0.631596939	-2.862610457
C	4.256836182	-0.185565532	0.076995478
C	3.142102992	-0.696935614	0.801653388
C	2.818697136	-0.268433038	-1.893794612
C	3.678060979	0.944971233	2.517767366
C	2.826346075	-0.087211892	2.020161349
C	1.782156618	4.507638385	2.749994862
C	3.078441850	2.082527424	3.144068202
C	1.658305435	2.126218382	3.243954738
C	1.280602087	5.416102307	1.765817753
C	0.025518107	5.125250921	1.154718234
C	1.000020417	3.358340808	3.061087422
C	1.019653893	5.809548430	-0.960636800
C	-0.108745587	5.327171108	-0.234666449
C	1.308535119	5.218337208	-2.229960722
C	0.449248427	4.182447215	-2.699296274
C	1.032718058	3.056779774	-3.318285781
C	0.274589070	1.853120398	-3.408478265
C	1.926735475	-1.175972820	-1.252370380
C	0.934205924	0.617878725	-3.167261338
C	0.163523441	-0.517389817	-2.811301441
C	2.190469910	-1.568957361	0.124957806
C	1.085932938	-2.141219389	0.953190418
C	0.673032906	-1.423168534	-1.835597586
C	1.480116013	-0.206165650	2.506307207
C	0.653127286	-1.255704495	2.073013995
C	-0.400550410	3.357065962	2.783407025
C	0.900098831	0.921727063	3.139975234
C	-0.505683097	0.969722770	3.297135982
C	-0.900587881	4.260931991	1.813283562
C	-2.155666888	3.985919039	1.206944828
C	-1.173889383	2.216839381	3.118579146
C	-1.164594948	4.658102905	-0.925442903
C	-2.290998647	4.190845889	-0.197978934
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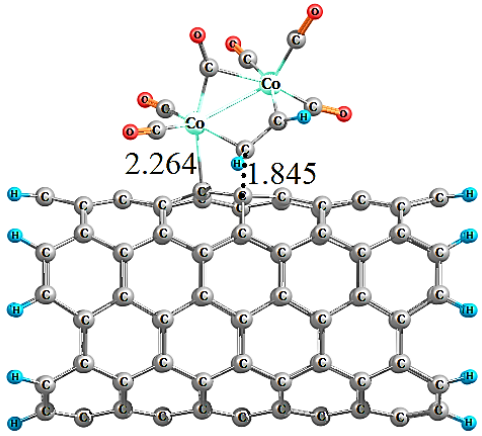

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C	-1.225242102	-0.523542020	-3.114460644
C	-2.013505510	-1.664554402	-2.771801300
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C	-1.235952797	-3.032798733	0.911952522
C	-1.531498016	-2.547614878	-1.787731024
C	-0.656755301	-1.361002030	2.582315884
C	-1.512283417	-2.435714158	2.164718368
C	-2.561172738	2.201025935	2.823688731
C	-1.250923706	-0.230605309	3.200492198
C	-2.668862448	-0.185682384	3.351381601
C	-3.062360736	3.102084506	1.852976656
C	-4.315506707	2.803503531	1.237029684
C	-3.331956179	1.043733572	3.149800698
C	-3.328120119	3.500107441	-0.884915222
C	-4.452267006	3.009180932	-0.152024930
C	-3.041837932	2.919880647	-2.143527669
C	-3.892739134	1.874961497	-2.620716564
C	-3.305304595	0.751653370	-3.239420652
C	-4.063790849	-0.448450184	-3.337000656
C	-2.453902274	-3.430701908	-1.166859357
C	-3.398309801	-1.691995085	-3.100915051
C	-2.310099671	-3.666073524	0.230916871
C	-2.827774732	-2.543035533	2.691895707
C	-4.728204084	1.027212788	2.875343012
C	-3.424069794	-1.391184100	3.304283391
C	-5.233468618	1.930646029	1.888787067
C	-5.503654888	2.334100734	-0.836133483
C	-5.215746494	1.751835787	-2.110043555
C	-5.502878264	-0.101128351	3.244771690
C	-6.906332880	-0.036106337	2.974992584
H	-7.581514865	-0.760935448	3.425629634
C	-6.493369233	1.664870005	1.294854494
C	-7.387870092	0.821790137	2.026656832
H	-8.435829454	0.762118354	1.738900199
C	-3.683300122	-3.586357418	2.241760138
C	-4.971390401	-3.684849974	2.860484746
H	-5.565579182	-4.588478458	2.736394635
C	-4.829989305	-1.343243147	3.472793683
C	-5.528377531	-2.594436989	3.462521840
H	-6.556000976	-2.646694829	3.817064327
C	-3.686051810	-3.738691465	-1.798210394
C	-4.543173757	-4.667563068	-1.125271405
H	-5.383869692	-5.113056183	-1.653826442
C	-3.418553567	-4.161512438	0.963355392
C	-4.416863943	-4.870364916	0.219399605
H	-5.161418004	-5.469138799	0.740899812
C	-5.478076536	-0.394535651	-3.248813845
C	-6.183720171	-1.629827215	-3.409377138
H	-7.258624978	-1.623003127	-3.580581790
C	-4.173816087	-2.840336576	-2.793517146
C	-5.549545905	-2.818579210	-3.190687461
H	-6.129194810	-3.739639568	-3.191213159
C	-6.634077915	1.876687155	-0.112735257
C	-7.676952347	1.254236346	-0.870413836
H	-8.657126369	1.100348020	-0.422800808
C	-6.072229427	0.738614241	-2.612625241
C	-7.404310761	0.701669644	-2.089077041
H	-8.171551368	0.116564750	-2.592712350
H	1.912256001	-3.215851032	2.877900496
H	0.733646908	-5.400251705	2.321454874

TS1'*perpendicular*

148
Co2C118H22O6

Co	-3.106984410	-3.469236954	-0.656731191
Co	-5.418971227	-3.100590907	0.675559775
C	-4.478256779	-4.681225245	-0.534847868
C	-1.830873078	-4.699954604	-0.794544742
C	-6.566005301	-4.375865493	1.197504087
C	-5.871108815	-1.902039488	1.865490294
C	-6.117433609	-2.381166722	-0.820019157
O	-1.102322242	-5.586621205	-0.912140448
O	-4.894868010	-5.717894595	-0.883697979
O	-7.344445153	-5.150635729	1.549172736
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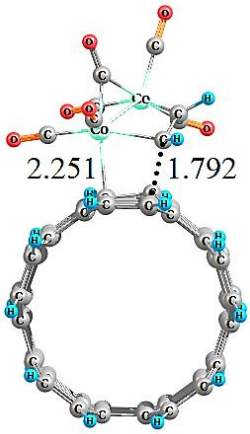

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CP4*oblique*

146
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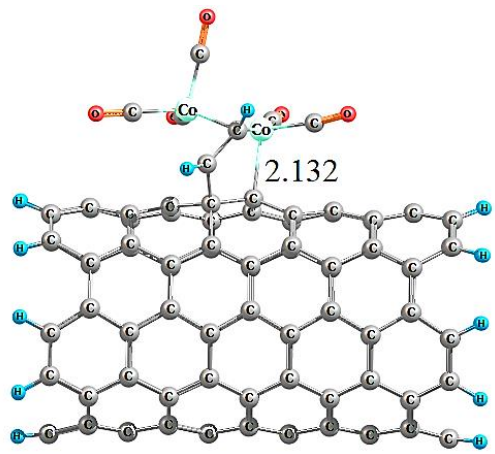

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CP4*_oblique_

146
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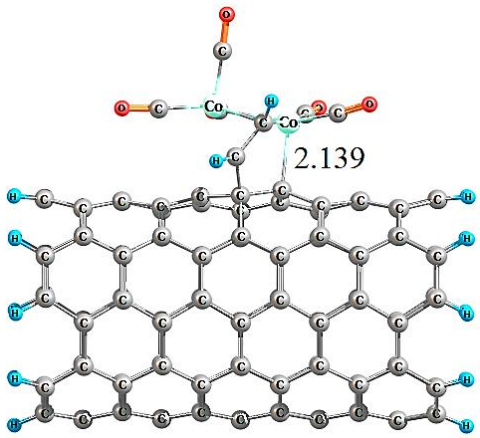

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C	3.176188221	2.069658403	2.722339788
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H	7.217992689	0.664107920	-3.599140490
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H	7.853744251	-1.249104968	-2.737205389
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CP4*perpendicular*

146
Co2C117H22O5

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O	-4.477566145	3.476032469	2.557142158
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H	-6.616396541	-1.502068866	2.606603809
H	-5.633482093	-3.422911133	3.719056718
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H	-3.719187054	-7.354452737	-0.336487145
H	-4.246193207	-6.385974768	-2.501128114
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C	-4.375774615	-1.405945850	-2.826223334
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C	-4.854173393	-0.451038010	-1.874917749
C	-5.538370378	-1.535359035	2.750453009
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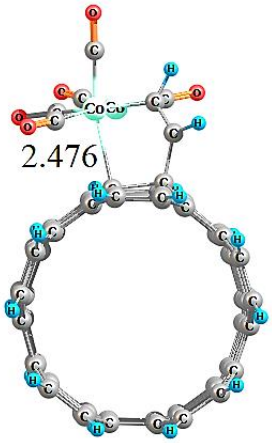

Note: Discarded in the main manuscript.

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CP4*perpendicular*

146
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O	-6.539058773	-3.801496816	-0.936595838
O	-0.964507176	-5.351374699	-1.575924203
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H	-3.829256266	7.479237526	0.735501674
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C	-2.787812585	-0.605606674	1.921986598
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C	-1.793378965	4.309537554	-2.736000352
C	-3.054447857	1.869288049	-3.105498477
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C	-0.826020894	-2.062541984	-0.861962358
C	-0.571682157	-1.786289199	1.888787688
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C	1.191776808	2.065628656	-3.179169138
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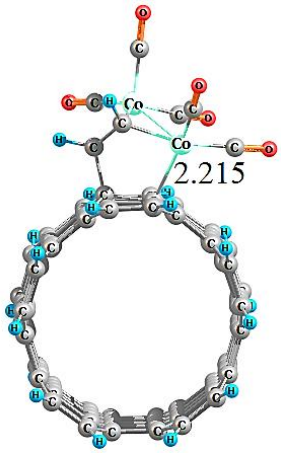

Note: Taken into consideration in the main manuscript.

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C	1.626063343	-2.538950180	-2.197548014
C	2.583372372	2.071144482	-2.903184150
C	1.310260401	-0.376575183	-3.294605153
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C	4.334265009	2.670758003	-1.305239456
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C	3.349164106	3.307748693	0.835589426
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C	3.075101642	2.694918719	2.088845596
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H	8.701761702	0.990769261	0.300847913
C	6.146361318	0.571661401	2.513062948
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H	8.245769844	-0.031202054	2.454648201
H	-2.731074534	-3.109253933	3.014315244
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CP5*oblique*

148
Co2C118H22O6

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H	3.359566619	-7.907408478	-0.588250510
H	3.579955260	-7.531591525	1.802250685
H	4.411599333	-6.146081574	3.278721318
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C	5.960872211	-1.816863517	2.127038403
C	4.576426026	-4.035453223	3.450686092
C	3.947400397	-2.772434250	3.257883111
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C	4.625501857	-1.667945431	2.626386738
C	6.011150417	-1.707926218	-2.014748006
C	5.160951723	-0.821332139	-1.282605485
C	3.966876984	-5.071943817	-3.315505519
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C	4.070580756	-2.572941628	-3.180629003
C	3.336637132	-6.119669130	-2.702289662
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C	1.799267298	-3.959706114	3.136723520
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C	0.425273336	0.858132183	2.506927681
C	1.772495712	0.771452019	-1.805693797
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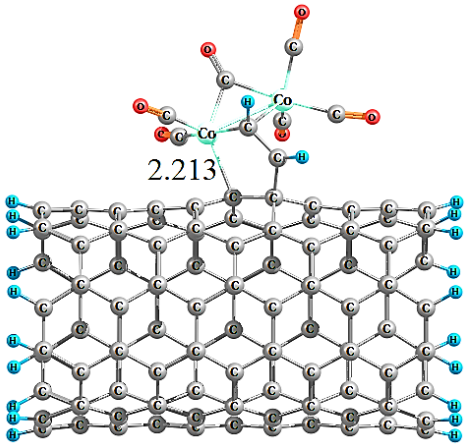

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C	-4.985588299	3.741914993	-2.940783371
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CP5*$_{oblique}$

148
Co2C118H22O6

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O	-5.538629461	-2.566950270	-2.299733454
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O	-3.264918210	-6.119614980	2.956004270
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C	-1.885520965	-4.732888428	-1.413061917
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H	-6.871962258	1.984078268	-2.552301888
H	-5.867211064	3.951494911	-3.567239111
H	-4.092152066	7.401807865	-1.476455682
H	-4.897885243	5.862773788	-3.171761167
H	-3.915513859	7.680020397	0.696184876
H	-4.416054197	6.615217364	2.821076992
H	-5.293177603	4.831686221	3.734205330
C	-4.675774606	3.954713704	3.548844365
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C	-0.838579982	0.973300116	-3.129703794
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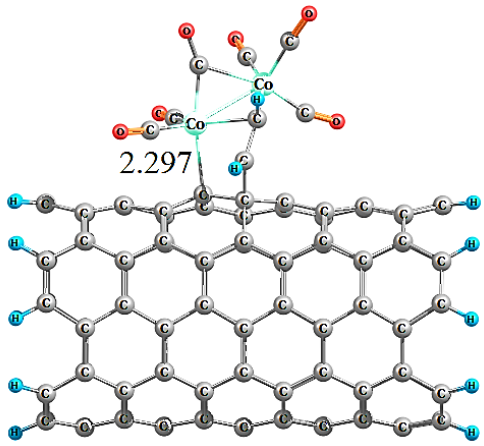

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C	1.616531860	-2.384303750	-2.241644389
C	2.597385410	2.312222813	-2.794257596
C	1.331757092	-0.138791269	-3.193940876
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C	2.937532390	-2.444626282	-2.750641609
C	4.782850027	1.174216411	-2.843875151
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CP5*perpendicular*

148
Co2C118H22O6

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H	-2.701017523	7.880985293	0.502052322
H	-3.367370503	6.921969073	2.632620638
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C	-4.697660592	1.143163211	1.790303358
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C	-1.905506854	-1.390941758	-0.207528236
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C	1.134319715	3.095177057	-2.863698915
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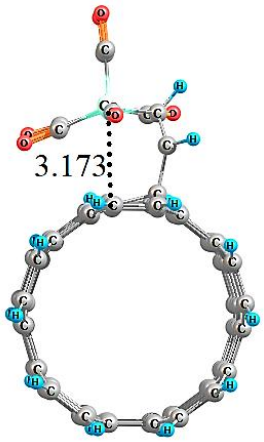

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C	5.572707141	0.954279344	2.186299828
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TS2*oblique*

148
Co2C118H22O6

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O	6.868500000	-1.253300000	1.655700000
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H	5.469900000	3.507400000	3.342100000
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C	3.879900000	4.255000000	-3.329900000
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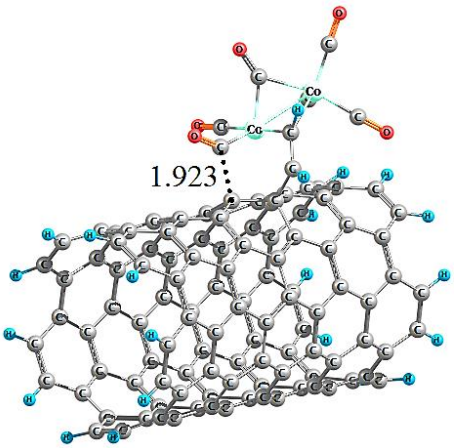

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C	-4.776400000	1.455000000	2.102900000
C	-3.294700000	-0.580600000	3.274600000
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C	-3.987800000	-1.560700000	-3.385200000
C	-2.155400000	-4.199800000	-0.977400000
C	-2.456000000	-3.794900000	1.736800000
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TS2*_oblique_

148
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C	-6.372441479	-4.807361031	0.926918198
O	-0.731297974	-5.456114176	-0.661213203
O	-4.491379398	-6.065023489	-1.202563735
O	-5.566244259	-1.713820162	2.688679093
O	-5.983198189	-1.961714655	-1.626757818
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H	7.616736510	-1.793819807	3.412476352
H	8.938522240	0.008830116	-0.372312213
H	8.330788682	-0.934032075	-2.529604153
H	7.211265895	-2.585017274	-3.425599170
C	6.139252571	-2.458312817	-3.286619235
C	4.110390746	-5.354515410	-1.106620301
C	5.362912215	-3.567025755	-3.072646516
C	3.991975946	-3.433254629	-2.705374421
C	3.967143855	-5.555602635	0.235846653
C	3.045841838	-4.755215604	0.986208536
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C	4.670278115	-4.405372175	2.853059590
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C	4.817469785	-2.054178536	3.428785645
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C	1.974071261	-4.179011088	0.264179900
C	0.974642839	-3.436941969	0.951812734
C	1.405233039	-2.831435953	-1.688843262
C	2.686405371	-3.013170650	2.647441496
C	1.379439106	-2.767966408	2.122626103
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C	5.618574623	1.193874570	1.929967112
C	4.808876449	2.176140496	1.286197303
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C	-1.246741920	-2.249899176	1.080042924
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C	-0.609266747	-1.315196153	2.082477553
C	2.982020472	1.746926812	2.846656393
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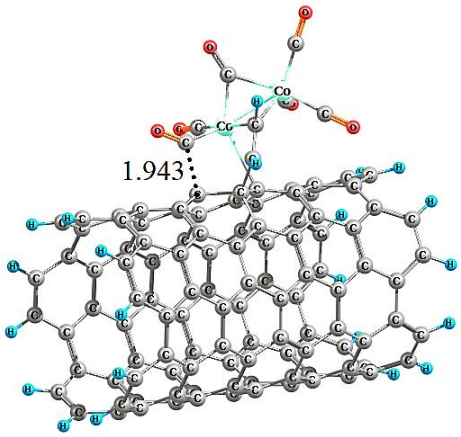

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C	-2.653929470	-0.089505925	-1.799212786
C	-1.321109289	-0.193800950	2.521896297
C	-2.674839026	0.040421124	2.081057486
C	0.963546378	3.138995821	2.810250658
C	-0.608310409	0.864961302	3.134257366
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C	-3.380744579	1.179246145	2.555345938
C	-1.077385115	4.525546422	2.779232406
C	-2.644348625	2.254983913	3.154387673
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C	-2.445287820	6.792687534	1.874713963
H	-2.966310391	7.696928900	1.565857881
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H	-3.326275319	7.051060348	-2.752157673
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TS2*perpendicular*

148
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C	-5.922018166	2.188275438	1.335093868
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O	-5.131807911	5.739697058	1.717807804
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O	-6.932978623	0.959424495	-2.082430492
O	-6.188308799	1.768805916	2.378014222
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H	-6.723567478	-2.087300947	-1.409359586
H	-6.078193780	-2.870685307	2.829417657
H	-4.766262498	-4.713673346	3.708343791
H	-2.605688999	-7.789112697	1.429930545
H	-3.531767231	-6.462512164	3.242607004
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H	-3.301292034	-6.873334139	-2.805655970
H	-4.490720989	-5.215300858	-3.596671175
C	-4.010271171	-4.260802397	-3.390092007
C	-5.917642063	-1.584630480	-0.877711822
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C	-5.000307232	-2.755477326	2.924146273
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C	-4.260929407	-3.793354670	3.421266207
C	-2.833851402	-3.738469630	3.410290181
C	-2.077107108	-6.896435575	1.759408994
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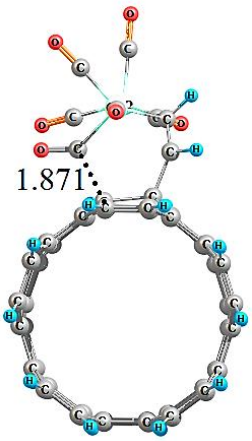

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C	1.216464401	3.262802162	1.109773493
C	1.321206027	3.087030240	-1.646550663
C	0.999623462	1.459721356	2.730355277
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C	3.335884268	-1.825009128	2.682996416
C	1.760595340	0.391491423	3.280998084
C	3.177870730	0.523369322	3.334986052
C	3.874373776	-2.594601662	1.614070908
C	5.023903451	-2.095601770	0.935159199
C	3.976377782	-0.600188803	3.026860437
C	3.972471361	-2.776613931	-1.159501344
C	5.073806318	-2.187937129	-0.472625586
C	3.513798328	-2.154539947	-2.353912707
C	4.184558177	-0.985218765	-2.812822124
C	3.417040968	0.082986803	-3.326014749
C	4.014360764	1.374436489	-3.405779778
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C	2.121231565	4.128282659	0.419680780
C	3.000705291	2.896496787	2.745339671
C	5.338283749	-0.384251595	2.660733557
C	3.770325901	1.818401558	3.279342100
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C	7.045939289	-0.697001124	0.927677743
C	7.878389207	0.205919312	1.652170329
H	8.883303016	0.425669602	1.296326073
C	3.658502510	4.077462534	2.329037776
C	4.957004785	4.312536000	2.858958992
H	5.430121127	5.284274754	2.730755707
C	5.178528266	1.952650791	3.375669028
C	5.698994465	3.276009579	3.368649714
H	6.740435135	3.453413723	3.630433740
C	3.313998304	4.524023214	-1.687228263
C	4.106066907	5.488934099	-1.000995442
H	4.866434312	6.053289643	-1.537604433
C	3.204906692	4.711140344	1.112085034
C	4.052349198	5.580319170	0.365973607
H	4.771032040	6.215640345	0.880194211
C	5.427325469	1.498753869	-3.415277084
C	5.955119263	2.813288482	-3.547651203
H	7.013788595	2.957078081	-3.755236859
C	3.849543544	3.738643728	-2.774667930
C	5.186050761	3.905507694	-3.234107940
H	5.654728647	4.887307959	-3.201071739
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C	7.985295896	0.008243827	-1.283458791
H	8.963808427	0.276310516	-0.889244918
C	6.206563986	0.413180081	-2.881808596
C	7.550810748	0.595357816	-2.442231955
H	8.195025560	1.315769909	-2.942899732
H	-2.339075920	3.108847333	-2.589395692
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CP6*oblique*

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Co2C118H22O6

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C	6.394499511	-1.886802593	-1.728060257
C	6.261922009	-2.022503690	0.939228375
C	7.361081836	-4.227019928	-0.693813759
O	1.617329670	-4.805726671	0.437603647
O	5.185511763	-5.529668540	1.149533994
O	6.647710827	-1.121930821	-2.554134599
O	6.652580373	-1.338161744	1.791967520
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H	4.935239443	4.423828128	-3.503296251
H	6.804514122	1.898050842	-0.549022096
H	6.108977008	2.817000654	-2.693069877
H	6.570472185	2.078412413	1.661507549
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H	2.937132381	7.083557907	2.632153572
H	4.238140335	5.282573233	3.606966049
H	2.291512599	7.983277714	0.731681027
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H	3.530630756	6.357695516	-3.118995256
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C	5.462111801	2.106560711	-2.182266030
C	3.867946998	4.274285975	-3.353921084
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C	3.517733125	2.616316025	3.083230132
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C	1.183718339	5.848724333	2.209931699
C	2.690613895	3.761457550	3.340069339
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C	2.100289403	0.484015845	-2.545325524
C	3.515780289	0.566604214	1.723110097
C	2.730247036	-0.430272025	1.050811688
C	1.285573875	3.620256306	3.223699144
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C	-0.789397128	4.380625130	2.161952018
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C	-0.894989843	4.586208542	-1.803304770
C	-0.275335550	3.757270461	-2.762390111
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C	-0.624861220	0.085106689	-3.147474518
C	2.118906891	-1.600675794	-1.151607593
C	1.153886870	-2.453137988	-0.252796107
C	0.139156373	-0.953337317	-2.542025464
C	1.472832262	-0.832231485	1.636019781
C	0.715797018	-1.842219072	1.044589459
C	-0.719955382	2.179590110	3.213187813
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C	-1.481827288	3.228709038	2.644017934
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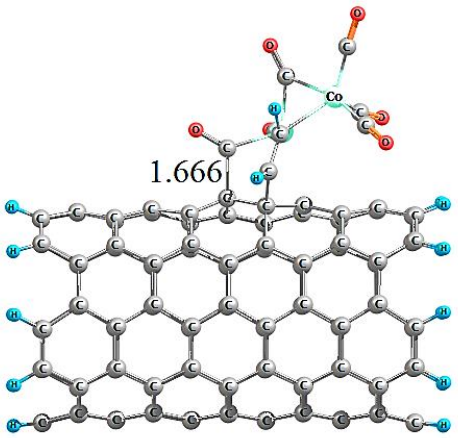

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C	-5.443074929	0.305391646	2.590588965
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C	-5.236690849	-2.042100993	3.289709840
C	-6.663795058	-2.132066758	3.240702901
H	-7.161688258	-3.052952453	3.537774876
C	-6.745879848	0.013469448	2.112094714
C	-7.397930087	-1.132587255	2.668052748
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H	4.323922371	-4.124964969	-1.989729501

CP6*_oblique_

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O	4.352985802	-6.168815276	1.106754016
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C	3.137594800	-3.886971562	-1.442641681
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H	-7.612418129	-1.762737978	-3.416800080
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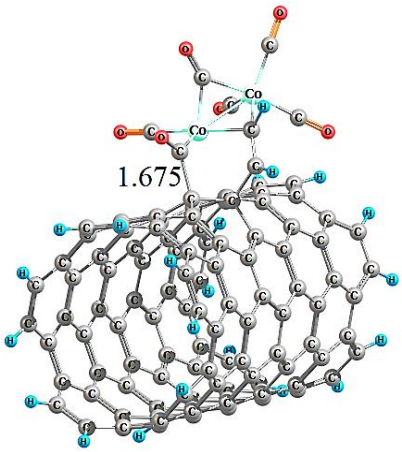

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C	0.518653732	5.208664399	2.197002296
C	2.447170664	4.731611288	-3.063714830
C	3.021451205	6.006798128	-2.763669881
H	3.990932102	6.278446027	-3.176768681
C	1.258439838	6.405592064	-1.146712311
C	2.443082499	6.822104588	-1.832091068
H	2.964442084	7.724120634	-1.517080921
C	4.705296774	1.473409597	-2.092116115
C	5.388672221	2.599216203	-2.655064015
H	6.462375680	2.708308576	-2.511409111
C	3.251645532	3.566943606	-3.275904436
C	4.683252461	3.614576636	-3.232001856
H	5.206184844	4.515180062	-3.548011107
C	4.738487405	1.253402922	1.916418533
C	5.989423415	1.597336953	1.302650220
H	6.756647814	2.109797658	1.880090754
C	5.085573864	0.913553270	-0.838359017
C	6.154562311	1.444270168	-0.042935551
H	7.046633344	1.843537539	-0.523010685
C	2.530282683	4.397011626	3.325949496
C	3.947031106	4.443830021	3.517182603
H	4.435641857	5.395964783	3.715956511
C	4.112584357	2.108411598	2.873909019
C	4.713735535	3.333638699	3.305096048
H	5.797661488	3.422388277	3.340444605
C	1.095721583	6.596251777	0.261336276
C	2.114579659	7.207520633	1.060295342
H	2.708682819	8.023878090	0.653447344
C	1.808456318	5.474819272	2.725900652
C	2.462391154	6.660858438	2.262200431
H	3.327569429	7.050706236	2.795289452
H	1.629076183	-3.488256087	-2.918147877
H	3.452326839	-4.755490625	-2.037084806

CP6*perpendicular*

148
Co2C118H22O6

Co	4.292125662	3.598656028	-0.603708085
Co	5.363924161	2.243247987	1.095147742
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C	2.690722897	3.048786998	-1.725384223
C	5.672194960	2.112768460	2.811019361
C	6.918387943	1.564801527	0.524162748
C	5.918664917	3.943985295	0.380801248
O	2.363374809	3.587868381	-2.736529366
O	4.101617077	6.396862494	-1.477323851
O	5.866920407	2.072708307	3.949042688
O	7.992964406	1.269320279	0.217704138
O	6.803859586	4.691856976	0.576586272
C	2.649562285	3.262395030	0.721975230
C	3.847764443	3.401039563	1.405880142
C	5.183027138	2.735377112	-1.862345579
O	5.817765957	2.228896694	-2.685625028
H	6.232497693	-2.388899905	2.571552648
H	6.624776770	-1.589159816	-1.723524670
H	6.816759540	-1.447895151	0.698302425
H	5.792507957	-2.767472833	-3.337239318
H	4.513400877	-4.762281704	-3.868627111
H	2.800159652	-7.648254605	-1.028990495
H	3.442354527	-6.509017084	-3.078816842
H	2.980369702	-7.498831140	1.166205783
H	3.906459621	-6.133784250	2.949903379
H	5.046964379	-4.326077422	3.439124011
C	4.484589386	-3.433570962	3.171079655
C	5.939620202	-1.036927511	0.202531350
C	5.150776097	-2.346337836	2.681009228
C	4.424166366	-1.227475812	2.162622131
C	5.830329347	-1.117365900	-1.148596152
C	4.603241236	-0.741171205	-1.791289953
C	4.837709138	-0.539489575	0.983878127
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C	4.047848956	-1.549132726	-2.830855182
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C	2.416091591	-6.640850416	1.527044213
C	1.236845660	-6.219211167	0.835204719
C	2.937307265	-5.872106071	2.529302185
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C	3.079302251	-1.080123488	2.570825603
C	2.320889598	0.052246045	2.129931153
C	3.769140031	0.178810157	-1.119602749
C	2.541230088	0.574115822	-1.704278108
C	2.765017953	0.792456715	1.035157678
C	2.663652817	-1.429225339	-3.091157095
C	1.966463720	-0.254192914	-2.674198834
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C	1.914489594	-2.596859809	-3.422858478
C	0.497615176	-2.537795450	-3.326594247
C	0.178860021	-5.475905191	-1.235700282
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C	-0.193766374	-3.660848672	-2.833731949
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C	0.987830552	0.223137454	2.636636679
C	0.225671538	1.353953864	2.233749172
C	1.819340323	1.751807921	-1.155309772
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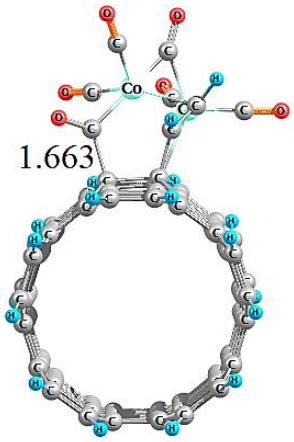

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CP7*oblique*

150
Co2C119H22O7

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O	1.943214516	4.615502745	-0.603343617
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O	6.140742055	0.772751791	2.729917326
O	8.158516746	2.476366453	-0.625995269
O	6.626535812	5.401971760	2.174633203
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H	5.197999219	-3.925429336	-3.300782472
H	2.507962197	-7.352036302	-2.500350037
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H	1.855422997	-8.177370474	-0.565066691
H	2.190175995	-7.791560471	1.813540302
H	3.275989144	-6.460637398	3.176748919
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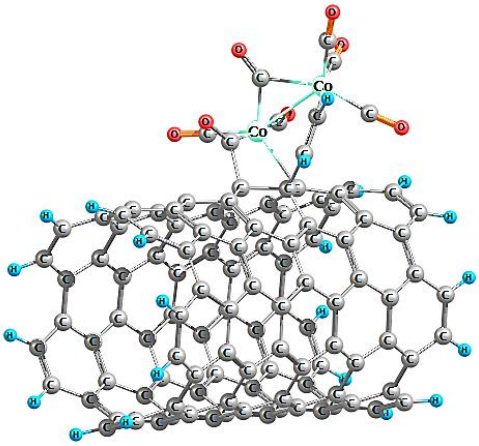

Note: Taken into consideration in the main manuscript.

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C	-4.226957158	5.305867656	2.170541062
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C	-2.899185871	5.105063903	0.153272916
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H	-4.438519447	6.623175922	0.518865737
C	-6.169337802	0.905682589	2.958196796
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H	-6.228391387	4.229486603	3.715765413
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C	-8.260023339	0.289332447	0.054646627
H	-9.122620021	0.732617966	-0.439671443
C	-6.856747255	0.079129687	2.018766465
C	-8.074178763	0.497511688	1.390759132
H	-8.792027647	1.102562577	1.941591056
H	2.129890513	2.856165974	2.738036866
H	4.170773778	3.799851625	2.841872861
C	5.290056415	1.559092120	-1.926037224
O	6.171433931	1.094961130	-2.509322651

CP7'*oblique*

150
Co2C119H22O7

Co	4.250898606	-2.474594635	0.976389467
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C	4.033148849	-5.366706469	-2.916901810
C	6.116239647	-4.196158826	-1.927637424
C	4.175524266	-6.243623956	-0.465968226
O	2.934229884	-3.410253222	-1.316950272
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H	-6.385479531	-3.635279809	-3.875592912
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C	-5.228728461	-3.824946828	3.165063220
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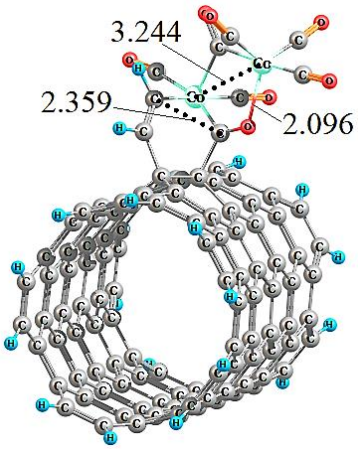

Note: Discarded in the main manuscript.

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O	6.035135509	-0.877588412	-0.737855982
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CP7*_oblique_

150
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O	1.182966541	5.236734809	-0.619725218
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O	5.385763799	1.293508575	2.739153939
O	7.391165292	2.958508935	-0.623881046
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C	3.290891251	3.705740875	1.998055908
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H	-8.330220268	1.352503862	-2.440535924
H	-7.111085394	2.911891637	-3.358505737
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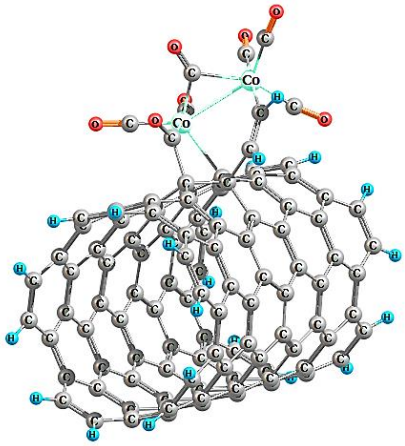

Note: Taken into consideration in the main manuscript.

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C	4.520920424	2.153435639	-1.957312704
O	5.392614096	1.689243133	-2.553999355

CP7'*_oblique_*

150
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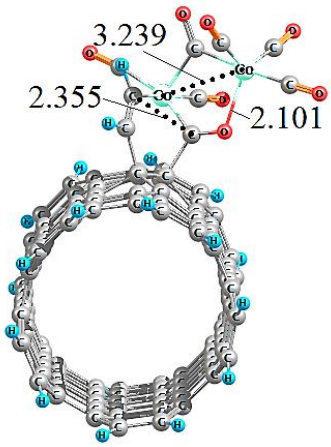

Note: Discarded in the main manuscript.

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CP7*perpendicular*

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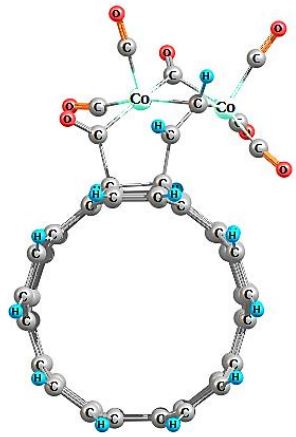

Note: Taken into consideration in the main manuscript.

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H	-2.074433489	3.814350560	0.390954017
C	-6.235736820	3.979252179	-2.118673313
O	-6.768667981	4.865549660	-2.630635981

CP7*perpendicular*

150
Co2C119H22O7

Co	-4.651960858	1.997226744	1.465142519
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C	-2.936374788	2.876229336	1.002549648
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C	-6.152919915	1.174331267	2.089124690
O	-2.565497411	4.006148122	1.124353731
O	-5.696473050	4.605238479	1.120038722
O	-5.168895428	1.098568642	-3.526360653
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O	-7.079750104	0.731623270	2.615926101
C	-2.686140702	2.918578436	-1.608464840
C	-3.967716901	3.299013087	-1.646205794
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H	-6.470850751	-2.028161119	-1.455822924
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H	-2.923959667	-6.747915850	-3.039382178
H	-4.162328964	-5.081452400	-3.731608502
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C	-4.494455918	-3.073269564	-3.130802351
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C	-1.942049701	1.672832528	0.585794404
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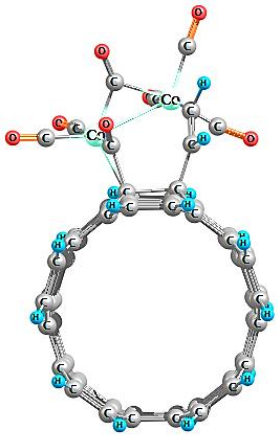

Note: Discarded in the main manuscript.

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C	8.111393655	0.429958720	1.614833083
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CP7'*perpendicular*

150
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C	-6.201850269	-2.872942401	-0.430230135
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O	-7.192718326	0.482987590	-1.952280952
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C	-4.388246119	-1.714866432	-2.137471632
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O	-5.938525420	-0.597364597	2.352999555
H	-5.510113831	4.001619681	2.440820950
H	-5.800920217	3.869618733	-1.917893772
H	-6.228153624	3.428344257	0.438810795
H	-4.499356661	5.054374626	-3.252353558
H	-2.693391036	6.671288942	-3.387720508
H	-0.521964023	8.533850661	-0.062607519
H	-1.268439765	7.917813741	-2.292441975
H	-0.908725796	8.141514355	2.072926126
H	-2.314877266	6.851415175	3.577810596
H	-3.940954132	5.387042637	3.669495769
C	-3.615223952	4.415600598	3.302260335
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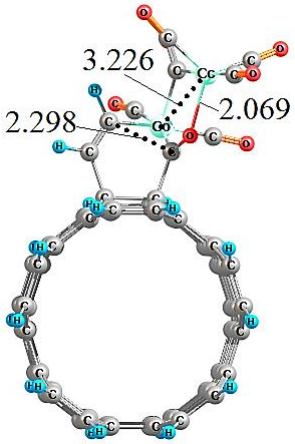

Note: Discarded in the main manuscript.

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C	-5.343665138	-5.191333738	-1.043324667
O	-5.584959701	-5.828134150	-1.977368502
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TS3*oblique*

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C	3.607277653	1.807016112	-0.098981509
C	5.546457501	4.001952857	2.393526354
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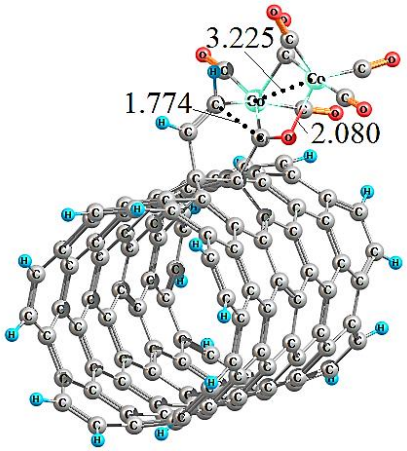

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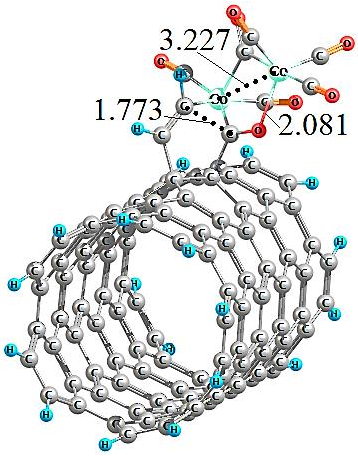

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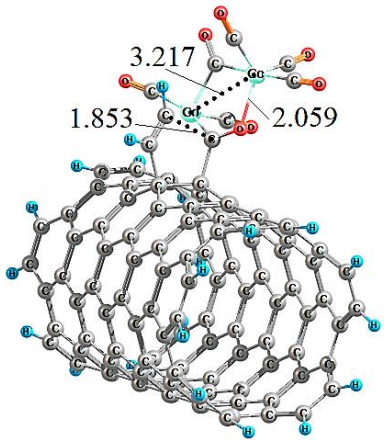

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PD*oblique*

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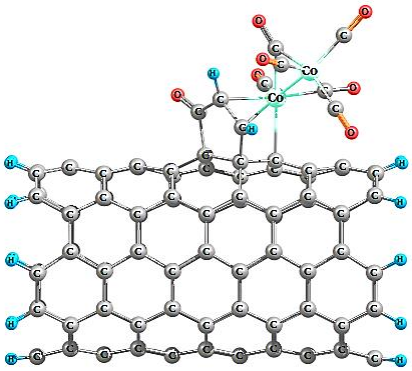

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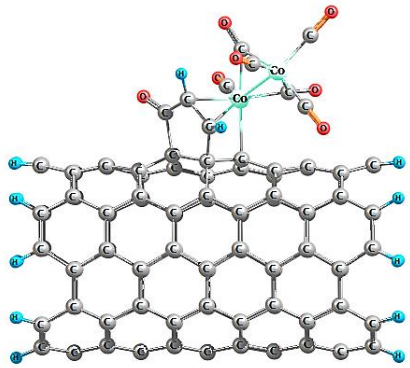

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H	8.561390218	-1.300497236	2.231369673
H	7.255944717	-2.772017829	3.653202087
H	9.015229118	-0.844899818	0.130035614
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C	3.971823639	-3.515946042	-2.925122327
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C	4.152672869	-5.012452106	2.587087592
C	2.969816445	-4.593772444	1.903673803
C	6.789455212	-1.875183565	3.249977707
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C	8.133067811	-0.434605545	-0.358096026
C	7.196412604	0.339618028	0.391978135
C	7.838990807	-0.820662992	-1.637504316
C	6.593471163	-0.451823518	-2.228701352
C	5.814643614	-1.381031798	-3.000689627
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C	1.715757736	-4.287125515	-0.163872109
C	0.761924097	-3.492610328	0.521530758
C	1.364514718	-2.762289924	-2.042761986
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C	3.092462165	-2.485161430	3.136598598
C	2.595346083	-1.157648627	3.267937901
C	5.667333006	0.502310893	2.290193537
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C	5.938243872	0.679958304	-1.683306382
C	4.713686512	1.133291785	-2.255886296
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C	2.566858893	0.488669331	-3.215013201
C	0.143928361	-2.303580164	-1.503167918
C	1.642422296	-0.587542708	-3.117129746
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C	-3.316416996	1.348265685	2.258228793
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H	-4.894204201	4.695776494	3.489762903
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H	-3.418846824	6.209492381	-3.648681587
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C	-3.924555042	4.155865910	-3.475413873
H	-4.988313224	4.358824523	-3.580953086
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H	-1.742180245	8.320324781	-0.185002727
C	-0.894866535	5.921798053	-2.448419468
C	-1.474576455	7.113860298	-1.910977177
H	-2.251357731	7.639824748	-2.462888734
H	-2.962918820	-3.110785166	1.977766998
H	-2.858942992	-5.299759249	0.440431480
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PD*perpendicular*

150
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C	-3.778840988	3.653428877	-1.895894540
C	-5.433152443	1.787362215	-2.714069115
C	-6.284543793	1.820880089	-0.247488806
O	-2.323992530	2.092170605	4.401199606
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O	-7.246904641	1.148493866	-0.133845229
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C	-5.765698306	1.945039342	2.461219849
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H	-6.146023124	-2.347157780	2.623813251
H	-6.735716619	-1.533368007	0.395039544
H	-5.021356124	-3.957278746	3.640606713
H	-3.653435260	-5.950030289	3.400269282
H	-2.421504502	-7.835869815	-0.362576623
H	-2.708912358	-7.353454706	2.003941279
H	-2.979115677	-7.085176114	-2.358521490
H	-4.195520749	-5.335990192	-3.526110756
H	-5.414846035	-3.512264280	-3.333186663
C	-4.816477365	-2.709392523	-2.906144651
C	-5.774084776	-1.274299352	0.832117020
C	-5.392260796	-1.842967851	-2.023511346
C	-4.585853224	-0.886169812	-1.325705923
C	-5.442846770	-1.727183438	2.070168079
C	-4.112049515	-1.521467760	2.574332420
C	-4.790922951	-0.583360579	0.044665909
C	-3.950326740	-3.850451293	3.479659423
C	-3.389554985	-2.555952470	3.242799305
C	-1.924272489	-6.844045222	1.447535581
C	-3.180258050	-4.971355793	3.346721519
C	-1.804435848	-4.864222839	2.973962493
C	-1.762301944	-7.115773406	0.118862835
C	-0.858826105	-6.333743565	-0.668949365
C	-1.192950379	-5.775287087	2.056558260
C	-2.486164391	-6.134892988	-2.555242364
C	-1.209095336	-5.858872219	-1.971763595
C	-3.170351589	-5.150959671	-3.210883017
C	-2.613488287	-3.837788659	-3.321862841
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C	-2.518148474	0.450989205	-1.305451489
C	-3.391723807	-0.426655442	2.053907849
C	-2.092742931	-0.147557607	2.520271738
C	-2.771817265	0.829993297	0.015373194
C	-1.981104774	-2.440056000	3.313903198
C	-1.367860868	-1.162791222	3.133406236
C	0.006481809	-5.375693512	1.415639997
C	-1.177378251	-3.609925976	3.187861859
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C	0.807432456	-4.347789936	1.990855876
C	-0.488838252	-4.756383631	-2.497636012
C	0.808003272	-4.452024582	-1.990545175
C	-1.205201525	-3.725421644	-3.180599780
C	-0.578313564	-2.455449285	-3.326844271
C	-1.360607735	-1.298120607	-3.145619426
C	-0.706038696	-0.058065749	-2.869660756
C	-1.858178379	1.764164685	0.758294094
C	-1.287350143	0.826588260	-1.940197299
C	-0.466734112	1.834702927	-1.356804461
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C	-0.660980552	2.201692381	-0.013831729
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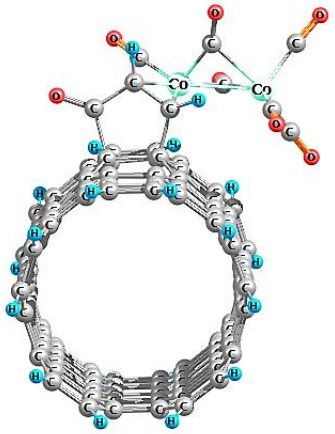

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C	2.445489716	4.177784163	0.628789430
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PK*oblique*

136
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C	-6.091139532	-1.435588809	-3.062515862
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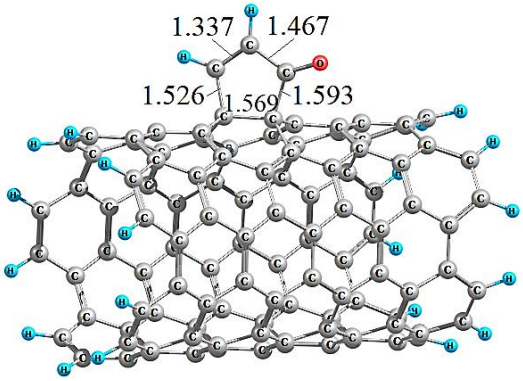

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C	1.234005378	3.351837844	1.493978188
C	2.461895954	2.939622236	2.101021736
C	2.448561774	1.831230238	2.973642780
C	3.672753268	1.160526314	3.249960886
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C	3.700180288	-1.390720584	-2.950466917
C	3.722983067	2.612799823	-2.414236660
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PK*_oblique_

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C113H22O

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H	-6.892433033	-4.249927297	-0.119640773
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H	-6.997312088	-1.440477888	-3.472971323
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C	-6.096285467	0.474691475	-3.296297840
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C	-4.813167521	-1.308504606	3.287032851
C	-5.957652315	-3.942735520	-0.584976872
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C	-4.805146602	-2.835472132	-2.407192087
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C	-3.683641067	0.560916982	-3.168235888
C	-2.467718475	1.250872809	-2.881716493
C	-3.794862005	3.207755295	-0.130698526
C	-2.562180964	3.228431944	0.574388715
C	-2.495746985	2.378552769	-2.029580998
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C	-2.300639753	-3.418986231	1.527277177
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C	-3.566516311	-3.244769368	-1.855813272
C	-2.348171292	-2.737452873	-2.396395315
C	-2.390662674	-1.522641432	-3.113046634
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C	-0.026429182	1.324303239	-2.884703164
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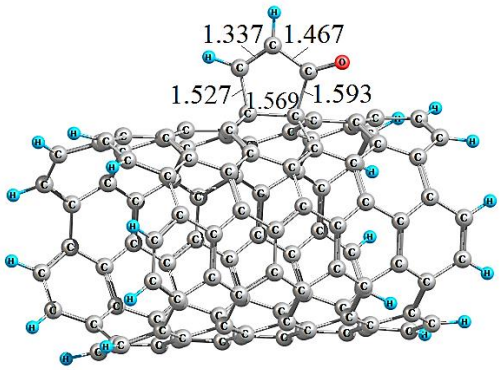

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C	6.076644214	3.132015351	-1.542737384
H	7.014180317	3.104683705	-2.094888979
C	4.895806206	3.363180147	0.562323838
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H	7.103964950	-1.002975308	-3.648806738
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H	7.236219906	-3.763204598	-0.215416003
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PK*perpendicular*

136
C113H22O

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H	-7.162528333	2.925647539	-1.560542976
H	-7.105365401	2.013579555	2.724010359
H	-7.014294887	-0.228727135	3.652816410
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H	-6.849181018	-4.218327056	-0.772924956
H	-6.897198206	-2.937885327	-2.837410735
H	-6.972998007	-0.915519712	-3.674432399
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C	-4.723640151	-3.768549174	1.020437178
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C	-5.945205154	-3.102915701	-2.336259135
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C	-3.688359523	1.060681380	-3.019336104
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C	-3.793887932	3.141195871	0.384242896
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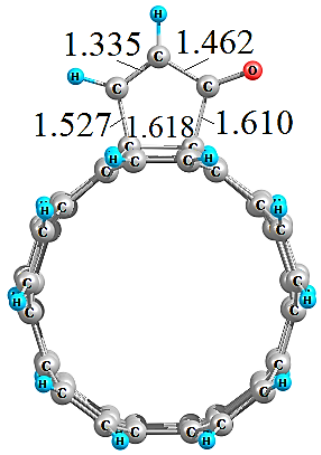

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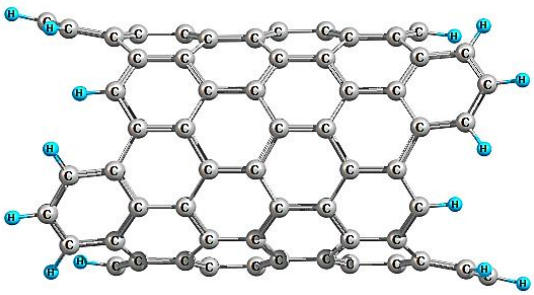

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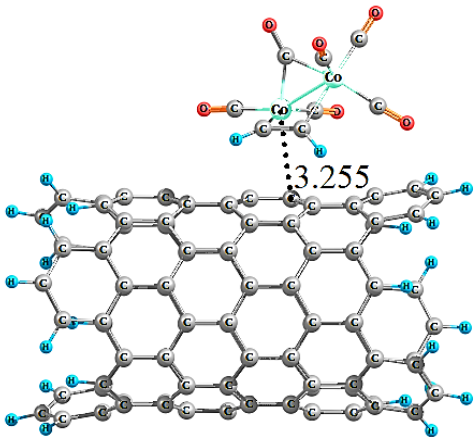

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H	0.462184139	8.121194256	1.596181268
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C	-6.237649226	-3.473591401	-0.342557717
C	-3.579632693	-3.594936693	-1.154263271
C	-7.451068906	-2.765080490	2.093332841
C	-7.080245408	-0.138737409	0.998317401
C	-8.220468129	-1.868349258	-0.489553765
O	-2.829702088	-4.338733560	-1.623763568
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O	-7.908041503	-3.286457840	3.015946372
O	-7.289325325	0.959998779	1.285163936
O	-9.133277937	-1.873143507	-1.197742467
C	-4.124763450	-2.761025702	1.353496313
C	-4.955779097	-1.734849377	1.487054434
H	-4.859021270	-0.863567500	2.142332023
H	-3.354741744	-3.319658807	1.878585477
C	-5.109636719	-1.345767286	-1.724840843
O	-5.385007289	-0.619380442	-2.579793679

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Co2C115H26O5

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C	-6.747838933	-1.802647424	0.368570100
C	-4.763325655	-1.069164359	1.537900828
C	-6.015540726	-1.691809206	1.548143101
C	-3.613624062	-2.498679212	3.180019796
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C	-1.790918527	-0.230600861	-2.866459599
C	-2.909849745	0.031545191	-2.039455125
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C	-4.328180411	-0.458214895	0.335321561
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C	-1.242624172	-2.122363350	3.553990011
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C	-0.147003687	-5.744393830	-1.541192842
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C	-1.272457492	-4.306861579	-3.148758918
C	0.783686909	-1.192636787	-3.503389157
C	-0.327277325	-2.062584690	-3.497712414
C	-1.661314196	-1.536307963	-3.412077737
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C	1.573902322	2.375564731	-2.789901463
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C	0.075081029	3.121236285	0.373850862
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C	0.827184666	3.299220560	1.565385149
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C	-0.372435662	1.379360567	2.546917575
C	3.054062880	2.751687829	3.192011691
C	1.934939509	1.868433318	3.187117929
C	2.106220003	0.509986290	3.545693237
C	0.995755601	-0.361698420	3.552044324
C	4.553665686	0.856342762	3.476963465
C	3.439758356	-0.017171236	3.460732297
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C	2.444957753	-2.202033450	2.895929834
C	5.792454314	-0.700616303	2.073388420
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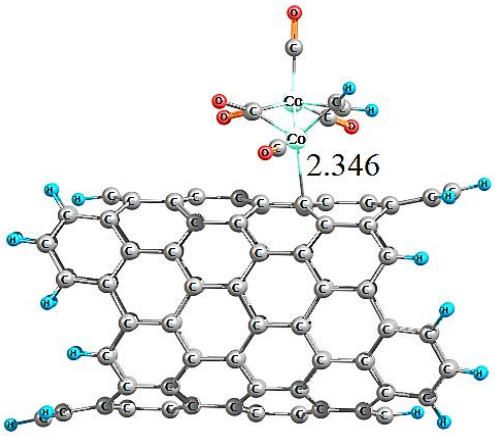

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C	3.907723613	2.878677759	-3.411167126
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C	2.297942971	4.827220660	0.387931745
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C	2.942938250	4.047898540	2.625674407
C	5.114023861	4.576491874	3.549146273
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C	5.756450917	0.434415448	2.894038519
C	7.932204056	-0.037380442	0.891471663
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C	5.393786628	0.939128196	-3.146221384
C	4.893500956	3.850912038	-3.597874676
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H	-6.694318059	-1.691136124	-1.789770012
H	-7.740767209	-2.251058591	0.392488479
H	-6.408603505	-2.103115966	2.477455066
H	-4.429082258	-3.207890875	3.057939346
H	-4.013067105	-5.170803396	4.196315189
H	-3.675591730	-7.463221151	3.310031070
H	-1.818131500	-7.913019318	1.727025894
H	-1.442386230	-6.951613928	-0.340879727
H	-2.075781276	-7.553292307	-2.474103221
H	-4.098867249	-6.870822032	-3.738232687
H	-4.511841739	-4.469967380	-4.204767063
H	5.477623801	5.892697760	-3.250556556
H	3.613045213	6.351935411	-1.678976351
H	3.228459260	5.389836452	0.378128896
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H	8.174686947	0.579994845	-2.446339944
H	6.208523733	1.648484946	-3.021776578
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C	-5.603705993	2.662472718	-0.419783200
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CP3'*parallel*

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Co2C116H26O6

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C	-5.394449866	4.593380049	3.726139010
C	-5.057790506	2.235689507	3.313283291
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C	0.089026132	2.726317934	1.718352231
C	-0.969350237	2.801812937	2.662153612
C	-1.855047576	3.906766874	2.644408795
C	-0.478448239	0.470804453	3.306903102
C	-1.367383469	1.564987585	3.271698069
C	-2.759244568	1.347989106	3.418046688
C	-3.658293899	2.454234572	3.392463713
C	-2.365924477	-1.063465317	3.321140975
C	-3.256893087	0.030100856	3.286783034
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C	-3.802308254	-2.270571335	1.772710222
C	-4.708996982	-1.167810312	1.755147948
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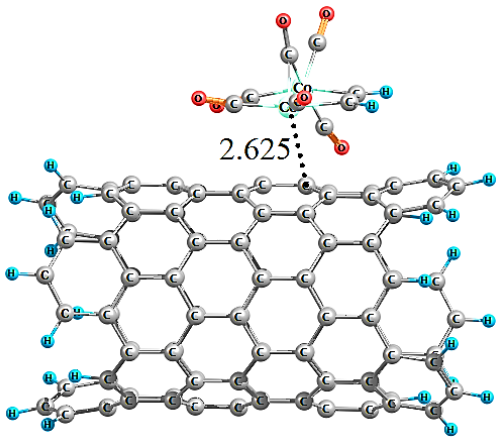

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H	1.287814911	-7.137901059	-3.542525026
H	3.696989364	-6.701436717	-3.943159689
H	4.627829657	-4.440064925	-3.530914246
H	4.686822932	-3.204613165	-1.593102505
H	6.281689839	-3.008566947	0.077808322
Co	4.275536002	2.287103188	1.228290542
Co	5.361618227	2.570969303	-1.045414998
C	5.669738991	3.426210592	0.685722122
C	4.326778933	2.006616097	2.955731196
C	6.894515214	3.219256301	-1.691412755
C	4.983833698	1.329805947	-2.266389257
C	4.091485582	3.725224068	-1.578744674
O	4.422615242	1.814700497	4.091190209
O	6.343659864	4.242807229	1.198341389
O	7.882594155	3.632486786	-2.118031033
O	4.932967779	0.546431519	-3.115019377
O	3.245487484	4.428574589	-1.926049347
C	5.660721284	0.898353017	1.106201983
C	6.177576058	1.001890846	-0.102269904
H	6.915646481	0.352916404	-0.585225469
H	5.919214633	0.168301186	1.878918208
C	3.193470461	3.720498982	1.277762345
O	2.598721555	4.704524823	1.383444120

CP3'*oblique*

150
Co2C116H26O6

C	-1.869392863	-5.004806593	-0.878737661
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C	-4.915165099	-4.839606383	-3.830553567
C	-4.433819651	-2.473473725	-3.716195305
C	-5.323845259	-3.516083622	-3.983922732
C	-6.038021102	-0.904408342	-2.715281275
C	-6.975099704	-0.110197614	-0.588629429
C	-8.109106828	-0.924145284	-0.552246416
C	-8.543083042	-1.461926122	0.658838332
C	-6.627795072	-0.523425414	1.796893274
C	-7.765546059	-1.333552511	1.808884594
C	-5.183916914	-1.923399631	3.208092837
C	-3.442363311	-3.658207731	3.185965539
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C	-3.978102411	-5.957090675	2.663339215
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C	-1.315645998	-4.633471232	0.356714063
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C	-0.699362113	-3.186408808	-1.979327046
C	-1.677326798	-4.210733448	-2.016025250
C	0.176638422	-1.042004211	-2.828946923
C	-0.806554042	-2.052520109	-2.853422423
C	-2.093337058	-1.772633454	-3.376271371
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C	-6.360493071	0.249815019	0.638212346
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C	-4.598013428	1.472857859	1.841339930
C	-4.519785670	0.366152778	2.753856759
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C	-3.239376992	0.095123347	3.305972966
C	-2.862723864	-1.264102289	3.472136063
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C	-2.239637311	-3.805130817	2.448492335
C	0.830818631	-1.825579173	1.627887149
C	-0.156215626	-2.826179320	1.582185307
C	-0.338674552	-3.613689589	0.390336880
C	1.666950360	-1.601720079	0.468648329
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C	2.240192792	-0.107432875	-1.862456992
C	1.264890067	-1.132375021	-1.898291644
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C	-0.866785339	2.946642734	-3.240034352
C	-1.855055004	1.941421977	-3.282798579
C	-0.118531379	5.166679801	-2.491074951
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C	-2.196340123	4.181972615	-1.617532435
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C	-1.032161849	5.986901405	-0.393160729
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C	-2.462383472	4.376075747	0.785123918
C	-3.447454681	3.343502754	0.750023319
C	-0.682495283	5.572974793	1.980250294
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C	0.109351988	1.782465178	3.532547572
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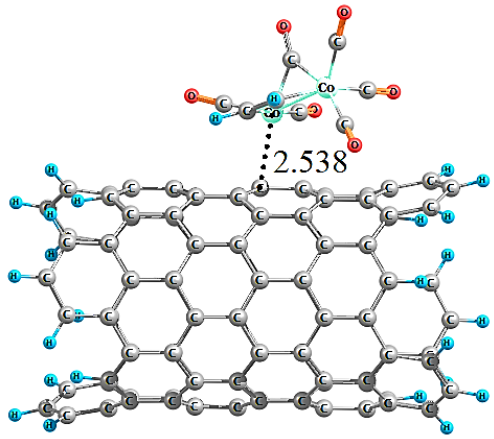

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C	5.411096476	2.691352798	-1.833264178
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C	2.825941701	3.289203515	-3.239845484
C	1.909290015	6.138615693	-3.382228072
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C	3.688221603	2.258361565	2.677567230
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C	5.402347334	-1.269102804	-1.985462734
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C	4.369853726	-3.452350890	-1.796590967
H	4.473838117	-3.585377688	-2.877774863
H	2.484286092	-4.392797078	-1.319569017
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TS1*parallel*

148
Co2C115H26O5

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C	4.115055276	-0.664723544	2.215860894
C	1.646871043	1.966951923	1.010487082
C	2.834099692	1.113252241	1.060307764
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C	2.775974575	-0.345188416	-2.360298730
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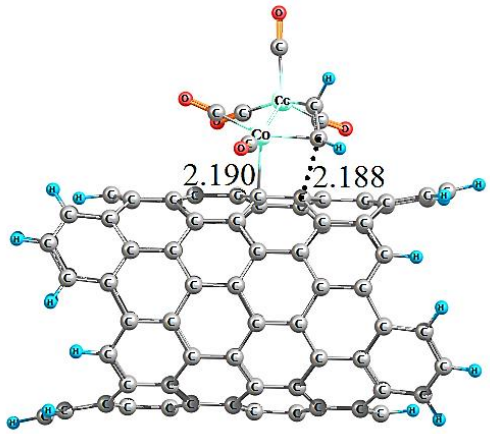

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C	5.022620361	5.529853808	-1.130465217
C	4.732898659	2.657354437	-1.817923941
C	2.736812900	4.322058838	-1.982527801
O	2.193085925	3.938582615	4.262684444
O	1.496662708	6.013773403	0.393942452
O	5.661777292	6.461121026	-1.388488937
O	5.250991152	1.871908833	-2.500988791
O	1.834232057	4.483034620	-2.691268196
C	4.436770042	2.498165619	1.607593823
C	4.921346342	3.399712295	0.723517514
H	5.848124937	3.913123968	1.028253096
H	4.853233653	1.892843104	2.414308500

TS1*oblique*

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Co2C115H26O5

C	4.789586266	0.795921197	1.015762599
C	3.924218066	1.883888206	3.039895444
C	5.032225987	2.687636402	3.320892220
C	4.852725793	3.972234365	3.829606547
C	2.453400207	3.747384953	3.642282235
C	3.577262102	4.528598577	3.916785923
C	1.089965657	5.484163957	2.556133272
C	0.439378244	6.446332838	0.392726089
C	1.371723835	7.484827353	0.344045694
C	1.980650183	7.818554597	-0.865035906
C	0.869814054	5.976318115	-1.967648737
C	1.797980235	7.019457388	-1.993092192
C	2.145384777	4.331043443	-3.272290477
C	3.676173704	2.408555186	-3.127945466
C	4.879074859	3.102514095	-3.277881029
C	6.012798862	2.694192585	-2.577340004
C	4.731976301	0.996900855	-1.430893875
C	5.925074259	1.699527526	-1.603963401
C	4.356150133	0.283582774	-0.212452769
C	1.571085576	-1.961196057	0.980827796
C	2.642074436	-1.000565957	0.984936156
C	2.825831849	-0.126283554	2.102221318
C	3.941867857	0.736036592	2.135099865
C	0.551238984	-0.712790449	2.856589057
C	1.666811628	0.155855454	2.890036520
C	1.511390422	1.485957386	3.352243343
C	2.635027940	2.361634723	3.391802311
C	-0.905209623	1.142470958	3.480690021
C	0.204168053	2.010979367	3.500162021
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C	-1.138097350	3.782318792	2.522984366
C	-1.023801091	4.822578742	1.562803302
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C	-1.084688458	4.962800737	-0.855530198
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C	-1.193589056	1.735176524	-3.381365146
C	-0.070494585	2.616039568	-3.363354737
C	1.242573237	2.086801565	-3.463340187
C	2.358949449	2.956618021	-3.447081634
C	0.297284070	-0.175435611	-3.149537458
C	1.400340424	0.701630988	-3.116444916
C	2.539858176	0.359339989	-2.357997571
C	3.669081425	1.227822031	-2.340909959
C	1.362733098	-1.601299079	-1.482781626
C	2.441088663	-0.702080768	-1.424499301
C	3.242929868	-0.586286633	-0.242357976
C	1.099031805	-2.476994465	-0.346143527
C	-1.953012297	-4.368645940	0.802696872
C	-0.813378627	-3.512152061	0.830880219
C	-0.553764578	-2.706950235	1.989660058
C	0.566544702	-1.872253787	2.029312120
C	-2.799670323	-3.332524385	2.828191961
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C	-1.829944720	-1.133445677	3.328519643
C	-0.709553511	-0.256998522	3.335143442
C	-4.258196548	-1.478058394	3.440078479
C	-3.145832113	-0.606618762	3.452712940
C	-3.310850162	0.782400789	3.133243562
C	-2.204731960	1.656223193	3.168567672
C	-5.581271969	0.252336690	2.356870614
C	-4.461583624	1.132127327	2.387413121
C	-4.365598432	2.189037241	1.449257981
C	-3.260245646	3.063342711	1.489122180
C	-6.256924646	1.182709190	0.214702409
C	-5.136567765	2.047732408	0.245455014
C	-4.477948677	2.398875151	-0.963224776
C	-3.347509075	3.270617836	-0.930808363
C	-5.828339438	0.715282611	-2.135353465
C	-4.708057635	1.579429056	-2.100732847
C	-3.567052732	1.316304495	-2.932780384
C	-2.457498630	2.186539764	-2.915955162
C	-4.535884244	-0.889346998	-3.426937098
C	-3.411474205	-0.013391165	-3.391829222
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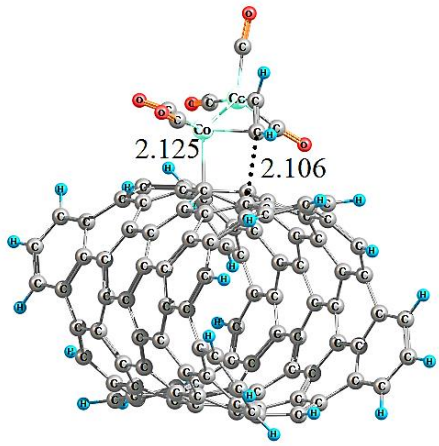

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C	-3.918540879	-6.328253710	0.846981435
C	-3.713058620	-5.536903483	1.980387767
C	-2.775784709	-4.506113512	1.950834105
C	-4.041706733	-2.853451637	3.253323053
C	-6.778398934	-1.640285868	3.275546042
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C	-6.638821638	0.474035115	1.436482109
C	-6.662841133	0.640184754	-1.011783248
C	-6.932429136	-1.214098863	-3.346802066
C	-5.822281127	-0.414970285	-3.063841792
C	-6.755459263	-2.494493924	-3.868251362
C	-5.480401484	-3.051105456	-3.960372400
C	-4.354778088	-2.272841607	-3.681345721
C	-3.004991817	-4.007806709	-2.586002936
C	-3.319297164	-5.993389696	-0.363269646
H	5.580009500	1.542227607	1.009003372
H	6.035954853	2.312672053	3.124292293
H	5.722132527	4.576097287	4.087707557
H	3.455529071	5.578784195	4.179830074
H	1.997687592	6.078704594	2.484324336
H	1.638278667	8.016857538	1.256731693
H	2.671586170	8.659974718	-0.906506352
H	2.394586161	7.191963347	-2.888241315
H	3.014247588	4.967980752	-3.123440592
H	4.924038462	3.973028155	-3.931426729
H	6.958856687	3.210963309	-2.735567189
H	6.779084117	1.480820547	-0.964876382
H	-4.621986300	-7.159090060	0.890163562
H	-4.309972282	-5.701411454	2.876958633
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H	-6.819315179	-2.514113017	3.924771148
H	-8.854919070	-1.762745834	2.724127857
H	-8.675075058	-0.038106131	0.948899272
H	-7.434550402	-0.125973323	-1.000267702
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H	-7.625992134	-3.095016848	-4.130228673
H	-5.360644607	-4.099768774	-4.230186488
H	-3.914803292	-4.599892117	-2.523737181
H	-3.601326251	-6.515167546	-1.277202896
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C	2.677225623	-4.027527397	2.530007471
C	6.132917957	-4.719297447	-0.909686788
C	4.205696109	-2.873292989	-2.389107542
C	6.149238222	-2.103995827	-0.780599304
O	2.337109693	-4.556737657	3.501313100
O	6.895523448	-5.579595397	-1.048472730
O	3.806206167	-2.615149308	-3.445624911
O	6.968552573	-1.287250197	-0.722393134
C	2.175781316	-4.285856334	-0.280949095
C	3.474935094	-4.579018312	-0.554853321
H	3.711004929	-5.652016194	-0.478166730
H	1.303575073	-4.934289695	-0.216673117
C	4.802028069	-2.660435095	1.567755746
O	5.694753366	-2.237105268	2.181158788

TS1*_oblique_

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Co2C115H26O5

C	2.373757675	-4.893292077	0.424565922
C	2.969232617	-4.081627701	2.666880483
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C	5.114265231	-4.593837964	3.656142045
C	4.313160836	-2.312794223	3.686925458
C	5.315010512	-3.247828905	3.956507962
C	5.763022262	-0.453196414	2.993514639
C	6.759361513	0.669859249	1.050779880
C	7.992547272	0.014562412	1.050988774
C	8.592846746	-0.342680041	-0.155724088
C	6.667049754	0.449926015	-1.383183290
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C	2.778109656	-4.510814419	-1.962179768
C	3.779032105	-5.464562871	-2.151357548
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C	0.870596398	-3.360712303	1.556792396
C	1.984527995	-4.237173583	1.597597719
C	-0.367000991	-1.430409493	2.479064136
C	0.746683777	-2.298475266	2.521873161
C	1.933819241	-1.898818503	3.172786493
C	3.057627606	-2.778984355	3.219695783
C	0.986236160	0.330896070	3.492325467
C	2.096083064	-0.534893991	3.526365395
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C	4.544317192	-0.876600220	3.537803913
C	2.452383053	2.178189640	2.896495283
C	3.574871666	1.299627242	2.943780554
C	4.710196332	1.555526582	2.128778481
C	5.823717124	0.683886474	2.174965485
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C	4.486767280	2.384137502	0.976519790
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C	6.204644722	1.068597466	-0.192946715
C	3.298283085	3.051605986	-1.482425053
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C	-2.592918991	0.329274249	2.425747564
C	-1.415852403	0.711635660	3.113693520
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C	-1.251493579	2.085496110	3.443411564
C	0.079979063	2.610952645	3.340789721
C	1.191839757	1.744677918	3.387320351
C	-0.905994782	4.778181734	2.731184257
C	0.215019265	3.899988236	2.772311292
C	1.362060806	4.178415412	1.988493938
C	2.472137199	3.311556183	2.037644482
C	0.064178264	5.930954195	0.824447279
C	1.168916100	5.047002822	0.860830140
C	1.800404554	4.650230676	-0.348461242
C	2.913802400	3.757997875	-0.310036234
C	-0.028583169	5.711193671	-1.597817838
C	1.075987265	4.827539592	-1.557842853
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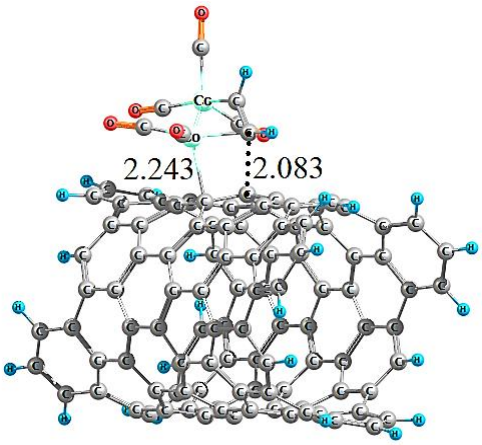

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C	-4.850091569	0.768704687	-1.049502192
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C	-2.137446225	4.395504691	3.323853082
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C	-1.848211686	6.929634128	2.148693759
C	-0.848135606	5.973223084	1.967612014
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C	-2.033218142	6.478412878	-2.939416988
C	-1.020119901	5.558514173	-2.662581418
C	-3.170754618	6.073542116	-3.636031950
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C	-3.839890791	1.920111673	-2.969214337
C	-6.088476973	1.409653905	-1.042941059
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H	5.882877601	-5.323441397	3.908973513
H	6.261418137	-2.918035383	4.383696529
H	6.567757344	-1.180483521	2.915761873
H	8.471924683	-0.237590604	1.996349346
H	9.575755832	-0.812845736	-0.150381287
H	8.310532192	-0.623778758	-2.276348000
H	6.354273427	-1.694919735	-2.885230906
H	5.964657170	-3.646883146	-4.021109021
H	5.619671711	-5.946799049	-3.159694471
H	3.721445194	-6.420331778	-1.631556662
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H	-6.393752237	2.045246800	2.287400118
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H	-4.051711639	5.119728005	4.005818354
H	-3.693331774	7.417012536	3.144731850
H	-1.786437210	7.883858796	1.626338888
H	-1.353473984	6.921890318	-0.433984570
H	-1.940721893	7.506940652	-2.591924400
H	-3.936400804	6.806248100	-3.889014212
H	-4.338022607	4.401163927	-4.337151322
H	-4.645827948	2.645740127	-2.888284430
H	-6.579363085	1.650390992	-1.985570486
Co	-3.230578983	-3.440809273	-1.048909629
Co	-5.052896390	-3.282001596	0.928458597
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C	-6.226604398	-4.613008661	1.045722867
C	-4.438187712	-2.576174028	2.408657966
C	-6.264316285	-2.038685912	0.562510875
O	-2.056723411	-4.894909888	-3.270313148
O	-6.991104540	-5.459443114	1.250836440
O	-4.154366758	-2.209107127	3.473050774
O	-7.102214652	-1.277678683	0.321296050
C	-2.254156234	-4.212426567	0.447946274
C	-3.561520761	-4.459533228	0.759150055
H	-3.775828585	-5.539036275	0.818507229
H	-1.396777394	-4.882704081	0.515744878
C	-4.720020827	-2.747944351	-1.761837235
O	-5.576627917	-2.304609394	-2.408779293

TS1'*parallel*

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Co2C116H26O6

C	1.419001317	-4.909220123	1.640106864
C	2.955452737	-3.858391649	3.245419453
C	3.784022194	-4.959057395	3.473753772
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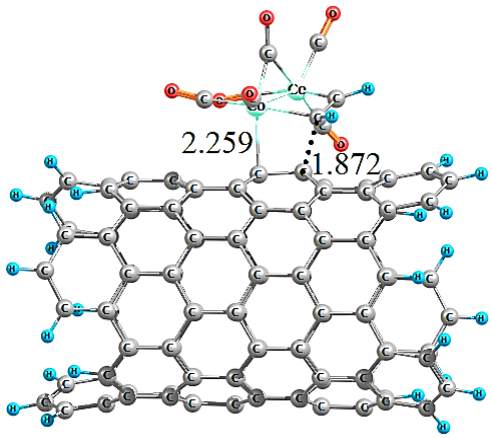

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TS1'*oblique*

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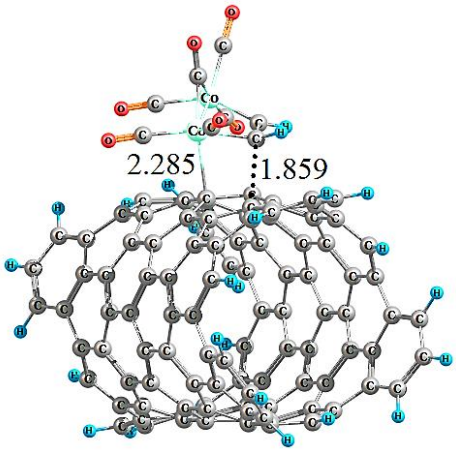

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TS1'*oblique*

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C	2.252831687	4.244934340	1.527098608
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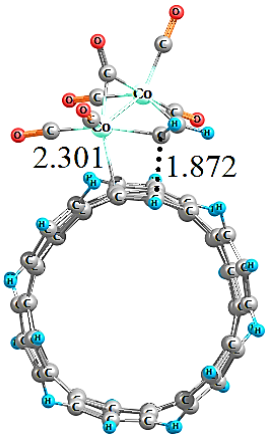

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H	8.639263897	-1.160013788	1.367600979
H	9.415363887	-2.099353170	-0.794878556
H	7.959261614	-1.941472214	-2.798633717
H	5.818035559	-2.778145384	-3.056154833
H	5.042369022	-4.772126356	-3.867872638
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CP4*parallel*

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Co2C115H26O5

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C	4.947292737	-1.212700111	-3.379052502
C	6.288860835	-0.924468845	-3.640803584
C	5.295661353	-3.144490387	-1.894006214
C	5.451425565	-3.844019381	0.454548671
C	6.840216550	-3.791503219	0.589421410
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C	3.590412655	2.099868214	-2.526024897
C	0.298477640	0.356732948	-3.090166983
C	1.687397393	0.632929194	-3.117896222
C	2.611758419	-0.416665217	-3.353235803
C	4.011893486	-0.145091676	-3.371823774
C	0.771130522	-2.027414030	-3.291128859
C	2.157754045	-1.753260081	-3.282732616
C	3.082626047	-2.737622535	-2.801284777
C	4.472594399	-2.470680852	-2.806814335
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C	2.552875201	-3.728275757	-1.930884787
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C	2.648576770	-4.350750516	0.407815613
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C	4.647466683	-3.524443797	1.579130235
C	1.030518957	-3.556957520	2.562898009
C	2.412216987	-3.270240655	2.573826830
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C	-3.023622595	-4.806418139	-1.943217013
C	-1.624781333	-4.528469703	-1.930219744
C	-0.826829344	-4.961437192	-0.845246253
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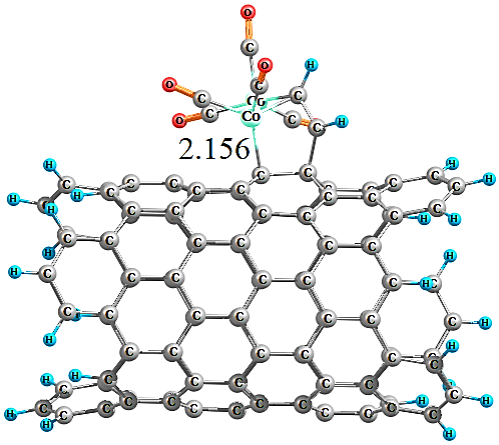

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CP4*oblique*

148
Co2C115H26O5

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C	2.803509276	-7.528770293	0.708787310
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C	0.360496640	0.751943097	-2.947835396
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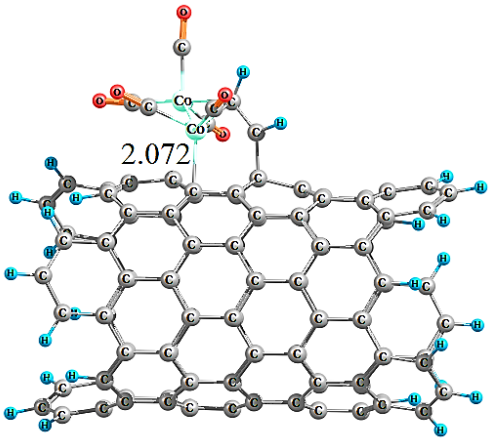

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CP4*_oblique_

148
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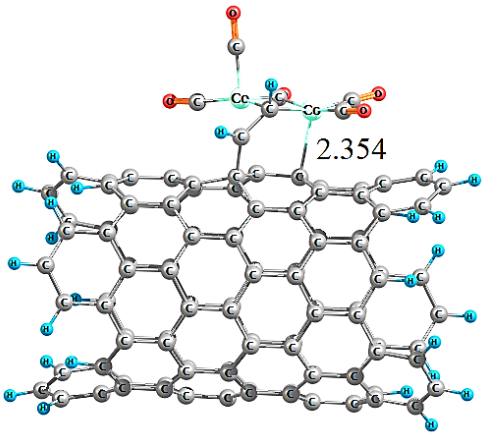

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CP5*parallel*

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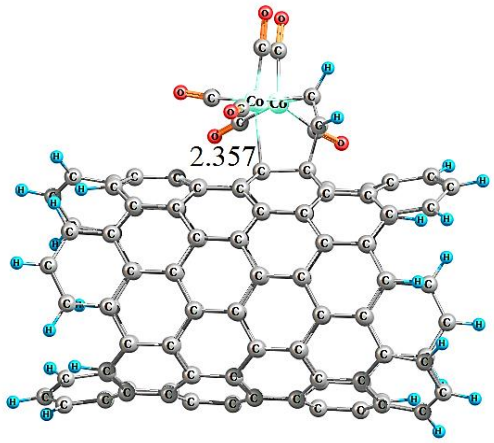

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CP5*oblique*

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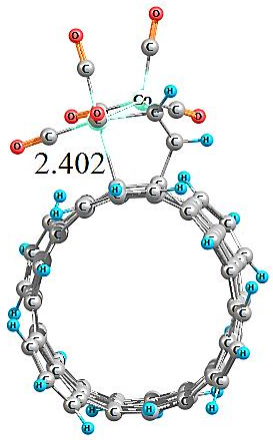

Note: Taken into consideration in the main manuscript.

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H	-5.840237075	2.791173392	1.796016592

CP5*oblique*

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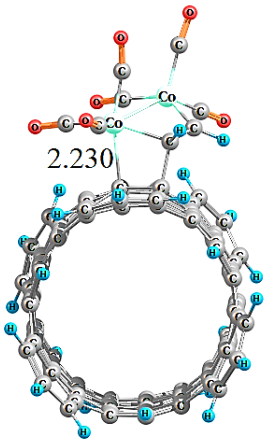

Note: Discarded in the main manuscript.

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CP5*_oblique_

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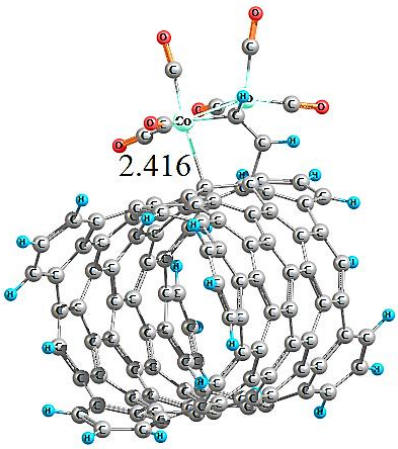

Note: Taken into consideration in the main manuscript.

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CP5*_oblique_

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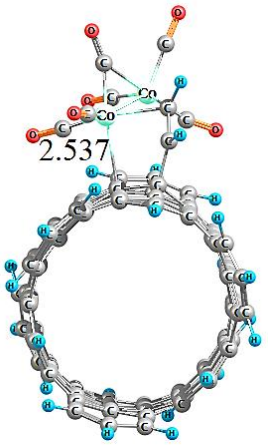

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CP5*_oblique_

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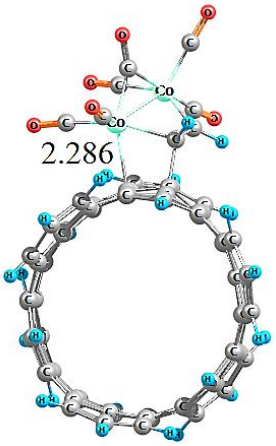

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TS2*parallel*

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C	1.324376919	6.025737461	-0.832171669
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C	2.264111268	4.067199975	-1.979412801
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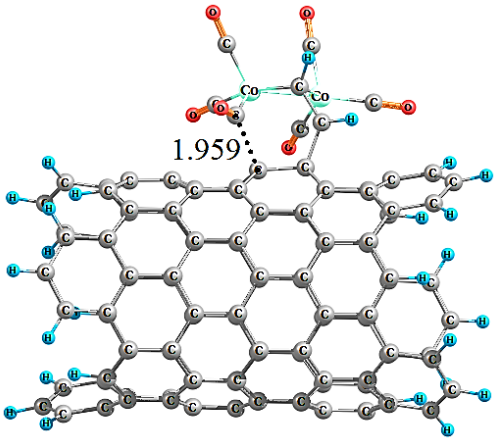

Note: Taken into consideration in the main manuscript.

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TS2*parallel*

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C	2.995374304	4.906765978	1.926780980
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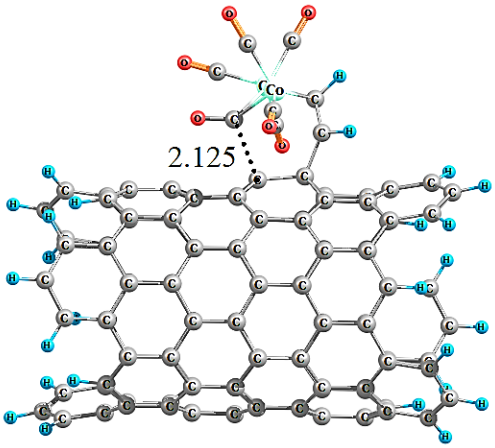

Note: Discarded in the main manuscript.

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TS2*oblique*

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C	4.997588816	2.359673049	3.023284999
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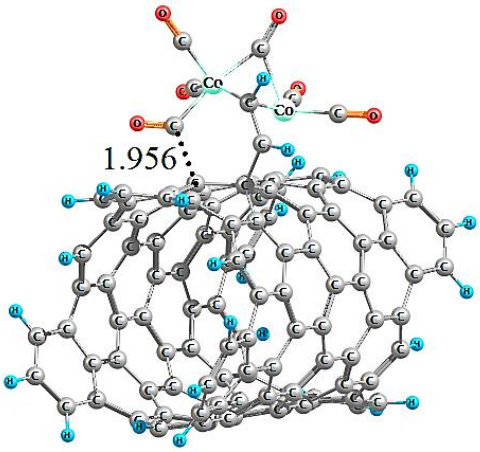

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TS2*_oblique_

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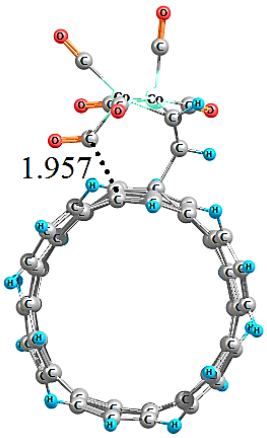

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CP6*parallel*

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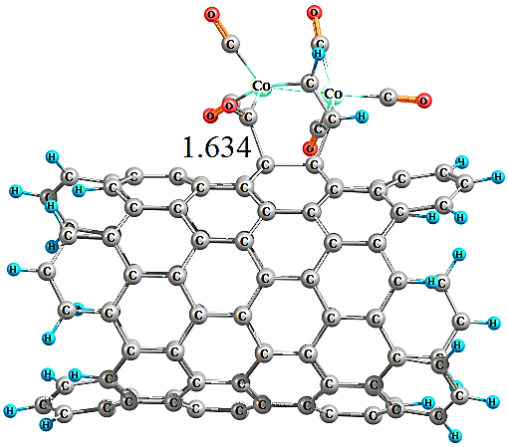

Note: Taken into consideration in the main manuscript.

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C	3.558658659	4.627869177	3.274140410
C	2.720114869	3.534732592	3.039902223
C	4.114495324	2.410843954	1.342773419
C	5.558635365	3.027331695	-1.209378485
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H	4.674811713	3.338079042	1.250069205
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CP6*parallel*

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Co2C116H26O6

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C	-1.701079628	-1.177541522	1.551210074
C	-1.146239311	-2.486737366	1.564420169
C	-0.145747099	-2.842948015	2.502307368
C	0.359021649	-4.175071916	2.537286749
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C	4.189493647	-1.170654616	2.825562687
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C	5.683430149	-2.131545722	-1.534423343
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C	0.440825446	1.964239163	3.317207679
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C	0.829129589	4.389019404	3.307359414
C	1.332962534	3.060831850	3.280598278
C	2.649053537	2.794533442	2.777851163
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C	3.192507235	3.756239784	1.893226064
C	3.998317617	3.303359685	0.822309491
C	4.507928826	1.986056486	0.834669429
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C	3.859657117	4.017863875	-0.417980881
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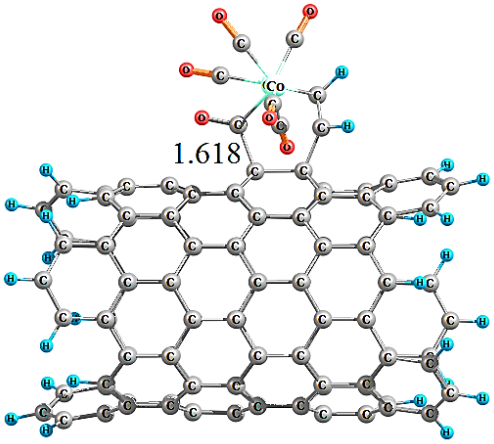

Note: Discarded in the main manuscript.

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C	-3.115790976	3.580869799	-1.904240002
C	-4.595979196	4.534494127	0.517457469
H	0.443920437	-6.041249658	1.504090303
H	1.420980851	-6.570789931	3.514522687
H	3.812259856	-6.890434415	4.091281372
H	5.418479903	-5.025254673	3.783951774
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C	-5.834850058	0.101183245	-0.062681005
H	-6.810277864	0.587481907	0.089159325
H	-5.086584985	1.472671218	1.368438188
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O	-3.711266703	-3.121404806	0.681916632

CP6*oblique*

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Co2C116H26O6

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C	5.386454662	1.820723290	-3.013728651
C	6.671659198	1.055004790	-1.066977601
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C	8.124024075	2.572841968	0.127968660
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C	5.014212071	2.322910358	2.996410615
C	3.045933650	3.768158096	3.266492791
C	3.724524856	4.979172613	3.438201016
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C	2.080187567	6.119819998	2.077209743
C	0.516207465	4.632712100	0.752226328
C	-1.691634830	1.782083979	-0.317557745
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C	0.055104333	2.149436586	-2.521759253
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C	4.837956628	-1.040454294	1.441996121
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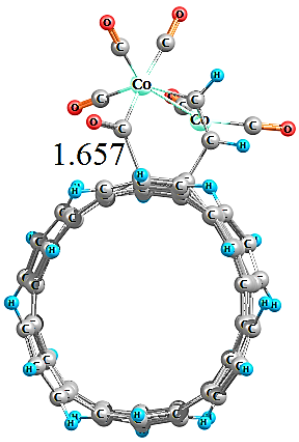

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H	1.606946419	5.946992290	-0.532844662
H	1.988362711	6.627198770	-2.697371576
H	4.087978054	6.501486987	-4.012707402
H	5.146492592	4.298770504	-4.441247589
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CP6*_oblique_

150
Co2C116H26O6

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C	8.238548640	1.018339580	-0.685524193
C	8.690084695	1.551796871	0.520278034
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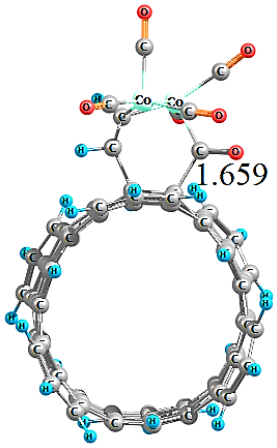

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C	-1.029714808	-4.907825009	-3.110285772
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C	-1.075952728	-6.491703622	3.191599776
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H	-7.052727550	-3.314746631	-0.572423169
H	-5.596245183	-3.170259420	-2.585770398
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CP7*parallel*

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Co2C117H26O7

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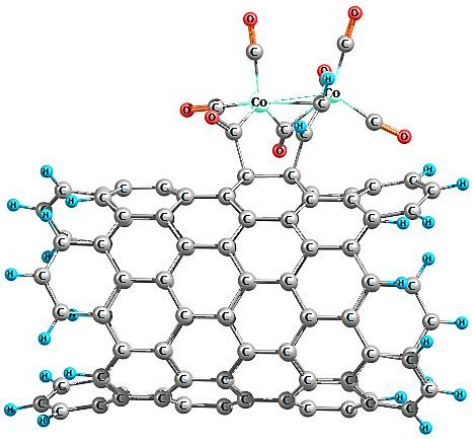

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H	-6.700100000	3.570500000	-3.948400000
H	-4.512700000	4.064500000	-3.439800000
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H	-2.944600000	7.808400000	-1.981700000
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H	5.922500000	-4.681700000	2.559200000
H	3.827600000	-4.733900000	3.875000000
H	1.667100000	-5.223400000	3.405200000
H	0.467800000	-7.181100000	3.623500000
H	0.020400000	-8.987600000	1.982400000
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H	-0.445600000	-6.909600000	-1.737200000
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H	3.381200000	-6.730700000	-3.733400000
H	4.374700000	-4.544600000	-3.120800000
H	4.430100000	-3.352700000	-1.195700000
H	6.084200000	-3.193500000	0.568600000
Co	4.570900000	2.922700000	0.318200000
Co	6.517400000	1.251200000	-0.469300000
C	4.636000000	1.871900000	-1.263000000
C	3.709300000	4.135100000	-0.588700000
C	7.957800000	1.793500000	0.463200000
C	6.628000000	-0.466100000	-0.852900000
C	7.134300000	1.869900000	-2.021700000
O	3.172400000	4.957200000	-1.198000000
O	4.193400000	1.729200000	-2.342400000
O	8.884400000	2.092800000	1.082900000
O	6.890800000	-1.566900000	-1.099300000
O	7.527700000	2.276600000	-3.025600000
C	4.277300000	0.847900000	1.701100000
C	5.575000000	1.063800000	1.274500000
H	6.218600000	1.275000000	2.136900000
H	4.137400000	0.947500000	2.789700000
C	2.935600000	2.848000000	1.417700000
O	2.695200000	3.630000000	2.289300000
C	5.659500000	3.995400000	1.309800000
O	6.367600000	4.718500000	1.860600000

CP7*parallel*

152
Co2C117H26O7

C	0.054956227	-5.074113766	-1.486827385
C	-1.544753507	-4.468514166	-3.250897293
C	-2.006503992	-5.751719289	-3.548560079
C	-3.344016105	-5.953954615	-3.888698987
C	-3.826095723	-3.616710538	-3.506346696
C	-4.264011099	-4.912813889	-3.792005443
C	-5.721879204	-2.916077747	-2.104910777
C	-6.483323129	-2.707230682	0.217066307
C	-7.158351086	-3.924780746	0.318384440
C	-7.079108667	-4.670240591	1.494581429
C	-5.514978707	-3.081662860	2.430366347
C	-6.199970014	-4.296902101	2.509627386
C	-3.372623158	-3.829506697	3.378573644
C	-1.124087296	-4.690060636	2.868752506
C	-1.411046532	-6.051650098	3.014794655
C	-0.797433063	-6.987797026	2.187541116
C	0.296050549	-5.222432263	0.950978184
C	-0.013271503	-6.572604686	1.109845928
C	0.688373870	-4.599460472	-0.315865515
C	1.644545273	-1.152604582	-1.431162463
C	1.109097977	-2.469579270	-1.460096470
C	0.153647257	-2.845042969	-2.436921822
C	-0.331438381	-4.184288036	-2.485419525
C	-0.085780013	-0.471828611	-2.997684002
C	-0.570831127	-1.793701202	-3.067593719
C	-1.937063544	-2.036702054	-3.379650223
C	-2.430014181	-3.373238786	-3.427866530
C	-2.346134833	0.369402093	-3.323885773
C	-2.840042807	-0.955110882	-3.353691653
C	-4.185953238	-1.232706740	-2.937803416
C	-4.680091201	-2.557496203	-2.973593324
C	-4.299448794	1.070651660	-2.060979622
C	-4.792950576	-0.269869824	-2.087197875
C	-5.596767860	-0.747562746	-1.019894103
C	-6.083377902	-2.078251510	-1.042751835
C	-5.003222278	1.287402136	0.251181917
C	-5.466954921	-0.044697772	0.227372371
C	-5.356409917	-0.851254752	1.386765236
C	-5.830931977	-2.195741361	1.368428975
C	-4.032303652	0.910296526	2.444885649
C	-4.497136250	-0.421763500	2.424883554
C	-3.786499424	-1.451023424	3.132895327
C	-4.270915826	-2.780866623	3.138206360
C	-1.926604668	0.141666950	3.383021684
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C	-1.504154839	-2.281348981	3.319880024
C	-1.988425396	-3.612221972	3.345453045
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C	0.382446056	-2.966168681	1.945943744
C	-0.111270276	-4.306635327	1.955291149
C	1.815098746	-1.249216014	0.945038882
C	1.278416838	-2.545975706	0.935000702
C	1.203065795	-3.298424112	-0.301391432
C	2.614070796	-0.829545391	-0.283632640
C	3.019138086	2.904473362	-1.333585676
C	2.570933050	1.556055229	-1.345926593
C	1.600990398	1.172685642	-2.243909457
C	1.123296111	-0.186720099	-2.280574630
C	1.384762645	3.524381305	-3.012607743
C	0.891594533	2.199464900	-2.965210934
C	-0.460625828	1.947874570	-3.299919624
C	-0.952601296	0.607305517	-3.311270829
C	-0.878951197	4.367390540	-3.314798103
C	-1.366930212	3.033434482	-3.301356686
C	-2.697950543	2.752152545	-2.847917669
C	-3.192424766	1.433159337	-2.874086678
C	-2.789456876	5.047142517	-1.971785126
C	-3.287331156	3.710160161	-1.989234301
C	-4.128342385	3.251289756	-0.948345015
C	-4.619855256	1.927352131	-0.973978231
C	-3.567882686	5.304540745	0.310612117
C	-4.048123009	3.973214003	0.292852542
C	-3.974339845	3.175658483	1.466957111
C	-4.453873113	1.829553830	1.446216638
C	-2.585954832	4.920698993	2.502457356
C	-3.070513165	3.590232387	2.482101793
C	-2.329333411	2.544916525	3.129239313
C	-2.814150509	1.222574773	3.131038493
C	-0.457327209	4.123539565	3.370046058
C	-0.951239314	2.787911417	3.344117281
C	-0.050211265	1.705392226	3.249300134
C	-0.536527686	0.385215177	3.253269689
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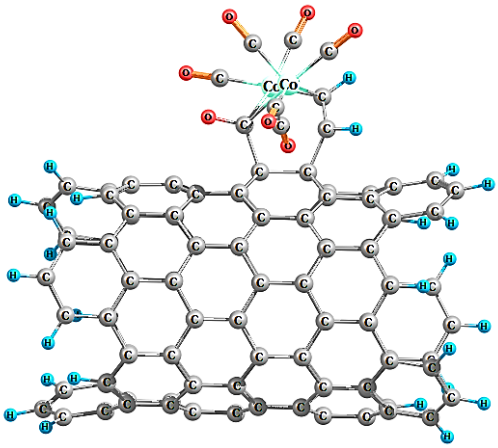

Note: Taken into consideration in the main manuscript.

C	1.888692925	1.019983248	1.933445152
C	1.377855382	-0.326896509	1.905880705
C	3.319734765	2.765328916	1.047729413
C	2.850935602	1.439131222	1.010592848
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C	3.750717206	3.402760424	-0.212977069
C	4.277570850	5.382457654	-1.489641017
C	3.330173975	5.039604039	-2.439825796
C	2.632544945	3.820456062	-2.339685815
C	0.498913054	4.578975650	-3.310261610
C	-1.486790751	6.806244103	-3.000272723
C	-1.765099835	5.444759976	-2.869264247
C	-2.120794715	7.731833324	-2.171218424
C	-2.904407463	7.301872500	-1.101886266
C	-3.198008819	5.944216321	-0.952962380
C	-2.968028640	5.796438428	1.478759045
C	-0.879961160	6.500573231	3.507028823
C	-1.351353130	5.215913608	3.231604153
C	0.467605883	6.700601066	3.804225528
C	1.383995363	5.657659899	3.681408126
C	0.939332486	4.362748402	3.403761269
C	2.861850936	3.642193907	2.040260238
C	4.421029106	4.607547100	-0.324182218
H	-0.436571418	-6.043400291	-1.442869348
H	-1.323147198	-6.598344492	-3.492644475
H	-3.686085780	-6.952669067	-4.158416097
H	-5.327681871	-5.107562254	-3.924305237
H	-5.991287906	-3.967665397	-2.039965858
H	-7.723474696	-4.303295689	-0.532786773
H	-7.643293872	-5.598050360	1.583926369
H	-6.026798603	-4.962006256	3.354933562
H	-3.731570899	-4.847764581	3.249905019
H	-2.131373388	-6.374767009	3.765441007
H	-0.996979029	-8.049072576	2.332458915
H	0.337114050	-7.298185484	0.376235280
H	4.845283025	6.306073923	-1.597519586
H	3.118495157	5.713054155	-3.269630182
H	0.864082522	5.596816418	-3.198134890
H	-0.754117542	7.141746466	-3.733456791
H	-1.931630829	8.796109710	-2.307847128
H	-3.267636086	8.018310946	-0.365680268
H	-2.480448347	6.767319722	1.430080339
H	-1.563486683	7.348241055	3.470570242
H	0.819647135	7.699093675	4.061527446
H	2.450447488	5.853734733	3.785735367
H	3.134714840	4.691527663	1.957912574
H	5.008570923	4.984495388	0.513655390
Co	5.566087885	-0.969659471	-1.258834613
Co	5.466267765	-1.514251457	1.275738307
C	6.398440775	-2.547590420	-1.105583539
C	4.606717704	-1.034647397	-2.774380356
C	7.157921393	-1.461256824	1.878739549
C	4.449575771	-0.837833962	2.532373546
C	5.129029811	-3.234373343	1.694109886
O	4.034814378	-1.045941841	-3.772400523
O	6.938003175	-3.566382023	-1.133757237
O	8.207789144	-1.359008514	2.346511453
O	3.984416196	-0.415368708	3.502901714
O	4.900685572	-4.326198105	1.969999592
C	4.700835421	0.697864369	-0.443696616
C	5.681770018	0.158418443	0.408493943
H	6.594543848	0.747803645	0.550659349
H	5.005146152	1.604263671	-0.972505537
C	3.850082618	-1.852440188	-0.420736412
O	3.658857648	-3.036901836	-0.596991106
C	7.012128310	-0.110191302	-1.895000306
O	7.923551905	0.456826609	-2.313027533

CP7'*parallel*

152
Co2C117H26O7

C	3.451743864	3.406469468	0.709751829
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C	2.809104584	5.091284082	3.092367104
C	2.034573432	6.086366957	3.688102756
C	0.081686222	4.664349648	3.592442670
C	0.664928484	5.904827916	3.864189637
C	-2.048728489	5.485405402	2.678467443
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C	-2.440739294	7.221230680	-1.819508556
C	-0.851988137	5.095687057	-3.213215504
C	1.454600962	4.232623943	-3.246547323
C	2.108361013	5.454958587	-3.438817124
C	3.342999274	5.690213075	-2.841624562
C	3.241560731	3.549410922	-1.726781226
C	3.868376544	4.778155381	-1.923788851
C	3.377882431	2.723504232	-0.522821559
C	2.039752806	-0.585802773	0.623092831
C	2.533504317	0.748834191	0.665951758
C	2.275957494	1.578066401	1.787243132
C	2.793921162	2.903042673	1.829089922
C	0.658365936	-0.101245578	2.555232602
C	1.184142245	1.205523584	2.625865395
C	0.407467311	2.252333832	3.193727714
C	0.926899956	3.578372845	3.244849287
C	-1.473610727	0.707236066	3.399629669
C	-0.963724452	2.025500414	3.431845012
C	-1.851055408	3.145031356	3.288011424
C	-1.341657800	4.464110646	3.330108307
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C	-3.594311727	3.857422597	1.752871696
C	-3.077941769	5.176649514	1.780335576
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C	-3.846182689	3.980975987	-0.650650210
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C	-4.244446594	1.878494370	-1.831175519
C	-3.709471939	3.183463644	-1.810549202
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C	-2.144745880	4.871970932	-2.720135726
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C	-1.877072096	2.489980799	-3.239026812
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C	2.909244499	1.404065835	-0.547219474
C	2.327300486	-1.382071305	-0.662733899
C	0.408112713	-4.553314164	0.562960484
C	0.961909161	-3.244708246	0.563336366
C	0.679040603	-2.388523604	1.606170327
C	1.199198331	-1.045266507	1.622754404
C	-0.854278218	-4.082807771	2.579296189
C	-0.362620362	-2.757544204	2.532339373
C	-1.125833369	-1.712034624	3.106878059
C	-0.612704784	-0.378981887	3.119662901
C	-3.006509735	-3.265962434	3.378439527
C	-2.496741068	-1.940462779	3.367624404
C	-3.378103331	-0.824963773	3.177655120
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C	-4.608443181	-1.093919054	2.532879141
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C	-5.811075858	-0.603662633	0.490901004
C	-5.482478255	0.050967170	-0.727146829
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C	-3.696259808	0.905373089	-2.728175759
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C	-1.508344682	0.059558294	-3.364919422
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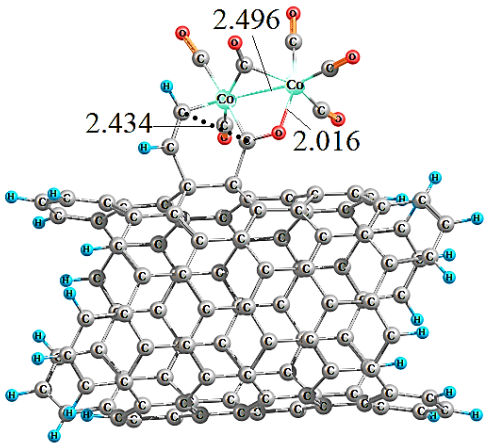
C	-1.141058472	-2.362631378	-3.169077365



Note: Discarded in the main manuscript.

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C	1.751138587	-2.853418525	-0.696412018
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C	-0.295144515	-7.241507700	0.623071811
C	-0.549977115	-6.448440232	1.729349291
C	-0.270200298	-5.068649408	1.691914034
C	-2.134692327	-4.322114511	3.116841139
C	-5.102522352	-4.687300713	3.365031179
C	-4.445659975	-3.467061181	3.198028074
C	-6.338442920	-4.904993457	2.756063580
C	-6.851789376	-3.980638983	1.848300015
C	-6.213093513	-2.751528957	1.667214445
C	-6.460876601	-2.580098022	-0.761425626
C	-5.817358610	-4.296891510	-3.130095907
C	-5.265461825	-3.045319319	-2.852497632
C	-5.023322625	-5.302686258	-3.680009767
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C	-3.069744477	-3.884465387	-3.540047942
C	-0.932205115	-4.705330266	-2.634147411
C	0.065748421	-6.650500819	-0.601399380
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H	2.489793672	7.041987165	3.946239225
H	0.041792277	6.733319776	4.199154216
H	-1.574702313	6.460523970	2.595011289
H	-2.932848015	7.967864388	1.463463188
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H	-2.051767681	7.680077043	-2.727871410
H	-0.423038189	6.087155414	-3.089423853
H	1.638444324	6.228767255	-4.044878079
H	3.863049589	6.629157793	-3.028484378
H	4.751748263	5.036503426	-1.340177203
H	-0.472866471	-8.315227504	0.672451673
H	-0.973573820	-6.887378465	2.631842823
H	-2.552144519	-5.320145337	3.009475176
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Co	5.042149754	-2.423203450	0.458795804
Co	6.262647074	-0.430436102	-0.417454906
C	6.318782704	-2.374095788	-0.938592786
C	4.205297708	-1.976654803	1.989867965
C	5.726157865	0.855278856	0.777731387
C	7.633136688	-0.824782342	0.587111508
C	7.122076405	0.343206622	-1.801021330
O	3.811243372	-1.705977691	3.040052105
O	6.926652845	-3.017328633	-1.711894802
O	5.627362425	1.611382326	1.641693381
O	8.554387941	-1.057314197	1.245308987
O	7.727563058	0.855392026	-2.634319552
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C	4.120788580	-3.836788803	-0.497853972
H	4.778472555	-4.653045229	-0.814203350
H	2.532966009	-4.782270219	-1.441173736
C	3.899223070	-1.419796266	-0.678914107
O	4.494142875	-0.566423070	-1.375671057
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CP7*oblique*

152
Co2C117H26O7

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C	1.685404022	6.302115928	-3.974465900
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C	6.487208716	4.735926221	-0.660578905
C	6.581542529	5.445187726	0.535483887
C	5.466992147	3.656351030	1.720206513
C	6.002375289	4.945870211	1.701883226
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C	1.118674484	4.684812496	3.097798271
C	1.252276273	6.070247255	3.228621695
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C	-0.675129434	5.037282351	1.469571231
C	-0.521600497	6.416652457	1.617713207
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C	-1.055606434	2.761051386	-2.017631553
C	-0.751687835	4.136017797	-2.096205644
C	-0.644061548	0.434264859	-2.743716428
C	-0.344446646	1.810665923	-2.834096759
C	0.895493911	2.227676029	-3.362936219
C	1.202638743	3.617666480	-3.451541104
C	1.622312634	-0.104267080	-3.473099532
C	1.926687637	1.265877179	-3.542847370
C	3.275939151	1.715558665	-3.361575435
C	3.584104689	3.095680449	-3.443798812
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C	4.151615107	0.832776404	-2.673826728
C	5.086080936	1.401740433	-1.766656913
C	5.388008535	2.781349860	-1.837698850
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C	5.349439078	1.441789212	0.641253344
C	5.643409941	2.835045775	0.576764207
C	4.514453863	-0.489328941	1.885736912
C	4.798155401	0.889994972	1.822840366
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C	4.453340563	3.189130807	2.666531561
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C	-1.668549726	-0.029987711	-1.853808720
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C	-1.257998211	-2.325063289	-2.591378925
C	-0.023839488	-1.907456471	-3.155489455
C	0.282466037	-0.522939513	-3.230812699
C	0.684177569	-4.248518776	-3.282099855
C	1.000992811	-2.874991378	-3.333256902
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C	4.447038593	-3.491945136	-0.348336815
C	4.529180113	-2.727788534	0.847085418
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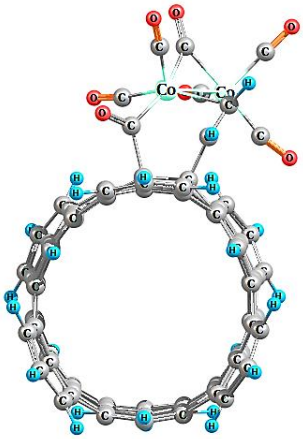

Note: Taken into consideration in the main manuscript.

C	-1.281891010	-1.360402571	2.553315940
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C	-2.292991657	-1.892155998	1.731742161
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C	-3.757662836	-5.979623107	-0.511991570
C	-3.141489081	-5.486039459	-1.658438998
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C	1.752716171	-5.208395600	-3.029812576
C	2.513210569	-7.440112474	-2.489527299
C	3.451388427	-6.923124416	-1.595477343
C	3.604656854	-5.542336467	-1.465549154
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C	2.630441556	-5.121357990	3.036966154
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C	-1.877170969	-4.089278903	2.676429083
C	-3.711371497	-5.239931902	0.669531151
H	-0.610494064	5.978725449	-1.005515077
H	-0.279767935	6.678591069	-3.170639127
H	1.845599426	7.339904346	-4.264979285
H	3.714694573	5.715070422	-4.415821639
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H	5.943310992	5.569728949	2.593112335
H	3.703084697	5.168850312	2.963334138
H	2.049868692	6.481203553	3.846588639
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H	-1.092524420	7.095767847	0.985202398
H	-4.183223208	-6.982497304	-0.510957209
H	-3.016716217	-6.125473759	-2.531729625
H	-0.854815345	-5.685401672	-2.880708747
H	0.793465212	-7.015322355	-3.717519769
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H	4.044171691	-7.594741432	-0.975232184
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Co	-5.248515408	1.883056194	1.091139546
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C	-6.663265111	2.426690006	2.045384261
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O	-4.253098126	1.517367282	-2.915911992
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C	-5.343495877	-0.048400513	1.354696546
C	-4.381652088	-1.534172481	-1.461983010
O	-4.747803095	-2.181993456	-2.392710274
H	-4.797149220	-2.049591975	1.092117352
H	-6.252388568	-0.406865595	1.849200748
C	-4.089682633	1.864745385	2.448156840
O	-3.576110753	1.910970938	3.480900855

CP7'*oblique*

152
Co2C117H26O7

C	-1.840472356	5.237098887	-0.381627846
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C	-4.194369141	5.981880247	3.061587056
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C	-4.614949566	4.761898483	3.591547015
C	-5.690186078	2.011459173	3.123401146
C	-7.079393960	0.842149346	1.469574111
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C	-1.427227736	4.704251094	0.856497604
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C	3.182905574	-1.602690422	2.072655221
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C	0.167935214	0.499685902	2.821820092
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C	-1.015378077	-2.546362817	-3.190643849
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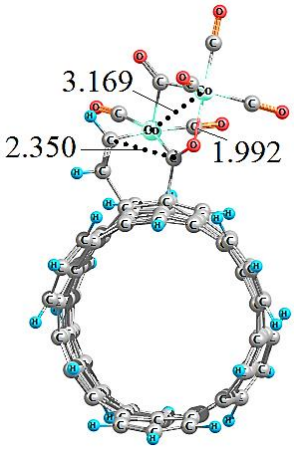

Note: Discarded in the main manuscript.

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C	1.940471196	-5.364724646	3.884190346
C	1.132824421	-4.248654238	3.639631310
C	1.454200063	-6.646181531	3.638385757
C	0.230934139	-6.827907083	2.991824126
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H	-4.777352470	6.882363275	3.252042744
H	-5.556218975	4.698121173	4.136380314
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H	-9.657576162	2.686332006	0.233462176
H	-8.690155622	1.901311793	-1.911762036
H	-6.658562261	2.423690172	-2.846035492
H	-6.046293906	4.057501130	-4.320156814
H	-5.215194254	6.348231783	-3.861970589
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Co	5.780576837	3.368596416	0.674839907
C	6.612479286	2.555485987	-0.912163132
C	6.706874336	0.125386076	0.415500576
C	5.833501343	2.832375487	2.397340959
C	7.302996223	4.191311027	0.828952664
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O	7.244677502	-0.227430482	1.374104311
O	7.397351649	2.900441225	-1.727032633
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O	4.273887878	5.810763022	-0.085320839
C	3.385010630	1.230610566	-2.619095650
C	4.703506027	1.384443778	-2.476537227
H	5.220101655	1.957213488	-3.255395040
H	2.866625883	1.604297874	-3.509735833
C	4.323565645	1.196364536	-0.164925718
O	4.153356079	2.233475699	0.500954403
C	7.001292848	0.051089198	-2.300605194
O	7.618597714	-0.473356651	-3.120419114

CP7*_oblique_

152
Co2C117H26O7

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C	-0.488330561	-4.790003066	-2.813621011
C	-0.804310118	-6.122995116	-3.088291270
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C	-2.702537983	-4.124125429	-3.606085071
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C	-6.200223453	-3.159490608	-0.651519690
C	-6.812377037	-4.414123125	-0.609101955
C	-6.980521211	-5.066835789	0.611282449
C	-5.776572960	-3.307299189	1.750901917
C	-6.393813419	-4.559972388	1.770148616
C	-3.868666233	-3.835501315	3.204349635
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C	-3.316238316	-1.740749456	-3.317430938
C	-3.714096321	-3.099155599	-3.350681976
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C	1.699182356	-0.233889739	-1.773308807
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C	1.447734399	2.043601501	-2.649197243
C	0.205154680	1.671464396	-3.219468185
C	-0.193213692	0.307616092	-3.203947422
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C	-2.130630515	2.339736466	-3.255567299
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C	-3.157514622	2.574548166	2.705012144
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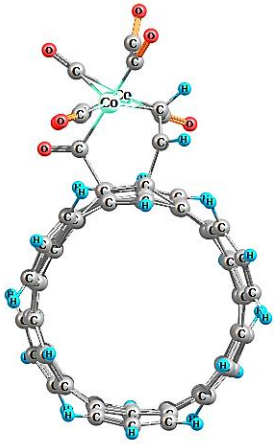

Note: Taken into consideration in the main manuscript.

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C	-1.147127080	6.450491748	-3.461008544
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C	-0.845560317	6.968577944	3.655807126
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C	2.048686425	3.996808517	2.716241746
C	3.990305144	4.939011212	0.613457236
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H	-0.105056397	-6.912201773	-2.814218358
H	-2.241819071	-7.479035283	-3.941157729
H	-3.991601555	-5.741344075	-4.213038582
H	-5.120390092	-4.534691634	-2.620788787
H	-7.134127568	-4.891258921	-1.534199003
H	-7.499381971	-6.024355749	0.643860768
H	-6.392468242	-5.150190273	2.685896596
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H	-2.563875713	-6.246210960	4.055472078
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H	0.666861399	-7.179430471	1.384703328
H	4.683683604	6.528758687	-0.657628839
H	3.520087329	5.668633590	-2.677050451
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H	2.274224673	5.057636057	2.635743615
H	4.347349165	5.404353630	1.531841265
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O	8.749385862	0.155715273	-1.186835284
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H	5.464635794	-1.333878791	-2.398077054
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C	6.062181563	-3.294026416	-0.863574331
O	6.683497625	-4.029649317	-1.493383685

CP7*_oblique_

152
Co2C117H26O7

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C	4.722759908	2.594182612	-3.716891929
C	5.630637113	3.611105796	-4.013448708
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C	7.326528219	0.090432756	-0.757093952
C	8.473700996	0.888214748	-0.743494057
C	8.958870540	1.390595257	0.462439300
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C	2.684884004	4.989845053	1.690012705
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C	2.090818449	4.402853225	-1.889161709
C	0.122775128	1.282208118	-2.624433465
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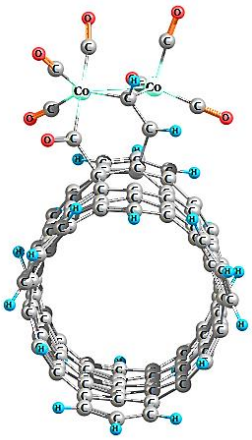

Note: Discarded in the main manuscript.

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H	6.627407651	3.358266458	-4.373373304
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H	5.802544428	4.591058001	3.984449329
H	5.291343825	6.781678449	2.941166929
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Co	-6.004326849	1.663886205	-1.458421092
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C	-5.820996199	1.059132254	2.388470372
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C	-5.594681850	0.832416586	-2.948597340
C	-7.133023004	0.428978035	-0.869049027
O	-6.051813636	0.295365118	3.221353658
O	-8.424896526	2.928644413	0.768925777
O	-7.647889531	3.848863497	-2.564381383
O	-5.326078293	0.324320336	-3.952137162
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C	-3.900100740	1.870815977	-1.237622788
C	-4.658496941	2.829274285	-0.554325978
C	-3.527166035	2.137664275	1.546665411
O	-3.068735450	2.766014482	2.459727013
H	-3.462599888	2.190315649	-2.189187274
H	-4.608660831	3.878951723	-0.856829156
C	-5.425710523	3.933496408	1.984923168
O	-5.383440257	4.955098478	2.512792575

CP7'*_oblique_*

152
Co2C117H26O7

C	0.302687523	-5.122068676	-1.463301709
C	-1.243236620	-4.596847615	-3.297989533
C	-1.627303286	-5.904746770	-3.607691293
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C	-6.363979640	-3.174101075	0.085370796
C	-6.970536538	-4.431143476	0.147809903
C	-6.900538576	-5.181084093	1.320518876
C	-5.471737780	-3.516366863	2.336414856
C	-6.090031794	-4.767594240	2.377620078
C	-3.329997654	-4.150885052	3.358557713
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C	0.219268618	-6.651167018	1.119263133
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C	0.347292408	-2.900783626	-2.448838292
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C	-4.069353011	-1.520263434	-2.987524377
C	-4.485586222	-2.872649465	-3.053150892
C	-4.337496133	0.753542439	-2.076318362
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C	2.781438472	1.522993711	-1.454123185
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C	-0.530671531	1.867630918	-3.254207580
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C	-4.329407565	2.921338717	-0.926513033
C	-4.739186452	1.574674903	-0.984649499
C	-3.942184004	4.988717314	0.372648201
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C	-4.657065956	1.455075641	1.439620752
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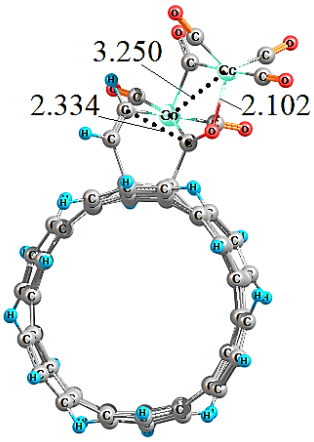

Note: Discarded in the main manuscript.

C	1.635733607	1.036849882	2.092711402
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C	2.510864964	1.540867409	1.116961366
C	2.877984708	0.718016779	-0.079228959
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C	3.889012016	5.597419486	-1.205491466
C	3.042593373	5.191902653	-2.234182710
C	2.491419908	3.902808170	-2.222007422
C	0.300149184	4.536203923	-3.157248075
C	-1.803871664	6.648361143	-2.823722083
C	-2.020497044	5.269159347	-2.731017247
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C	-3.329808767	7.035192354	-0.985494934
C	-3.556248970	5.663677082	-0.867485079
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H	-0.142548992	-6.114395429	-1.451316680
H	-0.899507379	-6.712523461	-3.539306845
H	-3.221969373	-7.189118906	-4.269125972
H	-4.966713944	-5.437996646	-4.057314976
H	-5.731801773	-4.370793182	-2.174467201
H	-7.478507963	-4.831778355	-0.728833661
H	-7.415042342	-6.139742287	1.378944697
H	-5.917361722	-5.429840994	3.225319936
H	-3.624815451	-5.186039651	3.204086027
H	-1.944766962	-6.631765474	3.745858379
H	-0.686208031	-8.206192081	2.302891163
H	0.627090314	-7.341697843	0.381692610
H	4.368346135	6.574808742	-1.246533710
H	2.789125456	5.881295750	-3.039049698
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H	2.684838887	4.766168474	2.141221049
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O	5.204872367	0.897935253	0.687606036
C	4.446317544	-2.650471232	-2.167865105
O	4.212883931	-3.413932041	-2.994979312

TS3*parallel*

152
Co2C117H26O7

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C	3.467872221	2.585059459	-0.606546385
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C	2.917323843	2.777330601	1.754174954
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C	-1.568030020	0.126721146	-3.364928586
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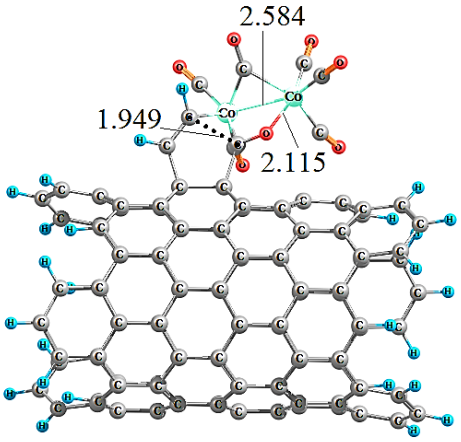

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C	-6.450411683	-4.719679420	2.802708997
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C	-1.158395556	-4.661802286	-2.668130401
C	-0.167633998	-6.661372612	-0.678874699
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H	2.811217340	6.902434576	3.916225442
H	0.361316280	6.674803437	4.230707525
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H	-4.746411189	-5.365627149	3.957565769
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H	2.428632257	-4.780210930	-1.655579764
C	3.834876959	-1.657790983	-0.819084679
O	4.488829901	-0.833280789	-1.516989865
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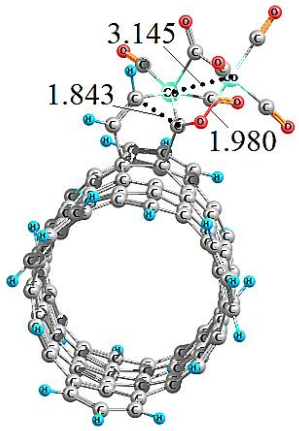
TS3*oblique*



152
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TS3*_oblique_

152
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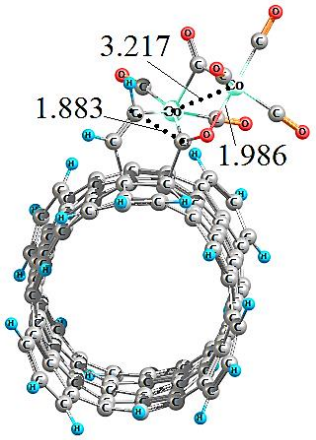

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C	3.203417636	-3.244881189	-1.864379694
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H	5.547241405	1.097958370	2.669563176
H	4.291970373	-0.850761024	3.440681865
C	4.358613070	0.559927690	0.283440514
O	5.295579292	0.068446737	-0.410451422
C	3.828091404	3.604731592	2.098463966
O	3.455195444	4.369187789	2.876462282

PD*parallel*

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Co2C117H26O7

C	-1.919565438	5.054142821	2.036547898
C	-3.547558309	3.859476613	3.436677516
C	-4.408808570	4.926858997	3.695194220
C	-5.784105775	4.711768667	3.782699577
C	-5.487145582	2.381415611	3.214704603
C	-6.327665136	3.468828864	3.467072510
C	-6.827671024	1.309923685	1.451763517
C	-7.094815606	1.107917248	-0.978534164
C	-8.073633698	2.086992702	-1.156625771
C	-8.025133485	2.927181170	-2.268767264
C	-5.927922861	1.941774001	-2.957822576
C	-6.919140587	2.913351406	-3.116913993
C	-3.978246654	3.353453798	-3.449760006
C	-2.207906065	4.760992080	-2.478449169
C	-2.854553127	5.994134390	-2.614108959
C	-2.687227886	6.980446119	-1.646714186
C	-1.342008869	5.485293222	-0.306964266
C	-2.003022659	6.702370165	-0.461831379
C	-0.990468922	4.886286530	0.984686318
C	0.729898745	1.762031798	2.122066028
C	-0.154816692	2.872690223	2.106765164
C	-1.332923758	2.865721551	2.898500471
C	-2.191557235	4.001546698	2.906834580
C	-0.962302229	0.473700853	3.302323003
C	-1.815216996	1.596008886	3.331955041
C	-3.224858050	1.414872309	3.385697275
C	-4.088916354	2.548234691	3.393538089
C	-2.897086079	-0.994846384	3.158901141
C	-3.753248934	0.129978654	3.145811269
C	-5.029568275	0.056961899	2.492237313
C	-5.889081790	1.180118149	2.486390618
C	-4.312996855	-2.093585775	1.518865817
C	-5.173791355	-0.953835038	1.504252836
C	-5.889418120	-0.624705626	0.324084477
C	-6.742871273	0.506022293	0.308177795
C	-4.515495853	-2.280535303	-0.892054687
C	-5.348945409	-1.142643868	-0.903227646
C	-5.289121815	-0.235360554	-1.989220977
C	-6.138187739	0.910131051	-2.007506990
C	-3.342659002	-1.442198822	-2.846923788
C	-4.179820397	-0.306176820	-2.864711778
C	-3.700036942	0.942980867	-3.388491607
C	-4.550122361	2.074357412	-3.430455937
C	-1.435019536	-0.023793909	-3.356834719
C	-2.291616108	1.116386061	-3.408444748
C	-1.772409639	2.402816970	-3.108834311
C	-2.618909270	3.536586731	-3.162300327
C	0.292506139	1.322045730	-2.294359618
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C	-1.294862870	4.591471372	-1.407906003
C	1.227565525	2.106796702	-0.195453210
C	0.357631436	3.200979395	-0.222552430
C	-0.118794994	3.792438359	1.013927088
C	1.894422581	1.807092330	1.133709402
C	3.231301638	-1.716768266	2.081307515
C	2.388996631	-0.579003036	2.064079030
C	1.223446517	-0.560322189	2.795201219
C	0.378580478	0.607485732	2.811958734
C	1.594317899	-2.937464256	3.398004660
C	0.744634990	-1.807219369	3.330506624
C	-0.657319322	-1.975007002	3.426772949
C	-1.513703068	-0.830905605	3.402025184
C	-0.343255502	-4.404420917	3.259561881
C	-1.192682376	-3.266789430	3.214447057
C	-2.451407444	-3.327394239	2.529615324
C	-3.305420345	-2.206726981	2.513828750
C	-1.718096002	-5.463548657	1.558519679
C	-2.578861188	-4.326278502	1.535267513
C	-3.324115536	-4.023955531	0.371542332
C	-4.177576951	-2.899390838	0.356670319
C	-1.977063733	-5.707434384	-0.838754470
C	-2.821342350	-4.571685263	-0.859220614
C	-2.782479576	-3.677151108	-1.962875567
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C	-0.782308566	-4.852062531	-2.777018715
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C	-1.139633127	-2.454702081	-3.258400946
C	-1.989680619	-1.331109528	-3.305616519
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C	0.777059537	-0.990351025	-2.938820441
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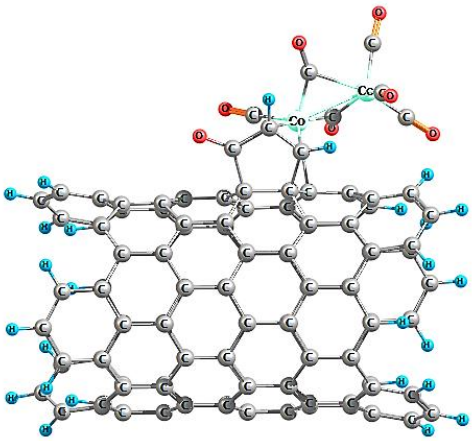
C	2.028827770	-0.916499770	-2.242244591



Note: Taken into consideration in the main manuscript.

C	2.184589916	0.104576754	-1.274478211
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C	2.836725136	0.559036569	1.175459182
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C	5.136796632	-3.714776449	2.381854954
C	3.974128005	-3.765872274	3.135900110
C	2.968485851	-2.801257060	2.953677778
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C	-0.156622674	-6.878659674	2.744905438
C	-0.790770139	-5.641817643	2.617002468
C	-0.344471183	-7.863347707	1.774616805
C	-1.021443316	-7.569468477	0.592180303
C	-1.665422457	-6.338674408	0.444547035
C	-1.062556268	-5.894556771	-1.885170631
C	1.463666099	-5.781166002	-3.488716463
C	0.591184331	-4.714883087	-3.264066377
C	2.840760966	-5.563649882	-3.535773713
C	3.372539177	-4.318336409	-3.209364915
C	2.521727900	-3.232926588	-2.982546049
C	3.894155303	-2.123701213	-1.267311436
C	5.247813019	-2.815253839	1.309050971
H	-2.658996941	5.846005982	1.941414236
H	-4.004761929	5.932275376	3.808024551
H	-6.444806393	5.543220376	4.026176085
H	-7.408013115	3.343947540	3.402999659
H	-7.380601455	2.243638804	1.379744131
H	-8.858569948	2.210211608	-0.411085869
H	-8.816148596	3.659797987	-2.425915570
H	-6.813058672	3.674013779	-3.889594609
H	-4.640782088	4.209661541	-3.348593554
H	-3.502523333	6.173884652	-3.471114027
H	-3.161780192	7.952159093	-1.779468801
H	-2.003856655	7.425626840	0.353099491
H	5.929903139	-4.440376619	2.558468182
H	3.835458469	-4.556298961	3.872838248
H	1.678603878	-5.081238933	3.398241346
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H	0.116458584	-8.842126122	1.903530002
H	-1.028925639	-8.286542805	-0.228175669
H	-0.328282802	-6.690029563	-1.781605082
H	1.066615754	-6.788623545	-3.609510409
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H	4.446246100	-3.054873074	-1.177303883
H	6.061948490	-2.930231646	0.597168731
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C	5.558082233	0.668738782	-1.882450604
C	4.016757505	2.919285064	-1.348133863
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C	7.092143137	-1.312662069	-1.239651852
C	8.416101126	1.115326486	-1.573217646
O	3.561986289	3.771792498	-1.977722092
O	5.140142935	0.382576467	-2.945857001
O	7.586217713	-0.179203508	2.145416133
O	7.146987864	-2.413546272	-1.600556929
O	9.345449523	1.513329499	-2.129208515
C	4.192486440	1.093915528	1.665570929
C	4.196290947	2.465017577	1.721045317
H	4.993341150	3.091614144	2.116010126
H	4.928309814	0.430510919	2.116439557
C	2.866249740	3.022997253	1.469834301
O	2.528244113	4.186618586	1.532040764
C	6.424747712	2.388939811	-0.016334886
O	7.062493630	3.293659174	0.369507482

PD'*parallel*

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Co2C117H26O7

C	-1.982669151	-4.655017993	0.435078159
C	-0.839221434	-4.628365247	2.610497918
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C	0.157600341	-6.627099023	3.537481445
C	1.423401127	-4.567710204	3.545060794
C	1.340995142	-5.939943707	3.796703905
C	3.761460153	-4.500659274	2.783953222
C	5.188754073	-4.520007708	0.789639376
C	5.458928845	-5.888913029	0.746396191
C	5.499584522	-6.553296931	-0.479317905
C	4.834331935	-4.533555014	-1.628962511
C	5.107701090	-5.903429904	-1.648532365
C	2.925826676	-4.536965593	-3.178350188
C	0.472505598	-4.626437577	-3.367239160
C	0.351596726	-6.004943654	-3.573894522
C	-0.735648538	-6.697444621	-3.049521112
C	-1.539817018	-4.686891571	-1.976252325
C	-1.632286983	-6.061124415	-2.188710726
C	-2.078431120	-3.984520449	-0.805566476
C	-2.178209396	-0.435843219	0.372790702
C	-2.134755942	-1.853767619	0.405890930
C	-1.656349518	-2.531814819	1.557038182
C	-1.638187162	-3.953793874	1.587677562
C	-0.856990319	-0.372718533	2.407333943
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C	0.229163383	-2.458279533	3.094404555
C	0.252275181	-3.882748026	3.128367782
C	1.359223845	-0.313380213	3.404206731
C	1.390222122	-1.727252897	3.420996243
C	2.644992015	-2.421188222	3.347369176
C	2.676256252	-3.835348159	3.373579579
C	3.706747526	-0.266897097	2.779221113
C	3.735393439	-1.695671298	2.796116248
C	4.625844473	-2.394664149	1.940166493
C	4.653440440	-3.811374482	1.953355082
C	5.078254095	-0.261832521	0.776604816
C	5.083976904	-1.672387564	0.784928900
C	5.072507360	-2.385105566	-0.439211702
C	5.086199679	-3.810770093	-0.434611604
C	4.716971170	-0.277424786	-1.624887070
C	4.724355485	-1.687932091	-1.619769956
C	3.965225726	-2.423000931	-2.594021724
C	3.997523616	-3.837900807	-2.606500224
C	2.837929123	-0.309721562	-3.165532319
C	2.874600417	-1.735685401	-3.187286264
C	1.689431127	-2.467513618	-3.457394451
C	1.725230433	-3.883181539	-3.486685012
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C	0.445379617	-1.778644075	-3.259122457
C	-0.624145913	-2.516894610	-2.708628199
C	-0.589893712	-3.944305876	-2.724438933
C	-1.672134726	-0.440171089	-1.966152626
C	-1.600637419	-1.838446282	-1.942312605
C	-2.142265131	-2.587070821	-0.821518957
C	-2.605906510	0.203442371	-0.937987821
C	-2.186175414	3.848297981	0.341617064
C	-2.170175718	2.433176424	0.330353524
C	-1.660461231	1.739502749	1.405253530
C	-1.641880234	0.299841690	1.417988950
C	-0.983475001	3.886890452	2.447788213
C	-0.922012556	2.473692379	2.398842815
C	0.136359236	1.793310257	3.049405425
C	0.169431127	0.364579928	3.052932518
C	1.254891419	3.948315380	3.409070521
C	1.293992818	2.527997751	3.394434706
C	2.544972929	1.834598920	3.280822936
C	2.582052072	0.425298023	3.303064614
C	3.582651511	3.986199734	2.698623301
C	3.618660578	2.559654176	2.711804573
C	4.540554485	1.864682992	1.893874830
C	4.572797350	0.452815747	1.912974620
C	5.030557727	4.002930626	0.752442374
C	5.049457991	2.587752691	0.759974595
C	5.078725723	1.871485808	-0.467156077
C	5.093157242	0.442948945	-0.458756635
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C	4.682149896	2.568948496	-1.639870742
C	3.872009739	1.829612340	-2.566604586
C	3.904423691	0.421456992	-2.575921343
C	2.729696539	3.935210833	-3.128143119
C	2.757837104	2.510711853	-3.113444341
C	1.579219640	1.779433205	-3.377842560
C	1.614591034	0.371217066	-3.389125276
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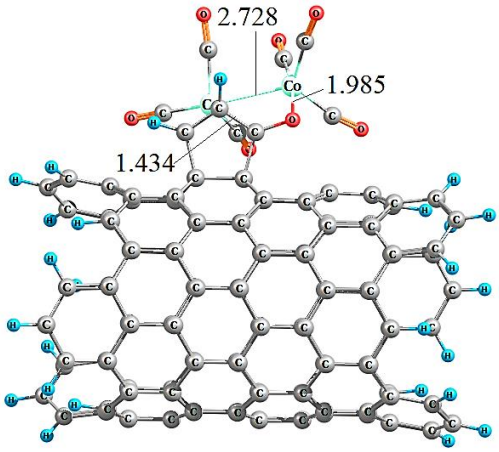

Note: Discarded in the main manuscript.

C	-0.769862823	1.745240717	-2.713004277
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C	-2.633680649	1.770774262	-0.955671814
C	-2.375024561	4.562656445	-0.878689700
C	-2.645769406	6.583463750	0.413265564
C	-2.154007786	5.948008449	1.542836409
C	-1.847640093	4.575913060	1.506971258
C	0.066498627	4.594602812	3.066031145
C	2.647187012	6.062155276	3.513661247
C	2.517400949	4.685273946	3.323248561
C	3.746759966	6.740457649	2.987630112
C	4.634424022	6.090774478	2.132021436
C	4.524780362	4.713264621	1.927841709
C	4.981211104	4.676456361	-0.476471468
C	3.891392701	6.045074704	-2.906185020
C	3.841581492	4.674104485	-2.648773128
C	2.813135790	6.678842458	-3.522429673
C	1.621046037	5.992293550	-3.746711577
C	1.544862532	4.619785939	-3.497465265
C	-0.807967989	4.546857052	-2.761518303
C	-2.662965541	5.915414090	-0.824627090
H	-1.824199462	-5.730941422	0.420817964
H	-1.764514437	-6.573386130	2.557536087
H	0.084873977	-7.686667470	3.780700460
H	2.209644792	-6.472206976	4.182703940
H	3.702655595	-5.581902853	2.683523789
H	5.610306272	-6.440849533	1.673515527
H	5.755134597	-7.611986755	-0.510551679
H	4.990323544	-6.466083112	-2.574080248
H	2.903168712	-5.618038124	-3.064170061
H	1.120289619	-6.537303320	-4.132907744
H	-0.842846615	-7.763381612	-3.247923698
H	-2.389587463	-6.640962244	-1.661646528
H	-2.924177479	7.635615171	0.461674523
H	-2.000143828	6.510780089	2.463107355
H	0.078665992	5.677258770	2.965644399
H	1.875405188	6.609773629	4.053339985
H	3.864081321	7.806786708	3.178144839
H	5.398311064	6.657789923	1.600748964
H	4.826344358	5.752768706	-0.460866749
H	4.766218689	6.621188224	-2.606277299
H	2.876845230	7.739976809	-3.761177768
H	0.742217806	6.528088140	-4.103216554
H	-0.756310278	5.626647659	-2.643494394
H	-2.836690630	6.475853296	-1.743919458
Co	-5.339862318	1.244096787	0.167125643
Co	-5.897261124	-1.412897210	-0.101220847
C	-7.078021816	1.330996035	-0.260025599
C	-4.697387544	0.382898065	1.587964767
C	-5.095857546	-2.713973382	0.833753525
C	-7.078193501	-1.133901794	1.139035840
C	-7.097026602	-1.818393759	-1.365324919
O	-4.387382954	0.008218160	2.642834170
O	-8.200217624	1.480064330	-0.504859609
O	-4.768093204	-3.650053109	1.425206928
O	-7.872848091	-0.985570043	1.965708374
O	-7.866686588	-2.187298018	-2.143177990
C	-4.093032489	2.106763398	-1.296309839
C	-4.758658729	0.988780751	-1.806544698
H	-5.588829114	0.959130086	-2.507901775
H	-4.340932558	3.126631017	-1.585967200
C	-4.071500392	-0.180665633	-1.341692432
O	-4.450607304	-1.396237317	-1.460272627
C	-5.240378371	2.806562152	0.953572669
O	-5.179674859	3.837125607	1.472913570

PD*oblique*

152
Co2C117H26O7

C	-3.276867751	-3.642879156	1.213536426
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C	2.926772551	-7.799267129	-0.878443829
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C	-3.201790146	-3.801048540	-1.235708633
C	-3.765852687	-5.067460292	-1.383103169
C	-3.278033339	-2.992086666	-0.020308696
C	-2.216087723	0.467322282	1.062398483
C	-2.546260974	-0.937336296	1.113040994
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C	-2.592758520	-3.076852632	2.304966755
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C	2.194017506	-3.034435617	3.214941915
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C	0.660439155	4.114765118	2.751809734
C	0.257618666	2.750467285	2.747418596
C	1.150649537	1.754160184	3.218606046
C	0.724071199	0.402684913	3.279122354
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C	2.531989514	2.073838854	3.317418766
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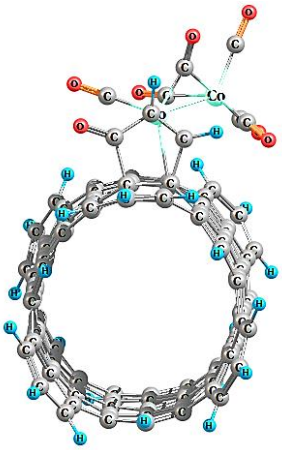

Note: Taken into consideration in the main manuscript.

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C	5.997524473	3.136189980	1.260795062
C	6.029325323	2.997174874	-1.181572435
C	5.054243569	4.694432507	-3.443748918
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C	-0.663540375	6.618011123	-0.319421911
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H	-3.779417476	-6.895188632	-2.522350648
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H	-3.874642398	3.317877364	-1.427968107
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O	-2.967356824	4.128641702	2.918878071
C	-6.048014491	2.035423082	0.093059502
O	-6.972560303	2.753340811	0.022229948

PD'*oblique*

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C	8.983599137	-1.617355296	-0.459911336
C	7.128068263	-0.645757028	-1.667733018
C	8.261188715	-1.461225554	-1.642634565
C	5.751692251	-2.013844285	-3.174475198
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C	3.516547283	-6.137824351	-1.865710674
C	1.821980086	-4.816441963	-0.527266638
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C	1.744219324	0.357718384	3.428824873
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C	4.114856036	-0.304260753	3.357985394
C	5.106041285	-1.313268152	3.436193115
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C	4.405282327	0.926552880	2.710556374
C	5.520819558	0.963105486	1.830057415
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C	5.827652382	1.138358132	-0.567466476
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C	4.135891818	2.377986307	-1.822887960
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C	-1.188054486	-1.827851224	-0.702024442
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C	-1.862396708	0.732497446	2.475628864
C	-0.604195056	1.018668525	3.074527412
C	0.391721641	0.009509337	3.142682864
C	-1.246891644	3.374611032	3.249353247
C	-0.251613393	2.377539118	3.295944015
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C	2.125421870	1.718499347	3.202306030
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C	1.408893643	3.935705072	2.462754957
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C	2.932726179	4.250377856	-0.757186969
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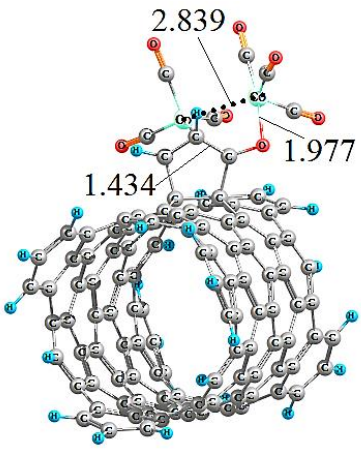

Note: Discarded in the main manuscript.

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H	6.576431220	-3.500263250	4.381863386
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H	8.984053417	-1.350879947	1.680898218
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H	8.564607406	-1.995121475	-2.542544535
H	6.470715068	-2.814270242	-3.017470091
H	5.789394857	-4.768324049	-3.996584389
H	5.218280701	-6.929228078	-2.921944052
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H	-3.413635073	4.529193890	-4.370949067
H	-3.832999442	2.956309831	-2.747837184
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C	-6.982474667	-0.504875085	2.464384955
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O	-7.407990323	0.415575469	3.011239272
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H	-3.177300878	-2.925870368	-1.913844565
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C	-5.354908731	-1.236212510	-2.589561925
O	-5.298294636	-0.827300470	-3.671191212

PD*_oblique_

152
Co2C117H26O7

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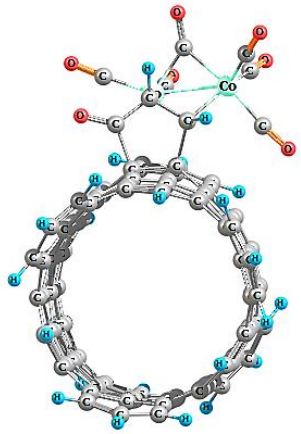

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H	-6.676916938	-2.576222431	2.790222860
H	-6.122841453	-4.538549931	3.809734676
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H	6.868804250	2.974243914	0.219897147
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PK*parallel*

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C	-4.713638283	-0.600695602	-3.501384755
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C	-3.812392249	2.754847599	-2.275902380
C	-0.237214129	3.244745136	-1.220392293
C	-1.653919362	3.313910586	-1.234806240
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C	-0.243194667	3.293337533	1.182032810
C	-1.641654077	3.340881338	1.173215379
C	-2.386746614	2.630485897	2.143365427
C	-3.810814141	2.722361152	2.161544548
C	-0.323238458	1.572315280	2.890350487
C	-1.729971181	1.657451998	2.926153809
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C	-3.929633672	0.645562213	3.432992983
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C	-1.890607529	-0.719870782	3.402885374
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C	1.873855644	2.418662905	2.121854230
C	0.432129473	2.488803494	2.105873086
C	3.922311840	1.338048425	2.951187065
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C	1.722555577	0.284909230	3.301353152
C	0.316877765	0.369990327	3.321380040
C	3.771170147	-1.070360132	3.316439209
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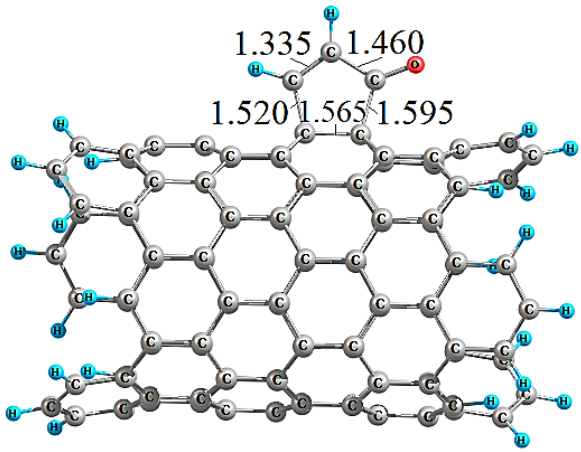

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C	4.303150412	-4.032828130	-1.209252020
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H	-6.791181195	-2.501296760	3.270111045
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H	-5.898662135	-2.526947110	-2.144382106
H	-6.687031927	-1.344246215	-3.951808427
H	-7.713905457	0.912255291	-4.036756707
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H	6.748674804	3.731923572	0.731901302
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H	6.534101507	0.858967130	3.832594132
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H	5.614751197	-0.050926284	-3.224420095
H	6.639025521	1.957355375	-3.176607228
C	2.490639670	5.321257981	-0.100883896
O	3.644447935	5.695588957	-0.074581236
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C	1.287424599	6.146626260	-0.160602766
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PK*oblique*

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C	-4.534147137	1.455688862	-3.326494065
C	-4.550251590	3.453275790	-1.898787527
C	-5.921040021	3.716092922	-1.942026737
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C	-4.555391611	3.929637174	0.498132907
C	-5.926641626	4.187217417	0.431718865
C	-4.546854497	2.622518860	2.575384802
C	-4.609337725	0.343909469	3.502921180
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C	-6.665964467	-0.926245858	3.565830722
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C	-3.959866912	-2.842540452	1.787946966
C	-0.398016229	-3.692091617	0.763178148
C	-1.857807409	-3.385260483	0.668821460
C	-2.536722324	-3.394856362	-0.563155780
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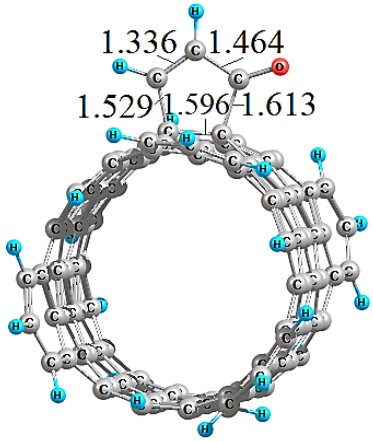

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PK*_oblique_

138
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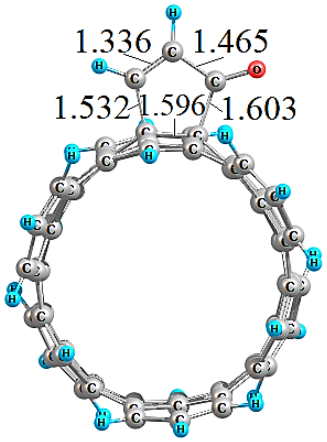

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RC*me*

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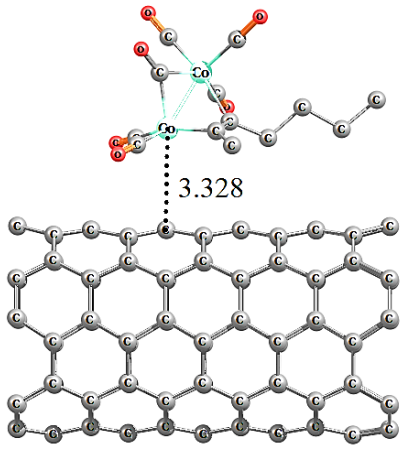

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RC*bu*

163
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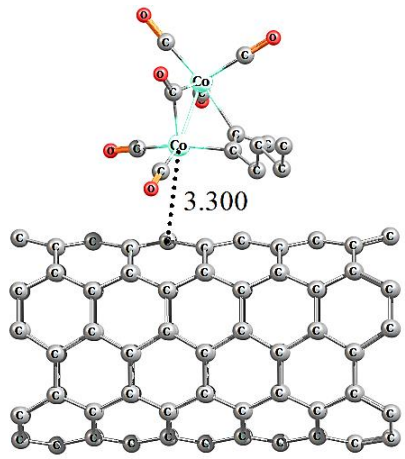

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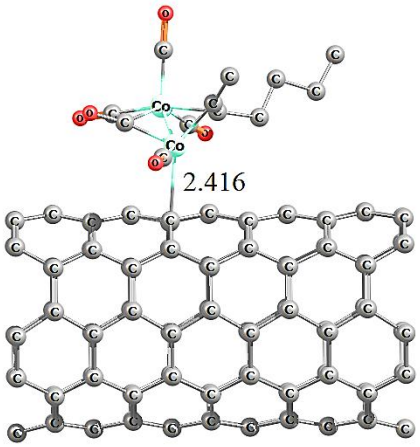

161
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C	4.512826335	5.259815755	-2.585471796
C	3.246569841	5.375614001	-1.932142815
C	4.837119105	4.117057952	-3.262137070
C	3.912886558	3.028248925	-3.325845112
C	4.334316136	1.665914859	-3.182184277
C	3.361073468	0.700363698	-2.821204520
C	3.984847431	-0.862740372	0.822975924
C	3.706366643	-0.315958822	-1.875843889
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C	2.217540373	1.012091137	3.388080905
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C	1.398618463	3.655303541	3.116172946
C	1.963718607	5.640090780	0.131521984
C	0.784908984	5.189788680	-0.529837421
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C	1.345205227	-1.018581266	-1.779457959
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C	-1.298828562	3.952600363	2.282991757
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C	-0.787625574	1.594546457	-3.134335200
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C	-1.336988484	-0.739632109	-2.643242312

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C	-2.052261441	-2.428238627	-1.028777078
C	-0.844598453	-1.724834404	2.306200878
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C	-1.915278329	-2.710572297	0.346841245
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C	-2.595533128	3.924039132	1.705409740
C	-1.918362679	1.952255700	3.550999458
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C	-3.913134188	3.746104260	-0.345873058
C	-3.642832282	3.213237758	2.366577492
C	-2.492716162	3.086192347	-2.220648490
C	-3.791241877	3.183273498	-1.633758624
C	-2.158378285	1.905165496	-2.928924341
C	-3.136188163	0.867662198	-3.023619002
C	-2.719831900	-0.472953619	-2.880976490
C	-3.696282103	-1.459602285	-2.560193801
C	-3.085596519	-3.007269498	1.098998564
C	-3.349676859	-2.471349975	-1.608451759
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C	-3.855835711	-0.122638850	3.785235551
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C	-4.514664571	1.174758005	-2.836486493
C	-5.999673600	2.526854850	2.482125212
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H	-8.176596765	2.304175489	2.462815900
C	-6.273046938	3.064862518	-0.259011513
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H	-8.412954168	2.769384430	0.089264077
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C	-4.248869674	-3.472150546	0.433782912
C	-5.376443686	-3.787563654	1.256228831
H	-6.212736495	-4.348214151	0.842526645
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H	-6.419895693	-3.379239722	3.058394913
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H	-8.222852295	1.887162735	-1.910636541
C	-5.487943536	0.152227171	-2.970190018
C	-6.856225354	0.539398758	-2.816976828
H	-7.650983706	-0.137633229	-3.124730669
C	-0.308686516	-5.222207011	-0.867996342
H	-0.524072305	-4.282728269	-1.390244843
H	-1.031119770	-5.291012797	-0.034509470
C	-0.571976558	-6.360341245	-1.848602642
H	0.182816823	-6.345801953	-2.651835594
H	-0.472893899	-7.334092705	-1.337942724
C	-1.967587745	-6.205937965	-2.450352272
H	-2.712897025	-6.175847097	-1.635581181
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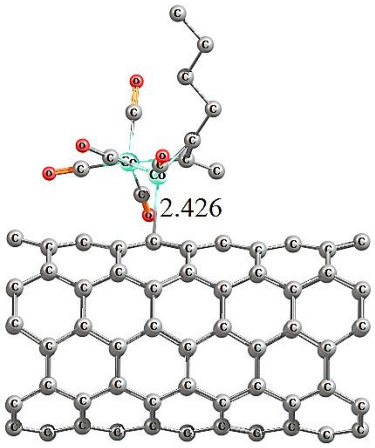
H	2.018542610	-7.527197332	1.550685944
H	1.395580743	-6.499528741	2.877318971
H	0.277085714	-7.222174517	1.666034316
C	-2.319278475	-7.311859888	-3.438237295
H	-1.601566265	-7.331812195	-4.272752221
H	-2.295669520	-8.298970527	-2.950798118
H	-3.324130681	-7.164324463	-3.859951408

CP3*bu*



161
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C	-6.370767443	-3.066722365	1.859575934
C	-4.026811537	-1.586047067	3.069762755
C	-5.972568785	-0.366794830	2.017467109
O	-3.967370631	-2.374356078	-3.417992535
O	-6.286009466	-0.651044075	-0.830303784
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O	-3.393072450	-1.415120376	4.023931001
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H	-0.231619355	8.474752082	-0.719779574
H	-1.158116047	7.737583515	-2.842022549
H	-0.446931428	8.294917344	1.459365627
H	-1.746407798	7.244526172	3.223176581
H	-3.424144843	5.894809317	3.619783784
C	-3.177412195	4.878224421	3.319194485
C	-5.275727821	3.190152281	0.179931882
C	-4.144880877	4.098306153	2.748506605
C	-3.807133211	2.831087103	2.179250704
C	-5.145302782	3.301701908	-1.175630749
C	-4.088262251	2.618625343	-1.856450338
C	-4.351308217	2.395444915	0.926955564
C	-3.562196317	4.590093160	-3.305995761
C	-3.318680699	3.243649407	-2.891155993
C	-0.428106317	7.110126695	-2.334004582
C	-2.517342897	5.433644911	-3.561963819
C	-1.169969964	4.978469268	-3.418214338
C	0.093201391	7.524981467	-1.140734209
C	0.915911798	6.645146529	-0.369766512
C	-0.154994640	5.793155919	-2.820446728
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C	0.777974986	6.529288775	1.050767245
C	-0.921837103	6.695615951	2.772177791
C	-0.723154061	5.315612916	3.090147616
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C	-1.600092304	3.037326707	3.236503063
C	-3.664670286	1.382841356	0.217927892
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C	-2.233115595	0.944337899	2.134445556
C	-3.534178034	1.491677426	-1.203063288
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C	-0.957760007	3.577837656	-3.476322680
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C	-0.699650928	-0.984055915	2.152206941
C	-2.003092475	-0.448096287	-1.211586740
C	-0.970325004	-1.195954329	-1.855593511
C	-1.237034679	-1.421576884	0.909698247
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C	2.829483326	3.439949431	1.679528818
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C	1.483680287	-0.799401218	3.234563584

C	-0.572546625	-2.452734990	0.202716242
C	0.481133223	-1.607805495	2.637159796
C	0.849179037	-2.893072196	2.139264244
C	-0.434220792	-2.335423929	-1.208903804
C	0.586536690	-3.092545554	-1.855215963
C	0.315600943	-3.320451897	0.902661938
C	1.047837575	-1.129477124	-3.233921963
C	1.337884522	-2.481026341	-2.882772096
C	4.097475145	1.330131593	-2.330702751
C	2.129973821	-0.252979974	-3.504204268
C	3.459625274	-0.765147548	-3.411286912
C	4.634932653	1.758374221	-1.089826507
C	5.507586503	0.875038703	-0.385604114
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C	5.371638921	0.759917524	1.013885842
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C	5.643326553	-0.593014853	-2.341995181
C	3.686292230	-2.168275861	-3.510442832
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C	6.022512948	-1.857400582	-2.856771777
C	7.249390188	-2.409447703	-2.373523789
H	7.704966510	-3.254875835	-2.885764190
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H	8.622586355	-2.522949533	-0.758727962
C	2.865192128	-4.406523322	-2.925632301
C	4.124942622	-4.928055970	-3.353000847
H	4.302208885	-6.001820070	-3.340496378
C	5.010129049	-2.672363569	-3.460386828
C	5.168941245	-4.083884399	-3.613271053
H	6.155605637	-4.502841799	-3.802088724
C	1.829053595	-5.257421437	0.905417278
C	2.428914268	-6.312172077	0.149921484
H	2.908525051	-7.144074671	0.662369219
C	2.102317702	-5.026781236	-1.881246480
C	2.562276356	-6.199466023	-1.206348811
H	3.144298009	-6.944559932	-1.745609641
C	4.357036150	-3.224955176	3.341006573
C	4.505843914	-4.645376075	3.299490348
H	5.447402236	-5.102773184	3.597550276
C	2.371574668	-4.823515480	2.160538610
C	3.539517913	-5.423491064	2.724349983
H	3.732258177	-6.484352874	2.575825574
C	6.944831237	-1.128534995	1.022112885
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H	-6.573377750	-4.895553724	-0.601428755
H	-5.983726783	-4.024639818	-2.024177069
C	-6.251391499	-6.145090897	-2.345816214
H	-5.529716579	-6.207217699	-3.178652751
H	-6.152804210	-7.082241764	-1.771419502
C	-7.667791659	-6.019091376	-2.898308014
H	-8.404487340	-5.971347389	-2.081763826
H	-7.771340476	-5.101258948	-3.497301495
H	-7.925063233	-6.874284337	-3.539799925
C	-2.936357506	-4.074953212	2.088035918
H	-2.349732492	-4.878113921	1.615870251
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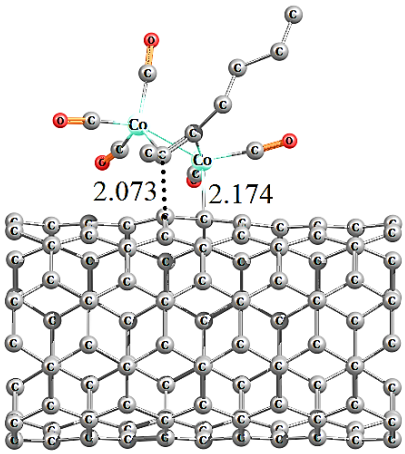

161
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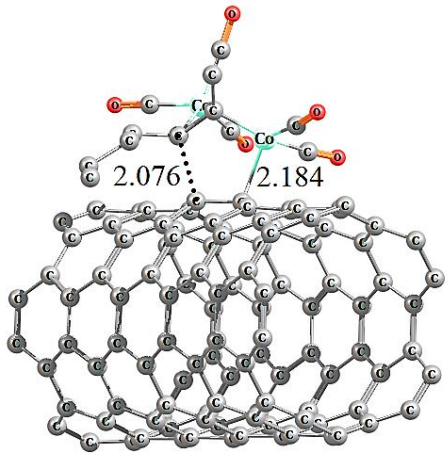
C	-2.692836083	-3.248196454	2.598188210
C	-1.470308852	-4.805363506	0.811959635
C	-4.995411940	-2.181472757	1.383755695
O	-6.785641706	-1.371532835	-1.621649444
O	-6.319810325	-5.521968255	0.394147549
O	-2.727295611	-3.179284002	3.751827903
O	-0.794462167	-5.750044648	0.828058912
O	-5.275880365	-1.616340460	2.359290319
C	-3.497939529	-2.537035363	-1.485344425
C	-3.196670878	-3.790659372	-0.996578673
H	5.919177360	-4.123471081	-3.609683666
H	4.254977693	-6.292031939	-0.175246213
H	4.797002447	-5.580808421	-2.433313191
H	4.576003979	-5.858477825	1.964346503
H	5.737576863	-4.360614180	3.485329621
H	8.372945378	-1.037138666	2.305998831
H	7.091289984	-2.650640712	3.591077405
H	8.881388725	-0.397655711	0.265966210
H	8.489687827	-0.889138001	-2.081221332
H	7.422357866	-2.222175881	-3.462553473
C	6.348759317	-2.056180296	-3.393884825
C	3.979538705	-5.093132831	-1.905503420
C	5.502593837	-3.126890100	-3.476949325
C	4.107239368	-2.965879322	-3.212662139
C	3.674446693	-5.494064481	-0.634604600
C	2.730767316	-4.754600886	0.145668602
C	3.359472552	-3.930833538	-2.464287611
C	4.123318532	-4.901412152	2.217467833
C	2.948126075	-4.463593669	1.530083872
C	6.599810086	-1.748507821	3.231800623
C	4.777461932	-4.058712709	3.071236316
C	4.296574472	-2.727224536	3.277754270
C	7.322166297	-0.839717140	2.509811064
C	6.666522815	0.262061746	1.877744054
C	5.183441032	-1.605326827	3.362968111
C	8.000804660	0.014444633	-0.223498485
C	6.999703031	0.681824658	0.549646941
C	7.780819340	-0.261918328	-1.543852768
C	6.545380898	0.112003839	-2.159313394
C	5.847461954	-0.762306886	-3.052891860
C	4.464503014	-0.535918286	-3.265937623
C	2.127775091	-3.525613636	-1.892802830
C	3.577671908	-1.655590750	-3.339182254
C	2.186252938	-1.431273512	-3.133779168
C	1.805081771	-3.953092498	-0.568015682
C	0.804499701	-3.234394403	0.139334356
C	1.442447999	-2.384665907	-2.403128613
C	2.238602676	-3.375196637	2.100872040
C	1.030685821	-2.926566100	1.497227447
C	4.649671792	-0.309592564	3.153385585
C	2.931756359	-2.484988918	2.982321129
C	2.377998358	-1.192372992	3.208296142
C	5.405806631	0.643770661	2.402711545
C	4.723058510	1.767507518	1.854327929
C	3.250621362	-0.088117558	3.306304826
C	6.049924613	1.453966932	-0.164278740
C	5.052192126	2.182398336	0.546322312
C	5.817654579	1.162923587	-1.544581652
C	4.604037455	1.619495215	-2.132851931
C	3.913642104	0.750617079	-3.004775208
C	2.529891469	0.990037669	-3.253849209
C	0.180627824	-2.006288527	-1.843222255
C	1.652440056	-0.118859257	-3.308672886
C	0.264122969	0.098779507	-3.113964549
C	-0.182666000	-2.495952515	-0.576255877
C	-1.294960808	-1.930873863	0.164767584
C	-0.488630365	-0.849879487	-2.363731200
C	0.309052963	-1.828907538	2.061018551
C	-0.911541524	-1.411560237	1.475151578
C	2.720116573	1.226623632	3.143399617
C	0.996624114	-0.953378270	2.937945664
C	0.447900728	0.325223920	3.199491433
C	3.472652265	2.176951878	2.408574303
C	2.805527740	3.308457540	1.869195642
C	1.326884431	1.440926423	3.312802398
C	4.119978567	2.992477641	-0.169966072
C	3.138199582	3.729888322	0.547705471
C	3.891882629	2.706506769	-1.539018612
C	2.690003566	3.165541280	-2.140871592
C	1.992201002	2.285976123	-3.019196993
C	0.613200015	2.514457950	-3.254010848

C	-1.724333247	-0.462743835	-1.823211787
C	-0.263875968	1.400205395	-3.301373301
C	-1.654138418	1.615679083	-3.099023192
C	-2.257307934	-1.113139283	-0.630797472
C	-3.128788576	-0.218671125	0.130492486
C	-2.392341972	0.670759421	-2.357339903
C	-1.603041615	-0.310994731	2.032442934
C	-2.838363227	0.131310498	1.449197519
C	0.795662370	2.744777747	3.135930234
C	-0.922183562	0.561837665	2.908479344
C	-1.477773116	1.851698406	3.171379523
C	1.548345510	3.696622024	2.406852467
C	0.865244730	4.821984555	1.854566886
C	-0.609617079	2.954243273	3.284741417
C	2.200100512	4.520211874	-0.167813871
C	1.197927115	5.241876349	0.549919128
C	1.970674556	4.232499287	-1.538098088
C	0.748231092	4.675021841	-2.127550187
C	0.058124623	3.802413578	-2.995572628
C	-1.326321505	4.037906315	-3.240635383
C	-3.692512808	1.037669162	-1.882310601
C	-2.207412666	2.915138489	-3.303270684
C	-4.063362972	0.587310030	-0.571630217
C	-3.562872825	1.199633800	2.061083755
C	-1.149171971	4.263900994	3.134947191
C	-2.862151560	2.086592140	2.935443561
C	-0.388825605	5.226045819	2.399829746
C	0.262065400	6.049933729	-0.159232681
C	0.027024346	5.755120856	-1.538466803
C	-2.535858100	4.479240305	3.330614698
C	-3.001517025	5.824227189	3.206128217
H	-3.998689376	6.088863172	3.552712875
C	-1.044230900	6.370175472	1.881973220
C	-2.275325761	6.745513405	2.502978283
H	-2.710090145	7.722884538	2.301980424
C	-4.802441995	1.610471292	1.516131043
C	-5.499143411	2.655110274	2.198060672
H	-6.538573391	2.864640004	1.951753121
C	-3.420827011	3.354661537	3.236352108
C	-4.826279639	3.505682432	3.031765484
H	-5.343857435	4.374592876	3.433744811
C	-4.373123586	2.130431936	-2.453721913
C	-5.665962717	2.437820566	-1.917160661
H	-6.336907335	3.103473244	-2.456995345
C	-5.052242320	1.306601526	0.137348798
C	-5.992234593	2.044145230	-0.650051817
H	-6.913872604	2.408355087	-0.199181005
C	-1.868398008	5.330037409	-3.025982412
C	-3.248101032	5.508450678	-3.332708898
H	-3.671354429	6.510577631	-3.367333901
C	-3.603152758	3.111623958	-3.178178868
C	-4.091223155	4.429686055	-3.410072056
H	-5.160825819	4.604478681	-3.507310458
C	-0.705147955	6.798279646	0.556327033
C	-1.580671741	7.622865571	-0.215114690
H	-2.181192046	8.387286370	0.274620509
C	-1.163612690	6.221617326	-2.147835888
C	-1.804504135	7.341225625	-1.534581952
H	-2.578645021	7.887397338	-2.070420304
C	-2.955488670	-5.015872577	-1.830598789
H	-1.863300193	-5.043584175	-2.015940768
H	-3.424275630	-4.897593046	-2.823037364
C	-3.395515953	-6.332523796	-1.198446742
H	-3.275396990	-6.276910417	-0.103879480
H	-4.472184683	-6.485090081	-1.376704075
C	-2.607778625	-7.527948451	-1.723412714
H	-2.703775321	-7.577249229	-2.822389997
H	-1.537494595	-7.365603386	-1.507910475
C	-3.065093918	-8.842249489	-1.100354215
H	-4.128398591	-9.030574861	-1.315255189
H	-2.484355179	-9.694015591	-1.483371594
H	-2.944976931	-8.813802459	-0.006218242
C	-3.732462520	-2.135125240	-2.906501523
H	-2.796806765	-2.105335344	-3.486578233
H	-4.388353026	-2.903397315	-3.348327537
H	-4.250289105	-1.172918080	-3.008403468

TS1*butyl,oblique*



161
Co2C122H32O5

Co	4.321788584	-3.869409193	-0.137672821
Co	1.967935476	-4.063959475	-0.957908089
C	4.848504628	-5.549074103	-0.441682275
C	5.696401396	-3.076502780	0.622584608
C	1.913661976	-3.839020099	-2.736525649
C	0.648623541	-5.174335417	-0.782682067
C	4.450621159	-3.098163416	-1.733687699
O	6.569028374	-2.530337011	1.155805619
O	5.170504712	-6.650488022	-0.593482726
O	1.862025183	-3.803054049	-3.891040004
O	-0.131935459	-6.027295595	-0.676829943
O	4.729885314	-2.620819373	-2.755628855
C	3.130972184	-3.249712709	1.300179395
C	2.645498877	-4.442640037	0.801112670
H	-6.460124308	-3.175619438	3.684547701
H	-5.252844784	-5.615349055	0.250493332
H	-5.622122005	-4.809110536	2.511517880
H	-5.534861812	-5.149430053	-1.885482254
H	-6.452546446	-3.487084864	-3.402650542
H	-8.465999641	0.244104215	-2.221810933
H	-7.498452475	-1.573819075	-3.509570437
H	-8.819936854	0.971326038	-0.176950355
H	-8.473023066	0.434868779	2.167257821
H	-7.622588367	-1.049328815	3.538759407
C	-6.537510416	-1.067357356	3.454236289
C	-4.743569346	-4.471436732	1.965020337
C	-5.883016430	-2.264948520	3.536549907
C	-4.484736006	-2.344378300	3.251105645
C	-4.535811213	-4.926071373	0.692660812
C	-3.494892543	-4.363273374	-0.110580441
C	-3.924171530	-3.428145300	2.501461526
C	-4.930894753	-4.285140191	-2.155948699
C	-3.685512543	-4.049096626	-1.493639627
C	-6.854928587	-0.765983798	-3.166324580
C	-5.447861298	-3.349906995	-3.007377360
C	-4.751588173	-2.121417828	-3.235529543
C	-7.400376875	0.257855916	-2.443073636
C	-6.556193954	1.236727958	-1.832472247
C	-5.437007139	-0.866537180	-3.320178929
C	-7.873443376	1.231708500	0.293395823
C	-6.788750852	1.715606804	-0.502981350
C	-7.678541517	0.930205749	1.612223454
C	-6.386500453	1.093850829	2.202827829
C	-5.830464295	0.120579808	3.093603283
C	-4.425349283	0.111294102	3.283029925
C	-2.652521629	-3.241502698	1.904731832
C	-3.738944700	-1.141658598	3.356317391
C	-2.333216894	-1.157422319	3.125816935
C	-2.431660757	-3.728056342	0.579111013
C	-1.335143045	-3.199349973	-0.153124294
C	-1.775344128	-2.227401152	2.389743286
C	-2.811569415	-3.101252078	-2.086833616
C	-1.532856365	-2.862536108	-1.508880559
C	-4.687970624	0.321435519	-3.133683267
C	-3.360176155	-2.111968608	-2.964251463
C	-2.599535293	-0.934009971	-3.212030556
C	-5.258773802	1.395449901	-2.382088508
C	-4.386202875	2.391418501	-1.856792632
C	-3.274495372	0.301081897	-3.310230692
C	-5.708735204	2.320034599	0.187292876
C	-4.615975371	2.864801695	-0.547340431
C	-5.502834503	2.002417189	1.565907931
C	-4.218789094	2.250573596	2.129216352
C	-3.669493599	1.283862032	2.999241439
C	-2.261044424	1.287429492	3.223806665
C	-0.481787000	-2.068815835	1.800527261
C	-1.582404624	0.046161200	3.276961048
C	-0.181022778	0.024768497	3.051856204
C	-0.223526488	-2.633099962	0.538585427
C	0.956582646	-2.271966602	-0.224796522
C	0.384118785	-1.038516592	2.294828405
C	-0.647454518	-1.903629295	-2.091564253
C	0.639533500	-1.697828386	-1.531479557
C	-2.526960303	1.508414056	-3.171200000
C	-1.193211383	-0.930207549	-2.964443810
C	-0.441197617	0.234893263	-3.249811444
C	-3.095086209	2.579052427	-2.436059881
C	-2.236718366	3.585308213	-1.919743491
C	-1.120777360	1.482043964	-3.364543213
C	-3.546840388	3.509291824	0.145056299
C	-2.468471782	4.065639545	-0.596793648
C	-3.344445727	3.197244783	1.512619454
C	-2.071113082	3.449970237	2.089008557
C	-1.516135865	2.471794010	2.965066094
C	-0.114446260	2.465706386	3.175075658

C	1.666943644	-0.887137317	1.744211097
C	0.563298456	1.218648768	3.219593126
C	1.964309939	1.193682136	2.990621960
C	2.065362800	-1.634175065	0.549724703
C	3.051009769	-0.886091951	-0.237094930
C	2.520637591	0.127418208	2.252170371
C	1.494176520	-0.729950149	-2.109793372
C	2.795615269	-0.495319692	-1.550611599
C	-0.374480131	2.679244929	-3.212903985
C	0.953901049	0.238799462	-2.983515788
C	1.713731147	1.414170423	-3.271946555
C	-0.942287837	3.751094363	-2.482685390
C	-0.068890399	4.748580639	-1.953594351
C	1.042736263	2.646331086	-3.386781554
C	-1.397060692	4.690308830	0.094604810
C	-0.301201076	5.227324571	-0.647438925
C	-1.193548185	4.376212252	1.463375361
C	0.096569348	4.609507358	2.027065029
C	0.645045410	3.638584787	2.892213945
C	2.053285579	3.637942949	3.111671166
C	3.856707902	0.270671449	1.753863200
C	2.732552881	2.382572912	3.174109262
C	4.119626834	-0.239599009	0.439714841
C	3.677900542	0.432020524	-2.187151440
C	1.798141367	3.847648962	-3.261815438
C	3.121713540	1.414849455	-3.061520531
C	1.225102960	4.930391647	-2.524298052
C	0.771251559	5.869552941	0.037460246
C	0.979018776	5.547815794	1.415010945
C	3.197034757	3.824113561	-3.483408370
C	3.885078520	5.072187081	-3.382073595
H	4.905828320	5.162048894	-3.748875302
C	2.073858984	5.950994039	-2.029629936
C	3.338374116	6.108374078	-2.676172430
H	3.935615907	6.999775973	-2.493333779
C	4.979320553	0.631581406	-1.670753979
C	5.829559948	1.536239253	-2.377424534
H	6.893819998	1.569467780	-2.151012075
C	3.880945658	2.566888029	-3.389683184
C	5.294838476	2.480266715	-3.210894543
H	5.944023809	3.245554299	-3.632111212
C	4.720912307	1.236668904	2.304067263
C	6.035781833	1.322047633	1.740546155
H	6.818915351	1.869343971	2.261931403
C	5.200046286	0.301122341	-0.292803949
C	6.265368527	0.874952920	0.469975586
H	7.225367493	1.078078322	-0.001657726
C	2.801985888	4.818377820	2.875489295
C	4.196230465	4.763506688	3.160690456
H	4.783534678	5.679716248	3.177155174
C	4.139265269	2.339622556	3.030116819
C	4.846051218	3.558089413	3.240504971
H	5.931194834	3.550632517	3.321137770
C	1.837269497	6.438857345	-0.702077576
C	2.854043896	7.107744841	0.046176591
H	3.566302371	7.755945640	-0.461133984
C	2.242498430	5.810051767	1.999455561
C	3.051843327	6.800649839	1.364356667
H	3.917573581	7.210910217	1.881017266
C	3.503291921	-2.943165850	2.724115048
H	3.912109870	-1.927304907	2.822044838
H	4.355979516	-3.605233188	2.957063986
C	2.358315120	-3.179156562	3.730502339
H	1.393827907	-3.154623875	3.202020981
H	2.436301170	-4.201264676	4.138717268
C	2.323981777	-2.179881850	4.883470028
H	3.228613831	-2.302627301	5.504632626
H	2.367507621	-1.152607696	4.485624675
C	1.069893508	-2.334857037	5.737817757
H	0.164147915	-2.173349877	5.130503086
H	1.004534445	-3.345990027	6.169598096
H	1.053459459	-1.608139876	6.562839670
C	2.424010992	-5.694597626	1.600353558
H	1.421516292	-5.665802633	2.058297850
H	2.482656229	-6.589562630	0.965961084
H	3.164698313	-5.790209798	2.409248494

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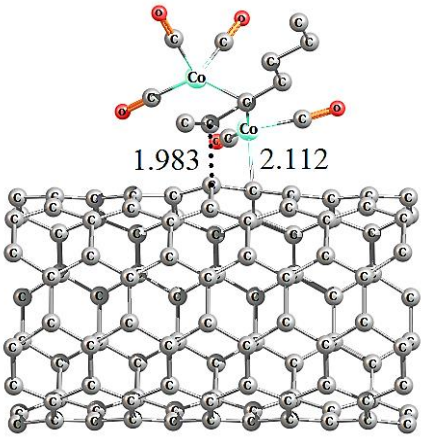

161
Co2C122H32O5

Co	3.855935903	-4.398848090	0.255060590
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C	4.239164144	-5.636663307	-0.933455381
C	3.129626281	-2.573424915	2.894039983
C	5.135946588	-1.162589622	1.594218870
C	2.409672791	-5.070884721	1.074076972
O	4.509260524	-6.451871123	-1.712497081
O	6.152559639	-4.733495731	2.051353890
O	2.796543685	-2.860118230	3.961706066
O	6.122706400	-0.595154745	1.817512180
O	1.473970457	-5.489581133	1.609350463
C	3.052333827	-2.992209921	-0.950036878
C	4.330433901	-2.645274803	-0.543382278
H	-5.164887054	-5.068490905	3.377814937
H	-3.161596433	-6.878434658	-0.071968713
H	-3.803677528	-6.315132373	2.205057429
H	-3.570218434	-6.420477195	-2.207396688
H	-4.964273185	-5.075062429	-3.675858391
H	-8.100960512	-2.235948106	-2.433058439
H	-6.573676929	-3.601933561	-3.737611916
H	-8.709331597	-1.728546202	-0.379491637
H	-8.225339717	-2.229151238	1.950140124
H	-6.950261655	-3.424744338	3.279332694
C	-5.916093345	-3.091723166	3.214457979
C	-3.082942293	-5.688024853	1.683788086
C	-4.912311585	-4.015568344	3.268673724
C	-3.556316241	-3.629466630	3.018972718
C	-2.721634635	-6.005213064	0.406536926
C	-1.909486596	-5.101836732	-0.354871835
C	-2.662961423	-4.445586558	2.262936741
C	-3.280728373	-5.393724489	-2.424519262
C	-2.185017703	-4.797092320	-1.720451346
C	-6.233372543	-2.640758288	-3.357129243
C	-4.065407212	-4.637316776	-3.245727474
C	-3.802859294	-3.237661192	-3.410079838
C	-7.093359745	-1.871830179	-2.625053393
C	-6.623436086	-0.691062418	-1.968072254
C	-4.856161759	-2.271415774	-3.473704228
C	-7.898321057	-1.202971922	0.121346663
C	-7.016167980	-0.364120039	-0.632172386
C	-7.626044083	-1.484453621	1.429634545
C	-6.458048871	-0.940984465	2.053775727
C	-5.624491654	-1.723726989	2.911122827
C	-4.293220544	-1.287713274	3.132568836
C	-1.502267183	-3.842892601	1.710159826
C	-3.239988809	-2.254706555	3.179141295
C	-1.903360879	-1.808241852	2.981223521
C	-1.108854211	-4.192721631	0.383541657
C	-0.221589492	-3.321617569	-0.303988182
C	-1.016747633	-2.612904658	2.234570466
C	-1.659324828	-3.586640195	-2.253891718
C	-0.537780111	-2.978625850	-1.637513665
C	-4.537961985	-0.909667248	-3.240426324
C	-2.495410175	-2.789719102	-3.104273540
C	-2.157287618	-1.420253528	-3.290592319
C	-5.439400434	-0.101756922	-2.479269294
C	-4.943960898	1.103040258	-1.902260522
C	-3.192517218	-0.466524101	-3.377867643
C	-6.197857743	0.528795858	0.104596148
C	-5.331132148	1.425826128	-0.584475529
C	-5.912339177	0.233618471	1.474168224
C	-4.780959055	0.855207870	2.072851377
C	-3.955137857	0.077031784	2.911304243
C	-2.624424663	0.524649479	3.165265585
C	0.169038081	-2.023074939	1.683574122
C	-1.584785822	-0.430394704	3.183884113
C	-0.246948689	0.010602863	3.003952175
C	0.627252974	-2.441405336	0.431217060
C	1.682990969	-1.715569215	-0.297581058
C	0.644043005	-0.784117285	2.233890533
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C	-0.834775077	-0.968164150	-2.999379176
C	-0.492747345	0.383697449	-3.240943590
C	-3.771805090	1.717326027	-2.439860136
C	-3.290089686	2.927502382	-1.871083970
C	-1.536814375	1.349092407	-3.346327213
C	-4.532813603	2.351112921	0.155795328
C	-3.681083070	3.254809070	-0.539131155
C	-4.251808576	2.059264361	1.512079735
C	-3.133164702	2.683679822	2.127313001
C	-2.299180537	1.896933472	2.972716048
C	-0.974384560	2.335131608	3.219723728

C	1.822171842	-0.198372875	1.737917501
C	0.068897686	1.374666854	3.235835859
C	1.408324476	1.815585838	3.057844389
C	2.442541547	-0.703768332	0.524740119
C	3.162496805	0.325424685	-0.219002385
C	2.292913639	1.019386608	2.301183016
C	1.643185950	0.033768571	-2.103858776
C	2.818016396	0.643451938	-1.536017158
C	-1.215706036	2.714116488	-3.141337564
C	0.822521818	0.820979785	-2.953042630
C	1.171091724	2.183535569	-3.192262315
C	-2.109166636	3.520491216	-2.393785326
C	-1.606920141	4.722296912	-1.810183075
C	0.140257737	3.140930756	-3.279390306
C	-2.874410017	4.160828921	0.199565163
C	-1.997595102	5.049463197	-0.495066675
C	-2.594799279	3.870006081	1.559699105
C	-1.455633937	4.482271286	2.164222914
C	-0.633119696	3.703143154	3.005032664
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C	1.744404419	3.179936565	3.301106446
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C	3.349245332	1.834765568	-2.120803339
C	0.469379119	4.514459397	-3.097462435
C	2.505714249	2.625047496	-2.964139086
C	-0.430244715	5.328407292	-2.340449381
C	-1.195176896	5.971640653	0.238188439
C	-0.914904948	5.679182416	1.609451270
C	1.804115210	4.948373214	-3.290199825
C	2.055940229	6.345680555	-3.129221252
H	2.997776013	6.772295767	-3.468916756
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C	1.198971866	7.122664733	-2.399542872
H	1.477904951	8.149767981	-2.171628496
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H	6.017447364	3.959170914	-1.968570660
C	2.853505656	3.972698215	-3.232888413
C	4.219866115	4.339468549	-3.033595870
H	4.590362596	5.287300291	-3.419566187
C	4.001181701	2.789137548	2.431416317
C	5.218723811	3.321823179	1.899621543
H	5.768488453	4.080882009	2.452758846
C	4.794091989	2.156041759	-0.183098233
C	5.598627483	3.022498328	0.620898539
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C	1.024287974	5.517058112	3.091025330
C	2.356227101	5.906902684	3.421416471
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C	0.188822777	6.309505645	2.235422992
C	0.648647255	7.530965658	1.653065294
H	1.328426501	8.176462606	2.206199608
C	5.557884670	-2.183510716	-1.260131046
H	6.440790913	-2.377905985	-0.630283069
H	5.479191058	-1.081612652	-1.353661424
C	5.772068241	-2.770545703	-2.652931501
H	5.825363428	-3.870793705	-2.586959364
H	4.912583950	-2.520707821	-3.295856430
C	7.046559579	-2.233417576	-3.297928001
H	6.992729116	-1.131413089	-3.330641507
H	7.910205732	-2.486472940	-2.659075936
C	7.262693299	-2.781289896	-4.704926604
H	7.335946802	-3.879847710	-4.690983440
H	6.422667909	-2.509493634	-5.363028376
H	8.185525791	-2.385643683	-5.153603268
C	2.552246146	-3.476150891	-2.284742303
H	1.651363455	-4.096470007	-2.191360788
H	2.347017991	-2.645291857	-2.976474068
H	3.336892395	-4.100806746	-2.729484805

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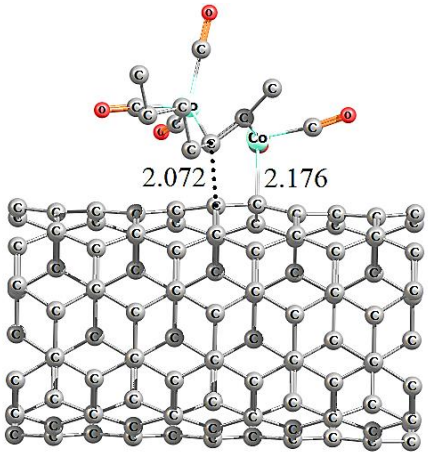

161
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C	3.882465713	4.465224646	-0.141350631
C	-0.246714894	4.306798397	2.841552193
C	-1.585323006	5.387816732	0.816789143
C	2.413578606	4.211116281	2.043265837
O	4.898225859	4.107959189	-0.572494630
O	2.497807708	7.862198577	0.884398026
O	-0.411544913	4.225084248	3.982680500
O	-2.518216344	6.065737991	0.683040302
O	2.708744305	3.782047969	3.083603326
C	1.416337484	4.105437338	-1.109370924
C	0.622205884	5.129975376	-0.643074472
H	6.582438609	-1.952510490	3.784990598
H	7.447251962	0.370626553	0.164369740
H	7.137505318	-0.277175134	2.486381439
H	7.320052690	-0.362293267	-1.925860056
H	6.814340408	-2.313832076	-3.281250898
H	5.623924204	-6.282085166	-1.769436562
H	6.219019627	-4.419830652	-3.210755674
H	5.351635627	-6.882903773	0.328180729
H	5.475604493	-6.052995066	2.609550020
H	5.913660123	-4.287250590	3.832419675
C	5.156972352	-3.520124157	3.679080252
C	6.275494998	0.042164454	1.903562604
C	5.532764968	-2.207222667	3.651311849
C	4.593736193	-1.191952566	3.283983104
C	6.449708611	0.405766942	0.598602223
C	5.312449019	0.659042935	-0.234538657
C	4.955593163	-0.093742366	2.444656193
C	6.283954739	-0.581324158	-2.177928144
C	5.226861327	0.173691731	-1.574936661
C	5.191270216	-4.516939387	-2.866050541
C	5.999172123	-1.679897294	-2.937137242
C	4.641022189	-2.090110390	-3.140136143
C	4.856380866	-5.565711961	-2.056477952
C	3.563006298	-5.622618703	-1.448541004
C	4.251326184	-3.467322636	-3.112392620
C	4.496256900	-6.359869203	0.751923598
C	3.387519623	-6.009092434	-0.082021574
C	4.566001598	-5.892804761	2.033691694
C	3.530361483	-5.051237555	2.550194127
C	3.818445344	-3.895265083	3.341411441
C	2.824678936	-2.888592031	3.445492531
C	3.920771156	0.621893839	1.788698824
C	3.217363285	-1.513651737	3.411727320
C	2.230344023	-0.536343432	3.097950046
C	4.108317261	1.009268771	0.426381767
C	2.957010962	1.329227071	-0.340611347
C	2.586000163	0.551501111	2.274297622
C	3.938604501	0.053937402	-2.165983315
C	2.858910165	0.812970460	-1.648915744
C	2.881841053	-3.775778048	-2.912777266
C	3.641494726	-1.105119044	-2.955873641
C	2.275096014	-1.432468225	-3.185657233
C	2.530088518	-4.875668594	-2.069382448
C	1.206943201	-4.926840451	-1.543039786
C	1.889825388	-2.789251546	-3.178388371
C	2.191565082	-5.622373156	0.573318686
C	1.033938589	-5.308145724	-0.195708575
C	2.265147461	-5.132023893	1.914464975
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C	0.458120026	-2.209974901	3.317226103
C	1.551797749	1.293007166	1.617706977
C	0.846783044	-0.852727855	3.258506057
C	-0.136761723	0.129829298	2.959997183
C	1.756702862	1.740706698	0.309231165
C	0.667727664	2.271966238	-0.500857259
C	0.212107733	1.219873729	2.116968098
C	1.548939862	0.702665958	-2.227669981
C	0.487761505	1.498113735	-1.738530985
C	0.507351324	-3.113157443	-3.021178661
C	1.266417725	-0.434702604	-3.019555778
C	-0.083954644	-0.756841645	-3.296119291
C	0.157641433	-4.205144798	-2.189767112
C	-1.163420852	-4.273907174	-1.670238033
C	-0.474415198	-2.127694615	-3.303163875
C	-0.182288879	-4.955030822	0.465076184
C	-1.338496932	-4.657698003	-0.308147640
C	-0.108202806	-4.467962332	1.792572060
C	-1.193959498	-3.706068953	2.302419174
C	-0.902880175	-2.548236928	3.079293157
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C	-0.813745758	1.977302159	1.509194135
C	-1.508107747	-0.186294496	3.144996713
C	-2.492711775	0.796095690	2.844609515
C	-0.584842804	2.637793306	0.233817749
C	-1.794889427	2.749168049	-0.576555908
C	-2.142904635	1.881407007	2.017569758
C	-0.779559122	1.385018006	-2.337338007
C	-1.872150210	2.191938675	-1.860686826
C	-1.846521095	-2.439932023	-3.130157358
C	-1.075568789	0.240449516	-3.120574286
C	-2.438394135	-0.082333693	-3.392668837
C	-2.199082684	-3.533798966	-2.302399728
C	-3.522953975	-3.579808140	-1.770243005
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C	-2.541921375	-4.288101917	0.350436476
C	-3.697694661	-3.965224401	-0.424768394
C	-2.468130803	-3.801792328	1.680154091
C	-3.552695458	-3.018306070	2.178407293
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C	-3.872631754	0.498097167	3.046773100
C	-3.022465085	3.058314960	0.070773998
C	-3.148619393	2.085629798	-2.494356774
C	-4.210449546	-1.747192962	-3.245244294
C	-3.439612601	0.922494906	-3.274985505
C	-4.568048726	-2.850803992	-2.409337170
C	-4.912514317	-3.606958711	0.228719713
C	-4.837874874	-3.117978620	1.570209305
C	-5.186833387	-0.769071399	-3.557804977
C	-6.555330332	-1.161652146	-3.427936792
H	-7.342458488	-0.544221927	-3.856550940
C	-5.890408651	-2.931214997	-1.907110995
C	-6.897786922	-2.213442820	-2.624245821
H	-7.950009400	-2.410697451	-2.427745962
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C	-5.462582720	2.783722331	-2.751688925
H	-6.245818638	3.521896646	-2.588551565
C	-4.787143507	0.607062087	-3.582466402
C	-5.735413074	1.673410806	-3.500789272
H	-6.729733165	1.550682441	-3.926163970
C	-4.494759809	2.609285058	1.978143263
C	-5.491060449	3.411069303	1.334205927
H	-6.437912425	3.608809013	1.833029199
C	-4.166954280	3.375440947	-0.695718506
C	-5.335193423	3.773850754	0.026351596
H	-6.161890779	4.252376617	-0.495896117
C	-5.628748003	-1.209074868	2.877824554
C	-6.589067856	-0.174450048	3.090972209
H	-7.648301764	-0.419068988	3.143336159
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H	-6.976437674	1.911862820	3.092952880
C	-6.068717609	-3.323808463	-0.540962270
C	-7.265467565	-3.021088926	0.180597076
H	-8.225723227	-3.024529715	-0.331925703
C	-5.923313428	-2.371035846	2.092027119
C	-7.194238405	-2.555896380	1.463910535
H	-8.099757845	-2.198638585	1.950847518
C	2.035518783	3.823540954	-2.441087124
H	1.270990638	3.422528565	-3.129315101
H	2.804583363	3.045635010	-2.333987016
C	2.720987719	5.030176315	-3.105905988
H	1.966212784	5.667675059	-3.592233549
H	3.227144181	5.648352401	-2.347986464
C	3.736386162	4.553546301	-4.140758386
H	4.503345016	3.949300734	-3.626649669
H	3.236944952	3.881263425	-4.859486529
C	4.397841256	5.710480111	-4.881482512
H	3.650624486	6.310538047	-5.423749363
H	4.918876018	6.377429768	-4.177188865
H	5.134451191	5.346294123	-5.612340877
C	0.116444153	6.303067119	-1.434692656
H	0.863881367	6.667501335	-2.151540323
H	-0.779822258	5.996115059	-2.000050480
H	-0.164212539	7.134631420	-0.774241435

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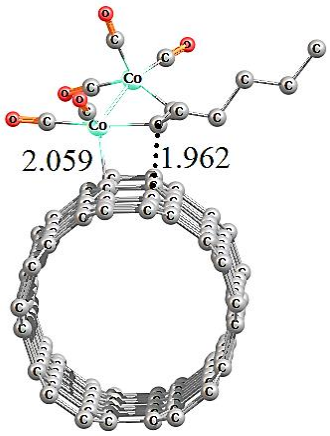

161
Co2C122H32O5

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C	2.299580860	4.104049282	-1.673588474
C	5.518560611	4.420624760	-0.959818608
C	7.052411157	2.458723290	0.628437002
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O	1.720811949	5.082111657	-1.901369517
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O	6.633848874	1.081594136	-2.563195242
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H	5.438616103	1.235544863	2.426074249
H	3.792909583	1.711870593	2.922023749
C	5.282257165	3.225981666	3.250784847
H	6.167516216	3.643777398	2.747724248
H	4.540480411	4.038719216	3.314630320
C	5.656326366	2.752556371	4.652631881
H	4.769120795	2.310766495	5.137415167
H	6.402260636	1.944051591	4.566533405
C	6.212342122	3.882012993	5.513646903
H	7.112864584	4.317892706	5.054222253
H	5.471109846	4.687447242	5.632255844
H	6.483372197	3.521331520	6.516611016
C	2.516141763	4.134925750	1.284418122
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H	5.926636108	-3.009889017	2.736882538
H	6.528372731	-2.051360064	-1.534492399
H	6.644025241	-1.973899538	0.899611300
H	5.627289003	-3.253536887	-3.172158311
H	4.233462680	-5.162510252	-3.730976348
H	2.282687174	-7.911175230	-0.915133703
H	3.039668532	-6.823694756	-2.951779284
H	2.388206964	-7.817893138	1.280793380
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C	3.955784328	-1.919638708	-2.725576226
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C	2.339858789	-4.128991166	-3.382692933
C	1.730287598	-7.054791021	-1.297494091
C	0.685177080	-6.471057252	-0.514730211
C	1.560831725	-5.213573882	-2.866695717
C	1.874280180	-6.927487445	1.638263651
C	0.756020267	-6.407797352	0.913412916
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C	3.761389545	-0.211815523	0.470846913
C	2.883754602	-1.462499716	2.765207794
C	2.198157323	-0.295972347	2.307831158
C	3.694114290	-0.260983143	-0.958954233
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C	2.656225182	0.351170961	1.160080057
C	2.586596269	-1.710411323	-3.032469460
C	1.946690647	-0.501503127	-2.630077793
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C	1.768872099	-2.830210005	-3.372189800
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C	-2.041492025	-3.994405966	1.621100865
C	-3.206363271	-3.493389739	0.978892733
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C	-3.626863090	0.201771611	-3.255631249
C	-4.165363886	-2.680721964	-1.119702752
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C	-4.089959343	-0.591305086	3.117691019
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C	-3.391353474	2.620734636	-2.949307515
C	-5.716848923	-0.593493954	-2.283738486
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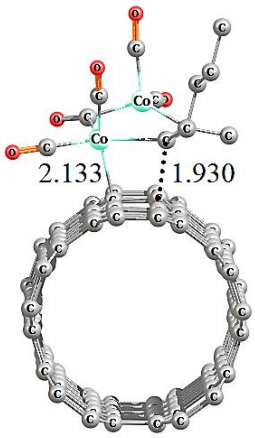

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H	-2.394862806	-8.080170897	0.867293843
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H	-2.433748087	-7.995318684	-1.329510510
H	-3.325536248	-6.760867058	-3.221437957
H	-4.570884536	-5.061174729	-3.808305368
C	-4.092282986	-4.120145500	-3.543317298
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C	-1.776733872	-5.350907065	2.810339977
C	-1.909438824	-7.107929895	-1.679367955
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C	-2.411707623	-6.412451351	-2.743768509
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C	-2.207936199	-0.650323276	2.460403498
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C	1.985542187	-4.150911974	-1.551036864
C	3.120563329	-3.631925587	-0.870594770
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C	-4.467539317	2.085237117	-2.950520849
H	-5.225489551	2.730734924	-3.423009612
H	-3.536341517	2.112336954	-3.539306527
H	-4.874659853	1.060091681	-2.987000273

TS1'*methyl,oblique*

163
Co2C123H32O6

Co	-3.559419335	3.603844088	1.280415102
Co	-5.101583889	2.591240207	-0.651057740
C	-4.657357026	4.962719050	1.694649410
C	-1.992943650	4.279297106	1.593817977
C	-5.734460915	1.469946174	-1.845086498
C	-5.519871764	1.760034613	0.877641789
C	-6.300222637	3.910499183	-0.756895754
O	-1.025952736	4.841569282	1.906331041
O	-5.283765940	5.880879859	2.013223633
O	-6.143309411	0.742249972	-2.649178636
O	-6.005813255	1.113804009	1.712560133
O	-7.059900361	4.776135917	-0.859821725
C	-3.246961753	2.581121308	-1.460294735
C	-3.299119041	3.730235557	-0.676205460
C	-3.632022863	2.582390290	2.743826285
O	-3.616114398	1.943979207	3.707713208
H	-4.947816060	-4.707927337	-3.564065370
H	-6.749899470	-2.549825653	-0.262378082
H	-6.159742245	-3.218268166	-2.527134013
H	-6.394727665	-2.993976271	1.884802076
H	-5.197774209	-4.471935943	3.398917389
H	-2.498416969	-7.769634932	2.285678285
H	-3.821914013	-6.163372569	3.536163579
H	-1.942414838	-8.422823355	0.261423384
H	-2.322479642	-7.938056785	-2.089665002
H	-3.425873856	-6.586763365	-3.404840530
C	-3.021042448	-5.577061415	-3.369771343
C	-5.499082131	-2.549648478	-1.978264660
C	-3.882328909	-4.513721813	-3.458344944
C	-3.419614425	-3.186103203	-3.228494740
C	-5.831862551	-2.171308889	-0.708980415
C	-4.904622071	-1.425202041	0.084825472
C	-4.209473413	-2.218471201	-2.507499866
C	-5.363190200	-2.765517784	2.146594122
C	-4.670922832	-1.716504322	1.466922433
C	-2.828235662	-5.879610829	3.194602488
C	-4.689724147	-3.596654390	2.998420069
C	-3.290343301	-3.418211551	3.223816508
C	-2.082707704	-6.784954684	2.491458351
C	-0.855394174	-6.385284840	1.877773752
C	-2.387141395	-4.526401527	3.325707967
C	-1.351387946	-7.648252919	-0.223917822
C	-0.499579631	-6.805406930	0.554485810
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C	-1.125373933	-4.073190034	-3.266991074
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C	-2.025945141	-2.966531554	-3.346293242
C	-1.498853652	-1.657283458	-3.148309981
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C	-3.016206104	0.144915146	0.099183877
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C	-1.003126619	-4.285549329	3.139592239
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C	-0.488210321	-2.966849278	3.298642000
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C	1.374990391	-5.215269306	0.563170717
C	0.236525329	-5.755087595	-1.536330005
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C	0.251938064	-3.811508387	-3.007040417
C	0.787892175	-2.516232376	-3.268745822
C	-1.617137641	0.415957056	-1.877052074
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C	0.394479268	-0.107872604	-3.152897091
C	-2.142208663	1.047954398	-0.660229312
C	-1.118475270	1.742521813	0.118696267
C	-0.380767018	0.823888387	-2.404348896
C	-1.528704885	0.274071090	2.038054950
C	-0.836836533	1.373043512	1.462574093
C	0.913940403	-2.731960703	3.155894389
C	-0.842042845	-0.578286494	2.925039850
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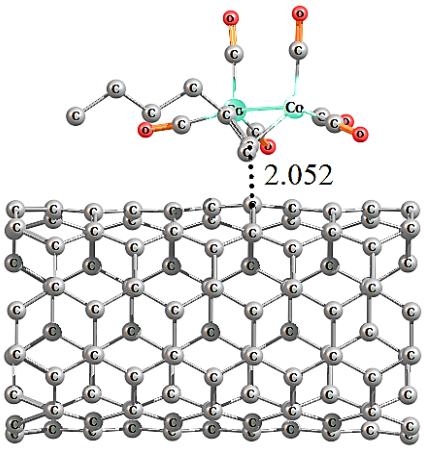

Note: Taken into consideration in the main manuscript.

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C	0.850454130	3.214142011	0.132383659
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C	1.082808282	2.912476020	1.487839845
C	2.813554888	-1.182081050	3.178623223
C	1.056268591	0.970037239	2.966192824
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C	3.672514399	1.715007850	-3.325079702
C	1.824872925	3.969201915	-0.574896823
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C	6.170182206	-1.351357225	-0.108499499
C	5.943706959	-1.060278684	-1.489605459
C	5.233006257	1.687543777	3.407674349
C	6.648778173	1.849452051	3.294503402
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C	6.756617345	-0.159515108	1.942425253
C	7.391755386	0.949591443	2.582208880
H	8.442611445	1.159573810	2.391391326
C	2.961358117	4.496063371	1.524176895
C	4.130027337	4.954288327	2.208213516
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C	4.330877820	2.795342962	3.299277524
C	4.794519746	4.128382237	3.071904915
H	5.752948425	4.446373342	3.477934020
C	3.385108884	3.992860311	-2.464972582
C	3.961768333	5.178950233	-1.909701488
H	4.760171502	5.696115994	-2.439219489
C	2.727862219	4.794609068	0.141625194
C	3.642783104	5.568510417	-0.638393795
H	4.193375816	6.388510619	-0.180032577
C	5.954352631	0.868655680	-2.993922235
C	6.433401467	2.173232945	-3.322136946
H	7.504424360	2.363620466	-3.361500541
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H	5.967531587	4.232424726	-3.539351978
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C	7.883848102	0.395062433	-1.469574385
H	8.587120332	1.034564629	-1.999841171
C	-3.037988905	5.085123059	-1.305706540
H	-3.441937135	5.890060177	-0.675369060
H	-3.552934285	5.144995107	-2.280817875
C	-1.533438641	5.290042026	-1.524605533
H	-1.010820080	5.246068929	-0.557410840
H	-1.139201636	4.456139481	-2.128514808
C	-1.176924855	6.602965702	-2.212063600
H	-1.677006552	6.652681576	-3.194722946
H	-1.564041907	7.447119260	-1.615988827
C	0.334474207	6.740029055	-2.387912205
H	0.843172623	6.716508128	-1.411138507
H	0.735695394	5.908811576	-2.990277006
H	0.601383761	7.682289394	-2.888970063
C	-3.068414773	2.545765856	-2.951869096
H	-2.029787831	2.742706863	-3.260201988
H	-3.377988510	1.584603287	-3.384732715
H	-3.706393078	3.325287964	-3.396956816

TS1'*methyl,oblique*

163
Co2C123H32O6

Co	4.460062183	2.277470928	-1.247212049
Co	5.609285782	0.915072875	0.738036699
C	5.942188037	3.143195967	-1.781672356
C	3.181389094	3.438717687	-1.393802557
C	5.855141810	-0.381313472	1.893700429
C	5.726582255	0.075268167	-0.845728706
C	7.180923865	1.745706095	0.860034812
O	2.429841354	4.312929111	-1.530015144
O	6.837593514	3.731580626	-2.215985766
O	6.023656416	-1.214749822	2.681875845
O	6.019991944	-0.687995149	-1.675093423
O	8.199410284	2.284020338	0.971572819
C	3.812809013	1.466290700	1.511999068
C	4.233159068	2.536970006	0.728915412
C	4.107912821	1.341157251	-2.719820249
O	3.851016396	0.787402071	-3.701693479
H	3.331833447	-6.043969312	3.433181501
H	5.652641181	-4.406102060	0.159289171
H	4.915740640	-4.937061429	2.418101810
H	5.167671576	-4.665521954	-1.993501462
H	3.585671540	-5.688265010	-3.530412910
H	0.054402126	-8.098226548	-2.468642046
H	1.777057140	-6.905755885	-3.696271069
H	-0.645785574	-8.620558883	-0.451319496
H	-0.121150670	-8.334522383	1.904328701
H	1.332253258	-7.399220264	3.241686162
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C	4.471018115	-4.092091344	1.895620534
C	2.367074340	-5.548168649	3.346350038
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C	4.244040264	-4.141770772	-2.233143334
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C	-0.059833665	-7.029599769	-2.641018791
C	-1.114095068	-6.310853788	-1.996899867
C	0.878996079	-4.931213379	-3.418179084
C	-0.984452915	-7.723302623	0.063491804
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C	1.035280551	-3.528425727	3.301409534
C	0.907132234	-2.117440425	3.145777316
C	3.490963799	-1.814100991	0.603324336
C	2.855234718	-0.738654937	-0.073052886
C	1.903312037	-1.419761279	2.426071312
C	2.844675018	-2.168165812	-2.048653544
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C	1.919713185	-2.765500623	-2.958582268
C	0.676684644	-2.110754789	-3.187170676
C	-1.389805039	-5.008377342	-2.481733013
C	-2.457582870	-4.254004557	-1.913450818
C	-0.487702928	-2.891413670	-3.319167467
C	-2.256933266	-5.660567133	0.063995653
C	-2.900283805	-4.586167788	-0.616045819
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C	0.546337422	0.603206062	2.482673796
C	1.449847835	-0.131974560	-1.979082698
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C	0.543436095	-0.720696576	-2.881036280
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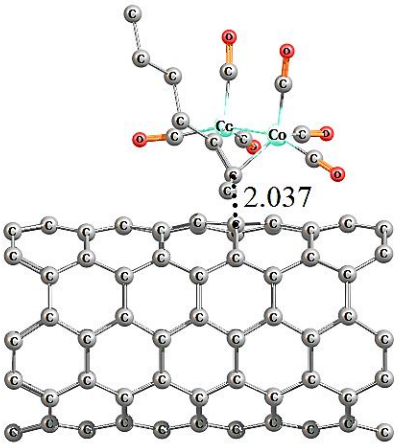

Note: Discarded in the main manuscript.

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C	0.045191485	3.323948258	0.028648173
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C	-3.129662802	-0.232560706	-3.099430359
C	-0.822719833	1.311830183	-2.855360982
C	-2.066580329	1.967257215	-3.103673512
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C	-1.119445114	3.958964275	2.083833714
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H	-6.113479109	4.800276864	-3.409659260
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C	-6.884477740	3.117344412	-2.371893465
H	-7.825642898	3.619268079	-2.155184599
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C	-2.602702204	5.993095711	-1.969637768
H	-2.743954825	7.033017737	-1.680821717
C	-3.428198513	4.014492892	-3.104519025
C	-3.481399868	5.419388164	-2.845598248
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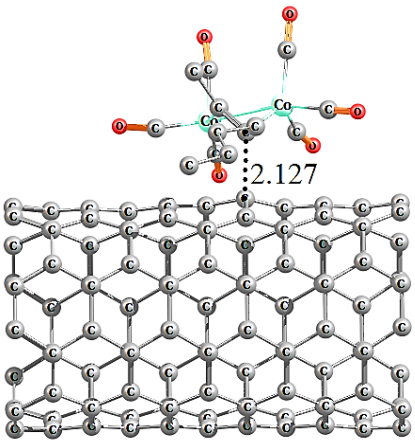
H	-8.499041123	3.114865776	-0.126430201
C	-6.437698552	1.848012879	2.270549494
C	-7.496785083	2.598817531	1.672147570
H	-7.981209690	3.397898633	2.230247630
C	4.347158665	3.909988925	1.348747982
H	4.590865322	3.797501933	2.418492079
H	3.327240577	4.344319209	1.322688281
C	5.327597193	4.888326854	0.724607213
H	6.327117029	4.426515254	0.670773146
H	5.025200865	5.115451066	-0.309690653
C	5.412686259	6.191448836	1.513822498
H	4.405852243	6.638911668	1.582614611
H	5.728676205	5.971125587	2.548386654
C	6.380240952	7.185297102	0.879325847
H	7.393469211	6.758879157	0.819712676
H	6.064244569	7.438058939	-0.144549291
H	6.437019901	8.118612857	1.458017190
C	3.606032268	1.510302134	3.000341272
H	2.703452979	2.078223458	3.279611535
H	3.535671431	0.505280552	3.436968511
H	4.474376393	2.002497609	3.463338908

TS1'*butyl,oblique*



163
Co2C123H32O6

Co	2.938148468	4.101798657	-1.196482613
Co	4.956389146	2.897668384	0.099286562
C	3.963139088	5.487745580	-1.691362023
C	1.423178425	4.909189694	-0.889386252
C	5.915281298	1.758057341	1.032906825
C	4.949092950	2.192627670	-1.548803932
C	6.148569644	4.221376548	-0.033590806
O	0.534270198	5.632359322	-0.707828753
O	4.530887885	6.436812855	-2.027658648
O	6.546225976	1.047104187	1.695758962
O	5.192529999	1.670601396	-2.556472514
O	6.921637522	5.080556345	-0.067859923
C	3.388452094	2.727433984	1.365556169
C	3.242556014	3.964485872	0.752562995
C	2.625647662	3.374297980	-2.801457671
O	2.391495303	2.920780711	-3.837647884
H	5.215355507	-4.517928282	3.379204350
H	6.864381143	-2.261248489	0.062777314
H	6.344853921	-2.984366443	2.325425724
H	6.493896086	-2.672493191	-2.079438347
H	5.328394631	-4.168594972	-3.598456146
H	2.771485452	-7.585769469	-2.511270188
H	4.012082667	-5.910364380	-3.756947128
H	2.288162171	-8.280766668	-0.481281808
H	2.696181800	-7.814696297	1.868288346
H	3.763981842	-6.449853329	3.198096171
C	3.320678042	-5.455874899	3.188472516
C	5.653105433	-2.324619321	1.804824720
C	4.142091289	-4.362140898	3.289626553
C	3.626834839	-3.049159159	3.090801483
C	5.945595540	-1.916984710	0.534583479
C	4.979564514	-1.188544911	-0.226984977
C	4.367305852	-2.042039736	2.369545405
C	5.450445327	-2.477457734	-2.320305312
C	4.731840198	-1.466729937	-1.611148653
C	3.015587858	-5.669106966	-3.391595038
C	4.794296975	-3.319826647	-3.175352585
C	3.386304047	-3.191373199	-3.374951599
C	2.316856238	-6.613287833	-2.691253497
C	1.088376926	-6.268797430	-2.047260419
C	2.523389272	-4.330799559	-3.488142966
C	1.676411400	-7.537542904	0.026892201
C	0.776492341	-6.719149310	-0.722359004
C	1.906353837	-7.274579883	1.349433083
C	1.247357577	-6.181455177	1.990129710
C	1.937488127	-5.297212236	2.887530617
C	1.370102636	-4.022044375	3.137122123
C	3.658743744	-0.953609727	1.824149300
C	2.228479658	-2.883177791	3.227938719
C	1.648796553	-1.589749596	3.059805785
C	3.983718319	-0.498949891	0.502389152
C	3.028698563	0.304070535	-0.177576399
C	2.363073824	-0.612307856	2.332249748
C	3.485301343	-1.066372553	-2.143548468
C	2.741277948	-0.025104973	-1.504398980
C	1.135117441	-4.145172073	-3.275041249
C	2.804222490	-1.940896728	-3.043724933
C	1.416369470	-1.726030719	-3.274414046
C	0.403902022	-5.131606215	-2.542316297
C	-0.849589603	-4.758304515	-1.975250092
C	0.569132091	-2.843721809	-3.399629284
C	-0.196686734	-6.000168708	0.015053535
C	-1.156216391	-5.200857497	-0.671602077
C	0.044568275	-5.725375480	1.397271243
C	-0.694767142	-4.673548586	2.013967195
C	-0.019622405	-3.808828397	2.902020086
C	-0.600455528	-2.541121818	3.198925081
C	1.672137673	0.519114462	1.830011581
C	0.255458086	-1.409573089	3.274255701
C	-0.303313257	-0.117014916	3.119257686
C	2.146935967	1.176070022	0.606185234
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C	0.420326421	0.855751793	2.373017036
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C	-0.837826723	-2.663862113	-3.231412510
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C	-1.561421824	-3.639740215	-2.504547422
C	-2.818457503	-3.283695334	-1.945439276
C	-1.395510416	-1.367426773	-3.382581526
C	-2.164140769	-4.510406566	0.067639631
C	-3.125568989	-3.728923661	-0.625590380
C	-1.928716754	-4.242949167	1.441159910
C	-2.666565807	-3.205065675	2.071527295

C	-1.984462528	-2.334040256	2.971573172
C	-2.550676315	-1.057619540	3.244148588
C	-0.280281260	2.000030700	1.879166071
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C	-2.257302011	1.371636954	3.178183471
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C	-0.953018607	3.226065448	-0.105048787
C	-1.538612437	2.348389640	2.449652010
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C	-1.180493846	2.948856659	-1.466508804
C	-2.791013688	-1.184226914	-3.194047743
C	-1.108725242	1.026008498	-2.969558015
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C	-3.514550841	-2.159173260	-2.461650370
C	-4.766163486	-1.784060582	-1.886821216
C	-3.349468304	0.121743021	-3.329707008
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C	-5.070895005	-2.223852653	-0.580767529
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C	-3.939132377	-0.840419341	3.000292502
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C	-2.253407659	3.477559883	1.949083429
C	-3.652354280	1.564182153	3.388032590
C	-1.953130761	3.923978324	0.625050677
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C	-5.839957336	-1.259152040	1.534743748
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C	-6.731526863	1.710489554	-3.191361556
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C	-6.741262193	-0.320842813	-1.867146861
C	-7.426982095	0.775584862	-2.476314977
H	-8.479840371	0.946821119	-2.259937312
C	-3.120693407	4.457401611	-1.455608040
C	-4.309466098	4.888641271	-2.124406754
H	-4.778822280	5.830450492	-1.846118876
C	-4.449011323	2.737509645	-3.236654518
C	-4.954314622	4.053119537	-2.992293640
H	-5.924161550	4.345431488	-3.390434442
C	-3.486348987	3.853344191	2.537302404
C	-4.131279817	5.011934220	1.999694733
H	-4.953414065	5.476844219	2.540574590
C	-2.895266624	4.725394247	-0.067164507
C	-3.843840589	5.436660172	0.732422307
H	-4.442175328	6.231004009	0.290049415
C	-5.904549420	0.631400891	3.084701521
C	-6.431257078	1.908091433	3.451692973
H	-7.507814924	2.051403694	3.523951405
C	-4.208841005	2.865708905	3.281843452
C	-5.606419604	2.994188815	3.550879658
H	-6.043339046	3.979866130	3.699050708
C	-7.050239009	-0.766567560	-0.541839136
C	-8.059027247	-0.135170233	0.250881832
H	-8.951951526	0.266756979	-0.224437790
C	-6.587697741	-0.238129394	2.175355956
C	-7.834414878	0.121499310	1.574483982
H	-8.552721065	0.723130169	2.128252904
C	3.584183075	2.477666393	2.839867675
H	4.516888300	2.990839615	3.132022874
H	3.793793930	1.410512010	3.008818335
C	2.422144249	2.936769707	3.742379810
H	2.629327296	3.948596648	4.129364785
H	1.506242592	3.041606215	3.141305359
C	2.156216867	1.997383370	4.916826077
H	2.077248511	0.959837269	4.551109132
H	3.024336688	2.010214775	5.599203861
C	3.242009823	5.237689595	1.564992212
H	2.204886956	5.490237661	1.840431134
H	3.818165387	5.122176137	2.494998344
H	3.655109025	6.079446208	0.995359756
C	0.884071330	2.362615826	5.674546601
H	0.941103232	3.385454809	6.079107926
H	0.006318642	2.319272347	5.009585803
H	0.703885657	1.672532401	6.511474603

TS1'*_methyl,oblique_

163
Co2C123H32O6

Co	2.211759716	4.162377479	-0.016523581
Co	4.408509927	3.119495764	-1.098422820
C	3.807273877	5.026273780	-0.036176030
C	1.511636297	5.082263112	1.326386477
C	6.093146621	3.684222692	-0.994515935
C	4.676876558	1.532853225	-1.794753504
C	3.836224882	3.831055640	-2.652253387
O	1.107103981	5.744933883	2.181705093
O	4.484497027	5.939385715	0.239920562
O	7.201432083	4.010495425	-0.996851747
O	5.088057209	0.575245487	-2.297847581
O	3.494882694	4.256550879	-3.669632125
C	3.008473585	2.668726928	1.230090602
C	4.238266791	2.372514427	0.652131866
C	1.475429015	5.021176575	-1.415448769
O	0.998237334	5.605317084	-2.285958871
C	5.328566362	1.627006790	1.351858474
H	5.937669276	1.069826197	0.621601903
H	4.893606167	0.887501546	2.047033929
C	6.256494206	2.551262359	2.163073750
H	6.676636657	3.331277430	1.510406585
H	5.672237959	3.067907597	2.940801126
C	7.385063522	1.755604675	2.813787314
H	6.949497598	0.952483477	3.432919139
H	7.974309313	1.258243644	2.024306959
C	8.294622255	2.633401052	3.666995819
H	8.753048605	3.429943217	3.061112525
H	7.727120430	3.112935984	4.479523681
H	9.104142056	2.044442611	4.122281075
C	2.896885121	2.827487214	2.726742880
H	3.494098931	3.691654957	3.052441017
H	1.860053202	2.999036363	3.046023846
H	3.260882602	1.927937929	3.254212816
H	-4.974067018	5.147556109	-3.240215583
H	-3.227230205	6.694756662	0.448368232
H	-3.706018859	6.298850974	-1.899251022
H	-3.739275792	6.115551990	2.524724260
H	-5.212742453	4.676551012	3.813467823
H	-8.243422766	1.925390779	2.187296930
H	-6.812864532	3.196555740	3.680549702
H	-8.711762876	1.571692999	0.072534768
H	-8.098296937	2.224308790	-2.185048254
H	-6.756094668	3.504927809	-3.347769373
C	-5.726458188	3.162265069	-3.263411507
C	-3.007926773	5.642312418	-1.383324823
C	-4.719566296	4.090237327	-3.201489300
C	-3.384760182	3.689413282	-2.902542579
C	-2.737075395	5.866930076	-0.061020350
C	-1.969314864	4.921847212	0.685392121
C	-2.538050308	4.454202622	-2.024265074
C	-3.450324496	5.080411323	2.698311660
C	-2.315588615	4.536326310	2.025313231
C	-6.442374897	2.263981513	3.259208555
C	-4.282073011	4.269537748	3.422979410
C	-4.023662825	2.868010027	3.507148683
C	-7.249471420	1.547113740	2.419054700
C	-6.732478440	0.418825290	1.711319774
C	-5.074487042	1.892375655	3.437692686
C	-7.876138715	1.073090406	-0.415209465
C	-7.039959562	0.185963590	0.329639252
C	-7.530365066	1.440823086	-1.686732850
C	-6.331097568	0.940186949	-2.278901623
C	-5.450984307	1.782185928	-3.039970100
C	-4.106225468	1.364145236	-3.204559092
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C	-0.276289552	3.140082480	0.611719774
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C	-1.824442665	3.292445861	2.488735202
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C	-2.697971770	2.443150509	3.237589080
C	-2.361791288	1.063919387	3.350038056
C	-5.577289485	-0.198972523	2.249781125
C	-5.036372864	-1.358548465	1.619891252
C	-3.393070144	0.105106777	3.311323778
C	-6.170918176	-0.648851195	-0.415068213
C	-5.340001479	-1.589437663	0.262120320
C	-5.809097267	-0.262587664	-1.743327317
C	-4.640235159	-0.843758554	-2.316476128
C	-3.772746243	-0.012432426	-3.056407750
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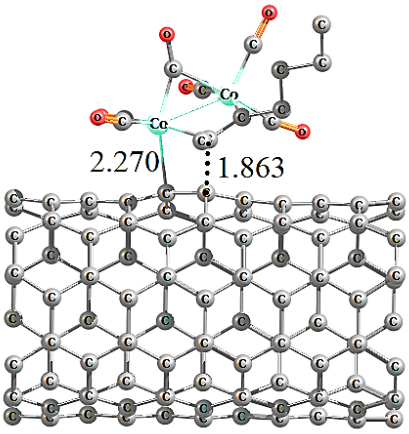
C	0.283492358	2.015893869	-1.473514198



Note: Taken into consideration in the main manuscript.

C	-1.389039337	0.523471470	-3.169775993
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C	0.747737520	2.432511660	-0.149461869
C	1.665866146	1.529955880	0.620951299
C	0.777435209	0.844533826	-2.069431906
C	-0.150584510	1.465372411	2.364698913
C	1.037838640	0.929189355	1.836732570
C	-3.057992646	-1.257140483	3.046626665
C	-1.019393635	0.637405122	3.119431971
C	-0.685415005	-0.726642819	3.294734049
C	-3.897842610	-2.007504615	2.186329460
C	-3.370957499	-3.169953038	1.562803471
C	-1.727807807	-1.698954134	3.260038636
C	-4.496354664	-2.462476511	-0.489860081
C	-3.680109921	-3.404104682	0.190352240
C	-4.140476726	-2.079950419	-1.809719717
C	-2.982912124	-2.654708066	-2.397292064
C	-2.109001156	-1.811582429	-3.142792377
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C	1.605668151	-1.728736662	-3.005983361
C	2.295075329	0.459866482	-0.185415674
C	3.092865074	-0.502323208	0.499738500
C	2.429576864	-1.004339309	-2.125493395
C	1.519998582	-0.298419617	2.339783310
C	2.727140792	-0.869384575	1.816019788
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C	0.650882247	-1.141523129	3.076558003
C	0.991384152	-2.517861604	3.243740073
C	-2.219509707	-3.795448551	2.114446311
C	-1.672528215	-4.951407047	1.479313059
C	-0.037982415	-3.481144414	3.179686165
C	-2.819470351	-4.252982606	-0.560473611
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C	-2.467457860	-3.872490092	-1.876914791
C	-1.293577826	-4.443768705	-2.459780357
C	-0.429684434	-3.609608738	-3.200030675
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C	3.915980638	-1.394837272	-0.235883091
C	3.231011065	-2.087974282	2.341442245
C	0.311966344	-4.834771932	2.914337007
C	2.340617253	-2.939617896	3.077357487
C	-0.527988231	-5.590070264	2.037460608
C	-1.132308106	-6.054040446	-0.623574778
C	-0.781025234	-5.672565527	-1.956269087
C	1.634863822	-5.280338616	3.163849522
C	1.908817166	-6.661523956	2.910601325
H	2.827264512	-7.111428867	3.282722779
C	-0.008884227	-6.760285923	1.427296142
C	1.109968322	-7.381037893	2.067247582
H	1.409105849	-8.387827973	1.781628723
C	4.411797818	-2.658158925	1.788753794
C	4.902963173	-3.855832922	2.404072948
H	5.913231384	-4.201141610	2.190962581
C	2.676385605	-4.303973890	3.256362441
C	4.059817846	-4.655060110	3.119781941
H	4.412848121	-5.621525352	3.474825671
C	4.129414759	-2.782212443	-2.247163649
C	5.312309169	-3.346932972	-1.670381561
H	5.899952897	-4.068967920	-2.234490580
C	4.759988195	-2.305213794	0.450249005
C	5.619592164	-3.117689441	-0.358870240
H	6.441196558	-3.665516634	0.099385413
C	1.230377137	-5.416747010	-3.319883892
C	2.583061440	-5.788607919	-3.607862386
H	2.835522752	-6.834667313	-3.771758982
C	3.290977796	-3.516845886	-3.136316059
C	3.584066941	-4.865234053	-3.520467659
H	4.618475867	-5.189759511	-3.616449703
C	-0.324651369	-7.002446850	0.053794501
C	0.462798216	-7.878402731	-0.760067792
H	0.909969712	-8.770240830	-0.324671482
C	0.361596385	-6.258026162	-2.560124124
C	0.795694651	-7.517174276	-2.034026537
H	1.502918536	-8.126648225	-2.593586278

TS1'*$_{methyl,oblique}$

163
Co2C123H32O6

Co	-4.240931959	1.140796221	-0.145295093
Co	-6.322673277	-2.476031309	-0.853081763
C	-6.974223885	-0.943554718	-1.512601325
C	-5.189609998	1.944177955	-1.403540199
C	-4.903612119	-3.479997591	-1.232885560
C	-7.091624330	-2.713275764	0.760610538
C	-7.429738054	-3.507473459	-1.795710065
O	-5.648127934	2.613291703	-2.232094775
O	-7.458506933	0.026120578	-1.907278370
O	-4.000130654	-4.157271236	-1.483227455
O	-7.646138670	-2.869364321	1.760045930
O	-8.121967349	-4.182627314	-2.423136255
C	-3.984812485	-0.656781288	-1.082175852
C	-4.721320215	-1.312308756	-0.148078081
C	-4.924864688	1.898398338	1.311297735
O	-5.448478959	2.266107037	2.277658039
C	-4.510726896	-1.443446478	1.335964694
H	-5.406184027	-1.076727765	1.865127097
H	-3.703874898	-0.769545604	1.657074030
C	-4.184496823	-2.854780603	1.845845527
H	-5.035191265	-3.534146653	1.688326767
H	-3.352369896	-3.285199306	1.270275195
C	-3.835302784	-2.825353535	3.330024137
H	-2.982271230	-2.144152986	3.495684126
H	-4.684041181	-2.393223027	3.889005702
C	-3.501375846	-4.208598627	3.877686107
H	-4.356333384	-4.893469310	3.764079871
H	-2.647010530	-4.648057628	3.340574702
H	-3.240041691	-4.161039800	4.944784884
C	-3.998903481	-0.786631876	-2.566334175
H	-5.022455997	-0.679618987	-2.950064814
H	-3.390110453	-0.005049750	-3.039928228
H	-3.612452762	-1.767552324	-2.892239606
H	-0.931032753	6.866212677	3.750062476
H	-3.370557832	6.593981127	0.141934753
H	-2.658530686	6.616434740	2.466367827
H	-2.711592859	6.749429316	-1.954641763
H	-0.722131419	7.152749134	-3.289597717
H	3.364162588	7.857615359	-1.782748263
H	1.424253493	7.554034487	-3.209874583
H	4.039055311	7.900729994	0.305604951
H	3.245202182	7.671751084	2.591068153
H	1.455792596	7.299959844	3.801124164
C	1.106270527	6.278008440	3.666604168
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C	-0.240308317	6.033034785	3.636215679
C	-0.733809314	4.741496311	3.282722552
C	-2.985687134	5.678784753	0.588693365
C	-2.738689085	4.533433608	-0.226613571
C	-1.884601525	4.571214496	2.439840953
C	-2.057559790	5.913494470	-2.196491607
C	-2.269962220	4.645535242	-1.581106952
C	1.970398169	6.677848071	-2.865455400
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C	3.690779715	5.721780332	-1.447051619
C	1.444827308	5.370183280	-3.099422496
C	3.951320157	6.906901129	0.740784110
C	4.122350730	5.749298624	-0.080198749
C	3.504432869	6.777957645	2.026552201
C	3.206503869	5.484972865	2.557351307
C	2.035441965	5.242552981	3.349069832
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C	-0.275440501	2.330511956	3.118535192
C	-2.522339152	3.311529745	0.443474523
C	-2.415127652	2.093866419	-0.326820650
C	-1.411106877	2.153200473	2.294228389
C	-1.578793320	3.535337082	-2.132779175
C	-1.799883731	2.227754629	-1.609494114
C	2.326505848	4.281284251	-2.889159575
C	-0.405925902	3.777547232	-2.914487456
C	0.492370820	2.697982703	-3.143662234
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C	4.524300657	3.325125473	-0.168567832
C	3.831692666	4.378099263	1.931772755
C	3.615962242	3.064150338	2.439696359
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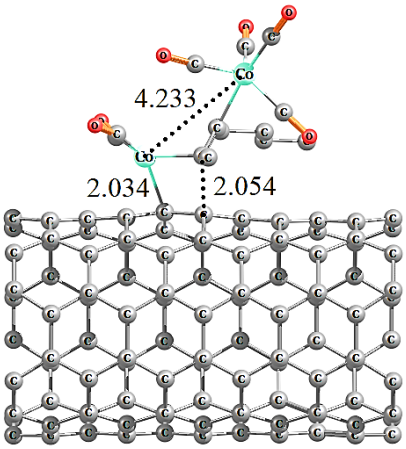

Note: Discarded in the main manuscript.

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C	-1.333452159	-0.188279739	-1.683151860
C	2.779693886	1.858217919	-2.978911353
C	0.040722363	1.358197452	-2.975324800
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C	4.555059293	0.882333079	-1.616463810
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C	5.170629263	-0.329578678	0.418092667
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C	4.481864159	-1.774801779	2.265125117
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C	-1.160036496	-3.997269425	0.168024208
C	-0.268641640	-3.719914357	-2.433021809
C	3.639036594	-2.980425752	-3.164969205
C	0.904879793	-3.472651499	-3.217795861
C	4.779326961	-2.807732466	-2.319289660
C	5.601514582	-2.758010563	0.322948515
C	5.133681650	-2.889930315	1.667805992
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C	4.154555737	-5.346495604	-3.324048974
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H	-0.864159972	-7.353212100	-0.364654738
C	3.779868943	-4.423719522	3.005213635
C	3.278938847	-5.743496338	3.247838466
H	3.970734211	-6.579924631	3.329414479
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C	1.936136570	-5.987002815	3.219183231
H	1.580455878	-7.014014710	3.277501590
C	5.853394843	-3.930300984	-0.434414207
C	6.108635997	-5.132030762	0.301501720
H	6.537933120	-5.996704600	-0.201389042
C	4.939684220	-4.188733379	2.205317207
C	5.664847995	-5.257737640	1.586530275
H	5.748733495	-6.220413446	2.087380908

TS1'*butyl,oblique*

163
Co2C123H32O6

Co	4.316100400	1.857351636	0.238119714
Co	3.499537625	4.222418921	1.155403575
C	5.369678364	3.332472645	0.252231406
C	5.242331537	0.987186318	-0.998429311
C	4.182027647	5.840487944	0.876599755
C	1.923485302	4.600517803	1.831790116
C	4.185443791	3.770973712	2.760095911
O	5.921122885	0.464215863	-1.774401929
O	6.382024134	3.876619681	0.031366679
O	4.574357469	6.913742961	0.709759405
O	0.992897992	5.080876397	2.324378964
O	4.603803757	3.501538383	3.801116402
C	2.984458888	2.755236366	-1.119080850
C	2.806393390	4.037984413	-0.618295973
C	4.953036971	1.112914228	1.743728670
O	5.383963442	0.623317612	2.693584726
H	4.387165552	-5.352398349	3.573514392
H	6.276262309	-3.842670217	-0.057168853
H	5.726925407	-4.236805040	2.275414787
H	5.742925421	-4.319146283	-2.154466485
H	4.215713095	-5.651940395	-3.493821330
H	1.084867004	-8.350198100	-1.968299633
H	2.569382907	-7.084855438	-3.412602803
H	0.587558871	-8.744759324	0.132721640
H	1.199985307	-8.166448116	2.410727485
H	2.561191322	-6.949138571	3.617602407
C	2.334265241	-5.890409282	3.506608261
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C	3.365874725	-4.988302023	3.480352969
C	3.123924301	-3.623234611	3.149221498
C	5.484272202	-3.258146169	0.407762941
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C	2.530923709	-4.274363191	-3.284171463
C	0.825541025	-7.325474180	-2.227971463
C	-0.272928978	-6.681333709	-1.580234660
C	1.446920622	-5.214939622	-3.250964395
C	0.159176954	-7.853249549	0.587113744
C	-0.599702934	-6.940333195	-0.207712147
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C	3.517926952	-1.716447982	1.668098164
C	1.799273371	-3.151419172	3.297782932
C	1.493727567	-1.784708478	3.014004460
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C	3.071718283	-0.531203892	-0.418913939
C	2.365246325	-1.043062327	2.184255976
C	3.139880116	-2.117522179	-2.268633178
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C	-0.739129471	-5.475847017	-2.159635709
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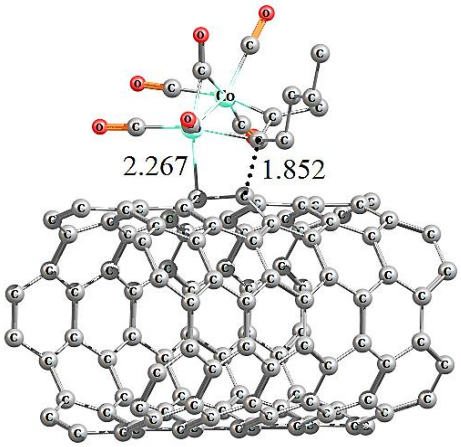

Note: Taken into consideration in the main manuscript.

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C	-0.532039322	2.864946558	-1.843975824
C	-3.085669860	-1.014203803	-3.061991171
C	-0.973049624	0.804850336	-3.088099541
C	-2.295232951	1.287377771	-3.324852955
C	-3.960204179	-1.754230361	-2.230060611
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C	-1.370558433	3.848431815	1.517717411
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C	-4.684304125	0.862179438	-3.102060287
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C	-5.565433738	0.119372768	-2.255379208
C	-6.213025150	-0.391676644	0.386411828
C	-5.856052831	-0.060513555	1.730959851
C	-4.973778598	2.221193956	-3.384861433
C	-6.328065912	2.643837869	-3.201148800
H	-6.659134862	3.599791648	-3.602253973
C	-6.700693472	0.768574817	-1.707025990
C	-7.167554645	1.937899028	-2.386246437
H	-8.148586397	2.346695121	-2.151495944
C	-2.133737173	4.727948965	-1.919279521
C	-3.244763429	5.332062075	-2.593192732
H	-3.490697199	6.376127967	-2.406962779
C	-3.888519507	3.152019218	-3.439662741
C	-4.096910543	4.566255345	-3.334571343
H	-5.004147135	5.013376046	-3.736556456
C	-2.470429117	4.523321387	2.107276920
C	-2.879395891	5.750555389	1.493328094
H	-3.560698193	6.418986316	2.016625994
C	-1.805427494	5.059652967	-0.569834344
C	-2.559225586	6.011899062	0.190947050
H	-2.996564094	6.878849460	-0.301207683
C	-5.447957134	1.935080449	3.080702931
C	-5.685765929	3.323682075	3.336838034
H	-6.705260543	3.688199446	3.448774133
C	-3.331966208	3.779730232	2.966648499
C	-4.657727661	4.219693331	3.283221494
H	-4.874373615	5.283972253	3.352992418
C	-7.038497091	0.500798183	-0.343451741
C	-7.861767849	1.389155085	0.420063648
H	-8.681066715	1.920295260	-0.061140212
C	-6.342661022	1.147669652	2.293549161
C	-7.524459849	1.702913821	1.705386733
H	-8.080663391	2.478502231	2.228632290
C	3.206923725	2.548166722	-2.602061933
H	2.298568137	2.849541711	-3.158070415
H	3.336067234	1.473875301	-2.807459176
C	4.412274275	3.302429839	-3.154701796
H	4.231495137	4.389344227	-3.107017569
H	5.296568689	3.110581459	-2.525662409
C	4.718307264	2.890898247	-4.591602465
H	4.920207257	1.805992810	-4.612691047
H	3.822508331	3.053287903	-5.215858112
C	5.904680806	3.648304094	-5.177722915
H	6.812099302	3.476586695	-4.578361721
H	6.113530744	3.329024962	-6.209066360
H	5.711540412	4.732341947	-5.191090079
C	2.213815450	5.167274425	-1.388768901
H	2.985566666	5.929789355	-1.593273200
H	1.770723628	4.845202791	-2.343551201
H	1.435411805	5.674136937	-0.794021370

TS1'*butyl,oblique*

163
Co2C123H32O6

Co	-4.436470090	0.225852124	0.165857805
Co	-6.465779509	-2.357064185	0.645807019
C	-7.052969156	-1.154509269	-0.572786249
C	-4.931687993	1.203754478	-1.270421445
C	-5.423415628	-3.735385868	0.283743507
C	-6.739733757	-1.643396391	2.277458708
C	-7.963531920	-3.323685576	0.616857067
O	-5.316525489	1.816842242	-2.174033824
O	-7.582710896	-0.437631740	-1.306800176
O	-4.756474742	-4.652610069	0.037776431
O	-6.940438199	-1.186024771	3.317215712
O	-8.908526253	-3.985585050	0.601723104
C	-3.809968316	-1.445054824	-0.513457604
C	-4.404453383	-1.659734486	0.749899723
C	-5.046281935	1.051096429	1.613644380
O	-5.435487367	1.545535122	2.585833325
H	-1.585233343	6.818968493	3.532957689
H	-4.084939872	6.070269096	0.024807951
H	-3.315980706	6.297019227	2.319255714
H	-3.496442672	6.212387144	-2.101752484
H	-1.621046111	6.778821910	-3.539081597
H	2.398118157	8.045028868	-2.239126027
H	0.466050930	7.434933435	-3.578190748
H	3.109368931	8.275854645	-0.172295052
H	2.411865270	8.067819859	2.146025605
H	0.729911145	7.542421831	3.452153447
C	0.503868397	6.480332743	3.377715872
C	-3.138725091	5.363079363	1.789377602
C	-0.801664335	6.072016759	3.421609384
C	-1.145642493	4.713317215	3.148511104
C	-3.571647144	5.235450426	0.498781770
C	-3.196980659	4.093170961	-0.274553039
C	-2.295447900	4.362275717	2.365757591
C	-2.752242341	5.450771923	-2.327828872
C	-2.787644744	4.197594396	-1.644654200
C	1.123536635	6.650641602	-3.207867139
C	-1.695358040	5.770640030	-3.135924112
C	-0.614804493	4.850837924	-3.308251436
C	2.211870494	6.994583599	-2.454963919
C	2.988152100	5.983954051	-1.807189803
C	0.752727508	5.278150881	-3.354724985
C	3.157582538	7.302235069	0.311941096
C	3.449796036	6.134074487	-0.459035961
C	2.764701833	7.184931286	1.616200673
C	2.645312317	5.893826427	2.217900037
C	1.540781584	5.550768610	3.064897650
C	1.246769270	4.176794502	3.256613262
C	-2.344061508	3.072639612	1.782523964
C	-0.116774852	3.750407147	3.287438721
C	-0.401523764	2.369722496	3.065229218
C	-2.814895686	2.939983708	0.446029297
C	-2.514247923	1.733805170	-0.263288502
C	-1.540635134	2.013213777	2.307417387
C	-1.983440532	3.153082556	-2.171608729
C	-2.009750574	1.865470269	-1.572165601
C	1.766949612	4.315140239	-3.125904162
C	-0.880583904	3.489890168	-3.018281703
C	0.132592952	2.511927506	-3.222289153
C	2.907702676	4.674213491	-2.342077760
C	3.691996997	3.628455203	-1.772889507
C	1.477099584	2.930939915	-3.292725289
C	3.799154920	4.964336060	0.260692614
C	4.147343309	3.776260515	-0.445922118
C	3.386701825	4.842133042	1.624030683
C	3.351646709	3.540063023	2.201017569
C	2.259327223	3.202784821	3.027950103
C	1.978225710	1.826072989	3.265276601
C	-1.647276191	0.697141842	1.770465392
C	0.623302822	1.404726448	3.269076820
C	0.333008455	0.032402645	3.063062573
C	-2.314353217	0.508079899	0.491246613
C	-1.985241395	-0.729440208	-0.281965218
C	-0.798979829	-0.316675260	2.274629971
C	-1.235513268	0.796552679	-2.122274151
C	-1.317115543	-0.502189179	-1.580765205
C	2.509372266	1.962774007	-3.110489761
C	-0.147136434	1.135890430	-2.971037907
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C	3.642523771	2.317766855	-2.336734052
C	4.434993280	1.281743578	-1.774132619
C	2.213603806	0.588813736	-3.300233638
C	4.538453977	2.608589664	0.277581624
C	4.894558571	1.430915408	-0.432639049
C	4.130261630	2.489015825	1.630442532
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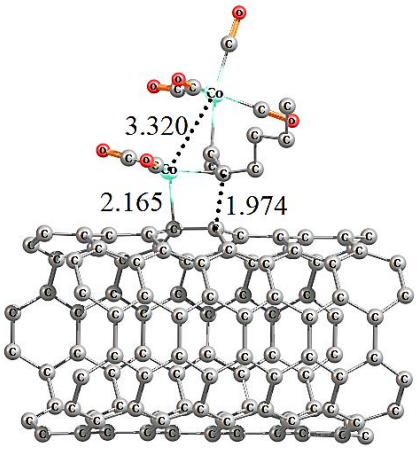

Note: Discarded in the main manuscript.

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C	-0.836290796	-1.639693447	1.726640400
C	1.355598674	-0.933778496	3.278545959
C	1.068552342	-2.320217698	3.096899756
C	-1.362732587	-1.822613018	0.447569505
C	-0.993903302	-3.001662431	-0.265047415
C	-0.046567424	-2.675607124	2.310346852
C	-0.527299781	-1.530377854	-2.145816096
C	-0.578384716	-2.860761360	-1.605458315
C	3.230579328	-0.379433496	-3.098285143
C	0.567836961	-1.197641579	-2.980839893
C	1.576647931	-2.177676381	-3.228705594
C	4.361737055	-0.027706130	-2.322763787
C	5.140354777	-1.076978940	-1.747152901
C	2.925050384	-1.763272533	-3.277710788
C	5.261095558	0.262404953	0.290874969
C	5.599570777	-0.928977424	-0.421267999
C	4.855966222	0.144137659	1.642026958
C	4.812980148	-1.157941628	2.229430513
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C	-0.118095481	-3.998091267	1.789369216
C	2.080865456	-3.291795954	3.329752336
C	-0.594314032	-4.161451445	0.451672251
C	0.181647015	-3.905498074	-2.191366778
C	3.945250362	-2.739080569	-3.094921453
C	1.291340850	-3.558070206	-3.029203300
C	5.083661548	-2.386552817	-2.304622755
C	5.984265255	-2.097701346	0.296357013
C	5.580610154	-2.214830472	1.663169137
C	3.656483627	-4.108988021	-3.320021494
C	4.737331133	-5.032038838	-3.157206677
H	4.642589163	-6.051500334	-3.526070232
C	5.886767788	-3.418821261	-1.756743854
C	5.821890173	-4.696650000	-2.396938182
H	6.569247646	-5.455464274	-2.172675726
C	0.133082741	-5.210752252	-1.626782893
C	0.875019123	-6.234009905	-2.301529115
H	0.692034645	-7.281343701	-2.068094113
C	2.289382351	-4.527889603	-3.291765045
C	1.922158446	-5.901326643	-3.110694927
H	2.554014196	-6.689822530	-3.515290615
C	0.654922041	-5.033913386	2.375378460
C	0.517032648	-6.342390310	1.806611297
H	0.892466646	-7.210855038	2.344653821
C	-0.261110807	-5.342167381	-0.261795397
C	0.076153997	-6.492878631	0.523047340
H	0.110350686	-7.477412796	0.059975871
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H	4.932119563	-5.930414959	3.531757056
C	1.784351276	-4.671580664	3.171631141
C	2.837491394	-5.596346308	3.460880710
H	2.614096873	-6.655364697	3.575654055
C	6.352869667	-3.269014185	-0.412876933
C	6.779902090	-4.389518724	0.368847682
H	7.294102918	-5.221604433	-0.108680572
C	5.567410558	-3.497141043	2.269581261
C	6.397733660	-4.500472578	1.675282720
H	6.614565462	-5.419048067	2.217361022
C	-3.794139689	-2.154662596	-1.831682722
H	-3.459132425	-3.197385292	-1.680189944
H	-3.040859303	-1.667013313	-2.466577922
C	-5.072133534	-2.159196387	-2.676973922
H	-5.864539203	-2.745008449	-2.191433103
H	-5.439142454	-1.126388126	-2.782563296
C	-4.786949936	-2.742281956	-4.058171145
H	-3.995255766	-2.147641556	-4.545579475
H	-4.386603781	-3.764301322	-3.945914329
C	-6.033552901	-2.764274580	-4.936576358
H	-6.432951716	-1.747392501	-5.072174699
H	-5.814853259	-3.179086784	-5.931254789
H	-6.825419974	-3.377205037	-4.478951216
C	-3.789034131	-2.072193213	2.068339224
H	-4.550190557	-2.244619011	2.834190367
H	-3.219040987	-3.011632526	1.967450732
H	-3.135259854	-1.290082587	2.471718111

TS1'*methyl,perpendicular*

163
Co2C123H32O6

Co	3.187104398	-2.946494264	1.310984659
Co	5.605579306	-2.314617004	0.315043654
C	4.584148453	-4.080539363	1.256376191
C	1.990985909	-4.246688656	1.402063348
C	6.822976738	-3.558118534	-0.083940197
C	6.449763193	-1.027269844	-0.521295414
C	5.915090438	-1.672450183	1.979900966
O	1.337412366	-5.192469457	1.504908473
O	5.031520640	-5.139809940	1.481251503
O	7.625832467	-4.331887737	-0.379063754
O	7.129549340	-0.323073721	-1.137835379
O	6.145699030	-1.191689688	3.004222777
C	3.100382994	-2.811629397	-0.728458398
C	4.366199811	-2.389369681	-1.129044386
C	3.271093527	-2.510683996	3.070317237
O	3.246229445	-2.221939236	4.183302353
C	4.626979662	-2.007156447	-2.550791600
H	4.858212316	-0.925343830	-2.589810721
H	3.709997103	-2.139777307	-3.150260334
C	5.779674439	-2.768266597	-3.216241280
H	6.717692113	-2.584508860	-2.670443130
H	5.584864816	-3.852742294	-3.157295663
C	5.951078183	-2.341950688	-4.671132978
H	5.010620043	-2.526944257	-5.217589279
H	6.120620415	-1.251733873	-4.704882745
C	7.101775014	-3.069722960	-5.357827478
H	8.054742313	-2.871389043	-4.843385913
H	6.937449512	-4.158300341	-5.352146607
H	7.207991819	-2.748968383	-6.404202405
C	2.472213701	-3.934274970	-1.522129663
H	3.115644336	-4.825664185	-1.457657267
H	1.480234025	-4.209136614	-1.141361775
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H	6.308301651	2.505152756	1.579341679
H	6.395292796	2.562501046	-0.850787220
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H	3.921829731	5.285271095	3.950011755
H	1.845150037	8.040043931	1.212060623
H	2.657726370	6.910245569	3.202204330
H	1.940572914	8.047442205	-0.982287770
H	2.937777582	6.920498328	-2.889117601
H	4.274061626	5.290968509	-3.505447619
C	3.829011632	4.327254184	-3.264373529
C	5.593659775	2.016332109	-0.357534814
C	4.628664873	3.316628639	-2.809473174
C	4.046721430	2.107251246	-2.314359035
C	5.547823162	1.980142985	1.004182330
C	4.404888944	1.422889803	1.663918387
C	4.526225893	1.461316167	-1.132539263
C	4.335554936	3.299276014	3.320704533
C	3.808124429	2.083401145	2.790380905
C	1.788671824	6.510351020	2.683044960
C	3.497240862	4.319545625	3.682332887
C	2.084687235	4.176193165	3.537697430
C	1.331045276	7.147114544	1.562842420
C	0.311944440	6.547538453	0.759533091
C	1.251113374	5.241866851	3.062680865
C	1.465867361	7.151136355	-1.377400907
C	0.377898283	6.548996834	-0.671519400
C	2.027297193	6.516694613	-2.450232766
C	1.532567851	5.243176895	-2.872445434
C	2.408170288	4.178073321	-3.258981268
C	1.904037788	2.852378132	-3.226605774
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C	2.485294090	-0.102112361	1.527329322
C	2.643653396	-0.121289166	-1.228310436
C	2.454961667	1.791382470	3.075476874
C	1.877300001	0.574393685	2.599548154
C	-0.033436843	4.916879840	2.560341182
C	1.580800508	2.851995128	3.465108138
C	0.176495349	2.635560198	3.384320919
C	-0.513505699	5.582379927	1.389280515
C	-1.578850142	4.978862675	0.659669633
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C	0.207129037	4.915411418	-2.493067406
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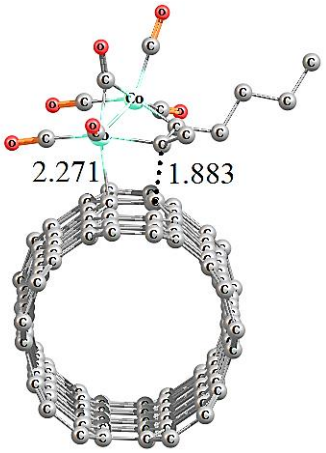

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C	0.566820111	-1.663250542	1.437046921
C	0.728474744	-1.698281306	-1.332289206
C	0.530303771	0.257472526	2.950486507
C	-0.035285472	-0.972900643	2.520954879
C	-1.959543819	3.375643433	2.462838553
C	-0.331797818	1.301954573	3.359360331
C	-1.736490617	1.092452367	3.314229761
C	-2.437258738	4.036752483	1.304869375
C	-3.507166797	3.450237172	0.576335995
C	-2.570659866	2.154911463	2.855840214
C	-2.302415961	4.034383433	-1.472142124
C	-3.438126643	3.449365445	-0.849406372
C	-1.715661440	3.372268870	-2.576686141
C	-2.281813879	2.150398727	-3.024927723
C	-1.405931060	1.088254735	-3.398291774
C	-1.909912512	-0.233671684	-3.415255762
C	-0.146187670	-2.603814391	-0.689866830
C	-1.085708502	-1.285181950	-2.935926874
C	-1.707125461	-2.508620033	-2.563951221
C	-0.220337847	-2.608491450	0.738481531
C	-1.368596418	-3.173558941	1.354765287
C	-1.239028556	-3.168777782	-1.409296853
C	-1.377694346	-1.283845719	2.885024092
C	-1.952371188	-2.512678201	2.458795927
C	-3.868813925	1.838768724	2.376547767
C	-2.241269381	-0.231710904	3.285117127
C	-3.651018773	-0.444113569	3.219234072
C	-4.346396123	2.499814200	1.214174997
C	-5.403640247	1.889723357	0.475553782
C	-4.474740515	0.604702737	2.756545584
C	-4.208733771	2.496673029	-1.564872748
C	-5.334750435	1.889028302	-0.933961407
C	-3.620773048	1.836530518	-2.676262179
C	-4.185667777	0.601718763	-3.111026093
C	-3.319916886	-0.446051205	-3.491383973
C	-3.835617542	-1.773063700	-3.533272930
C	-2.088722207	-4.126296794	-0.779881036
C	-3.006069514	-2.834971477	-3.057592041
C	-2.156657755	-4.129846542	0.648984144
C	-3.293854228	-2.836115268	2.819560635
C	-5.782781807	0.284749201	2.288841109
C	-4.166466413	-1.772444529	3.208187861
C	-6.259691287	0.944907303	1.113354001
C	-6.124539455	0.944957424	-1.652521243
C	-5.534226196	0.283177444	-2.774316137
C	-6.404310620	-0.918168196	2.704689222
C	-7.730946207	-1.154828099	2.232077682
H	-8.336481343	-1.939965676	2.680979053
C	-7.337897200	0.374713958	0.392224203
C	-8.186736515	-0.524845308	1.106408853
H	-9.144125687	-0.822290502	0.682631153
C	-3.852760562	-4.073448965	2.415872801
C	-5.182684181	-4.353012087	2.847374817
H	-5.587195592	-5.358565451	2.746807442
C	-5.568997518	-1.983074728	3.182433818
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C	-3.124980059	-4.739861948	-1.523474096
C	-3.918137877	-5.711175601	-0.841276672
H	-4.583817077	-6.363471546	-1.403525433
C	-3.266141951	-4.737898383	1.283356207
C	-3.985990665	-5.710842269	0.525896669
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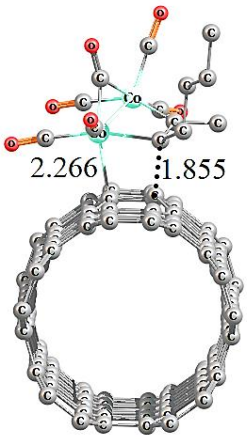
C	-5.233053181	-1.983303131	-3.644286158
C	-5.675035952	-3.337135543	-3.724582964
H	-6.699723210	-3.558324070	-4.017503695
C	-3.600140235	-4.070465160	-2.704247373
C	-4.879920026	-4.354229007	-3.268386047
H	-5.290834883	-5.360180525	-3.207607611
C	-7.268714417	0.375913742	-1.040957216
C	-8.042344218	-0.524734733	-1.834359705
H	-9.036920454	-0.821815965	-1.506756664
C	-6.112033077	-0.919907613	-3.248280374
C	-7.479794352	-1.154714417	-2.910829612
H	-8.038932022	-1.939154385	-3.417407147

TS1'*butyl,perpendicular*

163
Co2C123H32O6

Co	-3.353021280	2.803068929	1.077815101
Co	-5.704292075	2.161614050	-0.056983259
C	-4.787037705	3.890391271	1.045029894
C	-2.194523915	4.132269451	1.228480895
C	-6.876848446	3.416017888	-0.544359087
C	-6.466857659	0.881448431	-0.979607944
C	-6.119511149	1.479151777	1.570004344
O	-1.569082069	5.094012170	1.360440707
O	-5.298963018	4.897403671	1.356187411
O	-7.637172424	4.198744589	-0.918332030
O	-7.093728041	0.186094007	-1.658696728
O	-6.398943354	0.978234717	2.572121828
C	-3.148074772	2.686786023	-0.972458480
C	-4.410065165	2.319461312	-1.438509823
C	-3.498963616	2.323831404	2.818792009
O	-3.511453854	2.008958670	3.925139868
H	-5.559174427	-3.647395416	-3.135665277
H	-6.443063453	-2.688832585	1.093831941
H	-6.387694997	-2.727897087	-1.338468490
H	-5.630455822	-3.668925082	2.861866522
H	-4.161043341	-5.459867819	3.586767789
H	-1.876968249	-8.176258043	0.983108224
H	-2.826144831	-7.066827863	2.924133210
H	-1.845661040	-8.167930127	-1.214763686
H	-2.746281536	-7.040323759	-3.168624373
H	-4.064601876	-5.425917553	-3.854724609
C	-3.648481508	-4.456891689	-3.585025656
C	-5.623075958	-2.176633563	-0.794656081
C	-4.488435845	-3.457649801	-3.180904975
C	-3.955300388	-2.241037615	-2.649542209
C	-5.656436795	-2.151441323	0.567386203
C	-4.558617306	-1.587807869	1.295480538
C	-4.518399015	-1.602685484	-1.501569602
C	-4.562005684	-3.477080327	2.939685627
C	-4.019832220	-2.250846251	2.449222819
C	-1.933978899	-6.651372507	2.459225657
C	-3.733949680	-4.487127897	3.350305592
C	-2.317097556	-4.323687145	3.297647184
C	-1.399557281	-7.276565152	1.366966832
C	-0.343309206	-6.657678089	0.628647739
C	-1.440052051	-5.375996677	2.874063567
C	-1.361411916	-7.262360711	-1.575694542
C	-0.324826782	-6.650623146	-0.803685329
C	-1.868514834	-6.627441988	-2.674956119
C	-1.367618047	-5.344446470	-3.059589912
C	-2.233040456	-4.288659751	-3.491663296
C	-1.749514813	-2.956391816	-3.424240557
C	-3.747744052	-0.630631630	-0.819798561
C	-2.622206193	-1.914833843	-2.986766963
C	-2.056270596	-0.677032619	-2.536919891
C	-3.758059618	-0.646103645	0.618603123
C	-2.653049941	-0.040780268	1.281818772
C	-2.660411442	0.012651733	-1.479783701
C	-2.691010420	-1.942543619	2.819185691
C	-2.101642947	-0.716153643	2.384600310
C	-0.131629622	-5.030923368	2.453257780
C	-1.828470679	-2.992346630	3.260779670
C	-0.424984768	-2.756016773	3.269243522
C	0.428640841	-5.684268717	1.311286726
C	1.526676682	-5.061398201	0.649709017
C	0.440178758	-3.792974414	2.866028983
C	0.462904725	-5.669654971	-1.455632212
C	1.543521498	-5.053803684	-0.760456544
C	-0.070989035	-5.001956159	-2.601751490
C	0.506236309	-3.757002499	-2.983801931
C	-0.348654409	-2.716331689	-3.396048454
C	0.135280407	-1.372094521	-3.378524523
C	-2.038638899	1.205250221	-0.852244368
C	-0.729187583	-0.336225455	-2.959573675
C	-0.166606799	0.897649948	-2.535921821
C	-1.953070155	1.068214465	0.671716142
C	-0.754507448	1.546857050	1.319236643
C	-0.750765823	1.600278553	-1.452598601
C	-0.784471481	-0.381592159	2.821915910
C	-0.211019065	0.858980681	2.435396762
C	1.774157954	-3.461705180	2.478911489
C	0.065092668	-1.415551821	3.280600290
C	1.466743228	-1.185866370	3.323723949
C	2.330777291	-4.110346963	1.349505853
C	3.433575972	-3.504574318	0.689139106
C	2.342471861	-2.234325484	2.913144882
C	2.361788381	-4.093819421	-1.430254889
C	3.449961573	-3.496797279	-0.738139320
C	1.832160960	-3.433109924	-2.564144003
C	2.406974492	-2.201377337	-2.972392305



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C	1.744630081	2.446537425	-2.531119339
C	0.060683244	2.507699518	0.675881216
C	1.160305611	3.085912650	1.364517872
C	1.200661019	3.092776877	-1.402647743
C	1.101459474	1.187500926	2.883428143
C	1.684047154	2.426939050	2.499316259
C	3.662343543	-1.897184911	2.514446867
C	1.953591824	0.145442153	3.331309820
C	3.361743896	0.377810907	3.352894350
C	4.218665971	-2.545368989	1.380396186
C	5.309505612	-1.916588651	0.709467963
C	4.226643507	-0.656851257	2.935925968
C	4.248038418	-2.529298307	-1.401756404
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C	4.292221797	-0.627535500	-2.939256104
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C	1.996314820	4.058700274	-0.718712352
C	3.066283116	2.792879319	-2.944236286
C	1.976638763	4.056061011	0.711836318
C	2.996296989	2.766829994	2.942981462
C	5.555898161	-0.316546083	2.549618830
C	3.858362966	1.713057763	3.379593394
C	6.111956239	-0.963443526	1.401894314
C	6.143873672	-0.951237113	-1.367210248
C	5.613678437	-0.292751053	-2.520597722
C	6.134334592	0.892368176	3.007995386
C	7.483785723	1.149564422	2.617450403
H	8.050583298	1.939759297	3.106321411
C	7.223296427	-0.374393932	0.749539148
C	8.015071465	0.532492672	1.518076780
H	8.992259984	0.844981482	1.154505897
C	3.561813564	4.013578328	2.578999142
C	4.859019476	4.309059756	3.092445842
H	5.254452631	5.320771945	3.021829028
C	5.256861577	1.942774932	3.439610677
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H	6.716167700	3.534361551	3.772562776
C	3.067152236	4.690190265	-1.395397092
C	3.803787484	5.668510009	-0.661619041
H	4.493257652	6.332891740	-1.179329568
C	3.036827275	4.675799941	1.415404356
C	3.788263529	5.662051657	0.707205123
H	4.466863527	6.320113888	1.246822659
C	5.335700193	1.973228096	-3.399035929
C	5.763758721	3.333154979	-3.445905304
H	6.801351065	3.569089470	-3.675114566
C	3.621466446	4.033827158	-2.548895102
C	4.929222450	4.337196867	-3.033257666
H	5.322525909	5.347946567	-2.942641826
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H	9.018342222	0.852715275	-1.039094784
C	6.203165154	0.919722432	-2.954655913
C	7.544884871	1.170885772	-2.534014859
H	8.123553053	1.964055595	-3.003791411
C	-2.451094902	3.814087247	-1.710532836
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C	-3.288503300	5.084879546	-1.805294938
H	-4.216751889	4.888994887	-2.369905197
H	-3.603884143	5.395943300	-0.795771921
C	-2.507518103	6.221601201	-2.456712848
H	-1.585806405	6.397635680	-1.875497883
H	-2.184369899	5.910772707	-3.465313644
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H	-3.623867610	7.846853549	-1.540830952
H	-2.738253690	8.317968675	-3.011398779
H	-4.232498927	7.359451067	-3.139050479
C	-4.656488068	2.051463679	-2.880184115
H	-5.695716603	2.246087962	-3.178495683
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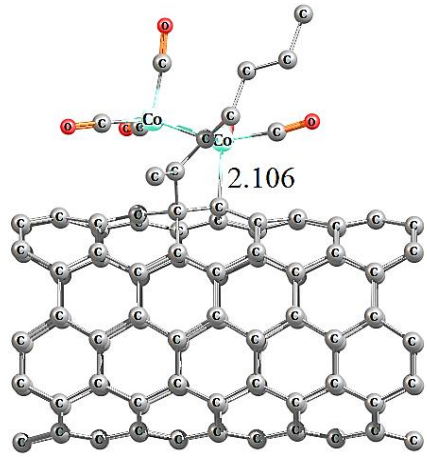
CP4*methyl,oblique*



161
Co2C122H32O5

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C	6.167525037	-1.496685732	0.641339292
C	2.668036124	-3.295359805	-2.594705311
C	1.754554700	-4.776207323	-0.590211594
C	4.862280903	-1.823880417	-1.706151234
O	6.940431570	-0.795705265	1.146940696
O	6.598774572	-4.903785706	-0.655455448
O	2.536528317	-3.283472305	-3.741124516
O	1.182316279	-5.779817773	-0.481389649
O	4.978057881	-1.340254613	-2.756557906
C	3.569661253	-2.059113363	1.478852713
C	3.490001686	-3.378835821	0.995344710
H	-5.540698880	-4.422089222	3.812553707
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H	-4.317442002	-5.827410798	2.673444402
H	-4.042442894	-6.203466491	-1.732518024
H	-5.297828572	-4.824320876	-3.293356192
H	-8.188817255	-1.678621483	-2.211287073
H	-6.775191564	-3.225365934	-3.441088836
H	-8.757687896	-1.031453917	-0.186313105
H	-8.336896133	-1.437716107	2.173213314
H	-7.180620535	-2.641142492	3.604886084
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C	-3.535196690	-5.297913769	2.132699252
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C	-2.999941370	-4.077810931	2.661533159
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C	-6.357063667	-2.280403237	-3.099483049
C	-4.369684992	-4.442999183	-2.871960093
C	-3.987329407	-3.081215345	-3.099410719
C	-7.152861125	-1.410321483	-2.410012114
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C	-7.676469728	-0.771577039	1.621192129
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C	-5.714925185	-1.084173555	3.141980602
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C	-3.383740014	-1.797357317	3.454362684
C	-2.014069272	-1.478909309	3.239504691
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C	-0.475708067	-3.290938526	0.060478929
C	-1.192175296	-2.401629626	2.555305018
C	-1.894960980	-3.552026420	-1.898366102
C	-0.727975724	-3.008143693	-1.298198404
C	-4.519997695	-0.695101689	-3.044429279
C	-2.646250325	-2.731439841	-2.798890066
C	-2.188583545	-1.406570330	-3.044249056
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C	-2.538069095	0.912896305	3.287302652
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C	-0.214716383	0.195781499	3.159596073
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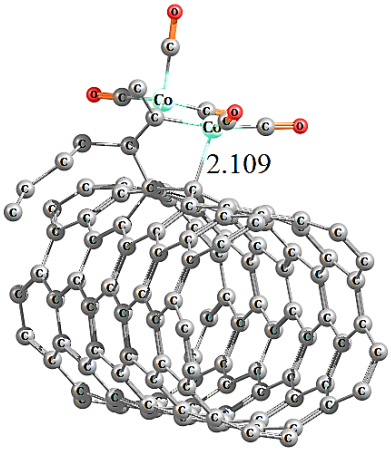
C	-0.834149339	-1.055295550	-2.754068522
C	-0.378619191	0.255548875	-3.040610211
C	-3.544579343	1.895604919	-2.365549658
C	-2.971947642	3.093038832	-1.856568931
C	-1.334967156	1.294956743	-3.209588862
C	-4.275686436	2.730789982	0.180597341
C	-3.348353871	3.526304326	-0.552257014
C	-4.030333739	2.492943197	1.553358550
C	-2.866953147	3.055414417	2.144690463
C	-2.101271107	2.245111385	3.030465860
C	-0.747935680	2.582184604	3.260984411

C	1.847766347	-0.276792449	1.965770681
C	0.213551833	1.534982193	3.319803842
C	1.581075788	1.848934083	3.128841295
C	2.570107320	-1.054192342	0.856808642
C	3.290273315	-0.010329363	0.023504737
C	2.404089262	0.928201097	2.438523063
C	1.704115082	-0.197969559	-1.837603913
C	2.899770062	0.348747136	-1.262146505
C	-0.907542666	2.640971251	-3.076576538
C	0.964566893	0.601414473	-2.739018185
C	1.423493781	1.918511379	-3.041775637
C	-1.741332181	3.559293107	-2.394355825
C	-1.150991194	4.749693445	-1.873304994
C	0.479420316	2.948063286	-3.212344023
C	-2.479404428	4.405850393	0.145752647
C	-1.527679024	5.181408592	-0.584525493
C	-2.231670213	4.164539118	1.523050781
C	-1.047144596	4.707406095	2.102510636
C	-0.291594520	3.901092371	2.981234352
C	1.070976741	4.241814897	3.221670043
C	3.694601669	1.379346176	1.990347492
C	2.032028459	3.189827406	3.312166815
C	4.132809866	0.911665693	0.708217166
C	3.541364458	1.455720628	-1.907165317
C	0.919041217	4.298598228	-3.106863253
C	2.783284632	2.262671858	-2.805296273
C	0.078331235	5.227001715	-2.417710134
C	-0.657061009	6.073379593	0.108502791
C	-0.405680973	5.826573029	1.494117891
C	2.288419805	4.608131614	-3.295667784
C	2.652333122	5.986634685	-3.213065767
H	3.633257880	6.312056011	-3.554213816
C	0.641276331	6.432174760	-1.931694262
C	1.850450305	6.875279168	-2.550353663
H	2.211643944	7.887041391	-2.375701356
C	4.762906855	1.956818173	-1.400409128
C	5.379839936	3.026349988	-2.117015448
H	6.405391686	3.310702120	-1.887629730
C	3.252651026	3.554704826	-3.155754546
C	4.643441100	3.808554448	-2.965331426
H	5.097695158	4.699715432	-3.394240452
C	4.268305589	2.543298002	2.532958037
C	5.538745391	2.944906292	2.004476480
H	6.142566268	3.681105329	2.531614791
C	5.046422176	1.705798494	-0.017061080
C	5.909690259	2.548966480	0.750734246
H	6.797009662	2.983417926	0.293078993
C	1.514421740	5.568032770	2.990993265
C	2.872307490	5.854601710	3.304772455
H	3.220888409	6.885482301	3.320042859
C	3.410552243	3.487531644	3.210402677
C	3.793049670	4.842105279	3.415063173
H	4.844862123	5.100304347	3.520095353
C	0.258090676	6.872094279	-0.620935878
C	1.067468117	7.775111522	0.133892975
H	1.616040941	8.567817984	-0.371513320
C	0.745849660	6.390094723	2.095901949
C	1.306095281	7.538939726	1.460245107
H	2.039374740	8.149120641	1.984419273
C	3.534244486	-4.581690875	1.892347759
H	2.483845263	-4.721765154	2.223807718
H	4.096641789	-4.356449983	2.813344817
C	4.040121308	-5.885342683	1.281151408
H	3.806900170	-5.912739869	0.203961370
H	5.139104516	-5.925967301	1.349062526
C	3.434382881	-7.115218219	1.947873788
H	3.646397999	-7.087078270	3.031301369
H	2.336532918	-7.068923384	1.842204585
C	3.954598080	-8.416924875	1.348109872
H	5.047746426	-8.490965676	1.456376745
H	3.504113969	-9.293966699	1.835192094
H	3.720936647	-8.468207602	0.273320151
C	4.132144348	-1.737752390	2.839663961
H	3.332368428	-1.751536712	3.600999254
H	4.898272724	-2.471701380	3.117910558
H	4.603114970	-0.745221082	2.873555187

CP4*butyl,oblique*



161
Co2C122H32O5

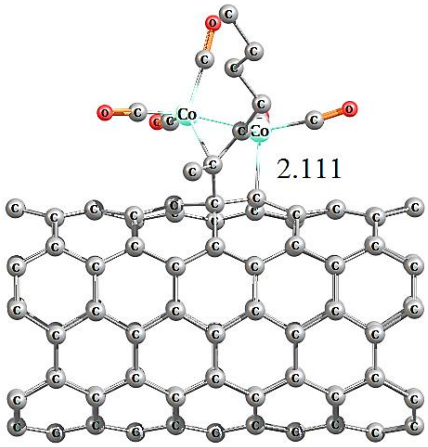
Co	4.264599356	-3.635990184	-0.735272273
Co	1.928880274	-4.084299953	-1.145792075
C	4.793541092	-5.296827235	-1.005961077
C	5.748061266	-2.862479016	-0.176333670
C	1.550331871	-3.957042311	-2.915080546
C	0.693743579	-5.248913882	-0.745433018
C	4.100793658	-2.954621438	-2.360313047
O	6.724947783	-2.377228101	0.216147543
O	5.158293109	-6.380714076	-1.193703540
O	1.267862043	-3.927944278	-4.033607950
O	-0.012572110	-6.131884229	-0.488200232
O	4.163041417	-2.518840831	-3.435515513
C	3.174480521	-2.976120131	1.040280301
C	2.807956601	-4.231004797	0.533116355
H	-6.052717821	-3.321537490	4.109653330
H	-5.004069431	-5.761573104	0.622427003
H	-5.251524314	-4.947131515	2.899009717
H	-5.410085498	-5.315781811	-1.512549763
H	-6.453557293	-3.676929599	-2.975438675
H	-8.501131999	0.013489014	-1.693691894
H	-7.556584461	-1.791842908	-3.017735859
H	-8.758400564	0.750945834	0.369133528
H	-8.252478974	0.230092407	2.689654559
H	-7.276796871	-1.224913166	4.017348268
C	-6.200152157	-1.220227958	3.857236815
C	-4.417563014	-4.593733260	2.295493468
C	-5.512243013	-2.398500368	3.909172068
C	-4.131195078	-2.446940616	3.535923433
C	-4.278763683	-5.052269140	1.016983407
C	-3.298341746	-4.470182817	0.149743782
C	-3.590146922	-3.524983970	2.773834175
C	-4.848494184	-4.431982954	-1.810228545
C	-3.573900363	-4.162188127	-1.215536877
C	-6.917493256	-0.964842202	-2.714210853
C	-5.435233889	-3.511121428	-2.629029923
C	-4.785219827	-2.261608883	-2.891195646
C	-7.449518057	0.050613473	-1.971969282
C	-6.598550572	1.059164679	-1.417435090
C	-5.506046139	-1.028917991	-2.944205341
C	-7.790576186	1.032827239	0.779966247
C	-6.767659150	1.542450698	-0.083275669
C	-7.506507201	0.740078997	2.082979455
C	-6.181978366	0.937552871	2.590430399
C	-5.545874194	-0.017691129	3.440709816
C	-4.131118026	0.009897834	3.539834768
C	-2.354508648	-3.322818718	2.106605954
C	-3.408167775	-1.224078647	3.578700516
C	-2.021358640	-1.208910557	3.260103073
C	-2.204179244	-3.818368633	0.776139519
C	-1.162634609	-3.277967361	-0.019905872
C	-1.473717193	-2.280803692	2.519831165
C	-2.757150024	-3.190807406	-1.856901255
C	-1.455606687	-2.923355403	-1.353779816
C	-4.780284419	0.182134525	-2.811503569
C	-3.380649352	-2.214855499	-2.697720677
C	-2.666556751	-1.018570571	-2.985212376
C	-5.339344532	1.250326429	-2.043216954
C	-4.469561027	2.277560202	-1.578727723
C	-3.378786322	0.197039732	-3.060587626
C	-5.667072599	2.184528125	0.538896447
C	-4.637304822	2.756826331	-0.261965155
C	-5.367172939	1.874437323	1.901846047
C	-4.058651554	2.156967220	2.382186477
C	-3.428166596	1.201154888	3.207773885
C	-2.008343762	1.239504343	3.333263706
C	-0.214751662	-2.109908077	1.854183800
C	-1.297036977	0.020747442	3.338528765
C	0.087069470	0.036881267	3.027708575
C	-0.016112493	-2.695487411	0.601102515
C	1.125857288	-2.351163876	-0.252161410
C	0.650552023	-1.024090498	2.262996210
C	-0.633064436	-1.924332025	-1.962402753
C	0.687333643	-1.693687591	-1.476104477
C	-2.657979301	1.426211582	-2.972930531
C	-1.249940825	-0.972609800	-2.801356372
C	-0.544035588	0.211471562	-3.132598831
C	-3.216013159	2.492439505	-2.228592545
C	-2.358753461	3.531258230	-1.772778534
C	-1.261932916	1.434874993	-3.236490983
C	-3.545531608	3.433635298	0.363152983
C	-2.527959160	4.018450636	-0.444314744
C	-3.250533870	3.128237342	1.712398039
C	-1.949976325	3.415941318	2.207700977
C	-1.313238606	2.448121904	3.035729689
C	0.094523692	2.481087724	3.159767985

C	1.902924023	-0.861524209	1.682732516
C	0.807677694	1.248986398	3.148875139
C	2.190389520	1.261661772	2.848449884
C	2.351986725	-1.767927366	0.526491294
C	3.214185744	-0.892382155	-0.370534481
C	2.738055771	0.191910524	2.100245760
C	1.477924459	-0.695751272	-2.093018435
C	2.802998833	-0.428511787	-1.618678014
C	-0.543856920	2.654980462	-3.148155836
C	0.860621588	0.254543551	-2.940150974
C	1.569232717	1.442795414	-3.288564290
C	-1.102511836	3.725395860	-2.408343720
C	-0.227827956	4.751805212	-1.940842866
C	0.861300049	2.654806173	-3.393694706
C	-1.435900871	4.677556488	0.179055696
C	-0.398515841	5.237407908	-0.627649846
C	-1.139069479	4.368515765	1.533071115
C	0.176405474	4.633748291	2.014915466
C	0.803728725	3.672191965	2.836723277
C	2.221892680	3.706351641	2.969615327
C	4.058460676	0.360043490	1.552312839
C	2.935243775	2.469351050	2.992602058
C	4.283020260	-0.172562887	0.241820545
C	3.616839980	0.519915555	-2.319087484
C	1.591395821	3.876078300	-3.331366218
C	2.985114218	1.480894466	-3.161474102
C	1.029575733	4.956855219	-2.582964814
C	0.697620743	5.908415216	-0.009545145
C	0.996971495	5.594046512	1.352688920
C	2.976241731	3.882273099	-3.629279777
C	3.636701208	5.147803689	-3.583493111
H	4.634744653	5.256725054	-4.003738927
C	1.878128071	6.004046719	-2.148330819
C	3.102121802	6.181406358	-2.863747237
H	3.687195986	7.088533961	-2.724005056
C	4.955515933	0.736673080	-1.916813590
C	5.731784209	1.651523658	-2.690056481
H	6.809813274	1.702333097	-2.546490804
C	3.695864015	2.642593789	-3.559057504
C	5.119034315	2.583598310	-3.484100775
H	5.721455122	3.357136538	-3.956611811
C	4.911250020	1.364364418	2.045953536
C	6.191192332	1.493398991	1.414392850
H	6.978540640	2.077167966	1.887372647
C	5.284175475	0.418828189	-0.557262232
C	6.365353827	1.048305826	0.134495959
H	7.284035487	1.292635449	-0.396378361
C	2.924236716	4.906943336	2.697585806
C	4.331596876	4.888438915	2.907099840
H	4.895866044	5.818973449	2.890481583
C	4.333974379	2.461886293	2.786086029
C	5.015824686	3.699101377	2.955106542
H	6.103443713	3.721717643	2.980484647
C	1.704516936	6.498818220	-0.812748741
C	2.747893883	7.193709644	-0.128054321
H	3.414615763	7.854869886	-0.678665315
C	2.286822440	5.886165873	1.859595688
C	3.032364351	6.893719990	1.176251875
H	3.919544720	7.323190633	1.638078227
C	3.931572893	-2.842913865	2.342751897
H	4.432337330	-1.864586776	2.394324804
H	4.741827888	-3.585858498	2.356941842
C	3.013380707	-3.029893833	3.575109787
H	1.957920987	-2.964374924	3.265537025
H	3.133773878	-4.053374343	3.969828779
C	3.261910502	-2.020200956	4.692589305
H	4.264687761	-2.187688078	5.123455821
H	3.276121944	-1.002253989	4.268664717
C	2.194256807	-2.091757760	5.779359468
H	1.201455415	-1.863426962	5.358203960
H	2.146045124	-3.097330955	6.226206514
H	2.391627855	-1.369095833	6.584353769
C	2.872427765	-5.488672103	1.348820208
H	1.982303755	-5.539560720	1.998818178
H	2.891227061	-6.386991007	0.718225517
H	3.761317614	-5.508204867	1.999105102

CP4*_methyl,oblique_

161
Co2C122H32O5

Co	2.557410987	-4.474819354	0.456454251
Co	3.824071773	-2.519560019	0.989181639
C	3.972600559	-5.332705596	1.065562791
C	1.556702084	-5.686105195	-0.353766682
C	3.686832724	-2.302492686	2.779486851
C	5.369732077	-1.732890749	0.784478333
C	1.719726144	-4.280759907	1.999156308
O	0.872129469	-6.441151678	-0.903444874
O	4.832512634	-5.952532937	1.534898550
O	3.633291735	-2.165442477	3.924762671
O	6.454265053	-1.341696425	0.654838389
O	1.215590485	-4.279655020	3.042747587
C	2.422759406	-3.122686036	-1.301127949
C	3.705883340	-3.260785183	-0.758521352
H	-5.464295372	-4.496699178	3.377079472
H	-3.999633664	-6.378523410	-0.273173469
H	-4.372718143	-5.851713977	2.071703970
H	-4.490791313	-5.750983651	-2.360568449
H	-5.803919340	-4.140084764	-3.623993818
H	-8.431999011	-0.991364790	-1.992667576
H	-7.198870218	-2.477128250	-3.464967079
H	-8.816989287	-0.509394085	0.120805229
H	-8.223179159	-1.200139833	2.375612094
H	-7.014487633	-2.634176852	3.512067945
C	-5.953195964	-2.433032187	3.378809397
C	-3.616254755	-5.301212351	1.515658706
C	-5.080434810	-3.481305287	3.300372214
C	-3.709056623	-3.261566829	2.957482392
C	-3.404581930	-5.599864454	0.201108716
C	-2.530142189	-4.781497423	-0.588158304
C	-2.987752827	-4.152502788	2.103250579
C	-4.085626429	-4.757198290	-2.543596535
C	-2.866989972	-4.355664026	-1.906336332
C	-6.707310860	-1.587163362	-3.076727269
C	-4.824028132	-3.851741342	-3.248210137
C	-4.389098033	-2.490160309	-3.356706613
C	-7.402292097	-0.750091541	-2.249870063
C	-6.734272027	0.327178769	-1.586865851
C	-5.306065455	-1.393593862	-3.287703022
C	-7.906731225	-0.122008741	0.574899101
C	-6.980601096	0.634714093	-0.211488943
C	-7.572671576	-0.510483742	1.840887228
C	-6.296469831	-0.160816117	2.385916230
C	-5.507135406	-1.098722390	3.122771031
C	-4.115567017	-0.853472657	3.243577211
C	-1.802414208	-3.684514924	1.481809411
C	-3.202997270	-1.950025442	3.145905307
C	-1.841258879	-1.666750568	2.841728334
C	-1.550471672	-4.040166999	0.118887495
C	-0.602163253	-3.270218961	-0.601823877
C	-1.136124988	-2.531970283	1.985181202
C	-2.225662609	-3.190195036	-2.413737009
C	-0.981170044	-2.783094166	-1.867904001
C	-4.793186354	-0.098539187	-3.023104156
C	-3.014138118	-2.235336393	-3.137734290
C	-2.511992151	-0.911168956	-3.279609309
C	-5.522330700	0.782151686	-2.164587513
C	-4.831062900	1.883655798	-1.581140569
C	-3.413997768	0.171821622	-3.244894433
C	-5.996992906	1.373376927	0.493634105
C	-5.073198798	2.186919226	-0.224796055
C	-5.646615946	0.965150230	1.818395327
C	-4.395786403	1.397468831	2.343522182
C	-3.615745458	0.467154797	3.061587287
C	-2.219847876	0.720752180	3.211995006
C	0.068273262	-2.068240392	1.360762371
C	-1.321506300	-0.359968195	3.080043697
C	0.044556131	-0.091109245	2.801333011
C	0.434273983	-2.572393810	0.109389077
C	1.563414390	-1.984236254	-0.718763026
C	0.757266181	-0.952391681	1.923763210
C	-0.342231591	-1.574649532	-2.338974368
C	0.908759902	-1.179595386	-1.844625700
C	-2.906461954	1.489634315	-3.026759107
C	-1.124696930	-0.650873640	-3.072953462
C	-0.624509459	0.657449053	-3.275658086
C	-3.630010269	2.366598047	-2.184032611
C	-2.950321842	3.475186798	-1.607102128
C	-1.534233830	1.753854914	-3.268413320
C	-4.103076400	2.959030559	0.486401321
C	-3.192467117	3.780155083	-0.236742433
C	-3.756536301	2.553956036	1.797694031
C	-2.514708867	2.986900479	2.338984963
C	-1.727989261	2.045645680	3.059276644
C	-0.336860905	2.286687181	3.202726900



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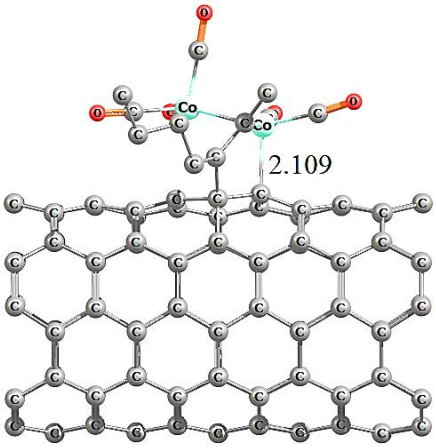
C	0.560815099	1.200986144	3.073422520
C	1.934378291	1.467033755	2.811783454
C	2.508838767	-1.096523401	0.152103108
C	3.262525101	-0.089667877	-0.616227736
C	2.650318546	0.601149320	1.964623402
C	1.524210990	-0.030543734	-2.339498447
C	2.829547178	0.373583867	-1.862759050
C	-1.019751173	3.054517887	-3.039028527
C	0.754494229	0.906597354	-3.075461906
C	1.263930042	2.219651731	-3.291669359
C	-1.741384236	3.935069134	-2.198065186
C	-1.039715877	5.030707708	-1.609534338
C	0.367816717	3.306292826	-3.266230782
C	-2.213256439	4.530394812	0.471775907
C	-1.281145476	5.335107603	-0.253681323
C	-1.866801275	4.124631825	1.784362009
C	-0.607363984	4.542117641	2.314374258
C	0.168615601	3.609212162	3.033033455
C	1.561106528	3.857469486	3.199247684
C	3.904101395	1.046649079	1.448795398
C	2.468282262	2.757734630	3.101991952
C	4.188133485	0.730673955	0.081113374
C	3.455459104	1.524528958	-2.434662384
C	0.890536525	4.614011236	-3.062502829
C	2.659743468	2.467027950	-3.161168306
C	0.166199795	5.501687180	-2.207142560
C	-0.304023850	6.098482830	0.450054298
C	0.044788516	5.688295785	1.774590292
C	2.254961457	4.874836174	-3.342043059
C	2.705403090	6.217623607	-3.147764428
H	3.668620773	6.532247864	-3.544845071
C	0.841069566	6.614086680	-1.646175709
C	2.017910606	7.063754060	-2.322698340
H	2.449307745	8.032432115	-2.077100279
C	4.725504503	1.942381968	-1.959163252
C	5.340434245	3.054880832	-2.615703320
H	6.393803831	3.270287529	-2.444292272
C	3.163269196	3.768540137	-3.407965075
C	4.580328161	3.943976914	-3.320318454
H	5.041198088	4.851066769	-3.706673802
C	4.587945349	2.122418560	2.057939799
C	5.826798166	2.525453063	1.457546343
H	6.514189344	3.168329766	2.004071192
C	5.089640036	1.550578854	-0.634870345
C	6.062448195	2.261073791	0.139313780
H	6.930843307	2.701986681	-0.347550547
C	2.058349917	5.178807374	3.067087955
C	3.452061544	5.370937833	3.308160503
H	3.849986496	6.377739528	3.420375366
C	3.848731893	3.007945279	2.911780532
C	4.320599211	4.315992213	3.235845672
H	5.390054402	4.507590477	3.297009468
C	0.596360024	6.923807880	-0.269379666
C	1.518184262	7.698617185	0.502425006
H	2.065978692	8.515886222	0.036737182
C	1.274307399	6.124395052	2.329061710
C	1.849355617	7.307857938	1.769394542
H	2.654223577	7.822256027	2.291262394
C	4.873567049	-3.727550638	-1.603022857
H	5.809720218	-3.400600829	-1.125406580
H	4.814702824	-3.180640147	-2.562254528
C	5.010315917	-5.227173420	-1.897177267
H	5.340388067	-5.750220074	-0.987279206
H	4.037650531	-5.667907122	-2.164638987
C	6.015631663	-5.488251401	-3.015237137
H	5.668292609	-4.990983094	-3.937667324
H	6.978883835	-5.017099365	-2.752710967
C	6.220907151	-6.977247360	-3.274611564
H	6.598136398	-7.483522090	-2.372737286
H	5.272212206	-7.459869283	-3.556666436
H	6.942349143	-7.148133244	-4.086783481
C	2.046900238	-3.666740304	-2.650378715
H	1.012178377	-4.037778056	-2.683980736
H	2.130291842	-2.865440686	-3.405613342
H	2.706388368	-4.489271660	-2.943803291

CP4*$_{butyl,oblique}$



161
Co2C122H32O5

Co	-1.762928155	-4.878383554	0.590775627
Co	0.601317675	-4.563299981	1.095040896
C	-1.760838983	-6.626811877	0.803124945
C	-3.428194842	-4.618002574	0.066271178
C	0.919236343	-4.310030159	2.859389725
C	2.141372977	-5.298295843	0.756288573
C	-1.770687017	-4.259633497	2.249007552
O	-4.521767565	-4.502661857	-0.298575848
O	-1.777219909	-7.774881648	0.952671830
O	1.182050639	-4.177988411	3.975794700
O	3.118857915	-5.887733362	0.550477775
O	-1.991905381	-3.891202933	3.328695197
C	-0.852550965	-3.978604790	-1.191618394
C	-0.121769864	-5.023546917	-0.612451985
H	-6.746562792	1.211637344	3.758814029
H	-7.417188708	-1.106383968	0.120926021
H	-7.146342266	-0.488682748	2.456987266
H	-7.354264852	-0.342035692	-1.976985201
H	-7.025836898	1.690906384	-3.270919704
H	-6.229244340	5.728703923	-1.677573516
H	-6.641733321	3.831518480	-3.135682920
H	-6.011637928	6.327045264	0.429433261
H	-6.050777380	5.434524749	2.690513439
H	-6.311996883	3.597569721	3.859261222
C	-5.482934552	2.913639490	3.687633199
C	-6.264736579	-0.715322201	1.860443790
C	-5.727423054	1.570376336	3.628701897
C	-4.695819010	0.660305895	3.237007575
C	-6.417312867	-1.064487731	0.549579609
C	-5.267064537	-1.205097699	-0.293886363
C	-4.955750928	-0.463173173	2.390914406
C	-6.342442762	-0.015790243	-2.211643449
C	-5.222236861	-0.685430663	-1.621385631
C	-5.627234504	4.026313282	-2.793296741
C	-6.157829448	1.127425966	-2.933880101
C	-4.842333930	1.669281914	-3.107924723
C	-5.395133971	5.095484017	-1.974151456
C	-4.111762299	5.275716796	-1.369027984
C	-4.589224870	3.077288796	-3.052662010
C	-5.107901908	5.882799813	0.842561414
C	-3.971139789	5.660909718	0.002174934
C	-5.129907092	5.380568026	2.112773097
C	-4.016004994	4.632144498	2.608745473
C	-4.189520994	3.428403049	3.362548816
C	-3.101949688	2.520786866	3.433988616
C	-3.865973329	-1.068581796	1.716149824
C	-3.358251958	1.115888548	3.356796739
C	-2.281224486	0.253274389	3.002881398
C	-4.037489224	-1.472179978	0.356048080
C	-2.872645316	-1.707783438	-0.417954697
C	-2.531259643	-0.847286377	2.160548377
C	-3.943715293	-0.430654122	-2.191851799
C	-2.805855590	-1.115082301	-1.691808755
C	-3.256951020	3.516781565	-2.848163990
C	-3.754083217	0.780884926	-2.935231067
C	-2.424757995	1.246606215	-3.138977463
C	-3.012013964	4.640679401	-1.998741773
C	-1.698298888	4.819539176	-1.475429849
C	-2.174291844	2.633484829	-3.118651916
C	-2.741127288	5.383929632	0.650472906
C	-1.558891815	5.199977388	-0.124181836
C	-2.765140384	4.856497226	1.979121763
C	-1.605236414	4.179622493	2.452141716
C	-1.780238803	2.987056018	3.185004858
C	-0.682117022	2.082710100	3.287613733
C	-1.435211416	-1.475199172	1.483346529
C	-0.937672357	0.697952944	3.174079356
C	0.131842376	-0.174597462	2.842578269
C	-1.644999613	-2.080570526	0.234045808
C	-0.507476726	-2.564503857	-0.654970759
C	-0.113679314	-1.275413883	1.977387170
C	-1.493672830	-0.838476777	-2.232878263
C	-0.368243049	-1.552324593	-1.797410827
C	-0.830060738	3.091697904	-2.962550960
C	-1.324791029	0.351480083	-2.980102765
C	-0.012539926	0.808064550	-3.246703315
C	-0.585234230	4.210178576	-2.130576512
C	0.725940362	4.402754825	-1.614104362
C	0.241943853	2.210011414	-3.253125845
C	-0.311573118	4.956131735	0.529385047
C	0.867364071	4.786050248	-0.249336228
C	-0.336654542	4.433293221	1.844888909
C	0.818205978	3.763525488	2.334302094
C	0.638514283	2.558319950	3.068469478
C	1.724394898	1.648823889	3.162160304

C	0.981648343	-1.939954513	1.374224086
C	1.465066858	0.264054994	3.047028744
C	2.540709668	-0.614748390	2.732336093
C	0.822213759	-2.691243013	0.149434101
C	2.038957284	-2.639953641	-0.676364069
C	2.299586740	-1.715194598	1.892164644
C	0.883150072	-1.282745852	-2.353002307
C	2.054736155	-2.019643278	-1.930458961
C	1.577802097	2.652161213	-3.085334917
C	1.072020516	-0.088996356	-3.096615200
C	2.393744668	0.365673487	-3.375598572
C	1.826805075	3.771863150	-2.256284077
C	3.142995163	3.940042978	-1.728854792
C	2.650757676	1.750840566	-3.362027710
C	2.103844494	4.520706314	0.402410665
C	3.284306226	4.323658867	-0.378981780
C	2.078209959	3.998308024	1.718725573
C	3.232740786	3.305702401	2.197630136
C	3.052676394	2.113598107	2.929016513
C	4.146089442	1.208761413	3.045836587
C	3.419464183	-2.390421956	1.323733934
C	3.884142440	-0.193285112	2.959927587
C	3.293777378	-2.818920115	-0.036932097
C	3.310137399	-1.759169229	-2.561642066
C	3.996237446	2.191924298	-3.220945146
C	3.485964377	-0.543618015	-3.297414284
C	4.249820445	3.318475432	-2.377913095
C	4.529214844	4.069431498	0.267470160
C	4.502618021	3.543254990	1.596734322
C	5.059418352	1.314807392	-3.549845678
C	6.385146737	1.833195022	-3.417090707
H	7.226109912	1.297113449	-3.852683114
C	5.560573807	3.518187892	-1.878028548
C	6.629055041	2.904785328	-2.603929076
H	7.658570104	3.197428046	-2.406110574
C	4.468656368	-2.460691669	-2.136843509
C	5.684106017	-2.217307036	-2.851940819
H	6.533415084	-2.885547662	-2.719900937
C	4.793519494	-0.091819935	-3.604414841
C	5.842529558	-1.064248109	-3.565635342
H	6.813993459	-0.834226705	-3.999018989
C	4.711343627	-2.222118731	1.872381632
C	5.786437405	-2.913678912	1.221708622
H	6.746237381	-3.023925438	1.722730698
C	4.465916030	-2.986515461	-0.809343456
C	5.672033453	-3.270245937	-0.090865327
H	6.543914827	-3.653114880	-0.618784420
C	5.469511400	1.678449692	2.849704709
C	6.524320443	0.735299013	3.042276512
H	7.554856806	1.079188156	3.107907660
C	4.953976148	-1.088351751	2.716531901
C	6.273050379	-0.607993737	2.980372591
H	7.109674420	-1.303457391	3.003214676
C	5.705080561	3.908955047	-0.507949971
C	6.926882524	3.705407243	0.207713212
H	7.881714892	3.811820926	-0.303944150
C	5.653107047	2.884827193	2.099419717
C	6.901259309	3.205160218	1.479011185
H	7.836705336	2.923141787	1.958769554
C	-1.599686291	-4.026317144	-2.502612832
H	-0.897765556	-3.705098582	-3.297385002
H	-2.368693248	-3.240104428	-2.477444425
C	-2.310923799	-5.315294974	-2.918786235
H	-1.637416950	-5.964961346	-3.500405647
H	-2.612482036	-5.886737238	-2.025747281
C	-3.552587858	-5.006502653	-3.752836163
H	-4.234172377	-4.382647748	-3.149083491
H	-3.261802521	-4.397472371	-4.626500884
C	-4.276878607	-6.266790561	-4.210929516
H	-3.621266242	-6.894640741	-4.834421088
H	-4.595124383	-6.868532237	-3.345369468
H	-5.172047893	-6.022313966	-4.800897410
C	0.298973126	-6.260349090	-1.354791249
H	-0.498252707	-6.668933345	-1.987613473
H	1.146602841	-5.998194485	-2.011376718
H	0.626852267	-7.052852895	-0.669903808

CP4*methyl,perpendicular*

161
Co2C122H32O5

Co	1.841377460	-3.683569537	1.189859047
Co	3.992618206	-4.077834426	-0.355390286
C	1.051647809	-5.181694269	1.635935717
C	2.529647841	-3.320001031	2.805772662
C	5.366126218	-2.928983212	-0.216564068
C	4.597323729	-5.171645297	-1.584309692
C	4.244596884	-5.165300837	1.014103834
O	3.027718131	-3.092580693	3.821356766
O	0.505391526	-6.162241874	1.919087311
O	6.406662829	-2.418438027	-0.188840086
O	4.997431081	-5.899714359	-2.393815549
O	4.478617238	-5.917920910	1.866199508
C	2.454710327	-3.122267806	-1.559120430
C	2.032160123	-4.197498248	-0.728725433
H	6.525322382	2.296044116	-3.249504264
H	7.259925030	0.862310583	0.850473846
H	7.170077297	1.017488486	-1.577993955
H	6.760737077	1.941220693	2.674941056
H	5.821465868	3.986417850	3.584656729
H	4.230664657	7.370181093	1.293301510
H	4.920429981	5.920327131	3.116073453
H	4.147506075	7.500441315	-0.901609058
H	4.682668976	6.292576873	-2.939242802
H	5.519506889	4.446861528	-3.766796483
C	4.875224609	3.599153228	-3.541084406
C	6.299125552	0.661299046	-1.030581448
C	5.440991066	2.389794650	-3.248951793
C	4.632494385	1.308648091	-2.776295276
C	6.348079004	0.579217459	0.328228182
C	5.156982380	0.285395547	1.068586117
C	5.058854451	0.447150330	-1.715600481
C	5.682254872	2.018846726	2.798149754
C	4.830272108	1.004985547	2.267138647
C	3.938324332	5.779333779	2.668687437
C	5.153137509	3.171601787	3.313067398
C	3.740912313	3.372058350	3.327297582
C	3.549830256	6.596269536	1.643022725
C	2.350600983	6.317925476	0.917320193
C	3.148176547	4.642635147	3.021895803
C	3.436978864	6.772974823	-1.289798014
C	2.295579337	6.403816955	-0.512089035
C	3.738571580	6.091921097	-2.436246136
C	2.915022809	5.005603175	-2.866826109
C	3.468310674	3.792427356	-3.389745221
C	2.659213130	2.626811988	-3.374331292
C	4.083511590	-0.333661561	-1.051673788
C	3.247959076	1.367229998	-3.053319187
C	2.397141732	0.285467368	-2.650137415
C	4.130392554	-0.398772188	0.389016990
C	2.926481521	-0.739147855	1.069305179
C	2.845939814	-0.613609318	-1.685173960
C	3.479199619	1.015492059	2.681568812
C	2.588153213	0.002895353	2.212301960
C	1.782832109	4.673445198	2.645817204
C	2.927755391	2.215070938	3.227098656
C	1.511101367	2.342313364	3.293383613
C	1.374252911	5.529028780	1.575785099
C	0.135303686	5.251628566	0.928426777
C	0.926936840	3.591969903	3.004518311
C	1.267084351	5.696437007	-1.182560315
C	0.081029707	5.337355425	-0.478257930
C	1.584448898	4.981854871	-2.379598782
C	0.696854570	3.951092016	-2.801658557
C	1.244783072	2.753165031	-3.297101925
C	0.428756487	1.579638254	-3.330415940
C	1.975018733	-1.701487393	-1.109780774
C	1.005503295	0.336163949	-3.009285111
C	0.145896170	-0.736589875	-2.639391562
C	1.958623041	-1.599318891	0.438226850
C	0.712775387	-1.816632777	1.124437755
C	0.554234251	-1.636098910	-1.635574055
C	1.239909488	-0.012167217	2.690901772
C	0.363126434	-1.035044465	2.275923120
C	-0.458943402	3.640609381	2.665732391
C	0.695295403	1.173812991	3.243382226
C	-0.714569485	1.302307808	3.339084105
C	-0.864792050	4.489375608	1.606481177
C	-2.104207039	4.230033734	0.961503475
C	-1.307471277	2.566001781	3.044970817
C	-0.972621571	4.660745589	-1.164737994
C	-2.161738453	4.320470762	-0.461123268
C	-0.658408545	3.954176879	-2.348321304
C	-1.544012601	2.938395541	-2.796728145
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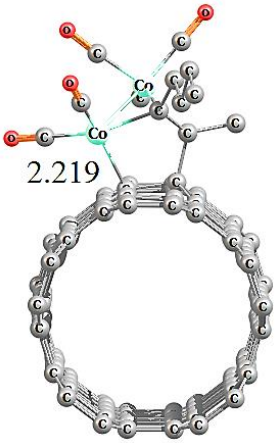
C	-1.809040880	0.574002688	-3.344757204



Note: Taken into consideration in the main manuscript.

C	-0.423484551	-2.385776081	-0.977449431
C	-1.232574168	-0.677326861	-3.002548969
C	-2.093584157	-1.741087569	-2.633209370
C	-0.323543987	-2.551468087	0.458887442
C	-1.536680862	-2.837948160	1.163604011
C	-1.691195756	-2.590799835	-1.582863325
C	-0.972395772	-1.050992846	2.738806741
C	-1.856287368	-2.091199550	2.316852378
C	-2.680708960	2.602752707	2.690881793
C	-1.523545867	0.138875948	3.279251584
C	-2.941024184	0.265052161	3.353453150
C	-3.088102264	3.452747035	1.629236407
C	-4.323904157	3.174037729	0.974913649
C	-3.527416509	1.512327517	3.051399245
C	-3.201425904	3.637593078	-1.142715872
C	-4.382412456	3.269797779	-0.431885742
C	-2.888130404	2.933231785	-2.336466017
C	-3.774150228	1.906227227	-2.772727576
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C	-4.055181738	-0.450266551	-3.333455665
C	-2.678989271	-3.388076040	-0.933082242
C	-3.473776324	-1.711058101	-3.000976821
C	-2.598073050	-3.516641428	0.491561816
C	-3.200236743	-2.110858126	2.797877230
C	-4.910840933	1.547688348	2.710927344
C	-3.756697702	-0.901956960	3.320845777
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C	-5.761677488	0.489074528	3.113897959
C	-7.144015672	0.612824653	2.781338716
H	-7.876936546	-0.047233542	3.241526606
C	-6.567961341	2.170386229	1.013554143
C	-7.537014700	1.432070115	1.757518628
H	-8.573125436	1.404324413	1.425119910
C	-4.069647955	-3.161230621	2.411003073
C	-5.383366630	-3.149333213	2.964147348
H	-6.022952426	-4.024369655	2.865600264
C	-5.164024973	-0.777385217	3.433952119
C	-5.916951310	-1.987048246	3.456272855
H	-6.967821136	-1.967750478	3.739286147
C	-3.898141252	-3.665685147	-1.585438326
C	-4.828453281	-4.492424726	-0.885283170
H	-5.675653300	-4.929725694	-1.410694293
C	-3.759986851	-3.885200199	1.206054261
C	-4.764900844	-4.593851854	0.477783388
H	-5.567187605	-5.102699480	1.009602660
C	-5.466928832	-0.312836638	-3.313434707
C	-6.231578369	-1.510222541	-3.405165943
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C	-4.312519787	-2.798130320	-2.662101291
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C	-7.667892319	1.651447185	-1.173971952
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H	-0.508017471	-5.135455481	-0.480767356
H	-0.341200765	-4.786109029	-2.208279373
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H	-0.193325999	-7.245119366	-2.674856383
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C	2.641148556	-3.223478418	-3.053782609
H	1.723693742	-2.919780179	-3.589215876
H	3.453754746	-2.558033050	-3.384236704
H	2.892932753	-4.243540096	-3.366323021
C	-2.142732676	-6.845262699	-1.811343819
H	-2.576176149	-6.502782547	-0.857698525
H	-2.479977876	-6.151130171	-2.597552653
H	-2.554524038	-7.841059203	-2.033634161

CP4*methyl,perpendicular*

161
Co2C122H32O5

Co	3.460924713	2.466076662	-1.546416679
Co	5.682261895	2.683365342	-0.305615626
C	2.675494577	3.940841141	-1.961985133
C	5.705723832	4.391570137	-0.795023846
C	6.997036388	2.251034701	0.779545014
C	6.381882456	1.813939702	-1.703684434
O	2.183598576	4.949114082	-2.254285610
O	5.698655891	5.525175482	-1.039461411
O	7.857509605	1.935590749	1.492202022
O	6.880733300	1.206242801	-2.557793299
C	3.076083065	2.781334793	0.432778382
C	4.391819536	2.490803293	0.972855996
C	4.014972869	2.030100822	-3.213588380
O	4.285546657	1.781927290	-4.308401720
C	4.560651477	2.184953891	2.430978374
H	5.219964389	1.309608271	2.567015926
H	3.594249903	1.955669611	2.911100317
C	5.179634262	3.380520936	3.183237795
H	6.135244226	3.661417052	2.715967098
H	4.514467101	4.255326515	3.092163269
C	5.398758320	3.042354856	4.654827900
H	4.438308520	2.742305829	5.107475817
H	6.064443835	2.164686793	4.722012622
C	5.997936933	4.209372373	5.432792529
H	6.970231021	4.504791907	5.009170499
H	5.334516176	5.087352255	5.397076719
H	6.153735802	3.945697492	6.489078920
C	2.539244735	4.133907413	0.877288914
H	3.303995810	4.905823597	0.713299158
H	1.629875014	4.433500491	0.338782940
H	2.294334142	4.099717211	1.954144013
H	6.019112603	-2.985334411	2.549485909
H	6.546805191	-1.926267981	-1.724933953
H	6.711214591	-1.885801690	0.709967248
H	5.587898630	-3.185378831	-3.300172294
H	4.200781896	-5.105726543	-3.827405503
H	2.319058908	-7.896769273	-1.010543806
H	3.031827014	-6.785035903	-3.050872035
H	2.468670772	-7.817321295	1.186537844
H	3.458738594	-6.553125962	3.011318108
H	4.727437983	-4.829224415	3.463931828
C	4.221822661	-3.897361371	3.217662810
C	5.831063873	-1.468664395	0.223070587
C	4.948766043	-2.860537813	2.703856588
C	4.287612252	-1.694116326	2.203289822
C	5.739201297	-1.493616342	-1.137165246
C	4.517294402	-1.092635157	-1.779439561
C	4.710693809	-1.034148067	1.010138627
C	4.505411296	-3.073263436	-3.301096971
C	3.916339802	-1.862918670	-2.820043986
C	2.155827294	-6.414845701	-2.521492933
C	3.722954089	-4.155199971	-3.597285222
C	2.302559909	-4.092707560	-3.443346866
C	1.754753678	-7.040295035	-1.375041550
C	0.721075439	-6.469164000	-0.567324162
C	1.543241068	-5.186458367	-2.923575576
C	1.960433440	-6.928452823	1.555891737
C	0.822967742	-6.412672075	0.858058542
C	2.517347344	-6.217028073	2.580623069
C	1.967110943	-4.952537903	2.961853370
C	2.794348036	-3.826398026	3.268162751
C	2.212841594	-2.533482564	3.206295258
C	3.793203904	-0.169415746	0.375752636
C	2.966956162	-1.455379579	2.658426724
C	2.266681366	-0.285342673	2.226159020
C	3.699347451	-0.186109518	-1.060759414
C	2.471133850	0.275858515	-1.642530574
C	2.710234924	0.382745773	1.093749022
C	2.531746588	-1.673444406	-3.096463583
C	1.886021341	-0.480068883	-2.684233287
C	0.245443323	-4.921620788	-2.410494316
C	1.717523528	-2.800555128	-3.421377763
C	0.302531884	-2.665014117	-3.327036458
C	-0.172356497	-5.575173258	-1.210017875
C	-1.252995128	-5.006743879	-0.475199319
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C	0.612909035	-4.714949586	2.616401105
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C	0.218785668	-1.076055051	3.280390884
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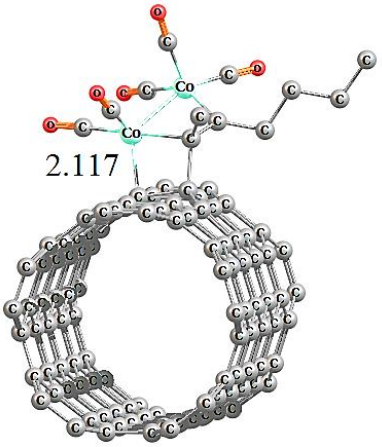

Note: Discarded in the main manuscript.

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C	0.519235186	-0.254669632	-3.001949099
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C	-1.767000729	-3.496307135	-2.325410489
C	-0.288141156	-1.367309047	-3.341301894
C	-1.702417613	-1.238089108	-3.266214219
C	-2.176997425	-4.138155534	-1.130989206
C	-3.261496534	-3.586011460	-0.394895318
C	-2.460124831	-2.328788123	-2.746543290
C	-1.970213554	-4.017935580	1.638915807
C	-3.155241968	-3.524277075	1.027247355
C	-1.390996848	-3.277740805	2.695352173
C	-2.015301255	-2.071912157	3.111698548
C	-1.193509544	-0.946717803	3.415058423
C	-1.772327369	0.343411962	3.399522844
C	-0.194700518	2.740552836	0.562622095
C	-1.023851906	1.425743758	2.861042115
C	-1.721432935	2.595904725	2.466210094
C	-0.314692763	2.672447559	-0.879631368
C	-1.517981091	3.128337803	-1.473870054
C	-1.314874744	3.246955136	1.282028405
C	-1.472205837	1.172928854	-2.930244831
C	-2.100685284	2.378324114	-2.525956546
C	-3.762874366	-2.071023807	-2.246119738
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C	-3.960553448	-2.590910004	1.727538204
C	-5.134504743	-2.073174771	1.106459916
C	-3.379892429	-1.850729589	2.793759437
C	-4.002588087	-0.634181073	3.195578943
C	-3.189170232	0.476601162	3.507242575
C	-3.780927564	1.772585613	3.514396146
C	-2.241954825	4.123541837	0.641823165
C	-3.028189773	2.862442316	2.981398749
C	-2.347957741	4.065021412	-0.782454854
C	-3.469023072	2.610099193	-2.859103610
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C	-4.287373466	1.486331525	-3.187580391
C	-6.168531948	-1.266762084	-0.947473526
C	-5.957917435	-1.146136645	1.810543265
C	-5.377021000	-0.406832224	2.887553394
C	-6.460695793	0.523297014	-2.600134852
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C	-4.084632331	3.831434814	-2.495520651
C	-5.435617462	4.018073819	-2.899716619
H	-5.896662800	5.000917108	-2.822296974
C	-5.698137330	1.618386127	-3.137203460
C	-6.223343345	2.938709854	-3.212728861
H	-7.288316893	3.093235041	-3.375125591
C	-3.294740084	4.701202616	1.388900724
C	-4.160628757	5.594923600	0.694472868
H	-4.854070533	6.224247317	1.249151955
C	-3.503076451	4.582691169	-1.408918015
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C	-5.185188821	1.906718172	3.661954950
C	-5.702397761	3.232473626	3.708632200
H	-6.731841798	3.405269219	4.016820207
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C	-4.978474269	4.277452917	3.194815149
H	-5.451349569	5.253852127	3.107313244
C	-7.150536873	-0.670626735	1.212680107
C	-7.952879236	0.214899024	1.992063322
H	-8.970642222	0.443854875	1.681535784
C	-6.011826440	0.777115278	3.333524551
C	-7.397617555	0.920124358	3.026157991
H	-7.987100339	1.693367812	3.515291150

CP4*butyl,perpendicular*

161
Co2C122H32O5

Co	-2.048998746	3.637841258	1.259006660
Co	-4.294774843	3.801965292	-0.217292413
C	-1.376971149	5.217960118	1.606755278
C	-2.618775933	3.278381055	2.921295746
C	-5.533315083	2.518697937	-0.049612464
C	-4.973159440	4.868487671	-1.433938747
C	-4.620151798	4.838721828	1.178487743
O	-3.033547847	3.038078032	3.970703616
O	-0.902919885	6.250376016	1.826509958
O	-6.485799251	1.858879992	-0.012804899
O	-5.426134302	5.572976923	-2.236743380
O	-4.908025998	5.547534840	2.051117229
C	-2.773641598	2.893280914	-1.433797381
C	-2.361507466	4.033288488	-0.679321663
H	-6.324573629	-2.999499070	-2.653422968
H	-6.949973653	-1.500945349	1.454536047
H	-6.991550797	-1.751512692	-0.965401568
H	-6.215997503	-2.434034424	3.286932990
H	-4.990353176	-4.325797229	4.187808443
H	-3.176884465	-7.595716460	1.890082770
H	-3.906508843	-6.164449992	3.712050934
H	-3.225106699	-7.798587312	-0.298934820
H	-4.022811995	-6.745995786	-2.336322754
H	-5.116102008	-5.041422361	-3.178178217
C	-4.559161457	-4.119274648	-3.022694206
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C	-5.238994439	-2.970356336	-2.726884008
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C	-6.111606309	-1.135673901	0.864490878
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C	-5.129924519	-2.385699776	3.335438613
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C	-2.568246782	-6.736914465	2.167058199
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C	-2.823456815	0.588535679	1.326643240
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C	-0.222579069	-3.408940271	3.251272436
C	-0.592383014	-5.698859830	-0.838017210
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C	-1.064234439	-5.076184562	-2.035600705
C	-0.327678413	-3.972257949	-2.553158579
C	-1.039313346	-2.865972763	-3.054014338
C	-0.365772132	-1.610500613	-3.179512220
C	-2.126739044	1.547421932	-0.949297086
C	-1.058277207	-0.430023198	-2.851849230
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C	-2.001006876	1.518222508	0.596305718
C	-0.745472967	1.901744817	1.186331582
C	-0.744347387	1.624822599	-1.566316906
C	-0.963736624	0.121307826	2.850483756
C	-0.236806254	1.215185106	2.338655846
C	1.134429820	-3.315209569	2.818014102
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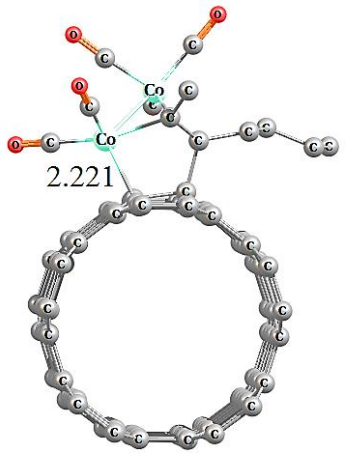

Note: Taken into consideration in the main manuscript.

C	0.175223829	2.518060103	-1.008053042
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C	1.114894428	1.399066568	2.707318458
C	1.845653083	2.512229234	2.189657024
C	3.220820988	-2.036411325	2.658580557
C	1.831347002	0.302379093	3.250097460
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C	4.802497597	-2.483612631	0.850699649
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C	3.873521082	-1.438016386	-2.891762658
C	3.162413026	-0.331974764	-3.404728668
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C	2.295887272	3.773803676	-1.151425311
C	3.144218300	2.111129684	-3.212505322
C	2.300369736	3.937492947	0.273119999
C	3.205323740	2.702320276	2.580653771
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C	5.259706047	3.986442721	2.569556204
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C	5.344848169	1.625928771	3.128517860
C	5.953034608	2.913513040	3.064545618
H	7.013689637	3.025480770	3.282347728
C	3.434634298	4.154805777	-1.893289542
C	4.318195780	5.095800313	-1.281096717
H	5.082205384	5.593993889	-1.874929495
C	3.458964488	4.456582236	0.894424620
C	4.333131718	5.238913733	0.079257481
H	5.111264746	5.844779272	0.539850335
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H	6.930834247	2.268582960	-4.056736057
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H	-3.926244188	2.256931718	-5.512588716
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H	-2.152771753	5.407071464	-2.347352141
H	-2.026621614	6.177031450	-0.745475208
C	-5.412590031	0.723431126	-5.124770974
H	-5.618733708	-0.060122042	-4.378246119
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H	-5.288596604	0.233102996	-6.101286175

CP4*butyl,perpendicular*

161
Co2C122H32O5

Co	3.515255055	2.558322605	-1.093867274
Co	5.669861970	2.773819668	0.191583957
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C	5.663531796	4.352674175	-0.630784598
C	6.931203265	2.785946410	1.412972769
C	6.512916295	1.738417423	-0.996607068
O	2.027890089	4.923537647	-1.811079355
O	5.711511253	5.396142518	-1.137286183
O	7.743029050	2.808549811	2.241755109
O	7.073868194	1.046019383	-1.739469009
C	3.020161653	2.763277065	0.842638046
C	4.329268115	2.487081945	1.404799241
C	4.221805310	2.151198256	-2.713352556
O	4.623427692	1.932221203	-3.773321146
H	5.895384223	-3.083964884	3.009488986
H	6.676019781	-1.997831418	-1.205791773
H	6.684841862	-1.992444113	1.232674262
H	5.855542784	-3.177166574	-2.887089005
H	4.519118167	-5.088444267	-3.559243297
H	2.472552878	-7.948341044	-0.931425086
H	3.309789638	-6.791597025	-2.897915565
H	2.481306993	-7.908685339	1.271566141
H	3.338149777	-6.678895991	3.184282908
H	4.555437490	-4.959540732	3.777600763
C	4.061668686	-4.025222931	3.517003053
C	5.845886298	-1.550562616	0.697443195
C	4.815478885	-2.970504511	3.085301549
C	4.183383033	-1.796314436	2.565369943
C	5.838761692	-1.560517344	-0.665434978
C	4.668059492	-1.134359721	-1.378764480
C	4.683939446	-1.111115310	1.416493253
C	4.775034436	-3.069349095	-2.958182643
C	4.147042026	-1.876653153	-2.485031458
C	2.398676240	-6.436672751	-2.419854757
C	4.021018833	-4.146499171	-3.336922420
C	2.594481136	-4.092835512	-3.277408536
C	1.927466582	-7.087606157	-1.314648240
C	0.840067908	-6.538327508	-0.564943329
C	1.807404320	-5.202435689	-2.834718399
C	1.941938403	-7.032046887	1.625686755
C	0.848550078	-6.509638402	0.865562901
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C	1.839435419	-5.088076355	3.072506171
C	2.634249280	-3.964197899	3.463087606
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C	3.801746479	-0.245424048	-0.701807799
C	2.622784583	0.237139599	-1.358137291
C	2.679976662	0.306547086	1.395633855
C	2.786970743	-1.682939586	-2.849039506
C	2.109830103	-0.499576452	-2.447609849
C	0.478429674	-4.953834135	-2.402449991
C	2.003314312	-2.803503217	-3.259746598
C	0.585185271	-2.675359719	-3.257824419
C	-0.014232763	-5.635092006	-1.246340306
C	-1.144130574	-5.087120578	-0.572957548
C	-0.192585143	-3.771351387	-2.824169764
C	0.003190543	-5.577434375	1.519233141
C	-1.134000397	-5.057027108	0.837642562
C	0.509968882	-4.851407780	2.641658577
C	-0.150121920	-3.645461130	3.015135490
C	0.632541718	-2.537270425	3.390507762
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C	0.666952694	1.791152611	1.400710916
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C	0.105945678	0.926496569	-2.473322903
C	-1.542271202	-3.538373473	-2.419823227
C	-0.008778021	-1.378984225	-3.280754032
C	-1.425836902	-1.258636806	-3.302280221
C	-2.027561090	-4.208642743	-1.270395160
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C	-2.211071250	-2.364356828	-2.860786822
C	-2.007310738	-4.148238225	1.509117920
C	-3.151959935	-3.647264123	0.830076906
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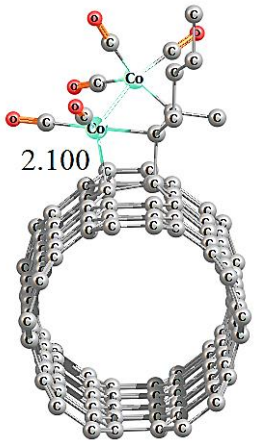

Note: Discarded in the main manuscript.

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C	-1.385393569	3.118755570	1.359615278
C	-1.233412040	1.144454787	-2.898747032
C	-1.897259865	2.337238488	-2.514402319
C	-3.546103870	-2.124015847	-2.444484806
C	-2.012889286	0.030817057	-3.317100905
C	-3.432032092	0.155930914	-3.314056903
C	-4.030502265	-2.793571587	-1.286909095
C	-5.152603265	-2.239163772	-0.604507797
C	-4.209090134	-0.936239734	-2.868351813
C	-4.009293625	-2.734608341	1.494880949
C	-5.141742099	-2.208750252	0.806715790
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C	-3.240985567	2.570241770	-2.935701816
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C	-6.017811525	-1.302934057	1.473599738
C	-5.517670614	-0.587113630	2.605651040
C	-6.229941661	0.463903807	-2.924521355
C	-7.586663012	0.623285704	-2.514348654
H	-8.218956057	1.364566713	-2.999430626
C	-7.180309916	-0.849474135	-0.630943559
C	-8.049923208	-0.016233073	-1.395467914
H	-9.039827895	0.231118455	-1.016473724
C	-3.888185985	3.779428356	-2.586280875
C	-5.209662290	3.968894792	-3.077881211
H	-5.680930658	4.947608624	-3.010097200
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H	-4.929646748	6.081766903	1.149559394
C	-3.387751538	4.508018152	-1.445265491
C	-4.202349794	5.441006413	-0.739961228
H	-4.941220962	6.033721177	-1.275976911
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H	-6.973892872	3.191168748	3.723456076
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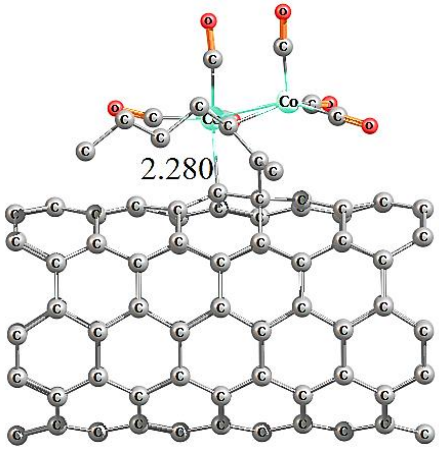
H	-9.025992222	0.272794702	1.174801262
C	-6.190124148	0.582332741	3.034381793
C	-7.552391765	0.725171965	2.635253610
H	-8.179772799	1.483089693	3.100717851
C	2.377871350	4.040587584	1.383321750
H	2.033580876	3.820028216	2.414509706
H	1.470074651	4.285532494	0.810828611
C	3.271592006	5.272210069	1.412429798
H	4.192113717	5.067985493	1.984074959
H	3.593330367	5.523910907	0.391313122
C	2.544158002	6.471680333	2.011209569
H	1.624261392	6.660513677	1.431076076
H	2.221517138	6.230168818	3.038803657
C	3.416268177	7.723090100	2.019894144
H	3.728881789	7.986673678	0.997749757
H	2.881276898	8.584193606	2.445961646
H	4.328077774	7.560506080	2.615503517
C	4.457837387	2.104597611	2.848240775
H	4.965435325	2.934047261	3.373765448
H	3.493347776	1.927434895	3.349125704
H	5.105117842	1.222572868	2.977825644

CP5*methyl,oblique*



163
Co2C123H32O6

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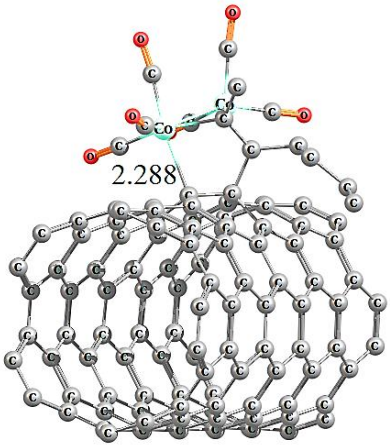
C	-4.956774489	-3.826399930	-1.723175287
C	-2.555104900	-4.307709880	-1.100374692
C	-6.361923656	-0.106145999	0.560639658
C	-5.483872197	-0.572797382	-1.847373620
C	-6.983668775	-2.588102403	-0.193344288
O	-2.130670463	-5.383433781	-1.129971162
O	-5.761199171	-4.568306736	-2.091110438
O	-6.852379598	0.758223924	1.155438451
O	-5.493769570	0.016713829	-2.844907626
O	-7.927126255	-3.247635432	-0.070191332
C	-3.985020174	-1.298362163	1.151335902
C	-4.199978955	-2.597638537	0.632981674
C	-3.209502264	-2.228418185	-2.898436262
O	-3.008073313	-1.861902079	-3.968817869
H	-4.022030418	5.994687708	3.165741029
H	-6.094390962	4.358349934	-0.246343631
H	-5.500854207	4.874885301	2.056432848
H	-5.450437055	4.639149535	-2.374283404
H	-3.751694438	5.769700497	-3.694774684
H	-0.377001495	8.288098283	-2.338842166
H	-1.990606166	7.054454559	-3.666048302
H	0.193249165	8.807311749	-0.277870515
H	-0.516176325	8.436606105	2.017694670
H	-2.058778180	7.410738084	3.173661259
C	-1.926453312	6.330678479	3.154229442
C	-5.017072481	4.038293909	1.555799957
C	-3.039661277	5.527088560	3.145598865
C	-2.923386348	4.125526583	2.932474675
C	-5.356319384	3.743289488	0.266312892
C	-4.622064988	2.750152902	-0.457625030
C	-3.897445937	3.381846956	2.165889978
C	-4.484846060	4.158639672	-2.522187349
C	-4.164813212	2.969453454	-1.798871187
C	-1.124631732	6.530744324	-3.265597156
C	-3.527671190	4.795511530	-3.264195556
C	-2.203641175	4.269569353	-3.341792733
C	-0.213770350	7.227175218	-2.519109857
C	0.830262717	6.538274296	-1.828121661
C	-1.039709704	5.108653087	-3.366043963
C	0.518270978	7.907014723	0.240499119
C	1.186792347	6.869098504	-0.478524273
C	0.118559723	7.697742430	1.531805628
C	0.371199468	6.443575781	2.165865977
C	-0.630631732	5.777574339	2.953544892
C	-0.487938687	4.384343594	3.170684777
C	-3.533099858	2.129700340	1.639661746
C	-1.647651778	3.551519621	3.137640347
C	-1.461462323	2.151118924	2.942237580
C	-3.956414526	1.771818874	0.312974003
C	-3.261724745	0.709624323	-0.329268926
C	-2.388523251	1.432603789	2.155561927
C	-3.026535326	2.240854894	-2.215830143
C	-2.689397085	1.008882900	-1.561206891
C	0.221001158	4.525250850	-3.086486876
C	-2.036743786	2.901800903	-3.004845628
C	-0.755515460	2.298234477	-3.141573576
C	1.175460985	5.251850370	-2.308591926
C	2.234514900	4.524037352	-1.687654138
C	0.387561523	3.116394430	-3.204458867
C	1.853397830	5.885324011	0.293353427
C	2.580269727	4.845646904	-0.358692106
C	1.434203202	5.667611269	1.642977990
C	1.775713728	4.426435565	2.257935321
C	0.794347707	3.775129327	3.035104947
C	0.946738194	2.384381993	3.301633010
C	-2.043027879	0.149120687	1.684796137
C	-0.208456794	1.558328772	3.238253259
C	-0.049772604	0.162900961	3.069482700
C	-2.828640780	-0.468723915	0.525227502
C	-1.978978508	-1.472861573	-0.294044820
C	-0.991113465	-0.542356752	2.264987732
C	-1.553499607	0.262791681	-2.038896249
C	-1.238773459	-0.976913710	-1.462895148
C	1.670704255	2.530863913	-2.977093261
C	-0.594753325	0.913092341	-2.846971998
C	0.668684673	0.304927738	-3.059294641
C	2.613987778	3.247398040	-2.201702319
C	3.676376192	2.529930970	-1.586003832
C	1.827910450	1.129276613	-3.122885977
C	3.286735340	3.875894658	0.417767934
C	4.017703532	2.850888923	-0.239343092
C	2.872729438	3.662027413	1.759280657
C	3.209731412	2.431734094	2.387303399

C	2.217972366	1.777932134	3.173490970
C	2.348472738	0.378401088	3.413790450
C	-0.653509236	-1.870683149	1.809573347
C	1.199064211	-0.437058498	3.369458730
C	1.348017282	-1.854557427	3.238962958
C	-1.073205625	-2.278035991	0.545950250
C	-0.263535431	-3.258931981	-0.099434275
C	0.412118347	-2.575210531	2.465793321
C	-0.146516799	-1.714490574	-1.969407376
C	0.174522928	-2.997636764	-1.414974669
C	3.092752290	0.536084398	-2.871164533
C	0.820843565	-1.072137287	-2.777609131
C	2.091058919	-1.694496095	-2.967666525
C	4.033693903	1.248767391	-2.088355384
C	5.081208454	0.511314009	-1.456503123
C	3.241535138	-0.878630177	-3.004148921
C	4.695565996	1.867281690	0.536862323
C	5.417806982	0.826028587	-0.122733861
C	4.281566644	1.652894414	1.872692791
C	4.606452902	0.405256098	2.493840087
C	3.626267040	-0.240320747	3.277156590
C	3.768874697	-1.629864508	3.552255526
C	0.774562798	-3.876811008	2.018432239
C	2.599904421	-2.456327350	3.548142115
C	0.443717181	-4.217704756	0.670553345
C	1.254541815	-3.758930486	-1.932911948
C	4.509490541	-1.480699334	-2.765549336
C	2.242069791	-3.091085831	-2.729561471
C	5.455424098	-0.765145882	-1.966936080
C	6.111109229	-0.152727504	0.647270030
C	5.689444953	-0.371267651	1.995970967
C	4.670109510	-2.877777375	-2.944732078
C	5.980112585	-3.409167443	-2.727062212
H	6.221986419	-4.416131402	-3.061708220
C	6.520065874	-1.479910363	-1.360949453
C	6.880869169	-2.729167780	-1.956744934
H	7.820696362	-3.208120177	-1.688221540
C	1.581477865	-5.009337747	-1.337338969
C	2.647242029	-5.752084289	-1.939325099
H	2.795854634	-6.798010398	-1.676497049
C	3.502318927	-3.705373335	-2.929525249
C	3.577335526	-5.119521957	-2.713570366
H	4.446980919	-5.674998880	-3.059554604
C	1.808424330	-4.597660754	2.668863298
C	2.107636440	-5.900873702	2.149751238
H	2.704601450	-6.596495671	2.737210168
C	1.171387057	-5.240197501	0.012375771
C	1.803638472	-6.213063430	0.855208872
H	2.164210534	-7.149963466	0.433484735
C	5.046574074	-2.235777598	3.442911193
C	5.140042911	-3.618033853	3.800532157
H	6.117060023	-4.075447881	3.945477181
C	2.748723412	-3.866982292	3.457327990
C	4.025674478	-4.407668804	3.811955107
H	4.136619364	-5.479306415	3.966186349
C	6.858780224	-1.163067675	-0.007916860
C	7.568595546	-2.084909536	0.826487433
H	8.339957202	-2.722987011	0.398980973
C	6.034405648	-1.589877560	2.636853550
C	7.166622653	-2.293235333	2.114981152
H	7.625426026	-3.093122225	2.693251301
C	-4.460737566	-3.797215114	1.500475218
H	-4.907641179	-4.612404462	0.910907472
H	-5.179166503	-3.549975678	2.300352987
C	-3.143123182	-4.269404174	2.133481840
H	-2.385899680	-4.377893114	1.342160679
H	-2.761158481	-3.484914816	2.808776484
C	-3.232361178	-5.591960757	2.882950251
H	-3.919352080	-5.491686671	3.740642670
H	-3.663794940	-6.359789019	2.217812187
C	-1.851533183	-6.039580762	3.359555908
H	-1.178807901	-6.196124211	2.500824061
H	-1.390336607	-5.274348796	4.003813407
H	-1.902717682	-6.980047336	3.927550458
C	-4.409764835	-0.979322489	2.568711745
H	-3.612116810	-1.242312681	3.283404920
H	-4.633837188	0.087483249	2.704484780
H	-5.312469181	-1.544045362	2.832065537

CP5*butyl,oblique*



163
Co2C123H32O6

Co	-2.366723761	-3.977077684	-1.170072621
Co	-4.807562003	-3.184339103	-0.504999872
C	-3.381657379	-5.342089207	-1.719733909
C	-1.032666390	-5.067578879	-0.739377335
C	-5.973389034	-2.112874537	0.240508735
C	-4.797573132	-2.407879928	-2.102363216
C	-5.803340635	-4.664304559	-0.439570637
O	-0.327655639	-5.950163927	-0.498136559
O	-3.911536268	-6.289082926	-2.114182553
O	-6.756773241	-1.445006902	0.771381757
O	-4.892830683	-1.927147026	-3.152346152
O	-6.544200773	-5.551176868	-0.365126383
C	-3.390832733	-2.534998761	1.068840473
C	-3.212217792	-3.854143195	0.598434986
C	-2.022295563	-3.433548517	-2.874866437
O	-1.828367998	-3.117569437	-3.962603695
H	-5.786640829	4.451806405	2.692102002
H	-7.098409700	2.075863572	-0.660685399
H	-6.786457717	2.864318888	1.620267820
H	-6.516320600	2.423439678	-2.794228360
H	-5.232953915	3.962468224	-4.170521641
H	-2.894223445	7.508870144	-2.932611012
H	-3.978583695	5.750303867	-4.205599418
H	-2.599926065	8.284610551	-0.893292162
H	-3.227277889	7.825500973	1.409638418
H	-4.386293329	6.425337453	2.621105713
C	-3.912126455	5.446926211	2.669829450
C	-6.043385710	2.203321885	1.178209334
C	-4.705761211	4.327077505	2.706247317
C	-4.137759864	3.028836603	2.580008781
C	-6.222219470	1.755005016	-0.099331110
C	-5.183746201	1.016823056	-0.750780736
C	-4.795699268	1.971445366	1.846171531
C	-5.443357841	2.273230994	-2.900704229
C	-4.779795203	1.296769281	-2.097632577
C	-3.004976927	5.556617446	-3.759319031
C	-4.720498698	3.140190271	-3.674574924
C	-3.296051084	3.067191275	-3.703455152
C	-2.392894683	6.549099890	-3.043527480
C	-1.207620247	6.272326524	-2.294672588
C	-2.463995224	4.234735100	-3.768515619
C	-2.017666031	7.568354087	-0.316348490
C	-1.024720038	6.769124237	-0.961266640
C	-2.371080635	7.308937093	0.979561202
C	-1.746896600	6.241561780	1.693213847
C	-2.502558483	5.332303631	2.511970308
C	-1.924304004	4.074841627	2.817377165
C	-4.030513780	0.880004148	1.398542755
C	-2.751342684	2.910430004	2.827806677
C	-2.116805326	1.637204183	2.716720455
C	-4.266572046	0.345232107	0.086355716
C	-3.247148461	-0.470290431	-0.479285831
C	-2.738928592	0.613856099	1.968230716
C	-3.454858736	0.952934062	-2.452229608
C	-2.759663701	-0.065074797	-1.716426704
C	-1.092650973	4.106716617	-3.435759754
C	-2.708300116	1.849259221	-3.274359612
C	-1.297864653	1.684279138	-3.357258849
C	-0.449655803	5.143952068	-2.690880129
C	0.765960554	4.832513485	-2.011081917
C	-0.477816144	2.822891977	-3.461072675
C	-0.102732903	6.096288086	-0.121503241
C	0.943565596	5.317347944	-0.698696589
C	-0.474171302	5.825311905	1.232353127
C	0.230486073	4.797805020	1.927180435
C	-0.511078366	3.907379197	2.732418359
C	0.073641637	2.658701346	3.088230580
C	-1.989578833	-0.519026099	1.584977416
C	-0.750185430	1.499352123	3.062299294
C	-0.143539374	0.224163170	2.978767872
C	-2.499760009	-1.415876529	0.450773927
C	-1.339589150	-2.129420716	-0.293591166
C	-0.779465895	-0.789476516	2.206601443
C	-1.432551668	-0.434426330	-2.133110813
C	-0.756994340	-1.474771950	-1.476803446
C	0.917100938	2.697443255	-3.181187317
C	-0.709890579	0.444687496	-2.970576396
C	0.686977023	0.266622570	-3.129952020
C	1.553883920	3.722203746	-2.440553855
C	2.769149191	3.420455560	-1.766601418
C	1.520758235	1.416007517	-3.235443572
C	1.898680464	4.671166771	0.145381909
C	2.943344323	3.905596950	-0.437254955
C	1.530973298	4.405356724	1.491119584
C	2.226958110	3.387778551	2.198773672

C	1.475506461	2.492105530	3.012375778
C	2.043694062	1.227052238	3.343172519
C	-0.016611095	-1.962494864	1.843396349
C	1.221872540	0.080794798	3.334432467
C	1.827324906	-1.214549079	3.293029313
C	-0.247932833	-2.558241029	0.604041584
C	0.860159119	-3.250612904	0.025639348
C	1.202818760	-2.240324706	2.551652543
C	0.530822092	-1.844972675	-1.925210643
C	1.229671395	-2.929011374	-1.297439277
C	2.900376422	1.278595399	-2.932682639
C	1.264198536	-0.969473238	-2.760485720
C	2.671884491	-1.157088181	-2.902653625
C	3.536322064	2.298564083	-2.183910652
C	4.743582416	1.973725627	-1.493134460
C	3.499839506	-0.016945199	-2.976686160
C	3.875921406	3.237406989	0.407296170
C	4.916722615	2.451921648	-0.176785352
C	3.509365498	2.972994862	1.747887470
C	4.200391238	1.936381726	2.451262687
C	3.457153583	1.052818747	3.262742355
C	4.033488608	-0.195960816	3.628014040
C	1.987571142	-3.371087473	2.185300474
C	3.196225914	-1.356783033	3.657723366
C	1.824928369	-3.874633138	0.858345977
C	2.513387311	-3.323095605	-1.759932653
C	4.885760478	-0.163332995	-2.685945758
C	3.256808758	-2.415211771	-2.583635184
C	5.524364746	0.860433434	-1.918543071
C	5.862702667	1.793717472	0.661523818
C	5.491806634	1.527454783	2.016646232
C	5.492721497	-1.441020507	-2.779558469
C	6.895555034	-1.509795536	-2.508863749
H	7.459048897	-2.401420459	-2.777042054
C	6.741210567	0.560406917	-1.254485431
C	7.503266279	-0.536339345	-1.766848245
H	8.536971909	-0.672728617	-1.454387062
C	3.211828308	-4.364952141	-1.089078019
C	4.473244050	-4.758802170	-1.641362112
H	4.939070627	-5.689326543	-1.321562946
C	4.653067944	-2.599136172	-2.734811191
C	5.171510335	-3.902364812	-2.442699783
H	6.180182424	-4.167278303	-2.754233327
C	3.181483412	-3.676739831	2.889034535
C	3.914807037	-4.827640546	2.447849690
H	4.696780542	-5.247660453	3.077762335
C	2.867033702	-4.634693295	0.270069442
C	3.766777579	-5.291380874	1.172226468
H	4.433170653	-6.070925834	0.807194887
C	5.441701042	-0.357565291	3.573949283
C	5.966978591	-1.610863372	4.022143255
H	7.033395007	-1.714715572	4.213858774
C	3.800667003	-2.642564303	3.653121557
C	5.169765777	-2.718424211	4.064579758
H	5.615346594	-3.685285264	4.290540368
C	6.916145023	1.043968712	0.080296914
C	7.858843485	0.450737864	0.979887631
H	8.807576654	0.073219041	0.602595979
C	6.192196249	0.526193387	2.738681900
C	7.506569596	0.198923294	2.275127691
H	8.181203296	-0.374039382	2.908612706
C	-3.986790782	-2.325826511	2.455429146
H	-4.879249766	-2.960903319	2.545491930
H	-4.352202149	-1.293877372	2.556815455
C	-2.993852073	-2.654114163	3.597288611
H	-3.269347542	-3.618536141	4.056894935
H	-1.985885474	-2.813683120	3.180907656
C	-2.916159956	-1.590022910	4.690411252
H	-2.781240810	-0.596078783	4.235288019
H	-3.879237665	-1.548869106	5.229098860
C	-3.300343437	-5.064029644	1.480872569
H	-2.328409921	-5.214449016	1.981815850
H	-4.060859094	-4.942480863	2.266142179
H	-3.533724040	-5.973409795	0.912317373
C	-1.773628451	-1.854164193	5.665693884
H	-1.885157017	-2.834118947	6.156126304
H	-0.805063038	-1.853326513	5.139196831
H	-1.729230826	-1.082736097	6.447971031

CP5*_methyl,oblique_

163
Co2C123H32O6

Co	-4.125738786	1.651397329	0.429091878
Co	-6.635371793	1.100507473	-0.033954897
C	-6.552832804	2.665152059	0.794164547
C	-3.468691131	3.067180859	1.138496964
C	-5.749269093	0.597702635	-1.493439711
C	-7.008416163	-0.281258930	1.040633555
C	-8.182194802	1.354742469	-0.826035865
O	-3.063238317	4.020220990	1.655350848
O	-6.637850558	3.705400051	1.310937594
O	-5.339581948	0.247709709	-2.523671763
O	-7.343927994	-1.175413774	1.697363022
O	-9.200029863	1.523635846	-1.352960771
C	-2.473061709	2.774541229	-1.543998764
C	-3.765735581	2.746908011	-1.151272050
C	-4.598434235	0.882248142	1.987872934
O	-4.856101770	0.554770996	3.064953641
H	4.909697795	5.733438273	3.330845164
H	3.227204589	7.182737676	-0.441400425
H	3.637123218	6.823525880	1.929827392
H	3.847539510	6.586927889	-2.502299241
H	5.433334741	5.201232619	-3.720446502
H	8.559195968	2.634777875	-1.955928383
H	7.103331897	3.818492748	-3.498871878
H	8.975021762	2.323526026	0.182553655
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C	4.720770252	4.663781909	3.264284703
C	3.416431188	4.191015527	2.905555446
C	2.770204264	6.330039449	0.057860890
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C	7.117324634	1.049990356	-1.513569095
C	5.432727026	2.419763134	-3.293191776
C	8.143671834	1.791817981	0.641715814
C	7.387922187	0.846756564	-0.124280303
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C	0.513367706	1.741139310	-2.366905636
C	-0.654765593	1.147706051	-1.868761136
C	3.582974393	-0.836062738	-2.944044228
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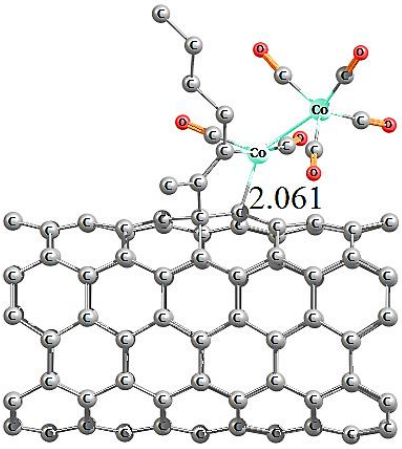

Note: Taken into consideration in the main manuscript.

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C	2.860636689	-3.417674079	-2.031447181
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C	-3.354710371	-4.571894445	-3.196795816
H	-3.642627311	-5.560411895	-3.550399317
C	-3.729403397	-2.652716570	2.062101059
C	-4.880727718	-3.275851390	1.477643141
H	-5.456674315	-4.002992705	2.046380339
C	-4.336322681	-2.215154880	-0.629327269
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H	-1.396292459	3.030074231	-3.423807781
H	-2.843393325	4.033641015	-3.240760238
H	-1.371524512	4.443428448	-2.345470638

CP5*_methyl,oblique_

163
Co2C123H32O6

Co	-4.646653719	0.079604318	-0.241139425
Co	-6.406182527	-2.045316740	-0.214998813
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C	-4.859002958	1.309100448	-1.556443339
C	-5.603069847	-3.526581251	-0.749514808
C	-6.865555097	-1.742234098	1.515914549
C	-8.053129876	-2.576330391	-0.631923373
O	-5.066013792	2.066126981	-2.404528918
O	-6.950278845	-0.309255568	-2.501034917
O	-5.145277543	-4.517129357	-1.133642059
O	-7.241009484	-1.569246869	2.591815479
O	-9.101424933	-2.967225251	-0.907181715
C	-3.555766228	-1.415371316	-1.005057317
C	-4.333993020	-1.742165849	0.177776029
C	-5.235983653	0.848288048	1.256319129
O	-5.533331461	1.339742321	2.259764430
C	-3.942581038	-2.225334144	1.548547122
H	-4.724647459	-1.949695302	2.267876700
H	-3.068211256	-1.661787249	1.894792763
C	-3.657433138	-3.720171888	1.687877064
H	-4.583424343	-4.288864340	1.496818422
H	-2.937557659	-4.043478984	0.917906441
C	-3.138151334	-4.073543850	3.077975198
H	-2.233779319	-3.480653524	3.298101302
H	-3.888626461	-3.775196080	3.831152139
C	-2.823566319	-5.559138851	3.215845700
H	-3.728087751	-6.168681041	3.062042761
H	-2.081046738	-5.872019411	2.465212950
H	-2.417780981	-5.792116469	4.211152373
C	-3.733275435	-1.937673411	-2.403727552
H	-4.780968670	-2.127954908	-2.660168470
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H	-4.267401354	5.946379721	-0.026061975
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H	-3.539116142	6.241909946	-2.097697880
H	-1.592696336	6.937676395	-3.377756649
H	2.283141220	8.213061206	-1.717118549
H	0.470195696	7.642989876	-3.228167586
H	2.814055466	8.319886379	0.409834103
H	1.956278947	7.937153957	2.648738545
H	0.216574189	7.279216689	3.801993154
C	0.032589640	6.217221114	3.650770759
C	-3.456453654	5.123942647	1.756040544
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C	-3.775181046	5.087617909	0.427217873
C	-3.308274611	4.014500917	-0.392964312
C	-2.636894828	4.098515111	2.326014292
C	-2.761960339	5.513096393	-2.321469658
C	-2.806810363	4.219894790	-1.719423143
C	1.122833299	6.852728402	-2.862006998
C	-1.666249360	5.905528046	-3.040802251
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C	2.902369598	6.144382020	-1.373873125
C	0.802196880	5.484306232	-3.118692396
C	2.867288381	7.318871109	0.833789743
C	3.257845016	6.216086398	0.014230890
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C	-2.562476335	1.675460132	-0.484433019
C	-1.803423414	1.779810367	2.142246151
C	-1.945505293	3.227154945	-2.249887535
C	-1.980364244	1.901397339	-1.732081083
C	1.823761273	4.533874586	-2.875545299
C	-0.800422954	3.640771413	-2.998333849
C	0.250874523	2.699146324	-3.179965495
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C	3.670991735	3.809529864	-1.435922423
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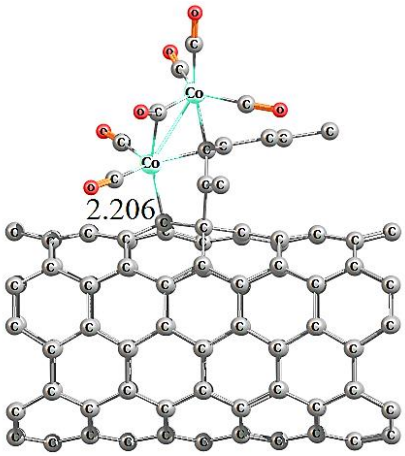

Note: Discarded in the main manuscript.

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C	2.628229978	2.203268295	-2.948888479
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C	1.033487544	0.379721680	-3.282386289
C	3.698440536	2.537394605	-2.082815009
C	4.480680079	1.486805874	-1.532614162
C	2.383304213	0.838611648	-3.241484932
C	4.404060783	2.679546705	0.599861571
C	4.843038588	1.560432473	-0.156556771
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C	0.894298243	-2.518700326	2.811148074
C	-1.368537308	-1.928061582	0.038813232
C	-0.926452358	-3.047073462	-0.723515710
C	-0.134296829	-2.848677160	1.911588567
C	-0.391911195	-1.422630102	-2.450302581
C	-0.442274643	-2.802971381	-2.027908239
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C	5.246818958	-0.852417642	-1.607406103
C	3.156053220	-1.489254529	-3.324508425
C	5.190615321	0.353225936	0.515291944
C	5.612350512	-0.780073726	-0.246414513
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C	6.068244018	-4.404710955	-2.440987631
H	6.817900265	-5.160153406	-2.213165622
C	0.369001558	-5.120230847	-2.144155538
C	1.188126948	-6.072262094	-2.837988102
H	1.018906541	-7.138474411	-2.696215863
C	2.607603228	-4.256852576	-3.593670877
C	2.273011142	-5.652861778	-3.547870286
H	2.952779101	-6.388626348	-3.973546791
C	0.626106845	-5.190258411	1.893239161
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C	0.222294598	-6.543648879	-0.082629714
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C	4.322869530	-3.938834185	3.008276370
C	4.016432072	-5.323631094	3.217023617
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H	2.530618541	-6.835808150	3.150605034
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C	6.830674991	-4.258022590	0.399312841
H	7.400389891	-5.043508556	-0.093917166
C	5.466127739	-3.521970941	2.263093635
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H	6.571903776	-5.409816949	2.162868931

CP5*$_{butyl,oblique}$

163
Co2C123H32O6

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Co	6.238730247	2.619412816	-0.377992732
C	5.804865308	4.042228278	-1.337860682
C	2.662691670	3.828754326	-1.536626795
C	5.534022194	2.046889520	1.146185865
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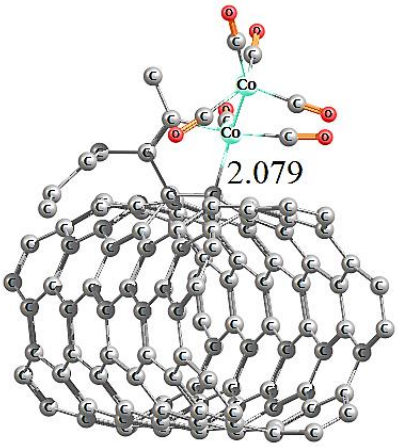

Note: Taken into consideration in the main manuscript.

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163
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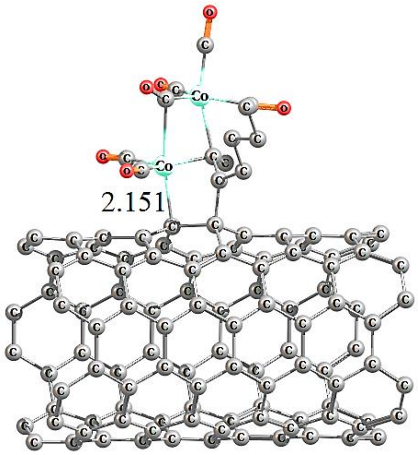

Note: Discarded in the main manuscript.

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H	4.692965595	-3.721095450	4.009337516
C	6.294263313	-2.507595381	4.819352336
H	6.585833672	-1.448253985	4.889333688
H	6.212756050	-2.905508361	5.841217711
H	7.108657294	-3.045431538	4.309523814
C	3.547917966	-2.515035642	-1.997079651
H	4.329069309	-2.876118335	-2.671921641
H	2.888803422	-3.371002989	-1.782952510
H	2.982902653	-1.755500630	-2.557677352

CP5*methyl,perpendicular*

163
Co2C123H32O6

Co	-3.600923751	2.813469476	-1.497008699
Co	-2.957250840	4.286048266	0.555538303
C	-2.410983587	3.163220673	-2.833429763
C	-4.565696831	4.288243934	-1.833611927
C	-1.984536077	4.438209693	2.009746519
C	-1.760292708	4.966790345	-0.554478446
C	-4.204977362	5.532727443	0.832004688
O	-5.227342939	5.189500791	-2.117604327
O	-1.686801024	3.429392017	-3.685110124
O	-1.384415513	4.562864096	2.991827391
O	-0.995453735	5.515227274	-1.230875053
O	-4.954594201	6.378014035	1.082984928
C	-3.366497102	2.224436305	1.316011021
C	-4.277465612	2.704003847	0.350103897
C	-4.712432283	1.697268611	-2.308991997
O	-5.474388138	1.074180565	-2.909887045
H	-5.805788719	-3.666833371	-2.963166417
H	-6.650375615	-2.753000340	1.227691750
H	-6.660607718	-2.684624776	-1.203288836
H	-5.786590756	-3.791388673	2.968691119
H	-4.303298905	-5.590706569	3.645607262
H	-2.041031087	-8.292223244	1.017556126
H	-2.970471947	-7.196175256	2.976652700
H	-2.056422722	-8.245402806	-1.183900435
H	-3.000416292	-7.076829811	-3.092500670
H	-4.331422885	-5.447870154	-3.699249638
C	-3.904690905	-4.479835412	-3.443470336
C	-5.879088638	-2.158396016	-0.657799163
C	-4.736337105	-3.474843262	-3.026583916
C	-4.198242391	-2.258601208	-2.508464598
C	-5.873092735	-2.196560210	0.706772466
C	-4.755074172	-1.672290402	1.430734112
C	-4.761571836	-1.602448719	-1.361501636
C	-4.716746800	-3.601030510	3.031626526
C	-4.181191436	-2.368308391	2.544958020
C	-2.085893682	-6.775244587	2.502225726
C	-3.881288781	-4.614403249	3.414194920
C	-2.465050077	-4.448378020	3.346994346
C	-1.562457591	-7.392685294	1.400541504
C	-0.516932408	-6.766005801	0.653247976
C	-1.591867589	-5.498436307	2.913990407
C	-1.577484867	-7.334782382	-1.539149773
C	-0.523764558	-6.738473028	-0.779138555
C	-2.109357088	-6.675956814	-2.612834250
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C	-1.996487783	-2.992787641	-3.301530180
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C	-2.271887548	-0.731549623	-2.380695555
C	-3.966834603	-0.699285376	0.772895375
C	-2.856661913	-0.113592446	1.429740226
C	-2.849074030	-0.053036195	-1.300584513
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C	-1.977532910	-3.116633837	3.308544609
C	-0.575922769	-2.875613297	3.303766925
C	0.262736351	-5.797786658	1.333621236
C	1.351488013	-5.168188453	0.663363708
C	0.284403858	-3.910203223	2.892149491
C	0.252040054	-5.747265032	-1.430582060
C	1.346781569	-5.142914866	-0.746493703
C	-0.305842492	-5.058114248	-2.552459956
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C	-0.592665716	-2.759545400	-3.299749113
C	-0.099098569	-1.420036971	-3.273161735
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C	-0.946304281	-0.394141042	-2.801861387
C	-0.369629591	0.831292719	-2.376943123
C	-2.301628949	1.190352556	0.881871187
C	-0.955682028	1.518532249	1.490090123
C	-0.938301655	1.524938064	-1.277656125
C	-0.942230194	-0.486940824	2.911626867
C	-0.376941882	0.765180669	2.532624718
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C	3.255738082	-3.586469019	-0.733402950
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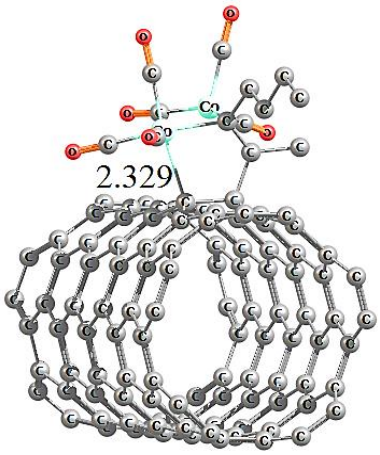

Note: Taken into consideration in the main manuscript.

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C	-0.142577497	2.451167208	0.833464783
C	0.993604452	2.993539864	1.495425277
C	0.983217889	3.035821605	-1.266993056
C	0.949415112	1.070008504	2.970401468
C	1.532552305	2.309184924	2.603483633
C	3.507504972	-2.021911256	2.534538584
C	1.807242945	0.016590930	3.384419493
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C	5.133829127	-2.024757943	0.709793381
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C	3.700257018	1.698046872	-3.287800965
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C	2.836488130	2.742841520	-2.834896930
C	1.800773712	3.971173042	0.841074874
C	2.855140019	2.639631200	3.034263086
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C	5.939447177	-1.030488919	-1.364426606
C	5.391815482	-0.354434291	-2.499068187
C	5.990340246	0.755010931	3.032421995
C	7.334663823	1.013269533	2.630436540
H	7.908057188	1.798658498	3.119305655
C	7.050939630	-0.487131382	0.746525238
C	7.851165877	0.409132785	1.515335475
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C	3.413713705	3.890681975	2.683664847
C	4.717223630	4.175398403	3.181854167
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C	5.118493739	1.802950790	3.490706633
C	5.547883573	3.157657302	3.575735738
H	6.585153351	3.386326042	3.813183366
C	2.857690956	4.628616215	-1.271264834
C	3.608113290	5.593678956	-0.536933404
H	4.295227769	6.259655504	-1.055537939
C	2.868093923	4.580685171	1.539218175
C	3.614376002	5.569398440	0.833556572
H	4.306758634	6.216143807	1.369326146
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C	5.526413473	3.284733468	-3.376535312
H	6.562205098	3.523281073	-3.610319446
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C	4.696197625	4.285901676	-2.939209175
H	5.095820792	5.293222001	-2.837560328
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C	7.842604834	0.464831555	-1.429424412
H	8.815144926	0.772030705	-1.049236751
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C	7.319549275	1.109644024	-2.518561782
H	7.889208961	1.914375224	-2.979581001
C	-5.747861902	2.841466313	0.651846378
H	-6.231331852	3.535934464	-0.051532814
H	-5.884044802	3.270312370	1.659219762
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H	-6.031681134	0.828156164	1.383617731
C	-7.963672978	1.598051900	0.809720433
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H	-8.391328588	2.235647929	0.016882703
C	-8.641446935	0.231117524	0.797513872
H	-8.246082893	-0.403955381	1.605586684
H	-9.729706652	0.317887997	0.931553176
H	-8.451637059	-0.287772070	-0.154840390
C	-3.718698548	2.182063912	2.788266285
H	-2.807720187	2.098259595	3.400381946
H	-4.253570416	3.089394682	3.095491245
H	-4.352135702	1.309008968	3.017750987

CP5*methyl,perpendicular*

163
Co2C123H32O6

Co	3.177911544	-2.939417917	1.314064425
Co	5.554444921	-2.253700775	0.292988509
C	4.425504169	-4.218856530	1.301747396
C	1.921375482	-4.200895090	1.393153174
C	6.713205267	-3.587913632	0.053366668
C	6.550477618	-1.057264924	-0.512017257
C	5.786122649	-1.635754775	1.981250432
O	1.273785051	-5.148136724	1.514992271
O	4.924967581	-5.259263681	1.455418300
O	7.484155487	-4.404332505	-0.214379225
O	7.284874262	-0.386132522	-1.101450374
O	6.000965751	-1.175386825	3.018784167
C	3.054996933	-2.662997640	-0.705195146
C	4.370005455	-2.235170404	-1.108631302
C	3.237527639	-2.495411541	3.072954841
O	3.174391624	-2.188767734	4.179434280
C	4.628355379	-1.891008434	-2.540342880
H	5.038306022	-0.868409547	-2.612394106
H	3.689647949	-1.897523992	-3.120054579
C	5.634579404	-2.853593900	-3.196467232
H	6.601255540	-2.786451874	-2.673327399
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C	5.822670130	-2.524903227	-4.674211613
H	4.848750161	-2.590894155	-5.188025534
H	6.153924858	-1.476337524	-4.767905882
C	6.828848091	-3.452696392	-5.346979828
H	7.815398993	-3.379581806	-4.863931249
H	6.500158787	-4.501436527	-5.283219436
H	6.951988315	-3.200862895	-6.410174045
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H	1.637645528	-4.270530544	-1.129972974
H	2.467474815	-3.629867515	-2.563163558
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H	6.333388249	2.495969530	1.540759342
H	6.425091562	2.500624997	-0.892277681
H	5.426017587	3.512710743	3.253345878
H	3.941600577	5.339357981	3.852305570
H	1.868115422	8.054144531	1.067694533
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H	1.959537472	8.022196542	-1.128032576
H	2.955846081	6.852496162	-3.009912581
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C	3.841689674	4.248694062	-3.326851203
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C	4.056020475	2.046031892	-2.335917421
C	5.569278903	1.966585351	0.974301333
C	4.419737610	1.430940339	1.643132898
C	4.541414813	1.414722231	-1.149351276
C	4.351259886	3.340980852	3.261041532
C	3.820997825	2.117020509	2.750795244
C	1.811676904	6.548607625	2.563293317
C	3.515338198	4.370168784	3.600224789
C	2.102491328	4.227686380	3.455071705
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C	1.271650981	5.287424140	2.964466589
C	1.483363666	7.118706890	-1.504610505
C	0.393488912	6.533528424	-0.786822392
C	2.044126503	6.460410242	-2.562992916
C	1.546909866	5.178740437	-2.957582322
C	2.420104009	4.103708131	-3.318440354
C	1.912048051	2.780442562	-3.256341862
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C	3.649969459	0.485291397	0.937393845
C	2.506732673	-0.106654991	1.541372549
C	2.655467337	-0.160843015	-1.212940965
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C	-0.015868600	4.958663548	2.471563453
C	1.595101407	2.903326352	3.402934564
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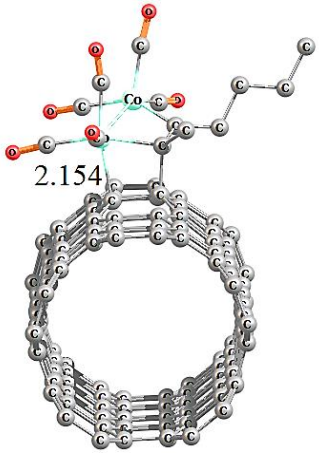

Note: Discarded in the main manuscript.

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C	0.536264382	0.302344763	2.935702462
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C	-1.728575011	1.152806987	3.290964143
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C	-2.561133806	2.210532342	2.819992205
C	-2.293631366	4.009769871	-1.537364769
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C	-1.707458061	3.322499834	-2.625427405
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C	-5.330932093	1.883524548	-0.956556230
C	-3.616831346	1.790396381	-2.697001488
C	-4.183908478	0.548966926	-3.106330403
C	-3.320828251	-0.508953599	-3.464918133
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C	-2.167356976	-4.119606012	0.731980402
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C	-8.188600232	-0.480553297	1.131820832
H	-9.145926029	-0.786145836	0.713635005
C	-3.862170338	-4.019175124	2.500605609
C	-5.190830341	-4.285858366	2.937872158
H	-5.600492821	-5.290779785	2.853143943
C	-5.572377771	-1.909511384	3.232341310
C	-6.024576881	-3.258509011	3.298405697
H	-7.074283011	-3.472693878	3.489896107
C	-3.135858853	-4.771723475	-1.426976751
C	-3.933657887	-5.722978042	-0.725137354
H	-4.606426243	-6.380486738	-1.272705638
C	-3.275803016	-4.711296146	1.379704806
C	-4.000724815	-5.694258070	0.643020017
H	-4.725037997	-6.329829749	1.149066324
C	-5.239184706	-2.043087129	-3.593638266
C	-5.684642612	-3.394988348	-3.650187289
H	-6.711674210	-3.618524404	-3.932922507
C	-3.610181345	-4.120511049	-2.622566124
C	-4.890868891	-4.407801101	-3.177834519
H	-5.307463544	-5.410009467	-3.096176682
C	-7.269239173	0.374097531	-1.034263630
C	-8.043991006	-0.539939581	-1.808952281
H	-9.038104140	-0.830787500	-1.474360556
C	-6.115918425	-0.968000925	-3.216759461
C	-7.482752803	-1.192675602	-2.873599900
H	-8.043687546	-1.987323390	-3.361987502

CP5*butyl,perpendicular*

163
Co2C123H32O6

Co	1.299463899	-4.427744161	-1.833822412
Co	-0.163446809	-5.261970230	0.119302064
C	0.334162881	-3.838519470	-3.255662350
C	1.081821142	-6.153577729	-2.264115776
C	-1.090773529	-4.891496723	1.565709143
C	-1.454977625	-4.976039647	-1.055401053
C	0.022974317	-7.023584297	0.328991404
O	1.009834729	-7.246239522	-2.629025660
O	-0.258840404	-3.498991536	-4.179548949
O	-1.686499560	-4.719473857	2.543055640
O	-2.350044993	-4.901630367	-1.788673578
O	0.066947409	-8.162832005	0.528981208
C	1.437616196	-3.917462714	1.001568316
C	1.858025000	-4.829729270	0.017280369
C	2.963605873	-4.316408667	-2.425821067
O	4.034792682	-4.408136562	-2.841631615
H	6.724167927	-0.489691051	-3.526381997
H	7.109593041	-1.897711461	0.615696111
H	6.927471902	-1.821544146	-1.809197745
H	7.153896805	-0.688020233	2.449615276
H	7.113285588	1.616288648	3.217085860
H	6.799060558	5.232499440	0.702982599
H	6.995473932	3.717240784	2.589847003
H	6.634675765	5.319892159	-1.488132312
H	6.547310003	3.919770601	-3.471765703
H	6.577366886	1.843706342	-4.181563030
C	5.672532058	1.320722256	-3.877567661
C	6.021730226	-1.812159228	-1.205616205
C	5.755074310	0.005405906	-3.505930548
C	4.628747203	-0.655160362	-2.929899746
C	6.123534307	-1.858422372	0.155968334
C	4.961287024	-1.657022517	0.966794906
C	4.754541433	-1.554427821	-1.817990035
C	6.195103017	-0.189920517	2.582028846
C	4.993878748	-0.820303496	2.131500101
C	6.007645275	3.944209927	2.193062893
C	6.172165513	1.107537559	3.015551968
C	4.946650656	1.839770346	3.040914127
C	5.897238456	4.798206445	1.130698628
C	4.640070640	4.973209238	0.473524313
C	4.866659980	3.218282319	2.655662998
C	5.679915890	4.901397232	-1.801399323
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C	5.630607941	4.112824912	-2.917506564
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C	3.707100806	-1.922314849	0.368951869
C	2.509363637	-1.762068389	1.115969259
C	2.301974380	-1.655624670	-1.609568488
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C	2.493201436	1.739474612	3.144120935
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C	2.190370609	4.838908824	0.638400237
C	2.414424503	3.098728969	2.787545850
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C	2.086508874	4.883999776	-0.767147749
C	3.225253112	3.908948372	-2.704576999
C	1.988944743	3.277133398	-3.024892277
C	2.013196143	1.936946207	-3.457192448
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C	1.132593496	-2.246133795	-0.963472868
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C	-0.270215700	-0.837263728	-2.498185299
C	1.241076338	-2.431638828	0.613465855
C	0.013661577	-1.888572879	1.312011767
C	-0.165937417	-1.788651668	-1.447413988
C	1.308418470	-0.361352108	2.732637482
C	0.076161233	-0.990311802	2.396153327
C	1.133393537	3.662096202	2.497699442
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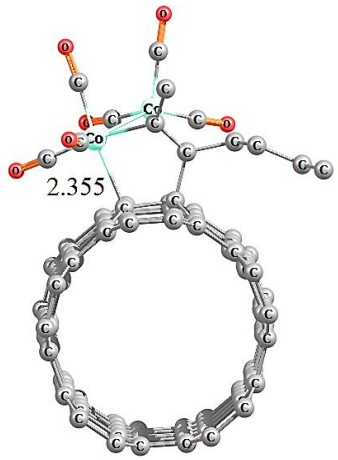

Note: Taken into consideration in the main manuscript.

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C	-1.146130265	0.884856384	3.414597183
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H	-7.076226579	3.175401007	3.628569198
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H	-7.277540972	4.664902743	1.722340795
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H	-6.951016952	1.076025177	4.209207895
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C	-6.196321810	-2.302723584	-0.345266129
H	-7.176846951	-2.396085779	-0.808366692
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H	-7.339020153	-1.068083896	-2.525811054
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H	1.259584538	-5.185116413	2.724204088
H	0.984871324	-3.483168861	3.036913934
C	3.076035372	-4.055575831	3.053340550
H	3.544822469	-5.053431238	3.098982454
H	3.715864897	-3.461534666	2.387556767
C	3.087853874	-3.429001306	4.445304233
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H	2.487019977	-4.051976106	5.131223725
C	4.498398964	-3.248959009	4.994728416
H	5.030020410	-4.212147191	5.050413135
H	5.081611607	-2.576193053	4.346033175
H	4.480862274	-2.809849336	6.002793206
C	2.905498941	-5.869267858	0.298729944
H	2.815236719	-6.261849630	1.322016520
H	2.865271697	-6.714009237	-0.400530902
H	3.900982205	-5.398468961	0.215557415

CP5*butyl,perpendicular*

163
Co2C123H32O6

Co	3.372026774	-2.753255233	1.110155467
Co	5.675858011	-2.063041224	-0.021632233
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C	2.188256056	-4.075110126	1.241200308
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C	6.562619343	-0.834988974	-0.902975252
C	6.013698210	-1.403379402	1.635387578
O	1.584067471	-5.049377341	1.376102106
O	5.298617091	-4.893329009	1.471922617
O	7.562331662	-4.188856180	-0.746752447
O	7.234189852	-0.146295488	-1.543883772
O	6.269373942	-0.916207886	2.650807712
C	3.141714880	-2.541641883	-0.920481258
C	4.437529324	-2.149503724	-1.384622278
C	3.473724432	-2.264799401	2.852100181
O	3.442553075	-1.942377471	3.955639398
H	5.556460140	3.651880980	-3.092578892
H	6.408193566	2.746224529	1.155968510
H	6.384639863	2.751206463	-1.278471668
H	5.561434846	3.739460318	2.905391258
H	4.065654386	5.524756201	3.591707992
H	1.784800127	8.195410850	0.934448941
H	2.724894800	7.112737598	2.894894099
H	1.777174195	8.162689946	-1.264128307
H	2.711725240	7.018797421	-3.192524265
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C	1.305543792	7.248326467	-1.619524209
C	0.265130188	6.636720511	-0.852211347
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C	2.073537843	0.658652526	-2.483638492
C	3.751372475	0.667255420	0.677758125
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C	2.679073136	-0.015957455	-1.424414149
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C	2.066598241	0.747716407	2.404790387
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C	-0.502773329	5.686845570	1.264638239
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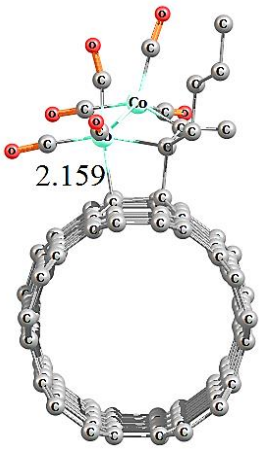

Note: Discarded in the main manuscript.

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C	-3.715144798	1.884037548	2.475785108
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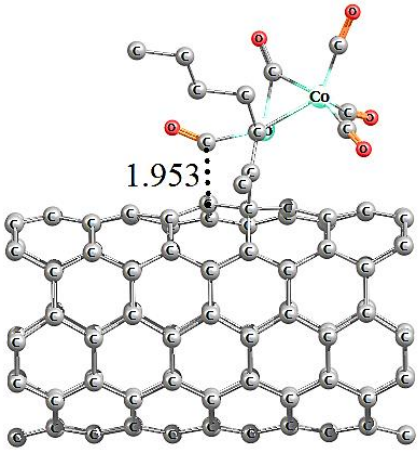
C	-7.243678438	0.310139174	0.690740219
C	-8.033853165	-0.595894296	1.459951095
H	-9.002742731	-0.924445896	1.088321541
C	-3.558844484	-4.026374153	2.604819413
C	-4.857162870	-4.327191442	3.107297221
H	-5.244503671	-5.342367660	3.041358297
C	-5.282642796	-1.961488192	3.425575334
C	-5.697158996	-3.321837332	3.511417080
H	-6.730063453	-3.562486942	3.755794908
C	-3.011594411	-4.750349897	-1.356750755
C	-3.750055573	-5.723002629	-0.619661299
H	-4.432413066	-6.395962574	-1.135774642
C	-3.012996383	-4.701024091	1.453990574
C	-3.749637713	-5.699613597	0.750076010
H	-4.432360628	-6.353832194	1.289211743
C	-5.285076589	-2.071010723	-3.409846212
C	-5.699949015	-3.433438781	-3.447107110
H	-6.734048822	-3.681112930	-3.679295089
C	-3.560254566	-4.108941983	-2.525009104
C	-4.859646524	-4.427066769	-3.017150258
H	-5.246975767	-5.439359318	-2.917658487
C	-7.244532596	0.287770392	-0.745397945
C	-8.034239627	-0.642985868	-1.484587425
H	-9.003483535	-0.958635355	-1.102729045
C	-6.168100658	-1.018966986	-2.987244816
C	-7.510628192	-1.278350116	-2.578235942
H	-8.075400991	-2.084815598	-3.042291663
C	2.585318864	-3.748886106	-1.674409476
H	2.292332509	-3.415449672	-2.690347388
H	1.651537824	-4.084864765	-1.200610196
C	3.537070865	-4.933291335	-1.772122385
H	4.473187271	-4.640092885	-2.278627124
H	3.825287482	-5.263709205	-0.761304844
C	2.899562308	-6.106206740	-2.510434822
H	1.964296084	-6.385385938	-1.995086257
H	2.611202196	-5.784063347	-3.525848072
C	3.827698274	-7.313354443	-2.590685351
H	4.101458543	-7.663238491	-1.583368328
H	3.352566525	-8.149733606	-3.123107739
H	4.758522400	-7.058563032	-3.120851747
C	4.682528285	-1.872328889	-2.827027937
H	5.675188855	-2.225228968	-3.143820050
H	3.903485591	-2.288347115	-3.482877204
H	4.680366516	-0.776367842	-2.982864626

TS2*methyl,oblique*



163
Co2C123H32O6

Co	4.044331120	2.224654924	-1.059412574
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C	5.529133656	3.243261769	-1.391868857
C	2.540634413	3.259000448	-0.861238584
C	6.295100610	0.837062689	1.374489938
C	6.241446278	0.637564972	-1.343838669
C	7.816896197	2.654728955	-0.016254771
O	2.084994263	4.315412273	-1.114298693
O	5.899053913	4.185532082	-1.992741087
O	6.366792247	0.205438143	2.337526264
O	6.487219263	-0.161903676	-2.147554417
O	8.891971790	3.080163370	-0.022867110
C	3.227642511	2.084784958	1.625258133
C	4.195838111	2.707050040	0.892709468
C	3.748653331	1.884493913	-2.787454638
O	3.530772471	1.719506190	-3.907676043
H	4.158159418	-5.036692973	3.687961513
H	6.290047737	-3.078570263	0.504716272
H	5.541890593	-3.689684383	2.740109095
H	5.949962538	-3.417138396	-1.671288494
H	4.616635144	-4.806606083	-3.158168459
H	1.572616572	-7.862712732	-2.163087290
H	3.100577411	-6.368465297	-3.312478050
H	0.866341100	-8.488660730	-0.174859831
H	1.250707722	-8.019409019	2.180414186
H	2.467836610	-6.757123087	3.490935196
C	2.163239567	-5.713569670	3.439397413
C	4.991250556	-2.936436962	2.180097236
C	3.121558721	-4.737726226	3.546901281
C	2.801057940	-3.371503936	3.305320529
C	5.416947883	-2.586709514	0.930814575
C	4.621449773	-1.711688283	0.125731367
C	3.720927451	-2.471107137	2.652037796
C	4.938093680	-3.107750209	-1.925623092
C	4.344751571	-1.999435527	-1.252723848
C	2.120412592	-5.998393152	-3.017794852
C	4.186848992	-3.888286710	-2.762160464
C	2.811608474	-3.589127273	-2.992399041
C	1.258456831	-6.841735871	-2.371692968
C	0.043703139	-6.340408792	-1.810128393
C	1.813068969	-4.609190846	-3.141812201
C	0.345410950	-7.655939847	0.294192106
C	-0.401705733	-6.736730869	-0.505912384
C	0.561950053	-7.391441854	1.618135457
C	0.038382339	-6.199090938	2.205200079
C	0.823281312	-5.381594879	3.087800556
C	0.428471471	-4.033579128	3.273251339
C	3.222557820	-1.282846906	2.076470106
C	1.431260564	-3.019594220	3.360456768
C	1.039509052	-1.669965271	3.132795362
C	3.737048614	-0.848948434	0.807000411
C	2.971336615	0.110307815	0.068746868
C	1.921638092	-0.798919150	2.452770043
C	3.159200354	-1.462148479	-1.804247757
C	2.556125040	-0.301757966	-1.208460923
C	0.450098129	-4.244104089	-3.012490788
C	2.385169822	-2.270250625	-2.691858640
C	1.046771500	-1.885378196	-2.981999105
C	-0.453403783	-5.124899387	-2.340140433
C	-1.680755440	-4.586860432	-1.849374465
C	0.067945531	-2.880724647	-3.163552591
C	-1.303314346	-5.882781658	0.176129492
C	-2.114883886	-4.972412091	-0.563960426
C	-1.076445421	-5.607676838	1.561043404
C	-1.683905730	-4.445312623	2.120147246
C	-0.914127508	-3.644784613	2.991388443
C	-1.322832540	-2.300449113	3.221833080
C	1.416933489	0.403154085	1.928838674
C	-0.320668000	-1.294291177	3.273953232
C	-0.691645869	0.055728162	3.068465830
C	2.225948380	1.152250782	0.891373504
C	1.301111374	1.992786937	-0.040220626
C	0.201503581	0.912750938	2.365294247
C	1.365389644	0.239746422	-1.807184675
C	0.782187685	1.395738317	-1.271435706
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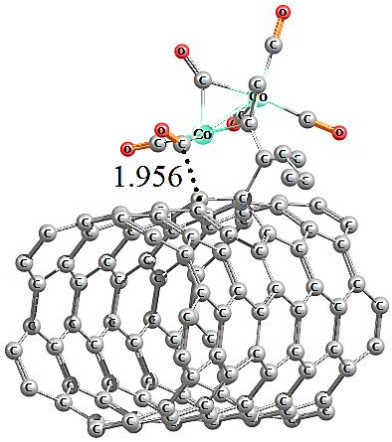
C	-3.432403521	-2.857340378	-1.928940025
C	-1.678092493	-1.157206698	-3.258150658
C	-3.053504038	-4.138765748	0.118974928
C	-3.865855825	-3.242787816	-0.626073580
C	-2.831384804	-3.869883214	1.495406953
C	-3.434711531	-2.717841327	2.068887845

C	-2.656370510	-1.913042230	2.950188448
C	-3.043072884	-0.557924403	3.158021629
C	-0.279424953	2.183980985	1.880367618
C	-2.045871743	0.439064191	3.224271481
C	-2.409379254	1.810660822	3.056986713
C	0.228665224	2.689530333	0.671601647
C	-0.647574265	3.531348779	-0.080904593
C	-1.519772944	2.686207935	2.390628433
C	-0.337493831	1.967726530	-1.915704614
C	-0.907861560	3.190280133	-1.427255685
C	-3.042525109	-0.781093519	-3.155423547
C	-1.090173093	1.178175329	-2.817133904
C	-2.413902973	1.585025237	-3.159910012
C	-3.935936150	-1.645895723	-2.478561963
C	-5.154694092	-1.095645010	-1.975814399
C	-3.404013411	0.591736581	-3.318057533
C	-4.779085065	-2.391690292	0.059255229
C	-5.584017435	-1.475811140	-0.686428413
C	-4.557525066	-2.123689295	1.431093815
C	-5.151673028	-0.953138103	1.999576343
C	-4.382176763	-0.159261714	2.876729908
C	-4.779527404	1.186148394	3.115766037
C	-2.043072184	3.914157461	1.888735463
C	-3.768833988	2.194040973	3.220970127
C	-1.609103275	4.331281759	0.593533209
C	-2.040712616	3.754018581	-2.070262969
C	-4.771026113	0.976104228	-3.229389951
C	-2.813716843	2.935768391	-2.957904656
C	-5.671152599	0.108517320	-2.535441292
C	-6.510766087	-0.632022796	-0.008175358
C	-6.285659550	-0.361329400	1.377548317
C	-5.134927865	2.330758857	-3.438225793
C	-6.530220471	2.641215889	-3.371586747
H	-6.893004609	3.599197216	-3.739005658
C	-6.898952203	0.634979442	-2.059042314
C	-7.388200760	1.816904289	-2.700569667
H	-8.417113709	2.134734376	-2.542218620
C	-2.638874181	4.929826761	-1.535697119
C	-3.731966781	5.493756880	-2.269841452
H	-4.069413233	6.504848919	-2.048458034
C	-4.127005223	3.336495488	-3.308306110
C	-4.452845020	4.720971657	-3.132606674
H	-5.350452055	5.130045608	-3.592423240
C	-3.254855978	4.441318506	2.407656486
C	-3.713703578	5.679541589	1.847769390
H	-4.487773601	6.252384343	2.354905632
C	-2.430841156	5.215252182	-0.155083404
C	-3.319384200	6.052663031	0.595604536
H	-3.787244157	6.914202109	0.122330505
C	-6.120858259	1.572730763	2.865397607
C	-6.479114315	2.918005199	3.197265245
H	-7.528031331	3.205888566	3.238062207
C	-4.139263619	3.560243288	3.098412277
C	-5.517467602	3.880542876	3.313956062
H	-5.818317238	4.917842443	3.447796230
C	-7.332813110	0.251779190	-0.751957966
C	-8.275216790	1.035274797	-0.010771476
H	-9.087488068	1.542550386	-0.528238572
C	-6.894819893	0.778492968	1.964628031
C	-8.061782285	1.292077741	1.313092151
H	-8.708026689	1.999274251	1.829883705
C	4.893072281	3.930571630	1.476327296
H	5.786096847	4.214770743	0.906240731
H	5.258168130	3.699853989	2.491329793
C	3.956994865	5.143483319	1.510790501
H	3.704084714	5.428170593	0.477494681
H	3.004714305	4.860462077	1.992595827
C	4.580347278	6.331288230	2.233940970
H	4.820954808	6.041536675	3.272154124
H	5.539652003	6.586356778	1.750902607
C	3.663447997	7.550825134	2.235611441
H	2.706819111	7.320122146	2.729315967
H	4.123459589	8.398829383	2.763443481
H	3.438917423	7.870217292	1.206439010
C	3.027687131	2.296971941	3.092701304
H	3.714856614	3.049137978	3.490933246
H	1.998585822	2.604453555	3.333113361
H	3.211544969	1.351906198	3.635646810

TS2*butyl,oblique*



163
Co2C123H32O6

Co	-3.857978725	2.631940397	1.163225487
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C	-2.288994959	3.556063269	0.931389835
C	-6.145082752	1.539141201	-1.400573889
C	-6.352246777	1.255695520	1.287603674
C	-7.446381889	3.566974647	-0.110137768
O	-1.775308874	4.600760217	1.115184016
O	-5.617450850	4.631028229	2.186660831
O	-6.250181410	0.961474620	-2.394552558
O	-6.742524715	0.463438442	2.038927917
O	-8.421031792	4.182185572	-0.199754192
C	-3.051972415	2.511348768	-1.529939103
C	-3.916473240	3.230299209	-0.752894390
C	-3.599650741	2.241578361	2.884385320
O	-3.403655445	2.044765346	4.004006321
H	-4.684612076	-4.460649611	-3.737490422
H	-6.625449692	-2.353137722	-0.524405446
H	-5.929325760	-3.000294625	-2.766896266
H	-6.346461955	-2.746069727	1.651169829
H	-5.172013304	-4.293627542	3.117273476
H	-2.448768409	-7.630270462	2.070659141
H	-3.824464508	-6.008755756	3.239387243
H	-1.789498464	-8.293251594	0.077907219
H	-2.103311836	-7.748211523	-2.271554815
H	-3.177483113	-6.346415396	-3.564631757
C	-2.769698771	-5.339940389	-3.492478105
C	-5.309316144	-2.314984613	-2.192274500
C	-3.623994614	-4.270622375	-3.586130431
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C	-5.705020744	-1.944659770	-0.938858887
C	-4.830722844	-1.167692321	-0.115963486
C	-3.996490655	-1.971840168	-2.651073912
C	-5.308727906	-2.549547832	1.913365521
C	-4.598993514	-1.498711035	1.260874735
C	-2.809035007	-5.735856066	2.958169657
C	-4.647020481	-3.418668427	2.738057530
C	-3.249133618	-3.268225087	2.977329327
C	-2.032963169	-6.651106426	2.301042334
C	-0.768420917	-6.267156248	1.757080745
C	-2.361689998	-4.388250216	3.111567776
C	-1.183293040	-7.509366631	-0.372639062
C	-0.354498632	-6.683930526	0.448846440
C	-1.360054052	-7.202186233	-1.693291966
C	-0.714174038	-6.058739382	-2.255280327
C	-1.405563788	-5.151041523	-3.127950215
C	-0.875584623	-3.846709875	-3.286601842
C	-3.383786011	-0.850468356	-2.052148009
C	-1.770352511	-2.735380079	-3.360970917
C	-1.245861350	-1.436172864	-3.107187561
C	-3.858219288	-0.389371269	-0.777792526
C	-3.007417580	0.479731620	-0.020264901
C	-2.039588694	-0.493027333	-2.415385460
C	-3.367639645	-1.096170206	1.826009344
C	-2.643845878	0.005612569	1.252514239
C	-0.967430019	-4.162946836	2.997220026
C	-2.687225470	-1.995177668	2.703056561
C	-1.318724626	-1.755696663	3.007667161
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C	0.448699488	-5.593615770	-1.592947019
C	1.174524963	-4.488474860	-2.126855343
C	0.497036408	-3.599913952	-2.989144578
C	1.041506217	-2.300340000	-3.194741122
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C	0.146205026	-1.197226769	-3.236311487
C	0.650302601	0.104467188	-3.005276892
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C	-1.152657107	2.176652931	0.135567729
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C	-0.763212619	-0.467209711	2.769847260
C	0.580310536	-0.213626886	3.137297990
C	1.766406702	-3.569831039	2.431995853
C	3.044631226	-3.161183933	1.962897389
C	1.463692688	-1.315871857	3.314859564
C	2.551702903	-4.357372873	-0.111917618
C	3.445582010	-3.563080995	0.654539237
C	2.368348425	-4.041808000	-1.484144613
C	3.089713947	-2.946898991	-2.032809259

C	2.404907923	-2.053771178	-2.906739705
C	2.928752061	-0.741679803	-3.090378770
C	0.455116637	2.233652302	-1.769044140
C	2.037350627	0.351984737	-3.148163756
C	2.536130651	1.677201052	-2.954937497
C	-0.004868646	2.764887197	-0.553633425
C	0.944112212	3.504879354	0.215905058
C	1.737699013	2.622614088	-2.269608545
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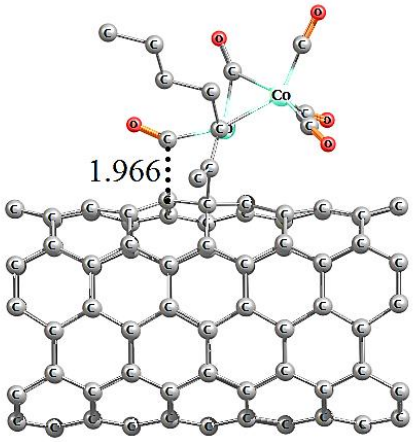
C	1.158095025	3.117841040	1.558075693
C	2.860226277	-1.080148063	3.228124394
C	1.121674328	1.074790285	2.912912731
C	2.477609545	1.337546076	3.270943403
C	3.665518017	-2.019157196	2.539604587
C	4.937798219	-1.587391113	2.054262542
C	3.359085484	0.245088353	3.418490236
C	4.444855904	-2.795744645	-0.009435819
C	5.333929702	-1.982247062	0.758640183
C	4.261270778	-2.480159235	-1.376856650
C	4.975004509	-1.365265690	-1.919531811
C	4.298307663	-0.484025352	-2.790194650
C	4.831618939	0.818282792	-3.003605024
C	2.376840588	3.783831325	-1.744701030
C	3.928687638	1.924719758	-3.103607550
C	1.983012449	4.216796529	-0.441301749
C	2.339443175	3.550478390	2.215108465
C	4.759163388	0.487849265	3.346593455
C	3.016876071	2.642672059	3.093736626
C	5.571213141	-0.454636299	2.641658732
C	6.345486182	-1.222929396	0.102167442
C	6.157438197	-0.902207838	-1.278466568
C	5.258767175	1.793763919	3.582244970
C	6.679588684	1.958697954	3.533933163
H	7.136208073	2.865694882	3.925365456
C	6.849975803	-0.047814373	2.182452214
C	7.453976478	1.063108544	2.852828160
H	8.512174485	1.274176905	2.710058262
C	3.059724176	4.666157517	1.702237491
C	4.201683161	5.100838419	2.449597016
H	4.645578779	6.073479047	2.244563225
C	4.361511361	2.900009254	3.459426581
C	4.831487669	4.244892476	3.305331340
H	5.764241775	4.550850909	3.775192228
C	3.635541479	4.198714538	-2.252602446
C	4.214166930	5.373312984	-1.666950061
H	5.042626004	5.876761236	-2.161728137
C	2.887676916	4.997558957	0.326578683
C	3.857908226	5.756433689	-0.406225501
H	4.409269870	6.556316344	0.085164422
C	6.201748759	1.064552010	-2.731829983
C	6.697018733	2.372021139	-3.036734698
H	7.769905292	2.553941250	-3.058817148
C	4.432447354	3.244924794	-2.954300636
C	5.838569082	3.428082024	-3.149485876
H	6.244340211	4.431734076	-3.260429038
C	7.249309081	-0.444090847	0.868282213
C	8.269886968	0.256445416	0.147950057
H	9.125825243	0.668187960	0.679598486
C	6.883208511	0.181383818	-1.838999444
C	8.091018761	0.561905059	-1.170774705
H	8.808280077	1.211337778	-1.669163133
C	-2.844483814	2.816745277	-2.983919629
H	-3.821153605	3.065687522	-3.427983561
H	-2.499375585	1.908628958	-3.499603209
C	-1.835906702	3.964581098	-3.275635344
H	-2.383035943	4.904363441	-3.453199607
H	-1.201921882	4.142552053	-2.392391564
C	-0.947780061	3.663840233	-4.481229232
H	-0.443805763	2.693002262	-4.333185665
H	-1.581936649	3.543190218	-5.377356369
C	-4.395747123	4.576434342	-1.267430322
H	-4.990089771	5.127144169	-0.532115592
H	-3.525277403	5.200840972	-1.519501973
H	-5.007712474	4.465577805	-2.177352558
C	0.097265531	4.748926440	-4.714893594
H	-0.377920862	5.723684539	-4.907425414
H	0.746951115	4.862120501	-3.832373235
H	0.738447529	4.504487163	-5.574255721

TS2*_methyl,oblique_

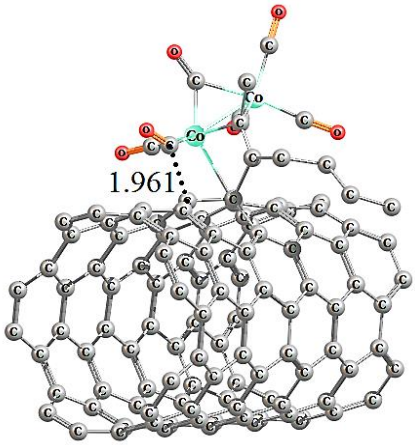


163
Co2C123H32O6

Co	-3.775515883	-2.365958355	-1.033075768
Co	-5.887711561	-1.666020269	-0.087717233
C	-5.375526303	-3.204346669	-1.318419628
C	-2.439708423	-3.621642808	-0.803212244
C	-5.847769862	-0.546912077	1.326584178
C	-5.619106071	-0.498588727	-1.381344743
C	-7.598405329	-2.109539158	-0.112931691
O	-2.164956751	-4.747244082	-1.013678327
O	-5.894155623	-4.115217793	-1.852322610
O	-5.874356805	0.155201870	2.241311631
O	-5.725680393	0.304491080	-2.211329108
O	-8.735556048	-2.303342403	-0.193240771
C	-2.903913865	-2.344213318	1.659850303
C	-4.001953586	-2.745716423	0.962063628
C	-3.425440069	-2.136920255	-2.767015013
O	-3.175906030	-2.037013909	-3.888330986
H	4.328854650	-5.761118927	-3.342342400
H	2.586380528	-7.203674906	0.338833530
H	2.973664876	-6.814758846	-2.032499233
H	3.310973794	-6.652971872	2.380086614
H	5.038512804	-5.360003828	3.499358153
H	8.263716182	-2.928040830	1.712512603
H	6.770288327	-4.075496528	3.242605598
H	8.677628209	-2.567497298	-0.418252387
H	7.833755011	-3.156933827	-2.621689208
H	6.259539289	-4.320899965	-3.599047136
C	5.280659885	-3.868225665	-3.452555760
C	2.389461389	-6.095677755	-1.461691477
C	4.189007343	-4.682800037	-3.303516663
C	2.923261736	-4.142065458	-2.930782234
C	2.165353625	-6.318116246	-0.134535758
C	1.530907088	-5.309357694	0.663501934
C	2.026555112	-4.835803667	-2.044874202
C	3.158893187	-5.586914906	2.540368875
C	2.034617036	-4.931695790	1.946431826
C	6.486969753	-3.096233217	2.861531175
C	4.131732044	-4.859119872	3.165612416
C	4.033898721	-3.434877148	3.240655770
C	7.330078735	-2.448804535	2.001128088
C	6.908952047	-1.251758907	1.342888443
C	5.178953110	-2.580749070	3.115287407
C	7.859703084	-1.991280481	-0.847085116
C	7.167042728	-1.028109886	-0.048953456
C	7.384921734	-2.322864661	-2.085284840
C	6.196814919	-1.705757814	-2.585517910
C	5.171803020	-2.461678357	-3.246580733
C	3.871164164	-1.903209717	-3.314540389
C	1.010110367	-4.102826672	-1.396791387
C	2.737219842	-2.754035691	-3.133901739
C	1.494414504	-2.149679850	-2.787631467
C	0.702476350	-4.389129883	-0.023225207
C	-0.022286353	-3.407609095	0.707310404
C	0.637217687	-2.810497970	-1.881615157
C	1.720583187	-3.627600875	2.410953714
C	0.570420252	-2.954803504	1.899544581
C	4.973188760	-1.204776908	2.844585306
C	2.748127700	-2.868044146	3.060160921
C	2.580214173	-1.461147040	3.194828866
C	5.854969836	-0.524461163	1.948133078
C	5.411792622	0.699609487	1.364003142
C	3.704891255	-0.617359739	3.109818810
C	6.345932794	-0.100184510	-0.736601272
C	5.661358435	0.916698175	-0.007406703
C	5.849776502	-0.448082719	-2.031873203
C	4.705949189	0.248950512	-2.519516869
C	3.699420643	-0.495657440	-3.170020276
C	2.396697454	0.070653721	-3.280085190
C	-0.393471680	-2.067723948	-1.245030803
C	1.278581918	-0.774989326	-3.069178510
C	0.030425296	-0.194776441	-2.741758176
C	-0.986406460	-2.562324632	-0.009423434
C	-1.777465887	-1.589609608	0.907709728
C	-0.809205695	-0.857270159	-1.808238987
C	0.280523739	-1.618245466	2.362756095
C	-0.863002952	-0.949035830	1.932243210
C	3.506638564	0.780029542	2.886533429
C	1.286184002	-0.889386016	3.042698262
C	1.107351304	0.500060755	3.245537595
C	4.378534648	1.455037002	1.997343465
C	3.946018665	2.678977493	1.417129357
C	2.243816598	1.357030467	3.173558889
C	4.863562144	1.877065702	-0.703378637
C	4.194687250	2.894867401	0.029528371
C	4.375365182	1.534277305	-1.990976176
C	3.238673779	2.224635309	-2.493087141

C	2.225293110	1.471156909	-3.151371138
C	0.913844132	2.018557148	-3.234760637
C	-1.902075045	-0.141175504	-1.214726463
C	-0.196974388	1.171992667	-3.035022834
C	-1.468154196	1.747113398	-2.729309156
C	-2.376281654	-0.476880636	0.064858106
C	-2.975539513	0.606697241	0.801258390
C	-2.330668532	1.086768279	-1.831804852
C	-1.187666602	0.312066961	2.441541010
C	-2.402780496	0.979419048	2.037697397
C	2.029506604	2.737620840	2.930089999
C	-0.186102276	1.058887874	3.108801195
C	-0.373744901	2.457049195	3.306845001
C	2.897991316	3.413030703	2.038788271
C	2.440484591	4.629524655	1.446443688
C	0.747154960	3.306861424	3.204989104
C	3.377420386	3.832791643	-0.663091015
C	2.687043630	4.844735113	0.074078931
C	2.890247679	3.490354021	-1.947168583
C	1.732399086	4.172848991	-2.437782462
C	0.730119570	3.425774467	-3.090927813
C	-0.576401404	3.979729338	-3.204642278
C	-3.413757971	1.819232907	-1.271398156
C	-1.705130733	3.117935528	-3.033764128
C	-3.721273635	1.592804848	0.107657488
C	-2.715478696	2.256652888	2.577428058
C	0.527508002	4.693894482	2.979247313
C	-1.682388712	3.013842565	3.225673521
C	1.399696768	5.374962461	2.073745890
C	1.880147238	5.797173034	-0.613877379
C	1.385018980	5.448179905	-1.909191640
C	-0.729300340	5.267051659	3.299680456
C	-0.868353065	6.673861070	3.083306093
H	-1.715406519	7.209140140	3.507845066
C	0.973059824	6.601624063	1.505675655
C	-0.039891553	7.323708214	2.212173238
H	-0.245743680	8.361430594	1.956498050
C	-3.876468158	2.945541660	2.126180126
C	-4.183842622	4.192055351	2.760810311
H	-5.166213205	4.641274665	2.624761384
C	-1.862464560	4.402907945	3.436304216
C	-3.206049505	4.899286744	3.398271035
H	-3.426363588	5.898172854	3.769718084
C	-3.865411196	3.011404886	-1.886872787
C	-4.963013189	3.688553649	-1.258182623
H	-5.515003511	4.452892643	-1.802045772
C	-4.381295990	2.615252070	0.834778329
C	-5.206401936	3.506765879	0.072451525
H	-5.940532929	4.135250595	0.574216666
C	-0.753440403	5.382019034	-3.093163800
C	-2.079323661	5.883316180	-3.280226448
H	-2.240817491	6.951257002	-3.414934046
C	-2.982480563	3.684124862	-2.787017888
C	-3.159991487	5.059608083	-3.138177634
H	-4.160060610	5.487564842	-3.164447229
C	1.224218115	6.821253849	0.114528858
C	0.469103553	7.771440799	-0.644728939
H	0.149959552	8.705100821	-0.185070275
C	0.257653737	6.139377308	-2.423113962
C	-0.002462702	7.439012636	-1.882450769
H	-0.689045550	8.113695331	-2.390447185
C	-4.935253771	-3.783300315	1.570703575
H	-5.925045249	-3.796391166	1.093336930
H	-5.132479529	-3.527660766	2.624666988
C	-4.346090987	-5.191417127	1.458342143
H	-4.240387666	-5.452503343	0.393077209
H	-3.323221987	-5.189604389	1.874971071
C	-5.204975886	-6.235389063	2.161547697
H	-5.309617055	-5.965271437	3.227202498
H	-6.221844249	-6.214997062	1.732533763
C	-4.621195886	-7.639482982	2.037989779
H	-3.614586127	-7.684427816	2.481704470
H	-5.251380397	-8.383084470	2.547139771
H	-4.533322394	-7.932573573	0.980633281
C	-2.670108641	-2.656995235	3.105886301
H	-2.650096120	-1.726045450	3.699885066
H	-3.453943175	-3.299632348	3.517296485
H	-1.701115612	-3.155332322	3.263061554

TS2*butyl,oblique*



163
Co2C123H32O6

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C	4.583026874	-4.322446349	1.498753824
C	1.579045671	-4.214904081	0.860188759
C	5.498113792	-1.926593365	-1.241432998
C	5.567861982	-1.821977644	1.450818268
C	6.788542831	-3.996793382	-0.025143806
O	1.103830863	-5.283734381	1.001630839
O	4.922895986	-5.261966990	2.123250933
O	5.682826579	-1.264165936	-2.168946174
O	5.896923386	-1.067110396	2.265676166
O	7.790272214	-4.568630090	-0.101461424
C	2.331356464	-3.104828950	-1.539688906
C	3.277271629	-3.764377421	-0.804900832
C	2.802238034	-2.971438596	2.890138560
O	2.568234259	-2.836196310	4.011873354
H	-5.597195253	-4.829549716	3.218048079
H	-4.124426368	-6.576253465	-0.451295909
H	-4.479449573	-6.142372029	1.916955628
H	-4.648283180	-5.851997973	-2.495094050
H	-6.009192343	-4.190086132	-3.632918669
H	-8.650250203	-1.116966383	-1.882171801
H	-7.413311672	-2.550672046	-3.399820924
H	-9.030001917	-0.701981629	0.245255441
H	-8.404137715	-1.493024229	2.458080897
H	-7.160629819	-2.994512511	3.455774582
C	-6.101378584	-2.772359276	3.340653065
C	-3.732355922	-5.566239757	1.374660846
C	-5.217249565	-3.810114178	3.202172976
C	-3.852669173	-3.563839419	2.869489364
C	-3.527532435	-5.815331013	0.048915647
C	-2.660116985	-4.966021225	-0.713977307
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C	-4.255266333	-4.846340266	-2.634326752
C	-3.029626677	-4.468324414	-2.002005699
C	-6.926679595	-1.666528303	-2.992552784
C	-5.021721189	-3.910866517	-3.270464919
C	-4.603273771	-2.545196587	-3.319130449
C	-7.624903219	-0.857562814	-2.139132455
C	-6.962450065	0.203846494	-1.447643508
C	-5.529625335	-1.456454216	-3.205664550
C	-8.115956495	-0.330254561	0.704839759
C	-7.201608992	0.461193918	-0.058081173
C	-7.763740738	-0.775338198	1.948468530
C	-6.482098665	-0.448495749	2.489742209
C	-5.673134332	-1.424135170	3.163037513
C	-4.282565656	-1.174372612	3.273468672
C	-1.938758067	-3.935563192	1.380499742
C	-3.364675590	-2.256587660	3.103627869
C	-2.008931793	-1.943224834	2.797519039
C	-1.665839855	-4.264781217	0.009443424
C	-0.717832995	-3.463027162	-0.685056345
C	-1.298666265	-2.766887695	1.897964690
C	-2.417056676	-3.263622145	-2.435303009
C	-1.159287219	-2.873361608	-1.883679602
C	-5.026205074	-0.166497993	-2.903775765
C	-3.228023574	-2.285319004	-3.097763539
C	-2.743732493	-0.951588211	-3.205011921
C	-5.755501631	0.682322512	-2.013857452
C	-5.062930300	1.765635843	-1.395385376
C	-3.651496176	0.122872144	-3.129589428
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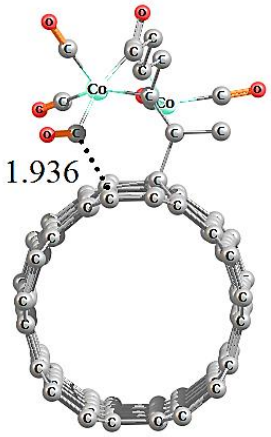
C	-5.295073982	2.015361838	-0.026596660
C	-5.844562547	0.704479873	1.967478744
C	-4.587882468	1.119744477	2.496772804
C	-3.794206128	0.159753077	3.159416106
C	-2.400995527	0.416060353	3.312144622
C	-0.111877859	-2.266238931	1.298771359
C	-1.496639458	-0.656969891	3.110073557
C	-0.142029544	-0.368242368	2.820475164
C	0.391612578	-2.867822055	0.071893025
C	1.408369948	-2.089087726	-0.817078580
C	0.550569824	-1.188535244	1.891752033
C	-0.562124479	-1.632632843	-2.319977272
C	0.694359635	-1.245914558	-1.854586145
C	-3.149348593	1.436292319	-2.874575870
C	-1.358131738	-0.688441281	-3.012575137
C	-0.865962331	0.627261604	-3.188894018
C	-3.869144986	2.276622942	-1.989991268
C	-3.187042390	3.362251149	-1.375737618
C	-1.782678817	1.718147026	-3.125180739
C	-4.321609128	2.762177071	0.706439814
C	-3.419614604	3.611021663	0.009263799
C	-3.961127183	2.303226404	1.999895196
C	-2.713563942	2.713723751	2.543759371

C	-1.915155011	1.743103555	3.213768409
C	-0.516831119	1.979114757	3.338461641
C	1.793286913	-0.732513554	1.336850281
C	0.379649350	0.907002566	3.145966801
C	1.755479424	1.183734826	2.880239177
C	2.220255823	-1.152512643	0.062847974
C	3.059828689	-0.210545459	-0.634363800
C	2.470891268	0.358487685	1.989845614
C	1.301301967	-0.077275540	-2.324545574
C	2.619004370	0.300883028	-1.873115174
C	-1.269306163	3.010995250	-2.847784863
C	0.515058153	0.880012290	-3.009268314
C	1.017990857	2.202642990	-3.179630543
C	-1.985008783	3.849917803	-1.959221564
C	-1.281333242	4.923153986	-1.331995749
C	0.114470550	3.281717631	-3.085033546
C	-2.432398405	4.331778809	0.739104412
C	-1.510802991	5.170092069	0.037943697
C	-2.073108539	3.874079763	2.029436688
C	-0.806044369	4.271870621	2.561711729
C	-0.016870294	3.310044445	3.225781518
C	1.377141747	3.552686972	3.381486894
C	3.708218236	0.834797864	1.473264959
C	2.287097092	2.460679260	3.220007393
C	3.990376765	0.571603780	0.095469457
C	3.230425156	1.475927316	-2.387519459
C	0.634493516	4.580266048	-2.824156449
C	2.415160122	2.450153690	-3.055427964
C	-0.083998567	5.424846068	-1.921022030
C	-0.530485739	5.907791797	0.763499756
C	-0.164977615	5.441563477	2.064906130
C	1.995412718	4.860967398	-3.106169211
C	2.442529247	6.195838544	-2.854502366
H	3.399558843	6.533015990	-3.247890587
C	0.592557849	6.515036512	-1.317990630
C	1.760098946	7.000936338	-1.986147028
H	2.188443164	7.960459100	-1.702275858
C	4.502971781	1.878572649	-1.895258317
C	5.101772043	3.029847620	-2.500120061
H	6.155057175	3.246170708	-2.328731630
C	2.908839799	3.765401597	-3.236065737
C	4.327608035	3.945833617	-3.152397460
H	4.778142987	4.874191566	-3.498442916
C	4.398842266	1.886139518	2.123500210
C	5.634487225	2.311424912	1.532309716
H	6.328263480	2.925730368	2.103316381
C	4.882455480	1.428369033	-0.595365727
C	5.864419700	2.101695885	0.203318603
H	6.731980425	2.560043299	-0.268924303
C	1.868352509	4.880188357	3.301756281
C	3.266891571	5.066496517	3.533079148
H	3.660555669	6.068300729	3.695389564
C	3.665464727	2.727377928	3.016989959
C	4.137817164	4.021974532	3.401676544
H	5.207356142	4.212359112	3.464106342
C	0.359328357	6.766725816	0.071143995
C	1.286048068	7.513244782	0.867014814
H	1.819426167	8.357406202	0.433618830
C	1.073447224	5.854469438	2.620346684
C	1.634584232	7.068415176	2.110347552
H	2.439616624	7.565522074	2.648531243
C	2.084346896	-3.390168304	-2.990997051
H	1.017306424	-3.292510763	-3.231376190
H	2.359883455	-4.427916000	-3.218421370
C	2.894844307	-2.416625879	-3.892668741
H	3.257594588	-1.567418786	-3.293952581
H	3.806007076	-2.921992670	-4.254598115
C	2.085481888	-1.870430780	-5.066715494
H	1.861306509	-2.686977995	-5.775233766
H	1.110188120	-1.507780292	-4.698524532
C	2.807663352	-0.728729380	-5.774577747
H	2.983769034	0.108542437	-5.079768984
H	3.787123492	-1.053204151	-6.159332554
H	2.216898888	-0.345474596	-6.619043018
C	3.850534871	-5.059705994	-1.358268537
H	4.384408016	-5.639703028	-0.598648421
H	3.035724212	-5.696321210	-1.740095135
H	4.553774980	-4.869646328	-2.183109640

TS2*methyl,perpendicular*

163
Co2C123H32O6

Co	-3.467351067	-3.877184950	1.047263416
Co	-2.357928344	-4.159341483	-1.043981578
C	-2.159541776	-4.410952107	2.155351528
C	-4.928166561	-4.309007393	1.958133904
C	-2.286756395	-4.476034705	-2.776823693
C	-1.079289084	-5.281233118	-0.601482198
C	-3.543620087	-5.409890706	-0.078904368
O	-5.883275328	-4.622872486	2.522771197
O	-1.329108312	-4.749725027	2.879445611
O	-2.272940720	-4.712869626	-3.907679653
O	-0.298756854	-6.085528300	-0.326365147
O	-3.972540071	-6.466577848	-0.350479138
C	-3.440616977	-2.105758238	-1.330322383
C	-4.162092865	-3.010147051	-0.570104012
C	-3.469654515	-2.103539785	1.709436389
O	-4.046976110	-1.601158928	2.609608795
H	-5.762543181	4.050741586	2.883583560
H	-6.683780941	2.977524361	-1.242888651
H	-6.678912021	2.990629994	1.190622108
H	-5.765390327	3.981254232	-2.989571737
H	-4.236245953	5.735086272	-3.679967189
H	-1.893083504	8.462588866	-1.155240009
H	-2.864437200	7.325634624	-3.070408067
H	-1.888790153	8.491544770	1.049403463
H	-2.864816209	7.391716519	2.984871277
H	-4.247951902	5.808672823	3.589746578
C	-3.844696426	4.824229277	3.359979934
C	-5.907177515	2.437519902	0.657972102
C	-4.698787640	3.832877551	2.957981615
C	-4.191408433	2.587953235	2.477116006
C	-5.913115763	2.425636270	-0.706980419
C	-4.805969981	1.856405397	-1.420924538
C	-4.788967316	1.891770389	1.372901865
C	-4.699945134	3.765083643	-3.041553618
C	-4.198698359	2.525991983	-2.534311990
C	-1.986665149	6.899173044	-2.588417877
C	-3.837942478	4.753036279	-3.431632366
C	-2.425650175	4.556333806	-3.358129163
C	-1.439448719	7.539717016	-1.512158027
C	-0.402443874	6.912755883	-0.752346143
C	-1.525854913	5.597923937	-2.961350849
C	-1.436659907	7.575542175	1.425396142
C	-0.400723782	6.930340096	0.679550085
C	-1.985942564	6.956207515	2.512924857
C	-1.526501237	5.662710470	2.912776549
C	-2.431814635	4.626873380	3.314926333
C	-1.973582265	3.285758161	3.266436167
C	-4.024409943	0.914640075	0.703361721
C	-2.859807045	2.260218171	2.821087631
C	-2.296481104	1.020618557	2.384090389
C	-4.045388248	0.881234942	-0.737152899
C	-2.937942656	0.263066789	-1.371254578
C	-2.876342511	0.346989823	1.314622087
C	-2.860854232	2.193481041	-2.848818701
C	-2.310892806	0.947105046	-2.401484493
C	-0.226644401	5.232515748	-2.528950078
C	-1.968615087	3.215349194	-3.286983846
C	-0.572866093	2.942164205	-3.277751171
C	0.349738781	5.905621135	-1.406692052
C	1.427296670	5.270985520	-0.723088149
C	0.313681897	3.967909862	-2.902183199
C	0.351239606	5.937494182	1.356492465
C	1.428059557	5.286391340	0.686788425
C	-0.224698294	5.290078231	2.494164390
C	0.314883014	4.033117814	2.893612927
C	-0.576156305	3.013904244	3.278683557
C	-0.117006075	1.660243442	3.279411937
C	-2.297383977	-0.878939594	0.773571091
C	-0.987270369	0.648897411	2.826330800
C	-0.454348939	-0.613244795	2.448729989
C	-2.408316301	-1.041183232	-0.794921619
C	-1.068580097	-1.414380423	-1.386038835
C	-1.043971893	-1.324462123	1.370958373
C	-0.993499839	0.572770005	-2.828269817
C	-0.459019326	-0.686058072	-2.427578862
C	1.642030980	3.619229533	-2.507139815
C	-0.115428619	1.586890715	-3.256673899
C	1.284711465	1.331452831	-3.298339212
C	2.210365389	4.282888563	-1.395692115
C	3.296010751	3.665735648	-0.714986317
C	2.181309675	2.368664999	-2.910455802
C	2.212015582	4.312931855	1.380428007
C	3.296835712	3.680684290	0.712249481
C	1.642932102	3.672666784	2.506270586
C	2.180822204	2.427559383	2.931086174



Note: Discarded in the main manuscript.

C	1.279970229	1.396997678	3.331214439
C	1.731260729	0.055482750	3.333714674
C	-0.297745783	-2.342521810	0.752319674
C	0.849338340	-0.968663372	2.893407945
C	1.391738236	-2.227656913	2.522842731
C	-0.308598570	-2.384974622	-0.705868915
C	0.851036911	-2.934184480	-1.343718903
C	0.826805417	-2.903094331	1.417848492
C	0.861699597	-1.029176614	-2.848037885
C	1.414194237	-2.276342791	-2.453750925
C	3.494362077	2.014647879	-2.505832277
C	1.742557575	-0.007571065	-3.287219540
C	3.146365602	-0.269095639	-3.301060861
C	4.060592839	2.674272546	-1.382174589
C	5.131437308	2.032922683	-0.692025166
C	4.031146917	0.753696174	-2.897829142
C	4.061475890	2.701649000	1.397816214
C	5.130091685	2.044791409	0.718942561
C	3.491812372	2.061323062	2.531210923
C	4.022445621	0.803149115	2.941291962
C	3.131928867	-0.212043787	3.352049412
C	3.594618149	-1.559655734	3.377777920
C	1.624130515	-3.895290057	0.768711061
C	2.702427361	-2.594729374	2.958968703
C	1.646190465	-3.899434153	-0.661403388
C	2.730186993	-2.645063446	-2.876099862
C	5.353072681	0.393169673	-2.500238413
C	3.617199389	-1.613887279	-3.310216455
C	5.916895674	1.049677307	-1.361840950
C	5.911848896	1.069244773	1.405088561
C	5.342659958	0.430595667	2.550926281
C	5.908901024	-0.833823881	-2.935403566
C	7.250664539	-1.110334304	-2.534269926
H	7.804864613	-1.919429374	-3.006295526
C	7.008724083	0.446891055	-0.690728118
C	7.785372172	-0.488574761	-1.438190479
H	8.752452553	-0.817107283	-1.061747091
C	3.260328107	-3.900492711	-2.498393819
C	4.556398738	-4.228102182	-2.991239362
H	4.931917109	-5.245660464	-2.900756655
C	5.011098743	-1.873001298	-3.359462141
C	5.409095639	-3.239572973	-3.410012857
H	6.440445274	-3.497378318	-3.643352204
C	2.672161357	-4.531962938	1.467593376
C	3.398637331	-5.536935857	0.759759803
H	4.064157370	-6.208561650	1.299087134
C	2.698316752	-4.550361306	-1.340765635
C	3.413016011	-5.545191870	-0.609670703
H	4.087599762	-6.224639939	-1.127571737
C	4.987078923	-1.823882540	3.436767996
C	5.380006344	-3.190189088	3.518575163
H	6.409464388	-3.447125864	3.760739027
C	3.229070036	-3.862396398	2.616930910
C	4.523004106	-4.182762917	3.117972274
H	4.893987299	-5.203943513	3.052528378
C	7.004333993	0.454515547	0.745675321
C	7.774631729	-0.474985791	1.507113148
H	8.740296980	-0.814310043	1.136851859
C	5.891145321	-0.793601328	3.003011232
C	7.231307196	-1.082947092	2.606881309
H	7.779023753	-1.891025236	3.088163065
C	-5.576773272	-3.335831965	-0.963005891
H	-5.900841979	-4.311542514	-0.575501198
H	-5.717243657	-3.349599264	-2.055217209
C	-6.438502983	-2.208529510	-0.363294445
H	-6.320311390	-2.202376985	0.733270060
H	-6.045824882	-1.236474383	-0.714015006
C	-7.915781238	-2.311683825	-0.720726514
H	-8.026543996	-2.317787417	-1.818776337
H	-8.317384906	-3.272355493	-0.355583996
C	-8.708687907	-1.151915126	-0.124006396
H	-8.310391414	-0.188288834	-0.479334544
H	-9.772432574	-1.206763332	-0.397220267
H	-8.636719047	-1.155446884	0.974433622
C	-3.829073658	-1.835545509	-2.771225300
H	-2.945927900	-1.543163399	-3.358353018
H	-4.266381997	-2.723051927	-3.241293072
H	-4.561345331	-1.014536510	-2.840788724

TS2*methyl,perpendicular*

163
Co2C123H32O6

Co	4.689536719	-2.443585645	1.232378479
Co	5.376236204	-1.195991204	-0.758933112
C	5.064242912	-4.065604771	1.877219413
C	3.085517446	-2.235394247	2.390935250
C	5.421501033	-1.228882359	-2.508820201
C	6.796822804	-0.117197932	-0.589015720
C	6.393504233	-2.417981069	0.271239773
O	2.783832234	-2.625570776	3.452932899
O	5.386841472	-5.089458906	2.298752898
O	5.439460031	-1.285911736	-3.662551583
O	7.811904859	0.435619877	-0.585829695
O	7.489568910	-2.837952166	0.345755522
C	2.953964757	-2.710254691	-0.075454029
C	4.148004240	-2.726488048	-0.808520990
C	5.425453463	-1.260547722	2.335233884
O	5.997014291	-0.555330064	3.049463761
H	5.700249061	3.316059581	-2.408970801
H	5.917840282	2.999077102	1.998422227
H	6.252255893	2.726365988	-0.396063251
H	4.823450994	4.160643188	3.441727419
H	3.222109269	5.968034161	3.690068546
H	1.294206902	8.233034631	0.441818731
H	1.961924356	7.425571721	2.634676114
H	1.619014460	7.917041208	-1.713647181
H	2.849566106	6.563565479	-3.312224278
H	4.288098092	4.925605082	-3.570810563
C	3.857614821	3.988407138	-3.223039964
C	5.436238997	2.202808783	0.096767033
C	4.648720009	3.087680197	-2.570803194
C	4.066835246	1.931247336	-1.959921980
C	5.246988427	2.357169711	1.431330897
C	4.057062577	1.837687107	2.043689541
C	4.485481403	1.459288884	-0.687378693
C	3.760354007	3.938614419	3.374439305
C	3.324845844	2.636168268	2.977099996
C	1.162673734	6.914821094	2.100783667
C	2.858718396	4.956603213	3.518349756
C	1.468905573	4.728456527	3.279040397
C	0.786938113	7.369508940	0.868090344
C	-0.128010696	6.612014452	0.070745824
C	0.641635008	5.681310453	2.602743158
C	1.219172800	6.948930865	-2.009717217
C	0.082541388	6.407397263	-1.329808876
C	1.911642187	6.187187162	-2.908236987
C	1.505054849	4.841431343	-3.174265810
C	2.447241229	3.774586208	-3.307893526
C	1.986131750	2.443979694	-3.124702222
C	3.680370341	0.495689537	0.000859308
C	2.802163927	1.504907784	-2.426146908
C	2.215501066	0.301973437	-1.912363749
C	3.419045030	0.749372463	1.412731506
C	2.213686011	0.220948779	1.952211010
C	2.709843862	-0.261350200	-0.726352192
C	1.960867863	2.323853091	3.178496889
C	1.477132466	1.026620164	2.839009227
C	-0.582408607	5.231385030	2.046089015
C	1.020456298	3.384760126	3.347397837
C	-0.361485151	3.092255112	3.184930896
C	-0.977103705	5.707026628	0.757019442
C	-1.944836922	4.954542386	0.029840821
C	-1.181060469	4.033441586	2.530580239
C	-0.570737481	5.312325919	-1.948889988
C	-1.736956776	4.753471760	-1.350572747
C	0.157010164	4.512422609	-2.883578232
C	-0.325355281	3.203375742	-3.166665723
C	0.605449188	2.151999067	-3.279281692
C	0.154954897	0.803860815	-3.148568785
C	2.043353547	-1.434094196	-0.022570730
C	0.967409045	-0.133113660	-2.472944736
C	0.366026786	-1.326905937	-1.987513477
C	1.679159070	-1.029916989	1.456371408
C	0.386631396	-1.439655846	1.953477677
C	0.788642052	-1.874561236	-0.757811997
C	0.117317677	0.695520465	3.125537459
C	-0.356361018	-0.612021965	2.841903217
C	-2.434074827	3.599219701	2.000758439
C	-0.814172454	1.744187706	3.301852775
C	-2.201995409	1.466044034	3.177819227
C	-2.825803511	4.069750797	0.724342299
C	-3.797922483	3.332563286	-0.005129963
C	-3.031097265	2.414539107	2.507873482
C	-2.415824721	3.674498661	-1.994599759
C	-3.588047919	3.130476244	-1.402604325
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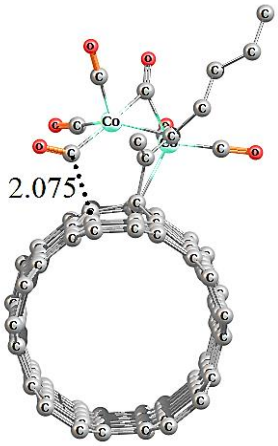
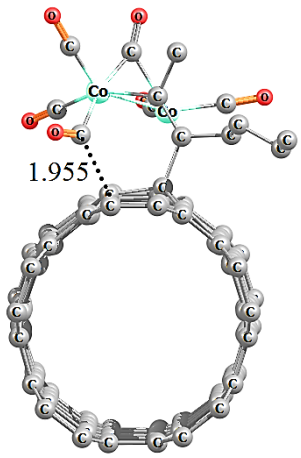
C	-2.169965332	1.585536935	-3.235043898



Note: Taken into consideration in the main manuscript.

C	-1.225939050	0.524000359	-3.360018756
C	-1.684537822	-0.808153062	-3.246138342
C	-0.121751256	-2.694292710	-0.072152982
C	-0.879177536	-1.745526643	-2.549524341
C	-1.496486290	-2.930581065	-2.070178715
C	-0.307372350	-2.507393635	1.338805189
C	-1.498321156	-3.021478807	1.919587532
C	-1.127049630	-3.395362522	-0.793004923
C	-1.715370169	-0.926292608	3.130177056
C	-2.207504589	-2.229969858	2.850042913
C	-4.266292935	1.971558016	1.969255082
C	-2.651489425	0.129325973	3.295979399
C	-4.041058738	-0.157768326	3.145485269
C	-4.656479581	2.438885263	0.685557364
C	-5.612467488	1.676530443	-0.048686231
C	-4.857084880	0.773474955	2.466957492
C	-4.247787052	2.047548463	-2.038178945
C	-5.407014838	1.479836964	-1.430997604
C	-3.527888277	1.263085085	-2.979121329
C	-4.005550055	-0.044805395	-3.283510603
C	-3.072417380	-1.093979842	-3.427526301
C	-3.539588964	-2.436941467	-3.329694371
C	-1.999183268	-4.293501870	-0.112428729
C	-2.729725275	-3.382997493	-2.629707236
C	-2.192914462	-4.100312884	1.290745670
C	-3.565257197	-2.561512397	3.138637678
C	-6.103020826	0.326144227	1.937174878
C	-4.506931765	-1.496564893	3.287188748
C	-6.489377330	0.788263045	0.640279734
C	-6.088623025	0.405517175	-2.073492693
C	-5.370468885	-0.375982366	-3.032058875
C	-6.717040858	-0.834059411	2.468064438
C	-7.981281069	-1.203009918	1.917357221
H	-8.596618233	-1.948214457	2.418079394
C	-7.471083819	0.068295332	-0.083981478
C	-8.348614738	-0.764436341	0.673922843
H	-9.246949377	-1.170944454	0.212990871
C	-4.041215271	-3.869690679	2.879378655
C	-5.392955196	-4.147452551	3.234724052
H	-5.750628621	-5.175378287	3.252739376
C	-5.892580230	-1.775688434	3.173109542
C	-6.295836346	-3.127110225	3.380166175
H	-7.349225207	-3.367573826	3.510887627
C	-2.940575183	-5.050861752	-0.848132347
C	-3.762863718	-5.948840765	-0.104570536
H	-4.356981694	-6.700142563	-0.621652787
C	-3.332882335	-4.663024078	1.909208802
C	-3.953645199	-5.759363798	1.238511599
H	-4.696351883	-6.363512519	1.756314861
C	-4.911690122	-2.724795146	-3.540848407
C	-5.300862073	-4.094405121	-3.465064081
H	-6.284201507	-4.401144578	-3.816495281
C	-3.316848395	-4.580539734	-2.156337609
C	-4.524921523	-4.998232655	-2.788665628
H	-4.910113285	-6.001811874	-2.617827848
C	-7.264795368	-0.128066860	-1.491272907
C	-7.927247587	-1.165339366	-2.214120222
H	-8.936613512	-1.463485588	-1.936403879
C	-5.859640524	-1.657443103	-3.382693929
C	-7.243640276	-1.908545072	-3.137867383
H	-7.724392927	-2.781434912	-3.575492989
C	4.470984818	-3.922798868	-1.670307712
H	4.018554256	-3.649741048	-2.646865844
H	3.894839705	-4.797787500	-1.336274019
C	5.909987492	-4.355510127	-1.907682819
H	6.541557490	-3.495007617	-2.176579461
H	6.332003929	-4.771918047	-0.978517040
C	5.999707088	-5.399322104	-3.017636530
H	5.363203629	-6.263943904	-2.761370811
H	5.585008875	-4.970519448	-3.946433256
C	7.432342873	-5.863723972	-3.257464102
H	8.074901291	-5.015802884	-3.540606348
H	7.856018485	-6.314429020	-2.346879905
H	7.483025273	-6.611091793	-4.062162935
C	2.289291624	-4.043381418	0.252304774
H	1.661328926	-3.971737448	1.148607446
H	1.664881901	-4.412827190	-0.574635007
H	3.055354181	-4.797013668	0.463719052

TS2*butyl,perpendicular*



163
Co2C123H32O6

Co	0.330744327	-5.178147530	-1.390509609
Co	-0.763607402	-4.737205078	0.695851721
C	-0.929368122	-4.635442664	-2.547037177
C	1.200101929	-6.421396391	-2.312761639
C	-0.993501998	-5.034941718	2.416340451
C	-2.469831501	-4.893747163	0.307000749
C	-0.697298921	-6.418017807	-0.437785989
O	1.736858850	-7.262770950	-2.888813404
O	-1.735759358	-4.294766761	-3.296840376
O	-1.134246094	-5.283830355	3.536351706
O	-3.576429685	-5.131686331	0.080625415
O	-1.139888186	-7.487363479	-0.248262872
C	1.504968632	-3.902719627	1.060389473
C	1.326065556	-5.056824431	0.313051169
C	1.565629651	-3.827531083	-1.904776656
O	2.460108978	-3.825435211	-2.674285185
H	6.937253423	-0.151925255	-3.328131825
H	7.245996291	-1.658479646	0.755164277
H	7.127916493	-1.562965860	-1.673357585
H	7.190962310	-0.437705826	2.588932258
H	7.049850451	1.859423908	3.368254388
H	6.692712739	5.524205231	0.938371036
H	6.882797264	3.965529594	2.791069899
H	6.591953782	5.651622149	-1.257978838
H	6.614938937	4.261544774	-3.252234271
H	6.740847594	2.185343080	-3.949386804
C	5.842642514	1.630646684	-3.684449135
C	6.206473911	-1.582829969	-1.094272840
C	5.953363871	0.313333463	-3.329798409
C	4.828990033	-0.395362081	-2.807375367
C	6.272314132	-1.643484541	0.268306223
C	5.081055804	-1.483198560	1.047702595
C	4.948044706	-1.342478070	-1.736370249
C	6.212884841	0.028153409	2.693949832
C	5.048510965	-0.638497738	2.203111215
C	5.900638400	4.170928439	2.369306473
C	6.133118772	1.321543924	3.133096465
C	4.883729746	2.012034183	3.128868294
C	5.793725327	5.049267725	1.327217047
C	4.550909389	5.200277668	0.636260977
C	4.770300130	3.395971208	2.776152556
C	5.663210255	5.201320285	-1.603812321
C	4.487235718	5.273647539	-0.792746640
C	5.676024217	4.418954762	-2.724426648
C	4.514212603	3.671455819	-3.092746762
C	4.597668017	2.314795057	-3.547194159
C	3.432131857	1.511545393	-3.462131973
C	3.786352375	-1.699712793	-1.018903202
C	3.550062829	0.146220933	-3.065648234
C	2.381484280	-0.527138947	-2.588302938
C	3.855290891	-1.797182917	0.415376426
C	2.632952108	-1.694365588	1.130874881
C	2.495457107	-1.454978194	-1.556795138
C	3.792705861	-0.122446922	2.593030809
C	2.588217172	-0.788785325	2.185465057
C	3.492123043	3.895401498	2.421807504
C	3.711827923	1.213312151	3.082148852
C	2.433027096	1.828978771	3.153759749
C	3.379153992	4.819452828	1.336559765
C	2.103334341	4.983369671	0.722537351
C	2.320895175	3.193435682	2.829334968
C	3.257188448	4.955319678	-1.420894570
C	2.040539509	5.051844528	-0.684366088
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C	2.068600551	3.464819282	-2.954684993
C	2.152206594	2.128297465	-3.388028253
C	0.977051631	1.316729722	-3.354825251
C	1.330713397	-2.119914668	-0.981355353
C	1.091466738	-0.029219842	-2.951150093
C	-0.068161595	-0.738532762	-2.540102947
C	1.395722741	-2.397027821	0.582008759
C	0.130645134	-1.894620909	1.246307363
C	0.034944960	-1.707657517	-1.504607687
C	1.332257128	-0.310133342	2.687376009
C	0.129837827	-0.981117052	2.318094659
C	1.031602791	3.722775253	2.516543082
C	1.257080071	1.015594058	3.160612363
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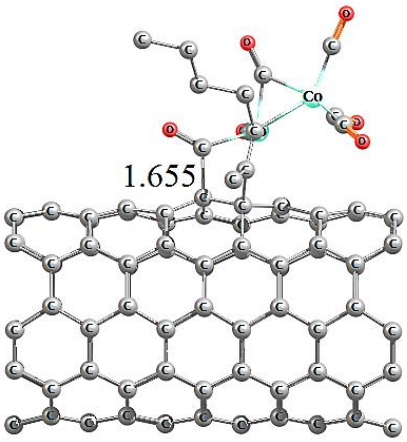
C	-0.127572301	3.028627226	2.953036271
C	0.795794829	4.767635700	-1.327339118
C	-0.416219913	4.883271418	-0.592452612
C	0.811052038	3.955305300	-2.485725764
C	-0.384272691	3.292007824	-2.873313638

C	-0.299088754	1.941358277	-3.323083360
C	-1.460851094	1.134203184	-3.295377021
C	-1.145742652	-2.093111185	-0.843404827
C	-1.344824642	-0.228218796	-2.908152040
C	-2.514943767	-0.925879198	-2.508745505
C	-1.093665355	-2.200723321	0.612328483
C	-2.320170857	-1.952106641	1.317822963
C	-2.413771148	-1.841175811	-1.438694148
C	-1.110990658	-0.477583001	2.815701484
C	-2.320701490	-1.130312125	2.458237320
C	-1.409280381	3.546058685	2.632054571
C	-1.181407421	0.850816210	3.305709189
C	-2.459198705	1.481190663	3.407731092
C	-1.523632910	4.454363614	1.546063487
C	-2.798768075	4.605650123	0.924331706
C	-2.573878478	2.843646786	3.059100235
C	-1.648025374	4.579182895	-1.228385694
C	-2.861716340	4.665069972	-0.484084945
C	-1.631872672	3.766308305	-2.393345668
C	-2.828443669	3.087644130	-2.768501972
C	-2.742478498	1.757141020	-3.231687133
C	-3.919551646	0.954601754	-3.231775688
C	-3.614863741	-2.177474824	-0.743050673
C	-3.803972860	-0.422856689	-2.868113489
C	-3.567445513	-2.218093278	0.685046121
C	-3.572414619	-0.653346250	2.961959707
C	-3.866359076	3.360343101	2.745779355
C	-3.640912635	0.686453241	3.449723516
C	-3.981493185	4.263111012	1.642636825
C	-4.104638110	4.372874610	-1.119639559
C	-4.088101250	3.562152824	-2.297609317
C	-5.023444842	2.694950320	3.217231241
C	-6.282027177	3.289455785	2.899696607
H	-7.185446538	2.956817312	3.407359557
C	-5.249136351	4.455041926	1.040481849
C	-6.392438494	4.144326854	1.836487947
H	-7.381173435	4.471851424	1.520355709
C	-4.767740512	-1.326122954	2.618389100
C	-5.974826931	-0.831528172	3.191662174
H	-6.889287178	-1.417944314	3.124634440
C	-4.907243601	1.311204654	3.586502803
C	-6.042000394	0.453737305	3.663433198
H	-7.008347462	0.855988251	3.961629968
C	-4.867876297	-2.041827407	-1.379063294
C	-6.015123644	-2.439085879	-0.628136950
H	-6.974807390	-2.563420058	-1.126541342
C	-4.765497560	-2.137352971	1.427037747
C	-5.966466213	-2.483146457	0.740187814
H	-6.887793955	-2.643410622	1.297405434
C	-5.194560148	1.575891846	-3.206081881
C	-6.329744004	0.717682306	-3.268826799
H	-7.318253633	1.134697048	-3.451524414
C	-4.967558963	-1.136410566	-2.496264746
C	-6.218357531	-0.603918567	-2.921947239
H	-7.122241845	-1.204325780	-2.837090223
C	-5.313300335	4.507599918	-0.393413417
C	-6.523527060	4.247226436	-1.104203040
H	-7.480554299	4.536650261	-0.674095407
C	-5.281056567	2.923881251	-2.714505838
C	-6.507009356	3.475474780	-2.234816022
H	-7.452342457	3.170864521	-2.679897858
C	1.991779972	-4.003295296	2.498503379
H	1.459701163	-4.814507161	3.012514386
H	1.712940453	-3.084296218	3.034210581
C	3.511518133	-4.245729863	2.643174652
H	3.707606691	-5.329654657	2.679415035
H	4.047991526	-3.873632613	1.757974990
C	4.082265022	-3.586189661	3.895402440
H	3.840288184	-2.511200039	3.882821374
H	3.584714920	-4.002852080	4.788919259
C	5.592777753	-3.766491653	4.002079648
H	5.863561806	-4.831685833	4.073342727
H	6.092356740	-3.354492898	3.111234068
H	5.994134375	-3.251106968	4.886628295
C	1.937633932	-6.348496429	0.804285541
H	1.928698294	-6.440716280	1.899836721
H	1.450985540	-7.234374899	0.383386922
H	2.990898328	-6.359131799	0.478649756

CP6*methyl,oblique*



163
Co2C123H32O6

Co	4.106121224	-2.096747235	1.067296048
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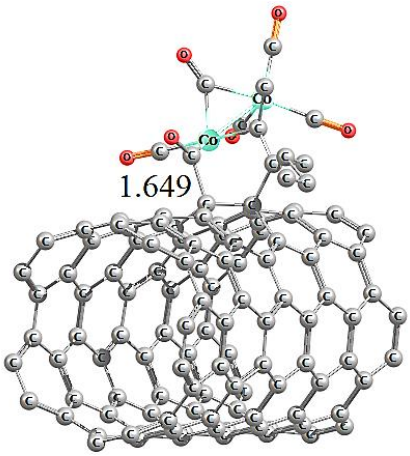
C	5.521419386	-3.195602501	1.356599779
C	2.534032675	-3.075601248	0.646894304
C	6.519525412	-0.598526239	-1.199406438
C	6.105160529	-0.524744423	1.482343286
C	7.918233309	-2.425196242	0.269358518
O	2.212505189	-4.205425437	0.871158795
O	5.868530248	-4.196806604	1.866784875
O	6.673470386	0.086945574	-2.115226732
O	6.300303216	0.266609628	2.309637256
O	9.005761755	-2.803290254	0.383186732
C	3.333258023	-1.939733661	-1.679550688
C	4.342525356	-2.498848523	-0.959100463
C	3.637708112	-1.959997435	2.774456338
O	3.319531859	-1.935567654	3.883613020
H	4.030644628	5.204187735	-3.678860845
H	6.216959451	3.290195697	-0.509801357
H	5.452646505	3.893176058	-2.741477223
H	5.855901676	3.602174388	1.669665286
H	4.479569013	4.928360483	3.174731077
H	1.349120792	7.901222835	2.215719998
H	2.918346360	6.439419333	3.350981583
H	0.637683773	8.521737691	0.225900657
H	1.042322645	8.085436812	-2.131855308
H	2.292209011	6.873672368	-3.459327486
C	2.017679961	5.821303099	-3.417967467
C	4.925021934	3.119511897	-2.187197605
C	3.003471521	4.874272973	-3.537928457
C	2.722817319	3.497457928	-3.309325498
C	5.359217693	2.775557914	-0.939856708
C	4.590779766	1.868140027	-0.142983534
C	3.670154783	2.617453021	-2.665644577
C	4.855028553	3.256795637	1.920852623
C	4.298264842	2.137152992	1.235965998
C	1.950822049	6.043436265	3.048428964
C	4.079499068	4.001716161	2.767327065
C	2.714334886	3.656111263	2.992849078
C	1.065388339	6.868565872	2.410290226
C	-0.131893603	6.337888998	1.838810008
C	1.685319265	4.644252960	3.153362241
C	0.140103615	7.680141227	-0.252639784
C	-0.583942381	6.733735486	0.536239735
C	0.368275221	7.433974536	-1.578455898
C	-0.120407314	6.233912326	-2.178555697
C	0.688977755	5.447451031	-3.068230979
C	0.333225838	4.090526696	-3.266306547
C	3.209476653	1.409327372	-2.102930357
C	1.364567678	3.106783299	-3.363129142
C	1.011926916	1.743917815	-3.143569076
C	3.737645604	0.983468613	-0.834321240
C	2.993804648	0.003001254	-0.107716134
C	1.920132628	0.892060789	-2.475076056
C	3.131287882	1.554801348	1.781651470
C	2.570860348	0.379710919	1.173300718
C	0.334389361	4.240279874	3.015979174
C	2.329203782	2.329186646	2.674246664
C	1.000724479	1.901051472	2.951230803
C	-0.593919948	5.102210102	2.353160701
C	-1.804222549	4.534257810	1.853656310
C	-0.006719513	2.863771666	3.146309427
C	-1.458548780	5.860963875	-0.156856446
C	-2.246620256	4.920841039	0.571623010
C	-1.219197906	5.605133727	-1.543099246
C	-1.792911678	4.431904301	-2.115329575
C	-0.998302218	3.661717362	-2.990736945
C	-1.368060122	2.308869317	-3.233980812
C	1.448855766	-0.328853224	-1.954809337
C	-0.336928994	1.332266047	-3.288042491
C	-0.669705742	-0.027940336	-3.089660537
C	2.294748341	-1.061230970	-0.937769152
C	1.449538334	-2.007665632	-0.001824575
C	0.246328948	-0.862015300	-2.389190333
C	1.382414471	-0.203199478	1.752451495
C	0.848743857	-1.379365012	1.227297805
C	-1.374356785	2.459019548	3.062890058
C	0.620040431	0.559426862	2.666776150
C	-0.680169505	0.118190563	3.008089229
C	-2.294034838	3.311072090	2.403940131
C	-3.504882457	2.753305537	1.909759571
C	-1.702007850	1.088589448	3.216193412
C	-3.160045554	4.068478203	-0.122139942
C	-3.947905900	3.141612920	0.611303917
C	-2.926335944	3.819448787	-1.500510566
C	-3.495420221	2.656754120	-2.087031353

C	-2.690707666	1.882476448	-2.970949046
C	-3.037104476	0.517450572	-3.189486235
C	-0.207681531	-2.147327449	-1.904652087
C	-2.012413133	-0.447867999	-3.254203448
C	-2.339102357	-1.831233410	-3.098669292
C	0.329986888	-2.677583154	-0.736171434
C	-0.512423107	-3.561373454	0.007655137
C	-1.431972920	-2.684051699	-2.433626475
C	-0.256610835	-1.988272078	1.848104322
C	-0.785921440	-3.234669084	1.357023589
C	-3.053726969	0.673277307	3.107285743
C	-1.043573072	-1.223771176	2.744629782
C	-2.354069492	-1.673401050	3.082780984
C	-3.973065241	1.520661812	2.443728138
C	-5.174620396	0.940811439	1.933425526
C	-3.373202665	-0.711989350	3.251177737
C	-4.835239454	2.271403625	-0.085430337
C	-5.614832670	1.324571964	0.648864963
C	-4.603497085	2.024748452	-1.458841493
C	-5.162461435	0.842910896	-2.040890015
C	-4.367022725	0.078904875	-2.920843672
C	-4.724326653	-1.274999244	-3.172859545
C	-1.912711626	-3.936952633	-1.959071786
C	-3.684635721	-2.252652152	-3.278740289
C	-1.460094418	-4.368057583	-0.675061307
C	-1.906675856	-3.827326054	1.988714945
C	-4.727614410	-1.135518870	3.158242832
C	-2.710993658	-3.034961942	2.874825859
C	-5.653810338	-0.286050402	2.476594219
C	-6.516083967	0.462290251	-0.040107269
C	-6.280825341	0.213231525	-1.428166504
C	-5.050004237	-2.502914672	3.351161994
C	-6.434964484	-2.855229272	3.278060054
H	-6.768516157	-3.828783948	3.632014266
C	-6.865170936	-0.843142914	1.993197381
C	-7.317702006	-2.048560313	2.617817484
H	-8.336283884	-2.395758436	2.454037488
C	-2.474867960	-5.015895695	1.443697349
C	-3.552644464	-5.617001388	2.173114888
H	-3.856110224	-6.638027070	1.947827799
C	-4.011868164	-3.476373765	3.217802208
C	-4.296641707	-4.871078282	3.037988468
H	-5.179641731	-5.308914616	3.499495352
C	-3.108719805	-4.492756807	-2.487916002
C	-3.530788023	-5.753828042	-1.947401862
H	-4.284142369	-6.343509413	-2.466334956
C	-2.262210738	-5.279805711	0.062722698
C	-3.128398046	-6.131986194	-0.700200428
H	-3.569736049	-7.014043107	-0.239291024
C	-6.054454860	-1.702616320	-2.930364909
C	-6.372601273	-3.055827082	-3.274079850
H	-7.412945796	-3.372223335	-3.324966352
C	-4.015693971	-3.630121259	-3.167598755
C	-5.384115934	-3.988731979	-3.393793651
H	-5.653413566	-5.032881046	-3.540746276
C	-7.311849583	-0.454561253	0.692403447
C	-8.231483067	-1.255718569	-0.058814136
H	-9.030876551	-1.789916031	0.451799937
C	-6.854167903	-0.939279789	-2.027106208
C	-8.008756240	-1.491935935	-1.384614563
H	-8.634469463	-2.210351847	-1.911257053
C	5.123563979	-3.659103749	-1.561607105
H	6.078908939	-3.835116568	-1.050569313
H	5.395459773	-3.416837487	-2.602548249
C	4.319415629	-4.961143203	-1.506110996
H	4.129351052	-5.220698024	-0.452834420
H	3.327603746	-4.797674350	-1.962545182
C	5.037302470	-6.110637276	-2.202829742
H	5.223703195	-5.840427086	-3.257358977
H	6.027860458	-6.253530843	-1.737165645
C	4.242688180	-7.411409432	-2.134318711
H	3.257834652	-7.293273799	-2.612066524
H	4.770674498	-8.232525946	-2.640659157
H	4.072020608	-7.707935610	-1.088201492
C	3.058144366	-2.238078669	-3.122200487
H	3.795854640	-2.926527871	-3.544336819
H	2.059162030	-2.680597684	-3.263172922
H	3.081970310	-1.308568580	-3.716840852

CP6*butyl,oblique*



163
Co2C123H32O6

Co	3.899121660	2.554339562	-1.253794694
Co	6.116345573	2.456466547	-0.361755440
C	5.208996993	3.765263195	-1.613541619
C	2.263222697	3.394649581	-0.774218902
C	6.426629744	1.448054344	1.088186372
C	6.078603240	1.191619904	-1.595006900
C	7.626900488	3.360859002	-0.437629652
O	1.872452171	4.514405810	-0.941168612
O	5.451622783	4.754765727	-2.202114046
O	6.641342188	0.840745885	2.045966207
O	6.364673604	0.393173221	-2.387810000
O	8.660085518	3.870369366	-0.546404107
C	3.176897599	2.451461132	1.530325362
C	4.060526235	3.113459561	0.734931285
C	3.403426908	2.328139656	-2.942219781
O	3.059357315	2.248387845	-4.041618310
H	4.620656632	-4.514123267	3.823275124
H	6.604405866	-2.490621531	0.590889094
H	5.897478687	-3.089990220	2.842489224
H	6.293975209	-2.921770370	-1.573458434
H	5.082123578	-4.445727181	-3.032491990
H	2.288642020	-7.706735846	-1.972318509
H	3.697162107	-6.124610900	-3.156119391
H	1.634131303	-8.327375986	0.037810658
H	1.974036887	-7.760443061	2.377861224
H	3.076335508	-6.370342631	3.659650131
C	2.688942437	-5.356478561	3.579129649
C	5.292083229	-2.399519523	2.258618962
C	3.564660049	-4.303631057	3.667353375
C	3.137140970	-2.974679643	3.388181164
C	5.693267134	-2.057028521	1.000043193
C	4.834039903	-1.270581813	0.168006681
C	3.987103195	-2.019996427	2.715655604
C	5.262932136	-2.698238803	-1.840322317
C	4.581963580	-1.621618320	-1.199806712
C	2.689850717	-5.826146536	-2.871967055
C	4.580142436	-3.554371500	-2.660733162
C	3.186940267	-3.368864269	-2.903018525
C	1.895201101	-6.719301918	-2.206520740
C	0.642740903	-6.302073158	-1.659253141
C	2.273665230	-4.469099258	-3.030182255
C	1.045148646	-7.527265820	0.482529036
C	0.227615816	-6.695816304	-0.343779506
C	1.236828641	-7.207549622	1.798418920
C	0.616658845	-6.045956462	2.351090998
C	1.329857150	-5.142931602	3.212144674
C	0.827086404	-3.826446963	3.358368461
C	3.401628139	-0.890258585	2.108475132
C	1.744122764	-2.732918468	3.422767413
C	1.246899737	-1.424888465	3.153328247
C	3.885459485	-0.458909325	0.823894189
C	3.042210670	0.405059835	0.060118227
C	2.062140220	-0.502387282	2.458997926
C	3.362389616	-1.190726036	-1.770030177
C	2.673220690	-0.061015482	-1.208338012
C	0.885686016	-4.210878911	-2.912993461
C	2.656597799	-2.081204417	-2.635224205
C	1.291478895	-1.811909771	-2.932643813
C	0.052356431	-5.144154808	-2.221286169
C	-1.215999673	-4.693438341	-1.747022534
C	0.397230006	-2.885764620	-3.096029053
C	-0.741187593	-5.897952664	0.313477433
C	-1.622027411	-5.077424010	-0.452286009
C	-0.539778353	-5.564975924	1.689350536
C	-1.241277881	-4.440246691	2.214906957
C	-0.541340238	-3.556063960	3.063045177
C	-1.058235499	-2.243975063	3.255955887
C	1.465866849	0.642553561	1.893214177
C	-0.140007620	-1.159040858	3.279068394
C	-0.618172219	0.148246234	3.030389970
C	2.230845883	1.421207213	0.847926422
C	1.288844460	2.230980608	-0.129521444
C	0.205021136	1.050563770	2.298949790
C	1.430722539	0.364490323	-1.812520662
C	0.769896209	1.495945323	-1.337399590
C	-1.006948795	-2.630274105	-3.032843247
C	0.764018828	-0.510483167	-2.700205616
C	-0.573565473	-0.226936327	-3.064305748
C	-1.832522626	-3.552660334	-2.344920777
C	-3.100228779	-3.112351002	-1.875836051
C	-1.481300764	-1.310747918	-3.239537240
C	-2.626962247	-4.303556659	0.206147691
C	-3.506207243	-3.496586260	-0.564132009
C	-2.430332852	-3.978224012	1.574327563
C	-3.126387870	-2.863252234	2.114690705

C	-2.417636678	-1.974449210	2.972525165
C	-2.913340166	-0.648972951	3.141510678
C	-0.392931826	2.249288477	1.756025697
C	-2.000145261	0.424331582	3.176332131
C	-2.475778646	1.757102050	2.969283741
C	0.089980072	2.790006705	0.571435672
C	-0.833869541	3.554820970	-0.204854909
C	-1.666408739	2.674074600	2.266198206
C	-0.391014476	1.955482934	-1.985062468
C	-1.058499393	3.153422732	-1.543232866
C	-2.871063295	-1.042546205	-3.151736848
C	-1.083321263	1.076152903	-2.854306676
C	-2.432915305	1.366301488	-3.213463553
C	-3.696847889	-1.960072098	-2.458691575
C	-4.957856630	-1.496463923	-1.973919975
C	-3.339150372	0.292963625	-3.349399320
C	-4.487077379	-2.702063519	0.096508724
C	-5.360813733	-1.875411274	-0.675731735
C	-4.292221850	-2.379309278	1.459851181
C	-4.980955063	-1.244736295	1.995205649
C	-4.281110695	-0.367684271	2.850929998
C	-4.786577651	0.947203989	3.052922593
C	-2.275054483	3.850190682	1.746075132
C	-3.860371859	2.036109993	3.130470089
C	-1.865901462	4.279024292	0.446365362
C	-2.234154501	3.594965430	-2.198174497
C	-4.732816933	0.567673112	-3.277658375
C	-2.939687005	2.686894130	-3.057270198
C	-5.565132814	-0.351914516	-2.566179712
C	-6.354701788	-1.090513899	-0.022758703
C	-6.156692001	-0.764089041	1.355097735
C	-5.202428618	1.882749062	-3.523740626
C	-6.618690106	2.081801232	-3.470598004
H	-7.055103924	2.997108304	-3.865571828
C	-6.833451685	0.086829538	-2.107623273
C	-7.412118208	1.208783436	-2.782025462
H	-8.464386905	1.446334296	-2.636902089
C	-2.934007265	4.731831524	-1.697109313
C	-4.067696726	5.182357289	-2.449894118
H	-4.485263643	6.170007692	-2.261406056
C	-4.278866677	2.969018253	-3.420580215
C	-4.718025101	4.328646334	-3.290465354
H	-5.641455795	4.648878054	-3.769100093
C	-3.524726846	4.294904084	2.254877228
C	-4.078100874	5.481044968	1.665418126
H	-4.892856977	6.006087747	2.160606467
C	-2.758562113	5.069485014	-0.326455489
C	-3.714561545	5.851511334	0.403707869
H	-4.247484211	6.661918866	-0.090935622
C	-6.153084073	1.218247025	2.786726826
C	-6.619434664	2.540694310	3.077798411
H	-7.688375399	2.743842961	3.109041449
C	-4.337466090	3.364779034	2.965416659
C	-5.739468568	3.579660691	3.169520316
H	-6.122960550	4.592780881	3.273751751
C	-7.241849175	-0.296041576	-0.792517521
C	-8.247513692	0.429053781	-0.075127365
H	-9.096669199	0.853249654	-0.607983598
C	-6.856951142	0.340348589	1.907892819
C	-8.060097571	0.739215885	1.240935743
H	-8.763586689	1.405157635	1.737309192
C	2.926579378	2.820903912	2.968002657
H	3.892231772	3.042657193	3.446725195
H	2.528029115	1.942731668	3.497808012
C	1.947402162	4.007584527	3.169261675
H	2.517194558	4.944191147	3.289050068
H	1.338150002	4.151055598	2.262770709
C	1.027730026	3.817906271	4.372601913
H	0.486577486	2.860312759	4.273587284
H	1.639488891	3.724892494	5.287564304
C	4.617609077	4.451298448	1.174627371
H	5.708132659	4.532730101	1.090664403
H	4.190856977	5.225233150	0.513844032
H	4.334702114	4.698308182	2.204542225
C	0.024837157	4.956347521	4.522508878
H	0.537256053	5.918754997	4.677896012
H	-0.595879094	5.052143679	3.617435355
H	-0.648670364	4.784660865	5.374790297

CP6*_methyl,oblique_

163
Co2C123H32O6

Co	3.786221068	-2.322850164	1.036161907
Co	5.891781895	-1.602986013	0.119370623
C	5.356951690	-3.201473239	1.289887837
C	2.352762235	-3.508982976	0.641009429
C	5.920128406	-0.444717682	-1.249540529
C	5.561359140	-0.472931603	1.438092966
C	7.591095927	-2.076188082	0.162201373
O	2.186519970	-4.672511905	0.861017275
O	5.866031291	-4.140854900	1.781327998
O	5.972653241	0.277805692	-2.148226950
O	5.650844620	0.321589494	2.279360128
O	8.724297319	-2.290535410	0.253433540
C	2.954877679	-2.273360770	-1.694742450
C	4.052886260	-2.673993738	-0.998379239
C	3.341454124	-2.260824066	2.752617884
O	3.044274730	-2.280230823	3.868161156
H	-4.222096885	-5.825861898	3.313388960
H	-2.471188090	-7.240538409	-0.353615989
H	-2.846329587	-6.863121259	2.023227075
H	-3.216127697	-6.682480195	-2.387116156
H	-4.969913873	-5.410770885	-3.488889632
H	-8.233062330	-3.024860229	-1.711424653
H	-6.722824851	-4.150508847	-3.241140924
H	-8.639683138	-2.681890416	0.425307682
H	-7.771916921	-3.271824163	2.618629313
H	-6.174367058	-4.417942958	3.572611379
C	-5.203006204	-3.947956636	3.431151913
C	-2.275850806	-6.135840867	1.449231485
C	-4.097094977	-4.745646733	3.279770397
C	-2.840815029	-4.186029114	2.911457985
C	-2.057817346	-6.351787823	0.120551655
C	-1.438375698	-5.332801286	-0.676562244
C	-1.926559320	-4.869891864	2.029520909
C	-3.081656242	-5.613275900	-2.541544325
C	-1.965722838	-4.944977869	-1.948411667
C	-6.453128449	-3.167673728	-2.859357731
C	-4.069082355	-4.897058323	-3.158554358
C	-3.993384438	-3.472884808	-3.230640603
C	-7.306071354	-2.532248039	-1.999001893
C	-6.901329254	-1.331159302	-1.338762428
C	-5.151966039	-2.634800770	-3.109854173
C	-7.829420887	-2.093946874	0.852712442
C	-7.156846334	-1.116544524	0.056122358
C	-7.340507918	-2.426277935	2.085932000
C	-6.159446019	-1.794932903	2.581844214
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C	-3.825141749	-1.962817870	3.294010042
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C	-2.679103720	-2.795308378	3.108843552
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C	-0.572347788	-2.822134034	1.859588034
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C	-6.344721793	-0.181103213	0.743840300
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C	-2.382829264	0.033572364	3.265162975
C	0.446517223	-2.065015731	1.237049412
C	-1.251642667	-0.795582224	3.040792714
C	-0.015302815	-0.193620280	2.712215711
C	1.115704580	-2.599777561	0.004988682
C	1.820358686	-1.548929603	-0.930111716
C	0.832531394	-0.845852967	1.777747139
C	-0.263545454	-1.601895642	-2.349235912
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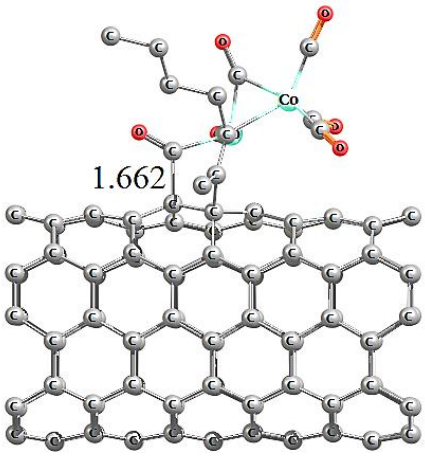

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C	2.333697294	1.125363239	1.812684154
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C	2.389467317	1.030303806	-2.057737973
C	-2.077020281	2.725531354	-2.921730765
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C	-2.511180187	4.608866397	-1.435375926
C	-0.803741278	3.312573311	-3.199913880
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C	-2.756700263	4.816978198	-0.061793455
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C	-0.765010229	3.413190717	3.086632854
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C	3.400247721	1.879165932	1.249718301
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C	0.763680725	6.702468063	-3.078054885
H	1.601137525	7.250673042	-3.505141018
C	-1.069909977	6.599916824	-1.493091162
C	-0.069635231	7.338095651	-2.201332300
H	0.122695044	8.377852706	-1.943340680
C	3.830002389	3.020389315	-2.146346952
C	4.115455085	4.272071175	-2.782790657
H	5.092837963	4.734205630	-2.654424565
C	1.787024613	4.447200467	-3.443748480
C	3.124086442	4.963779216	-3.414767144
H	3.327318494	5.964618894	-3.790790630
C	3.832367058	3.079122426	1.866067922
C	4.915267278	3.778011023	1.234135800
H	5.455688963	4.550465074	1.777977022
C	4.344603718	2.698842248	-0.858330953
C	5.157384747	3.603405918	-0.097369966
H	5.879370543	4.244589103	-0.600566415
C	0.688240095	5.391190778	3.093628130
C	2.006979525	5.912812815	3.281794295
H	2.151048429	6.982024946	3.426186952
C	2.942644896	3.731418587	2.771474788
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H	4.093324401	5.549903938	3.162066373
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C	4.982730498	-3.706999466	-1.618749731
H	5.968499996	-3.730065594	-1.136591618
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H	4.262746422	-5.386437514	-0.471064396
H	3.372589257	-5.109875298	-1.965245890
C	5.257169529	-6.150886764	-2.233422750
H	5.379974441	-5.867551040	-3.293838207
H	6.266823613	-6.137143407	-1.787483791
C	4.670418935	-7.556014289	-2.137738813
H	3.670407263	-7.593605471	-2.596977759
H	5.307277230	-8.293622572	-2.647459630
H	4.566035760	-7.862789178	-1.085826292
C	2.689804802	-2.614446007	-3.129220207
H	2.578227334	-1.693505644	-3.727540342
H	3.501300107	-3.203596771	-3.566176084
H	1.753352717	-3.183740148	-3.244410829

CP6*_butyl,oblique_

163
Co2C123H32O6

Co	3.111719883	-3.261666960	1.140393266
Co	5.312427567	-3.049224693	0.181919332
C	4.507228119	-4.397763584	1.451071124
C	1.473711930	-4.112041707	0.676559669
C	5.542979438	-1.944910626	-1.210262020
C	5.481114885	-1.874393583	1.481194101
C	6.757562995	-4.054184392	0.000706017
O	1.074126282	-5.227196487	0.837439863
O	4.816873200	-5.373472954	2.033807401
O	5.733309985	-1.268703508	-2.127430441
O	5.791518540	-1.130714917	2.314546774
O	7.753175172	-4.639719881	-0.059291715
C	2.356037749	-3.071710662	-1.596101961
C	3.274898752	-3.759463045	-0.857371797
C	2.667459399	-3.107572667	2.850085720
O	2.356964210	-3.065498211	3.962076940
H	-5.558442441	-4.864613061	3.165903570
H	-4.100366227	-6.580786556	-0.502106206
H	-4.437376167	-6.171830214	1.874772034
H	-4.635557722	-5.824581933	-2.534929884
H	-6.008866522	-4.150446261	-3.638897178
H	-8.652717595	-1.091808472	-1.865322542
H	-7.416328746	-2.514609131	-3.393340573
H	-9.022796167	-0.700741357	0.268902873
H	-8.379307592	-1.522858705	2.464850796
H	-7.125594211	-3.037285075	3.423140586
C	-6.067017137	-2.809765659	3.312940416
C	-3.694829907	-5.590605441	1.331872995
C	-5.179227346	-3.844852951	3.162551201
C	-3.816995792	-3.593445954	2.833399478
C	-3.499453438	-5.826140626	0.002791678
C	-2.634420616	-4.969592867	-0.755137810
C	-3.069807986	-4.456783491	1.951435640
C	-4.246858565	-4.815507161	-2.660457333
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C	-5.019929752	-3.872960943	-3.279021947
C	-4.605463800	-2.507084956	-3.314621481
C	-7.628343376	-0.828833831	-2.122594479
C	-6.965901482	0.227648257	-1.424546568
C	-5.533875641	-1.419658539	-3.194543092
C	-8.106883107	-0.332431329	0.727531794
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C	-4.253202784	-1.208213370	3.255686938
C	-1.899396028	-3.964129103	1.344600598
C	-3.333890810	-2.286052715	3.070932387
C	-1.980047820	-1.966496911	2.761765299
C	-1.629220162	-4.287321679	-0.032094731
C	-0.692961887	-3.469366970	-0.722527472
C	-1.264469265	-2.787003720	1.860345588
C	-2.418288882	-3.227217901	-2.436888097
C	-1.156314668	-2.839715435	-1.880571679
C	-5.031517054	-0.131566412	-2.884728969
C	-3.230895130	-2.246199362	-3.087951072
C	-2.747924272	-0.911521263	-3.187541192
C	-5.760333420	0.710894725	-1.988719674
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C	-0.081066085	-2.280993609	1.275698279
C	-1.470161391	-0.683454039	3.082073612
C	-0.118845730	-0.386413462	2.790113163
C	0.475673346	-2.935497778	0.049485671
C	1.437094693	-2.070404487	-0.855345312
C	0.570798814	-1.200137530	1.852508436
C	-0.560794289	-1.595840429	-2.315327083
C	0.699715809	-1.215460683	-1.860840130
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C	-0.872370871	0.668139688	-3.170413048
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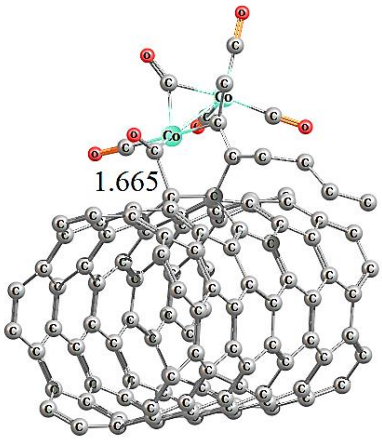

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C	3.078852572	-0.187550126	-0.662946063
C	2.498685967	0.349888781	1.969725763
C	1.302106337	-0.042313133	-2.330551005
C	2.626033708	0.333422023	-1.893613140
C	-1.277197431	3.048668606	-2.814296909
C	0.509370201	0.920463866	-2.999617923
C	1.009579878	2.245321440	-3.165126274
C	-1.990859791	3.879631189	-1.917067600
C	-1.285469546	4.947192086	-1.282402451
C	0.105094204	3.322456784	-3.055535730
C	-2.426569170	4.332990036	0.787272182
C	-1.509420363	5.180075693	0.090992489
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C	0.003974780	3.284486518	3.246825136
C	1.397898753	3.527384982	3.399285851
C	3.730302979	0.838235028	1.451552794
C	2.309614622	2.439286228	3.220385698
C	4.009003263	0.589205929	0.071138332
C	3.229944070	1.514746701	-2.399227663
C	0.624377614	4.619380076	-2.785554054
C	2.407050876	2.494596424	-3.050086062
C	-0.090633179	5.454403665	-1.870976832
C	-0.526217369	5.910184065	0.819894962
C	-0.154216769	5.429686414	2.114171512
C	1.983279150	4.904930279	-3.072357830
C	2.430600649	6.237635182	-2.808751752
H	3.385002579	6.580010998	-3.203893363
C	0.588346842	6.538737296	-1.259454121
C	1.752241398	7.032724917	-1.928257610
H	2.181178973	7.989524155	-1.636272445
C	4.504859449	1.916996951	-1.909172153
C	5.097266742	3.075536131	-2.508387773
H	6.151855371	3.291005657	-2.344472120
C	2.896828690	3.812462379	-3.220240927
C	4.316717346	3.994946677	-3.146694930
H	4.762581552	4.926317514	-3.490544587
C	4.419142994	1.887095383	2.108933410
C	5.650749795	2.323825440	1.516070222
H	6.344513704	2.934861767	2.090444908
C	4.893282872	1.457630176	-0.616516237
C	5.876531335	2.127742566	0.184514350
H	6.740921154	2.592807337	-0.286766516
C	1.885970413	4.856939667	3.334268615
C	3.285277473	5.043998939	3.564878904
H	3.676132684	6.044304167	3.742346744
C	3.687327560	2.713441958	3.014714783
C	4.157997831	4.003994259	3.416956006
H	5.227269157	4.194798272	3.481670239
C	0.360500483	6.776505319	0.132564037
C	1.290261687	7.515525210	0.932462687
H	1.820431212	8.365146658	0.505883958
C	1.087326349	5.837154423	2.667977379
C	1.644675584	7.057924146	2.169210091
H	2.451317002	7.550081898	2.709466160
C	2.090528430	-3.342366852	-3.047421049
H	1.019056413	-3.249847638	-3.272739898
H	2.369542632	-4.375055035	-3.291610601
C	2.882457975	-2.352802655	-3.948483115
H	3.259478377	-1.515065223	-3.341761925
H	3.785771653	-2.852858600	-4.336772827
C	2.051361010	-1.787957706	-5.098391442
H	1.814930039	-2.593434203	-5.815586023
H	1.082119757	-1.432895070	-4.707526093
C	2.758267535	-0.634466785	-5.802623866
H	2.945065822	0.193576932	-5.099584520
H	3.731569101	-0.951067531	-6.208986800
H	2.152032451	-0.240815700	-6.631248974
C	3.834359696	-5.055507856	-1.417605824
H	4.316207740	-5.668558797	-0.649304807
H	3.021551132	-5.659998622	-1.851524604
H	4.580199962	-4.865026727	-2.204367666

CP6*methyl,perpendicular*

163
Co2C123H32O6

Co	4.551043368	2.544251181	-1.295985227
Co	5.457109111	1.234487830	0.548615514
C	4.754557391	4.172931853	-1.992772426
C	2.781778343	2.218692368	-2.259740546
C	5.735798076	1.177520463	2.275769010
C	6.863341091	0.218333982	0.108836303
C	6.323886959	2.568356082	-0.539936085
O	2.459343925	2.764485935	-3.269699860
O	4.956597598	5.211769848	-2.451049463
O	5.910608237	1.169399986	3.419611438
O	7.879572548	-0.293899634	-0.098552798
O	7.406777154	3.011714077	-0.661961283
C	2.956962560	2.751738776	0.091854044
C	4.191754197	2.718127557	0.769911042
C	5.142164356	1.417820250	-2.529282111
O	5.604950756	0.734917837	-3.339095615
H	5.721182024	-3.181569447	2.495798581
H	5.936898310	-2.978794623	-1.903616602
H	6.268345759	-2.633009922	0.481513972
H	4.873441141	-4.136376764	-3.375363744
H	3.288492427	-5.965317461	-3.595365723
H	1.378787821	-8.204707518	-0.307199027
H	2.045546318	-7.420566143	-2.508937952
H	1.696650215	-7.850041659	1.843856412
H	2.906579521	-6.456132588	3.423292464
H	4.323890319	-4.795370533	3.666954194
C	3.881941452	-3.869465295	3.303576366
C	5.450222542	-2.127945786	-0.027222453
C	4.665044799	-2.966050159	2.644430083
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C	0.141272290	-6.366521601	1.434895639
C	1.964027524	-6.098727393	3.012831767
C	1.539350216	-4.754880736	3.258263506
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C	1.991082005	-2.353470096	3.171821519
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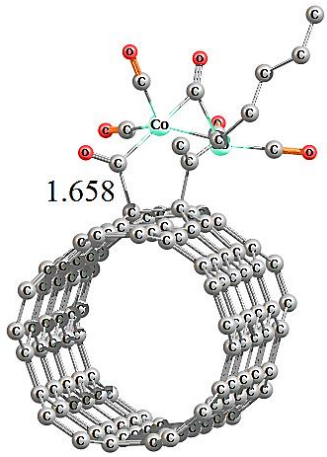

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C	-5.605842712	-1.724355729	0.062960064
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C	-4.031359890	0.067478367	3.271504308
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H	-9.273697453	1.072970400	-0.258360282
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H	-7.385380118	3.247699682	-3.572179943
C	-3.002885294	5.054059301	0.758100415
C	-3.833095152	5.931669070	-0.000136318
H	-4.437376828	6.683326794	0.504387183
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H	-8.973931220	1.406144253	1.887419525
C	-5.903180935	1.661514579	3.336413220
C	-7.288635536	1.892517088	3.083985178
H	-7.780098293	2.768341984	3.503543182
C	4.553492585	3.852628978	1.700226257
H	4.231566218	3.470189857	2.691437175
H	3.907058774	4.722617340	1.516909693
C	5.990085671	4.341511553	1.812978478
H	6.685680050	3.498441017	1.941179663
H	6.283293540	4.844385031	0.876505023
C	6.160376494	5.304605690	2.984354454
H	5.459750946	6.150064597	2.870720830
H	5.876499119	4.786773263	3.917067888
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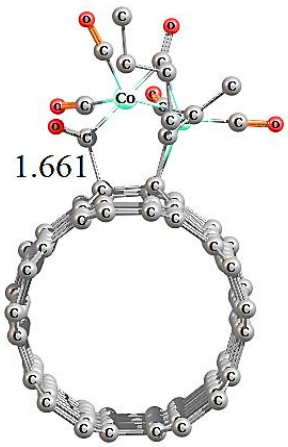
H	8.297597654	4.996873970	3.237909379
H	7.882261028	6.366238204	2.183871246
H	7.698916775	6.515078027	3.948563535
C	2.262974660	4.101717472	-0.058973697
H	1.588111841	4.121627947	-0.924128581
H	1.681594976	4.375404846	0.834613861
H	3.013104540	4.880318162	-0.233959627

CP6*butyl,perpendicular*



163
Co2C123H32O6

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C	-2.829582903	2.597853731	1.706591756
C	-5.811561720	1.134408022	-2.726934063
C	-6.941382503	0.605045172	-0.396994728
C	-6.188086400	3.055663314	-0.319338694
O	-2.492858817	3.257350467	2.642749874
O	-5.111028633	5.452112579	1.966753267
O	-6.033468148	0.973190458	-3.850836526
O	-7.979039945	0.220811591	-0.061097103
O	-7.140239405	3.715156674	-0.529526960
C	-2.888336758	2.864945515	-0.717624062
C	-4.093130565	2.760337112	-1.428472161
C	-5.266949460	1.859398490	1.898888034
O	-5.821084320	1.276335722	2.730473020
H	-5.855525371	-3.155989365	-2.581148143
H	-6.276095331	-2.451569945	1.745019640
H	-6.481191573	-2.336690332	-0.677659723
H	-5.365776510	-3.483657500	3.401701297
H	-3.908042507	-5.354987674	3.933004700
H	-1.969069885	-8.065773800	1.043584323
H	-2.698726436	-6.994788601	3.100110930
H	-2.162306916	-7.938607515	-1.148063986
H	-3.203045050	-6.672021119	-2.940401185
H	-4.498875999	-4.975762189	-3.460861377
C	-4.020270656	-4.038461744	-3.183134416
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C	-2.595805262	-3.933781705	-3.191156356
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C	-2.834179357	-1.566876430	-2.567887648
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C	-0.220575868	1.116547560	-2.236454878
C	-1.842166949	1.380155772	1.159265506
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C	3.784376523	0.195421751	3.230174135
C	4.354880226	-2.678534751	1.086781150
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C	6.538570598	0.619466395	2.665695753
C	7.856132619	0.844383513	2.165848815
H	8.493574291	1.595391135	2.628673760
C	7.374190922	-0.592437846	0.272374937
C	8.263106071	0.254946789	0.999087977
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C	6.230624060	3.016711490	3.318427667
H	7.290184994	3.199649626	3.486999731
C	3.257432078	4.725423653	-1.266636369
C	4.097548436	5.640131476	-0.565114600
H	4.771754329	6.294120744	-1.115053790
C	3.466194834	4.597139724	1.533215514
C	4.199790978	5.576623200	0.799825330
H	4.954119157	6.180394336	1.300984600
C	5.217958226	2.006293832	-3.581247197
C	5.697704980	3.347198366	-3.612871211
H	6.720258651	3.552312832	-3.924090198
C	3.678921920	4.094842653	-2.493785180
C	4.948202935	4.364897153	-3.081888245
H	5.394386840	5.352894280	-2.984968018
C	7.263028150	-0.527276895	-1.158451854
C	8.037737372	0.385956097	-1.934475655
H	9.049337040	0.642085674	-1.624950441
C	6.077642140	0.897996507	-3.267681074
C	7.460242160	1.079285419	-2.963837417
H	8.025777972	1.871270694	-3.451201798
C	-2.076344309	4.162224652	-0.812011508
H	-1.549924366	4.155345628	-1.782184065
H	-1.284896585	4.111445312	-0.056218587
C	-2.750674485	5.530045451	-0.597744615
H	-2.589176901	6.159191155	-1.489773469
H	-3.839815633	5.435640384	-0.486614150
C	-2.170611637	6.251018609	0.619174835
H	-2.318335536	5.628650481	1.517130886
H	-1.077713054	6.340923086	0.486640577
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H	-2.614408139	8.271671328	-0.050745321
H	-3.868998484	7.557335790	0.990319814
H	-2.344764855	8.130384967	1.703780209
C	-4.431036941	3.742757999	-2.518207997
H	-3.895828633	4.694815867	-2.446342886
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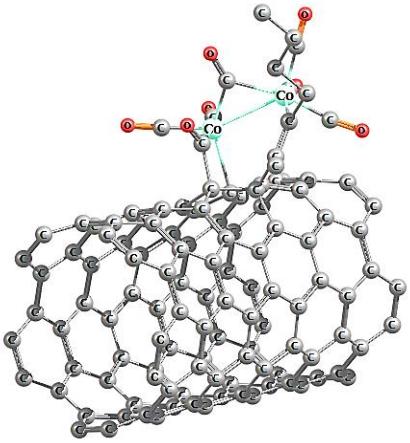
CP7*methyl,oblique*



165
Co2C124H32O7

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C	-5.836147095	-0.372758603	1.544415106
C	-6.569791854	-0.057784426	-0.926183553
C	-7.258763381	-2.388236184	0.223331018
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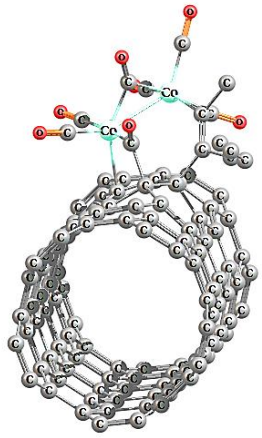

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C	-0.105361368	-6.429595710	-2.894230849
H	0.604410102	-7.254923365	-2.726677609
H	-0.627894622	-6.243477639	-1.942274560
H	-0.852376305	-6.763293197	-3.629407772
C	4.864291735	-4.137250312	-2.164066130
H	4.238602810	-4.532470450	-2.972169900
H	5.839873150	-3.872541212	-2.596694969
H	5.036400670	-4.955660271	-1.446687522

CP7*_methyl,oblique_

165
Co2C124H32O7

Co	-3.410464903	1.900774363	1.720942471
Co	-5.363397541	1.522977585	-0.179853429
C	-4.849051693	2.982548927	1.256452544
C	-2.271673724	3.399779918	0.757038891
C	-5.266308986	0.509343461	-1.621221136
C	-6.075792777	0.221134433	0.827055224
C	-6.881768265	2.453654165	-0.367040922
O	-2.387474174	4.588335472	0.796171685
O	-5.313579117	4.010701569	1.577409881
O	-5.391869458	-0.077308674	-2.612889943
O	-6.600523682	-0.662048092	1.354498594
O	-7.912613032	2.956216539	-0.496976342
C	-2.857383713	2.512459577	-1.651664854
C	-4.210649717	2.511617393	-1.539144359
C	-2.702003840	2.730059445	3.089489058
O	-2.263548637	3.276373146	4.006489271
H	4.488872343	5.716400821	3.279177046
H	2.644795319	7.237175336	-0.278562856
H	3.078654152	6.808882068	2.079390421
H	3.320428291	6.690192794	-2.347284844
H	5.021112170	5.403406653	-3.511399532
H	8.308793182	2.924597326	-1.911004305
H	6.761209735	4.108276259	-3.357769302
H	8.773522921	2.543148706	0.209103663
H	7.973521081	3.118775701	2.431247086
H	6.424336717	4.274169422	3.445041843
C	5.441541209	3.821391452	3.329134537
C	2.475901847	6.104468424	1.509749254
C	4.343596850	4.639255956	3.229857859
C	3.065849516	4.108734334	2.897293167
C	2.223119649	6.350263737	0.192098750
C	1.558291165	5.359828411	-0.604941091
C	2.125808092	4.830138614	2.071638444
C	3.164372915	5.624744235	-2.507504508
C	2.055787864	4.969214604	-1.888750647
C	6.488843467	3.122326176	-2.985967708
C	4.122305468	4.899343890	-3.161137007
C	4.021868842	3.478347146	-3.252181580
C	7.362827726	2.453967788	-2.172549195
C	6.961714778	1.247165810	-1.521002166
C	5.169435228	2.618109695	-3.194481755
C	7.967705837	1.960405093	0.651743313
C	7.258284481	1.004418812	-0.138190211
C	7.516248387	2.285005295	1.901562477
C	6.340139798	1.665315361	2.421775768
C	5.327043148	2.420135603	3.108670460
C	4.027962806	1.861500084	3.197521341
C	1.082663619	4.124626537	1.443880686
C	2.889988878	2.715964781	3.064136573
C	1.639904004	2.117203238	2.734671517
C	0.724083659	4.451598085	0.086505100
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C	1.746413339	3.657883353	-2.327890052
C	0.608755941	2.979759643	-1.787323799
C	4.968656665	1.238255655	-2.943864980
C	2.745061756	2.909160124	-3.022195566
C	2.562573318	1.507102273	-3.174028095
C	5.883602177	0.535260472	-2.099877607
C	5.456464401	-0.698324210	-1.522170322
C	3.686166611	0.661178839	-3.163239651
C	6.451376024	0.071983340	0.559802229
C	5.746866939	-0.937199031	-0.162733723
C	5.981635493	0.412262390	1.866692585
C	4.847192810	-0.288630404	2.372241391
C	3.853721749	0.454636661	3.044483897
C	2.555131671	-0.111798755	3.175974180
C	-0.288661357	2.064660167	1.257073954
C	1.434319703	0.739179106	2.985059834
C	0.182019255	0.161080891	2.673977512
C	-1.039896229	2.650967032	0.090682154
C	-1.814912951	1.661749636	-0.855451157
C	-0.679969816	0.847315229	1.781298918
C	0.280887179	1.659498640	-2.276954913
C	-0.885523812	1.008801967	-1.869666848
C	3.492731494	-0.739577623	-2.967147866
C	1.270915467	0.938236423	-2.986426569
C	1.081013837	-0.443133242	-3.222391558
C	4.398118356	-1.437555694	-2.131462971
C	3.980520078	-2.670413020	-1.559551833
C	2.217067751	-1.303359854	-3.215584362
C	4.965492705	-1.904500456	0.541994206
C	4.271870057	-2.909809456	-0.184727932
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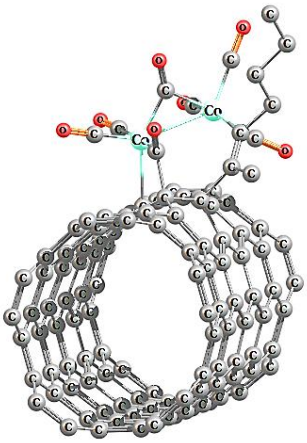

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C	-2.231053899	-1.090805226	1.853799299
C	-1.203860442	-0.253454553	-2.385288363
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C	2.008908529	-2.688592021	-2.999623141
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C	-0.402856379	-2.393484591	-3.294756681
C	2.907421736	-3.386996053	-2.158348985
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C	0.717231401	-3.247208101	-3.245186820
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C	3.009236673	-3.522054978	1.812792868
C	1.857313644	-4.204575216	2.321375727
C	0.869524740	-3.458128050	2.994549890
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C	-0.759990499	-5.206701187	-3.348821008
C	-0.896325528	-6.616622492	-3.154827456
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C	0.987397265	-6.577803231	-1.626434734
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C	-1.894993093	-4.337904035	-3.441855892
C	-3.236851826	-4.833077055	-3.382629321
H	-3.467132081	-5.824529132	-3.767732856
C	-3.772095895	-3.013814157	1.956472239
C	-4.881070065	-3.691823539	1.347731861
H	-5.413283548	-4.466756371	1.896084807
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C	-5.152553876	-3.502626853	0.023961680
H	-5.892266322	-4.133007271	-0.467154059
C	-0.620983583	-5.407722917	3.021151549
C	-1.941166754	-5.906712901	3.250013803
H	-2.100974797	-6.975279546	3.381715797
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H	0.195207476	-8.700288936	0.055859566
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C	-4.244786417	0.736506305	2.826473076
O	-4.744983953	0.120907791	3.662916097
C	-5.064458945	3.386175086	-2.432231714
H	-6.055533994	2.931457411	-2.568273552
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C	-5.235131577	4.795899318	-1.861469773
H	-5.614668773	4.736077986	-0.829483976
H	-4.247510945	5.281401660	-1.785307186
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C	-6.342522949	7.056537237	-2.136976087
H	-6.740738309	7.020661944	-1.111342320
H	-5.373562683	7.578062553	-2.100427031
H	-7.030116842	7.658446503	-2.748834556
C	-2.227321775	3.514996698	-2.597825674
H	-1.782533038	4.353309304	-2.038083349
H	-1.439943285	3.066418881	-3.217247971
H	-2.961070671	3.944562003	-3.282433582

CP7*butyl,oblique

165
Co2C124H32O7

Co	3.071505444	-2.525956701	1.734235161
Co	5.014060978	-2.623720700	-0.209113936
C	4.214686935	-3.913924898	1.244143462
C	1.613009730	-3.773522793	0.860579069
C	5.078621811	-1.666976091	-1.696015278
C	6.000737111	-1.450253786	0.726584875
C	6.329329859	-3.825776945	-0.387919314
O	1.447578310	-4.948406091	1.003774632
O	4.423142077	-5.032689433	1.528756938
O	5.271954985	-1.173471312	-2.725746905
O	6.704201870	-0.674020333	1.212181759
O	7.245720277	-4.514619126	-0.518468914
C	2.325855529	-3.106619484	-1.632297841
C	3.621213836	-3.461328353	-1.444782995
C	2.249437775	-3.138091128	3.151085188
O	1.733119654	-3.549428282	4.097373519
H	-5.383831656	-4.596435257	3.554246767
H	-3.986575996	-6.552956730	-0.002734213
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H	-4.578717779	-5.939054503	-2.085034329
H	-6.022705631	-4.352091525	-3.226966151
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H	-7.461057114	-2.726129836	-3.030316878
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C	-4.650534139	-2.663496489	-3.033211917
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C	-7.022084633	0.165025003	-1.284093763
C	-5.597105291	-1.585765817	-2.960838881
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C	-4.141346081	-0.922121962	3.364886039
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C	-0.627134905	-3.425752171	-0.530224135
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C	-1.380628641	-0.363362493	3.049044245
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C	0.568550628	-2.813251088	0.153915809
C	1.502828924	-2.031202770	-0.841904294
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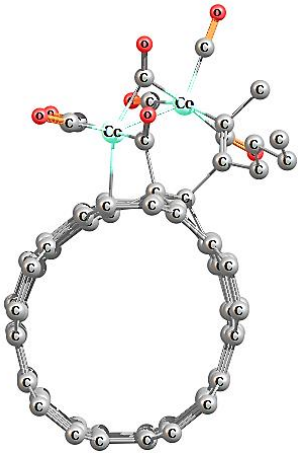

Note: Taken into consideration in the main manuscript.

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C	4.962969133	3.118763667	-2.911071575
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C	5.849247102	2.360101071	-0.188024659
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H	3.675167953	6.463322453	3.141491007
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C	4.181047962	4.411924333	2.948816473
H	5.248203245	4.622698625	2.976621107
C	0.227020702	6.926359459	-0.391181227
C	1.173590210	7.725154166	0.327138966
H	1.678564066	8.550695046	-0.171270213
C	1.057092463	6.154741099	2.168659763
C	1.579257274	7.348164879	1.575519539
H	2.400002546	7.880650624	2.052623562
C	4.166738724	-1.531032130	2.779377395
O	4.804397080	-1.009710100	3.585714589
C	1.545515690	-3.871427065	-2.701445576
H	2.177414669	-3.953941939	-3.599630041
H	0.692520921	-3.278952536	-3.045520859
C	1.043854141	-5.261723111	-2.298167026
H	1.892780284	-5.952320816	-2.159719373
H	0.551884849	-5.218980381	-1.313943444
C	0.062074822	-5.827806455	-3.319734630
H	-0.729668141	-5.081868442	-3.509715010
H	0.576817597	-5.979020437	-4.285432742
C	-0.575582035	-7.132168476	-2.852281123
H	0.186733199	-7.907758273	-2.678409162
H	-1.112894374	-6.977335568	-1.903037345
H	-1.291897042	-7.516399077	-3.593415869
C	4.250814795	-4.590203362	-2.217061027
H	3.608743222	-5.014893860	-2.996418051
H	5.186054597	-4.265349733	-2.695969127
H	4.506832865	-5.404031160	-1.519829630

CP7*butyl,oblique

165
Co2C124H32O7

Co	2.879342005	2.824673510	-1.773156207
Co	4.866078364	2.964997555	0.124891354
C	3.969663988	4.252402537	-1.268301049
C	1.379469116	3.979012021	-0.813678042
C	5.007056499	1.971986334	1.582637417
C	5.885511084	1.869163226	-0.869051420
C	6.124492123	4.223303066	0.318522915
O	1.166098462	5.151530074	-0.883520655
O	4.119139922	5.385366985	-1.532310738
O	5.241144278	1.464623948	2.597439779
O	6.611520520	1.141138446	-1.394528369
O	7.009519218	4.950945616	0.455287416
C	2.192075975	3.256623448	1.613292784
C	3.461190157	3.689278386	1.416231773
C	1.989167967	3.449396376	-3.142374321
O	1.431248957	3.868587920	-4.061390194
H	-5.701192553	4.477117231	-3.405636084
H	-4.363254601	6.401136412	0.185822975
H	-4.641006539	5.888191193	-2.178631755
H	-4.892717601	5.694593395	2.247368445
H	-6.213724960	4.006968441	3.392509370
H	-8.724528738	0.771732584	1.737293760
H	-7.556563766	2.306029980	3.209988944
H	-9.050851580	0.291577872	-0.387321532
H	-8.403612140	1.062304717	-2.600205413
H	-7.194990555	2.583416378	-3.599672622
C	-6.130168756	2.400361088	-3.469241407
C	-3.882442839	5.362157235	-1.602636024
C	-5.282883509	3.474053603	-3.353798569
C	-3.915806598	3.290898168	-3.003175969
C	-3.719086257	5.657550480	-0.280996872
C	-2.829053359	4.870577137	0.522796290
C	-3.205902715	4.225994996	-2.162363168
C	-4.467672055	4.705440513	2.408814310
C	-3.221385136	4.360927918	1.800992070
C	-7.032890021	1.426584876	2.840082477
C	-5.211197312	3.754537556	3.052096423
C	-4.746279910	2.407894713	3.143726903
C	-7.692732261	0.560114702	2.011756983
C	-6.984395099	-0.497720826	1.363239161
C	-5.630876037	1.279946532	3.067014508
C	-8.116692495	-0.060732081	-0.820975139
C	-7.192166923	-0.802815143	-0.023480934
C	-7.751613835	0.373791834	-2.065651584
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C	-2.024782845	1.735894293	-2.823158735
C	-1.779254940	4.213594967	-0.159431390
C	-0.826198880	3.455987976	0.574505049
C	-1.351273569	2.620098254	-1.947977054
C	-2.586605137	3.174113711	2.244234927
C	-1.307405882	2.815432254	1.713677562
C	-5.075659926	0.001158621	2.814926159
C	-3.362678708	2.190534179	2.929752961
C	-2.824261892	0.883412035	3.082619517
C	-5.765800642	-0.909040936	1.955185083
C	-5.026243965	-1.986329998	1.380500235
C	-3.690349697	-0.225090030	3.052511024
C	-6.163664234	-1.491819051	-0.712732761
C	-5.229346747	-2.286315394	0.017286771
C	-5.784796306	-1.037729484	-2.014561982
C	-4.502395665	-1.419300412	-2.507911681
C	-3.728024992	-0.441392402	-3.167678871
C	-2.325532114	-0.651129560	-3.283620553
C	-0.168590931	2.174196275	-1.316420404
C	-1.466050114	0.459866660	-3.074674346
C	-0.110701699	0.224380986	-2.748322257
C	0.396451583	2.935119870	-0.141391562
C	1.396284670	2.172937147	0.813335186
C	0.532334055	1.104906542	-1.841495217
C	-0.650264973	1.624606185	2.209169367
C	0.647705823	1.298908431	1.812412775
C	-3.138029784	-1.526590555	2.854650496
C	-1.426802207	0.670024134	2.909955920
C	-0.889057851	-0.616323975	3.146872403
C	-3.820122470	-2.429270371	2.002585316
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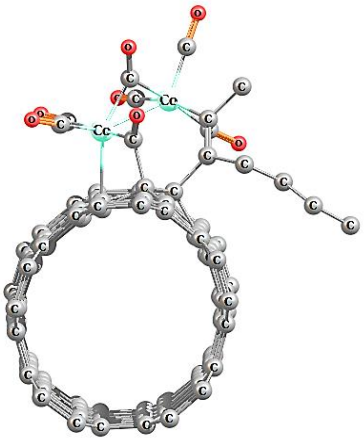

Note: Discarded in the main manuscript.

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C	2.535658321	-0.363613773	-1.903069837
C	1.275010943	0.156721327	2.327190288
C	2.613802175	-0.195618331	1.916649200
C	-1.200419732	-3.024862065	2.902696449
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C	2.121859143	-4.742426405	3.281474817
C	2.621312962	-6.067874189	3.085241034
H	3.582511496	-6.355981268	3.506526215
C	0.811090034	-6.508336761	1.531190499
C	1.984617120	-6.926541553	2.233469719
H	2.453261801	-7.878240875	1.989565720
C	4.548526755	-1.709275239	2.031100695
C	5.173530558	-2.817563137	2.685034617
H	6.237675373	-2.999953791	2.544330163
C	2.991571342	-3.610115165	3.391653211
C	4.416369471	-3.740805780	3.347360910
H	4.891210281	-4.640880638	3.733241425
C	4.521237488	-1.824580642	-1.987145353
C	5.759175120	-2.197618341	-1.364093689
H	6.479468050	-2.807343767	-1.906353387
C	4.942644725	-1.283951586	0.726289598
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H	6.828258915	-2.372104899	0.462516243
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H	3.950282154	-6.073736740	-3.448045934
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C	1.341522183	-5.933211844	-2.410157813
C	1.941047728	-7.109755182	-1.858013500
H	2.778341804	-7.585100293	-2.365819322
C	3.995817661	1.927142404	-2.878516717
O	4.641680096	1.468627589	-3.716175182
C	1.421812629	3.866960607	2.778327748
H	0.346860322	3.793140849	2.626561389
H	1.600597577	4.949334974	2.825316396
C	1.769543504	3.192824606	4.113722816
H	1.906563266	2.110519098	3.952991312
H	2.742199839	3.562263518	4.483351998
C	0.684325858	3.401246486	5.165823446
H	0.563883051	4.480691340	5.366149760
H	-0.280452119	3.051780173	4.755308903
C	4.057647492	4.808381027	2.230603929
H	4.297924542	5.652319381	1.564070448
H	3.406334678	5.184970289	3.026030234
H	4.997915111	4.488741318	2.702883633
C	0.979912158	2.651885925	6.460485315
H	1.053763178	1.569883560	6.269477227
H	1.933841620	2.982134429	6.900368227
H	0.187375799	2.810533717	7.206045735

CP7*methyl,perpendicular*

165
Co2C124H32O7

Co	-4.748348675	-1.881159697	-1.314582533
Co	-5.544150449	-1.366298394	1.272532044
C	-5.284062288	-3.280894928	-2.276959264
C	-2.970192598	-1.669103432	-2.444820891
C	-4.330333800	-1.184598649	2.558960893
C	-6.427531549	0.163762298	1.549280224
C	-6.496893129	-1.644132571	-0.520888617
O	-2.851702557	-2.050614010	-3.561820993
O	-5.651376533	-4.109234913	-2.991997594
O	-3.673086251	-1.262240765	3.507967227
O	-7.060536509	1.098791918	1.797974912
O	-7.622469643	-1.605728300	-0.859786846
C	-3.047139708	-2.471866380	-0.188250388
C	-4.232705458	-2.734437466	0.528358858
C	-5.233227588	-0.573329845	-2.418303265
O	-5.704937269	0.138601146	-3.196453208
H	-5.419431877	3.719663823	2.322094819
H	-5.576696623	3.550126395	-2.100556603
H	-6.014822376	3.159676241	0.271352000
H	-4.317678106	4.709751373	-3.478989277
H	-2.570142674	6.389922364	-3.649869571
H	-0.552514215	8.409352813	-0.300795949
H	-1.221423732	7.717656001	-2.533182345
H	-0.980668998	8.044622047	1.826762189
H	-2.354710960	6.742805467	3.348145397
H	-3.918630067	5.206075052	3.535906824
C	-3.546333767	4.247147239	3.179702909
C	-5.199529957	2.633908252	-0.221269318
C	-4.389474986	3.414578654	2.496680866
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C	-4.954884507	2.852246316	-1.543271224
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C	-4.288849903	1.842541940	0.553540325
C	-3.276294399	4.404643669	-3.397062070
C	-2.953916664	3.062362578	-3.018906427
C	-0.481853694	7.129541602	-1.992913145
C	-2.293753807	5.348584941	-3.494953991
C	-0.931307809	5.003452608	-3.233408203
C	-0.105553292	7.518562559	-0.738458470
C	0.723898646	6.668739061	0.059714497
C	-0.049202778	5.869538293	-2.514226514
C	-0.658656609	7.043866471	2.108774187
C	0.456228385	6.439493061	1.447117797
C	-1.432276446	6.310745800	2.964550323
C	-1.132849632	4.933587249	3.205755128
C	-2.156587641	3.936195153	3.288701499
C	-1.785709498	2.583211559	3.075323560
C	-3.505764080	0.890604151	-0.134713397
C	-2.647717958	1.729446248	2.329071324
C	-2.123962399	0.513157858	1.779943044
C	-3.221108500	1.151568899	-1.519591976
C	-2.068483574	0.537194447	-2.067459539
C	-2.644507889	0.010485406	0.582869598
C	-1.614352305	2.645256207	-3.201016350
C	-1.242803600	1.299984870	-2.894524340
C	1.120993072	5.309614523	-1.941736693
C	-0.590900233	3.629559533	-3.323126260
C	0.757646214	3.221389020	-3.137983938
C	1.518604588	5.719646492	-0.630951452
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C	-1.733429982	-0.845752474	-1.650480200
C	-0.388176816	-1.297500734	-2.098110116
C	-0.865744091	-1.750740329	0.620004736
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C	2.834840676	3.535480119	-1.896491329
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C	3.348337638	2.320654154	-2.421975644
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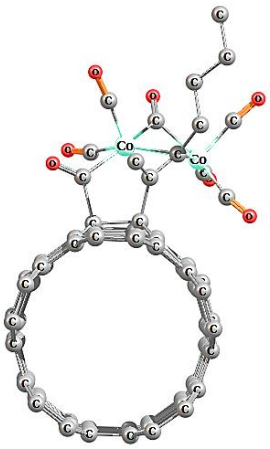

Note: Taken into consideration in the main manuscript.

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C	1.791997004	-0.889306211	-3.170276758
C	2.179015528	-2.231369983	-2.921815476
C	4.533997967	1.771404512	-1.871635875
C	2.811253743	0.094478912	-3.279844372
C	4.171586374	-0.302265054	-3.110182047
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C	5.808541299	1.323228188	0.164078922
C	5.040878365	0.544247279	-2.388957935
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C	1.739160344	-4.359725864	-0.034977367
C	2.486743062	-3.570015060	2.517132291
C	1.980158566	-4.141725493	-1.427097179
C	3.515455826	-2.659336699	-3.192137278
C	6.237615542	-0.011105464	-1.847113501
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C	5.337666006	-0.786977446	3.076317273
C	6.773448185	-1.200105560	-2.397726593
C	7.992840507	-1.679122718	-1.832025018
H	8.560247759	-2.456779994	-2.339763991
C	7.537895768	-0.423090558	0.192407322
C	8.364706620	-1.301824609	-0.569567128
H	9.218096819	-1.788853134	-0.101371387
C	3.880187559	-4.006993325	-2.965224490
C	5.214967481	-4.378767166	-3.296999505
H	5.493135262	-5.430223185	-3.338437843
C	5.895680805	-2.055572289	-3.148594965
C	6.197549316	-3.427174855	-3.386346410
H	7.232354210	-3.745805970	-3.497335606
C	2.604483349	-5.204584918	0.696574871
C	3.371195633	-6.143386742	-0.055338549
H	3.895323895	-6.951390311	0.451800767
C	3.085543391	-4.774185725	-2.038936755
C	3.605292664	-5.933117091	-1.388704055
H	4.310583056	-6.578698699	-1.908777887
C	4.689189039	-3.108379473	3.496300288
C	4.975223477	-4.499669023	3.386007840
H	5.925317895	-4.890254754	3.745622916
C	2.989275497	-4.797653499	2.025206962
C	4.147867131	-5.322690515	2.667076896
H	4.461251334	-6.346877262	2.473228324
C	7.284137684	-0.640225975	1.589561556
C	7.848505486	-1.743934705	2.296480039
H	8.839823876	-2.109212319	2.034478773
C	5.719489711	-2.111483764	3.398148716
C	7.086264749	-2.459780099	3.179683734
H	7.488450086	-3.378784468	3.601964510
C	-6.723098242	-2.460245527	2.067727082
O	-7.483031999	-3.058193002	2.701209119
C	-4.536131418	-4.142871243	1.014977620
H	-4.687428716	-4.055878320	2.103936305
H	-3.650727307	-4.785951942	0.904991873
C	-5.741991438	-4.858903033	0.408273828
H	-6.575699421	-4.155598800	0.254935015
H	-5.476232753	-5.238057601	-0.591489720
C	-6.219381608	-6.019130829	1.275710963
H	-5.381258826	-6.716931115	1.447138875
H	-6.511373308	-5.629177161	2.265428416
C	-7.394847977	-6.759368311	0.646894504
H	-8.246625783	-6.078309017	0.496809407
H	-7.119543258	-7.173411344	-0.335339309
H	-7.732707474	-7.590026242	1.283046213
C	-2.415592894	-3.730952467	-0.795897663
H	-3.209753446	-4.403471989	-1.137159795
H	-1.791294014	-3.532401454	-1.672450141
H	-1.799449482	-4.271521602	-0.061785126

CP7’*methyl,perpendicular*

165
Co2C124H32O7

Co	5.078908751	0.586463741	0.132964585
Co	5.164280261	3.558341745	1.376538935
C	6.322856152	-0.513538169	-0.622141369
C	3.488708525	1.533124298	0.383383750
C	4.217826930	4.874697507	2.136764792
C	5.901411635	3.040443764	2.898709128
C	6.231966768	2.107671039	0.552560848
O	3.365305435	2.668273650	0.852779418
O	6.979053326	-1.346266350	-1.074171365
O	3.638006347	5.734488932	2.635410631
O	6.475481306	2.792536268	3.872089858
O	7.395153157	2.033786617	0.336074805
C	3.221708397	1.096921455	-2.186309515
C	4.413148704	1.353327083	-1.613500204
C	5.234590836	0.063744573	1.837828238
O	5.299365617	-0.259123756	2.943610974
H	4.642136222	-4.655237266	2.846699341
H	5.278235530	-4.514126493	-1.485073135
H	5.543453565	-4.155052245	0.909187522
H	3.986232932	-5.533060509	-2.956658905
H	2.046275246	-6.963461763	-3.252452207
H	-0.536530075	-8.638361054	-0.119453939
H	0.434936209	-8.073545571	-2.274384683
H	-0.289333891	-8.315353352	2.047042671
H	1.109052455	-7.188454644	3.684511824
H	2.857468149	-5.889281933	3.937536494
C	2.656258831	-4.888957420	3.558567078
C	4.859382301	-3.523632635	0.344971260
C	3.660436027	-4.195775491	2.942730366
C	3.383917076	-2.958957471	2.279092622
C	4.707152436	-3.727498670	-0.994886869
C	3.677631225	-3.032824544	-1.711185975
C	3.987928400	-2.616365244	1.029848849
C	2.994578745	-5.084840573	-2.976133779
C	2.831833317	-3.701525635	-2.655340636
C	-0.267560228	-7.383508874	-1.810630086
C	1.902067686	-5.890070250	-3.144472520
C	0.583177172	-5.358349541	-3.011682877
C	-0.814584370	-7.701882871	-0.599614256
C	-1.595683941	-6.737581752	0.111977661
C	-0.472984463	-6.085117773	-2.373953349
C	-0.487455589	-7.272627367	2.288489379
C	-1.436575411	-6.528563853	1.519131388
C	0.299529830	-6.638510191	3.208094212
C	0.177677389	-5.227601059	3.407715955
C	1.320882330	-4.380926084	3.565012090
C	1.162966270	-2.992650665	3.321178696
C	3.403284532	-1.575573222	0.255869851
C	2.199851434	-2.279821724	2.650287210
C	1.887711616	-1.014345201	2.058154298
C	3.230345986	-1.810824210	-1.163699469
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C	2.511816747	-0.648309446	0.873034386
C	1.579165907	-3.114369186	-2.948533294
C	1.368403280	-1.722483062	-2.685796194
C	-1.604607822	-5.363364686	-1.918906650
C	0.442049193	-3.952812401	-3.142825213
C	-0.851051422	-3.362338704	-3.080842871
C	-2.180427871	-5.697707330	-0.653323596
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C	-0.282630481	-0.997954802	3.180119976
C	2.187307352	0.623306843	0.152857908
C	0.737843731	-0.290249209	2.519283623
C	0.442542918	0.983553107	1.956243161
C	2.056945150	0.386516272	-1.444962315
C	0.771351065	0.983858993	-1.961453235
C	1.048414984	1.376429426	0.748217252
C	0.121964030	-1.118022769	-3.058046662
C	-0.083772660	0.274056226	-2.828078710
C	-3.061610096	-3.374184987	-2.043051485
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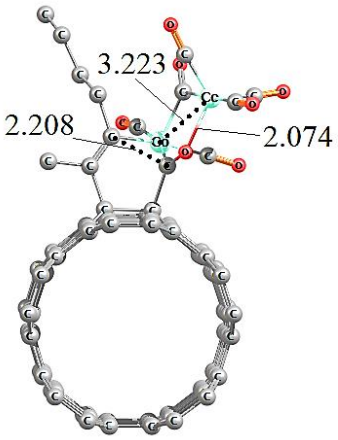

Note: Discarded in the main manuscript.

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C	-7.995838337	2.177772986	-1.258822899
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C	-4.211196473	4.769594759	-3.671436808
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H	-6.270235100	4.412453522	-4.050625791
C	-1.859175365	5.309099675	0.522593948
C	-2.427261217	6.328990516	-0.296461829
H	-2.881495743	7.206209492	0.160359510
C	-2.160401211	4.900982640	-2.237912011
C	-2.573834491	6.130032562	-1.643888843
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H	-7.205374650	4.204296884	2.946636552
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C	5.404791841	2.243636853	-2.324607756
H	5.779746783	3.000747559	-1.623072622
H	4.881659278	2.822546110	-3.102074812
C	6.598657437	1.525016441	-2.948883786
H	7.246252842	1.122435797	-2.155833771
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H	6.803694597	2.858799224	-4.635547750
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C	8.660918439	1.770074015	-4.399789288
H	9.314737804	1.397713465	-3.596010932
H	8.368939640	0.908227913	-5.019994384
H	9.250210367	2.455121063	-5.026501548
C	2.914474082	1.382308453	-3.634233883
H	2.374211159	0.532364553	-4.080790219
H	2.272984269	2.272661766	-3.747214341
H	3.826928949	1.527551621	-4.222963717

CP7*butyl,perpendicular*

165
Co2C124H32O7

Co	4.655512299	2.404320138	-0.974328795
Co	5.376167138	1.740697684	1.665754259
C	5.591427472	3.878528803	-1.270039897
C	2.849515267	2.221397521	-2.113980740
C	4.077232151	1.619742445	2.857055123
C	6.253284105	0.301179343	2.238220744
C	6.155014418	1.415136974	-0.125130151
O	2.673937970	2.793600626	-3.140652846
O	6.215086405	4.828122887	-1.485517057
O	3.301200172	1.689806462	3.713922646
O	6.886695492	-0.579663934	2.636253930
O	7.120835914	0.905458509	-0.560355778
C	2.912125697	2.827918751	0.135475178
C	4.071245811	3.102324100	0.897426687
C	5.122363007	1.551422863	-2.450558380
O	5.510175843	1.081854886	-3.431816046
H	5.825844392	-3.289937250	2.199876149
H	6.088298501	-2.654193125	-2.177833705
H	6.414242133	-2.456192698	0.237617775
H	4.971282729	-3.856888524	-3.658459026
H	3.426801000	-5.700027697	-3.999647159
H	1.569983395	-8.210817403	-0.905394802
H	2.209076344	-7.257062448	-3.047876576
H	1.899253139	-7.998306160	1.262488169
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H	4.477803309	-5.019371988	3.260252071
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C	3.451100727	-0.614775396	-1.457935657
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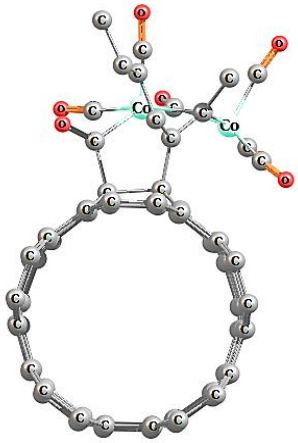

Note: Taken into consideration in the main manuscript.

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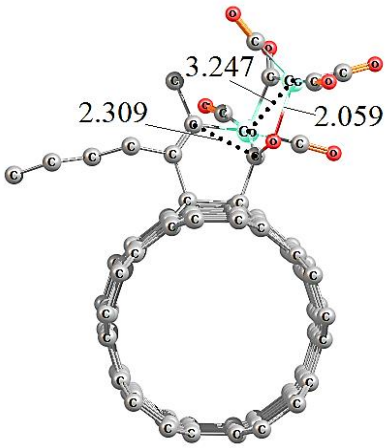
C	-2.274589963	2.253422179	-2.707541610
C	-4.189002090	-2.054192618	-2.071594816
C	-2.637627427	-0.086305044	-3.286252056
C	-4.036519076	0.145121279	-3.122789129
C	-4.562049521	-2.607244596	-0.816741591
C	-5.542300632	-1.920759900	-0.041057509
C	-4.819913790	-0.849923345	-2.499428725
C	-4.161836111	-2.356859946	1.923913718
C	-5.339982593	-1.794780845	1.349732793
C	-3.464200169	-1.600057797	2.904131819
C	-3.983042947	-0.326830271	3.278847091
C	-3.084854791	0.743283058	3.478483060
C	-3.596714069	2.073363468	3.457063067
C	-2.118355490	4.165136596	0.358585438
C	-2.818810735	3.084959788	2.815560050
C	-2.312898002	4.039512074	-1.052209860
C	-3.643656225	2.558114964	-2.980342692
C	-6.080776717	-0.475984765	-1.946361300
C	-4.548494214	1.472999136	-3.189516002
C	-6.449903549	-1.024818068	-0.678607400
C	-6.054970279	-0.780420235	2.051245383
C	-5.359345284	-0.028228535	3.048960039
C	-6.734764475	0.690714072	-2.410437981
C	-8.009901000	0.984156649	-1.840888023
H	-8.651023877	1.735418436	-2.298196915
C	-7.454411973	-0.381397644	0.084939309
C	-8.360117462	0.462929050	-0.624320724
H	-9.270868760	0.812114612	-0.141359035
C	-4.158122474	3.833490967	-2.648764034
C	-5.519185370	4.086438160	-2.985172006
H	-5.911357755	5.100803660	-2.942464755
C	-5.942409352	1.699119811	-3.059916899
C	-6.388845845	3.045835852	-3.185517132
H	-7.450186438	3.259486967	-3.297377321
C	-3.082524935	4.847428427	1.134259460
C	-3.935254554	5.757802709	0.442047694
H	-4.553117206	6.458622727	1.000392683
C	-3.469309101	4.599683205	-1.639572043
C	-4.123231846	5.636959471	-0.909776790
H	-4.886142472	6.244854547	-1.392514270
C	-4.977127737	2.303507860	3.684554097
C	-5.411289401	3.660538241	3.686215267
H	-6.405046845	3.913813469	4.050489424
C	-3.443574420	4.289267563	2.414272867
C	-4.665146618	4.628031049	3.064798399
H	-5.085197878	5.625505790	2.949926727
C	-7.250537881	-0.256265998	1.501597218
C	-7.944702507	0.716534008	2.281291250
H	-8.964331952	0.995640974	2.022239925
C	-5.890134971	1.214359258	3.470408965
C	-7.282088580	1.431554293	3.242321526
H	-7.790119606	2.263033649	3.727135796
C	6.620710323	2.932116273	2.198149138
O	7.434698670	3.599801048	2.674177320
C	2.126849964	4.067396144	-0.343906349
H	1.607914868	4.497872189	0.531516835
H	1.329058723	3.750766004	-1.017604378
C	2.815644050	5.188353353	-1.128254022
H	3.613754067	5.685839858	-0.562592528
H	3.276281022	4.776635476	-2.036324318
C	1.770144996	6.224749801	-1.542138134
H	0.968137082	5.718261648	-2.107549424
H	1.293858136	6.648345614	-0.640629219
C	2.370302540	7.341120480	-2.389308741
H	3.160807537	7.873377633	-1.837828341
H	2.818100701	6.933678081	-3.308593743
H	1.605975189	8.075728133	-2.680774545
C	4.275073918	4.462022335	1.529538683
H	3.476187341	5.174453650	1.300647040
H	4.278859132	4.330686420	2.622453502
H	5.241769122	4.908052135	1.258819152

CP7'*butyl,perpendicular*

165
Co2C124H32O7

Co	-5.115184767	-0.993050666	0.170895023
Co	-4.989749961	-4.040408018	1.286247248
C	-6.429438459	-0.061937915	-0.684006565
C	-3.471829565	-1.816220395	0.519962810
C	-3.989640695	-5.369760406	1.948719760
C	-5.859718122	-3.780953468	2.803237624
C	-6.149140069	-2.611665363	0.577929121
O	-3.276849128	-2.937954414	0.988072868
O	-7.162044264	0.601615010	-1.274228897
O	-3.379730009	-6.244086744	2.382422629
O	-6.501853724	-3.681471296	3.760349564
O	-7.320628983	-2.602507788	0.392260388
C	-3.186738772	-1.575669951	-2.063389521
C	-4.435984555	-1.708968802	-1.575695237
C	-5.369293413	-0.464499551	1.865874619
O	-5.488639930	-0.132618977	2.963792181
H	-5.136488992	4.377442813	2.571312724
H	-5.653538772	3.917979775	-1.750332501
H	-5.958534035	3.683433434	0.654546965
H	-4.398667966	4.948085229	-3.250255258
H	-2.564804259	6.504611563	-3.580562247
H	-0.191798476	8.559075167	-0.505364462
H	-1.065441380	7.792526565	-2.639718027
H	-0.467452239	8.350074908	1.672854761
H	-1.823530524	7.217961464	3.342463748
H	-3.479428911	5.806245347	3.623598303
C	-3.193846655	4.803096847	3.312395305
C	-5.213082837	3.074058643	0.146554778
C	-4.126491229	3.999947968	2.717762004
C	-3.741676378	2.749244205	2.139243749
C	-5.038630495	3.208335073	-1.199351020
C	-3.939261887	2.554324351	-1.848554285
C	-4.291055383	2.281847037	0.905287154
C	-3.375919568	4.577257438	-3.216718552
C	-3.118586663	3.232128617	-2.807472804
C	-0.324575445	7.187488922	-2.120373148
C	-2.342807826	5.453656062	-3.404983910
C	-0.991496329	5.034332975	-3.210501055
C	0.167412967	7.619342276	-0.920883096
C	1.000440874	6.762003552	-0.135084192
C	-0.008968429	5.876788910	-2.597631794
C	-0.200183320	7.340767041	1.980483063
C	0.821337283	6.626200809	1.278576607
C	-0.963294181	6.703684433	2.917942502
C	-0.743556296	5.319641287	3.203779958
C	-1.825034517	4.399488946	3.382755060
C	-1.557199562	3.015389103	3.227262370
C	-3.611181313	1.243229862	0.208802291
C	-2.518587343	2.188087111	2.576257786
C	-2.094970416	0.918429159	2.069364248
C	-3.418548963	1.402499015	-1.220010776
C	-2.351434004	0.685456858	-1.808517639
C	-2.658656406	0.435117956	0.897022149
C	-1.815885482	2.728369267	-3.026700758
C	-1.507422506	1.376779210	-2.672225919
C	1.162273236	5.272279390	-2.076174837
C	-0.741477215	3.638551039	-3.251168417
C	0.589986052	3.153718939	-3.128344828
C	1.679767281	5.724956504	-0.822311323
C	2.562014926	4.862987784	-0.108168854
C	1.560720104	3.985464313	-2.539951559
C	1.336044291	5.464490715	1.906876130
C	2.387183892	4.730245304	1.284448662
C	0.535196719	4.796492164	2.884817131
C	0.840186412	3.437967749	3.186963846
C	-0.224221778	2.533006307	3.352692068
C	0.036489556	1.131102435	3.242041208
C	-2.228698747	-0.851054201	0.268314636
C	-0.909060176	0.311013158	2.600472137
C	-0.507127733	-0.968821585	2.124185647
C	-2.084911809	-0.726149203	-1.353947270
C	-0.736228245	-1.233436155	-1.792517857
C	-1.054248314	-1.481043399	0.931954011
C	-0.214503798	0.847362543	-2.991959748
C	0.086425285	-0.510461714	-2.680884517
C	2.765561511	3.394965627	-2.047037923
C	0.843329942	1.748638701	-3.216405751
C	2.187644754	1.283356356	-3.140306630
C	3.277265993	3.842190121	-0.807419822
C	4.170906298	2.997180556	-0.092852268
C	3.168715745	2.124400844	-2.537562753
C	2.933147245	3.581016309	1.935603343
C	3.994538546	2.863266692	1.317648812
C	2.144633274	2.922914366	2.907234207
C	2.446686506	1.574534841	3.237347498



Note: Discarded in the main manuscript.

C	1.369234124	0.657861797	3.414076270
C	1.629209287	-0.728162201	3.308018589
C	-0.380225833	-2.508760889	0.266331821
C	0.675994968	-1.557062377	2.658409717
C	1.082444874	-2.835372422	2.199292458
C	-0.203010178	-2.368873736	-1.167662596
C	0.905280598	-3.040471429	-1.755150947
C	0.565632285	-3.303750482	0.971814340
C	1.379626599	-1.015191196	-3.007767475
C	1.691647844	-2.366255966	-2.714687886
C	4.356312004	1.530395986	-2.038379507
C	2.445115639	-0.103106358	-3.237344813
C	3.786003326	-0.577904928	-3.131773830
C	4.865913981	1.974754456	-0.787516930
C	5.738502087	1.106069499	-0.068065604
C	4.751904378	0.248176056	-2.517759373
C	4.522799050	1.713835313	1.959010241
C	5.565031951	0.974044169	1.326022735
C	3.734496543	1.056941730	2.943176875
C	4.031794045	-0.301253910	3.257025089
C	2.965670739	-1.205763878	3.448283818
C	3.230594142	-2.603390436	3.363253840
C	1.284158238	-4.332315986	0.290632566
C	2.265428904	-3.440896857	2.725694105
C	1.459797899	-4.196176289	-1.123136572
C	2.981586149	-2.891446773	-3.039592132
C	5.947709796	-0.354401785	-2.025308319
C	4.054675172	-1.972487200	-3.248671183
C	6.453120989	0.085718190	-0.762346825
C	6.113187283	-0.173261637	1.971948177
C	5.325701259	-0.828901282	2.969068003
C	6.370708423	-1.602687035	-2.541333820
C	7.595004836	-2.128672399	-2.031954970
H	8.077241253	-2.967003077	-2.531081110
C	7.356706874	-0.744454694	-0.055262187
C	8.075478738	-1.711207119	-0.819625330
H	8.927748694	-2.227562717	-0.381881078
C	3.275612539	-4.247286015	-2.767662327
C	4.561656582	-4.718972585	-3.155827221
H	4.773043183	-5.786595134	-3.153923900
C	5.391771778	-2.440191020	-3.180417604
C	5.593306043	-3.838059571	-3.357337313
H	6.597435847	-4.228612217	-3.510825517
C	2.147957493	-5.185204653	1.012674944
C	2.812340007	-6.205349191	0.270133787
H	3.319671185	-7.015880019	0.789911497
C	2.490119411	-4.920907620	-1.761294654
C	2.978716608	-6.076900488	-1.083694196
H	3.614021474	-6.788653974	-1.607340032
C	4.553905488	-3.081087005	3.540998648
C	4.739401066	-4.491721659	3.496181349
H	5.683595290	-4.927423304	3.817268424
C	2.649221876	-4.728918405	2.286766234
C	3.810886890	-5.294835580	2.884724558
H	4.041163393	-6.348191358	2.736468389
C	7.180655647	-0.878441345	1.364762911
C	7.714588779	-1.986030294	2.088591060
H	8.660293718	-2.430734548	1.784383267
C	5.639082510	-2.161130741	3.330803275
C	6.963418607	-2.610334855	3.048106529
H	7.329397024	-3.537080704	3.485962490
C	-5.550848536	-4.993861636	-0.090193799
O	-5.994961335	-5.643431123	-0.938877952
C	-2.801025623	-2.114441923	-3.422512834
H	-3.408872270	-3.001291649	-3.651964246
H	-1.760695250	-2.474012452	-3.391903217
C	-2.931629765	-1.098477916	-4.568908479
H	-3.995922751	-0.978609554	-4.838264467
H	-2.595936737	-0.104947595	-4.238705969
C	-2.116476251	-1.500078161	-5.793237033
H	-1.063363486	-1.630777249	-5.484983015
H	-2.459065976	-2.481760644	-6.165204352
C	-2.194839234	-0.456911687	-6.902668989
H	-3.233914357	-0.314511988	-7.238396341
H	-1.821967347	0.515134010	-6.543157344
H	-1.592290379	-0.750043323	-7.774548170
C	-5.466056773	-2.466855330	-2.386747506
H	-6.443429827	-2.530138788	-1.899967835
H	-5.613862568	-1.959237517	-3.353407893
H	-5.134235782	-3.495649492	-2.593312615

TS3*methyl,oblique*

165
Co2C124H32O7

Co	-4.712651689	0.265970028	-0.720027174
Co	-5.944653961	-1.271184654	1.863988153
C	-6.372853391	-0.307052617	0.179181453
C	-3.658408298	-0.872112375	0.289792587
C	-5.554622023	-2.157496810	3.370830289
C	-6.384318373	0.227376558	2.700608405
C	-7.172109150	-2.438599444	1.385980301
O	-3.938114313	-1.452417316	1.359557988
O	-7.415732382	-0.007772583	-0.300452037
O	-5.325431871	-2.725557535	4.345036780
O	-6.816680356	1.133310329	3.275001465
O	-8.064140860	-3.129624389	1.121564597
C	-3.079350259	-2.214929144	-1.742261340
C	-4.257735468	-1.649425323	-1.376408848
C	-5.313880958	0.971953180	-2.296392761
O	-5.527240235	1.483685543	-3.306349345
H	2.656472040	-6.766210928	-3.526923894
H	-0.304784435	-7.503595485	-0.462103613
H	0.749699299	-7.225189140	-2.638099537
H	0.014658242	-7.363211485	1.742974212
H	1.788038254	-6.923897126	3.348716636
H	6.031868454	-5.959769444	2.566333833
H	3.896388146	-6.449238853	3.608583685
H	7.040020813	-5.729315844	0.626585365
H	6.599018911	-5.844006393	-1.760821344
H	4.994381183	-6.226074007	-3.196294413
C	4.263878426	-5.419305521	-3.197855237
C	0.362859273	-6.351756868	-2.116848505
C	2.938542039	-5.725389913	-3.381479874
C	1.934288815	-4.733618804	-3.203861949
C	-0.237266797	-6.509132176	-0.900693591
C	-0.612844950	-5.359921768	-0.133344490
C	0.657799343	-5.033957984	-2.599295636
C	0.259318260	-6.333788717	1.998991051
C	-0.332836928	-5.259143101	1.267343120
C	4.113989437	-5.427324045	3.303824490
C	1.257636429	-6.086193420	2.899831256
C	1.707318879	-4.751487377	3.128991998
C	5.319244753	-5.151182425	2.717971774
C	5.564425029	-3.866464269	2.142930502
C	3.089383412	-4.433894677	3.349140121
C	6.645927615	-4.852358530	0.116191379
C	6.212745031	-3.719772376	0.871505349
C	6.397117843	-4.916925972	-1.227325648
C	5.704743751	-3.851988274	-1.879326000
C	4.659131121	-4.101489114	-2.833856914
C	3.730921863	-3.061591526	-3.089236687
C	-0.110531752	-3.978120259	-2.081587603
C	2.349964739	-3.384051091	-3.253097520
C	1.390688047	-2.339942090	-3.093144379
C	-0.826724689	-4.160928460	-0.849326497
C	-1.272283368	-2.992646914	-0.170786414
C	0.149984757	-2.623663025	-2.480616778
C	-0.209959874	-3.956291555	1.804512892
C	-0.849390751	-2.850072064	1.146218588
C	3.502746553	-3.086126149	3.212690212
C	0.829332827	-3.704128315	2.751517431
C	1.189299218	-2.355616410	3.028686982
C	4.763746526	-2.794440089	2.606091570
C	4.982993368	-1.476914562	2.103624658
C	2.537501733	-2.042389642	3.284241711
C	6.006953319	-2.514852542	0.154998694
C	5.617167293	-1.332930492	0.852304144
C	5.744211103	-2.584525122	-1.248682064
C	5.112402547	-1.464987923	-1.866990676
C	4.084353263	-1.711927467	-2.801170417
C	3.168503307	-0.664149304	-3.103052670
C	-0.669319683	-1.558759158	-2.042489072
C	1.790568316	-0.988840572	-3.235798960
C	0.821682540	0.034379318	-3.110535023
C	-1.770379705	-1.827804713	-1.028515138
C	-2.145146201	-0.611182144	-0.121758796
C	-0.428261900	-0.266927969	-2.490811021
C	-0.728196734	-1.535383501	1.734503815
C	-1.367583967	-0.445280515	1.152729087
C	2.958254737	-0.680055802	3.206474637
C	0.290858507	-1.304218581	2.692682737
C	0.627818018	0.027580072	3.034090809
C	4.207156738	-0.388718281	2.605171151
C	4.434563153	0.924072404	2.109402501
C	1.989746840	0.349367046	3.303335709
C	5.447218149	-0.107392453	0.137380765
C	5.068306450	1.067191802	0.840395539
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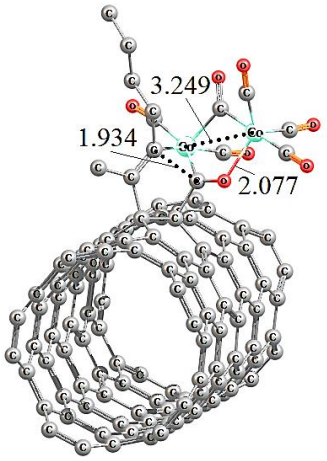
C	4.562059964	0.930795675	-1.888806905



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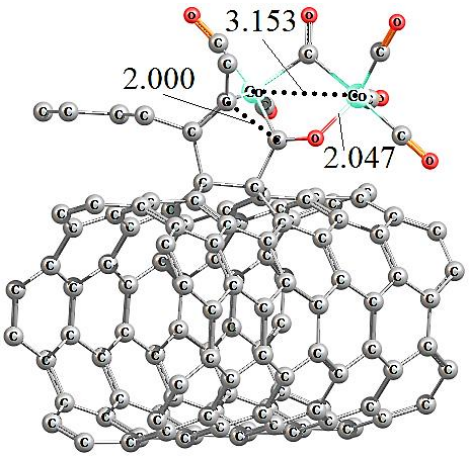
C	1.223336670	1.384764460	-3.259928905
C	0.243755224	2.421963899	-3.173017497
C	-2.045970051	0.687042512	-0.900928822
C	-2.322891492	1.896707676	-0.176831202
C	-0.999093089	2.142668265	-2.567626304
C	-1.282550809	0.823823862	1.748887014
C	-1.979183762	1.954885701	1.194005406
C	2.394755406	1.705129290	3.201067267
C	-0.270853061	1.069683373	2.708871772
C	0.058551039	2.414846699	3.049550828
C	3.639254029	1.999051441	2.593963690
C	3.842457689	3.316107752	2.079068234
C	1.410977387	2.737632439	3.287542182
C	4.867153794	2.279867371	0.120121225
C	4.468054682	3.458831823	0.822311297
C	4.608216678	2.208682021	-1.268606485
C	3.960926114	3.318389176	-1.897984448
C	2.937939173	3.065573994	-2.836275008
C	2.023977035	4.107176253	-3.156636364
C	-1.795296038	3.244181348	-2.140888772
C	0.644646002	3.776155760	-3.344235061
C	-2.446178941	3.126830792	-0.878318653
C	-1.907955366	3.221053159	1.821270813
C	1.808121514	4.100879879	3.200186600
C	-0.865881149	3.462296303	2.778563138
C	3.058298201	4.398351760	2.573414255
C	4.279696726	4.678392316	0.109285814
C	4.016528688	4.604718174	-1.294044250
C	0.836838636	5.125550024	3.334599759
C	1.309558304	6.474453583	3.269622476
H	0.664835337	7.293014942	3.583668111
C	3.284094537	5.710865686	2.085398293
C	2.499542115	6.759403111	2.662083550
H	2.778738704	7.798756673	2.499571581
C	-2.555265715	4.343649856	1.227900185
C	-2.512471345	5.577886784	1.954479439
H	-3.184051842	6.390266125	1.681982723
C	-0.538913513	4.793855606	3.128966065
C	-1.534782417	5.796467285	2.879564855
H	-1.443371480	6.778597514	3.339451279
C	-1.578947624	4.540341655	-2.678941345
C	-2.417877258	5.594514878	-2.184157423
H	-2.471138915	6.541995885	-2.717058005
C	-2.806827020	4.301997719	-0.171435545
C	-3.007742355	5.483323911	-0.958773182
H	-3.519794751	6.343435054	-0.530830925
C	2.386117733	5.455380331	-2.906586552
C	1.455593288	6.461900238	-3.319454189
H	1.767434341	7.503875425	-3.362868818
C	-0.325853895	4.812616290	-3.300684124
C	0.141789328	6.149285259	-3.516806731
H	-0.571086258	6.946933482	-3.716289232
C	3.916458985	5.855286350	0.811256236
C	3.790857536	7.055022389	0.039314369
H	3.754554680	8.021589859	0.538548385
C	3.406303691	5.711691985	-1.940603690
C	3.543163403	6.985632162	-1.301578227
H	3.314062638	7.897817316	-1.849390511
C	-4.912725626	1.691004828	0.322482729
O	-5.150604560	2.604283952	0.991454370
C	-5.531110482	-2.410510440	-1.682340055
H	-6.150414524	-2.412310851	-0.776053293
H	-5.284219828	-3.472063546	-1.841791533
C	-6.371787547	-1.913882943	-2.854865632
H	-6.792929522	-0.925442201	-2.621211327
H	-5.735990171	-1.784339349	-3.748302444
C	-7.522572889	-2.869021006	-3.157171727
H	-7.117653958	-3.862399941	-3.418560335
H	-8.119299436	-3.006646479	-2.238903711
C	-8.416507029	-2.360033649	-4.283264134
H	-7.840436217	-2.227437397	-5.212324519
H	-9.239341724	-3.059418517	-4.490767316
H	-8.856801183	-1.385879152	-4.020528598
C	-3.030417741	-3.328696030	-2.749777056
H	-3.917486087	-3.312327889	-3.392294326
H	-2.156967603	-3.216637559	-3.407262196
H	-2.962253282	-4.321323389	-2.273419972

TS3*butyl,oblique*



165
Co2C124H32O7

Co	3.895430562	3.310490506	-0.744005622
Co	5.360891774	2.093103089	1.767866196
C	5.581405173	3.355492259	0.240539101
C	2.839510459	2.578293227	0.733137816
C	5.128504936	0.880512596	3.064110597
C	6.171785280	0.923226350	0.724770970
C	6.261752908	3.243832017	2.778748675
O	3.334516317	2.368309771	1.859944179
O	6.519582082	3.993916815	-0.094965233
O	4.998970559	0.078977395	3.880203283
O	6.827316352	0.180655442	0.122317879
O	6.955557908	3.923429573	3.406058265
C	1.371554455	4.176174397	-0.638257749
C	2.517008829	4.434964612	0.063258255
C	4.419819092	4.604225885	-1.875601312
O	4.626442035	5.444057676	-2.641997853
H	-5.828879583	5.133074797	-2.482178061
H	-3.669495176	6.737258785	0.916303520
H	-4.431098343	6.350535796	-1.363054841
H	-3.842696022	6.093524248	3.043207802
H	-5.073620885	4.558791070	4.473602182
H	-8.197081597	1.684131160	3.269848143
H	-6.617397492	3.017159721	4.542567403
H	-8.940653111	1.332143061	1.231932493
H	-8.657526054	2.055756139	-1.068796784
H	-7.534541878	3.415079584	-2.356430652
C	-6.490690123	3.116050072	-2.430204761
C	-3.645408091	5.721477028	-0.948899552
C	-5.524465447	4.088424634	-2.499303580
C	-4.146560618	3.747187134	-2.403837583
C	-3.215106850	5.941271436	0.328257747
C	-2.301328097	5.027417133	0.943779027
C	-3.211205498	4.552370682	-1.656525216
C	-3.501916839	5.064015530	3.138308822
C	-2.456418473	4.579796757	2.294020722
C	-6.273295968	2.101853761	4.064575905
C	-4.195019017	4.200350209	3.940496095
C	-3.872387907	2.810355248	3.950216886
C	-7.164298867	1.349629246	3.348867402
C	-6.708446015	0.247434761	2.562113837
C	-4.879591485	1.791632470	4.031481382
C	-8.158750853	0.878385416	0.625742559
C	-7.194603289	0.016574491	1.231811814
C	-7.998198565	1.286750199	-0.670461144
C	-6.868575589	0.851344072	-1.426233141
C	-6.129433544	1.749015394	-2.272382801
C	-4.801985964	1.393629731	-2.621233320
C	-2.003677939	3.967666754	-1.242095103
C	-3.794728540	2.404706653	-2.665128262
C	-2.424347702	2.001127583	-2.602542580
C	-1.511134655	4.241625770	0.077423707
C	-0.513093177	3.374830624	0.602127651
C	-1.496200328	2.787435169	-1.880924224
C	-1.862564053	3.341297605	2.632417792
C	-0.758423612	2.842589859	1.860345374
C	-4.530060203	0.470064395	3.661646199
C	-2.587013854	2.446477469	3.476553419
C	-2.179166797	1.085119491	3.527487159
C	-5.461647545	-0.320749220	2.919551289
C	-4.966135077	-1.451470030	2.204030243
C	-3.159986458	0.082314043	3.642982019
C	-6.399521684	-0.766844263	0.359066943
C	-5.445213108	-1.680692375	0.897521703
C	-6.231447726	-0.337114182	-0.993943087
C	-5.123879927	-0.854371667	-1.728505381
C	-4.395706722	0.030833200	-2.551065399
C	-3.079248817	-0.330988173	-2.952593243
C	-0.218309092	2.261804069	-1.553904175
C	-2.073720701	0.675978542	-2.960970639
C	-0.713175575	0.294136997	-2.925512966
C	0.561927666	2.862907394	-0.373462397
C	1.520592009	1.830055215	0.336169253
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C	-2.808021043	-1.264370754	3.327294185
C	-0.870230407	0.723694941	3.097971325
C	-0.453562080	-0.621692710	3.221085437
C	-3.729764102	-2.050186711	2.592878364
C	-3.243363302	-3.182027258	1.884526179
C	-1.442599280	-1.641549020	3.338567798
C	-4.672550132	-2.501729691	0.020653986
C	-3.727465841	-3.412204366	0.563746235
C	-4.509444919	-2.075877752	-1.324070518
C	-3.414569478	-2.584601869	-2.072113199

C	-2.682184237	-1.686126639	-2.899235760
C	-1.354793409	-2.033971285	-3.279759795
C	1.465995333	0.474390139	-1.824418044
C	-0.362155522	-1.033232733	-3.296636936
C	1.012505621	-1.430381567	-3.304637256
C	2.019309202	0.748570051	-0.594194586
C	2.929989770	-0.199491907	-0.034848631
C	1.932547366	-0.671341030	-2.557116631
C	1.573278596	-0.083578691	1.976675260
C	2.739897591	-0.598252441	1.304403045
C	-1.080438658	-2.969620960	2.999238495
C	0.854637418	-0.971816417	2.814569614
C	1.281528993	-2.329803637	2.930935393
C	-1.996151491	-3.754634139	2.258680944
C	-1.489034703	-4.876050193	1.534615067
C	0.299419306	-3.339962372	3.004894630
C	-2.936869238	-4.207230597	-0.314692538
C	-1.970276393	-5.108540539	0.228733448
C	-2.780068080	-3.786167616	-1.655623686
C	-1.670431359	-4.289618356	-2.403836863
C	-0.951186449	-3.402992978	-3.233141998
C	0.359232548	-3.766281663	-3.651147161
C	3.171773717	-1.273246295	-2.207943406
C	1.366362451	-2.751245830	-3.694381440
C	3.669559387	-1.049271347	-0.891413827
C	3.357969810	-1.793633157	1.741954353
C	0.670779811	-4.674643506	2.679565166
C	2.615032178	-2.687262179	2.584987541
C	-0.247443622	-5.461565554	1.916319317
C	-1.190544113	-5.920397740	-0.644355096
C	-1.040116358	-5.500384284	-2.002693399
C	2.034872817	-5.057454183	2.737434031
C	2.335822392	-6.420573801	2.424057760
H	3.317960550	-6.828009784	2.655942697
C	0.236889798	-6.597783024	1.218960182
C	1.462488974	-7.168917137	1.685946757
H	1.767292575	-8.155613097	1.342198615
C	4.473793659	-2.313567134	1.024645765
C	5.103105596	-3.483945092	1.564957839
H	6.094896589	-3.773542040	1.221429199
C	3.033580831	-4.033642378	2.704391448
C	4.403998054	-4.319620629	2.384172867
H	4.848438894	-5.263938165	2.693137944
C	3.662457784	-2.382854423	-2.944017968
C	4.934191135	-2.912439946	-2.541127663
H	5.470567135	-3.593832427	-3.198993725
C	4.620905015	-1.943934871	-0.341247610
C	5.399805868	-2.702001890	-1.275278136
H	6.300309778	-3.215607665	-0.943597683
C	0.750800679	-5.129351702	-3.624361709
C	2.060515034	-5.437069537	-4.115991908
H	2.328638190	-6.468444516	-4.337792206
C	2.733837693	-3.140720952	-3.713167430
C	3.022764783	-4.471228353	-4.159937124
H	4.043991135	-4.746742490	-4.416446928
C	-0.253587407	-6.836809959	-0.103041553
C	0.455316942	-7.660729362	-1.034779272
H	1.000027761	-8.534911157	-0.682740405
C	0.034971781	-6.020695953	-2.769341178
C	0.594052717	-7.265027051	-2.334217807
H	1.246728606	-7.830413410	-2.996729879
C	4.442782880	1.926339938	-1.725820217
O	4.852365529	1.138028955	-2.466192187
C	0.808543849	5.272740189	-1.499145061
H	1.375607985	6.196382946	-1.312205818
H	-0.238451296	5.503889450	-1.266571431
C	0.926113280	4.913466782	-2.994671328
H	1.976127872	5.021164463	-3.312166378
H	0.659419375	3.857384841	-3.155488437
C	0.019339055	5.788516379	-3.854862357
H	-1.021036992	5.674026747	-3.502424836
H	0.287826464	6.850086979	-3.711390222
C	0.102488257	5.417150060	-5.331200864
H	1.130691417	5.526753867	-5.708972550
H	-0.203068783	4.370509019	-5.483242099
H	-0.554337672	6.054179077	-5.941021295
C	2.931622358	5.734333151	0.665333978
H	3.630652746	6.296465035	0.027057380
H	2.060166713	6.361367369	0.909021887
H	3.471168468	5.511956785	1.600470570

TS3*_methyl,oblique_

165
Co2C124H32O7

Co	5.063130071	0.614017471	-0.544464948
Co	5.449096531	2.971049662	1.676821390
C	6.345920991	1.883769380	0.286718091
C	3.589083460	1.469445153	0.227604575
C	4.662265874	3.962404821	2.944800696
C	6.409471477	2.025825777	2.823341077
C	6.079121692	4.382895868	0.829940805
O	3.594421442	2.201139641	1.248212612
O	7.478619705	1.866316779	-0.069180660
O	4.184449530	4.613394382	3.764894648
O	7.126554951	1.505330991	3.567056159
O	6.582622560	5.297276919	0.326916313
C	2.592280786	2.351715739	-1.783156537
C	3.885055372	2.177269614	-1.405648449
C	6.053543518	-0.034468496	-1.931405475
O	6.625681683	-0.578842423	-2.772569475
H	3.744408600	-5.396803325	3.300511262
H	5.513997343	-4.300910677	-0.484228100
H	5.114837509	-4.466312224	1.914458322
H	4.707052459	-4.849500517	-2.505138849
H	2.900622291	-6.130885822	-3.513095546
H	-0.332089961	-8.400848000	-1.512985308
H	1.157200510	-7.381266420	-3.134220891
H	-0.727136901	-8.623195007	0.641211461
H	0.165723884	-7.942009081	2.797684507
H	1.791090603	-6.778148266	3.682368383
C	1.656109148	-5.711766961	3.512090983
C	4.583646630	-3.715131632	1.333407809
C	2.761674901	-4.929920068	3.292114910
C	2.621721632	-3.573695612	2.884362865
C	4.817356297	-3.614051815	-0.006130923
C	4.030932427	-2.718704638	-0.800073612
C	3.516490056	-2.963974023	1.931976227
C	3.730464583	-4.386520824	-2.634082151
C	3.468739332	-3.106362735	-2.053157470
C	0.327608603	-6.798452793	-2.738554004
C	2.714159451	-5.106262518	-3.196668703
C	1.386526673	-4.580628750	-3.228688713
C	-0.513336849	-7.374282688	-1.825995706
C	-1.497702203	-6.586751119	-1.153008665
C	0.229463165	-5.403777050	-3.030175786
C	-1.011202150	-7.656719166	1.053580504
C	-1.740221802	-6.723502592	0.253811303
C	-0.508532600	-7.272934376	2.266135441
C	-0.713032887	-5.940219137	2.737281045
C	0.346943876	-5.179430094	3.339080727
C	0.219687059	-3.768069059	3.366187314
C	3.104997147	-1.795707504	1.271411542
C	1.369344219	-2.959596538	3.115504637
C	1.166814958	-1.598999208	2.740675977
C	3.439659195	-1.621375264	-0.121087541
C	2.702826743	-0.642675220	-0.856687209
C	2.024264068	-1.009025275	1.785064295
C	2.303959289	-2.420654546	-2.482967687
C	2.033982507	-1.101771385	-1.994165247
C	-1.003915105	-4.774805042	-2.726515383
C	1.248229372	-3.177797019	-3.078932849
C	-0.041479665	-2.586228284	-3.180804671
C	-1.887396313	-5.377758329	-1.778610062
C	-2.894766867	-4.562870809	-1.180610314
C	-1.183971299	-3.395515313	-3.026519003
C	-2.345549185	-5.636690797	0.932787839
C	-3.128790175	-4.693342490	0.204070532
C	-1.817859854	-5.235983674	2.199664207
C	-2.110745573	-3.917693262	2.659184788
C	-1.069325008	-3.171190571	3.250035223
C	-1.200534358	-1.754923966	3.324743586
C	1.640641649	0.204320675	1.170743516
C	-0.057455618	-0.955969042	3.048755459
C	-0.231945316	0.403438300	2.695110509
C	2.295497794	0.613578046	-0.113067822
C	1.492414143	1.575147301	-1.041816440
C	0.642339592	0.984952537	1.729870819
C	0.853222277	-0.414565142	-2.462362209
C	0.586165517	0.892366682	-2.056089314
C	-2.444530128	-2.773669494	-2.776177485
C	-0.179681681	-1.174333139	-3.071149891
C	-1.457599094	-0.590211502	-3.243104122
C	-3.320391949	-3.368346503	-1.834823183
C	-4.330009701	-2.562998543	-1.240398785
C	-2.617701514	-1.406049486	-3.101232530
C	-3.773027130	-3.619497979	0.892449175
C	-4.559658170	-2.690606255	0.160897189
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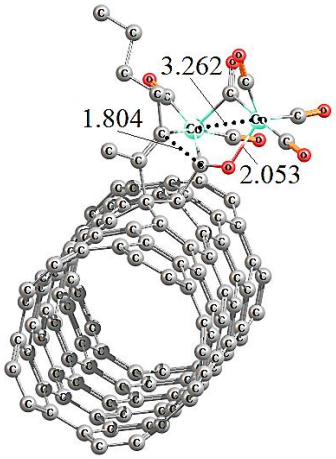
C	-3.534091881	-1.913454768	2.624081590



Note: Taken into consideration in the main manuscript.

C	-2.480314639	-1.163704261	3.220682837
C	-2.593568461	0.255708688	3.267748414
C	0.254432809	2.231497417	1.102668298
C	-1.455976188	1.045515092	3.006938588
C	-1.625560394	2.429393896	2.685104448
C	0.594326921	2.488622240	-0.216416386
C	-0.269425789	3.374136108	-0.933372906
C	-0.767820978	3.024979895	1.738919543
C	-0.555171083	1.558249236	-2.531272108
C	-0.837479465	2.917590364	-2.143663716
C	-3.858439735	-0.773130863	-2.832586000
C	-1.592054232	0.813895373	-3.145226138
C	-2.875140903	1.411965555	-3.322311317
C	-4.731154081	-1.360936926	-1.885645721
C	-5.724839338	-0.531940729	-1.280266788
C	-4.022159333	0.609447990	-3.152056757
C	-5.172514161	-1.600994455	0.844251045
C	-5.949106122	-0.654182784	0.107443826
C	-4.648746702	-1.205903435	2.097185107
C	-4.923954509	0.118619537	2.562772151
C	-3.881785901	0.858500171	3.159676136
C	-4.005480966	2.272556634	3.250421872
C	-1.170353909	4.257227015	1.153468386
C	-2.845263435	3.078788268	3.022713357
C	-0.941522186	4.418369220	-0.246535256
C	-1.961505297	3.594433099	-2.671228351
C	-5.267537896	1.250021282	-2.900538181
C	-3.009896865	2.828295666	-3.282790003
C	-6.141462396	0.664471468	-1.932201601
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C	-6.046973893	0.827857881	2.054242522
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C	-6.730260491	3.182473380	-3.011516440
H	-6.999081392	4.136188960	-3.461472128
C	-7.150557115	1.470121581	-1.345566730
C	-7.559890737	2.629080773	-2.077703191
H	-8.471635403	3.153891214	-1.798483800
C	-2.254196568	4.920665554	-2.238731338
C	-3.362530738	5.579810903	-2.864696122
H	-3.485598003	6.655983948	-2.754304894
C	-4.282359162	3.417496992	-3.470556375
C	-4.345283819	4.851232161	-3.466870502
H	-5.235512516	5.356614824	-3.836223478
C	-2.152907541	5.066450615	1.783509321
C	-2.511455991	6.286501292	1.117671654
H	-3.063555650	7.056333487	1.653465970
C	-1.745565498	5.334059633	-0.975670744
C	-2.323036956	6.413628817	-0.227300780
H	-2.731702323	7.279387684	-0.745636661
C	-5.289972752	2.867993344	3.169957258
C	-5.357211727	4.287797774	3.342986311
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C	-3.010370874	4.462372577	2.746737562
C	-4.250641665	5.060400935	3.143245660
H	-4.346670363	6.144186969	3.165786781
C	-7.375709893	1.348360075	0.061226310
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H	-7.919745728	3.642305439	2.521421935
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H	5.822286735	3.156023427	-1.391050558
H	4.534284800	4.140591965	-2.020542880
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H	5.076562405	1.613696725	-3.577311592
H	4.802165463	3.233844971	-4.189012455
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H	7.121857008	3.905259539	-3.533378305
H	7.404195388	2.296625354	-2.865976929
C	7.291071379	2.337238372	-5.024255982
H	7.064983348	1.265014837	-5.130927880
H	6.764062852	2.873793997	-5.828701038
H	8.371551896	2.472943151	-5.176808078
C	2.167382858	3.362061982	-2.802192503
H	1.690099344	4.232164551	-2.320781734
H	3.008953481	3.719869570	-3.399245862
H	1.434449946	2.927915978	-3.498247054

TS3*_methyl,oblique_

165
Co2C124H32O7

Co	3.914609821	-2.195032852	1.039065872
Co	6.078924600	-1.498264737	-0.108204021
C	5.893343310	-2.813294152	1.131517182
C	1.656798663	-3.904531166	0.016745404
C	5.302151124	-1.099723533	-1.652429265
C	6.640903457	-0.025601245	0.731103769
C	7.534795296	-2.194137511	-0.786394769
O	1.639095418	-5.018674395	0.402835393
O	6.256133010	-3.688694067	1.831652422
O	4.860228046	-0.866907299	-2.703588060
O	7.121528513	0.900364088	1.237188528
O	8.501578304	-2.649836935	-1.236863099
C	2.497421368	-2.815521259	-1.440596061
C	3.598487894	-3.140197306	-0.612873307
C	3.093462748	-3.216415750	2.192777923
O	2.658974063	-3.912180928	3.010640447
H	-4.901428694	-5.401180710	3.498775657
H	-3.434786448	-6.946685744	-0.267257300
H	-3.711359158	-6.554447353	2.117345069
H	-4.106114111	-6.356686513	-2.293479761
H	-5.698501292	-4.939936931	-3.459690011
H	-8.670017388	-2.229626044	-1.677637566
H	-7.314927312	-3.489971348	-3.249802722
H	-8.978144028	-1.890826280	0.474833881
H	-8.163326100	-2.544892279	2.667253480
H	-6.705253326	-3.796347174	3.710928855
C	-5.692211921	-3.431806309	3.551644238
C	-3.068517306	-5.893598754	1.539390291
C	-4.671252128	-4.339982028	3.428562465
C	-3.368620162	-3.918380875	3.039569763
C	-2.911190862	-6.115757082	0.202165669
C	-2.205837503	-5.163408250	-0.600718860
C	-2.556700248	-4.691233681	2.131086483
C	-3.854513253	-5.314011744	-2.478487627
C	-2.683374388	-4.748491311	-1.886737465
C	-6.934957795	-2.547861022	-2.859102272
C	-4.750591480	-4.515727425	-3.133882403
C	-4.523809217	-3.110385096	-3.242422700
C	-7.699113984	-1.837323001	-1.974774349
C	-7.156339600	-0.695061331	-1.309585684
C	-5.586909869	-2.154861304	-3.122263345
C	-8.116960105	-1.375476460	0.896174108
C	-7.363217019	-0.467080878	0.091578474
C	-7.656994906	-1.744496433	2.130811317
C	-6.424179921	-1.221007392	2.624458131
C	-5.464597098	-2.049301843	3.301771878
C	-4.120413331	-1.602248182	3.358229067
C	-1.489006464	-4.058250776	1.470066637
C	-3.061502102	-2.548403889	3.204019562
C	-1.766069660	-2.063074126	2.850325265
C	-1.292520559	-4.322048760	0.071232076
C	-0.535608303	-3.380541137	-0.672731111
C	-0.958357165	-2.820087653	1.969251374
C	-2.256782056	-3.489577278	-2.372991826
C	-1.053688802	-2.902035960	-1.860491390
C	-5.248839399	-0.808086649	-2.843980001
C	-3.192746102	-2.660396388	-3.059881241
C	-2.886147512	-1.278337624	-3.203328969
C	-6.052471951	-0.059271073	-1.928506832
C	-5.492470544	1.115148365	-1.344336269
C	-3.930697274	-0.339451748	-3.114658634
C	-6.455658997	0.384816488	0.768368224
C	-5.700898087	1.345165912	0.031300104
C	-5.975517706	-0.002992724	2.057836688
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C	-3.830259497	-0.218500890	3.189030024
C	-2.485443269	0.236532740	3.291254774
C	0.152516317	-2.202803585	1.350933315
C	-1.437973987	-0.704350133	3.089964909
C	-0.148448421	-0.231169501	2.745863118
C	0.645481595	-2.737836546	0.030530740
C	1.466718386	-1.772324077	-0.893224792
C	0.639658961	-0.986899753	1.828350478
C	-0.592616430	-1.637169491	-2.381808867
C	0.631651339	-1.096878648	-1.975070385
C	-3.606101114	1.032334900	-2.889702273
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C	-1.242473384	0.537565151	-3.268799760
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C	-4.818692352	2.234855660	0.716904796
C	-4.073870302	3.191812579	-0.023030375
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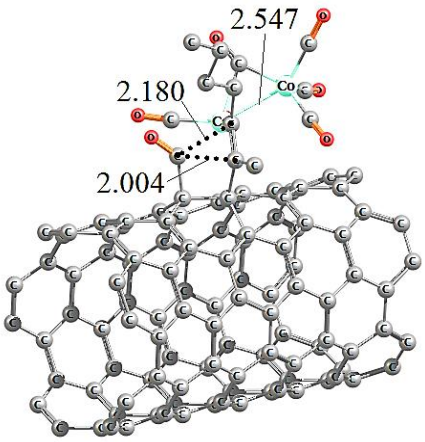
C	-3.154311270	2.447454432	2.491444251



Note: Discarded in the main manuscript.

C	-2.202081110	1.614547761	3.144590974
C	-0.850611522	2.055757212	3.220276468
C	1.760991834	-0.328412403	1.194940844
C	0.183831672	1.121578731	3.015658150
C	1.492057678	1.600805087	2.698713467
C	2.167364060	-0.687466653	-0.096934162
C	2.827815342	0.343598922	-0.852565144
C	2.272970587	0.882854737	1.778504935
C	1.042569604	0.141898768	-2.494343646
C	2.298914359	0.728912716	-2.098224604
C	-1.962123946	2.846502856	-2.945026121
C	0.097248048	0.974431765	-3.148990234
C	0.399467840	2.353563498	-3.357770669
C	-2.757635038	3.595421841	-2.045225527
C	-2.189407616	4.766835486	-1.459670393
C	-0.640038493	3.299050337	-3.238385709
C	-3.173332113	4.058547594	0.659707144
C	-2.405553963	5.006003137	-0.086231502
C	-2.707631379	3.679848313	1.940484260
C	-1.498163559	4.269300662	2.425719861
C	-0.557097209	3.445347834	3.077323450
C	0.788431568	3.895079719	3.186861190
C	3.397805165	1.531734029	1.194261934
C	1.842059206	2.946050696	3.002332811
C	3.665367766	1.270629961	-0.180980155
C	2.720420488	1.960602976	-2.665406751
C	-0.299172468	4.662466598	-3.018335299
C	1.750049220	2.798353727	-3.308962522
C	-1.093821699	5.415591793	-2.099090036
C	-1.516808296	5.888806821	0.592289362
C	-1.051157577	5.509722666	1.889875936
C	0.995677484	5.125182303	-3.362523329
C	1.263444697	6.512991848	-3.142467732
H	2.148589805	6.972255666	-3.578148029
C	-0.554381081	6.600431692	-1.537092067
C	0.510614729	7.229956263	-2.255335632
H	0.813483634	8.243548186	-1.999297392
C	3.936354747	2.556926522	-2.228601982
C	4.347234801	3.761101916	-2.889620311
H	5.369813838	4.117665751	-2.777678699
C	2.044097912	4.166038201	-3.529047698
C	3.427892188	4.543391303	-3.523270344
H	3.729251856	5.511552978	-3.918732627
C	3.954610450	2.686557191	1.797867015
C	5.079667030	3.284382146	1.141387830
H	5.694142176	4.011161887	1.668878284
C	4.407578625	2.219871585	-0.928068270
C	5.293379657	3.067913071	-0.187566623
H	6.068406250	3.631330884	-0.704244022
C	1.076344174	5.278829356	3.071422511
C	2.440184846	5.673745391	3.252589657
H	2.686295317	6.724058008	3.397702452
C	3.154502712	3.413506208	2.729593040
C	3.448116009	4.767675720	3.089407353
H	4.480599550	5.110741329	3.109771856
C	-0.777682352	6.847602597	-0.146150584
C	0.054698713	7.738353876	0.604701870
H	0.449120760	8.638783109	0.137145288
C	0.129793964	6.110471726	2.398125471
C	0.496017393	7.380009253	1.846040111
H	1.235013444	8.000749133	2.349295365
C	4.422494256	-1.064460184	2.314488007
O	4.744157158	-0.386246222	3.193974015
C	4.486363652	-4.266157997	-1.106792664
H	5.325001981	-4.408767897	-0.419245244
H	4.936254115	-3.900474276	-2.048668396
C	3.869990602	-5.649727152	-1.365490039
H	3.654486187	-6.136014129	-0.403326683
H	2.909004960	-5.582021790	-1.898273330
C	4.838502730	-6.512062291	-2.169308176
H	5.028724507	-6.031144977	-3.145394532
H	5.810801778	-6.545611032	-1.648196867
C	4.316141270	-7.928863292	-2.383275536
H	3.354690064	-7.915632315	-2.920139164
H	5.023985943	-8.532662119	-2.969512933
H	4.154180297	-8.435265899	-1.419288714
C	2.391424902	-3.150214471	-2.895221924
H	3.130287300	-3.893980633	-3.207536545
H	1.385381241	-3.503374653	-3.168699837
H	2.579046360	-2.224386736	-3.467784936

TS3*_methyl,oblique_

165
Co2C124H32O7

Co	-4.080362394	-1.865082930	-1.059303874
Co	-6.271235496	-1.484317839	0.302342259
C	-6.340937878	-2.546612686	-1.125115395
C	-1.617108712	-3.901661155	-0.632830011
C	-5.192694933	-1.270160048	1.691952105
C	-6.956748776	0.105144430	-0.143477144
C	-7.543493560	-2.311177427	1.186039047
O	-1.682164874	-4.876104952	-1.277544237
O	-6.639260132	-3.277184478	-1.988985493
O	-4.579575028	-1.160971203	2.674027929
O	-7.495149721	1.104050029	-0.376609981
O	-8.381469331	-2.855603062	1.773007748
C	-2.512471645	-2.934726158	1.038280185
C	-3.640727131	-3.176628839	0.252840219
C	-3.357578666	-2.651325127	-2.430891292
O	-2.954532093	-3.171607175	-3.384456907
H	5.204808550	-5.296856125	-3.492139453
H	3.395497951	-7.034639950	0.023366489
H	3.884042849	-6.508511907	-2.301146513
H	3.882604981	-6.559880512	2.138841597
H	5.383328131	-5.226339306	3.506859493
H	8.545218610	-2.471876049	2.176272905
H	7.028633194	-3.797889035	3.532824303
H	9.053667110	-2.024408550	0.078505429
H	8.420183414	-2.552961391	-2.206251954
H	7.041694809	-3.716686284	-3.446101838
C	6.023522486	-3.343804285	-3.352419675
C	3.196426582	-5.875265955	-1.744200042
C	4.983472382	-4.237871136	-3.375026584
C	3.656141897	-3.817130810	-3.078734431
C	2.919766527	-6.173065912	-0.441950226
C	2.149885247	-5.259970396	0.348499365
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C	2.521329001	-4.911200909	1.687331945
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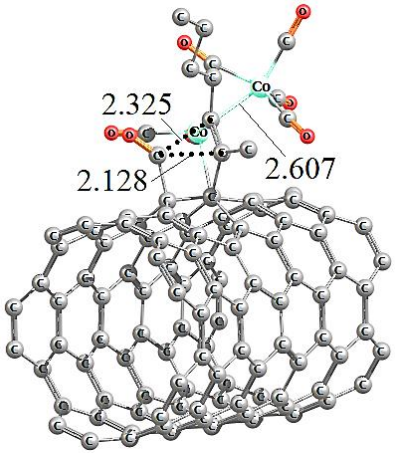
C	4.256118807	-3.369055926	3.279414939
C	7.554541086	-2.080983977	2.401469657
C	7.092397627	-0.892239203	1.756332195
C	5.336660239	-2.427668587	3.316535887
C	8.239291301	-1.472893174	-0.387763290
C	7.430799041	-0.592133519	0.395643797
C	7.881367032	-1.771169313	-1.673909870
C	6.703291537	-1.199480357	-2.243302923
C	5.793142989	-1.973784257	-3.040539979
C	4.464674590	-1.499694589	-3.185159277
C	1.629371137	-4.025854836	-1.709357408
C	3.382509381	-2.432994863	-3.179678627
C	2.068730219	-1.945961592	-2.911050157
C	1.299383797	-4.378414547	-0.355005569
C	0.482090604	-3.476001855	0.374169601
C	1.167081785	-2.742382778	-2.164220336
C	2.071616204	-3.666273987	2.192719940
C	0.922611367	-3.039563933	1.611162921
C	5.043663823	-1.060524847	3.089273182
C	2.953569749	-2.886821478	2.998776446
C	2.652033995	-1.509930350	3.188253354
C	5.942909212	-0.272404245	2.305291944
C	5.457264144	0.944540230	1.742279338
C	3.711155842	-0.585360986	3.257440596
C	6.600673433	0.312710751	-0.311494527
C	5.797237556	1.247668152	0.407397056
C	6.228074068	-0.000923564	-1.655748647
C	5.082812280	0.648634418	-2.200302238
C	4.182281923	-0.121617365	-2.967421600
C	2.857803391	0.362351169	-3.153819557
C	0.015877684	-2.140544741	-1.608336616
C	1.784728760	-0.566546564	-3.086366878
C	0.479032099	-0.086133457	-2.826921986
C	-0.612300760	-2.758489217	-0.392988299
C	-1.510630119	-1.854378801	0.521295004
C	-0.407898387	-0.874953231	-2.031183244
C	0.442240555	-1.785546175	2.137587968
C	-0.733532619	-1.203050241	1.649789152
C	3.425919697	0.802719036	3.085313026
C	1.332434962	-1.029722035	2.938970096
C	1.030993589	0.327317139	3.193434755
C	4.319852401	1.588351591	2.318259692
C	3.847140181	2.809150172	1.764285179
C	2.100305108	1.265709826	3.277675873
C	4.993455608	2.190177477	-0.304066530
C	4.196932347	3.120734357	0.417855195
C	4.628768547	1.880082939	-1.639834866
C	3.493026530	2.523187265	-2.200571118



Note: Discarded in the main manuscript.

C	2.585272247	1.738539202	-2.966918761
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C	-1.577159150	-0.254221807	-1.486132897
C	0.191879172	1.281195602	-3.055204044
C	-1.129017826	1.760675447	-2.829880666
C	-2.222447707	-0.774902078	-0.317025890
C	-2.871565750	0.274754932	0.459089477
C	-2.005627944	0.991130910	-2.035767837
C	-1.181087649	0.007604715	2.195972599
C	-2.405942868	0.617226180	1.742365033
C	1.803544972	2.637720963	3.089527731
C	-0.286653250	0.790848034	2.973219119
C	-0.593018914	2.158033570	3.235476688
C	2.694680288	3.427578426	2.324024754
C	2.199368369	4.641495714	1.759719950
C	0.462891419	3.091919365	3.276093481
C	3.375589353	4.040748568	-0.293839297
C	2.551698738	4.957737999	0.430429470
C	3.019594137	3.736587567	-1.629961658
C	1.864667919	4.369665619	-2.185439966
C	0.968211600	3.590929721	-2.948084094
C	-0.359308980	4.064729993	-3.142101823
C	-3.178456858	1.634226762	-1.538639637
C	-1.434867736	3.124589782	-3.092514091
C	-3.603206218	1.283216603	-0.227188269
C	-2.854077775	1.829742549	2.337278092
C	0.157979064	4.470807035	3.109161290
C	-1.930067312	2.622572753	3.094247431
C	1.050292655	5.266850739	2.325720234
C	1.739768444	5.891897450	-0.276119206
C	1.387601454	5.589151887	-1.628469036
C	-1.160432547	4.931310345	3.353835896
C	-1.392168969	6.333405277	3.193094770
H	-2.313549098	6.778833795	3.562896882
C	0.581547208	6.492268065	1.788455492
C	-0.546510156	7.091526867	2.432427729
H	-0.814429379	8.122401954	2.208528476
C	-4.034239013	2.460954336	1.852514703
C	-4.482855065	3.634693897	2.541571382
H	-5.491059378	4.008857326	2.370916359
C	-2.229662251	3.979914960	3.368841490
C	-3.604864280	4.374747101	3.277651040
H	-3.926189051	5.326182483	3.697120631
C	-3.658871023	2.829097931	-2.124918365
C	-4.849265255	3.393867986	-1.559403462
H	-5.399832997	4.160098889	-2.101664069
C	-4.397299309	2.202991263	0.500343086
C	-5.198944761	3.103703921	-0.273272408
H	-6.020371159	3.641522895	0.196028044
C	-0.638791483	5.446929758	-2.989706626
C	-1.976519063	5.871649383	-3.265071021
H	-2.198047853	6.931735671	-3.373342770
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C	-3.005948052	4.973711174	-3.234874732
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C	0.197210533	7.764995514	-0.329212048
H	-0.225725313	8.646666402	0.149029260
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H	-5.327715572	-4.444529054	-0.134847258
H	-4.976111490	-4.147755139	1.554596467
C	-3.833139340	-5.752419568	0.663889454
H	-3.580133087	-6.097001256	-0.349232036
H	-2.886139716	-5.711693978	1.224674947
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H	-5.000468254	-6.420500432	2.349876408
H	-5.729425326	-6.772151819	0.780445192
C	-4.178283078	-8.165081261	1.364800175
H	-3.228336850	-8.174990797	1.921782945
H	-4.863792225	-8.874298386	1.850854044
H	-3.973747886	-8.532809216	0.347493274
C	-2.328572798	-3.456998604	2.430088098
H	-3.151379691	-4.116695046	2.723323717
H	-1.375506640	-3.989434922	2.567609526
H	-2.323135824	-2.596575437	3.120441067

TS3*butyl,oblique

165
Co2C124H32O7

Co	-5.120442314	0.825635034	0.828928089
Co	-5.521596501	3.073980011	-1.512539139
C	-6.370441627	2.150044691	0.015758828
C	-3.660830360	1.571737577	-0.054595839
C	-4.748365685	3.924070631	-2.888035074
C	-6.549510723	2.057177355	-2.536376494
C	-6.118503994	4.567495246	-0.798357562
O	-3.674862131	2.288623518	-1.085882260
O	-7.463527622	2.238665253	0.468453194
O	-4.272018443	4.479457250	-3.776394421
O	-7.311022051	1.506469672	-3.210595241
O	-6.602570612	5.532404143	-0.376437215
C	-2.543095836	2.454718898	1.902061684
C	-3.858911099	2.335946843	1.582185325
C	-5.998057039	0.321042472	2.350945158
O	-6.467430479	-0.097142525	3.316688276
H	-4.306495768	-5.318523999	-2.969566502
H	-5.810941013	-4.088682332	0.884413239
H	-5.550450324	-4.307923862	-1.528291923
H	-4.934485443	-4.633144641	2.873020714
H	-3.140412603	-5.982655764	3.812057265
H	-0.132628027	-8.440012957	1.687041055
H	-1.482010518	-7.322379251	3.365118107
H	0.135866721	-8.716471931	-0.480821485
H	-0.833836538	-8.028403235	-2.601575088
H	-2.444548558	-6.800196310	-3.425378970
C	-2.249605022	-5.739223876	-3.281322512
C	-4.956608452	-3.571920610	-0.990158091
C	-3.303182057	-4.900589519	-3.019314448
C	-3.077162672	-3.546665282	-2.643739471
C	-5.112319298	-3.440339836	0.357957118
C	-4.247337829	-2.568037034	1.093030977
C	-3.891063184	-2.879270674	-1.657653125
C	-3.931703374	-4.215676700	2.942511549
C	-3.640397241	-2.960056864	2.323968316
C	-0.648122752	-6.787233503	2.914896141
C	-2.922593334	-4.973861680	3.466220639
C	-1.571951782	-4.512647468	3.418178608
C	0.114001578	-7.418394914	1.970196165
C	1.097779371	-6.691290827	1.231659399
C	-0.467992909	-5.394355829	3.174201459
C	0.444988155	-7.772474304	-0.926021179
C	1.259242888	-6.863293864	-0.182927542
C	-0.100877109	-7.384740091	-2.118536386
C	0.143008815	-6.071743964	-2.625026807
C	-0.909056907	-5.269350770	-3.185432902
C	-0.715673023	-3.866545405	-3.244824400
C	-3.390881096	-1.721754860	-1.039920996
C	-1.810371830	-2.998811854	-2.949462552
C	-1.522717899	-1.644575265	-2.608849816
C	-3.642177215	-1.511002025	0.364750347
C	-2.825196716	-0.555009313	1.043985189
C	-2.298937878	-0.999144788	-1.620433549
C	-2.424367797	-2.323548752	2.679981439
C	-2.119616077	-1.026251652	2.154305843
C	0.775442312	-4.831048971	2.793438104
C	-1.375573585	-3.120768672	3.233806092
C	-0.056070831	-2.590343714	3.254627162
C	1.577507755	-5.492449631	1.812705591
C	2.590396482	-4.738531810	1.148060033
C	1.036313413	-3.456955033	3.056064582
C	1.880502049	-5.819443209	-0.913064847
C	2.745643329	-4.903986911	-0.243935884
C	1.307249019	-5.414159397	-2.158515334
C	1.638838347	-4.119433329	-2.657288997
C	0.604845381	-3.331927427	-3.206511589
C	0.799882376	-1.924982529	-3.313170327
C	-1.823381063	0.201984614	-1.047434458
C	-0.287044558	-1.066959661	-2.991629109
C	-0.029196334	0.287586117	-2.671867918
C	-2.395579953	0.667144335	0.256154820
C	-1.509690720	1.610557229	1.131556559
C	-0.822380828	0.925802271	-1.672959251
C	-0.886618025	-0.387370084	2.550734256
C	-0.584272542	0.903398012	2.114072994
C	2.310014030	-2.901933021	2.728543356
C	0.142217355	-1.188171480	3.112209070
C	1.454628411	-0.665125098	3.205143641
C	3.106424476	-3.555361276	1.756135233
C	4.121772670	-2.811269269	1.095524710
C	2.565049096	-1.539057783	3.017394849
C	3.404341190	-3.874991004	-0.985115955
C	4.272211137	-2.974054052	-0.312899568
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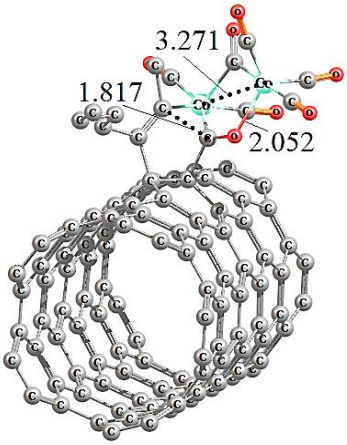
C	3.156923892	-2.187126661	-2.733361873



Note: Taken into consideration in the main manuscript.

C	2.110196666	-1.395570164	-3.286943833
C	2.288662317	0.015889885	-3.364404719
C	-0.345370186	2.162406233	-1.089073295
C	1.205904062	0.864193886	-3.058144664
C	1.457853190	2.243006195	-2.769845428
C	-0.605198807	2.458658382	0.240331607
C	0.342239624	3.310728551	0.890926835
C	0.679332184	2.894936222	-1.793123890
C	0.617797223	1.514230873	2.509409389
C	0.947938499	2.851324047	2.079828967
C	3.819333033	-0.972792476	2.673286203
C	1.651229162	0.728906778	3.075867478
C	2.970311454	1.265524935	3.172244688
C	4.613036664	-1.619445581	1.695644278
C	5.613266957	-0.851111630	1.024526950
C	4.066326136	0.405153647	2.957039327
C	4.900454579	-1.927507915	-1.047620229
C	5.759454142	-1.008097031	-0.370028594
C	4.330715027	-1.527009954	-2.278602204
C	4.643976111	-0.224608304	-2.781513767
C	3.608074030	0.556754001	-3.334616473
C	3.794330836	1.961809162	-3.455805985
C	1.168082203	4.117782276	-1.255335733
C	2.687992058	2.827360343	-3.181826705
C	1.023599283	4.311649972	0.151967873
C	2.132301130	3.480125269	2.532042479
C	5.327186054	0.979058376	2.630325606
C	3.172587780	2.672917265	3.100972537
C	6.120481957	0.334366024	1.630686957
C	6.403111804	0.031528185	-1.102346368
C	5.825803078	0.436146883	-2.346263680
C	5.589189735	2.333228999	2.958708137
C	6.886739240	2.837399853	2.629414083
H	7.224885109	3.784178337	3.046027896
C	7.136678543	1.078145762	0.978173264
C	7.639170232	2.227586796	1.665559291
H	8.559619759	2.701720918	1.329856151
C	2.462864922	4.783530991	2.061240341
C	3.633399775	5.397316310	2.614526847
H	3.804330427	6.463478623	2.474570063
C	4.480350550	3.201835479	3.210998727
C	4.611520210	4.630320343	3.176862069
H	5.544555094	5.097099761	3.486788702
C	2.152721782	4.868667533	-1.950388933
C	2.596893991	6.083682697	-1.327720849
H	3.152322904	6.819319289	-1.906694144
C	1.904043656	5.201405451	0.820448563
C	2.484696552	6.242709158	0.022966593
H	2.955828967	7.099265224	0.502292979
C	5.108534666	2.494565952	-3.454961738
C	5.234073681	3.906560991	-3.655614962
H	6.206255800	4.336825128	-3.889239133
C	2.932539868	4.205984070	-2.941778167
C	4.178030538	4.735677185	-3.411503323
H	4.325881119	5.812897515	-3.456984726
C	7.282558507	0.921324508	-0.435790887
C	7.931722105	1.911819571	-1.241010831
H	8.786357338	2.458807365	-0.846984322
C	6.153512806	1.711734290	-2.875763232
C	7.381838234	2.297048342	-2.429985519
H	7.807931508	3.143943916	-2.964733432
C	-5.872403879	-0.224835190	-0.374875179
O	-6.444100215	-0.868975301	-1.147939504
C	-2.039294043	3.500045120	2.859014112
H	-1.056725274	3.202696442	3.247144260
H	-2.694776028	3.529122837	3.744328814
C	-1.934834432	4.908483458	2.240161570
H	-1.629070673	4.827965135	1.183671738
H	-2.927978009	5.385901704	2.225910065
C	-0.948292512	5.799001988	2.989128943
H	-1.301480714	5.949387168	4.024851182
H	0.019921311	5.278016500	3.072886573
C	-0.742828712	7.143878582	2.301021276
H	-1.687971771	7.705185751	2.232657200
H	-0.017696275	7.764991175	2.847518255
H	-0.364692181	6.999392228	1.276296352
C	-4.808960030	3.402260342	2.090826720
H	-4.463984342	3.780134036	3.062768695
H	-4.813145831	4.250033422	1.391401596
H	-5.840786580	3.065704178	2.217439230

TS3*_butyl,oblique_

165
Co2C124H32O7

Co	3.549368559	-2.858705275	1.146734252
Co	5.773061931	-2.582709249	-0.054841321
C	5.359217154	-3.853425721	1.180743534
C	1.084194036	-4.173095255	0.065210976
C	5.070867815	-2.097287627	-1.612794395
C	6.557551936	-1.203987301	0.767451335
C	7.122391765	-3.494217266	-0.694834760
O	0.903444264	-5.299515768	0.377664463
O	5.568299091	-4.793442955	1.859417711
O	4.666706173	-1.819607971	-2.667794642
O	7.175942362	-0.358017355	1.263846308
O	8.021086279	-4.090767919	-1.121295633
C	2.070193783	-3.261489632	-1.365003327
C	3.063180023	-3.754713495	-0.486931380
C	2.561955146	-3.717928785	2.302327454
O	2.001917481	-4.331364038	3.109537618
H	-5.563121326	-4.516499760	3.740144876
H	-4.461101639	-6.333654950	-0.041424700
H	-4.623681207	-5.863079406	2.337948112
H	-5.048999118	-5.688453322	-2.084255187
H	-6.414246143	-4.044821813	-3.241952964
H	-8.854337418	-0.859934645	-1.401118177
H	-7.768266319	-2.345214936	-2.984215474
H	-9.061904103	-0.424395706	0.744301387
H	-8.320989667	-1.163313448	2.936391665
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C	-3.888449412	-5.329427705	1.738992278
C	-5.160284657	-3.509872784	3.648173810
C	-3.816021091	-3.317418572	3.221513022
C	-3.795494626	-5.596015458	0.403290974
C	-2.956961569	-4.787712356	-0.429399984
C	-3.168978664	-4.224518035	2.304073326
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C	-8.116643842	-0.054678325	1.137311988
C	-7.238889227	0.698308281	0.298573238
C	-7.698734845	-0.471429418	2.371728030
C	-6.384583639	-0.153899974	2.830247502
C	-5.561364284	-1.120313819	3.504139654
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C	-6.187961910	1.399313732	0.939989757
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C	1.215866997	-2.050485442	-0.850846348
C	0.598776787	-1.118193372	1.881981421
C	-0.820160432	-1.607590093	-2.309029466
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C	-3.360172614	1.513302373	-2.795565407
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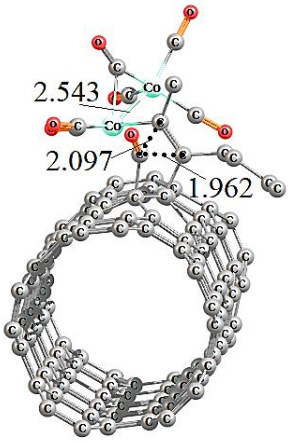

Note: Discarded in the main manuscript.

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C	1.894363364	1.303617861	2.689800370
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C	2.523996634	0.453263704	1.767093472
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C	0.275116154	0.842016834	-3.138541398
C	0.795758123	2.149813685	-3.375133440
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C	-1.311180265	4.980317889	-1.459321335
C	-0.070774537	3.255415272	-3.249303986
C	-2.345107894	4.472942910	0.693453787
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C	-1.918410793	4.041525581	1.970903175
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C	3.723996839	0.898703169	1.144797813
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C	3.905107709	0.586218985	-0.234383910
C	3.033509101	1.390438148	-2.715302786
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C	1.734580307	6.955833918	-2.359370358
H	2.204826944	7.910064317	-2.129152068
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H	5.998033713	3.081335460	-2.905931241
C	2.712454264	3.663633630	-3.607725823
C	4.139372712	3.808063434	-3.629672282
H	4.588457234	4.707979454	-4.045634699
C	4.479818847	1.952784055	1.716650226
C	5.671265357	2.347606829	1.024353048
H	6.411514178	2.967301612	1.526451111
C	4.777901191	1.388065370	-1.012620535
C	5.812265354	2.083064272	-0.305445558
H	6.657215835	2.503078709	-0.848323267
C	2.103303540	5.005769891	2.994847871
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H	2.696277400	7.650677845	2.216052524
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H	-1.787084059	-5.283336714	-3.951338835
H	-1.548478012	-5.021394460	-5.693995452
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H	3.894555996	-5.672898340	0.048840396
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TS3*methyl,perpendicular*

165
Co2C124H32O7

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Co	5.283842988	3.374578880	1.312959202
C	6.292611486	-0.675194765	-0.790673695
C	3.544031333	1.467207524	0.172511158
C	4.355166611	4.753563617	1.981834582
C	5.824848443	2.774567203	2.892606337
C	6.312282037	1.870801379	0.528828614
O	3.475589005	2.604259652	0.677775197
O	6.930916840	-1.475138810	-1.322241031
O	3.786796864	5.653888967	2.418308703
O	6.288786756	2.491401918	3.913350418
O	7.480181023	1.740159014	0.371039011
C	3.165594075	1.014756625	-2.271654697
C	4.308687535	1.322367436	-1.623248497
C	5.217654627	-0.118201891	1.737255139
O	5.279581014	-0.464433893	2.837525158
H	4.602569200	-4.783184260	2.630127909
H	5.072684773	-4.656693209	-1.722666598
H	5.448529322	-4.303079301	0.659205591
H	3.681241933	-5.644155891	-3.127056327
H	1.686678801	-7.009893319	-3.354092984
H	-0.826128595	-8.603032699	-0.129296967
H	0.074580027	-8.069583257	-2.323053041
H	-0.473188954	-8.285375885	2.023457763
H	1.026583385	-7.204292575	3.600723633
H	2.822539647	-5.962354971	3.788466329
C	2.638759113	-4.955911026	3.416944996
C	4.757854130	-3.655063006	0.122462487
C	3.639832255	-4.293880174	2.763730151
C	3.376983392	-3.047430681	2.112089933
C	4.543640863	-3.855856570	-1.208916382
C	3.502467846	-3.133474455	-1.880417218
C	3.941558237	-2.722423908	0.841485046
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C	-0.584098290	-7.356549260	-1.830662671
C	1.581420630	-5.932458160	-3.241622494
C	0.285741608	-5.358295979	-3.062279107
C	-1.091317827	-7.657139694	-0.598141794
C	-1.809635584	-6.667268111	0.144146854
C	-0.768430693	-6.051057007	-2.385269276
C	-0.628386638	-7.237182801	2.272485843
C	-1.584898881	-6.463115654	1.542793312
C	0.215622672	-6.628802857	3.158135257
C	0.146714782	-5.214873872	3.362164542
C	1.321192820	-4.405418906	3.474833923
C	1.198230952	-3.012179174	3.239193546
C	3.361677255	-1.660533090	0.091344809
C	2.231132906	-2.330274556	2.530600718
C	1.938802980	-1.053633888	1.954830882
C	3.116440506	-1.897500398	-1.317496605
C	2.112764453	-1.117081328	-1.933628316
C	2.529871141	-0.702414185	0.746847502
C	1.355519651	-3.148328141	-3.036666516
C	1.199394100	-1.751058665	-2.768227006
C	-1.856667790	-5.292816937	-1.885856916
C	0.185342927	-3.949044537	-3.189006351
C	-1.084426679	-3.316471247	-3.077719498
C	-2.391387191	-5.608837984	-0.597717585
C	-3.161471313	-4.615046080	0.073189442
C	-2.125567855	-4.001557260	-2.424197087
C	-1.961458488	-5.216956367	2.103728704
C	-2.943054945	-4.415481748	1.451618613
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C	0.829498070	-0.295275286	2.459054780
C	0.551735782	0.988558336	1.909443646
C	1.994358687	0.327353198	-1.542677309
C	0.719921583	0.974433224	-2.024383344
C	1.121268034	1.362097698	0.677874132
C	-0.038405492	-1.104760836	-3.095737039
C	-0.188599838	0.293833024	-2.860361284
C	-3.250791095	-3.256463476	-1.952090695
C	-1.190072818	-1.899770311	-3.249222208
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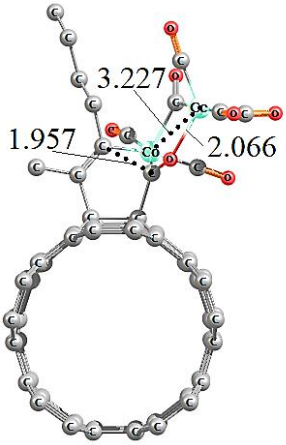

Note: Taken into consideration in the main manuscript.

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C	0.329328062	2.199928948	-1.468189989
C	-0.713460212	2.950435192	-2.083668164
C	-0.297645627	3.343110844	0.617891033
C	-1.427165197	0.913783919	-3.199711951
C	-1.587735595	2.306008757	-2.985456213
C	-4.635523478	-1.235720538	-2.037957531
C	-2.586730173	0.108834319	-3.359867105
C	-3.867384984	0.729974407	-3.266840091
C	-5.162664524	-1.545629182	-0.754448688
C	-5.923887817	-0.546626326	-0.078885455
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C	-2.853893621	1.668602695	3.252194877
C	-2.973002689	3.078712984	3.082374028
C	-0.916033638	4.398297689	-0.118197974
C	-1.938016729	3.769060884	2.381113224
C	-1.130863778	4.195173370	-1.518564982
C	-2.820552239	2.945346035	-3.327229960
C	-6.017852777	0.806166216	-2.120574310
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C	-6.541296808	0.499745838	-0.825860475
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C	-5.248972947	1.514680858	2.825578428
C	-6.316061179	2.059377796	-2.707367087
C	-7.467309452	2.743235332	-2.215172385
H	-7.867913724	3.596784262	-2.758851212
C	-7.337563544	1.462953324	-0.159808647
C	-7.965066269	2.453229169	-0.973085762
H	-8.749045006	3.083150111	-0.556866774
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H	-6.282174634	4.630952209	-3.837969088
C	-1.671409503	5.381072988	0.558809911
C	-2.237143681	6.419480116	-0.238372250
H	-2.644494526	7.310804292	0.235109594
C	-2.091337366	4.985091379	-2.187956787
C	-2.441686875	6.226457267	-1.579032112
H	-3.007148046	6.968677807	-2.139277995
C	-4.235387194	3.703316054	3.245437910
C	-4.273957023	5.120224245	3.112555057
H	-5.161358587	5.671968439	3.416753635
C	-2.193905060	5.060191734	1.864955490
C	-3.278934984	5.781449718	2.439265829
H	-3.401136719	6.841820727	2.226400919
C	-7.120142595	1.663044413	1.246423981
C	-7.521307325	2.862175410	1.907470089
H	-8.421888677	3.384374475	1.589698202
C	-5.414352450	2.891896876	3.107661017
C	-6.690110982	3.460328361	2.816138472
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O	7.073961265	5.107170564	-0.202466618
C	5.259460798	2.318205715	-2.243345738
H	5.525421377	3.054536898	-1.471124084
H	4.721139572	2.902147454	-3.007831769
C	6.531584317	1.741443376	-2.857320734
H	7.136696680	1.253351415	-2.079946723
H	6.268878895	0.958479837	-3.590622227
C	7.377870781	2.825549493	-3.517567260
H	6.792135300	3.317459061	-4.313716673
H	7.603627860	3.604075101	-2.768781646
C	8.677192930	2.272821088	-4.094367634
H	9.287096211	1.809344514	-3.303656071
H	8.472914327	1.502928175	-4.854780467
H	9.277386477	3.064647565	-4.565548930
C	2.906376608	1.321461394	-3.717720899
H	2.357134987	0.487833579	-4.184473470
H	2.281399373	2.224201741	-3.831813080
H	3.837955144	1.460607043	-4.278140885

TS3*methyl,perpendicular*

165
Co2C124H32O7

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O	-5.276367829	-1.762484406	-3.197808027
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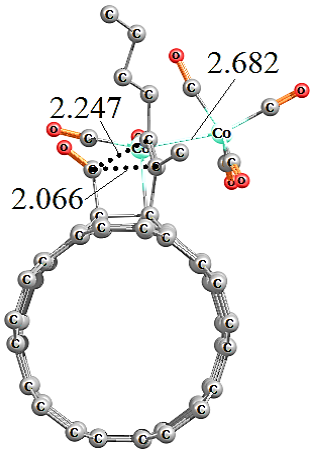

Note: Discarded in the main manuscript.

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TS3*butyl,perpendicular*

165
Co2C124H32O7

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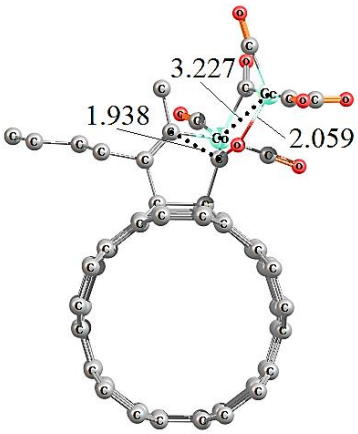

Note: Taken into consideration in the main manuscript.

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C	3.881559725	-0.214183346	-3.191368523
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H	7.288440079	-3.874342939	3.140314059
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O	-6.469194641	-5.933141356	-0.547033134
C	-2.950350043	-1.319708537	-3.810542363
H	-3.116210385	-2.339616839	-4.194210386
H	-1.913766843	-1.068178414	-4.079900409
C	-3.896670644	-0.327294419	-4.502992967
H	-4.943367881	-0.633046385	-4.333219340
H	-3.787284126	0.662828445	-4.027510355
C	-3.615191202	-0.195299594	-5.994754188
H	-2.555799248	0.082446399	-6.133740136
H	-3.750802547	-1.175098122	-6.485333423
C	-4.508251399	0.850617459	-6.654445518
H	-5.571781544	0.590060028	-6.538718466
H	-4.350849620	1.837612585	-6.192176120
H	-4.295123898	0.941377381	-7.729378451
C	-5.152690870	-2.704001230	-2.348288877
H	-5.097347147	-3.668231021	-1.821221444
H	-6.199559672	-2.374574395	-2.321199011
H	-4.866971040	-2.887690644	-3.392420553

TS3*butyl,perpendicular*

165
Co2C124H32O7

Co	5.206744754	-1.357704689	0.743541268
Co	5.516440565	-1.891836601	-1.811587854
C	5.790747506	-2.940557380	0.141374270
C	2.267229774	-1.824011560	3.131630742
C	3.985791268	-2.826114264	-1.914762146
C	5.147638644	-0.745496974	-3.113927545
C	6.464627440	-0.602015496	-0.848100431
O	2.290499061	-2.155603541	4.258316384
O	6.240753672	-4.013933436	0.315361831
O	2.997438188	-3.430058170	-1.928907127
O	4.964866212	-0.076886911	-4.039465976
O	7.323871150	0.205146489	-0.874985798
C	2.749882641	-2.763449267	1.334492809
C	3.999418201	-2.482130011	1.852767268
C	6.355976203	-0.885540475	1.987705347
O	7.118006541	-0.721116297	2.847340937
H	6.112528918	2.704325990	-1.563775101
H	5.712845482	3.005724143	2.795286070
H	6.446799032	2.234389530	0.579864602
H	4.422300337	4.516758331	3.716668745
H	2.899043705	6.387456596	3.451186827
H	1.553019312	8.221154068	-0.286046325
H	1.847686108	7.732921970	2.078477472
H	2.220755706	7.533406015	-2.274450101
H	3.622245283	5.891536750	-3.389557678
H	4.987978880	4.184896734	-3.145387797
C	4.451835702	3.329342280	-2.738984354
C	5.491144898	1.914671484	0.990542297
C	5.080743579	2.506467873	-1.846577041
C	4.352846099	1.474092230	-1.183774194
C	5.083358058	2.337286534	2.210791837
C	3.756280425	2.008290298	2.663588719
C	4.596128820	1.125827851	0.176906655
C	3.367470650	4.320409617	3.536475402
C	2.923049777	2.983641557	3.288530715
C	1.118130677	7.165357091	1.503713299
C	2.508994094	5.373247250	3.389003219
C	1.152760333	5.155792893	2.995341086
C	0.951629713	7.440373023	0.176165401
C	0.134028198	6.591574950	-0.635669724
C	0.475814550	6.026836146	2.085228667
C	1.818818025	6.543079540	-2.480470209
C	0.555494127	6.155968235	-1.931475410
C	2.607176422	5.618967291	-3.106641908
C	2.172598040	4.261834929	-3.223596812
C	3.061539009	3.160023397	-3.018401932
C	2.493778504	1.895586555	-2.711793271
C	3.645242206	0.305796032	0.864226015
C	3.134300710	1.050720763	-1.762627656
C	2.422989799	-0.054519661	-1.207792576
C	3.162559622	0.840026214	2.139520018
C	1.866881644	0.471436778	2.554505147
C	2.745321292	-0.506699943	0.084800202
C	1.527343165	2.752092014	3.318851669
C	1.029083734	1.429453793	3.126706445
C	-0.676977202	5.535420815	1.421567965
C	0.630252994	3.851559980	3.186786139
C	-0.727270852	3.577377661	2.866588126
C	-0.855325576	5.827408730	0.033568816
C	-1.737869832	4.999148572	-0.718285150
C	-1.395798660	4.436637338	1.973361753
C	-0.048767212	4.992278542	-2.471915380
C	-1.327437970	4.574584394	-1.999637204
C	0.776504829	4.026884507	-3.126613377
C	0.270157686	2.705460743	-3.280309808
C	1.144729484	1.623052470	-3.060724916
C	0.604190304	0.326867406	-2.810240347
C	1.886743576	-1.515256460	0.793760278
C	1.248455106	-0.518506615	-1.881272727
C	0.512134028	-1.613496940	-1.344018564
C	1.386065388	-0.907421694	2.246661114
C	-0.054952128	-1.149071528	2.544739811
C	0.727616392	-1.995786408	-0.005858953
C	-0.375525849	1.185303364	3.251365096
C	-0.872317060	-0.140275469	3.108419313
C	-2.580667470	3.968596569	1.327718205
C	-1.259808844	2.273148990	3.104474949
C	-2.631056513	2.024415339	2.813692479
C	-2.755598076	4.254776057	-0.046609914
C	-3.644793587	3.442539648	-0.803274376
C	-3.303966113	2.889175488	1.901059108
C	-1.953561510	3.425236793	-2.571135560
C	-3.233589079	3.017499451	-2.102639689
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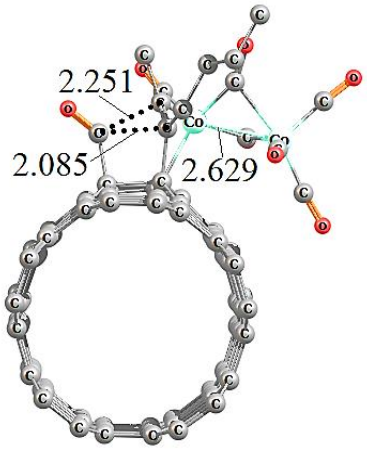

Note: Discarded in the main manuscript.

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C	-0.651000119	-2.071723521	-2.022192871
C	-1.391230838	-3.150394309	-1.475600521
C	-0.680458242	-2.279485548	1.988158429
C	-1.989840720	-2.639564244	2.419725027
C	-1.229783099	-3.445143171	-0.105323976
C	-2.277049363	-0.358778606	3.210571033
C	-2.791126818	-1.673499109	3.067175881
C	-4.470949873	2.411123123	1.252319239
C	-3.166942254	0.739916455	3.059694943
C	-4.532083245	0.477584165	2.742946674
C	-4.643793028	2.692740458	-0.131246454
C	-5.517640591	1.856499804	-0.884590524
C	-5.188719219	1.319926635	1.819511246
C	-3.845540775	1.867592432	-2.662809493
C	-5.113068308	1.438688692	-2.171017655
C	-3.028058818	0.916373741	-3.335036716
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C	-2.552227223	-3.641231017	-2.148983873
C	-2.640191823	-3.782767142	1.860665367
C	-4.196605860	-1.909751226	3.181398320
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C	-5.087259550	-0.806492252	3.010450777
C	-6.533200105	1.109749396	-0.217400785
C	-5.744358805	0.294354515	-2.741323175
C	-4.928556373	-0.653405805	-3.434318384
C	-7.114372688	-0.208393518	1.770330942
C	-8.300075593	-0.617430135	1.091914198
H	-9.020917846	-1.260750758	1.593005743
C	-7.433590902	0.318682342	-0.971343098
C	-8.454655050	-0.362114073	-0.245130976
H	-9.293582319	-0.809682372	-0.774880373
C	-4.698629541	-3.226981796	3.066173323
C	-6.100647580	-3.400341150	3.239087352
H	-6.515244581	-4.399550906	3.358391352
C	-6.454450214	-1.055557371	2.728103107
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C	-4.526484932	-3.067037825	-3.488541728
C	-4.996875636	-4.392851046	-3.272166647
H	-5.932664122	-4.718512657	-3.722443122
C	-3.263011001	-4.739611975	-1.611683759
C	-4.381987543	-5.208267397	-2.356544254
H	-4.845471534	-6.160080411	-2.104026929
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C	-7.622491887	-1.220648215	-2.937075150
H	-8.677026231	-1.442210695	-2.783446265
C	-5.427870251	-1.958289414	-3.659514872
C	-6.842931109	-2.124757192	-3.609164549
H	-7.296971282	-3.043453834	-3.975798595
C	6.843093209	-2.866893809	-2.493097007
O	7.674301195	-3.483699428	-3.005179846
C	2.184670352	-4.149697786	1.124329472
H	1.641256752	-4.108427328	0.167875540
H	1.407507685	-4.377039192	1.877918721
C	3.175148247	-5.309158941	1.015842220
H	4.046822752	-5.000684514	0.422097339
H	3.550837345	-5.615526972	2.002889723
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C	4.610982383	-3.359344568	2.900205270
H	5.439423854	-3.944959308	2.480367758
H	5.045825586	-2.714886641	3.681243711
H	3.893779050	-4.039124387	3.377276339
C	3.450852708	-7.695339183	0.214050329
H	4.347393423	-7.423166630	-0.363824008
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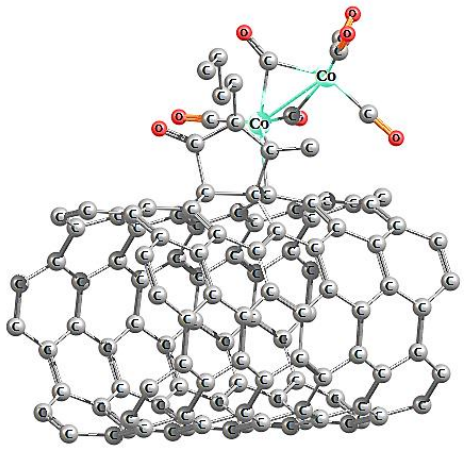
PD*_methyl,oblique_



165
Co2C124H32O7

Co	-3.986772455	1.896866098	0.948617486
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C	-5.608912112	3.047686590	0.932108536
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O	-1.672044198	4.551217233	1.758770607
O	-5.873820782	4.038665042	1.510003289
O	-5.795776610	-0.430446339	-2.191544831
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O	-6.918466647	3.726545411	-2.258732497
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H	4.809107072	5.395184668	3.581250458
H	2.861574846	7.095444796	0.118217284
H	3.406756969	6.547743869	2.425054726
H	3.362926700	6.700813662	-2.017344246
H	4.937003330	5.479627572	-3.410372581
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H	6.660007935	4.151153337	-3.411862723
H	8.810550738	2.407757400	-0.007254605
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H	6.731124602	3.920580794	3.534155952
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C	1.731649358	5.251796438	-0.240836264
C	2.398075063	4.601195414	2.394588961
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C	2.098210392	4.968819358	-1.596734597
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C	4.055518484	4.967121437	-3.029875090
C	3.918803748	3.556384248	-3.204410585
C	7.284983671	2.445311497	-2.315820664
C	6.894431315	1.218383846	-1.697126909
C	5.053249137	2.678164606	-3.238870443
C	8.031102362	1.802106124	0.451516566
C	7.262558378	0.901087203	-0.347131976
C	7.674150407	2.046218082	1.749564128
C	6.531125704	1.401596948	2.311400014
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C	1.711217745	3.715959344	-2.130646588
C	0.603062055	3.012130236	-1.554739460
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C	4.076824091	0.173549158	3.031704946
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C	2.041905000	-1.199284566	-3.275499071
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C	4.236822577	-2.978929404	-0.435903781
C	4.615913147	-1.768041012	1.651207982
C	3.519245576	-2.482958332	2.203297488

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C	-2.315331557	0.487727702	0.381171730
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C	-1.295021569	-0.162690823	-2.165008642
C	-2.472478780	-0.860622071	-1.703463681
C	1.827879564	-2.590420970	-3.110596825
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C	3.105167174	-3.703382806	1.603863604
C	1.986757916	-4.408221762	2.147801474
C	1.058627723	-3.700126631	2.941398675
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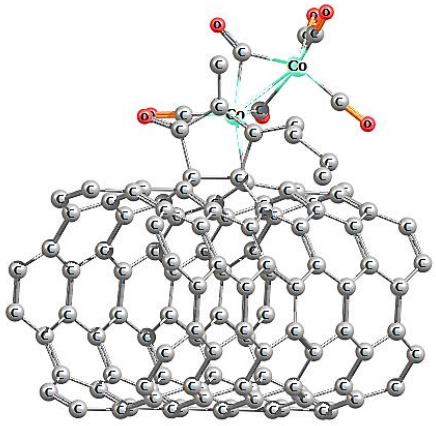
C	-4.363068558	-3.992020930	-2.521143470
H	-5.339897813	-4.435896878	-2.335824520
C	-2.115983827	-4.170827200	-3.409016619
C	-3.460275418	-4.654615051	-3.300451632
H	-3.730143812	-5.614990376	-3.735300347
C	-3.612948765	-3.164604655	2.174725029
C	-4.765173327	-3.791805794	1.595584630
H	-5.279590755	-4.587500675	2.130955178
C	-4.344078114	-2.583872406	-0.460599161
C	-5.113039324	-3.518884958	0.304400135
H	-5.893270973	-4.106174752	-0.177008614
C	-0.447679561	-5.638193478	2.943722590
C	-1.758096849	-6.138128082	3.216915502
H	-1.924141185	-7.211137063	3.294111130
C	-2.667141004	-3.903452413	2.951895309
C	-2.834640296	-5.295514834	3.229096885
H	-3.835009013	-5.714301761	3.316984661
C	1.203837587	-6.856277531	-0.531040672
C	0.504555938	-7.850633544	0.223970589
H	0.126784660	-8.743691383	-0.270635822
C	0.484769011	-6.353865869	2.128449847
C	0.155246946	-7.607089341	1.522001002
H	-0.494611649	-8.309946121	2.040027608
C	-5.136102663	0.574186087	1.359717525
O	-5.529975468	-0.312234747	2.016070040
C	-3.715001755	4.897997944	-0.369271729
H	-3.967149889	5.423911142	0.562681237
H	-4.650380333	4.706130700	-0.911366129
C	-2.781182749	5.765220441	-1.226857954
H	-1.844178797	5.944790972	-0.670415274
H	-2.503858720	5.212311156	-2.141821278
C	-3.413813298	7.099076430	-1.607000794
H	-4.356695314	6.912853670	-2.150102592
H	-3.683776996	7.644499992	-0.686587134
C	-2.481978203	7.951759766	-2.462519669
H	-2.221826467	7.430481345	-3.396954627
H	-2.945976324	8.912896916	-2.727570292
H	-1.544178544	8.161822033	-1.925211481
C	-3.399763525	2.412550006	-2.261884246
H	-4.246187860	3.084378390	-2.432852008
H	-2.582836461	2.700026594	-2.950642822
H	-3.693962880	1.388026335	-2.529044739

PD*$_{butyl,oblique}$



165
Co2C124H32O7

Co	-3.796818540	2.364040630	1.035078190
Co	-6.099461986	2.385738714	-0.118157117
C	-5.324406692	3.641827048	1.053695269
C	-1.527628186	3.988572719	0.980566817
C	-5.875243435	1.084475662	-1.324256239
C	-7.639992569	2.059032959	0.722506520
C	-6.447409875	3.651629359	-1.292760145
O	-1.208054046	4.813630343	1.812860544
O	-5.500842089	4.641325398	1.650934173
O	-5.740990902	0.299313223	-2.163291201
O	-8.681726476	1.868200927	1.183100371
O	-6.717929371	4.486116814	-2.051060716
C	-2.652634829	2.903650053	-0.792455972
C	-2.653030675	4.015450372	0.042880604
C	-3.248581555	2.656527994	2.695784920
O	-2.932180741	2.816074124	3.793877897
H	5.328798192	4.984995769	3.637023280
H	3.568811750	6.865515733	0.162583165
H	4.056984129	6.269091672	2.469995318
H	4.006621137	6.431889055	-1.976840126
H	5.439354412	5.062436423	-3.384822953
H	8.475687280	2.157252000	-2.052937464
H	7.020648925	3.566657957	-3.388755425
H	8.992340122	1.621225849	0.015656524
H	8.417135566	2.111360325	2.324440071
H	7.093368052	3.324724714	3.580203020
C	6.059474093	2.997007435	3.487311917
C	3.342846849	5.673384417	1.905059808
C	5.060382683	3.937509791	3.516394001
C	3.717871845	3.577426169	3.211270553
C	3.064925857	6.011780126	0.612475080
C	2.250575173	5.150301987	-0.190540340
C	2.849977002	4.439026953	2.445171538
C	3.707096881	5.411136563	-2.208417905
C	2.577996730	4.834042664	-1.549292154
C	6.650069380	2.604393772	-3.040449515
C	4.513295804	4.640325563	-2.998898286
C	4.233560283	3.251072891	-3.175087587
C	7.471666052	1.809249035	-2.289044331
C	6.960658418	0.629249366	-1.667235609
C	5.273770088	2.263037669	-3.211405433
C	8.158333565	1.095749056	0.477516475
C	7.299857812	0.277154586	-0.318292261
C	7.834450125	1.371937537	1.777879191
C	6.636080254	0.843277976	2.345275278
C	5.769175770	1.641184414	3.168228118
C	4.421894721	1.226115663	3.312249614
C	1.711036775	3.883631102	1.837879072
C	3.384154552	2.207003476	3.312163879
C	2.050943581	1.780587625	3.038399891
C	1.376330094	4.282051970	0.500069664
C	0.503267032	3.435981691	-0.230152452
C	1.194259033	2.616907275	2.282645605
C	2.062597050	3.627787522	-2.082114203
C	0.896154107	3.035971306	-1.497023996
C	4.921875067	0.907692426	-3.000344803
C	2.909503054	2.823156144	-2.903975682
C	2.552024650	1.461106556	-3.110911486
C	5.782862001	0.071817475	-2.222818946
C	5.247139133	-1.133966283	-1.681156661
C	3.571500824	0.492084800	-3.182829249
C	6.437524257	-0.606865109	0.375543828
C	5.583137266	-1.483555128	-0.356549558
C	6.097944389	-0.315517307	1.733140330
C	4.929381121	-0.924973551	2.276529983
C	4.074675980	-0.133908699	3.074644214
C	2.730251001	-0.559342377	3.263040070
C	0.022375661	2.069542711	1.715905133
C	1.700117674	0.420008335	3.221204966
C	0.371507249	0.008846262	2.964975802
C	-0.603307287	2.763484785	0.546011023
C	-1.540388822	1.904255350	-0.370234517
C	-0.473320250	0.845110495	2.173431495
C	0.363585717	1.810960234	-2.043282442
C	-0.826188278	1.266800767	-1.550277610
C	3.227836415	-0.884734206	-3.027555665
C	1.212948182	1.032861402	-2.867770817
C	0.855938874	-0.307283500	-3.140207202
C	4.084791217	-1.718692675	-2.267789059
C	3.561898255	-2.927594098	-1.734320157
C	1.885753939	-1.290063173	-3.232883355
C	4.744074736	-2.405105748	0.340822782
C	3.901359706	-3.280787704	-0.395427367
C	4.411467793	-2.118189563	1.691044903
C	3.251780781	-2.720657930	2.248067268

C	2.390576203	-1.915998112	3.047857246
C	1.038398798	-2.323154773	3.215457659
C	-1.677731643	0.288285677	1.627464956
C	0.019294464	-1.345430415	3.176135515
C	-1.324907238	-1.755832975	2.948362244
C	-2.263588457	0.823560392	0.441861765
C	-2.983115017	-0.174258977	-0.341773523
C	-2.173280038	-0.933486508	2.172952212
C	-1.324547380	0.079058734	-2.106902383
C	-2.565973779	-0.497791486	-1.645386847
C	1.532620531	-2.651634882	-3.062137681
C	-0.476927336	-0.722652339	-2.914020200
C	-0.840496102	-2.073081040	-3.197862652
C	2.386844343	-3.488701338	-2.304933935
C	1.841075831	-4.689610549	-1.759026601
C	0.175451803	-3.048690884	-3.258753470
C	3.044429984	-4.178573810	0.302679359
C	2.179438592	-5.043570648	-0.435716874
C	2.715240599	-3.892990418	1.649898974
C	1.534816388	-4.483227234	2.198965268
C	0.684919646	-3.685613396	2.995327646
C	-0.661296773	-4.101566433	3.191184543
C	-3.372569505	-1.512792768	1.658849322
C	-1.691557545	-3.110733244	3.178969500
C	-3.756965582	-1.151574063	0.335981453
C	-3.071026033	-1.681260216	-2.254817025
C	-0.185025119	-4.417350773	-3.113697581
C	-2.193072092	-2.488552679	-3.051039713
C	0.669984891	-5.259853486	-2.337044439
C	1.329569759	-5.955010318	0.255875630
C	0.996444835	-5.664213082	1.615306486
C	-1.519701899	-4.820658001	-3.365477090
C	-1.807540151	-6.214692179	-3.228446230
H	-2.744143708	-6.617221317	-3.609201922
C	0.150401484	-6.473316151	-1.819258799
C	-0.995833049	-7.018629760	-2.477705136
H	-1.304436579	-8.042024049	-2.272355315
C	-4.256851317	-2.284534542	-1.753940770
C	-4.765524702	-3.422550660	-2.457848341
H	-5.781578671	-3.765646748	-2.269490314
C	-2.550193303	-3.826758126	-3.350769203
C	-3.936312910	-4.172853494	-3.239157943
H	-4.302443598	-5.101212772	-3.673198382
C	-3.909787838	-2.687188703	2.234870883
C	-5.121871418	-3.194375686	1.660557268
H	-5.710769847	-3.935548024	2.197470996
C	-4.594079382	-2.028519534	-0.395589074
C	-5.448113870	-2.884413146	0.372110784
H	-6.285970903	-3.389412803	-0.105799380
C	-1.007213474	-5.463511279	3.003577538
C	-2.360584443	-5.829855477	3.280098375
H	-2.632588787	-6.880824901	3.360455308
C	-3.041793628	-3.515947992	3.011079162
C	-3.347366706	-4.883891455	3.291233467
H	-4.384531377	-5.200266193	3.381375609
C	0.495536616	-6.835026924	-0.478228367
C	-0.294126947	-7.757032439	0.279802147
H	-0.760512753	-8.608085743	-0.213411806
C	-0.153945750	-6.268885344	2.185785405
C	-0.609573178	-7.482655929	1.580247478
H	-1.321973753	-8.119076983	2.102040666
C	-5.050665880	1.153428614	1.474308629
O	-5.514232866	0.314237084	2.147046550
C	-3.191253535	2.883502137	-2.185024829
H	-4.166952251	3.378504634	-2.209838638
H	-3.355548683	1.848543185	-2.518990166
C	-2.207087926	3.601274496	-3.153128393
H	-2.624562552	4.585918691	-3.423022357
H	-1.260095163	3.821098930	-2.634266998
C	-1.904440192	2.804431887	-4.419934895
H	-1.624871228	1.773146697	-4.147392171
H	-2.821922570	2.721860508	-5.028267461
C	-0.777916248	3.430232219	-5.235978191
H	-1.026434770	4.460231615	-5.536382021
H	0.153118706	3.469913188	-4.647002412
H	-0.573988659	2.847882941	-6.146068885
C	-3.300655502	5.331760707	-0.235762367
H	-3.526554159	5.856487970	0.699818244
H	-2.580447170	5.945103667	-0.803604373
H	-4.214861266	5.231726046	-0.830446591

PD*methyl,perpendicular*

165
Co2C124H32O7

Co	-5.252174021	-1.419791287	-0.228386940
Co	-6.032983696	-1.508077757	2.182524242
C	-5.600271112	-3.006707985	0.475829878
C	-2.090170560	-2.521298722	-2.813215700
C	-4.455750181	-1.860612503	2.926594294
C	-6.332009429	-0.060506382	3.157435291
C	-6.862010324	-0.741486472	0.691946361
O	-2.081624308	-2.573865446	-4.024135235
O	-5.720466355	-4.173418071	0.498954831
O	-3.437422263	-2.064172010	3.438835527
O	-6.577969752	0.853979537	3.821079707
O	-7.762480375	-0.125827383	0.245374523
C	-2.461825442	-3.093920330	-0.597046918
C	-2.741300435	-3.423842682	-1.872656517
C	-5.622116790	-1.850371868	-1.887161291
O	-5.916585586	-2.173708307	-2.958857797
H	-6.144726750	2.608403110	1.193863826
H	-5.797793440	2.165194536	-3.090419816
H	-6.498216352	1.740242060	-0.796119740
H	-4.612264203	3.526762725	-4.304344423
H	-3.184128805	5.487708527	-4.399502963
H	-1.914592706	7.995930661	-1.037353007
H	-2.202103865	7.093930027	-3.277269908
H	-2.518345909	7.637426628	1.057261039
H	-3.818638988	6.153555478	2.473552820
H	-5.085865835	4.384655700	2.472031656
C	-4.517791484	3.483651086	2.248897229
C	-5.534215667	1.377144558	-1.143544204
C	-5.115120023	2.484780775	1.522256993
C	-4.354664871	1.379096694	1.063264740
C	-5.141384730	1.613726095	-2.419719665
C	-3.805817282	1.279533706	-2.829896399
C	-4.625444877	0.746087544	-0.205105914
C	-3.547857604	3.417972834	-4.106296738
C	-3.033649067	2.168568140	-3.636791667
C	-1.437027710	6.672671261	-2.627667374
C	-2.743531865	4.520914668	-4.163560542
C	-1.375626144	4.441072898	-3.757666121
C	-1.274685747	7.180513957	-1.369795206
C	-0.406166218	6.526717396	-0.439532287
C	-0.738244108	5.487610491	-3.019657672
C	-2.063552340	6.718196500	1.421998113
C	-0.790494271	6.303264163	0.921624551
C	-2.796092943	5.881818441	2.218249711
C	-2.294412724	4.587261382	2.554608476
C	-3.132143663	3.421591170	2.556720335
C	-2.508236919	2.149002326	2.460242687
C	-3.607444241	-0.095655744	-0.777583627
C	-3.119860023	1.121458226	1.688615562
C	-2.342654939	-0.024975613	1.301314432
C	-3.146122224	0.251216874	-2.124217713
C	-1.834699675	-0.118805203	-2.484779705
C	-2.636553423	-0.694860310	0.108666208
C	-1.629575819	2.002170768	-3.652833192
C	-1.062884142	0.759614259	-3.240017461
C	0.442753813	5.175359750	-2.300514699
C	-0.789154867	3.150320030	-3.728933119
C	0.582772488	3.001446140	-3.385267404
C	0.614146643	5.707970115	-0.985108576
C	1.544044242	5.064561644	-0.116811421
C	1.212949761	4.034229803	-2.666718893
C	-0.124296398	5.280313324	1.642112953
C	1.167767424	4.848098824	1.224278010
C	-0.893261578	4.404085930	2.468181373
C	-0.320836550	3.149804523	2.833264570
C	-1.141198089	2.006770103	2.824537278
C	-0.534152393	0.714863284	2.787094713
C	-1.713768105	-1.754322941	-0.456380939
C	-1.139647099	-0.308578382	2.026231061
C	-0.345191437	-1.437293070	1.664652295
C	-1.290628407	-1.406958971	-1.980710737
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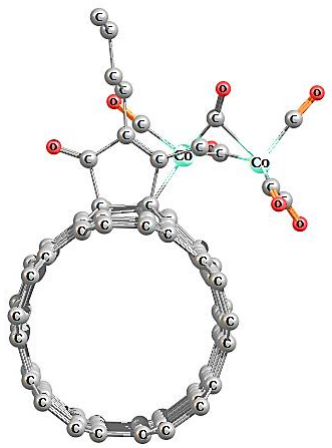
C	-0.532045411	-2.040972123	0.413136578
C	0.353665552	0.564584468	-3.340664268
C	0.922635348	-0.693088506	-2.986096695
C	2.425113369	3.742143995	-1.968639630
C	1.181285792	1.702607077	-3.404168645
C	2.566451926	1.576501716	-3.100287851
C	2.596086192	4.269878261	-0.667562157
C	3.531890112	3.646549156	0.202525542
C	3.199712449	2.618403492	-2.360437486
C	1.856636629	3.845609130	1.973713397
C	3.151656468	3.429342912	1.561524939
C	1.096483318	2.981395026	2.796864962
C	1.658248422	1.739198660	3.192921013



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C	1.437752324	-0.694154323	3.176252080
C	0.495627739	-2.822171278	-0.129939021
C	0.843255786	-1.721015122	2.398483904
C	1.632882775	-2.841205122	2.031427851
C	0.850051656	-2.617207604	-1.520295197
C	2.176664732	-2.976072585	-1.902565869
C	1.474357998	-3.381005190	0.736524861
C	2.336550914	-0.854020035	-3.075825666
C	2.921552222	-2.097063722	-2.717168593
C	4.394928267	2.319024433	-1.657506127
C	3.167556266	0.297433114	-3.130932836
C	4.548159835	0.163963048	-2.795639616
C	4.562826544	2.842900614	-0.347091528
C	5.484923245	2.192657717	0.524948699
C	5.166476849	1.184925329	-2.042391486
C	3.826195265	2.423481094	2.300431312
C	5.112969933	1.983172554	1.870140327
C	3.066034844	1.564979198	3.140234560
C	3.633210808	0.315906528	3.526255630
C	2.807259678	-0.828543408	3.553177074
C	3.423276240	-2.114367145	3.541238033
C	2.527463312	-4.181325456	0.201926605
C	2.822897604	-3.147765316	2.759984662
C	2.890956340	-3.970694819	-1.165678256
C	4.336882958	-2.276844090	-2.811501012
C	6.372942053	0.880648832	-1.345028495
C	5.169105518	-1.116863757	-2.847534764
C	6.533601332	1.396100910	-0.021105284
C	5.807502610	0.988370707	2.617954608
C	5.047260833	0.133267167	3.475073939
C	7.169972501	-0.211767276	-1.762242744
C	8.381401294	-0.437345012	-1.042088646
H	9.133062112	-1.116776105	-1.439609888
C	7.478795905	0.791351544	0.843370613
C	8.532425435	0.050873869	0.227944915
H	9.399095274	-0.252293732	0.812461912
C	4.910468796	-3.525705010	-2.478218144
C	6.319896578	-3.654853984	-2.640898456
H	6.784938460	-4.638002202	-2.597196358
C	6.549837973	-1.243284018	-2.547648846
C	7.119568567	-2.542319933	-2.675440018
H	8.200558264	-2.667535016	-2.657997694
C	3.441493111	-4.813653555	1.073681365
C	4.454591115	-5.616289445	0.470195329
H	5.053565507	-6.290299715	1.079847275
C	4.163513295	-4.397333988	-1.607158009
C	4.805752435	-5.413306084	-0.837931041
H	5.676782622	-5.929728813	-1.236996500
C	4.774199867	-2.252661246	3.949415826
C	5.313163652	-3.570881731	3.956657420
H	6.266685345	-3.766681579	4.443428810
C	3.588986415	-4.283485132	2.406639475
C	4.735852074	-4.560894514	3.204537033
H	5.245036647	-5.518395192	3.112097559
C	7.103047488	0.582710611	2.213873887
C	7.763256943	-0.376063054	3.039100544
H	8.827777484	-0.563881680	2.911115017
C	5.615442063	-1.088441895	3.909873476
C	7.038628380	-1.188083920	3.869264454
H	7.542747934	-2.003688202	4.384196640
C	-7.228691234	-2.699537080	2.771329106
O	-7.998143313	-3.428050982	3.230219763
C	-3.460915239	-4.625632976	-2.376921736
H	-3.974048339	-4.348475495	-3.312163781
H	-4.227486938	-4.940692666	-1.653082349
C	-2.480645190	-5.773366476	-2.654398071
H	-1.705115092	-5.416563940	-3.354287293
H	-1.961531968	-6.040477001	-1.716666786
C	-3.172849778	-7.003029811	-3.232099293
H	-3.959927165	-7.338893289	-2.534303184
H	-3.683999226	-6.719853051	-4.168424519
C	-2.196906852	-8.144549532	-3.500272377
H	-1.418944116	-7.833394030	-4.214402488
H	-1.693378702	-8.456327487	-2.571931000
H	-2.710815310	-9.022160089	-3.918517128
C	-2.648659954	-3.938785364	0.606227797
H	-1.684703785	-4.433049467	0.828167601
H	-2.903880096	-3.348418119	1.494047888
H	-3.401057982	-4.717989113	0.451537674

PD*butyl,perpendicular*

165
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C	-5.715200000	0.844600000	-2.755000000
C	-6.400900000	0.841100000	-0.263000000
O	-2.384400000	1.587400000	4.407800000
O	-6.279600000	4.029800000	0.965500000
O	-3.244900000	3.221100000	-2.697100000
O	-5.847300000	0.122700000	-3.649100000
O	-7.307400000	0.107700000	-0.069900000
C	-2.695500000	2.743500000	1.127300000
C	-3.158400000	2.695200000	2.417900000
C	-5.621300000	1.035100000	2.442800000
O	-6.134800000	0.780700000	3.446400000
H	-6.101600000	-2.639300000	-1.728900000
H	-5.729100000	-3.052400000	2.640600000
H	-6.409600000	-2.278300000	0.421000000
H	-4.472400000	-4.562200000	3.620000000
H	-2.941900000	-6.433700000	3.386900000
H	-1.573100000	-8.195400000	-0.383400000
H	-1.881500000	-7.754200000	1.989100000
H	-2.220700000	-7.469600000	-2.360300000
H	-3.590900000	-5.816900000	-3.496700000
H	-4.951400000	-4.103600000	-3.305700000
C	-4.420700000	-3.257100000	-2.873900000
C	-5.471400000	-1.940500000	0.854100000
C	-5.063400000	-2.443300000	-1.989300000
C	-4.338400000	-1.420900000	-1.295200000
C	-5.089900000	-2.371700000	2.081300000
C	-3.771500000	-2.055500000	2.563000000
C	-4.569500000	-1.136700000	0.070300000
C	-3.414200000	-4.366500000	3.458500000
C	-2.963300000	-3.029400000	3.219500000
C	-1.147500000	-7.176700000	1.430000000
C	-2.552900000	-5.418800000	3.330600000
C	-1.189800000	-5.197200000	2.959000000
C	-0.974000000	-7.424900000	0.098500000
C	-0.147800000	-6.562000000	-0.690300000
C	-0.505700000	-6.052000000	2.039800000
C	-1.809500000	-6.480700000	-2.554500000
C	-0.551800000	-6.105600000	-1.983500000
C	-2.580200000	-5.551000000	-3.192800000
C	-2.134300000	-4.195700000	-3.299800000
C	-3.020400000	-3.090100000	-3.122800000
C	-2.458400000	-1.824300000	-2.811700000
C	-3.640900000	-0.310500000	0.792800000
C	-3.118500000	-0.978100000	-1.870400000
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C	-3.154900000	-0.898700000	2.047400000
C	-1.878100000	-0.524600000	2.491100000
C	-2.716800000	0.502500000	0.035400000
C	-1.570200000	-2.795900000	3.291200000
C	-1.069000000	-1.473400000	3.107800000
C	0.652600000	-5.550000000	1.394400000
C	-0.670900000	-3.894300000	3.171400000
C	0.688800000	-3.612400000	2.867400000
C	0.838400000	-5.813300000	0.001600000
C	1.731300000	-4.976700000	-0.728000000
C	1.365900000	-4.459300000	1.969900000
C	0.068400000	-4.942200000	-2.506000000
C	1.341000000	-4.535400000	-2.009400000
C	-0.738200000	-3.969200000	-3.172500000
C	-0.221300000	-2.651400000	-3.317000000
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C	-0.547300000	-0.275800000	-2.846200000
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C	-1.198300000	0.555500000	-1.912000000
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C	-1.428200000	0.874800000	2.240300000
C	0.012200000	1.127500000	2.582100000
C	-0.655200000	1.948500000	0.016500000
C	0.331000000	-1.221100000	3.263400000
C	0.824000000	0.111800000	3.149600000
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C	1.216700000	-2.307700000	3.124300000
C	2.590600000	-2.056100000	2.854700000
C	2.745600000	-4.247100000	-0.034100000
C	3.648700000	-3.430800000	-0.768700000
C	3.273200000	-2.909900000	1.938500000
C	1.984300000	-3.385900000	-2.562400000
C	3.260100000	-2.991200000	-2.070500000
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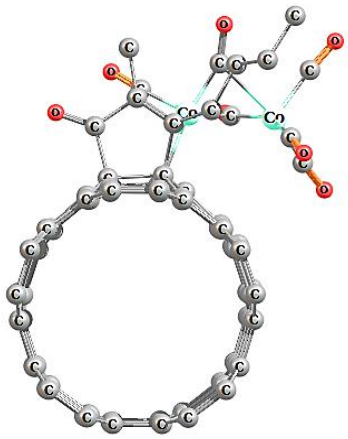

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C	1.455900000	3.155800000	-1.402800000
C	0.660300000	2.257400000	2.052900000
C	1.965600000	2.610400000	2.510400000
C	1.269700000	3.432500000	-0.030900000
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C	3.277100000	2.817300000	-3.009000000
C	2.270400000	4.183500000	0.653400000
C	2.628200000	3.654100000	-2.050300000
C	2.632300000	3.754100000	1.969400000
C	4.158300000	1.867200000	3.298400000
C	6.348500000	-0.857500000	1.282900000
C	5.048300000	0.764800000	3.121400000
C	6.537300000	-1.117900000	-0.110300000
C	5.802800000	-0.281600000	-2.644100000
C	5.006100000	0.676700000	-3.344700000
C	7.090200000	0.177300000	1.900800000
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H	9.318700000	0.790800000	-0.599900000
C	4.666800000	3.183000000	3.207400000
C	6.067800000	3.349900000	3.402700000
H	6.483000000	4.346000000	3.545100000
C	6.420200000	1.013100000	2.860400000
C	6.923000000	2.291700000	3.233000000
H	7.996200000	2.472900000	3.245800000
C	3.153100000	5.009800000	-0.077000000
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H	4.683800000	6.544500000	0.206800000
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C	4.619600000	3.093500000	-3.370100000
C	5.094300000	4.412400000	-3.121400000
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C	3.334400000	4.740200000	-1.483700000
C	4.468400000	5.214900000	-2.202000000
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PK*methyl,oblique*

151
C118H32O

C	-1.979547943	-4.470539350	1.310693505
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H	-7.197150258	-1.174101196	2.423158657
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H	-6.229120899	5.332723798	-0.528132746
H	-6.336092607	4.770807183	1.832988023
H	-6.587758817	3.094192112	3.211001176
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C	-6.285330921	-1.450743899	1.897672318
C	-5.908199617	1.084695940	3.317429309
C	-4.828899811	0.180054744	3.111663020
C	-6.372161444	-1.983229210	0.644029656
C	-5.182982858	-2.204302489	-0.121892601
C	-5.007116660	-1.081373211	2.432837506
C	-6.211799197	-1.330794712	-2.228822868
C	-5.095941443	-1.859983964	-1.509623334
C	-5.622898836	2.619984178	-3.366526759
C	-6.041552801	-0.291094459	-3.099921760
C	-4.745858620	0.274001500	-3.302000631
C	-5.463234821	3.805747827	-2.703024139
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C	-4.271977760	4.060780195	1.950255080
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C	-3.322591425	2.120632733	3.098849914
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C	-3.522584274	0.710672389	3.206026827
C	-2.395571791	-0.145193383	3.023893139
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C	-2.768545041	-2.615796033	-0.087968370
C	-2.562386670	-1.373974889	2.346513592
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C	-1.841468387	3.686839574	1.954426781
C	-2.006456916	2.604576490	2.844747667
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C	-1.421382742	-2.049732265	1.859805239
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C	0.022249353	-0.493736977	3.037471697
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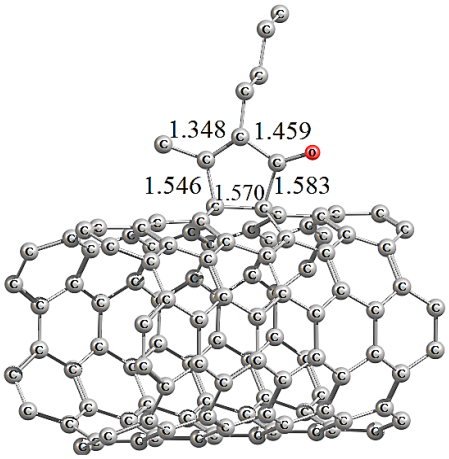

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C	1.870516673	3.542820223	1.396000707
C	3.027644736	2.974342851	2.016288539
C	2.857269440	1.894102759	2.907350203
C	3.974373526	1.063684276	3.201367905
C	3.465605175	-2.747104786	1.951619944
C	3.767043675	-0.348059355	3.309152093
C	3.416471999	-3.349026190	0.658047724
C	3.502390505	-2.701975871	-2.021486209
C	4.064020536	1.142879250	-3.179684213
C	3.662209543	-1.597000645	-2.923911802
C	4.240089410	2.377759219	-2.480659142
C	4.377693404	3.498321676	0.044758126
C	4.311113352	3.171930224	1.435271958
C	5.173418991	0.276920824	-3.350679411
C	6.473390943	0.862847431	-3.233611539
H	7.350766528	0.311439989	-3.565948253
C	5.520314284	2.693640665	-1.958464283
C	6.642255111	2.037075929	-2.556009084
H	7.650397037	2.396515542	-2.358369976
C	4.670259318	-3.266057373	-1.430361691
C	5.908651480	-3.076298788	-2.127859257
H	6.776545087	-3.679089356	-1.865517065
C	4.963714346	-1.132383104	-3.228579476
C	6.050597617	-2.042862387	-3.005492615
H	7.027699974	-1.839253883	-3.439355147
C	4.732546532	-2.448999539	2.521137958
C	5.860822907	-3.168653331	2.003780611
H	6.803844763	-3.162936779	2.547134063
C	4.629085698	-3.582216710	-0.043238289
C	5.814703815	-3.713442770	0.753642121
H	6.721753717	-4.128420643	0.317546181
C	5.287099870	1.555326725	2.988008340
C	6.369309298	0.697379148	3.367858746
H	7.378103352	1.098644049	3.446364515
C	4.886335031	-1.218262987	3.221035299
C	6.173999373	-0.647657210	3.485360867
H	7.029756133	-1.297446385	3.658050832
C	5.591210246	3.274147363	-0.653690071
C	6.788161366	3.222892703	0.130713978
H	7.759957315	3.293997694	-0.354390967
C	5.461277996	2.637100261	2.072558338
C	6.725196467	2.913441851	1.458972439
H	7.647541167	2.742871125	2.011159840
C	-1.695435322	-6.898969084	0.588380931
H	-1.859790464	-7.120405716	1.656457686
H	-0.879179767	-7.547746082	0.236561982
C	-2.986604035	-7.188221351	-0.188686807
H	-3.775338821	-6.503245873	0.168866630
H	-2.825724080	-6.953127800	-1.256196679
C	-3.449431866	-8.633106104	-0.036304236
H	-2.646527563	-9.310958871	-0.376431536
H	-3.607963856	-8.848351870	1.034680445
C	-4.729720893	-8.917978464	-0.815631891
H	-5.548772444	-8.268499146	-0.470275949
H	-4.584301052	-8.729921821	-1.890784611
H	-5.050165074	-9.962897977	-0.694187774
C	0.362979194	-5.560994568	-1.412951477
H	0.325043043	-5.005924753	-2.363522178
H	1.422817907	-5.618734266	-1.112265059
H	-0.001809306	-6.580954395	-1.585557791

PK*butyl,oblique*

151
C118H32O

C	-1.143595271	-4.623626958	2.246658738
O	-1.885990768	-4.794775102	3.192184450
C	0.502070174	-4.993994313	0.660753971
C	-0.275029112	-5.592686335	1.586620170
H	-7.104549964	-0.302263675	3.451952023
H	-6.836840171	-3.662474084	0.738986948
H	-6.954796282	-2.342965640	2.779149011
H	-6.728082515	-3.575308584	-1.475901950
H	-6.760454119	-1.999335452	-3.326951150
H	-7.097117232	2.388175638	-3.079021572
H	-6.902061060	0.102875084	-3.871166285
H	-7.246857513	3.616576425	-1.266571720
H	-7.315193520	3.457939334	1.156460406
H	-7.262650165	2.028527935	2.809099569
C	-6.278064589	1.574181616	2.902264411
C	-5.988583214	-2.509367276	2.307123323
C	-6.188280696	0.253380727	3.262805814
C	-4.939868115	-0.428317424	3.214168953
C	-5.922118124	-3.254753699	1.165781415
C	-4.687831026	-3.351628630	0.446932718
C	-4.832228310	-1.796183358	2.766000340
C	-5.802219101	-3.088455811	-1.777225390
C	-4.626168143	-3.241794934	-0.979909748
C	-6.000902777	0.643026746	-3.587362889
C	-5.820454107	-2.201055813	-2.816868976
C	-4.662603611	-1.421718427	-3.118149330
C	-6.110931662	1.931991094	-3.142392141
C	-4.976727711	2.604665428	-2.592731111
C	-4.751061809	-0.043512562	-3.506989379
C	-6.311878634	3.568982430	-0.711369711
C	-5.074710415	3.405973542	-1.406640008
C	-6.350246923	3.479186783	0.653236078
C	-5.154191720	3.224505303	1.389858950
C	-5.121372549	2.288787469	2.480655947
C	-3.865278338	1.751469145	2.857295266
C	-3.578494612	-2.275237547	2.348535663
C	-3.774429878	0.370658971	3.210073463
C	-2.490142506	-0.250045262	3.176203163
C	-3.505478753	-3.110372426	1.181644095
C	-2.242625737	-3.240939898	0.545713335
C	-2.377940474	-1.584033431	2.724300300
C	-3.397288515	-2.834634975	-1.551878229
C	-2.177132754	-3.023600321	-0.822344326
C	-3.587910673	0.758672735	-3.413252153
C	-3.420568251	-1.904230437	-2.634985036
C	-2.221987423	-1.203477281	-2.949686120
C	-3.700974244	2.108454290	-2.955479000
C	-2.525535115	2.760012221	-2.477537300
C	-2.306171935	0.139469660	-3.363246603
C	-3.890115139	3.651757311	-0.669241623
C	-2.620950837	3.548891330	-1.312445327
C	-3.931885415	3.557423948	0.756847403
C	-2.700347080	3.371567247	1.451882876
C	-2.669111322	2.447883578	2.518270036
C	-1.410157396	1.931902230	2.938589197
C	-1.106859946	-2.081603625	2.360225534
C	-1.321668182	0.548570688	3.256321105
C	-0.054389518	-0.080146855	3.242503859
C	-1.027429862	-3.266231464	1.438989009
C	0.308137120	-3.458745158	0.633388387
C	0.043821798	-1.421384535	2.768443199
C	-0.923660993	-2.629560230	-1.423926113
C	0.289768313	-2.883908244	-0.779511698
C	-1.129957823	0.947484762	-3.328623903
C	-0.965418567	-1.709776280	-2.503454948
C	0.221926603	-1.038995347	-2.881910457
C	-1.240198946	2.286345305	-2.878920389
C	-0.071878316	2.945740507	-2.411224828
C	0.140062608	0.320104502	-3.308144958
C	-1.427454957	3.838047350	-0.582477016
C	-0.168513175	3.742004606	-1.232503053
C	-1.470417858	3.747205907	0.833979173
C	-0.251441131	3.565737902	1.540748743
C	-0.224508828	2.631147335	2.615210443
C	1.030434594	2.088388698	3.014353672
C	1.350597386	-1.921787054	2.396308809
C	1.113878165	0.718336418	3.332614336
C	2.397898107	0.088116821	3.356432446
C	1.486352360	-2.812343665	1.345010177
C	2.748530819	-2.846681963	0.678462892
C	2.517010963	-1.236377658	2.892547991
C	1.496320952	-2.477657559	-1.378655034
C	2.762988323	-2.709917106	-0.728743351
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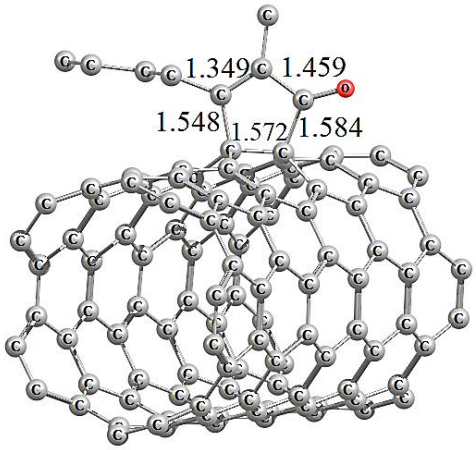

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C	2.589246558	0.478663732	-3.217415658
C	1.022033095	3.999556640	-0.494376731
C	2.291210001	3.883367889	-1.141387333
C	0.978518939	3.910143982	0.916403155
C	2.206083260	3.710133927	1.623320591
C	2.231150098	2.787763992	2.690361423
C	3.484179499	2.271286230	3.122510213
C	3.813439052	-1.716634498	2.559639445
C	3.567874839	0.887481826	3.476812338
C	3.933269383	-2.525122575	1.389842923
C	3.974915310	-2.346462612	-1.362376780
C	3.771039061	1.270311407	-3.177782166
C	3.933688126	-1.407558712	-2.447706834
C	3.665771859	2.615437614	-2.704255476
C	3.485429979	4.155849398	-0.413428621
C	3.440532902	4.067012644	1.012927801
C	5.040008752	0.638661075	-3.199594431
C	6.186856564	1.494098523	-3.190218726
H	7.169540367	1.089647418	-3.424799001
C	4.835477792	3.275774404	-2.248982171
C	6.087638894	2.775607463	-2.727109112
H	6.992957147	3.365942598	-2.598538450
C	5.213121362	-2.543357062	-0.684481633
C	6.408584783	-2.223849819	-1.409002873
H	7.372784694	-2.577105909	-1.047074103
C	5.120941389	-0.741383417	-2.833391080
C	6.364053930	-1.352437707	-2.456393020
H	7.292363699	-1.027698429	-2.922467940
C	4.971701505	-1.068587497	3.066521717
C	6.240683368	-1.614479891	2.678977817
H	7.143379282	-1.319747085	3.210791865
C	5.190981149	-2.616674216	0.736615498
C	6.350198185	-2.360269466	1.541438404
H	7.337547259	-2.644501336	1.181654426
C	4.674318506	2.981545584	2.823194840
C	5.895671021	2.447069268	3.346890483
H	6.796868883	3.057548601	3.352271114
C	4.844553618	0.268049679	3.541362715
C	5.977091461	1.131757575	3.699814586
H	6.941641138	0.714691937	3.982868587
C	4.741897970	4.072664738	-1.065440648
C	5.896835079	4.406655831	-0.287535957
H	6.849220281	4.593416683	-0.780338296
C	4.653818030	3.901075305	1.731021664
C	5.854068590	4.324099550	1.074658918
H	6.772712611	4.446726423	1.645421866
C	1.437950990	-5.675620467	-0.269135914
H	1.811968911	-6.601452280	0.194971151
H	2.319531563	-5.047180041	-0.458718733
C	0.768419775	-6.005877546	-1.618665414
H	0.057473761	-6.838493406	-1.476493264
H	0.173091812	-5.142904515	-1.959151203
C	1.801107319	-6.348402051	-2.687027191
H	2.485782066	-5.488967648	-2.799436447
H	2.416958654	-7.199341680	-2.346190246
C	1.157491970	-6.670420253	-4.031229418
H	0.481783805	-7.535737537	-3.948578410
H	0.566492352	-5.814835223	-4.392377224
H	1.916812884	-6.902966389	-4.791718317
C	-0.342305259	-7.027234867	1.972779448
H	-0.260734566	-7.117744517	3.066277041
H	-1.319774188	-7.447423117	1.688823994
H	0.449046890	-7.619414689	1.498866758

PK*methyl,perpendicular*

151
C118H32O

C	-1.402142823	-4.665890980	-1.154054424
O	-1.432326437	-5.067007822	-2.297556777
C	-1.391505985	-4.655188670	1.166629699
C	-1.426675875	-5.444623007	0.078776863
H	-7.094086607	-1.343199501	2.992942623
H	-7.172329988	-2.669785071	-1.188469343
H	-7.177089100	-2.660664496	1.245550660
H	-7.089320999	-1.362437289	-2.938638818
H	-6.984574883	0.952366438	-3.665515553
H	-6.833568358	4.520505790	-1.100845230
H	-6.895700951	3.045290866	-3.030819972
H	-6.835736348	4.527784301	1.098456101
H	-6.902367071	3.068314269	3.039663680
H	-6.990633169	0.979791296	3.693133738
C	-6.067868792	0.458935202	3.444305739
C	-6.228786310	-2.631081512	0.712069716
C	-6.126509342	-0.848020464	3.048323260
C	-4.959114029	-1.504636429	2.545864251
C	-6.226274890	-2.635171997	-0.651435218
C	-5.003925361	-2.403555583	-1.364140578
C	-5.008068417	-2.398015234	1.427876918
C	-6.121720451	-0.867727528	-2.997370480
C	-4.954782811	-1.520342120	-2.489452567
C	-5.940766450	3.255088809	-2.552485367
C	-6.062444675	0.434076243	-3.409386440
C	-4.831694423	1.157206826	-3.345902043
C	-5.905806613	4.085406139	-1.467849525
C	-4.699268906	4.232744328	-0.713636313
C	-4.771672630	2.528865019	-2.940942263
C	-5.908715698	4.095601515	1.470760190
C	-4.700749722	4.238027296	0.717980260
C	-5.946214288	3.273944657	2.561967493
C	-4.777891513	2.550335249	2.957900877
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C	-3.646388303	0.414406646	3.321286548
C	-3.799456663	-2.706531185	0.758588284
C	-3.707869260	-0.942764484	2.887177012
C	-2.502106999	-1.582661841	2.454744631
C	-3.796923263	-2.707049837	-0.689513160
C	-2.555999880	-2.498651534	-1.342898908
C	-2.559906992	-2.506669344	1.417374991
C	-3.703146137	-0.963021950	-2.838097353
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C	-2.317491158	2.396320078	-2.896348996
C	-3.489987568	3.929460820	1.387161630
C	-2.246701255	4.092385719	0.710260352
C	-3.530158829	3.065518059	2.526102326
C	-2.323708459	2.417613765	2.919009438
C	-2.383407789	1.068250820	3.314131013
C	-1.182760099	0.290743930	3.307365165
C	-1.328316888	-3.149575120	0.841933333
C	-1.238110802	-1.050609054	2.881050975
C	-0.031558599	-1.696624648	2.485556852
C	-1.327271000	-3.114313337	-0.771054506
C	-0.045697960	-2.630507195	-1.351851462
C	-0.046276750	-2.631593476	1.430254255
C	-1.232632477	-1.069368442	-2.823296134
C	-0.026822758	-1.714755421	-2.424430331
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C	-1.020315607	3.807099833	-1.381037857
C	0.216949016	3.995299099	-0.705453119
C	0.140889278	2.304430422	-2.914472630
C	-1.023590787	3.817405535	1.396384671
C	0.215217174	4.000602140	0.722250285
C	-1.063589268	2.963624227	2.522607967
C	0.133902727	2.327261730	2.944568670
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C	1.153380909	-2.925140039	-0.687326722
C	2.394386221	-2.675409058	-1.342375949
C	2.392946389	-2.661709567	1.419372409
C	1.218824564	-1.173117408	-2.851715250
C	2.424476502	-1.808528895	-2.455915054
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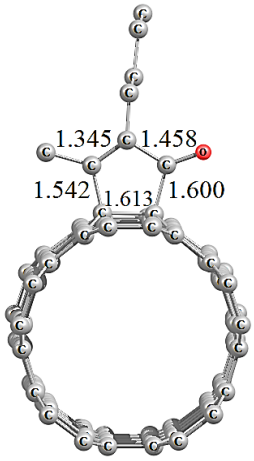

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C	1.425915315	3.711165218	1.401738825
C	2.668073019	3.864522665	0.717711879
C	1.384927700	2.859884880	2.539464630
C	2.586979522	2.211713313	2.947529606
C	2.526264046	0.865245646	3.365572766
C	3.729262067	0.101656566	3.385714715
C	3.625526433	-2.944717148	0.756230898
C	3.676441015	-1.260328801	2.958618022
C	3.626249961	-2.951764050	-0.674729859
C	3.682097473	-1.284508636	-2.887965855
C	3.855628443	2.721888071	-2.512610010
C	3.736514257	0.073669433	-3.326620158
C	3.894124136	3.579490124	-1.369179820
C	3.890718078	3.591635773	1.399055583
C	3.849511537	2.743088317	2.549160641
C	5.051024051	2.105625323	-2.954329026
C	6.276499533	2.715409901	-2.551512166
H	7.211910577	2.421909567	-3.024218215
C	5.126976689	3.783657517	-0.702713052
C	6.314037453	3.532704037	-1.453815754
H	7.278101529	3.869809756	-1.077539972
C	4.879546992	-1.941040585	-2.521692091
C	6.095117498	-1.394748269	-3.024333467
H	7.020541737	-1.962375762	-2.946191637
C	4.989984675	0.734266956	-3.381712939
C	6.149108557	-0.090828848	-3.444380746
H	7.115874443	0.345455698	-3.688358062
C	4.848223202	-2.786521164	1.446025207
C	6.037842488	-3.112771045	0.729571806
H	6.983428121	-3.213344177	1.259057886
C	4.850951484	-2.797111300	-1.361779781
C	6.038918572	-3.118061644	-0.640074058
H	6.985394599	-3.222672294	-1.167170847
C	4.982318594	0.763125996	3.437449255
C	6.141463228	-0.061256286	3.507411216
H	7.108002864	0.377571175	3.747894350
C	4.874107600	-1.919627612	2.598328912
C	6.088832486	-1.368921467	3.098894716
H	7.014737994	-1.936318571	3.025564071
C	5.125182400	3.790184661	0.734025294
C	6.310381559	3.545490231	1.490099800
H	7.275279932	3.879655590	1.113312338
C	5.044054205	2.130779627	2.998915163
C	6.270542818	2.737842471	2.594803357
H	7.204788727	2.448434447	3.072279176
C	-1.416382284	-6.932930487	0.004473382
H	-2.016644492	-7.237225996	-0.868752512
H	-1.883945408	-7.367995380	0.900986089
C	0.016469379	-7.456396175	-0.157528771
H	0.468294367	-6.981203049	-1.045773615
H	0.617252704	-7.134614659	0.712078646
C	0.072280946	-8.973763073	-0.298835949
H	-0.400586618	-9.439547198	0.583966059
H	-0.530529822	-9.275497964	-1.172930023
C	1.499682319	-9.489969578	-0.452580544
H	1.977749394	-9.054994327	-1.343646272
H	2.111289984	-9.217353483	0.421454723
H	1.522044711	-10.584650919	-0.554772658
C	-1.392165060	-5.062534920	2.590838645
H	-0.455955683	-4.737683043	3.076423841
H	-2.219181220	-4.569265685	3.129364507
H	-1.488284725	-6.148685592	2.704403558

PK*butyl,perpendicular*

151
C118H32O

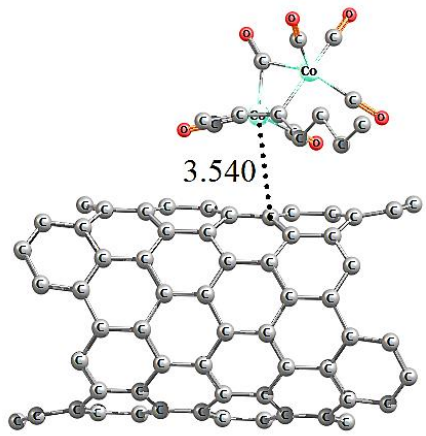
C	-1.475276809	-4.166941617	-2.577034850
O	-1.512798500	-4.238581067	-3.786625178
C	-1.499978013	-4.790364493	-0.340825722
C	-1.571315497	-5.249636764	-1.603258162
H	-7.032440620	-1.831798550	2.332767025
H	-7.114629092	-1.910985409	-2.055793997
H	-7.156122031	-2.587950191	0.280541188
H	-6.933406950	-0.174759549	-3.380083242
H	-6.693655636	2.241704082	-3.426882773
H	-6.396636442	4.931325285	0.042296362
H	-6.504742269	4.066110292	-2.226144257
H	-6.436463236	4.311264770	2.152136004
H	-6.611183604	2.372434951	3.605254428
H	-6.817904108	0.193357849	3.654772008
C	-5.919797974	-0.287401872	3.271316126
C	-6.198967027	-2.463089730	-0.222545357
C	-6.040755611	-1.427109774	2.526070209
C	-4.901445378	-1.978591728	1.858882506
C	-6.175770607	-2.082289616	-1.532298801
C	-4.932979594	-1.728136334	-2.152828113
C	-4.979498655	-2.508239904	0.530106904
C	-5.940130979	0.261949784	-3.294994796
C	-4.818567240	-0.570765741	-2.987516820
C	-5.548493365	4.077458011	-1.706339575
C	-5.804986846	1.621746443	-3.324280977
C	-4.539041454	2.228191284	-3.057204789
C	-5.487664526	4.564743768	-0.431174549
C	-4.288114641	4.424992908	0.335670715
C	-4.413466952	3.425303454	-2.282398403
C	-5.539233429	3.742893230	2.390266568
C	-4.313097265	4.025440191	1.710261418
C	-5.637524345	2.651496498	3.206812111
C	-4.515043606	1.783893289	3.386715404
C	-4.652779785	0.358814515	3.407080982
C	-3.502419455	-0.427861732	3.143738042
C	-3.778535954	-2.673633835	-0.199502889
C	-3.628331874	-1.604752009	2.346533586
C	-2.450762668	-2.158527339	1.749349561
C	-3.753907057	-2.273814577	-1.589769712
C	-2.493106354	-1.964145251	-2.160404341
C	-2.540664112	-2.738074157	0.488976006
C	-3.533116925	-0.008968940	-3.164051961
C	-2.371199162	-0.807254039	-2.921140568
C	-3.148169861	3.731167281	-1.721880347
C	-3.391545145	1.409332477	-3.212133187
C	-2.095387656	1.963999482	-3.022546300
C	-3.083219316	4.244691896	-0.388722435
C	-1.845633086	4.145818603	0.310904044
C	-1.970940779	3.148793108	-2.273400406
C	-3.131314231	3.475190165	2.266851179
C	-1.870076447	3.753836852	1.664942688
C	-3.235199648	2.330121717	3.117266601
C	-2.070478633	1.533643633	3.315270716
C	-2.206841337	0.132781160	3.318979174
C	-1.047965648	-0.675760976	3.094871402
C	-1.337351232	-3.263565319	-0.242616378
C	-1.166553934	-1.837782921	2.307680446
C	0.010047292	-2.409167434	1.743519952
C	-1.309102757	-2.785719921	-1.783634959
C	0.005554827	-2.230224135	-2.206123920
C	-0.038313942	-3.007455412	0.467196577
C	-1.072037042	-0.252731717	-3.178122437
C	0.090804971	-1.050621401	-2.975742986
C	-0.691007610	3.492835903	-1.737794187
C	-0.937705158	1.148188826	-3.224666369
C	0.353284611	1.732266717	-3.077967431
C	-0.626206363	4.002435111	-0.420524814
C	0.608018085	3.924506635	0.281812734
C	0.478717490	2.929902180	-2.313994555
C	-0.674288048	3.230817054	2.247311663
C	0.583426187	3.528200483	1.653225005
C	-0.777158035	2.099281624	3.088800455
C	0.378902038	1.306175018	3.316859471
C	0.240879207	-0.113127321	3.323774548
C	1.390164087	-0.908770867	3.110886115
C	1.154606952	-3.159094654	-0.251429890
C	1.274362367	-2.075048942	2.309081649
C	2.451610881	-2.643153221	1.758339467
C	1.177296435	-2.760983715	-1.647149295
C	2.440366521	-2.405949996	-2.204435737
C	2.395756199	-3.167258660	0.449275568
C	1.370149749	-0.479210648	-3.231071187
C	2.534254572	-1.265055237	-3.029600312
C	1.748596806	3.260138676	-1.774422608
C	1.501857546	0.933846462	-3.283856485

C	2.796875531	1.505801249	-3.110314811
C	1.813998143	3.764982637	-0.447160984
C	3.049876473	3.655165443	0.256412770
C	2.921649567	2.681820775	-2.340791437
C	1.766363739	2.993888332	2.224767305
C	3.025795196	3.264722503	1.612182328
C	1.662589087	1.861450064	3.077912634
C	2.822550900	1.060100381	3.288238396
C	2.684808539	-0.344065318	3.310685163
C	3.845289851	-1.147554511	3.115166487
C	3.621984828	-3.320558568	-0.265816764
C	3.727386467	-2.329050000	2.321413379
C	3.645101768	-2.925839764	-1.640787291
C	3.824410401	-0.711102546	-3.296571301
C	4.203310880	3.012216826	-1.808768364
C	3.957509808	0.710301509	-3.335217290
C	4.268545961	3.510265851	-0.470082088
C	4.221459329	2.744979321	2.190038251
C	4.117506658	1.611572855	3.055508859
C	5.371482041	2.479911964	-2.405557635
C	6.620840719	2.882694237	-1.846377152
H	7.547046380	2.682055273	-2.381612947
C	5.499617160	3.450611462	0.227555356
C	6.683747330	3.355093707	-0.562935769
H	7.658118127	3.518350460	-0.106199983
C	4.979389245	-1.509015320	-3.129045115
C	6.229972152	-0.911702515	-3.457268215
H	7.122703850	-1.528776244	-3.540538928
C	5.244838209	1.289618871	-3.202090001
C	6.359468182	0.452632021	-3.494142629
H	7.351786399	0.885675571	-3.605013675
C	4.840211490	-3.430726758	0.440953942
C	6.021909716	-3.608375105	-0.337897944
H	6.952115890	-3.906319417	0.142224178
C	4.886965370	-2.653017952	-2.256449223
C	6.044470708	-3.229018620	-1.653757885
H	6.992216910	-3.234302492	-2.188849857
C	5.130441822	-0.597250643	3.351159230
C	6.243440318	-1.470237750	3.186012409
H	7.227764382	-1.170675292	3.540933855
C	4.894065729	-2.925328014	1.790426952
C	6.128253146	-2.605240520	2.425733230
H	7.023926473	-3.179168558	2.195574847
C	5.475084722	3.053883434	1.608175943
C	6.633663858	2.542183789	2.265513435
H	7.620673400	2.915141277	1.998307855
C	5.270908515	0.832946467	3.315222289
C	6.533896957	1.460464563	3.098591009
H	7.443796465	0.997484753	3.475840174
C	-1.602907724	-5.582659909	0.914282240
H	-1.127139834	-5.031593117	1.743021660
H	-1.042862339	-6.525627329	0.795520797
C	-3.061049248	-5.899378918	1.292458591
H	-3.633459599	-4.959874890	1.360710964
H	-3.527755998	-6.491091729	0.485844953
C	-3.160226345	-6.640540681	2.620904764
H	-2.610006233	-7.595265520	2.553857731
H	-2.659393388	-6.041856533	3.401092513
C	-4.608963985	-6.897575631	3.023345857
H	-5.155732067	-5.947149472	3.123961929
H	-5.126610452	-7.505591537	2.265287601
H	-4.670389421	-7.427890138	3.984626345
C	-1.743765228	-6.653505224	-2.067840788
H	-1.432246405	-7.374901080	-1.302028332
H	-2.799940738	-6.841735893	-2.317828532
H	-1.159601181	-6.813671097	-2.985046253

RC*methyl*

165
Co2C121H36O6

C	1.369231021	-5.248869590	0.040464513
C	1.851494378	-4.820580108	2.410010164
C	2.521614632	-6.013440876	2.690214439
C	3.624368189	-6.011792247	3.543299754
C	3.514735633	-3.603977545	3.729031079
C	4.166863685	-4.810147191	3.995285743
C	5.507848764	-2.218818925	3.346601568
C	7.012188080	-1.326321372	1.621283833
C	7.999872575	-2.311444817	1.687710619
C	8.629567617	-2.747795059	0.522754338
C	7.185028017	-1.348630680	-0.818723192
C	8.171574526	-2.333014087	-0.727033540
C	5.937866997	-2.276860223	-2.720119950
C	4.016957609	-3.675090800	-3.345476455
C	4.698480119	-4.885063165	-3.493873204
C	4.097133722	-6.078151765	-3.096720963
C	2.185852589	-4.867302634	-2.244354202
C	2.887123082	-6.064366871	-2.404348346
C	1.190288056	-4.621751225	-1.200051610
C	-1.033749637	-1.775235659	-0.168183354
C	-0.241231162	-2.958366173	-0.098857133
C	0.224955698	-3.424702140	1.160573175
C	1.014056702	-4.597930833	1.230326512
C	-0.520774340	-1.292392560	2.162373515
C	0.277692337	-2.453775104	2.220219709
C	1.434405674	-2.471758772	3.038598372
C	2.242020464	-3.645447869	3.103188000
C	1.130805837	-0.083977474	3.480023158
C	1.933946733	-1.242860467	3.534983569
C	3.360912746	-1.129987854	3.660573976
C	4.163993486	-2.293402691	3.737340577
C	3.125596719	1.274684712	3.169147685
C	3.935408288	0.101121112	3.245994842
C	5.181169280	0.055041777	2.565036675
C	5.986556466	-1.106694079	2.641362982
C	4.560103079	2.146451360	1.408519997
C	5.345286653	0.977361014	1.476034489
C	5.954893035	0.470007346	0.303486335
C	6.759337404	-0.704785401	0.371458596
C	4.728251386	2.121738914	-1.017663102
C	5.515143672	0.953497591	-0.952290184
C	5.504902574	0.010661553	-2.035856711
C	6.313411323	-1.149950715	-1.976836885
C	3.552086534	1.212002764	-2.943046128
C	4.365919316	0.040093715	-2.884258772
C	3.854973772	-1.200607444	-3.349856488
C	4.661098389	-2.363111965	-3.291329286
C	1.621170125	-0.158108082	-3.505354302
C	2.424836375	-1.314881974	-3.423100639
C	1.861490352	-2.534607569	-2.975475446
C	2.670056166	-3.706389423	-2.900879707
C	-0.198568511	-1.345866147	-2.412773433
C	0.601535298	-2.503548523	-2.329353884
C	0.399449256	-3.450237789	-1.267774104
C	-1.184345481	-1.093316172	-1.405928677
C	-3.393657347	1.749310555	-0.375667472
C	-2.581114853	0.583212718	-0.305682072
C	-2.128707549	0.111214580	0.947873421
C	-1.354328886	-1.062373464	1.019076368
C	-2.934348471	2.214068647	1.968840610
C	-2.122796866	1.056306936	2.028261583
C	-0.994357080	1.019751662	2.888582534
C	-0.186846444	-0.156628226	2.952218892
C	-1.288604548	3.423242914	3.296519972
C	-0.484203137	2.259537795	3.359452852
C	0.946487837	2.369516232	3.432816436
C	1.747513801	1.210463235	3.510627289
C	0.706090153	4.761872463	2.912057491
C	1.511499046	3.587469672	2.983516003
C	2.768729448	3.552928474	2.333505122
C	3.567888119	2.393815001	2.412933132
C	2.182344924	5.675677832	1.209115801
C	2.971123577	4.502307821	1.274366211
C	3.609526562	4.011683771	0.104437816
C	4.406448088	2.829454193	0.171815022
C	2.346378446	5.647919367	-1.220221904
C	3.136064111	4.475321348	-1.151736000
C	3.080711496	3.503898214	-2.208599691
C	3.884371332	2.346479053	-2.154287732
C	1.117048743	4.694570121	-3.090138714
C	1.924998530	3.521602844	-3.026137697
C	1.428853852	2.293969025	-3.527142101
C	2.234962890	1.137068171	-3.472007076
C	-0.803508576	3.342326812	-3.730264111
C	0.002347850	2.180030976	-3.657503260



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C	0.241663053	-0.225928878	-3.171365782
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C	-1.817786568	0.989034988	-2.570617503
C	-1.971429536	0.072629257	-1.477322482
C	-3.660737451	2.356453393	-1.629395514
C	-5.286567074	3.765860858	-0.530340293
C	-4.809492384	3.376033377	0.720255842
C	-3.814979324	2.401544540	0.814232249
C	-2.563047972	3.339436385	2.716246690
C	-1.317369926	5.946681556	3.508437544
C	-0.641235754	4.733922789	3.356004287
C	-0.710208549	7.139252868	3.117624012
C	0.498913481	7.123130643	2.424009282
C	1.193173424	5.923015345	2.257943071
C	1.998610207	6.302570128	-0.030854981
C	0.844711154	7.064587258	-2.684186721
C	1.509327280	5.870093055	-2.399113422
C	-0.256073531	7.063229516	-3.539547206
C	-0.802690491	5.861537809	-3.987481541
C	-0.154976002	4.653645591	-3.717542198
C	-2.150054318	3.262748761	-3.345300654
C	-4.664914029	3.323628196	-1.696916841
H	2.089343726	-6.061604616	0.100483606
H	2.196043097	-6.940886633	2.220227480
H	4.116101355	-6.952072620	3.790760850
H	5.112060753	-4.806359708	4.537085275
H	6.072558835	-3.145755838	3.280021765
H	8.261484616	-2.752508212	2.648992690
H	9.431577215	-3.482602767	0.586267292
H	8.566157888	-2.790617957	-1.633653272
H	6.488114204	-3.200659997	-2.557891855
H	5.709177172	-4.890932449	-3.900677727
H	4.616592554	-7.022558533	-3.256042213
H	2.496872032	-6.983195816	-1.968056931
H	-6.102672786	4.484706389	-0.594846407
H	-5.199114867	3.845383764	1.623175661
H	-3.112031401	4.263995400	2.553711341
H	-2.328603431	5.955860728	3.913651507
H	-1.224585702	8.085583062	3.281934544
H	0.893624313	8.041376848	1.990260848
H	1.281858438	7.118326224	-0.088589812
H	1.175846694	7.992758502	-2.219509630
H	-0.742043575	8.004662774	-3.793793387
H	-1.745952901	5.860130660	-4.532470345
H	-2.717257050	4.188278132	-3.278093654
H	-4.944168098	3.747657012	-2.661167956
Co	-4.553025879	-2.299561085	-0.985420277
Co	-6.857478881	-1.770637183	-0.222422935
C	-6.086878827	-3.283314944	-1.288924347
C	-3.360095648	-3.352116645	-1.717465883
C	-7.556407415	-2.694551077	1.131191339
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C	-8.178471261	-1.804517457	-1.391988534
O	-2.563408593	-4.064336691	-2.162959568
O	-6.477128784	-4.275253360	-1.786277969
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O	-9.072393335	-1.828568761	-2.123453454
C	-4.280736429	-2.787803444	0.759579486
C	-5.098109648	-1.732010132	0.902409676
C	-4.714387715	-1.012169349	-2.240496923
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H	-7.019693241	-0.361299806	2.516152873
H	-6.119223270	-1.460274258	3.571625751
C	-5.729207792	0.650556640	3.921462608
H	-4.727511341	0.512399119	4.364366656
H	-5.669939683	1.569075177	3.311653990
C	-6.766313011	0.829324949	5.024142193
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H	-6.822771599	-0.068548727	5.658643441
H	-6.519828733	1.684457932	5.670359135
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H	-4.025618569	-4.502499968	1.961664349
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H	-3.049424411	-3.108773432	2.457771821

RC*butyl*

165
Co2C121H36O6

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C	1.656950343	-4.872558290	2.194067985
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C	3.433538944	-6.199476944	3.156753933
C	3.471084158	-3.797888302	3.436256933
C	4.072128556	-5.046809242	3.611357938
C	5.506142334	-2.502330555	2.964212671
C	6.938731697	-1.616245984	1.174755720
C	7.874893462	-2.651929508	1.134784846
C	8.401733779	-3.069476962	-0.086776794
C	6.947024609	-1.544376230	-1.270534888
C	7.883730966	-2.580173723	-1.285242587
C	5.522228448	-2.328862947	-3.111124905
C	3.488642254	-3.599129429	-3.649795148
C	4.092389447	-4.835070150	-3.892172124
C	3.455521633	-6.011602627	-3.501397186
C	1.673143915	-4.742171087	-2.472498296
C	2.297002791	-5.965429357	-2.727029297
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C	3.447790267	-1.317752561	3.468408402
C	4.189907796	-2.523742909	3.445341395
C	3.310031760	1.113946685	3.084353670
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C	5.393666839	0.774376299	1.233478266
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C	6.637420455	-0.930241037	-0.029807425
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C	5.399896191	0.844428014	-1.199862815
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C	6.009747954	-1.253849902	-2.355995880
C	3.321099659	1.285373822	-3.034104551
C	4.071431498	0.071226943	-3.076834301
C	3.461969340	-1.121629944	-3.549156152
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C	1.283352465	0.040699336	-3.505016210
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C	2.174849474	-3.580155324	-3.114404623
C	-0.520114748	-1.096505074	-2.333610132
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C	-2.659554801	0.853656495	0.006154289
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C	-2.020794388	1.203345803	2.319051666
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C	4.473815127	2.726701986	0.069457845
C	2.482934957	5.704615895	-1.067832269
C	3.209916047	4.490650750	-1.099100399
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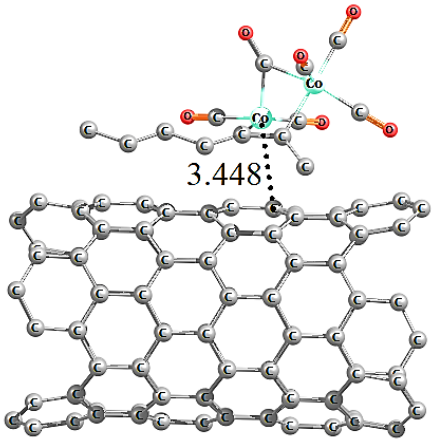

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H	8.191603978	-3.018653994	-2.233922509
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H	5.071741896	-4.875243739	-4.367821815
H	3.911674020	-6.973607686	-3.732831812
H	1.889231729	-6.880944656	-2.299886403
H	-5.960288190	4.954986259	0.106012186
H	-4.955824147	4.166833929	2.232637235
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H	1.377329925	8.030929567	2.325086530
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Co	-4.767754482	-1.822982572	-0.752063985
Co	-7.019145407	-1.197170170	0.078434317
C	-6.369607819	-2.735803370	-0.982494719
C	-3.709585040	-2.868275439	-1.681859482
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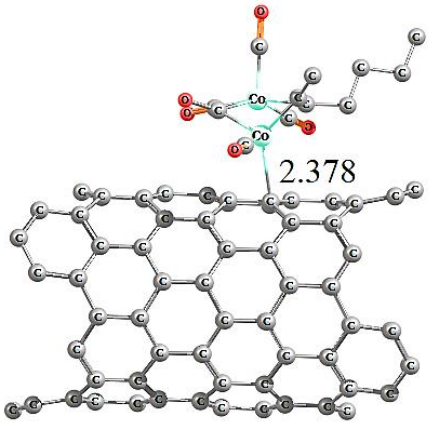
CP3*methyl*



163
Co2C120H36O5

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H	-5.733054368	-3.140170946	2.329485877
H	-3.593728511	-3.948641040	2.939472660
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H	-2.529752599	-7.479049918	-3.859805492
H	-3.312333875	-5.172668347	-4.330354064
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H	3.135243593	6.460400015	2.583455972
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H	5.984908757	3.798856544	4.380774377
H	6.556248441	2.122653086	2.922484212
H	8.580805087	1.496484154	1.995021264
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H	8.356774926	1.837229603	-2.279050927
H	6.257701685	2.579282076	-2.894671501
H	5.568373884	4.448392034	-4.022450661
Co	-3.851339727	2.229746253	-1.548072326
Co	-4.541850723	2.991019001	0.787192725
C	-3.416128378	3.809706074	-0.755262326
C	-3.300151321	2.527046593	-3.174840548
C	-5.851792865	4.198812440	0.808443919
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O	-6.725524630	4.951174267	0.906007957
O	-4.957782161	0.928132799	2.828251162
O	-2.464857056	4.212895352	2.436855755
C	-5.636777686	2.261796006	-1.816980701
C	-5.619123321	1.824705137	-0.548933073
C	-6.540119138	0.741759975	-0.039393357
H	-5.972897975	0.026375786	0.572105913
H	-6.918851989	0.173793808	-0.907417634
C	-7.722876196	1.243254417	0.785595966
H	-7.359570149	1.847338829	1.632239877
H	-8.353801995	1.911149642	0.173138962
C	-8.541730700	0.070032431	1.316622439
H	-8.897543116	-0.540181154	0.467679999
H	-7.873590241	-0.580381474	1.907933153
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H	-10.412439400	1.147735072	1.594397771
H	-10.293668693	-0.351418111	2.546847971
H	-9.379670060	1.093706241	3.040791740
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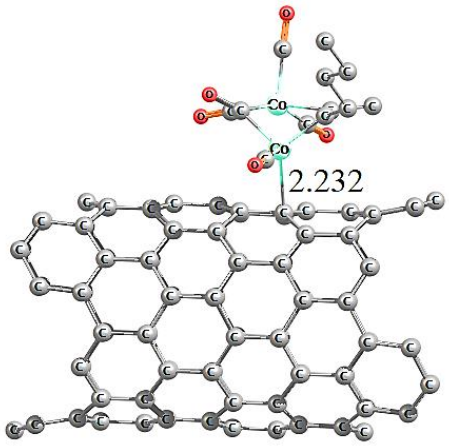
H	-6.120633239	2.328925885	-3.906406966
H	-7.475492559	1.909462297	-2.797920446
H	-6.882535536	3.578533958	-2.884279973

CP3*butyl*



163
Co2C120H36O5

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C	-3.763193998	-2.440883815	2.016611465
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C	-0.147695801	-5.167624143	3.228487156
C	-0.822761917	-6.377997767	3.402446971
C	-0.411176175	-7.514148419	2.707024341
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C	0.290615157	-5.515247327	-2.985021084
C	-0.490927063	-6.646325273	-3.229079274
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C	-2.698564088	-0.604679428	-1.577587407
C	-3.562602821	-1.721789257	-1.573937980
C	-1.696966148	1.328925701	-0.371797486
C	-2.556284201	0.194118282	-0.375143637
C	-2.784937060	-0.509876124	0.851091972
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C	2.386197415	-1.743871566	3.178400671
C	1.530570353	-2.865900048	3.173013594
C	1.884671330	-4.018165970	2.430563138
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C	3.095820587	-4.066736378	-0.944107125
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C	1.430837725	-5.477256560	-2.069418061
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C	0.827344805	2.091834054	2.838669784
C	-0.018988073	0.963880854	2.850853251
C	3.020734634	3.111049935	3.291315142
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C	2.708511247	0.678258550	3.471014500
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C	3.515389148	2.714938511	-3.613841613
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C	1.275317571	1.730586326	-3.252784689
C	2.953479620	4.031570978	-3.314974157
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C	4.596580855	5.367215112	3.647567339
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C	7.069844872	0.947080038	0.258754750
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H	0.775367017	-8.276523426	1.073656830
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H	-0.095168450	-7.636478233	-3.005426683
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H	-3.422511543	-5.149801558	-4.092226141
H	3.737300664	7.323234841	-2.960168207
H	2.044549665	7.139799340	-1.155174411
H	2.178763833	5.936914129	0.802079764
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H	6.229970699	4.008645842	4.022485299
H	6.721825390	2.526307863	2.338582725
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H	7.741116412	2.844361080	-3.073129854
H	5.515997797	3.411176219	-3.315336135
H	4.496226001	5.284702130	-4.152011095
Co	-4.193931485	1.681957076	-0.665971530
Co	-4.785338952	2.282745518	1.771328040
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C	-3.991261840	2.066586173	-2.343575364
C	-6.236072543	3.259348456	2.113531627
C	-4.599310136	0.952684023	2.933013973
C	-3.472117573	3.179579464	2.547753425
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O	-4.059852648	4.471130996	-0.120860286
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O	-4.535429261	0.121178996	3.737025708
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C	-5.939511779	1.003037141	0.623814658
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H	-6.359052913	0.392381824	-2.599603688
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H	-7.932081518	2.878532151	-1.713560912
H	-6.500783143	2.913886100	-2.751688831
C	-8.234710525	2.042945487	-3.697512977
H	-7.653220874	1.446776701	-4.422282973
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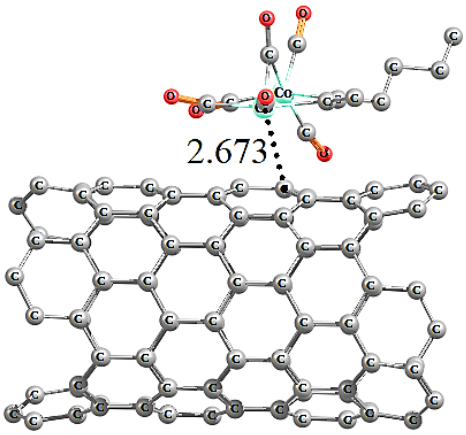
CP3'*methyl*



165
Co2C121H36O6

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C	5.960061425	4.521172804	-3.571267986
C	5.578078794	2.172358127	-3.147495715
C	6.457736550	3.239842742	-3.340562653
C	6.862781340	0.976860990	-1.429047048
C	7.123386125	0.672349852	0.993825160
C	8.148966431	1.597172331	1.201290068
C	8.158755654	2.381161880	2.354153379
C	6.034041875	1.453752206	3.040109768
C	7.070709994	2.371140472	3.225783518
C	4.159075479	2.911203609	3.674675163
C	2.424911103	4.424174234	2.814316067
C	3.117639420	5.626062440	2.979319570
C	2.992186061	6.640083622	2.031534050
C	1.611250881	5.217164209	0.649151378
C	2.312347883	6.409865580	0.836063575
C	1.264898496	4.654983183	-0.656519115
C	-0.553565043	1.626445398	-1.930060114
C	0.350567957	2.726747601	-1.866423091
C	1.462985598	2.781809606	-2.748638879
C	2.356277064	3.878982340	-2.692133448
C	0.990214700	0.446892531	-3.391379638
C	1.885568984	1.533651302	-3.317647705
C	3.281767939	1.302669225	-3.376995755
C	4.187753415	2.401579921	-3.312741216
C	2.860901668	-1.103522942	-3.268535670
C	3.758590432	-0.017398395	-3.197107028
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C	4.189964583	-2.298782349	-1.618128880
C	5.105128311	-1.204206780	-1.563430341
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C	6.736215288	0.139572523	-0.312715769
C	4.388089808	-2.582870692	0.788951200
C	5.272918309	-1.486262947	0.839968422
C	5.275807577	-0.635647170	1.971568431
C	6.176221977	0.467905120	2.029962564
C	3.308742738	-1.809145337	2.825873829
C	4.191102859	-0.710386467	2.877558617
C	3.781507464	0.521229478	3.493261955
C	4.678094334	1.614283748	3.565393480
C	1.479652082	-0.359336042	3.511822003
C	2.381881903	0.744676533	3.585354265
C	1.903795616	2.064879939	3.371526936
C	2.798667843	3.159552642	3.446486418
C	-0.231497239	1.103658291	2.584309637
C	0.667844976	2.188304619	2.648146628
C	0.601418481	3.214280902	1.675391743
C	1.507826419	4.313137890	1.737898038
C	-1.054004546	1.907684205	0.439651555
C	-0.147109564	2.982700659	0.495645806
C	0.376601851	3.557431223	-0.714280499
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C	-3.217083637	-1.687543198	-2.090642985
C	-2.322030860	-0.581535457	-2.033331703
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C	-0.336349800	0.581807934	-2.861983667
C	-1.718333829	-2.835780526	-3.620056314
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C	-1.205126169	-3.645801389	3.269335161
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C	-0.782733153	-1.226768659	3.142788707
C	0.107594212	-0.136127101	3.220039676
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C	-3.758234018	-1.381853577	0.255125744
C	-2.863741243	-0.290530088	0.314094061
C	-2.352503793	0.290010169	-0.904851818
C	-4.161582573	-1.897854962	-1.051877957
C	-5.205068846	-3.589784935	-2.427227156
C	-4.120854848	-3.576235376	-3.302929240
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C	-1.203176222	-4.136963826	-3.717483664
C	-0.161866575	-6.857658281	-3.007098485
C	0.526091582	-5.653283283	-2.842416534
C	-0.027351912	-7.873957512	-2.062093490
C	0.656085800	-7.644893397	-0.868813165
C	1.351553378	-6.448727347	-0.680645659
C	0.831591262	-6.110336614	1.694951303
C	-1.605833523	-6.027015184	3.426375201
C	-0.708945106	-4.974494791	3.232987439
C	-2.971958553	-5.769030064	3.530845430
C	-3.471681233	-4.491326328	3.283869408
C	-2.594478877	-3.421541692	3.090026281
C	-3.875417649	-2.229932630	1.362850699
C	-5.184574239	-2.822475431	-1.261649816
H	2.921542517	5.627599117	-1.598958248
H	4.230622376	5.808113556	-3.487079646
H	6.651124797	5.340870366	-3.764966808
H	7.532856411	3.071552509	-3.288333459
H	7.457376616	1.881076347	-1.323052305
H	8.928046681	1.719856734	0.449646160
H	8.985426266	3.068287907	2.531731814
H	7.016343543	3.092268064	4.040568142
H	4.850941903	3.745871071	3.590828305
H	3.773311488	5.759104172	3.839061247
H	3.500250429	7.590946198	2.188532446
H	2.346846164	7.148530505	0.036038290
H	-6.033089675	-4.275415698	-2.606461479
H	-4.070243071	-4.290986447	-4.124064902
H	-1.899625218	-4.968144132	-3.634073416
H	-0.818576920	-6.993566100	-3.865663551
H	-0.529469938	-8.827823653	-2.220812132
H	0.631600185	-8.388095135	-0.072411166
H	0.064736933	-6.872522926	1.578298369
H	-1.237062075	-7.051226451	3.472716994
H	-3.661740028	-6.589546236	3.726191383
H	-4.547008016	-4.327935248	3.220967718
H	-4.465513049	-3.136571806	1.250239877
H	-5.952066629	-2.967320781	-0.502022205
Co	-3.807298983	2.421574153	-1.601352565
Co	-5.060202939	2.551828789	0.734233093
C	-5.279114281	3.443918499	-1.223593221
C	-3.598492550	2.285565880	-3.338071290
C	-6.616363990	3.313585291	1.155545801
C	-4.801618480	1.316578980	1.959095744
C	-3.825950231	3.684928251	1.370480702
O	-3.493988611	2.239133466	-4.487934406
O	-6.023101416	4.210145574	-1.710300079
O	-7.583403076	3.845956250	1.498613825
O	-4.816689579	0.529556211	2.810689499
O	-3.002788813	4.377333223	1.793197662
C	-5.245670516	1.045747070	-1.637196924
C	-5.769145502	0.979479607	-0.413725845
C	-2.736717861	3.859488761	-1.408242966
O	-2.182399477	4.870491100	-1.367413998
C	-6.724312652	-0.046562148	0.108402341
H	-6.201782081	-0.684061253	0.844814185
H	-7.012836006	-0.705570739	-0.728496508
C	-7.991132436	0.485802736	0.771372797
H	-7.726173827	1.032785754	1.689700053
H	-8.491071981	1.205330832	0.100919571
C	-8.944020643	-0.651441934	1.129497519
H	-9.221761406	-1.195648007	0.209560910
H	-8.409892720	-1.374037088	1.772381083
C	-10.202530723	-0.164566956	1.840188688
H	-10.759614182	0.543066297	1.207195170
H	-10.873690841	-0.999909792	2.088091879
H	-9.946050917	0.354958483	2.776205784
C	-5.653236781	0.312976555	-2.873959437
H	-4.794143950	-0.127149227	-3.402304115
H	-6.365717252	-0.496553572	-2.650048890
H	-6.142295092	1.012200473	-3.572782489

CP3'*butyl*

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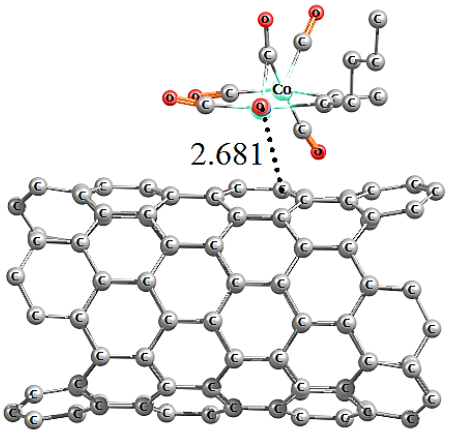
Co2C121H36O6

C	-1.625521802	-5.027922226	-1.474562309
C	-2.990062851	-4.065037290	-3.277749549
C	-3.792465924	-5.178819838	-3.534410077
C	-5.138165926	-5.010787936	-3.857662934
C	-4.953450521	-2.625070368	-3.515948942
C	-5.734923125	-3.754178064	-3.770632624
C	-6.535879851	-1.432857302	-2.064160506
C	-7.158593869	-1.028486718	0.276686674
C	-8.150707521	-2.004669901	0.390121673
C	-8.283288222	-2.730493332	1.573103579
C	-6.333467306	-1.639727519	2.496903916
C	-7.334194580	-2.609903774	2.587137186
C	-4.492155721	-2.945882138	3.468272592
C	-2.573134968	-4.387603184	2.943911912
C	-3.215674553	-5.620918478	3.076714644
C	-2.899363678	-6.669263347	2.214727083
C	-1.413149681	-5.231272419	0.963465294
C	-2.067693169	-6.454809567	1.116166805
C	-0.912731786	-4.710754234	-0.309062576
C	0.895757989	-1.633336925	-1.476090101
C	0.056592337	-2.786062930	-1.481383173
C	-0.911726449	-2.952360444	-2.507617484
C	-1.740649965	-4.100357426	-2.517681693
C	-0.482768258	-0.624854842	-3.206241212
C	-1.316808802	-1.761769309	-3.199543496
C	-2.700387602	-1.623141291	-3.468750395
C	-3.543186248	-2.773007286	-3.471319517
C	-2.435296466	0.807258249	-3.439787690
C	-3.271449914	-0.328997199	-3.433320172
C	-4.622139273	-0.233316491	-2.952976218
C	-5.465318166	-1.370159917	-2.966518891
C	-4.052152391	1.993601888	-2.062658054
C	-4.902649953	0.846845504	-2.074521278
C	-5.774436145	0.600673682	-0.980557794
C	-6.617859010	-0.536258102	-0.990541432
C	-4.606329408	2.378479771	0.273735391
C	-5.427411998	1.232230568	0.262190171
C	-5.545135219	0.438402731	1.428419185
C	-6.382936865	-0.714928538	1.422367750
C	-3.786411002	1.771166766	2.481078427
C	-4.606511790	0.623930964	2.471440543
C	-4.222920113	-0.548546851	3.207431469
C	-5.059937463	-1.690197583	3.215132174
C	-1.998364993	0.472278266	3.498310008
C	-2.840854281	-0.680227410	3.507246162
C	-2.266138707	-1.977152617	3.437036632
C	-3.101670567	-3.120124017	3.446470675
C	-0.093998329	-0.925943253	2.907784653
C	-0.934059610	-2.058875159	2.903446144
C	-0.672343431	-3.123801650	2.008959559
C	-1.518003819	-4.271622832	2.003184053
C	1.075292032	-1.780196030	0.951399588
C	0.227302767	-2.903967440	0.937027750
C	-0.086956018	-3.564058493	-0.301622081
C	1.622873851	-1.290172078	-0.291517962
C	3.361016340	1.835566409	-1.438097318
C	2.530157605	0.678619633	-1.447532714
C	1.585148526	0.496991574	-2.480380188
C	0.757309838	-0.649023752	-2.485414217
C	2.041400453	2.809291049	-3.231453493
C	1.202758398	1.669205757	-3.220225108
C	-0.179591468	1.803624750	-3.518156916
C	-1.024804257	0.652477193	-3.512130033
C	0.084938829	4.244469530	-3.453915053
C	-0.751451450	3.101199238	-3.446482921
C	-2.083802298	3.182825314	-2.915638164
C	-2.927116423	2.052600471	-2.929008764
C	-1.500865247	5.393878809	-2.010427178
C	-2.344343717	4.244608125	-2.016807919
C	-3.242320300	4.020934227	-0.945487227
C	-4.082948220	2.888734946	-0.959419784
C	-2.117491684	5.836889012	0.299067170
C	-2.943339916	4.687477285	0.291630776
C	-3.091557956	3.912576677	1.472791291
C	-3.924790505	2.753284491	1.463265192
C	-1.296669793	5.229211778	2.509240472
C	-2.123971716	4.080464847	2.498953041
C	-1.713915928	2.888386143	3.187616582
C	-2.544883450	1.749235691	3.196686447
C	0.512320078	3.901720939	3.449835181
C	-0.329173703	2.751113129	3.448036756
C	0.244036631	1.457818653	3.405924719
C	-0.588284287	0.319838500	3.417088925
C	2.435848294	2.499611597	2.937636823
C	1.591885530	1.364939607	2.919296280



C	1.869977973	0.286621640	2.038892586
C	1.029978089	-0.868526068	2.038912735
C	3.597819802	1.656084353	0.971969409
C	2.761524657	0.517726144	0.961931955
C	2.453958913	-0.141997606	-0.284269899
C	4.141095018	2.146823558	-0.293744285
C	5.270626993	3.839467121	-1.599904720
C	4.326428063	3.715066078	-2.617202411
C	3.315863563	2.755290534	-2.516567060
C	1.474521249	4.068131224	-3.479851720
C	0.190441091	6.748347528	-3.085590998
C	-0.445557391	5.512147124	-2.951082452
C	-0.133637825	7.797721558	-2.226571659
C	-0.965483319	7.582381245	-1.128721945
C	-1.612517596	6.354782411	-0.972733424
C	-1.411755444	6.158342534	1.466432946
C	0.756027657	6.308245624	3.522181762
C	-0.044700683	5.193613666	3.264974058
C	2.103764888	6.141209545	3.837153544
C	2.702740756	4.886008097	3.741777113
C	1.923205648	3.754989008	3.487459154
C	3.510051929	2.558059190	2.039868314
C	5.128469252	3.125486189	-0.409226067
H	-2.360348731	-5.827765882	-1.420201038
H	-3.368945155	-6.179849999	-3.460388879
H	-5.747120082	-5.881034730	-4.100458614
H	-6.814208709	-3.652320093	-3.879081811
H	-7.087574986	-2.367125418	-1.991339622
H	-8.805486471	-2.212500305	-0.455553535
H	-9.087972337	-3.458468856	1.671607106
H	-7.358122824	-3.285587372	3.441456239
H	-5.118491558	-3.824774099	3.335058026
H	-3.979820928	-5.753454809	3.841827770
H	-3.371630444	-7.641450812	2.351924786
H	-1.945607282	-7.231991524	0.362447210
H	6.076296442	4.566682973	-1.699217435
H	4.356344753	4.383037701	-3.477755233
H	2.103306056	4.945325991	-3.346184056
H	0.954261161	6.884338655	-3.850375654
H	0.331826102	8.772799250	-2.366833850
H	-1.095631110	8.362215924	-0.379027247
H	-0.679275860	6.960414086	1.414552821
H	0.329581240	7.308597093	3.454690756
H	2.711801751	7.011894424	4.080687322
H	3.782721028	4.787153790	3.845039971
H	4.060550397	3.492755347	1.963341658
H	5.773562682	3.350388367	0.439578275
Co	4.099079314	-2.207094429	-0.752598118
Co	5.172320070	-2.174925458	1.677400323
C	5.606262658	-3.108829272	-0.222553888
C	3.989456933	-2.137810605	-2.503333101
C	6.797186972	-2.614515376	2.247520407
C	4.597777714	-0.945287852	2.806058604
C	4.090826403	-3.475952772	2.275409882
O	3.922323724	-2.128532699	-3.657561607
O	6.439809133	-3.834317112	-0.617221698
O	7.845373612	-2.859037710	2.669901160
O	4.400582704	-0.151556417	3.627505319
O	3.362357047	-4.286866641	2.656895126
C	5.418295883	-0.721789047	-0.716446124
C	5.859790311	-0.604521126	0.533418959
C	3.114026639	-3.704131954	-0.561326184
O	2.613301901	-4.741264124	-0.492353871
C	5.872877380	0.018239065	-1.934120744
H	6.302181750	0.992197816	-1.639979365
H	5.017091112	0.247297510	-2.590827028
C	6.919213250	-0.754469522	-2.739933455
H	7.834374789	-0.860076932	-2.131597286
H	6.563298672	-1.779044249	-2.937905198
C	7.226802453	-0.056643509	-4.060738328
H	6.293610504	0.016991114	-4.646016772
H	7.546887603	0.980495993	-3.856555222
C	8.293021938	-0.777328680	-4.878447636
H	9.240880885	-0.838271620	-4.321477478
H	7.975926608	-1.805243310	-5.112789878
H	8.489668667	-0.258556417	-5.828231679
C	6.776806637	0.422128895	1.106807008
H	7.683060520	-0.054674358	1.514284194
H	7.087018141	1.149036005	0.339792480
H	6.300364850	0.966960752	1.937971806

TS1*methyl,parallel*

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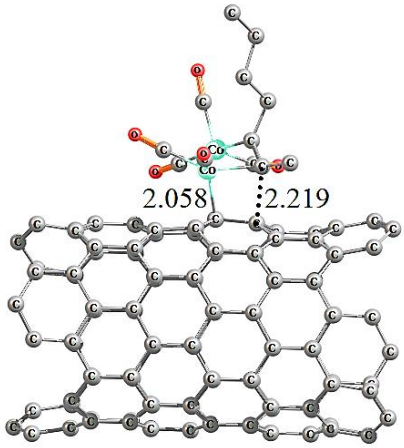
Co2C120H36O5

C	0.904698434	-4.952734712	-1.313584381
C	-0.598671809	-4.608209188	-3.220494760
C	-0.855839584	-5.949351937	-3.513490106
C	-2.128246769	-6.344038440	-3.923502705
C	-2.958214619	-4.095185021	-3.610091528
C	-3.190685934	-5.442650613	-3.895195352
C	-5.015315797	-3.656214921	-2.329825301
C	-5.977696142	-3.521312696	-0.073419976
C	-6.490421324	-4.817911496	0.004010847
C	-6.422039463	-5.524018645	1.204333712
C	-5.174600918	-3.722745787	2.226582578
C	-5.697532986	-5.016858588	2.282090862
C	-3.036855544	-4.162014027	3.349217245
C	-0.665435444	-4.702506129	2.984504586
C	-0.758031207	-6.089182974	3.126793111
C	0.031080643	-6.926820428	2.340633171
C	0.916056719	-5.022501801	1.142800572
C	0.803484236	-6.404850605	1.303964961
C	1.303830106	-4.361940576	-0.103287003
C	1.993430511	-0.839439571	-1.282362860
C	1.567684213	-2.225561376	-1.278783884
C	0.800972937	-2.753049015	-2.342725225
C	0.503653927	-4.141654077	-2.380241075
C	0.264599331	-0.434981096	-3.010067559
C	-0.023512536	-1.817800975	-3.059185062
C	-1.319405256	-2.257514967	-3.421116607
C	-1.617416129	-3.652713637	-3.465993920
C	-2.085980679	0.062410786	-3.448562502
C	-2.376241504	-1.316027483	-3.463902625
C	-3.684923312	-1.781720809	-3.105034326
C	-3.983127953	-3.164674882	-3.139832834
C	-4.178174634	0.489974719	-2.285837517
C	-4.472159992	-0.905701943	-2.310685469
C	-5.269870961	-1.478794848	-1.285539005
C	-5.564702791	-2.862910512	-1.312447803
C	-5.055391984	0.635380233	-0.024472706
C	-5.331852118	-0.747449273	-0.049790579
C	-5.215464056	-1.510748594	1.136810358
C	-5.506208715	-2.906297800	1.115107569
C	-4.234852047	0.431431845	2.254488829
C	-4.518603332	-0.950471676	2.234527330
C	-3.747121943	-1.862321798	3.033647788
C	-4.047942119	-3.245697635	3.028266685
C	-2.146677253	-0.026102237	3.412070242
C	-2.452312199	-1.420396727	3.414340226
C	-1.399066823	-2.372733733	3.413294768
C	-1.697103983	-3.757188405	3.410142199
C	0.190285730	-0.535367938	2.966188183
C	-0.119147061	-1.909411853	2.958555755
C	0.615735682	-2.780493859	2.123631022
C	0.323787174	-4.175594534	2.114932626
C	1.806376844	-0.867929066	1.179303161
C	1.456582290	-2.225659751	1.134624052
C	1.601488298	-2.983241127	-0.081744524
C	2.446984812	-0.257199701	0.009630416
C	2.567794324	3.397601604	-1.069249742
C	2.276974640	2.001771494	-1.093321546
C	1.593962117	1.437196637	-2.184620555
C	1.374027442	0.045725484	-2.242451619
C	1.110763686	3.736627954	-2.979640753
C	0.818303356	2.351582289	-2.981069846
C	-0.456060463	1.899954099	-3.397662059
C	-0.738233011	0.502588930	-3.392563449
C	-1.226728359	4.232289505	-3.448565911
C	-1.514943962	2.846522517	-3.448489912
C	-2.805765423	2.376878313	-3.034042111
C	-3.096954308	0.997933220	-3.053440990
C	-3.271879667	4.641830256	-2.199025481
C	-3.565545626	3.247274979	-2.216475940
C	-4.384993978	2.683957063	-1.208107979
C	-4.680741546	1.305543244	-1.235212874
C	-4.198641407	4.810819259	0.039293781
C	-4.484761088	3.424578868	0.019354637
C	-4.391769259	2.663886383	1.215643485
C	-4.682745900	1.265772175	1.194410522
C	-3.347743706	4.600828756	2.310202182
C	-3.643200455	3.216388003	2.289734118
C	-2.834164953	2.295711506	3.037563049
C	-3.139594520	0.919392811	3.040032217
C	-1.224090921	4.121459106	3.400199267
C	-1.529228417	2.729671319	3.376951462
C	-0.484555038	1.778493524	3.408160462
C	-0.793226138	0.404168611	3.406319358
C	1.144291939	3.609542156	3.106010743
C	0.829034682	2.229612721	3.038800734



C	1.612442989	1.353183277	2.241513487
C	1.267382099	-0.037729188	2.183112469
C	2.781742936	3.300639779	1.331746367
C	2.499314168	1.917801760	1.286240513
C	2.650921499	1.200867280	0.023568658
C	3.150046721	3.979979496	0.085645951
C	3.580702334	5.975223684	-1.205527179
C	2.790248629	5.495320471	-2.248105494
C	2.229426937	4.216658643	-2.171214303
C	0.108380364	4.645558971	-3.341348760
C	-2.189575756	6.561493940	-3.197090182
C	-2.275213093	5.174037459	-3.056859995
C	-2.987992076	7.393063021	-2.413266426
C	-3.752195336	6.865014322	-1.373131993
C	-3.853693735	5.481676012	-1.214557792
C	-3.760569594	5.397863485	1.234382427
C	-1.975579891	6.420788284	3.412766377
C	-2.239060425	5.077182415	3.138057690
C	-0.704140180	6.811088007	3.830200664
C	0.353484742	5.902801441	3.828363922
C	0.118762549	4.553356123	3.553660331
C	2.205094349	4.094445447	2.332835687
C	3.699212294	5.256388601	-0.012976360
H	0.558450857	-5.983175312	-1.292738295
H	-0.064188750	-6.688891096	-3.398303066
H	-2.310409846	-7.384217288	-4.191802216
H	-4.207360651	-5.788916371	-4.078000675
H	-5.140809106	-4.734205762	-2.260003618
H	-6.921503812	-5.283610730	-0.881640852
H	-6.865129551	-6.517138083	1.271832930
H	-5.515956037	-5.636884522	3.159378338
H	-3.244171888	-5.219880928	3.205903056
H	-1.462616023	-6.514185841	3.840854698
H	-0.016812039	-8.005455805	2.486853938
H	1.304186399	-7.073564213	0.604591467
H	4.047843395	6.955951724	-1.291880511
H	2.598618799	6.119106381	-3.121008421
H	0.306692591	5.705985450	-3.203024059
H	-1.481018881	6.991744636	-3.904004378
H	-2.949164254	8.472106045	-2.559406410
H	-4.250225992	7.528968167	-0.667207363
H	-3.411211794	6.427116558	1.197895699
H	-2.761255155	7.164454045	3.283463412
H	-0.518165808	7.853534504	4.086814430
H	1.368442626	6.247338910	4.022852290
H	2.335529679	5.171916624	2.262273052
H	4.195724437	5.701944958	0.849362566
Co	4.114044198	-0.915969190	-1.002063928
Co	4.864879177	-0.851888299	1.462346694
C	4.450553605	-1.065873894	-2.738288847
C	6.415839851	-1.686650801	1.634058880
C	4.677806952	0.557894040	2.507925724
C	4.066390864	-2.029732305	2.541220458
O	4.621957859	-1.123933551	-3.880326589
O	7.452664683	-2.142917751	1.878334847
O	4.805915005	1.395056619	3.299899582
O	3.592511765	-2.787247840	3.271390271
C	4.662211360	0.928748223	-0.873185917
C	5.474317095	0.335462406	0.057590795
C	4.421167701	-2.615508249	-0.555121090
O	4.718291486	-3.725595247	-0.395471859
C	6.975586477	0.573411306	-0.095283467
H	7.469431949	0.507002891	0.883970315
H	7.148328643	1.599376162	-0.460514139
C	7.603153265	-0.431545925	-1.062182638
H	7.290268660	-1.452034326	-0.787456563
H	7.208596564	-0.260732076	-2.078286589
C	9.126209220	-0.355427049	-1.080977704
H	9.439560018	0.672774915	-1.332794631
H	9.505408328	-0.560781507	-0.065247916
C	9.735859336	-1.343123613	-2.070468020
H	9.383907635	-1.141027423	-3.094011352
H	10.833943507	-1.285718683	-2.071487125
H	9.449436763	-2.375056794	-1.815760116
C	5.009962090	1.892797178	-1.949369002
H	4.243259702	1.937041653	-2.734511079
H	5.190754133	2.909278853	-1.564662644
H	5.934681597	1.536475069	-2.435310985

TS1'*methyl,parallel*

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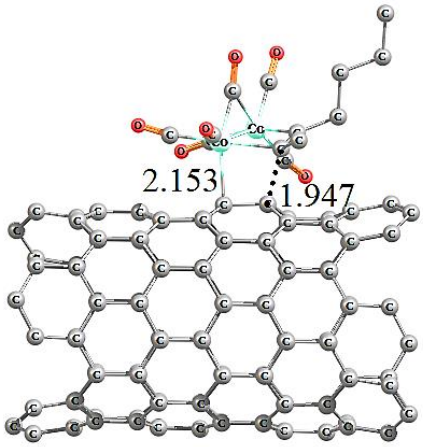
Co2C121H36O6

C	-1.562296474	4.919815967	1.685837659
C	-3.076386161	3.898189945	3.330503746
C	-3.871909309	5.016440399	3.588164615
C	-5.239502240	4.864483067	3.813115084
C	-5.078784841	2.492959317	3.373059883
C	-5.853238039	3.627186437	3.628215145
C	-6.592531405	1.394927990	1.779145519
C	-7.068712782	1.091570228	-0.610041610
C	-8.024475968	2.099410386	-0.753202591
C	-8.050525549	2.875795185	-1.911141890
C	-6.065503938	1.768441909	-2.735681540
C	-7.032514154	2.769288040	-2.857515554
C	-4.125259813	3.063329059	-3.508569317
C	-2.219726527	4.440840655	-2.794101363
C	-2.823276032	5.693860808	-2.934834279
C	-2.543238385	6.711439992	-2.025492604
C	-1.169746865	5.209347074	-0.723048668
C	-1.788217441	6.449889162	-0.882036907
C	-0.761232339	4.643060253	0.563213001
C	0.937221670	1.505621820	1.722499868
C	0.093666713	2.655283444	1.721365499
C	-0.967067216	2.776256722	2.656109402
C	-1.775955533	3.943193814	2.662573400
C	-0.633704681	0.410927741	3.229641033
C	-1.444314724	1.563918693	3.246741282
C	-2.846968242	1.443772957	3.421365867
C	-3.665665211	2.610933715	3.425684724
C	-2.627221066	-0.985961357	3.297654573
C	-3.441103420	0.168061105	3.293993715
C	-4.764014845	0.118763058	2.737375839
C	-5.581943777	1.273500938	2.743245335
C	-4.197781869	-2.093971505	1.808366403
C	-5.018815510	-0.925539393	1.808753051
C	-5.815536227	-0.621090186	0.673861072
C	-6.628380008	0.538520055	0.670989413
C	-4.614295269	-2.387242550	-0.566980388
C	-5.403180347	-1.218446866	-0.566255949
C	-5.413837444	-0.374350014	-1.703082746
C	-6.219645308	0.801628307	-1.709051652
C	-3.611149353	-1.709828082	-2.674161093
C	-4.401023751	-0.541209136	-2.677311037
C	-3.931898945	0.651729492	-3.326561434
C	-4.740065431	1.813716350	-3.352486151
C	-1.713534415	-0.411408083	-3.466456752
C	-2.527433254	0.760615928	-3.504621843
C	-1.930359810	2.038647529	-3.340869290
C	-2.737417810	3.202501662	-3.374921078
C	0.167237613	0.917285132	-2.663912806
C	-0.641546951	2.070884954	-2.708001320
C	-0.418971866	3.103709420	-1.769610812
C	-1.233567560	4.274842312	-1.789305196
C	1.269580511	1.726162555	-0.648188942
C	0.419290320	2.846362920	-0.662728581
C	0.049522412	3.491999334	0.572377878
C	1.897832396	1.334294768	0.626398170
C	3.318436044	-2.026316861	1.706718056
C	2.519943406	-0.852126200	1.694045987
C	1.455642810	-0.731302131	2.580478343
C	0.657223692	0.453356924	2.606122806
C	1.804761839	-3.084434068	3.279317555
C	0.991498232	-1.926695635	3.233592816
C	-0.405394403	-2.037183208	3.446973284
C	-1.222071444	-0.865057021	3.440357470
C	-0.189066674	-4.481011243	3.343190004
C	-1.000001199	-3.317238219	3.319555101
C	-2.306996435	-3.355264925	2.727740942
C	-3.121741294	-2.204891390	2.729305282
C	-1.728250270	-5.555877547	1.796537551
C	-2.546257881	-4.387729927	1.789975347
C	-3.375990895	-4.109939471	0.677660729
C	-4.187024545	-2.955287740	0.678142687
C	-2.214269015	-5.910240657	-0.555868075
C	-3.012247628	-4.741329568	-0.561279859
C	-3.051995301	-3.913891094	-1.715675143
C	-3.855378924	-2.733032607	-1.718388591
C	-1.202317805	-5.226398639	-2.660349635
C	-2.004675495	-4.059737043	-2.664375401
C	-1.509890452	-2.845960647	-3.251255159
C	-2.311731734	-1.687304043	-3.277765526
C	0.712064618	-3.898260484	-3.359258907
C	-0.104111110	-2.730362639	-3.371568475
C	0.486311365	-1.456561861	-3.208734864
C	-0.315770603	-0.298607929	-3.247487748
C	2.617601287	-2.559620925	-2.636789095
C	1.791644417	-1.413142373	-2.617003198



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C	3.747851558	-1.743368629	-0.641357206
C	2.944253416	-0.587534373	-0.638267923
C	2.787210165	0.151194773	0.644336027
C	4.231471455	-2.267730400	0.644012544
C	5.201191267	-4.047840852	1.957053709
C	4.131776184	-3.999876413	2.844858603
C	3.138332525	-3.021014534	2.696709523
C	1.197464280	-4.338346874	3.460677181
C	-0.123942123	-6.977645538	2.917593290
C	-0.724343923	-5.723831004	2.785094552
C	-0.427117072	-7.996115607	2.014361078
C	-1.193902593	-7.730583095	0.880884814
C	-1.803831679	-6.483620276	0.726487976
C	-1.425278545	-6.199780760	-1.677789950
C	0.914504574	-6.302320335	-3.538642682
C	0.115179068	-5.183771718	-3.296132065
C	2.288525963	-6.151555191	-3.722009153
C	2.900196430	-4.916763574	-3.512829803
C	2.122969158	-3.781277927	-3.270053333
C	3.652559529	-2.653947222	-1.699350543
C	5.205995751	-3.243639185	0.808651674
H	-2.277763037	5.735747786	1.612850376
H	-3.424406972	6.009700143	3.591634249
H	-5.846051563	5.736177007	4.056692522
H	-6.939024017	3.544065937	3.662732162
H	-7.115658886	2.345533404	1.705883157
H	-8.732789766	2.292789520	0.051785276
H	-8.826365628	3.630445381	-2.036690815
H	-6.975203584	3.480058914	-3.681189474
H	-4.740234838	3.952221671	-3.389170269
H	-3.529408663	5.865661625	-3.746519175
H	-2.985595451	7.697134594	-2.166061137
H	-1.699648492	7.203451085	-0.100011954
H	5.991932601	-4.783011148	2.104167389
H	4.057246319	-4.728568028	3.651778991
H	1.816552140	-5.225739006	3.351561408
H	0.598072475	-7.151484246	3.714612479
H	0.008748352	-8.985289990	2.150714986
H	-1.298919933	-8.484665276	0.101457573
H	-0.715675244	-7.020353078	-1.602849977
H	0.465034561	-7.294537119	-3.562623108
H	2.899546302	-7.023309464	-3.953922687
H	3.986583129	-4.837666117	-3.520972363
H	4.178810764	-3.601279736	-1.606137892
H	5.941062045	-3.419266284	0.022243564
Co	3.562080008	2.664679079	0.932663459
Co	4.927880737	2.113352748	-1.214285752
C	5.224734014	3.354726069	0.732675298
C	3.350768181	2.873513264	2.680126283
C	6.516797645	2.747490505	-1.709161502
C	4.736697080	0.784562035	-2.333977925
C	3.748653359	3.184319837	-2.042897438
O	3.236900040	3.066406985	3.812582138
O	6.177238339	3.927608270	1.089383277
O	7.527027863	3.132306286	-2.121176871
O	4.802791992	-0.035090489	-3.151325214
O	2.979990220	3.819384504	-2.628871111
C	4.531057710	0.847671529	1.157256354
C	5.420461617	0.807247653	0.107800804
C	2.797942538	4.217101966	0.426509948
O	2.479982544	5.292783016	0.159984702
C	6.680236795	0.008079706	0.090505227
H	6.928645667	-0.291424507	-0.941092906
H	6.548350729	-0.913729510	0.681886779
C	7.864589262	0.787668056	0.686379690
H	8.048825304	1.700563217	0.100652781
H	7.607552753	1.116001007	1.706909861
C	9.127977494	-0.067419247	0.724623505
H	8.922334916	-0.988967065	1.296882415
H	9.379115938	-0.384768229	-0.302419138
C	10.310310335	0.671443651	1.343030988
H	10.086146367	0.970408130	2.378693663
H	11.211748862	0.041607852	1.359770114
H	10.543354747	1.584024048	0.773509875
C	4.919468646	0.420052424	2.548254276
H	4.041621896	0.324577519	3.205391448
H	5.443019772	-0.551316713	2.549683803
H	5.588444048	1.173087388	2.993187424

TS1'*butyl,parallel*

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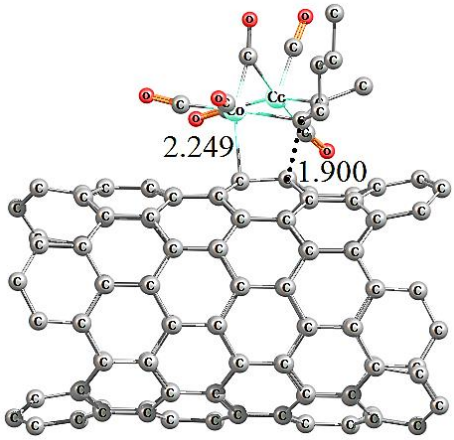
Co2C121H36O6

C	1.165700000	4.984800000	-1.567600000
C	2.611400000	4.071200000	-3.332600000
C	3.334700000	5.231800000	-3.615300000
C	4.690100000	5.151000000	-3.931600000
C	4.670600000	2.766200000	-3.535900000
C	5.372300000	3.941500000	-3.814600000
C	6.335100000	1.712600000	-2.067000000
C	6.979500000	1.385300000	0.279500000
C	7.893200000	2.436000000	0.384400000
C	7.958500000	3.188500000	1.556500000
C	6.087500000	1.967500000	2.481500000
C	7.011700000	3.011900000	2.564300000
C	4.144100000	3.149800000	3.410400000
C	2.134800000	4.448800000	2.852000000
C	2.687700000	5.726100000	2.982500000
C	2.303300000	6.746700000	2.115500000
C	0.920000000	5.206700000	0.868600000
C	1.489500000	6.472000000	1.016300000
C	0.456100000	4.647100000	-0.401700000
C	-1.168400000	1.454800000	-1.521300000
C	-0.379900000	2.643800000	-1.547400000
C	0.607000000	2.835200000	-2.548200000
C	1.357800000	4.039700000	-2.580100000
C	0.347500000	0.467000000	-3.153200000
C	1.100200000	1.658600000	-3.196900000
C	2.492300000	1.610400000	-3.464200000
C	3.253000000	2.816100000	-3.495000000
C	2.397200000	-0.829400000	-3.381600000
C	3.153800000	0.362700000	-3.404500000
C	4.511000000	0.367300000	-2.935400000
C	5.271100000	1.560800000	-2.967200000
C	4.113800000	-1.888900000	-2.023600000
C	4.875800000	-0.681500000	-2.049400000
C	5.729200000	-0.360900000	-0.961000000
C	6.483800000	0.837100000	-0.983300000
C	4.697300000	-2.208900000	0.312700000
C	5.427400000	-1.002800000	0.288800000
C	5.471600000	-0.182400000	1.442100000
C	6.219400000	1.031200000	1.424000000
C	3.800600000	-1.623800000	2.494400000
C	4.533200000	-0.418500000	2.475000000
C	4.051900000	0.736100000	3.181800000
C	4.805000000	1.935000000	3.184100000
C	1.899300000	-0.435700000	3.437800000
C	2.658500000	0.773200000	3.452900000
C	1.993000000	2.024400000	3.359500000
C	2.745600000	3.224900000	3.369700000
C	-0.091300000	0.818500000	2.793700000
C	0.665200000	2.008400000	2.812600000
C	0.335400000	3.048500000	1.914300000
C	1.094900000	4.256100000	1.908000000
C	-1.356600000	1.614700000	0.871700000
C	-0.558100000	2.773200000	0.856300000
C	-0.298900000	3.457800000	-0.384900000
C	-2.029200000	1.207100000	-0.368200000
C	-3.374000000	-2.187500000	-1.427700000
C	-2.633900000	-0.977100000	-1.441300000
C	-1.635200000	-0.789100000	-2.389900000
C	-0.900500000	0.434400000	-2.447900000
C	-1.917200000	-3.143500000	-3.115100000
C	-1.158700000	-1.948600000	-3.096900000
C	0.223400000	-1.985600000	-3.407600000
C	0.981400000	-0.774800000	-3.429300000
C	0.131300000	-4.438800000	-3.348800000
C	0.885600000	-3.237400000	-3.351500000
C	2.229600000	-3.223100000	-2.848300000
C	2.986000000	-2.033900000	-2.875300000
C	1.820500000	-5.468700000	-1.934500000
C	2.579900000	-4.261800000	-1.953200000
C	3.466100000	-3.965900000	-0.890200000
C	4.218500000	-2.772600000	-0.915600000
C	2.473900000	-5.845400000	0.372800000
C	3.213500000	-4.638900000	0.354500000
C	3.286500000	-3.832900000	1.522400000
C	4.031300000	-2.614400000	1.501600000
C	1.564400000	-5.252100000	2.550200000
C	2.309400000	-4.048200000	2.530800000
C	1.796200000	-2.872000000	3.175400000
C	2.543000000	-1.676700000	3.179300000
C	-0.362100000	-4.032500000	3.398400000
C	0.397300000	-2.827000000	3.386900000
C	-0.261500000	-1.579900000	3.294100000
C	0.486200000	-0.385700000	3.312300000
C	-2.372300000	-2.771900000	2.835500000
C	-1.603800000	-1.586500000	2.789700000



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C	-1.208800000	0.689200000	1.923900000
C	-3.674800000	-1.963000000	0.944700000
C	-2.928400000	-0.770400000	0.916500000
C	-2.899300000	0.003700000	-0.361100000
C	-4.215200000	-2.484900000	-0.319700000
C	-5.183600000	-4.281300000	-1.610900000
C	-4.169400000	-4.173200000	-2.556400000
C	-3.211000000	-3.155400000	-2.446800000
C	-1.265200000	-4.362200000	-3.367500000
C	0.215600000	-6.944400000	-2.982300000
C	0.762100000	-5.665300000	-2.858700000
C	0.626800000	-7.965300000	-2.125800000
C	1.452800000	-7.685600000	-1.038200000
C	2.010500000	-6.413200000	-0.893900000
C	1.771500000	-6.194600000	1.534600000
C	-0.439000000	-6.446700000	3.534100000
C	0.289300000	-5.286000000	3.267400000
C	-1.803600000	-6.366500000	3.808500000
C	-2.485000000	-5.158700000	3.668600000
C	-1.779700000	-3.982100000	3.403700000
C	-3.464200000	-2.893400000	1.969300000
C	-5.156600000	-3.497100000	-0.448400000
H	1.845900000	5.832300000	-1.523100000
H	2.841500000	6.202000000	-3.566600000
H	5.237600000	6.055700000	-4.193900000
H	6.456200000	3.912000000	-3.920500000
H	6.815900000	2.686100000	-2.005700000
H	8.536700000	2.680800000	-0.460000000
H	8.703800000	3.977800000	1.649400000
H	6.975500000	3.701500000	3.407000000
H	4.707800000	4.069600000	3.273600000
H	3.435800000	5.915400000	3.751500000
H	2.707900000	7.749300000	2.250000000
H	1.316200000	7.235700000	0.258800000
H	-5.950600000	-5.046600000	-1.727500000
H	-4.112500000	-4.883400000	-3.381200000
H	-1.832500000	-5.281000000	-3.238000000
H	-0.548600000	-7.137000000	-3.734500000
H	0.231400000	-8.972000000	-2.257500000
H	1.645200000	-8.449500000	-0.285400000
H	1.098400000	-7.047300000	1.485200000
H	0.057500000	-7.416200000	3.506400000
H	-2.356500000	-7.271500000	4.058600000
H	-3.571100000	-5.132600000	3.748800000
H	-3.950700000	-3.862800000	1.885300000
H	-5.838300000	-3.717700000	0.373900000
Co	-3.811700000	2.568300000	-0.528700000
Co	-5.046900000	1.794700000	1.679500000
C	-5.479200000	3.153800000	-0.147100000
C	-3.695900000	2.824800000	-2.277400000
C	-6.681000000	2.242200000	2.229000000
C	-4.670700000	0.469300000	2.756700000
C	-3.924600000	2.942000000	2.491800000
O	-3.610100000	3.046000000	-3.408400000
O	-6.464700000	3.736400000	-0.379200000
O	-7.733900000	2.479000000	2.643000000
O	-4.615000000	-0.359300000	3.565600000
O	-3.179500000	3.623700000	3.053900000
C	-4.655700000	0.615700000	-0.747500000
C	-5.507900000	0.511200000	0.332000000
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H	-5.354200000	-0.859600000	-2.149300000
H	-4.226100000	0.306300000	-2.828200000
C	-6.266300000	1.003600000	-2.695700000
H	-7.168400000	0.797400000	-2.095300000
H	-6.083100000	2.085600000	-2.608300000
C	-6.525300000	0.654300000	-4.158000000
H	-5.624300000	0.902100000	-4.745400000
H	-6.667300000	-0.436500000	-4.251800000
C	-7.733200000	1.387000000	-4.731600000
H	-8.649300000	1.128200000	-4.178100000
H	-7.597300000	2.477400000	-4.663400000
H	-7.892200000	1.130700000	-5.789100000
C	-6.707500000	-0.365300000	0.403000000
H	-7.617800000	0.259300000	0.415600000
H	-6.771600000	-1.071800000	-0.438400000
H	-6.712400000	-0.934400000	1.347500000

TS1'*methyl,oblique*

165
Co2C121H36O6

C	0.537084174	5.216710163	-0.111528573
C	1.301526288	4.844433188	-2.417997442
C	1.841709475	6.111013897	-2.651104052
C	3.013559683	6.245327609	-3.394378372
C	3.223348836	3.842234784	-3.550410588
C	3.743641734	5.119627589	-3.771332378
C	5.323697807	2.718597779	-2.948078280
C	6.739488099	2.020484452	-1.064284560
C	7.594379969	3.125016224	-1.038675355
C	8.040575515	3.633701779	0.180062243
C	6.655914498	2.056063382	1.380231238
C	7.513740280	3.158263209	1.380293296
C	5.117333543	2.812100639	3.138766983
C	2.989484255	3.963935453	3.553009747
C	3.503992624	5.246722448	3.759754560
C	2.811901034	6.360813781	3.289211272
C	1.156831645	4.933765405	2.253885202
C	1.692169402	6.204695241	2.472692642
C	0.314874556	4.572860494	1.112020837
C	-1.413081175	1.466860506	-0.097699438
C	-0.764720096	2.734270206	-0.104117296
C	-0.246780495	3.258961923	-1.314795727
C	0.388529274	4.520825638	-1.322437770
C	-0.638868015	1.049272798	-2.361143306
C	0.022708177	2.297524486	-2.349079182
C	1.242455940	2.459774139	-3.049410135
C	1.900242791	3.725200538	-3.052422342
C	1.282007354	0.051822255	-3.480099992
C	1.938139875	1.301998034	-3.472233740
C	3.371995034	1.368857428	-3.460709768
C	4.027857087	2.624148826	-3.472576080
C	3.392633446	-1.046585712	-2.971556173
C	4.051939348	0.218901605	-2.977945174
C	5.206525751	0.420008414	-2.175877107
C	5.861496211	1.675228568	-2.181967913
C	4.741721327	-1.738482006	-1.070758943
C	5.374931862	-0.478382185	-1.068057518
C	5.789573868	0.099061051	0.155739139
C	6.440529471	1.367065967	0.158915700
C	4.648112045	-1.697410920	1.358336014
C	5.283851529	-0.438726374	1.363456880
C	5.040130456	0.493008061	2.429053716
C	5.701949150	1.745259974	2.444800741
C	3.163984640	-0.943024367	3.131656883
C	3.830373146	0.320324963	3.151924048
C	3.125255276	1.486247366	3.554527000
C	3.787244191	2.738630727	3.575219355
C	1.027350844	0.176907659	3.474101157
C	1.692200135	1.426736835	3.479283803
C	1.036388330	2.574916601	2.976509895
C	1.702000379	3.836414650	2.972284008
C	-0.802562482	1.153170661	2.210061472
C	-0.136560370	2.398438114	2.204349493
C	-0.329717274	3.311445552	1.116069878
C	-1.634634384	0.795728817	1.111442702
C	-3.339558033	-2.340022846	-0.110671361
C	-2.683940902	-1.085890195	-0.108729950
C	-2.160884492	-0.570945760	-1.289972347
C	-1.566189566	0.728112217	-1.312416535
C	-2.591582969	-2.744669594	-2.383102983
C	-1.932384842	-1.493945306	-2.366163275
C	-0.734540508	-1.311617806	-3.103742683
C	-0.080213766	-0.040980077	-3.088549109
C	-0.681212971	-3.731358429	-3.527177849
C	-0.026867600	-2.471499267	-3.510533114
C	1.404700735	-2.403025681	-3.439328151
C	2.057005260	-1.153234704	-3.443709365
C	1.417371703	-4.811040993	-2.932009701
C	2.071483893	-3.543724458	-2.929689425
C	3.243875679	-3.355763639	-2.159516198
C	3.895703430	-2.104903593	-2.167585572
C	2.817238572	-5.539934719	-1.082964108
C	3.456069257	-4.277043100	-1.077711223
C	3.903050466	-3.713089056	0.146880863
C	4.547623247	-2.439314195	0.150311794
C	2.717225336	-5.495749488	1.349017873
C	3.358836385	-4.233895344	1.350900403
C	3.066240569	-3.275985512	2.380698401
C	3.719984391	-2.026876537	2.399268827
C	1.176650922	-4.699634709	3.053480146
C	1.835148624	-3.435509861	3.060391770
C	1.137507267	-2.277710109	3.479418357
C	1.797555737	-1.032189848	3.508454452
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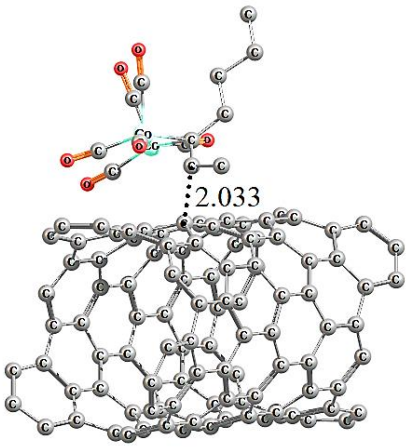
C	-0.296278085	-2.340063499	3.450124374



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C	-2.813147468	-2.606836401	2.236114948
C	-2.167595922	-1.356271613	2.232107101
C	-2.468705608	-0.381570285	1.152780201
C	-3.697914895	-2.960598403	1.117486118
C	-5.003976359	-4.559024569	-0.134115432
C	-4.428138987	-4.132105530	-1.322866575
C	-3.536870879	-3.050583751	-1.322455393
C	-2.005641963	-3.811415930	-3.087846327
C	-0.365863796	-6.237113150	-3.728185027
C	0.130522325	-4.950237248	-3.512834658
C	0.343678136	-7.346211882	-3.267496519
C	1.462000001	-7.182462225	-2.452446021
C	1.978870629	-5.904847903	-2.224744838
C	2.583739936	-6.187780527	0.137824442
C	1.247237798	-7.085847553	2.660918768
C	1.787249722	-5.818973126	2.431247041
C	0.065560813	-7.218740507	3.388616612
C	-0.671366087	-6.093208462	3.754694071
C	-0.151189674	-4.815230562	3.538389178
C	-2.254431939	-3.672415337	2.959237566
C	-4.572923161	-4.034259320	1.093822773
H	1.152292592	6.113356432	-0.112362898
H	1.357267937	6.991365321	-2.230225935
H	3.404999806	7.239015701	-3.609747223
H	4.730504117	5.231876680	-4.219032237
H	5.758258705	3.709165362	-2.836995876
H	7.894628393	3.599544518	-1.972275923
H	8.743990305	4.465658803	0.192161167
H	7.751830702	3.659126127	2.318103198
H	5.563713561	3.797446651	3.028508221
H	4.458503077	5.371333946	4.270038995
H	3.197055946	7.359757026	3.491267093
H	1.247485954	7.070840947	1.983814314
H	-5.735476245	-5.366381167	-0.146798656
H	-4.669939232	-4.631348290	-2.260779621
H	-2.452123411	-4.797284759	-2.979889178
H	-1.320041110	-6.371829086	-4.236342782
H	-0.027391698	-8.348735023	-3.478166544
H	1.922892748	-8.046191743	-1.974280597
H	1.972055487	-7.086865960	0.128856596
H	1.739733501	-7.967112917	2.251105433
H	-0.326652027	-8.212600589	3.601960315
H	-1.662592058	-6.208095321	4.191769172
H	-2.697616841	-4.657568226	2.833577853
H	-4.910485368	-4.483295017	2.027671293
Co	-5.755843361	0.339695613	0.448632900
Co	-4.451027035	1.899120963	-1.102385734
C	-7.346337145	1.168880113	0.573513215
C	-6.147832485	-1.009133334	1.495155426
C	-6.011509572	2.570917744	-1.609273718
C	-3.576403476	3.419976786	-1.098334675
C	-3.934447120	1.187212621	-2.690299992
O	-6.419426413	-1.838206204	2.258132773
O	-8.420501802	1.581306417	0.698945874
O	-6.999539830	3.020608262	-2.010668721
O	-3.096668734	4.474498731	-1.101569298
O	-3.698079091	0.873410082	-3.778952193
C	-4.140331361	0.689734762	1.587920404
C	-4.539668896	1.837586634	0.922215238
C	-5.696763500	-0.511580844	-1.103643355
O	-5.781194450	-1.159499244	-2.064580300
C	-4.778790808	3.121193166	1.685004995
H	-3.785982784	3.603892502	1.787683981
H	-5.086209881	2.867598430	2.713708194
C	-5.772140897	4.127704320	1.130043400
H	-5.450180012	4.497635627	0.146154331
H	-6.750638463	3.643797040	0.983058939
C	-5.940327177	5.324744235	2.063350576
H	-6.283052252	4.971968698	3.051609223
H	-4.955711171	5.797257985	2.224003675
C	-6.924320126	6.350594348	1.511013494
H	-7.916029667	5.897263864	1.359039442
H	-7.041678342	7.205166037	2.193117474
H	-6.581209039	6.736028523	0.538407440
C	-4.100121998	0.555980477	3.083173351
H	-4.120840394	-0.491498344	3.411610016
H	-3.201175952	1.037388081	3.506261207
H	-4.984171788	1.055143714	3.510221643

TS1'*butyl,oblique*

165
Co2C121H36O6

C	-1.825175083	5.063656165	-0.278173385
C	-2.565566335	4.679679123	2.034191786
C	-3.417060215	5.780384505	2.151266602
C	-4.614699867	5.666196224	2.855769778
C	-4.217751288	3.307386773	3.204710010
C	-5.051976088	4.422885840	3.308871394
C	-5.941750658	1.643144621	2.659595488
C	-7.061824873	0.467973678	0.814697082
C	-8.167234516	1.311898831	0.683168998
C	-8.679313292	1.598673883	-0.581261092
C	-6.893407256	0.344537428	-1.622496399
C	-8.001818849	1.187598986	-1.728584327
C	-5.526413685	1.337496604	-3.405293504
C	-3.742314963	2.958650135	-3.870744204
C	-4.554942787	4.049728044	-4.190242717
C	-4.183845383	5.334798625	-3.799833205
C	-2.263230662	4.455608411	-2.622646245
C	-3.092233802	5.529188955	-2.953993379
C	-1.401931067	4.406013036	-1.439894714
C	1.001952676	1.939515143	0.052069697
C	0.054588808	2.995884832	-0.057741828
C	-0.623725624	3.463563975	1.096293300
C	-1.555441565	4.519923424	0.988264738
C	0.266974364	1.509651756	2.325420660
C	-0.685925359	2.543185227	2.198805114
C	-1.934052108	2.441511894	2.858872638
C	-2.888889279	3.494614378	2.744806566
C	-1.381230547	0.142899191	3.485192522
C	-2.331059335	1.179798560	3.362030950
C	-3.733883772	0.877948125	3.317516330
C	-4.685120685	1.922055973	3.213180130
C	-3.123843055	-1.492299196	3.027668380
C	-4.081776220	-0.440190677	2.918452174
C	-5.217825538	-0.600813042	2.081464709
C	-6.168734077	0.442474229	1.972830652
C	-4.178980136	-2.644549171	1.164345071
C	-5.110099246	-1.591894588	1.047428386
C	-5.609208133	-1.231262300	-0.226915411
C	-6.559183046	-0.175276755	-0.345478795
C	-4.004612189	-2.760518419	-1.257990782
C	-4.937138764	-1.709582655	-1.377168767
C	-4.895152877	-0.827316437	-2.509884142
C	-5.850196913	0.210545498	-2.639374484
C	-2.691938184	-1.786209873	-3.059311694
C	-3.653827836	-0.738925946	-3.193417554
C	-3.249908719	0.534966764	-3.675420944
C	-4.204662266	1.572805282	-3.808997616
C	-0.894193853	-0.188140910	-3.450410221
C	-1.851630975	0.847299566	-3.568848352
C	-1.525509528	2.157600040	-3.147700974
C	-2.487169266	3.205502421	-3.258443563
C	0.582529769	1.310318688	-2.233468455
C	-0.375952574	2.342210407	-2.342583570
C	-0.462375792	3.352195327	-1.328710078
C	1.436804950	1.259868752	-1.092048939
C	3.823190214	-1.240987661	0.418550258
C	2.879654500	-0.189926272	0.301697167
C	2.200485195	0.264840716	1.428515345
C	1.295114714	1.365695959	1.330103950
C	3.117338501	-1.642382818	2.704640279
C	2.166893081	-0.604001241	2.572927196
C	0.930017978	-0.682808521	3.263739952
C	-0.025092994	0.372035588	3.128852170
C	1.471491297	-2.998567960	3.881319543
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C	-0.876727189	-2.257215668	3.641575202
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C	-0.259836138	-4.618929755	3.331950626
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C	-2.363368549	-3.739865504	2.408551699
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C	-1.355505778	-5.815572664	1.521298002
C	-2.292883251	-4.762034941	1.401407100
C	-2.820756573	-4.423524353	0.126936044
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C	-1.177414340	-5.928723152	-0.904254708
C	-2.117006674	-4.876268987	-1.020699367
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C	-2.984317907	-2.918821476	-2.251761775
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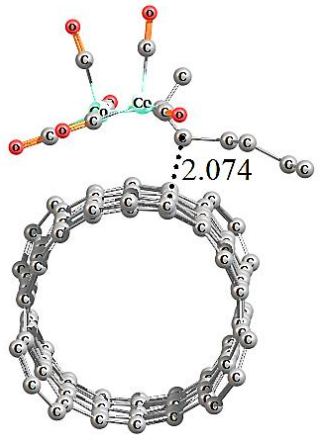

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C	2.529891425	-0.767058242	-2.018936506
C	2.538163591	0.330863225	-1.017437911
C	4.360980162	-1.854155873	-0.745880679
C	5.979285856	-2.971361429	0.653368720
C	5.280061396	-2.600554238	1.793873364
C	4.148892631	-1.779601225	1.688819284
C	2.790563105	-2.769504582	3.479244459
C	1.791221490	-5.480384404	4.279372397
C	0.995514602	-4.381939150	3.948771072
C	1.403786914	-6.764598220	3.896766052
C	0.314622315	-6.952142789	3.047889732
C	-0.497945259	-5.868931070	2.705228589
C	-0.918601211	-6.470928445	0.361860900
C	0.692324574	-7.186778339	-2.058212577
C	-0.157649839	-6.085289415	-1.941722464
C	1.894111593	-7.069747914	-2.755142843
C	2.335707567	-5.824937337	-3.201819507
C	1.502508015	-4.708676072	-3.099581783
C	3.223147134	-3.033851170	-2.561277705
C	5.468871994	-2.676603896	-0.619128642
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H	-3.153421379	6.721670993	1.670307331
H	-5.252905151	6.540417964	2.980211703
H	-6.052638900	4.313255792	3.725565368
H	-6.608141146	2.478768175	2.459318907
H	-8.614520811	1.761076787	1.569277185
H	-9.569807113	2.219545156	-0.674389543
H	-8.321706348	1.540906124	-2.708335477
H	-6.210731675	2.182240522	-3.383257427
H	-5.490016854	3.889610402	-4.725981685
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H	-2.898192565	6.513802642	-2.529962214
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H	3.339292693	-5.716643904	-3.611657993
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H	5.935532098	-3.106833501	-1.504976220
Co	5.541520114	1.882981152	-0.126644059
Co	3.657811410	3.293424024	1.130952291
C	6.813733128	3.145909978	-0.295660943
C	6.497394448	0.550163843	-0.748231905
C	4.956819157	4.412150348	1.587416422
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H	4.180855106	2.548612189	-3.485583974
H	2.948290287	1.322777614	-3.358665777
C	4.958336741	0.531710953	-3.492732332
H	5.960244520	0.987364540	-3.573990772
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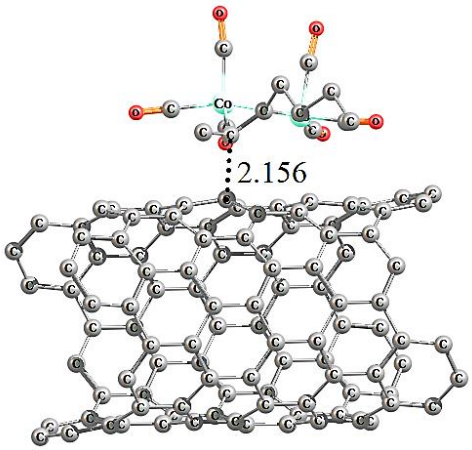

165
Co2C121H36O6

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C	-2.896681304	6.365957619	3.371015393
C	-3.128061021	3.966843543	3.552793680
C	-3.634813830	5.250724211	3.764396183
C	-5.244600787	2.859923529	2.977713528
C	-6.671537294	2.167158030	1.103550312
C	-7.510831762	3.282985018	1.069751400
C	-7.935980275	3.798703778	-0.153797317
C	-6.561153842	2.202203126	-1.339831205
C	-7.401375429	3.317896774	-1.348393597
C	-4.983863640	2.933678363	-3.077624973
C	-2.825825957	4.038203915	-3.500289446
C	-3.310673140	5.327094781	-3.733976212
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C	-0.960174636	4.993271310	-2.241369626
C	-1.463987831	6.272279188	-2.488716518
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C	1.765909556	1.624420374	0.193742200
C	0.950332216	2.825855375	0.155543523
C	0.355538053	3.334116945	1.331138950
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C	0.053776192	2.377957802	2.361865328
C	-1.164383219	2.558315044	3.051376357
C	-1.809411381	3.831777823	3.047469187
C	-1.230479730	0.158341782	3.509409800
C	-1.872317344	1.411370306	3.492830558
C	-3.304818913	1.493950599	3.488021459
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C	-4.621898263	-1.586977752	-1.298964663
C	-5.236009505	-0.317455563	-1.309926613
C	-4.966930119	0.611035040	-2.372921339
C	-5.600474095	1.875793267	-2.392853062
C	-3.114813360	-0.859757867	-3.063521530
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C	-0.955965978	0.220991705	-3.376935321
C	-1.589575631	1.477243355	-3.389571757
C	-0.900322068	2.614711977	-2.893246006
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C	0.273281607	2.425272914	-2.132234039
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C	1.791738370	0.823387157	-1.035628923
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C	2.326843486	-0.443226499	1.428205900
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C	-3.229856961	-3.238601725	2.223447685
C	-3.871086335	-1.983655500	2.226424338
C	-2.829639006	-5.434626488	1.163583305
C	-3.457330623	-4.166090456	1.151069733
C	-3.905806846	-3.606971672	-0.076076888
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C	1.012768317	-1.170484430	-2.879731130
C	0.374074970	0.099447847	-2.886770694
C	2.800205827	-2.641075753	-2.078380694
C	2.166941613	-1.373256999	-2.079578841
C	2.396116313	-0.431496115	-1.019436721
C	3.691838578	-2.991240314	-0.973490508
C	4.968622136	-4.615014462	0.278729250
C	4.442525545	-4.122721371	1.469844364
C	3.619497608	-2.993568395	1.456305006
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C	0.372720578	-6.133939408	3.788421096
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C	-1.982682408	-5.796136031	2.300859562
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H	-7.812554386	3.762598204	2.000320221
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H	-5.412153927	3.927705068	-2.971918830
H	-4.265910616	5.461954701	-4.240246537
H	-2.948742845	7.438492309	-3.523391418
H	-0.990409513	7.138561338	-2.027913697
H	5.657385097	-5.459038828	0.297259816
H	4.660678808	-4.621230295	2.413944694
H	2.474687587	-4.707409129	3.071797398
H	1.327587514	-6.272976166	4.293986300
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H	-1.944689197	-7.939155370	2.068645916
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H	-1.809317522	-7.904760984	-2.159414091
H	0.262861419	-8.186989547	-3.495975006
H	1.634580028	-6.204757557	-4.078518959
H	2.671014779	-4.677993311	-2.706462970
H	4.799402643	-4.603358696	-1.875989009
Co	4.672545387	2.744063545	-1.132768591
Co	5.377307054	0.376060760	-0.439397310
C	6.302841836	3.472761574	-1.373824809
C	3.738838802	4.195346786	-1.427601066
C	7.080487940	0.845191197	-0.655322756
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C	5.287674273	-0.628036722	-1.954574238
O	3.131108215	5.169418566	-1.573252071
O	7.293933918	4.038610811	-1.559754858
O	8.205169308	1.066866659	-0.802581313
O	6.105050185	-1.406449551	1.743024075
O	5.414854195	-1.260005932	-2.912157646
C	3.670316580	2.557875618	0.578635832
C	4.866158746	1.906148405	0.708767250
C	4.123963233	1.881793780	-2.586422438
O	3.766488425	1.416414713	-3.586381519
C	5.755785911	2.124817965	1.912256429
H	5.897794264	3.202527900	2.101709890
H	6.755210454	1.700538620	1.741307206
C	5.099698995	1.453957977	3.130660811
H	4.296517506	2.100177557	3.521379907
H	4.598285752	0.525939091	2.807462845
C	6.078832345	1.111823445	4.246140632
H	6.864092081	0.451954179	3.839204734
H	6.583857438	2.029002495	4.595766149
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H	4.880034052	-0.502862925	5.064555880
H	6.086483529	0.144824559	6.205391006
H	4.605379039	1.066994355	5.848937520
C	3.258129096	3.682064655	1.481740937
H	2.643951114	4.439243080	0.979552326
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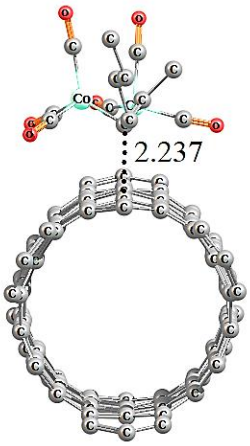
TS1'*butyl,oblique*



165
Co2C121H36O6

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C	3.040261472	-6.088519996	3.558594770
C	3.247073259	-3.680875683	3.633384774
C	3.772668110	-4.949244333	3.888685210
C	5.341734602	-2.571755069	2.981746659
C	6.741565494	-1.923904387	1.070444097
C	7.593787789	-3.030375596	1.063260805
C	8.015595318	-3.578325663	-0.147443530
C	6.612978615	-2.034775003	-1.369831538
C	7.466397629	-3.140334769	-1.351769636
C	5.028380525	-2.842598656	-3.065370617
C	2.884394923	-3.995111565	-3.410918272
C	3.388432580	-5.283009730	-3.605703908
C	2.697224604	-6.386398506	-3.108067935
C	1.065594867	-4.933108908	-2.073340700
C	1.589662929	-6.211214324	-2.280323095
C	0.238370426	-4.549953951	-0.930069194
C	-1.716221011	-1.539026777	0.252120997
C	-0.867121590	-2.711273376	0.259818213
C	-0.282920183	-3.182238456	1.457919449
C	0.363841181	-4.439825809	1.488136731
C	-0.639641131	-0.931664930	2.413102705
C	0.022397664	-2.180309208	2.444851123
C	1.256559252	-2.315844988	3.114745643
C	1.916465226	-3.581640390	3.151118839
C	1.305235563	0.100373596	3.469030835
C	1.960827193	-1.144244747	3.496300033
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C	4.050620225	-2.464450159	3.512178410
C	3.411210757	1.190761795	2.922772511
C	4.071898797	-0.071877064	2.958880016
C	5.223802142	-0.292358265	2.155881460
C	5.877714848	-1.546217404	2.188525723
C	4.748505290	1.837121136	0.997800288
C	5.380919271	0.576942933	1.022739463
C	5.778241648	-0.036085413	-0.190276896
C	6.424455407	-1.305760952	-0.166953965
C	4.620738647	1.726903348	-1.427826152
C	5.253030375	0.466674125	-1.405217226
C	4.983647696	-0.499529656	-2.433571322
C	5.636478761	-1.754495934	-2.421856726
C	3.096104142	0.917802234	-3.140924530
C	3.755768498	-0.345635735	-3.132553098
C	3.034860028	-1.520861308	-3.475258893
C	3.690655112	-2.776175215	-3.473331357
C	0.950179295	-0.206179853	-3.381189568
C	1.606071836	-1.450938817	-3.365925879
C	0.948061163	-2.582222558	-2.818127186
C	1.607411575	-3.849283038	-2.810756351
C	-0.875432144	-1.134896618	-2.052263310
C	-0.212216692	-2.382484015	-2.041662039
C	-0.407359832	-3.290207943	-0.945528575
C	-1.779298559	-0.783827862	-1.001474264
C	-3.487070486	2.347703732	0.168113834
C	-2.956557093	1.007691443	0.201994882
C	-2.281415679	0.568923638	1.408201222
C	-1.646208729	-0.670196557	1.432179055
C	-2.622250713	2.825354173	2.387411601
C	-1.958346164	1.573808812	2.382066832
C	-0.726450523	1.436061899	3.072839998
C	-0.064743990	0.178107626	3.089751162
C	-0.671957856	3.865395091	3.421729651
C	-0.014558538	2.616047069	3.429773965
C	1.416355373	2.550787731	3.351747402
C	2.074860106	1.304749573	3.390825940
C	1.419852235	4.942513887	2.792483081
C	2.080483471	3.681686952	2.820414794
C	3.256383292	3.479447626	2.055199302
C	3.910166748	2.231914065	2.091263423
C	2.816784857	5.634713547	0.927935736
C	3.459622763	4.373923059	0.949983070
C	3.895620704	3.777922385	-0.264296143
C	4.540251444	2.504861715	-0.240330989
C	2.688640492	5.524197801	-1.500316734
C	3.331605910	4.263469438	-1.475003819
C	3.019355818	3.274309333	-2.468083105
C	3.671844090	2.025643027	-2.459393271
C	1.112917216	4.674519795	-3.145279120
C	1.771459730	3.412603813	-3.125358322
C	1.062656921	2.242492208	-3.486544076
C	1.719522205	0.996012309	-3.482257605
C	-1.024728268	3.554671529	-3.473429050
C	-0.369139080	2.305510927	-3.431477722

C	-1.042007205	1.165004321	-2.906640073
C	-0.377004164	-0.090737928	-2.877364114
C	-2.858952687	2.621482051	-2.163158103
C	-2.207263393	1.365208607	-2.118840617
C	-2.431567060	0.450323090	-1.029841280
C	-3.737533720	3.006145893	-1.060263357
C	-4.977403774	4.695940013	0.144364056
C	-4.453676488	4.226200577	1.349866523
C	-3.632430059	3.098745283	1.362593375
C	-2.014841633	3.917978568	3.013634007
C	-0.379463042	6.376888891	3.540486449
C	0.127683109	5.086287628	3.362301153
C	0.326298906	7.478041829	3.060297826
C	1.453566854	7.302295609	2.257578097
C	1.978034732	6.024093197	2.061907189
C	2.569240193	6.249082075	-0.307126759
C	1.189998263	7.071928229	-2.829652854
C	1.736623363	5.813946135	-2.573000873
C	-0.010735779	7.180729636	-3.531275692
C	-0.755161916	6.044651128	-3.842148601
C	-0.227930528	4.772955450	-3.599573498
C	-2.318850128	3.650468732	-2.941016192
C	-4.537434850	4.152342813	-1.058495386
H	1.074520952	-6.083517853	0.309885501
H	1.366901704	-6.875628621	2.448635899
H	3.438576868	-7.073838418	3.798761574
H	4.766191048	-5.045127873	4.325430152
H	5.775658347	-3.564845540	2.891638902
H	7.908464312	-3.477904384	2.005480440
H	8.716359894	-4.412686248	-0.146408704
H	7.682948221	-3.672821552	-2.277282925
H	5.473590234	-3.825994722	-2.933614106
H	4.334653572	-5.420277802	-4.128006964
H	3.074435823	-7.390414609	-3.300045424
H	1.145564982	-7.067409529	-1.773621045
H	-5.656404352	5.547792794	0.141186559
H	-4.647049111	4.764021749	2.278020829
H	-2.466885893	4.897417189	2.879923626
H	-1.336548377	6.518253083	4.041103899
H	-0.052100871	8.483056218	3.244368802
H	1.910953770	8.157545922	1.761063749
H	1.953661668	7.145445390	-0.315362658
H	1.690462492	7.966044099	-2.459158630
H	-0.409224319	8.167204642	-3.766191123
H	-1.756311677	6.145387325	-4.259478913
H	-2.755081305	4.641360550	-2.846800515
H	-4.815183281	4.617403099	-2.003803085
Co	-4.974598384	-2.058350572	-0.945519482
Co	-5.409758060	-0.220987984	0.744915944
C	-6.548270332	-2.911238976	-1.103756794
C	-3.894442032	-2.898694084	-2.045065191
C	-7.102350176	-0.774164826	0.998582819
C	-5.030352877	0.381374523	2.362427521
C	-6.034329302	1.248603307	-0.098201179
O	-3.164921147	-3.496381119	-2.716083096
O	-7.515604498	-3.526871254	-1.258908655
O	-8.213290415	-1.061788729	1.123400941
O	-4.866459230	0.737532713	3.449142527
O	-6.637648077	2.114988908	-0.563611649
C	-3.669910206	-2.611489645	0.442072065
C	-4.756801815	-2.078722029	1.077786286
C	-5.119580846	-0.608174007	-1.948669295
O	-5.196860863	0.241203629	-2.737163825
C	-3.202424188	-4.033835918	0.639307652
H	-2.828479696	-4.147081745	1.673370243
H	-2.360505934	-4.262490768	-0.022511766
C	-4.244437662	-5.118456801	0.336443922
H	-5.178532868	-4.969515223	0.896144561
H	-4.509205382	-5.069953038	-0.732073335
C	-3.666264703	-6.496192210	0.650946488
H	-2.712146199	-6.614173157	0.107848008
H	-3.420438196	-6.551309247	1.725638129
C	-4.620432063	-7.625056973	0.275776268
H	-5.573196993	-7.531569532	0.819503211
H	-4.846116228	-7.603449153	-0.801472623
H	-4.190326346	-8.608999025	0.513302029
C	-5.467032941	-2.805716401	2.202627508
H	-6.468808471	-3.138809243	1.894732476
H	-4.895968625	-3.677666913	2.549040850
H	-5.595092094	-2.134850193	3.062759607

CP4*methyl,parallel*

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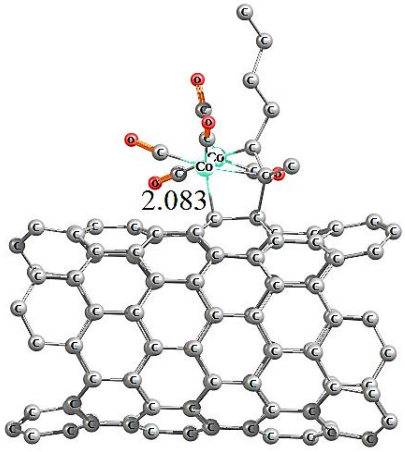
Co2C120H36O5

C	0.046980474	4.958183808	-1.577959660
C	1.678451695	4.310552742	-3.292319530
C	2.171348411	5.582909612	-3.588564049
C	3.525390208	5.760823630	-3.869118391
C	3.955687041	3.424982506	-3.419190115
C	4.424630600	4.709063726	-3.707530114
C	5.781531403	2.719235348	-1.924669146
C	6.473586072	2.512748132	0.423046613
C	7.166238999	3.719892484	0.535800797
C	7.075275491	4.467899471	1.709076394
C	5.462158054	2.909344394	2.612661254
C	6.168169729	4.111429713	2.705797998
C	3.307957626	3.704386639	3.478841571
C	1.103850795	4.597424076	2.852155498
C	1.402029782	5.956357879	2.988564474
C	0.839401256	6.887143000	2.117996933
C	-0.221890178	5.117180045	0.859951173
C	0.097404982	6.466925076	1.014203150
C	-0.586560127	4.489503202	-0.410870713
C	-1.645414392	1.064421102	-1.557694906
C	-1.055698611	2.375407031	-1.566780769
C	-0.080397691	2.727775579	-2.533395300
C	0.433833428	4.053886059	-2.569223193
C	0.151415723	0.330423065	-3.058958748
C	0.657176377	1.651430628	-3.118993475
C	2.038365267	1.871223648	-3.360010098
C	2.554120914	3.200445054	-3.406531951
C	2.424408156	-0.540152543	-3.253394603
C	2.929892237	0.778819035	-3.271229199
C	4.257326159	1.046763020	-2.799166304
C	4.770094295	2.365308183	-2.828533880
C	4.314984843	-1.249227744	-1.900921678
C	4.820293835	0.085335808	-1.917076068
C	5.592058559	0.561387802	-0.825943811
C	6.095953998	1.885003024	-0.843031931
C	4.931983811	-1.457397780	0.437744642
C	5.415633899	-0.132623304	0.420588514
C	5.286459449	0.679963854	1.572911346
C	5.786825161	2.015087034	1.560680475
C	3.897800506	-1.052913078	2.598345534
C	4.390801733	0.269549771	2.589202098
C	3.682070867	1.314936081	3.275226821
C	4.193547406	2.635070324	3.286707741
C	1.782147473	-0.241183988	3.477066591
C	2.299148477	1.089096516	3.503048830
C	1.413278614	2.191196331	3.372859324
C	1.922961055	3.513279857	3.393011068
C	-0.385316404	0.609404745	2.761139890
C	0.130872182	1.921089426	2.789365589
C	-0.376909575	2.880350740	1.886919441
C	0.132467993	4.211930320	1.894212594
C	-1.789852112	1.168036499	0.857395380
C	-1.212938111	2.449361802	0.835832993
C	-1.112873597	3.185415354	-0.398332583
C	-2.455797888	0.683216772	-0.366091626
C	-2.960353262	-3.003883791	-1.351668836
C	-2.463456875	-1.677149552	-1.372914267
C	-1.528182621	-1.295724164	-2.310315866
C	-1.089412504	0.065207984	-2.400926798
C	-1.328634486	-3.663308006	-3.020708143
C	-0.822200747	-2.343635190	-3.003056810
C	0.535615739	-2.104845722	-3.309342162
C	1.029554313	-0.765437393	-3.311198879
C	0.931941270	-4.529436591	-3.270483368
C	1.432654953	-3.201098138	-3.260317491
C	2.742009816	-2.925186071	-2.747589876
C	3.241907551	-1.607990044	-2.758389805
C	2.777330555	-5.213138830	-1.845163792
C	3.284157376	-3.880065291	-1.853198740
C	4.081489950	-3.419288272	-0.779314073
C	4.585203590	-2.100825482	-0.795678930
C	3.444457786	-5.454020584	0.473711568
C	3.940983762	-4.128780852	0.463564559
C	3.830666089	-3.320853416	1.627382030
C	4.333638623	-1.983396867	1.616307846
C	2.371071879	-5.034790224	2.616638460
C	2.880979306	-3.713473756	2.609029475
C	2.139396945	-2.652502447	3.229511344
C	2.653203958	-1.340161339	3.248396815
C	0.228008924	-4.194109568	3.410653811
C	0.750148815	-2.868835809	3.400606249
C	-0.126333643	-1.768241053	3.281286541
C	0.390447872	-0.458760832	3.307585747
C	-1.987659821	-3.324710041	2.848958244
C	-1.445518713	-2.019723102	2.775624453



C	-2.013237157	-1.050764394	1.902933440
C	-1.449965698	0.270564938	1.885151526
C	-3.461532436	-2.767292404	0.989861812
C	-2.969891413	-1.452624283	0.946027382
C	-3.088742456	-0.709491985	-0.392047212
C	-3.804812796	-3.428275506	-0.283587328
C	-4.347222852	-5.398855370	-1.568970407
C	-3.337341896	-5.114336772	-2.477828680
C	-2.591040529	-3.931397185	-2.354379998
C	-0.449737390	-4.729676009	-3.284169192
C	1.507068648	-6.971558032	-2.914820807
C	1.790566577	-5.611040770	-2.783105753
C	2.096293363	-7.894104402	-2.050091713
C	2.832827304	-7.460049490	-0.949163106
C	3.129863865	-6.103478754	-0.799311010
C	2.783996598	-5.925226549	1.617535186
C	0.601124554	-6.578940357	3.563044985
C	1.104866917	-5.303810787	3.300399406
C	-0.757614127	-6.751962146	3.823194781
C	-1.650156060	-5.691331773	3.677265468
C	-1.174977346	-4.404980283	3.409956861
C	-3.060970536	-3.641868857	2.012593248
C	-4.530391434	-4.598650533	-0.429016274
H	0.551778197	5.920479217	-1.535473851
H	1.497729819	6.439099006	-3.577599310
H	3.894565722	6.749191178	-4.141128138
H	5.496235978	4.887056832	-3.790460073
H	6.064636719	3.767298404	-1.860021174
H	7.756296288	4.086553257	-0.303531586
H	7.654176169	5.385481472	1.809898741
H	5.988283377	4.780991407	3.546247089
H	3.692212804	4.713341191	3.348882402
H	2.090633797	6.283695240	3.766799074
H	1.045965399	7.947935055	2.256477753
H	-0.217382258	7.187258642	0.259707266
H	-4.950873330	-6.296926353	-1.697685182
H	-3.123530206	-5.805707868	-3.292510666
H	-0.825029547	-5.742872706	-3.160483556
H	0.804904845	-7.307768544	-3.676979059
H	1.906268577	-8.958310706	-2.186195865
H	3.155382077	-8.171843794	-0.189887400
H	2.285823772	-6.889953408	1.555764331
H	1.268908684	-7.439650428	3.548150522
H	-1.135879593	-7.743044760	4.071723808
H	-2.722239018	-5.867208690	3.755965678
H	-3.358658913	-4.684900290	1.931703507
H	-5.207475435	-4.921639911	0.362567997
Co	-3.998577074	1.687631215	-1.340047415
Co	-4.713820061	1.525749897	1.239373577
C	-4.781557632	1.943452385	-2.906613227
C	-6.127173240	2.595177689	1.271226414
C	-4.884521449	0.134220230	2.299788585
C	-3.774543313	2.575909157	2.364194284
O	-5.231004719	2.087476027	-3.964596979
O	-7.089023691	3.216409271	1.442793010
O	-5.197935029	-0.678322915	3.064191795
O	-3.226647992	3.244373399	3.126424353
C	-4.541659116	-0.415731411	-0.935753810
C	-5.393549604	0.412950243	-0.186867058
C	-3.911537920	3.366574046	-0.823096179
O	-3.971887500	4.494017969	-0.548947228
C	-6.891550304	0.315686297	-0.386597643
H	-7.370970397	0.423072613	0.598324733
H	-7.156447884	-0.693189190	-0.742653553
C	-7.493178905	1.361291613	-1.331536670
H	-7.035695031	2.344802986	-1.139477622
H	-7.242445463	1.107510367	-2.373594424
C	-9.007157695	1.468341776	-1.186423183
H	-9.462232782	0.474477563	-1.341481062
H	-9.245256781	1.767068541	-0.151175541
C	-9.604425877	2.473617404	-2.165634966
H	-9.393153829	2.181514911	-3.205923631
H	-10.695101091	2.550052330	-2.048867721
H	-9.174271189	3.474174068	-2.005383255
C	-5.095363339	-1.174428825	-2.125095232
H	-4.341345284	-1.281516964	-2.917470390
H	-5.443063067	-2.184573464	-1.852257592
H	-5.939572286	-0.627023656	-2.559592498

CP4*butyl,parallel*

163
Co2C120H36O5

C	0.493160227	-5.065292636	1.572362515
C	1.903840587	-4.201203264	3.385080216
C	2.551512856	-5.392637181	3.717034682
C	3.895147120	-5.378555333	4.089633875
C	4.018141366	-3.001917726	3.664702233
C	4.644237657	-4.208580532	3.987697799
C	5.823527439	-2.035200859	2.297598469
C	6.634532360	-1.721388216	0.000751395
C	7.496555496	-2.817901304	-0.061750413
C	7.586814982	-3.566810676	-1.234717490
C	5.831057078	-2.247908051	-2.247182375
C	6.703663546	-3.338407466	-2.288835435
C	3.869012989	-3.333232407	-3.247641690
C	1.774944423	-4.531779423	-2.768713647
C	2.272238209	-5.833798729	-2.881421589
C	1.788771721	-6.842429632	-2.051411409
C	0.399828217	-5.252355642	-0.875398549
C	0.919018373	-6.541023659	-1.003140751
C	-0.133565746	-4.690589319	0.366822660
C	-1.727083797	-1.453301247	1.419096185
C	-0.969267696	-2.668109002	1.481379068
C	-0.008977127	-2.879060900	2.504809951
C	0.685485992	-4.119342046	2.580161691
C	-0.155435002	-0.479564274	3.029809149
C	0.527318994	-1.713844815	3.134195502
C	1.907616982	-1.736187732	3.470374199
C	2.602855777	-2.978628452	3.555927412
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C	4.019921233	-0.601663597	3.058808779
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C	5.217178442	0.748848929	-0.077831488
C	5.278996585	-0.068812920	-1.232376864
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C	3.731628469	1.456946768	-2.354377371
C	4.402309259	0.216058353	-2.306189505
C	3.891177412	-0.916165245	-3.029357983
C	4.581985876	-2.151514017	-3.002091386
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C	-0.000163537	-3.050466947	-1.912965845
C	0.692883417	-4.296930149	-1.883552576
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C	-1.498260390	2.027360855	2.889668536
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C	2.639946472	1.880748949	2.934932224
C	1.734568510	5.389879044	1.979648789
C	2.423303790	4.141848841	2.027627600
C	3.353402273	3.807013202	1.015725632
C	4.036066806	2.572810333	1.071602503
C	2.526474831	5.740638008	-0.284873106
C	3.202405466	4.498418202	-0.236243414
C	3.285216122	3.689397703	-1.401613947
C	3.968706053	2.435526495	-1.351209064
C	1.666086956	5.185369059	-2.491301871
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C	0.393481094	0.379310228	-3.272090611
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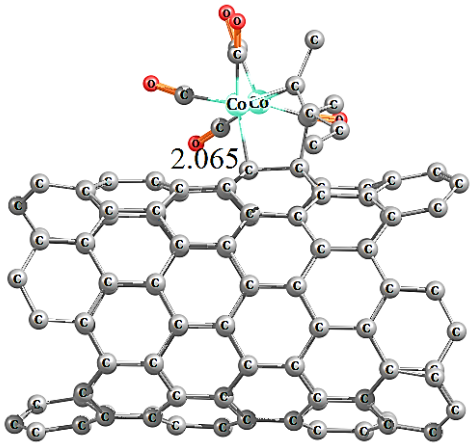

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C	-3.430621427	3.352337657	2.131710175
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C	0.154311465	6.942899874	2.948503279
C	0.635432314	5.636729720	2.841405655
C	0.669990565	7.946619423	2.128144086
C	1.539419453	7.629950049	1.085765684
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C	1.884626653	6.120990259	-1.472418173
C	-0.241399226	6.467509783	-3.555276972
C	0.418763946	5.275428754	-3.252692391
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C	-3.554585364	3.031107220	-2.223388620
C	-5.335192631	3.735005186	0.097285425
H	1.133922760	-5.943958666	1.564067464
H	2.009298847	-6.335911571	3.662011016
H	4.381967527	-6.306420508	4.388224431
H	5.722110609	-4.232916202	4.144265442
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H	6.673820286	-4.023598723	-3.135353516
H	4.381935534	-4.279061091	-3.090224440
H	3.053171221	-6.053336111	-3.608640446
H	2.154185802	-7.861650651	-2.172784444
H	0.660251157	-7.304206507	-0.269800196
H	-6.065036915	5.355854813	1.328435081
H	-4.270678280	5.138149274	3.018353333
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H	1.813779021	8.386211435	0.350794187
H	1.252854389	7.005886233	-1.447997634
H	0.297634984	7.413208735	-3.508041038
H	-2.090347457	7.376673408	-4.176194590
H	-3.414800143	5.297148253	-3.941213671
H	-4.005096743	4.019502261	-2.165365500
H	-5.998635361	3.964212046	-0.737420806
Co	-4.080975117	-2.476896180	0.753163016
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H	-5.413761592	-1.175705909	3.535214123
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H	-4.425377067	-0.518055614	5.876973143
H	-2.971691131	0.180235489	5.126472907
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C	-6.968021379	-1.494568516	-0.290008120
H	-7.264331277	-2.525595824	-0.510504074
H	-7.415241472	-1.213584589	0.671129099
H	-7.419297553	-0.852562664	-1.065318551

CP4*_methyl,oblique_

163
Co2C120H36O5

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C	2.258891801	4.754191947	-2.248437595
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C	4.293763682	5.852081093	-2.958151785
C	4.100820563	3.455035312	-3.200500025
C	4.856713338	4.624278690	-3.303427759
C	5.909683978	1.949087528	-2.479490132
C	6.986503499	0.923389408	-0.527124296
C	8.005054481	1.862377244	-0.347502140
C	8.378883316	2.246054411	0.939211304
C	6.610151524	0.897282972	1.887807171
C	7.634070729	1.833829650	2.043918572
C	4.996930408	1.873325104	3.460703950
C	3.045772010	3.361579610	3.683942559
C	3.730960710	4.525301056	4.044611993
C	3.273994517	5.768096160	3.612248928
C	1.529562325	4.709389452	2.316631606
C	2.229627872	5.856514764	2.692250362
C	0.757972445	4.576840169	1.080637941
C	-1.657546978	2.121402697	-0.563014924
C	-0.528890793	3.088964649	-0.362757268
C	0.286261212	3.478028377	-1.440273373
C	1.156000405	4.592851475	-1.304341624
C	-0.271586775	1.327331195	-2.550230063
C	0.566054396	2.466403841	-2.434804120
C	1.867360792	2.426281396	-2.967244031
C	2.730141612	3.559661728	-2.850178519
C	1.562377610	0.060482808	-3.541381479
C	2.406651864	1.175424853	-3.383909867
C	3.817947333	0.990541348	-3.242477313
C	4.674861820	2.111836763	-3.115105450
C	3.389201292	-1.418531276	-2.932713436
C	4.246723304	-0.288707147	-2.791928654
C	5.335150707	-0.334737437	-1.879681966
C	6.187304293	0.785940428	-1.743148615
C	4.393263260	-2.426592520	-0.961884397
C	5.228864027	-1.299177094	-0.819572440
C	5.589981930	-0.847191143	0.472828388
C	6.438684793	0.288363532	0.617507431
C	4.017153172	-2.451103993	1.440120272
C	4.852676505	-1.323694479	1.584168628
C	4.633405754	-0.387224569	2.652195725
C	5.484905992	0.732628956	2.807282266
C	2.463196070	-1.487673407	3.040133551
C	3.323347080	-0.360917290	3.199375558
C	2.776091067	0.902187349	3.550348400
C	3.627820393	2.020896805	3.717035074
C	0.528068454	-0.017922647	3.138174074
C	1.379522519	1.091347422	3.290831676
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C	1.825968180	3.486292829	2.970839224
C	-0.988956804	1.319989073	1.780554289
C	-0.143129368	2.426682300	1.934087750
C	-0.109379534	3.469120622	0.923121336
C	-1.986597424	1.317185703	0.720820241
C	-3.859308187	-1.523142012	-0.925900085
C	-3.039790160	-0.379044552	-0.774520621
C	-2.229367928	0.062718118	-1.864592832
C	-1.389154419	1.164823291	-1.707791319
C	-2.866082160	-1.994027328	-3.095079888
C	-1.995285404	-0.893212734	-2.910008570
C	-0.690498952	-0.923266526	-3.464608474
C	0.173212846	0.188565014	-3.284936778
C	-1.017205650	-3.289560136	-4.030839892
C	-0.156822921	-2.180240386	-3.866939613
C	1.249080997	-2.372679371	-3.659274990
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C	0.786944398	-4.760289202	-3.311721616
C	1.652900036	-3.638225287	-3.170778426
C	2.761854616	-3.701898660	-2.289333839
C	3.617844467	-2.589452172	-2.156536999
C	1.845574156	-5.816434072	-1.395845448
C	2.692478635	-4.691752637	-1.250851172
C	3.088083316	-4.262962976	0.045178804
C	3.938996254	-3.126118117	0.190212420
C	1.469621800	-5.840885633	1.008482958
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C	2.918125150	-2.638787212	2.340617968
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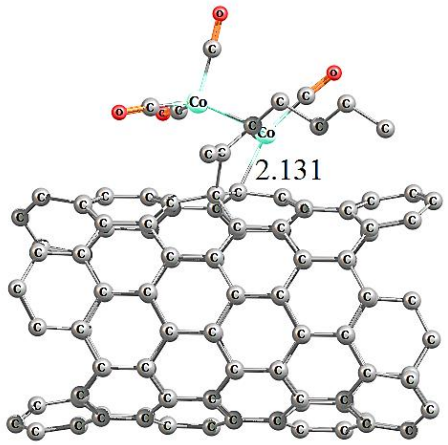

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C	-2.740133022	0.106593189	0.534870419
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C	-5.048771398	-3.059324532	-2.364402453
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C	-2.386699051	-3.131684595	-3.756758462
C	-1.140823301	-5.799181059	-4.341929691
C	-0.445249441	-4.634191266	-4.006272266
C	-0.684006217	-7.038161689	-3.897198051
C	0.367346342	-7.120647144	-2.984319081
C	1.076214346	-5.971853226	-2.630773212
C	1.362909845	-6.456060625	-0.246156727
C	-0.404481264	-7.183413851	2.055662243
C	0.368346180	-6.024674446	1.954275072
C	-1.672054766	-7.125756474	2.632276821
C	-2.244637001	-5.898754261	2.965407057
C	-1.493791810	-4.724648493	2.869999884
C	-3.302486624	-3.218679493	2.141737617
C	-5.448854271	-3.076032052	0.028144663
H	1.995218532	6.005175637	0.068974250
H	2.659409123	6.854233184	-1.970027455
H	4.874383749	6.765520811	-3.083084091
H	5.892660455	4.571553316	-3.636319606
H	6.495483041	2.839562146	-2.264177853
H	8.488098332	2.310838922	-1.215000339
H	9.204757946	2.943513708	1.075712465
H	7.831357128	2.261153749	3.026512035
H	5.614501115	2.768464757	3.454667307
H	4.631048472	4.455650373	4.654432691
H	3.786387252	6.673598234	3.935588857
H	1.970563470	6.817095113	2.248016497
H	-6.655684260	-4.128783628	-1.412135955
H	-5.243511219	-3.488576336	-3.346859290
H	-3.014118684	-4.020127988	-3.763848534
H	-2.050350862	-5.735097845	-4.937920996
H	-1.205279661	-7.945404154	-4.201052411
H	0.620216387	-8.075908633	-2.525414191
H	0.607760484	-7.228485119	-0.371518831
H	-0.021705299	-8.126165123	1.666126963
H	-2.251661689	-8.040571833	2.751830327
H	-3.285216922	-5.851526862	3.284232241
H	-3.892057471	-4.107817392	1.929993875
H	-5.943115401	-3.526026424	0.888952820
Co	-3.568272246	4.217257620	0.616069422
Co	-3.996976392	1.679962834	1.325997206
C	-2.604717221	5.495542657	-0.080570002
C	-5.199916517	4.913540885	0.767848916
C	-5.719491443	1.378730038	1.416552261
C	-3.689131631	1.505529778	3.084763937
O	-1.922046343	6.297615067	-0.570722407
O	-6.247564777	5.398760630	0.871294306
O	-6.849785099	1.124052728	1.440648351
O	-3.495603866	1.463455007	4.221757607
C	-2.921523409	2.934602930	-1.006487468
C	-4.157633087	2.561792833	-0.434261206
C	-2.753790436	4.193614637	2.188554938
O	-2.247049419	4.312442222	3.227244870
C	-5.416986223	2.538518747	-1.269538200
H	-5.364382363	3.319027294	-2.046272996
H	-6.296396943	2.773253080	-0.651667791
C	-5.623967594	1.183986775	-1.950070859
H	-4.731202734	0.937454279	-2.553269550
H	-5.707937793	0.398077890	-1.180219960
C	-6.858304533	1.138407719	-2.841664289
H	-7.748090004	1.398600725	-2.242985417
H	-6.771515939	1.906972888	-3.628902212
C	-7.043315579	-0.237536409	-3.475088774
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H	-7.927991577	-0.269612809	-4.128363348
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H	-1.865349303	4.074264966	-2.521939955
H	-2.908766404	2.787997503	-3.173953232
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CP4*_butyl,oblique_

163
Co2C120H36O5

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C	-4.012750704	5.539811211	3.434428533
C	-3.866901551	3.125211759	3.429432539
C	-4.600037731	4.293944613	3.648211615
C	-5.697157442	1.734670686	2.548081376
C	-6.774622181	0.926568943	0.496100486
C	-7.774278680	1.897077342	0.398466813
C	-8.126628094	2.411784815	-0.848508500
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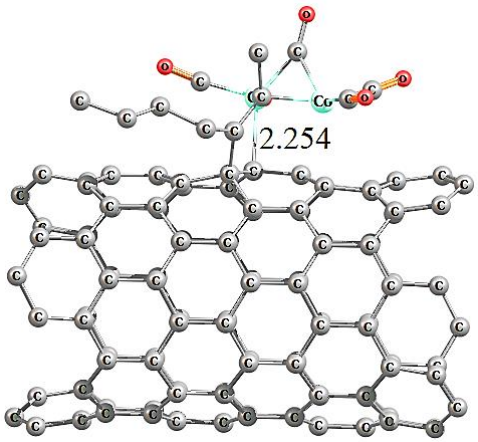

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165
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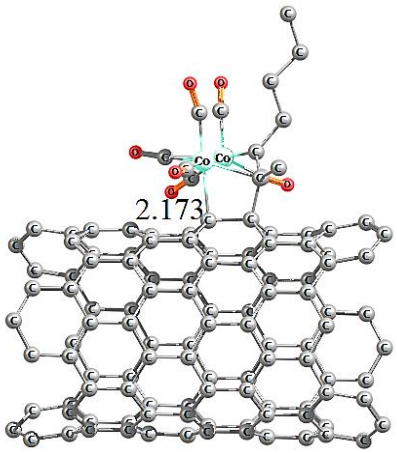

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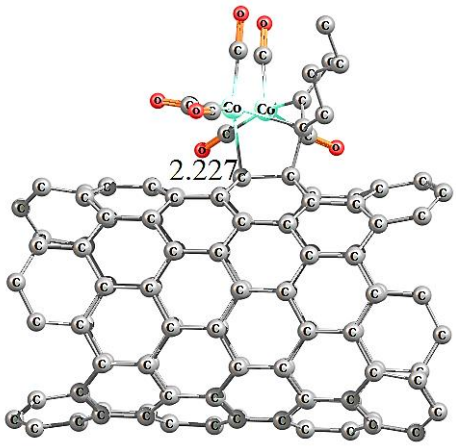
H	-10.339953241	2.031833177	-0.620429333
C	-4.960312967	-0.842185428	-2.373761441
H	-4.191041665	-0.714647313	-3.150542880
H	-5.206085458	-1.916333660	-2.329356520
H	-5.853707344	-0.293018841	-2.696046725

CP5*butyl,parallel*

165
Co2C121H36O6

C	-0.593452189	4.998430958	1.678372865
C	-2.140406749	4.161746737	3.400306159
C	-2.750722243	5.375788216	3.720238095
C	-4.104717519	5.413422830	4.051771123
C	-4.309628226	3.046109640	3.606912221
C	-4.896387959	4.274977276	3.919966297
C	-6.098593979	2.170833271	2.165407174
C	-6.806470353	1.941668846	-0.171982721
C	-7.617901479	3.074914781	-0.249382200
C	-7.613291779	3.857516085	-1.403845527
C	-5.863124141	2.489667002	-2.359863592
C	-6.685179934	3.618302984	-2.415913318
C	-3.813363243	3.507778880	-3.257545783
C	-1.683551282	4.606860490	-2.696840324
C	-2.120726429	5.930857388	-2.806900575
C	-1.620618286	6.907418719	-1.949383831
C	-0.341936276	5.243274172	-0.751455462
C	-0.800785114	6.554146058	-0.876734148
C	0.102351594	4.632971614	0.505400780
C	1.412567624	1.276496738	1.529109793
C	0.734454211	2.527748892	1.594382294
C	-0.257653726	2.767260181	2.575093852
C	-0.893068290	4.038766409	2.645756837
C	-0.228331950	0.366407979	3.081269187
C	-0.862575250	1.622374021	3.176520216
C	-2.250070250	1.697127315	3.469401386
C	-2.894158959	2.967056588	3.540561240
C	-2.380889058	-0.740032588	3.343662194
C	-3.023292836	0.518614894	3.401925351
C	-4.386917494	0.652288481	2.973266321
C	-5.031267332	1.910236911	3.037171568
C	-4.226379166	-1.623073833	2.032900622
C	-4.870078867	-0.349156367	2.088599656
C	-5.711842294	0.063732832	1.023215248
C	-6.349607479	1.327553314	1.075543118
C	-4.874883964	-1.851430244	-0.294766099
C	-5.488098069	-0.582752330	-0.241051056
C	-5.457334666	0.264224804	-1.375874231
C	-6.085710577	1.543031033	-1.327228981
C	-3.926274798	-1.301962609	-2.462230916
C	-4.542427669	-0.033292819	-2.413108058
C	-3.949807509	1.090397985	-3.085356763
C	-4.585904410	2.355033296	-3.059510934
C	-1.916217298	-0.270954219	-3.359860469
C	-2.557775215	1.003736028	-3.348355143
C	-1.778053880	2.184787123	-3.228487959
C	-2.413922580	3.451416629	-3.216897158
C	0.178490561	0.777019451	-2.683178387
C	-0.455799826	2.035514501	-2.691057189
C	0.000766011	3.039832379	-1.809601541
C	-0.639010973	4.315014304	-1.784098055
C	1.602454768	1.466082228	-0.830075324
C	0.912803932	2.687829976	-0.792440373
C	0.759257135	3.393118837	0.462453565
C	2.354153044	1.062559481	0.391235432
C	3.258428287	-2.567143713	1.328112664
C	2.632300859	-1.295311217	1.367255641
C	1.627418258	-1.055302469	2.274380011
C	1.007325252	0.241943833	2.365773144
C	1.693102192	-3.437853026	2.963637171
C	1.045027894	-2.180389065	2.959502983
C	-0.326781490	-2.093811053	3.295035815
C	-0.968551839	-0.816572154	3.345787308
C	-0.460396011	-4.544571176	3.226923343
C	-1.101241390	-3.276328695	3.253770302
C	-2.452932166	-3.134508329	2.794804806
C	-3.094474183	-1.880717903	2.851372138
C	-2.276079420	-5.399189826	1.854143298
C	-2.921631195	-4.127746075	1.902429959
C	-3.798844876	-3.737284629	0.863194373
C	-4.436092026	-2.478827176	0.918082060
C	-2.998546645	-5.677647548	-0.443153939
C	-3.624164125	-4.409250431	-0.396182640
C	-3.623100647	-3.573594468	-1.545815387
C	-4.252292000	-2.291784284	-1.495528331
C	-2.028398159	-5.117731135	-2.602047187
C	-2.662664773	-3.852342315	-2.555185518
C	-2.038699499	-2.711739715	-3.164104681
C	-2.673870296	-1.453740981	-3.141351037
C	0.009611848	-4.057799522	-3.406641995
C	-0.638855131	-2.789642029	-3.363264567
C	0.128787977	-1.612084944	-3.234849271
C	-0.507531127	-0.356018422	-3.222923680
C	2.137386224	-2.990930957	-2.847584253
C	1.471438631	-1.745802075	-2.752001411



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C	3.600138776	-2.298523775	-1.025480386
C	2.970866795	-1.045170643	-0.962567238
C	3.124973397	-0.266611565	0.346813787
C	4.102677334	-2.897868379	0.227609127
C	4.867849230	-4.821296070	1.468936651
C	3.844042672	-4.660572389	2.390500844
C	2.980348928	-3.552980199	2.302089736
C	0.934147445	-4.596717703	3.218672441
C	-0.789290584	-7.028318659	2.846157509
C	-1.217233960	-5.703178137	2.747966823
C	-1.313880353	-7.996948852	1.990139090
C	-2.134389898	-7.628703873	0.925282005
C	-2.574942636	-6.308320965	0.808178842
C	-2.328042839	-6.062800514	-1.612895921
C	-0.134106612	-6.464392095	-3.605867658
C	-0.754479083	-5.249012767	-3.311263191
C	1.232402660	-6.501304343	-3.879527990
C	2.020366727	-5.363250167	-3.716553150
C	1.426488763	-4.133811804	-3.419690290
C	3.251392421	-3.209361140	-2.033192483
C	4.944295902	-3.990736060	0.335300986
H	-1.193395994	5.905235929	1.652599222
H	-2.170090016	6.297047008	3.690597948
H	-4.562824989	6.358483115	4.341639614
H	-5.976627192	4.341863792	4.044857903
H	-6.487830046	3.185459431	2.125192501
H	-8.233000463	3.360242242	0.603524756
H	-8.281764326	4.714791561	-1.476642414
H	-6.582320075	4.322495907	-3.240785688
H	-4.289754138	4.472879024	-3.102629637
H	-2.868302566	6.192715696	-3.554855791
H	-1.937524020	7.943018382	-2.068226928
H	-0.538200899	7.294262269	-0.121307340
H	5.560223847	-5.656429471	1.571701409
H	3.706242561	-5.390368794	3.187883227
H	1.413962664	-5.562327797	3.077287203
H	-0.026757493	-7.299215664	3.575526033
H	-1.009648038	-9.037150991	2.101939486
H	-2.411426718	-8.361016677	0.167471334
H	-1.735337865	-6.974020572	-1.582056537
H	-0.716638215	-7.385157544	-3.603413532
H	1.701363914	-7.446362337	-4.151816657
H	3.103612262	-5.433415427	-3.806092681
H	3.656500917	-4.216909114	-1.970506353
H	5.616091216	-4.246378629	-0.485045212
Co	4.158887819	2.343677347	0.637741389
Co	4.746965735	1.607236707	-1.900519410
C	5.802629692	3.028533691	0.836288332
C	3.635700793	2.739046761	2.283353839
C	6.220575968	2.536432842	-2.332449274
C	4.692342634	0.122888546	-2.785559299
C	3.553041381	2.410103633	-2.963483147
O	3.343252784	3.076728606	3.348948254
O	6.850845622	3.498067537	0.944963873
O	7.161567207	3.014908564	-2.812028159
O	4.824185605	-0.794501421	-3.488016088
O	2.773177496	2.899294965	-3.661649247
C	4.634822881	0.093066003	0.646515538
C	5.443028843	0.621432141	-0.371100010
C	3.624893641	3.651183160	-0.453073255
O	3.317751188	4.646879780	-0.958075244
C	5.223413668	-0.411785959	1.959330212
H	5.770472157	-1.349806127	1.744655947
H	4.396291615	-0.705923596	2.621170646
C	6.120648253	0.509648697	2.783145949
H	6.930323840	0.949496274	2.183118343
H	5.519293403	1.348319055	3.166528723
C	6.727252127	-0.239976708	3.967455037
H	5.916621545	-0.716698965	4.545225438
H	7.362956616	-1.060411052	3.591171392
C	7.541625040	0.674236197	4.876179430
H	8.365626830	1.148468093	4.320743525
H	6.910809077	1.476233209	5.289565103
H	7.976865521	0.118028578	5.718958458
C	6.931935027	0.391903834	-0.323174377
H	7.511784531	1.324562448	-0.297724631
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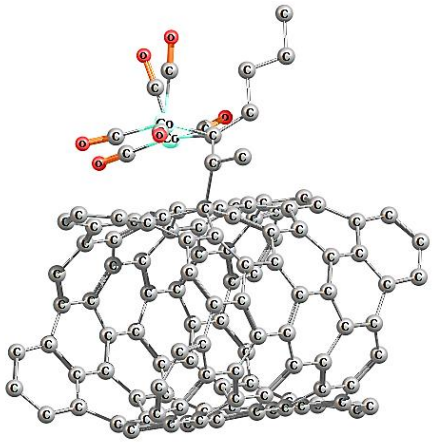
H	7.205141742	-0.110091528	-1.264658102

CP5*methyl,oblique*



165
Co2C121H36O6

C	-0.758618771	-5.184362040	0.033255923
C	-1.386712597	-4.827672424	-2.313425014
C	-1.986440612	-6.066021027	-2.547243826
C	-3.144807918	-6.146312735	-3.320162600
C	-3.221935257	-3.736363211	-3.501822851
C	-3.803129379	-4.987572769	-3.725451546
C	-5.278439972	-2.494516127	-2.978391002
C	-6.723533143	-1.679692960	-1.162344209
C	-7.638217791	-2.735367811	-1.145138237
C	-8.160131925	-3.186304733	0.066320265
C	-6.738673299	-1.656040871	1.284134747
C	-7.656517897	-2.708691081	1.275652797
C	-5.309631760	-2.454444489	3.112044698
C	-3.268602533	-3.720246616	3.606219759
C	-3.864242427	-4.967390034	3.814951421
C	-3.228632310	-6.126570483	3.375301084
C	-1.463332334	-4.815782171	2.367977798
C	-2.079812974	-6.049015631	2.587885322
C	-0.563990609	-4.525238030	1.249523545
C	1.396926551	-1.546991508	0.056069792
C	0.673033261	-2.776733552	0.045907083
C	0.204534957	-3.312419169	-1.178904564
C	-0.499392013	-4.532864545	-1.188025605
C	0.771415490	-1.149731325	-2.252473641
C	0.035534584	-2.350103910	-2.243784316
C	-1.182649532	-2.453617820	-2.961013067
C	-1.907455305	-3.683457646	-2.971450779
C	-1.082567101	-0.059136388	-3.410765279
C	-1.806031235	-1.269147087	-3.414908124
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C	-3.150520214	1.160002043	-3.005520139
C	-3.875809995	-0.067839005	-3.010812677
C	-5.067879260	-0.189439230	-2.249016690
C	-5.787453243	-1.408547574	-2.252992402
C	-4.530487671	1.968514217	-1.175606189
C	-5.228873249	0.743398160	-1.168730777
C	-5.718431228	0.218699110	0.050916971
C	-6.437302733	-1.012224879	0.056484698
C	-4.521118522	1.977882439	1.254942729
C	-5.227230686	0.757334389	1.264518890
C	-5.073626055	-0.161076430	2.358081598
C	-5.808400061	-1.372199399	2.377315597
C	-3.136581805	1.178227893	3.088206960
C	-3.878965713	-0.042576964	3.116257851
C	-3.256060897	-1.238138696	3.564917599
C	-3.991203595	-2.449071111	3.589200170
C	-1.078506670	-0.055859388	3.519967354
C	-1.819928988	-1.264383784	3.532220203
C	-1.223645181	-2.457811243	3.066448873
C	-1.961507185	-3.678090421	3.058363405
C	0.713564684	-1.158083663	2.323166963
C	-0.024228808	-2.361075123	2.321013294
C	0.146980414	-3.296824134	1.253737512
C	1.586549101	-0.870854136	1.242965105
C	3.521764088	2.171648451	0.055865762
C	2.809910652	0.944967466	0.043879284
C	2.323458102	0.432473225	-1.135440679
C	1.772215908	-0.907059978	-1.203625532
C	2.878877259	2.573285147	-2.244154248
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C	0.272318993	-0.034486273	-2.977322900
C	1.068631050	3.618875879	-3.486105469
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C	-1.081389485	2.399220189	-3.432537967
C	-1.794399045	1.184489113	-3.426705993
C	-0.989272438	4.818233908	-2.989473169
C	-1.705806900	3.585180257	-2.977501903
C	-2.912223273	3.478324041	-2.245363519
C	-3.627741609	2.263583952	-2.248155004
C	-2.403883200	5.661051862	-1.202035314
C	-3.110591287	4.434885583	-1.192019576
C	-3.626189290	3.922656692	0.028515068
C	-4.340309168	2.686356003	0.036220832
C	-2.374647542	5.659577450	1.231960443
C	-3.088507942	4.436989408	1.238295969
C	-2.880295446	3.484212669	2.293153004
C	-3.606774598	2.276026719	2.317349016
C	-0.929754109	4.808859256	2.992796644
C	-1.659728656	3.584821284	3.001880302
C	-1.042396537	2.397044367	3.459589457
C	-1.778125059	1.195802025	3.501699194
C	1.116795914	3.589126243	3.496665181
C	0.393056726	2.374880019	3.471242194

C	1.028279441	1.171653236	3.051821499
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C	2.972897431	2.463317359	2.385900469
C	2.272950575	1.247107014	2.383099427
C	2.642056207	0.187816343	1.334211523
C	3.904145227	2.766970379	1.287009688
C	5.314579401	4.295724677	0.059493771
C	4.738959210	3.894084829	-1.137852957
C	3.792748809	2.859421974	-1.151757039
C	2.374871513	3.649366557	-2.996766502
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C	0.319305327	4.877080895	-3.532445329
C	0.224100048	7.286083937	-3.348655525
C	-0.924726382	7.199614412	-2.564855104
C	-1.514370864	5.956019540	-2.325300821
C	-2.168724140	6.319299410	0.012899323
C	-0.851660337	7.187155712	2.559180820
C	-1.457076916	5.949225853	2.334166371
C	0.312782931	7.265634024	3.321498766
C	0.971652789	6.106791261	3.730822762
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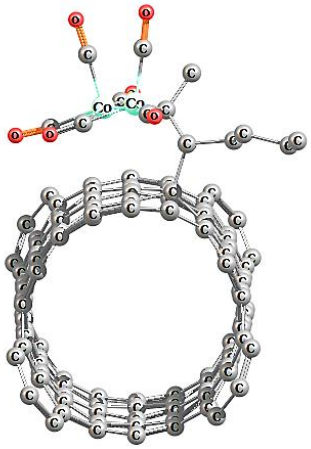
H	-1.562874661	-6.965223024	-2.101040297
H	-3.583577221	-7.119938613	-3.536060887
H	-4.782360853	-5.051281042	-4.198744553
H	-5.767725815	-3.458895241	-2.863536311
H	-7.926887322	-3.217420512	-2.078526699
H	-8.908877487	-3.977863142	0.069472620
H	-7.959062151	-3.171052721	2.214683796
H	-5.808352621	-3.414800887	3.005727132
H	-4.837170136	-5.028140234	4.301547463
H	-3.678621393	-7.097967139	3.577930177
H	-1.675813753	-6.947341395	2.122323094
H	6.086815969	5.064187028	0.059585932
H	5.026271866	4.373738152	-2.073294533
H	2.861354901	4.616043590	-2.889517928
H	1.863055614	6.203576869	-4.242848618
H	0.653375989	8.262782773	-3.569870613
H	-1.353647650	8.096860421	-2.119712953
H	-1.506655500	7.182051306	0.005087213
H	-1.279728423	8.087545815	2.119640250
H	0.755087586	8.239252519	3.530200377
H	1.953647872	6.173270000	4.197735457
H	2.944354567	4.535345484	2.918897072
H	5.182054446	4.220342880	2.219253491
Co	5.563249433	-0.689713375	0.375396897
Co	3.998022444	-2.029549066	-1.201456165
C	7.021508871	-1.706383888	0.594190590
C	6.119573308	0.591192774	1.432938952
C	5.593060281	-2.706786814	-1.560715181
C	3.211937391	-3.629507316	-1.232116103
C	3.767498342	-1.393159240	-2.868551744
O	6.529875409	1.361804084	2.192568698
O	8.028407950	-2.232480561	0.812741369
O	6.556825825	-3.207597057	-1.959281933
O	2.905272290	-4.740392128	-1.306779714
O	3.596923576	-1.055493130	-3.957462692
C	3.892874358	-0.741373379	1.658000485
C	4.175206360	-1.925551779	0.911141331
C	5.639574785	0.221906867	-1.150228697
O	5.799525246	0.864364996	-2.101928762
C	4.179478227	-3.260526382	1.609019665
H	3.144674582	-3.647106497	1.500784717
H	4.295461851	-3.103525294	2.693645987
C	5.161292189	-4.339327717	1.179049433
H	5.202307867	-4.432242898	0.085092295
H	6.177941669	-4.064750849	1.503981742
C	4.782882444	-5.699682627	1.758680935
H	4.713554223	-5.623572434	2.857690298
H	3.773634956	-5.966703462	1.400134471
C	5.775248339	-6.790763690	1.373288626
H	6.784800930	-6.551399606	1.741510448
H	5.483687621	-7.765315390	1.790775805
H	5.834188754	-6.894205314	0.278726355
C	4.145580871	-0.744167936	3.152098454
H	4.307513281	0.277890113	3.522823690
H	3.262104345	-1.148908050	3.680182562
H	5.023084550	-1.348300766	3.415021815

CP5*butyl,oblique*



165
Co2C121H36O6

C	-1.777796968	5.105368153	-0.151407460
C	-2.525114973	4.651478131	2.145184639
C	-3.367274128	5.755739924	2.296810741
C	-4.571513313	5.626984459	2.986355302
C	-4.201110967	3.251906477	3.245741458
C	-5.024157109	4.371238865	3.387757403
C	-5.941575491	1.627638566	2.633256026
C	-7.066290859	0.520526611	0.748930830
C	-8.157928614	1.385268967	0.633326408
C	-8.656133180	1.714064038	-0.626041751
C	-6.880113933	0.464267679	-1.689743389
C	-7.976157649	1.324922996	-1.779912113
C	-5.484011360	1.493330090	-3.427861843
C	-3.684989808	3.113696545	-3.823070483
C	-4.488550574	4.218651457	-4.120333938
C	-4.116306843	5.489282851	-3.687844501
C	-2.213425975	4.566187123	-2.515694567
C	-3.033150091	5.653047933	-2.824116203
C	-1.362379025	4.478309190	-1.327855819
C	1.053561853	1.972492629	0.088931980
C	0.088189669	3.021856914	0.012891306
C	-0.584004881	3.459900355	1.180340870
C	-1.507541225	4.523456560	1.102805340
C	0.270287684	1.435056393	2.325332655
C	-0.670333561	2.486146812	2.239655274
C	-1.924591261	2.372357874	2.878833191
C	-2.866558583	3.441759090	2.803440328
C	-1.406834098	0.045308234	3.421320489
C	-2.342843118	1.096348017	3.333238032
C	-3.746936976	0.814041927	3.276218067
C	-4.685594057	1.873105332	3.200889718
C	-3.170290114	-1.555677629	2.925108618
C	-4.112404967	-0.488545084	2.841327420
C	-5.247743598	-0.610591828	1.996487672
C	-6.181997316	0.449164871	1.911049257
C	-4.234203389	-2.645407336	1.030858170
C	-5.148514119	-1.575493043	0.936887780
C	-5.630885856	-1.169891802	-0.330257064
C	-6.564524612	-0.097365957	-0.425445704
C	-4.032944390	-2.685610103	-1.390748542
C	-4.950954973	-1.620060723	-1.487611431
C	-4.883102578	-0.701693178	-2.589724428
C	-5.827993421	0.348250586	-2.699851972
C	-2.676893114	-1.658127197	-3.128415578
C	-3.629986619	-0.601319693	-3.248971710
C	-3.207977850	0.682437918	-3.686861574
C	-4.154756882	1.729829619	-3.807006836
C	-0.856336556	-0.062794755	-3.441929842
C	-1.809232344	0.981929462	-3.554448548
C	-1.481612091	2.278766203	-3.100601557
C	-2.436026776	3.335677571	-3.190236250
C	0.624855649	1.403600456	-2.197236692
C	-0.335973856	2.437455880	-2.284333811
C	-0.427400382	3.413805089	-1.243797679
C	1.479964101	1.339300103	-1.066975033
C	3.865111199	-1.239596050	0.387441007
C	2.966998415	-0.143186429	0.300753923
C	2.218213176	0.225725184	1.413931716
C	1.340421651	1.350244621	1.367347138
C	3.077268873	-1.756561409	2.624297705
C	2.138126882	-0.707781786	2.507998816
C	0.893262491	-0.801058751	3.178018734
C	-0.047193690	0.269132404	3.074241389
C	1.405513690	-3.137225480	3.738034459
C	0.468703453	-2.078079561	3.627403450
C	-0.932547316	-2.363401078	3.516031980
C	-1.866512171	-1.311308086	3.432322257
C	-0.346557440	-4.724810510	3.155378992
C	-1.286423666	-3.656944160	3.062134993
C	-2.440606837	-3.798938827	2.254256591
C	-3.373170794	-2.744471731	2.171655419
C	-1.455083830	-5.863354213	1.317188106
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C	-3.820243773	-3.332327069	-0.142831212
C	-1.246313336	-5.896845390	-1.107350550
C	-2.173525976	-4.831188687	-1.200027491
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C	-2.996100775	-2.817598066	-2.370684663
C	0.151615152	-4.807488212	-2.770765533
C	-0.790878696	-3.743295286	-2.867057816
C	-0.371018709	-2.464259222	-3.301613003
C	-1.310422912	-1.422821479	-3.432415532
C	1.966757122	-3.227323971	-3.142539953
C	1.029481865	-2.171554962	-3.203252352

C	1.394636383	-0.861649154	-2.780894213
C	0.438447527	0.197169280	-2.930809387
C	3.489473945	-1.751161833	-1.943293717
C	2.582897786	-0.684237283	-2.034955455
C	2.722889678	0.498600937	-1.055587869
C	4.397645508	-1.835623328	-0.789256040
C	5.941848151	-3.081443154	0.587141141
C	5.236399870	-2.724806315	1.726660299
C	4.137907772	-1.856007201	1.634993189
C	2.729193132	-2.907455543	3.353691426
C	1.698036825	-5.631130288	4.074478657
C	0.914169825	-4.516026096	3.772010665
C	1.293856399	-6.901834944	3.665282013
C	0.199142623	-7.057829628	2.816920162
C	-0.601299826	-5.957694894	2.501512964
C	-1.012774000	-6.486637488	0.142114374
C	0.637688645	-7.124194259	-2.273553453
C	-0.205364714	-6.020957143	-2.128380946
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C	3.226319215	-2.962214380	-2.602439499
C	5.461460200	-2.715096627	-0.678727525
H	-2.593534319	5.821861929	-0.213117127
H	-3.089660565	6.711824809	1.854431037
H	-5.202327324	6.502000337	3.139579231
H	-6.028956160	4.255542582	3.792675755
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H	-9.536632316	2.350536135	-0.708396864
H	-8.283051398	1.711084933	-2.751387554
H	-6.161132205	2.343275492	-3.390570170
H	-5.417222630	4.079328852	-4.672743078
H	-4.725020205	6.351218063	-3.959203104
H	-2.839032031	6.623625292	-2.368853903
H	6.822229239	-3.717664716	0.668528164
H	5.523758760	-3.126510263	2.698212784
H	3.406945861	-3.756931925	3.316133380
H	2.637292024	-5.503774962	4.611459131
H	1.887996293	-7.771750660	3.943564367
H	-0.021443385	-8.031197880	2.379802096
H	-0.202352801	-7.207416971	0.221987513
H	0.351078048	-8.085065659	-1.847167586
H	2.489206773	-7.862218303	-3.085467013
H	3.329744512	-5.613578834	-3.706772647
H	3.887610447	-3.801818432	-2.404693682
H	5.910819692	-3.144933156	-1.574011072
Co	5.410582885	1.825134655	0.217271960
Co	3.575283213	3.315410480	1.084585665
C	6.763420974	2.970221256	0.019338035
C	6.460963438	0.446622638	-0.058485227
C	4.859320013	4.406719919	1.612661721
C	2.502240357	4.541494739	0.408309271
C	2.844121352	3.063592847	2.716500133
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O	7.695231327	3.653089245	-0.060016364
O	5.626969874	5.184291421	1.989999895
O	1.901828479	5.432737444	-0.016986750
O	2.459140429	3.080869904	3.806081286
C	3.814562283	1.579280970	-1.488188866
C	4.037568789	2.810743145	-0.863301678
C	4.957183287	1.382591007	1.867646800
O	4.925490673	0.911753499	2.934158050
C	4.211439977	1.385280733	-2.941769643
H	4.329819625	2.349541354	-3.451468254
H	3.370188887	0.884493648	-3.451475177
C	5.467131779	0.536297847	-3.143506578
H	6.358254672	1.139270026	-2.893948881
H	5.463014779	-0.301669175	-2.431230736
C	5.574981288	-0.030166709	-4.554414030
H	4.656805982	-0.605086773	-4.771146682
H	5.611691690	0.792359756	-5.289668701
C	6.792519441	-0.934539687	-4.713251435
H	7.724552182	-0.384002586	-4.512898100
H	6.742998568	-1.772754437	-4.000445541
H	6.854804679	-1.354852335	-5.727477524
C	4.474654897	4.002017806	-1.696009069
H	4.815392399	4.830353405	-1.063780073
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CP5*_methyl,oblique_

165
Co2C121H36O6

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C	3.766408532	-5.759127463	3.551452143
C	3.651358412	-3.345461344	3.633675515
C	4.334858402	-4.534256189	3.897545466
C	5.594096769	-1.972407739	3.018151053
C	6.918225681	-1.148951633	1.122387513
C	7.900940336	-2.141468001	1.122132300
C	8.391615666	-2.636682452	-0.085129137
C	6.813894767	-1.281414582	-1.317566647
C	7.796717093	-2.273417325	-1.292639506
C	5.347635270	-2.282084887	-3.019095455
C	3.363371393	-3.689029730	-3.397597187
C	4.025182852	-4.901549835	-3.606774410
C	3.469591678	-6.091465394	-3.140396957
C	1.660270710	-4.868520852	-2.105683783
C	2.339179739	-6.068938007	-2.325451464
C	0.788962654	-4.605318106	-0.962668662
C	-1.709833066	-1.977576205	0.247262264
C	-0.556644539	-2.955598216	0.230638799
C	0.107582358	-3.313233898	1.413750062
C	0.924351362	-4.470666399	1.448169253
C	-0.549409325	-1.123045255	2.362871831
C	0.269583430	-2.276917792	2.404161014
C	1.506050906	-2.251047574	3.078495381
C	2.328380157	-3.419395107	3.127052124
C	1.239839636	0.148536385	3.440311680
C	2.049193960	-0.998764406	3.474095550
C	3.477647050	-0.878051492	3.474853845
C	4.292271232	-2.035170465	3.527354394
C	3.193885508	1.506724125	2.934602913
C	4.012018374	0.341406831	2.978659197
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C	6.003908668	-0.884112916	2.232554482
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C	5.734044126	0.602695965	-0.146597146
C	6.532902503	-0.576866089	-0.117766326
C	4.374569684	2.207496987	-1.394146883
C	5.157686361	1.034762423	-1.365596726
C	5.014004229	0.038873010	-2.391639033
C	5.815040609	-1.126410895	-2.374110994
C	2.970561416	1.210520400	-3.109362415
C	3.778746607	0.038193786	-3.093986114
C	3.207623735	-1.217336008	-3.434921553
C	4.015035965	-2.380604769	-3.435895042
C	0.980650173	-0.172228045	-3.345177949
C	1.781984576	-1.325654003	-3.333878436
C	1.256106381	-2.535785560	-2.806829192
C	2.069948382	-3.712195827	-2.815506596
C	-0.733420786	-1.329204431	-2.034548353
C	0.062811052	-2.497614347	-2.057455517
C	-0.029679613	-3.447524985	-0.971451161
C	-1.716516786	-1.119634443	-1.021581778
C	-3.797642775	1.786122337	0.161398333
C	-3.188109989	0.453575159	0.180353443
C	-2.417711193	0.120374043	1.404125136
C	-1.609430054	-1.002828554	1.420228023
C	-3.020058592	2.330115669	2.387176865
C	-2.203010352	1.170779257	2.362790318
C	-0.950810417	1.202007594	3.037278823
C	-0.125573361	0.048709136	3.045157013
C	-1.209924955	3.615797731	3.404687766
C	-0.397219134	2.464243277	3.401554928
C	1.030100350	2.588725873	3.334173872
C	1.846696895	1.441668206	3.379235986
C	0.726895339	4.961323578	2.786505534
C	1.547591776	3.799323237	2.818357305
C	2.752674774	3.758047887	2.071134882
C	3.565179112	2.608093303	2.114025149
C	2.050546677	5.842113150	0.945383059
C	2.854496103	4.677185439	0.972763370
C	3.383786804	4.149144780	-0.236589213
C	4.185998412	2.968786691	-0.207390127
C	1.979583952	5.732080859	-1.485139602
C	2.778385863	4.563718251	-1.454083896
C	2.602140310	3.543517100	-2.449613833
C	3.403497613	2.385222905	-2.432787668
C	0.538652602	4.691964362	-3.141699854
C	1.349908707	3.523166193	-3.113695628
C	0.792234897	2.271811065	-3.465661046
C	1.595970306	1.115342536	-3.450997228
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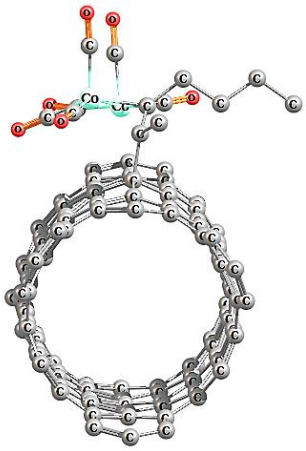
C	-0.634949464	2.156657297	-3.409370281



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C	-3.143720653	2.170679278	-2.141768444
C	-2.340209942	1.001035877	-2.091640718
C	-2.471296875	0.040045427	-1.034706153
C	-4.081727818	2.444909196	-1.052827301
C	-5.551111465	3.948347865	0.142244306
C	-4.990367342	3.528742675	1.345922943
C	-4.046779226	2.496803980	1.355423611
C	-2.552975075	3.489300292	3.010724085
C	-1.252830763	6.143617897	3.519433956
C	-0.578089168	4.931042405	3.345483402
C	-0.694012565	7.328882178	3.047339364
C	0.456697654	7.306624302	2.258491846
C	1.147935505	6.110211348	2.066254308
C	1.746650003	6.427385914	-0.290895527
C	0.310745877	7.080321990	-2.829952075
C	1.010449880	5.901849398	-2.568525969
C	-0.892001249	7.035492522	-3.535782112
C	-1.486715536	5.813952678	-3.844007613
C	-0.803603669	4.619312055	-3.596539481
C	-2.738371524	3.250268510	-2.928219056
C	-5.019819738	3.480932593	-1.058563240
H	1.837757491	-6.010345524	0.269000576
H	2.230599996	-6.754847180	2.410796569
H	4.286973537	-6.684174403	3.797290081
H	5.323984332	-4.499179714	4.352902102
H	6.153843654	-2.900902240	2.933668251
H	8.263713062	-2.544920558	2.066933963
H	9.189359913	-3.378836085	-0.079072705
H	8.079595299	-2.778708766	-2.215466573
H	5.910332633	-3.203306938	-2.886626949
H	4.987170763	-4.910232300	-4.118093442
H	3.969297989	-7.037612626	-3.345879925
H	1.996059030	-6.981440134	-1.838837892
H	-6.329019910	4.710931771	0.136230239
H	-5.261605724	4.018884909	2.280779891
H	-3.130491438	4.401048722	2.881997601
H	-2.224627486	6.157156062	4.011286949
H	-1.204552450	8.274465133	3.227257069
H	0.802853010	8.217108769	1.770300621
H	1.018429125	7.234799834	-0.306705572
H	0.692119285	8.030796975	-2.457977610
H	-1.411183147	7.963296965	-3.774084092
H	-2.492224150	5.786288444	-4.262095328
H	-3.295581355	4.179386969	-2.843043188
H	-5.324645805	3.928035941	-2.004271932
Co	-4.313368811	-3.027155802	-1.129515885
Co	-5.158683929	-0.829128154	-0.101432582
C	-5.718888345	-4.137149823	-1.126286886
C	-3.152768570	-4.184061389	-1.739089288
C	-6.699496300	-1.715235787	-0.257532058
C	-5.698963548	0.016367807	1.356474784
C	-5.635493936	0.168744102	-1.560724910
O	-2.413560127	-4.975675133	-2.145573978
O	-6.531160215	-4.959777683	-1.184365901
O	-7.768877085	-2.147075883	-0.305996386
O	-6.125166385	0.497677267	2.314156277
O	-6.071125150	0.704031210	-2.481279378
C	-3.001615937	-2.878358777	0.507994481
C	-4.300307385	-2.399688816	0.773706551
C	-4.163352204	-2.005403818	-2.574652989
O	-4.025730386	-1.435866319	-3.574183774
C	-5.045853307	-2.880225629	1.998865594
H	-5.006835749	-3.975623944	2.098619631
H	-6.111419262	-2.615446717	1.949697649
C	-4.412938480	-2.238367014	3.244577496
H	-3.427771428	-2.696816901	3.434708148
H	-4.204498711	-1.173673469	3.048503576
C	-5.285596173	-2.347585579	4.488107163
H	-6.259069803	-1.868278894	4.285477638
H	-5.494738674	-3.409806880	4.703868860
C	-4.627140194	-1.684983892	5.694473334
H	-4.429280917	-0.621218259	5.490767199
H	-5.263904075	-1.749590769	6.588596075
H	-3.662980833	-2.162659365	5.926662818
C	-2.669538762	-4.229879966	1.140346333
H	-1.939151598	-4.795363022	0.546577814
H	-2.247055592	-4.110117691	2.151363515
H	-3.573290309	-4.845591587	1.206471338

CP5*butyl,oblique

165
Co2C121H36O6

C	-0.528801167	5.210303534	0.207426161
C	-1.371637933	4.764904653	2.475673179
C	-1.937973844	6.016974169	2.728331824
C	-3.120512000	6.113374696	3.458802859
C	-3.287739390	3.703092404	3.557063410
C	-3.832074689	4.965394818	3.803485544
C	-5.370629177	2.555788271	2.933158969
C	-6.768587347	1.861370266	1.037918851
C	-7.630359628	2.960247079	1.014102814
C	-8.053134563	3.488934981	-0.204776030
C	-6.633475090	1.941692215	-1.402675768
C	-7.495974260	3.040388496	-1.401491584
C	-5.046462963	2.744384126	-3.099546144
C	-2.912235961	3.913746989	-3.465444603
C	-3.431393936	5.189807872	-3.696111098
C	-2.753263633	6.315679826	-3.232260938
C	-1.103944944	4.910424699	-2.162139827
C	-1.642996730	6.176439134	-2.401862073
C	-0.274150429	4.566141211	-1.010357444
C	1.926807682	1.707573771	0.242743102
C	0.874082238	2.791940211	0.211663252
C	0.254772873	3.241584779	1.388341398
C	-0.422923049	4.485670137	1.401308979
C	0.644754224	1.000690133	2.353217568
C	-0.035990069	2.240550883	2.384144945
C	-1.276754942	2.362488633	3.039507244
C	-1.958351039	3.619100603	3.069147315
C	-1.294315338	-0.047199825	3.418779636
C	-1.966328150	1.185767747	3.436926587
C	-3.398881366	1.230646865	3.424553989
C	-4.074832422	2.474628771	3.455098398
C	-3.389961539	-1.178604541	2.920239800
C	-4.067536070	0.074159127	2.940492545
C	-5.229616316	0.264538626	2.144250875
C	-5.898591569	1.510377513	2.159729492
C	-4.733899750	-1.879531189	1.020700464
C	-5.381659917	-0.626548656	1.027263714
C	-5.786250202	-0.035514806	-0.194640686
C	-6.443979590	1.228511701	-0.190187742
C	-4.607134792	-1.803379553	-1.405376243
C	-5.252074277	-0.548942818	-1.401315196
C	-4.985119412	0.409544731	-2.438154881
C	-5.649010925	1.658108429	-2.445795640
C	-3.077399091	-0.994344229	-3.111572102
C	-3.749012914	0.261027478	-3.123345365
C	-3.035905018	1.439173164	-3.472535862
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C	-0.956625530	2.538068059	-2.833743501
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C	0.885356910	1.129681421	-2.028876296
C	0.215177346	2.374613095	-2.069817074
C	0.402019080	3.321164010	-0.998422480
C	1.847029662	0.833081453	-1.014501928
C	3.571565429	-2.278606486	0.217003398
C	3.117071915	-0.886704135	0.227326178
C	2.354827742	-0.460943261	1.425113723
C	1.704575860	0.759713487	1.428795856
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C	2.008262859	-1.475309667	2.382388276
C	0.757455942	-1.353432399	3.044209907
C	0.075584299	-0.109979580	3.033091877
C	0.737279275	-3.774898554	3.445546301
C	0.061744471	-2.538062690	3.422382203
C	-1.369383078	-2.497678587	3.350655393
C	-2.046368055	-1.262494958	3.371845150
C	-1.340661965	-4.898250749	2.845236640
C	-2.021866473	-3.649092849	2.853196932
C	-3.209826544	-3.480911739	2.096922950
C	-3.882647271	-2.243490905	2.115138524
C	-2.743406010	-5.648991847	1.007533486
C	-3.407639677	-4.398865039	1.010548675
C	-3.858063467	-3.829649301	-0.212048536
C	-4.520149175	-2.564890631	-0.207098449
C	-2.624122856	-5.576646450	-1.422150816
C	-3.286246295	-4.325392961	-1.415606028
C	-2.981756465	-3.344062602	-2.418779005
C	-3.648766190	-2.103596509	-2.427635956
C	-1.049880057	-4.724919103	-3.065887288
C	-1.725256740	-3.472732521	-3.062821843
C	-1.026178853	-2.296851576	-3.421021376
C	-1.696167331	-1.058628226	-3.432475136
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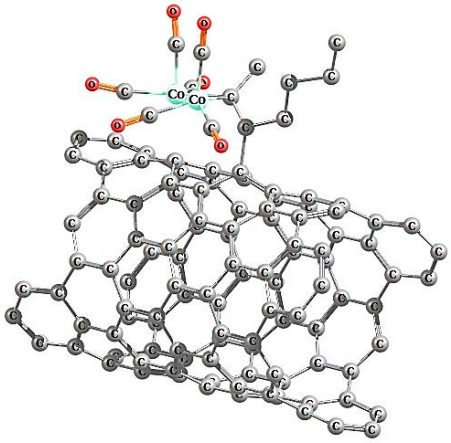

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C	2.232423627	-1.357395560	-2.051446711
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C	4.537285853	-4.136082478	1.432436975
C	3.715694629	-3.006837268	1.419618738
C	2.087277138	-3.810342155	3.056711813
C	0.487944940	-6.288151414	3.606202646
C	-0.041904470	-5.009094916	3.408119083
C	-0.203312822	-7.409278112	3.153095224
C	-1.341119852	-7.267909535	2.357768934
C	-1.888275507	-6.003028600	2.141530880
C	-2.490995395	-6.280311675	-0.217718718
C	-1.096450745	-7.119534684	-2.724738795
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C	0.296942364	-4.808702287	-3.505853722
C	2.372576680	-3.650709281	-2.854618914
C	4.589113551	-4.125289960	-0.971866590
H	-1.141252531	6.109095277	0.199160880
H	-1.463842134	6.915384917	2.334484930
H	-3.533412129	7.094421163	3.691782537
H	-4.824496089	5.048827956	4.245172602
H	-5.818590169	3.541427051	2.830790101
H	-7.950145503	3.418285003	1.949503301
H	-8.760176765	4.317902858	-0.216642897
H	-7.712388801	3.560063725	-2.334274081
H	-5.502986531	3.724855036	-2.985539056
H	-4.379668807	5.300040569	-4.221035045
H	-3.142233508	7.309217322	-3.452970212
H	-1.207040463	7.050725458	-1.919478022
H	5.736316809	-5.484276644	0.246291122
H	4.733017196	-4.650036426	2.373633356
H	2.557234922	-4.783958950	2.944972147
H	1.450697216	-6.404827067	4.102180373
H	0.193616574	-8.404202170	3.352354491
H	-1.788198712	-8.140372519	1.882237724
H	-1.859504557	-7.165575444	-0.213287023
H	-1.586898333	-8.016562703	-2.347893107
H	0.527956332	-8.201980480	-3.633221353
H	1.850742494	-6.167245294	-4.135868371
H	2.822757155	-4.634414047	-2.752807390
H	4.849206453	-4.614844298	-1.909831131
Co	4.809152480	2.168388256	-1.008556375
Co	5.264530946	0.127037804	0.429548930
C	6.292026928	3.166550920	-1.074496855
C	3.714235157	3.122898452	-1.981161326
C	6.887132614	0.872894038	0.482597141
C	5.272763487	-0.539206599	2.074017703
C	6.003040916	-1.169894545	-0.614643245
O	3.012863408	3.785177255	-2.621475604
O	7.193838851	3.876324889	-1.227320183
O	7.978629569	1.241130424	0.552215193
O	5.325714743	-0.917146236	3.161366630
O	6.640347227	-1.910694031	-1.221564291
C	3.318369926	2.504262770	0.450887709
C	4.497390729	1.921891492	0.956508358
C	4.913189407	0.883736338	-2.220731798
O	4.963531725	0.143813118	-3.112754592
C	3.109663090	3.993797011	0.804817284
H	2.795962008	4.045150042	1.865114370
H	2.257141153	4.382590858	0.236354595
C	4.226697851	5.003264973	0.539934226
H	5.213684576	4.663097182	0.881259930
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C	3.895907000	6.338529512	1.203992409
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C	4.914308761	7.421348438	0.865286974
H	5.925019749	7.122820891	1.184115598
H	4.947019499	7.601074567	-0.220353855
H	4.669630070	8.372359401	1.360216597
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H	6.237478080	2.399947851	2.208505789
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H	4.760451861	1.890907797	3.052130429

TS2*methyl,parallel*

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Co2C121H36O6

C	2.123153662	-4.939793615	1.832156894
C	3.635454459	-3.787927444	3.387251848
C	4.514330454	-4.846462678	3.628078483
C	5.878316412	-4.601673599	3.779619346
C	5.539894274	-2.256238505	3.300149013
C	6.399106892	-3.331763398	3.538707080
C	6.894930676	-1.100331326	1.607454970
C	7.225869699	-0.812911683	-0.808396737
C	8.233422818	-1.762881543	-0.987960135
C	8.247515881	-2.556248986	-2.134734652
C	6.158902128	-1.585401108	-2.870264115
C	7.178752709	-2.527625124	-3.028885051
C	4.269152889	-3.011645738	-3.527533299
C	2.504062502	-4.502202661	-2.697180564
C	3.188589841	-5.710249400	-2.853071161
C	3.039153367	-6.724220213	-1.908595127
C	1.636008819	-5.297421868	-0.551952876
C	2.336000427	-6.493163923	-0.727057237
C	1.252596589	-4.743059397	0.746334373
C	-0.602210576	-1.700065871	1.937819617
C	0.319665465	-2.792780194	1.913841004
C	1.428619460	-2.820222395	2.796673005
C	2.311603977	-3.932937654	2.784588514
C	0.962662432	-0.462189111	3.333559574
C	1.850434047	-1.563217793	3.336222215
C	3.248147896	-1.350227723	3.438425084
C	4.141420642	-2.462823159	3.426167437
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C	5.041518587	0.079200645	2.640523216
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C	4.296691168	2.237769486	1.711001485
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C	5.427879723	0.528940815	-1.832940139
C	6.304871363	-0.594479358	-1.865706974
C	3.491814478	1.729695677	-2.719393410
C	4.354281408	0.614113951	-2.751226166
C	3.928794134	-0.616028346	-3.358462428
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C	2.526412897	-0.818672345	-3.459605261
C	2.023446706	-2.130451187	-3.250765272
C	2.903164082	-3.239720236	-3.318591500
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C	0.774305603	-2.240150766	-2.552669504
C	0.672625203	-3.275951023	-1.592716142
C	1.566710211	-4.386570486	-1.639168822
C	-1.026396026	-1.979905130	-0.388963847
C	-0.110845718	-3.054090913	-0.439356726
C	0.362327567	-3.649731748	0.781234615
C	-1.571073916	-1.600816144	0.886540919
C	-3.217180244	1.672952717	1.973258022
C	-2.334667982	0.566578219	1.927715804
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C	3.260540533	2.296870440	2.681335703
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C	2.512905414	4.430196297	1.747318075
C	3.299664427	4.182952804	0.597569543
C	4.177236734	3.078576422	0.571484830
C	1.961043595	5.883227490	-0.598780760
C	2.828199092	4.764819743	-0.629444326
C	2.851214157	3.914882726	-1.768024214
C	3.725092783	2.785653780	-1.797159893
C	0.868133839	5.086944785	-2.620930810
C	1.741414775	3.973202283	-2.652282659
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C	-0.604086023	1.201494989	-3.010839505
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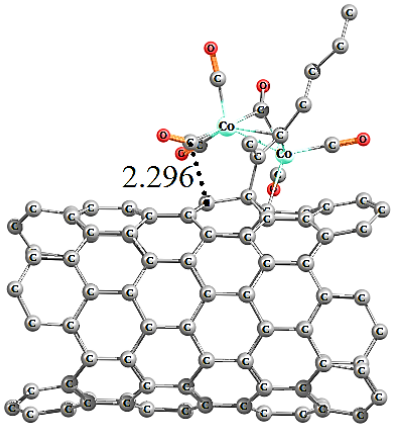

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C	-5.206081981	3.599922434	2.294556038
C	-4.074657061	3.641101032	3.099503156
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C	-1.144190858	4.172835657	3.569627046
C	-0.010608891	6.882077693	2.957269635
C	0.659590691	5.665869174	2.811161014
C	0.184456540	7.903744831	2.027989570
C	0.909947827	7.667942000	0.861151447
C	1.589253825	6.458986642	0.694538169
C	1.088565504	6.096465765	-1.675254633
C	-1.363366509	6.003659735	-3.390480050
C	-0.479806979	4.944790277	-3.171029323
C	-2.732098810	5.762447927	-3.497545072
C	-3.250280052	4.495185513	-3.235206840
C	-2.387596050	3.419587844	-3.015138979
C	-3.778000080	2.215337325	-1.382421541
C	-5.240998927	2.752124873	1.176335252
H	2.892504771	-5.702849013	1.737707632
H	4.132786377	-5.865859656	3.674551596
H	6.552122012	-5.426262806	4.010214318
H	7.477329801	-3.177248346	3.516369558
H	7.470791508	-2.018957122	1.522069024
H	8.992370260	-1.899411637	-0.218339616
H	9.060701325	-3.264769284	-2.289502336
H	7.124122130	-3.253867901	-3.839035540
H	4.946544026	-3.856970816	-3.433173078
H	3.859105848	-5.847126507	-3.700697736
H	3.545468607	-7.677541442	-2.056991101
H	2.349907938	-7.233696904	0.071938851
H	-6.026870836	4.293094019	2.474204482
H	-3.987291611	4.399368405	3.877526561
H	-1.820304598	5.019461029	3.476681644
H	-0.705168924	7.021331497	3.785029047
H	-0.305961224	8.865817301	2.173223597
H	0.927371799	8.413066573	0.066305827
H	0.334095308	6.872816927	-1.571713022
H	-0.981058602	7.021677737	-3.458555471
H	-3.409588606	6.588253542	-3.712110790
H	-4.328222621	4.346127535	-3.184775548
H	-4.357321532	3.127904777	-1.266069935
H	-6.035632178	2.859660590	0.438238791
Co	-4.386389039	-2.937845880	0.101872069
Co	-5.158699101	-0.797097265	-1.015136060
C	-3.488813249	-3.436106736	-1.363146758
C	-5.402430647	-4.229435464	0.789778677
C	-5.879764589	-2.510203572	-1.169210079
C	-6.512180935	0.312358480	-1.012419890
C	-4.712324699	-0.689415305	-2.759738918
O	-6.041278701	-5.104797518	1.186951865
O	-2.999682154	-3.831383184	-2.331080562
O	-6.726696767	-3.083114260	-1.748251426
O	-7.398707102	1.056792369	-1.004794511
O	-4.397651355	-0.586744271	-3.860787702
C	-3.968988530	-1.202027036	1.558708804
C	-5.212469597	-1.138084755	0.916833437
C	-2.890193665	-3.468783861	1.095907284
O	-2.349417639	-4.314350274	1.685378796
C	-6.484367223	-1.118679770	1.720683501
H	-6.661982118	-0.044198947	1.934241063
H	-6.307648997	-1.579917963	2.704988810
C	-7.749781851	-1.721355951	1.127729103
H	-7.942471365	-1.321206075	0.120820906
H	-7.627158422	-2.809678155	1.007138052
C	-8.969450637	-1.447404622	2.003401244
H	-8.791565972	-1.850741060	3.015244184
H	-9.090735052	-0.356275545	2.118861198
C	-10.243390604	-2.051106841	1.421956025
H	-10.147905142	-3.142942289	1.319646500
H	-11.114152899	-1.844739271	2.060689946
H	-10.449853944	-1.638784698	0.422234182
C	-3.861196658	-1.557784591	3.025237797
H	-2.831260984	-1.835234922	3.289922241
H	-4.144659480	-0.690771287	3.645072123
H	-4.514521541	-2.400699283	3.283013195

TS2*butyl,parallel*

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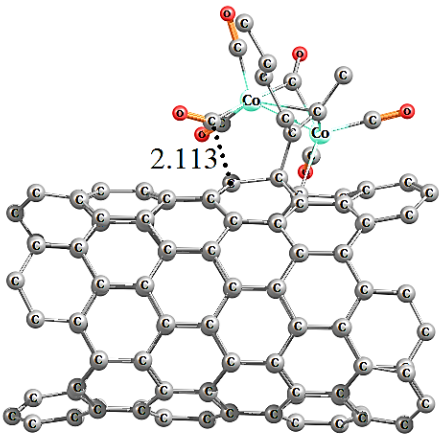
Co2C121H36O6

C	1.590502507	-4.986113473	1.723157587
C	3.099626958	-3.945610126	3.356872217
C	3.901142284	-5.057625729	3.623170048
C	5.269423719	-4.897789594	3.838641844
C	5.095111657	-2.531266723	3.376411754
C	5.876379850	-3.659764552	3.637962211
C	6.595905522	-1.435101221	1.766624888
C	7.057985412	-1.126798403	-0.625490776
C	8.013098380	-2.133653293	-0.777966498
C	8.032650927	-2.906483744	-1.938714783
C	6.042119817	-1.797580188	-2.747162306
C	7.009320397	-2.797586267	-2.878579012
C	4.100914114	-3.097156615	-3.506944452
C	2.215864968	-4.490138149	-2.773118471
C	2.832383718	-5.735286947	-2.922883775
C	2.577703054	-6.755001292	-2.008209883
C	1.199066577	-5.271007543	-0.688572709
C	1.833885335	-6.503014374	-0.855794271
C	0.781567609	-4.720572425	0.601520671
C	-0.956335766	-1.603755525	1.766035546
C	-0.095290061	-2.742691533	1.765915840
C	0.980624714	-2.839638144	2.684258185
C	1.797668002	-4.003912900	2.694299090
C	0.637394371	-0.463890435	3.218312606
C	1.454503153	-1.616791974	3.252084858
C	2.857930203	-1.490285629	3.423555835
C	3.682341445	-2.654239194	3.436545525
C	2.631536588	0.938030245	3.293585389
C	3.449239701	-0.214163656	3.292507057
C	4.770782455	-0.161198679	2.734893514
C	5.591227327	-1.314143177	2.737491059
C	4.205495576	2.056165266	1.816226173
C	5.024331613	0.886334432	1.809012373
C	5.815323047	0.584365305	0.669928414
C	6.626433994	-0.576863614	0.659778028
C	4.605678646	2.353667930	-0.559123523
C	5.394084504	1.184212900	-0.566261930
C	5.394599093	0.341059708	-1.704119840
C	6.202076870	-0.833722249	-1.718816386
C	3.574131922	1.670837774	-2.650220864
C	4.369628635	0.505919606	-2.665991471
C	3.897677817	-0.687410155	-3.311459857
C	4.711350594	-1.844851362	-3.351643254
C	1.670911051	0.361981711	-3.415660037
C	2.491046437	-0.803883053	-3.471246207
C	1.903540339	-2.085664689	-3.304007817
C	2.716526425	-3.245271964	-3.354853407
C	-0.195675749	-0.983030544	-2.604140224
C	0.623284640	-2.128770476	-2.656958228
C	0.415414641	-3.172348785	-1.725066767
C	1.239970339	-4.335983742	-1.756076139
C	-1.266822698	-1.805087859	-0.581689447
C	-0.414615262	-2.927528243	-0.610191308
C	-0.045472240	-3.582970547	0.618650721
C	-1.915096187	-1.472641211	0.679651693
C	-3.337639180	1.945493261	1.713835409
C	-2.521890032	0.784689467	1.686462276
C	-1.440097451	0.680268081	2.541165461
C	-0.656550866	-0.517680845	2.611472903
C	-1.794113996	3.035274589	3.242036753
C	-0.977844604	1.880419152	3.189645883
C	0.412870845	1.988343583	3.428432438
C	1.227370125	0.815277942	3.425228104
C	0.194945063	4.433268307	3.355331062
C	1.007432264	3.270547019	3.326676615
C	2.317352040	3.314062947	2.744302795
C	3.128941277	2.161629740	2.737106257
C	1.741921170	5.522618385	1.829774180
C	2.559950865	4.354421050	1.815268609
C	3.383579861	4.079390843	0.698276353
C	4.192296462	2.922934359	0.690272075
C	2.204537685	5.877178758	-0.523349404
C	3.003888894	4.709059928	-0.537210539
C	3.024031480	3.875832072	-1.688139492
C	3.830291343	2.696764237	-1.700600602
C	1.147874713	5.175105520	-2.598678362
C	1.955673245	4.012557289	-2.614200037
C	1.454115867	2.793287987	-3.183560462
C	2.263635895	1.639731540	-3.227938201
C	-0.773763373	3.832332874	-3.254084748
C	0.047991520	2.667972471	-3.274677651
C	-0.532061879	1.390072566	-3.111786689
C	0.275694539	0.238479321	-3.177741333
C	-2.669378080	2.479541952	-2.531616246
C	-1.833815395	1.327863989	-2.514150997



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C	-3.103464628	0.397715638	-0.623284727
C	-2.949051137	-0.333243867	0.725562890
C	-4.307404040	2.158676726	0.693902171
C	-5.226071058	3.974147717	1.990872578
C	-4.124070907	3.945852472	2.833539718
C	-3.130008469	2.965410115	2.674708005
C	-1.191395686	4.288615949	3.451328721
C	0.135000666	6.935177397	2.957636048
C	0.735616827	5.682688889	2.816834935
C	0.437093878	7.959705369	2.060508196
C	1.200832264	7.700188399	0.923515418
C	1.811649464	6.454369417	0.763156022
C	1.390144647	6.157076532	-1.629784360
C	-0.992738453	6.232970999	-3.442358178
C	-0.182924504	5.120591688	-3.204046351
C	-2.366797671	6.074049811	-3.614518208
C	-2.969305651	4.835145190	-3.401188233
C	-2.182122130	3.707101762	-3.161329670
C	-3.724912915	2.552597037	-1.633067454
C	-5.274232213	3.134546729	0.864837351
H	2.315382957	-5.793771046	1.650183661
H	3.457154033	-6.052387959	3.639532505
H	5.880909387	-5.764355217	4.088234290
H	6.961867459	-3.570885098	3.666194853
H	7.118326054	-2.385933989	1.690147065
H	8.725660565	-2.330007978	0.022492241
H	8.807859030	-3.660663916	-2.070918163
H	6.947555617	-3.505758709	-3.704125106
H	4.722435768	-3.982962534	-3.400375266
H	3.530605980	-5.898486127	-3.743052169
H	3.031296259	-7.734932095	-2.153564695
H	1.763742768	-7.258331836	-0.073758227
H	-6.012074237	4.711622042	2.149057496
H	-4.023417503	4.689019273	3.624257654
H	-1.810082826	5.177009807	3.348703528
H	-0.588989873	7.102114700	3.754495196
H	0.000672615	8.947794495	2.203350894
H	1.301133740	8.456727209	0.145757903
H	0.679690395	6.975936178	-1.543532913
H	-0.549401286	7.227691158	-3.476094709
H	-2.984779123	6.941488485	-3.843984991
H	-4.055229619	4.748866020	-3.405681131
H	-4.255532587	3.495426313	-1.524698916
H	-6.037468346	3.290277058	0.102013513
Co	-4.659364046	-2.662920204	-0.376717202
Co	-5.273825460	-0.324334357	-1.390985717
C	-3.705101237	-3.112120578	-1.799250512
C	-5.695259557	-3.962355128	0.245005951
C	-6.120427294	-2.051120550	-1.527838630
C	-6.625175003	0.773154651	-1.476976506
C	-4.760912163	-0.273382474	-3.116877525
O	-6.348776022	-4.856431327	0.573348635
O	-3.183795051	-3.497530320	-2.757450712
O	-7.081153667	-2.445649130	-2.081115215
O	-7.519777883	1.508100849	-1.502896377
O	-4.398151671	-0.214437114	-4.206999782
C	-4.306342506	-0.808880871	1.273214536
C	-5.472161183	-0.622538883	0.544276665
C	-3.168104742	-3.174532685	0.688672606
O	-2.703800413	-4.110998481	1.218499907
C	-4.320224718	-1.130203968	2.760689262
H	-4.827533774	-0.287461112	3.268790034
H	-3.286202964	-1.114780652	3.136229772
C	-4.949668638	-2.449725082	3.217355808
H	-5.917568448	-2.628146417	2.725699420
H	-4.297235527	-3.285061780	2.925326111
C	-5.134839151	-2.475995130	4.731786386
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H	-5.816617563	-1.659992969	5.029765541
C	-5.677365209	-3.813972133	5.222668352
H	-6.650379125	-4.037641836	4.758236251
H	-4.988136111	-4.632548071	4.964624804
H	-5.813057351	-3.815860109	6.313796664
C	-6.828396412	-0.597429804	1.180225617
H	-7.586393269	-1.105043121	0.568252342
H	-6.843973809	-1.021926972	2.191027084
H	-7.131838069	0.461083371	1.267771632

CP6*methyl,parallel*

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Co2C121H36O6

C	1.954427328	-4.990114123	1.744167383
C	3.471634402	-3.852333377	3.310166042
C	4.328987320	-4.923421909	3.566517847
C	5.691425970	-4.698987728	3.762662976
C	5.399066123	-2.342972352	3.308335454
C	6.236326715	-3.433797780	3.556860305
C	6.837922834	-1.163292036	1.700769771
C	7.254054541	-0.832132020	-0.693720516
C	8.253619119	-1.792149753	-0.859770452
C	8.284894804	-2.573733746	-2.014499470
C	6.223404575	-1.571629010	-2.783603054
C	7.234430814	-2.524965600	-2.929212292
C	4.328237946	-2.971163032	-3.483986151
C	2.517201396	-4.450212105	-2.718943404
C	3.191183470	-5.665380299	-2.879218694
C	2.979356281	-6.706080744	-1.979472725
C	1.526987210	-5.303686348	-0.650802929
C	2.218264402	-6.501440731	-0.827396180
C	1.088585466	-4.778299899	0.645940418
C	-0.730798143	-1.726284133	1.819187257
C	0.161713025	-2.830742363	1.813230496
C	1.285032633	-2.852942897	2.677379002
C	2.157249215	-3.979719257	2.680758117
C	0.853417152	-0.490323519	3.187645213
C	1.718232289	-1.604366593	3.213799864
C	3.117142985	-1.411247399	3.375759955
C	3.994652659	-2.534615131	3.379796044
C	2.770707741	1.005272656	3.260539608
C	3.641854423	-0.108701809	3.245254236
C	4.958574948	0.013947207	2.685530468
C	5.832197576	-1.098445259	2.676659909
C	4.278245382	2.207463517	1.783428518
C	5.153790482	1.078663555	1.765159715
C	5.948180969	0.819322635	0.618132605
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C	4.634612085	2.524528502	-0.595570100
C	5.480407868	1.395844307	-0.612723811
C	5.499324544	0.545736162	-1.745418762
C	6.361323712	-0.589619955	-1.769510498
C	3.596172033	1.777887598	-2.660424510
C	4.445893241	0.651667180	-2.683971011
C	4.015502160	-0.571151293	-3.303344524
C	4.881073823	-1.690386071	-3.352143830
C	1.741693399	0.372084836	-3.365518878
C	2.613367718	-0.755681416	-3.426135172
C	2.091139443	-2.062377779	-3.238562597
C	2.955139330	-3.183184736	-3.301045903
C	-0.039386500	-1.050178543	-2.504613348
C	0.824130401	-2.162305194	-2.570377218
C	0.655964520	-3.227690801	-1.658203562
C	1.532711426	-4.352471205	-1.704246745
C	-1.100700090	-1.968860054	-0.525166017
C	-0.210652902	-3.049203374	-0.554290776
C	0.199658230	-3.697349830	0.677982102
C	-1.831024613	-1.736812749	0.781031850
C	-3.287779159	1.707364281	1.810157113
C	-2.415989430	0.587030364	1.762273702
C	-1.304678732	0.546489463	2.572335153
C	-0.444226789	-0.608767234	2.591755743
C	-1.759483666	2.876841786	3.292370482
C	-0.886961286	1.765243303	3.214223344
C	0.501778657	1.943762650	3.420851761
C	1.376359396	0.813259774	3.396250566
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C	1.030029031	3.251679853	3.318085883
C	2.333424563	3.364105257	2.728744506
C	3.204054676	2.255599220	2.711881305
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C	2.514832418	4.417951283	1.801859468
C	3.342338822	4.187760018	0.677418769
C	4.209479503	3.073728807	0.659417875
C	2.058494871	5.922712207	-0.529069318
C	2.915789494	4.796698573	-0.553346375
C	2.957980751	3.960579062	-1.701688342
C	3.821994523	2.822979748	-1.723937465
C	1.001956851	5.159911784	-2.582235406
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C	-0.865244524	3.722105939	-3.190284551
C	0.011970204	2.598496760	-3.217176484
C	-0.502513177	1.296769596	-3.031990798
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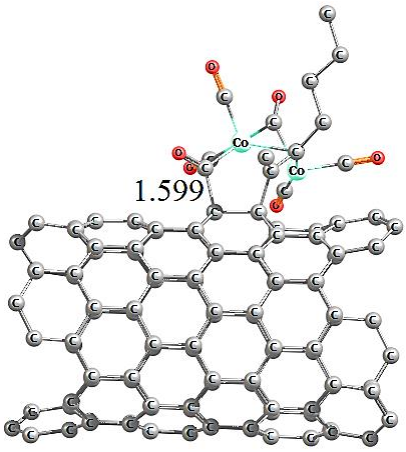

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C	-4.288960445	1.862050809	0.809060408
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C	-4.144622476	3.669761751	2.938773222
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C	0.980807840	7.692463788	0.931636339
C	1.651273604	6.478843950	0.762390921
C	1.213354445	6.158012315	-1.622803789
C	-1.202011201	6.108367646	-3.391702886
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C	-5.302159154	2.783148245	1.002220297
H	2.709929837	-5.767155318	1.654658414
H	3.933088220	-5.938024799	3.592770877
H	6.346173555	-5.535763453	4.003945383
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H	8.991728609	-1.947297842	-0.073441201
H	9.092848185	-3.290343127	-2.158741617
H	7.186713823	-3.244715590	-3.745633597
H	4.993328291	-3.825741982	-3.386749229
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H	-6.087583373	4.324604016	2.300921012
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H	-0.268546929	8.875587824	2.225303238
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H	0.464797114	6.941115907	-1.527404445
H	-0.807320397	7.122739549	-3.440544527
H	-3.232486712	6.717269498	-3.761852472
H	-4.188324512	4.478651708	-3.294041913
H	-4.315578808	3.216887860	-1.415081252
H	-6.091899243	2.895219602	0.259134993
Co	-4.531217903	-2.707238435	-0.057991932
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H	-8.977476046	-3.723247302	3.386680635
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CP6*butyl,parallel*

165
Co2C121H36O6

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C	6.101054509	-3.548578790	3.425542863
C	6.724507813	-1.214734686	1.656740364
C	7.162679424	-0.798027734	-0.720554975
C	8.160569321	-1.754915279	-0.912638026
C	8.199876444	-2.493785321	-2.094931206
C	6.148612596	-1.456899917	-2.845242551
C	7.157981350	-2.407747432	-3.016648746
C	4.256317218	-2.823997178	-3.613598057
C	2.436056968	-4.325583204	-2.918014857
C	3.108384974	-5.535843573	-3.117858036
C	2.887195109	-6.608352080	-2.258712079
C	1.427544530	-5.252306375	-0.890583101
C	2.117622328	-6.444346584	-1.105688552
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C	6.280312207	-0.513186327	-1.794597075
C	3.528878767	1.893582512	-2.621424186
C	4.376046256	0.766603095	-2.679252943
C	3.947755170	-0.431501208	-3.346534484
C	4.811030567	-1.550493281	-3.429549348
C	1.676504508	0.519186026	-3.391185785
C	2.546176528	-0.607674893	-3.487179527
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C	-0.114757382	-0.929669592	-2.598255906
C	0.747117950	-2.040529380	-2.698381823
C	0.569301228	-3.138472767	-1.827761181
C	1.443948593	-4.262880191	-1.908100776
C	-1.195286260	-1.919260283	-0.664972779
C	-0.306570060	-2.999126744	-0.725778103
C	0.091158036	-3.693889956	0.484907988
C	-1.940786267	-1.737362116	0.641371720
C	-3.401412712	1.669973590	1.782984951
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C	-1.420894298	0.483859066	2.510440816
C	-0.564315669	-0.674082526	2.499148827
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C	-1.006377366	1.677656044	3.198368364
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C	4.118382150	3.066571368	0.747745207
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C	2.840493463	4.837062085	-0.412550664
C	2.889067776	4.042308557	-1.589731715
C	3.750211799	2.903647947	-1.646187789
C	0.941709613	5.277207551	-2.440257976
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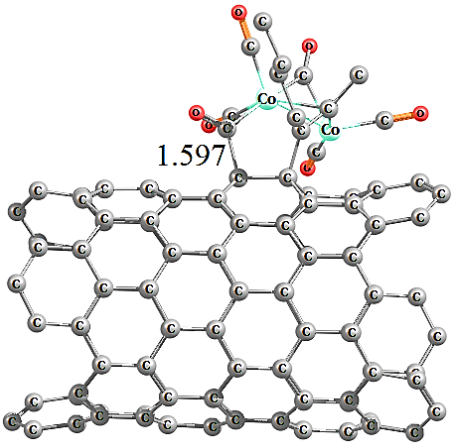

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C	-5.372746188	3.593446158	2.146058531
C	-4.256915359	3.599141252	2.968999443
C	-3.218997200	2.670857527	2.766379820
C	-1.331213953	4.060878394	3.558393460
C	-0.133181257	6.786461684	3.158215288
C	0.525887274	5.570296929	2.969527260
C	0.122738004	7.859517840	2.304365003
C	0.900007681	7.682213565	1.160863927
C	1.568846297	6.473762969	0.953040777
C	1.149327512	6.240455255	-1.445047554
C	-1.254847864	6.258952416	-3.229964659
C	-0.392876710	5.178191599	-3.031951899
C	-2.621499618	6.041499076	-3.394207178
C	-3.164477514	4.770059173	-3.213238668
C	-2.325263835	3.672745435	-3.011556130
C	-3.816269568	2.390078677	-1.529571386
C	-5.402422029	2.785697810	0.994403931
H	2.588524362	-5.802867752	1.407939557
H	3.792137033	-6.046736400	3.350845395
H	6.202238757	-5.665470056	3.798160772
H	7.181335672	-3.411519902	3.458593464
H	7.290774114	-2.136187495	1.542996728
H	8.890856132	-1.941521741	-0.125879577
H	9.006721181	-3.207561134	-2.258073761
H	7.115440733	-3.096931115	-3.859303692
H	4.918543027	-3.683406448	-3.543054527
H	3.819587455	-5.630478604	-3.937597175
H	3.384397932	-7.559821502	-2.444428744
H	2.072631152	-7.237954168	-0.360424801
H	-6.190301524	4.287652662	2.337848113
H	-4.179739961	4.324938708	3.778086395
H	-1.993521058	4.921452286	3.500390970
H	-0.865943132	6.887423917	3.958082953
H	-0.360058461	8.819408364	2.485043404
H	0.965618492	8.472975767	0.414081371
H	0.402163771	7.021799871	-1.327013424
H	-0.857568437	7.273439252	-3.240050222
H	-3.281125417	6.885407255	-3.593414505
H	-4.245228120	4.633798156	-3.214624798
H	-4.396027000	3.299399285	-1.390421814
H	-6.181830939	2.931788433	0.246155520
Co	-4.630930941	-2.685389443	-0.257798481
Co	-5.303098069	-0.600324384	-1.424310156
C	-3.669766952	-3.270689631	-1.628598100
C	-5.466993560	-4.094766119	0.436990529
C	-6.107616279	-2.333426186	-1.485515654
C	-6.631893976	0.531154703	-1.518220119
C	-4.730415751	-0.585415353	-3.127482332
O	-6.021789625	-5.035736240	0.809413058
O	-3.143778564	-3.701925804	-2.564721856
O	-7.041571551	-2.814604018	-2.014525681
O	-7.524994841	1.270579602	-1.546164437
O	-4.310946240	-0.533372273	-4.199678260
C	-4.283172398	-1.138540050	1.207445446
C	-5.478192037	-0.939916050	0.499015448
C	-2.913483065	-2.999881979	0.742427139
O	-2.612339843	-4.019321376	1.293430089
C	-4.278070064	-1.427226932	2.710384697
H	-4.735143727	-0.547504326	3.204090521
H	-3.232917279	-1.442064437	3.060546378
C	-4.933967472	-2.704617632	3.230865280
H	-5.953181913	-2.830053415	2.837534013
H	-4.357850077	-3.576686872	2.889454375
C	-4.982657547	-2.709776138	4.756999621
H	-3.961246841	-2.566533791	5.150152344
H	-5.574869301	-1.846009770	5.106983790
C	-5.572178501	-4.003001147	5.309862742
H	-6.599205212	-4.154786078	4.942749628
H	-4.973130305	-4.870744297	4.993853356
H	-5.602495095	-3.992687020	6.409035642
C	-6.818955105	-0.850504980	1.165629456
H	-7.621137281	-1.258049870	0.535972602
H	-6.849832300	-1.344247198	2.144672078
H	-7.038072485	0.218964236	1.334743895

CP7*methyl,parallel*

167
Co2C122H36O7

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C	-5.486069345	5.067156002	3.722790060
C	-5.389642218	2.698214510	3.251748071
C	-6.134177655	3.855772240	3.493853246
C	-6.887114424	1.665034573	1.598777818
C	-7.269610625	1.402034554	-0.809478411
C	-8.176445327	2.448655365	-0.984641657
C	-8.110598641	3.244478702	-2.128211043
C	-6.128004570	2.072883385	-2.865176934
C	-7.046979163	3.114111211	-3.019437040
C	-4.100628986	3.304351318	-3.513629719
C	-2.181230124	4.607902374	-2.698268058
C	-2.738973820	5.879921060	-2.860457261
C	-2.459568880	6.888526214	-1.942135820
C	-1.175560322	5.346525613	-0.595185307
C	-1.752547563	6.603653094	-0.773393551
C	-0.822515550	4.769322420	0.704455384
C	0.685781334	1.554869408	1.881766088
C	-0.103720973	2.734713969	1.867637735
C	-1.236055358	2.851810894	2.710058335
C	-2.005426557	4.051334254	2.705863534
C	-1.021090197	0.459255481	3.210036859
C	-1.786443304	1.642998547	3.227772358
C	-3.199909814	1.570985913	3.358523746
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C	-3.059784972	-0.864816456	3.221103580
C	-3.831588777	0.320316590	3.200813419
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C	-0.036789950	3.611164592	0.743074601
C	1.818473161	1.483709907	0.874970862
C	2.966286619	-2.067086206	1.944449593
C	2.209208248	-0.869987767	1.876422887
C	1.068923721	-0.747104921	2.640726650
C	0.294315499	0.467822930	2.641235355
C	1.294683789	-3.110026979	3.363149297
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C	-2.274917596	-5.460266405	1.744843645
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C	-4.606060126	-2.769754742	0.557813017
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C	-1.540024366	-5.102225261	-2.658643128
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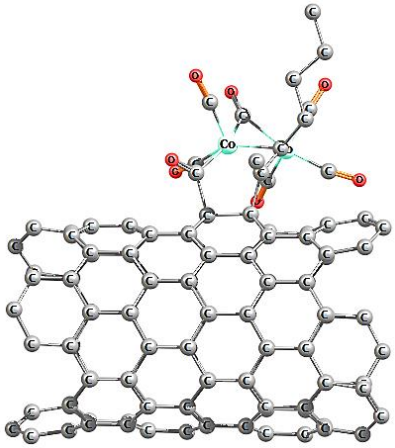

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C	3.933542828	-2.337788837	0.932966666
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C	3.600074270	-4.114861346	3.073569955
C	2.661410226	-3.084068117	2.880237937
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C	-0.755819222	-6.938492082	2.909659851
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H	-7.222607960	3.809690818	3.488217897
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H	-8.848453077	4.031537976	-2.280499529
H	-6.916690623	3.836657680	-3.824286548
H	-4.687743451	4.214585445	-3.419853938
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H	5.467648372	-4.966547125	2.445408118
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H	-1.888155365	-8.395137699	0.049944660
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H	0.100040800	-7.211977654	-3.513716109
H	2.560081027	-7.022534208	-3.768985525
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H	3.846287490	-3.690343892	-1.300235081
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C	5.317755439	3.688727802	1.102087240
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H	10.900794863	1.981172407	2.794802937
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CP7*butyl,parallel*

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Co2C122H36O7

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C	6.102948821	-3.818801883	3.351911452
C	6.815709720	-1.555674423	1.527463402
C	7.201434104	-1.209317848	-0.869723861
C	8.130378065	-2.230972318	-1.073589905
C	8.085395588	-2.991598643	-2.241834905
C	6.081704420	-1.838483289	-2.950343482
C	7.022712749	-2.855122571	-3.133189531
C	4.083488711	-3.091184000	-3.646063774
C	2.190256235	-4.460288075	-2.878945171
C	2.775554277	-5.714460090	-3.078932103
C	2.515467103	-6.757047653	-2.193477824
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C	0.660589762	-2.064175578	-2.646316516
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C	1.238353250	-4.316475688	-1.839133244
C	-1.197775202	-1.781470616	-0.554406522
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C	0.011782465	-3.620028851	0.584244157
C	-1.889835553	-1.537788380	0.772823231
C	-3.119722644	1.950648088	1.946931293
C	-2.334497475	0.774956696	1.843005896
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C	4.447611799	2.861989359	0.616010657
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C	1.342216481	5.228425088	-2.535898636
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C	2.361688516	1.680781982	-3.243878932
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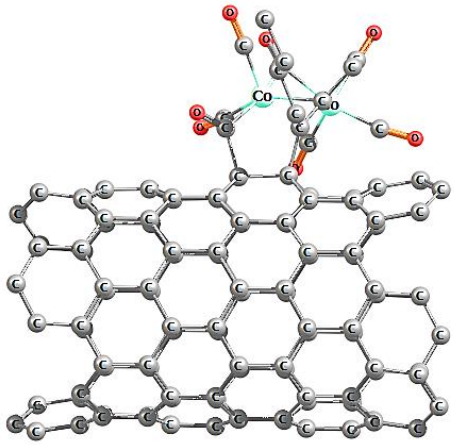

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C	-2.823926214	-0.274418133	0.828757575
C	-4.092790062	2.228321827	0.942516388
C	-4.924311017	4.024338871	2.328096733
C	-3.800591893	3.949376692	3.133961917
C	-2.837775678	2.946822742	2.911831955
C	-0.840061676	4.233084380	3.595405894
C	0.500628312	6.873117527	3.078943482
C	1.079074746	5.616191870	2.894343261
C	0.794147260	7.913611086	2.197321784
C	1.525412521	7.670449357	1.035988069
C	2.113819919	6.420256887	0.830782751
C	1.630968778	6.187120444	-1.556442121
C	-0.802974372	6.342636713	-3.288490806
C	-0.008348736	5.210544921	-3.098694018
C	-2.186389305	6.213083588	-3.401858039
C	-2.804525298	4.984235640	-3.176014169
C	-2.031872028	3.836549903	-2.984595175
C	-3.516088396	2.703672600	-1.382527470
C	-5.022459575	3.228419447	1.171506188
H	2.392583414	-5.876905377	1.467545230
H	3.642392103	-6.168655480	3.375803138
H	6.083026942	-5.932916249	3.751956086
H	7.190184225	-3.749215259	3.352745038
H	7.320126630	-2.512363885	1.413864866
H	8.872349597	-2.449720988	-0.306258602
H	8.839976054	-3.758134415	-2.415486769
H	6.910623448	-3.554434927	-3.961007697
H	4.689619379	-3.991289052	-3.578728019
H	3.451720714	-5.867693227	-3.919241093
H	2.943663675	-7.741655568	-2.378282121
H	1.728898769	-7.300521982	-0.257580431
H	-5.686955384	4.776096460	2.529463516
H	-3.653478026	4.668889464	3.938903779
H	-1.453246142	5.129937788	3.548906863
H	-0.199082174	7.032965582	3.898551110
H	0.375208099	8.903849628	2.373551791
H	1.617809896	8.444045542	0.274227302
H	0.937598611	7.016003754	-1.434695112
H	-0.340863549	7.328598358	-3.327195660
H	-2.796019599	7.095583187	-3.593291593
H	-3.891088041	4.919218469	-3.132788897
H	-4.022605100	3.655577771	-1.242803196
H	-5.786782358	3.448756572	0.429488442
Co	-4.607042361	-2.465311061	-0.029528944
Co	-5.909223359	-0.703908070	-1.521620886
C	-3.572271033	-3.143027741	-1.332489704
C	-5.444089523	-3.799785679	0.807036425
C	-6.014471792	-2.666698638	-1.417242747
C	-6.134473048	1.032186153	-1.352441391
C	-4.748584390	-0.677283487	-2.891171391
O	-5.954882377	-4.713451284	1.291706428
O	-3.082103361	-3.663184448	-2.240736440
O	-6.550196491	-3.565342233	-1.954223173
O	-6.512517640	2.130043016	-1.331317407
O	-4.024717964	-0.612438206	-3.788043542
C	-4.207749391	-0.821126897	1.305600113
C	-5.444213965	-0.783654290	0.626665821
C	-2.897848339	-2.735381731	0.985714592
O	-2.664847577	-3.706183786	1.642920528
C	-4.194770371	-1.035910103	2.831178034
H	-4.586171717	-0.100832660	3.277964551
H	-3.146178225	-1.089508157	3.165787233
C	-4.905655387	-2.237644286	3.450231872
H	-5.931652514	-2.354248541	3.073611153
H	-4.366251363	-3.158359034	3.187447578
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H	-3.915060152	-1.968826434	5.347706515
H	-5.503511598	-1.200495467	5.249553146
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H	-6.605499635	-3.479446961	5.290065463
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H	-5.593239914	-3.223564356	6.732077969
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H	-7.090630718	0.452344420	1.149864306
C	-7.628898817	-0.872114171	-1.930833994
O	-8.732991622	-0.949174523	-2.269578390

TS3*methyl,parallel*

167
Co2C122H36O7

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C	-4.499922775	3.519694245	3.043826206
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C	-6.837533411	4.137609439	3.075641634
C	-6.233420035	1.836356863	2.647496290
C	-7.205828433	2.834853765	2.748649724
C	-7.233916337	0.566647025	0.790415399
C	-7.186862884	0.244096788	-1.641829843
C	-8.232639610	1.104724292	-1.979751618
C	-8.137943812	1.902269844	-3.119897255
C	-5.881895709	1.124854548	-3.510210836
C	-6.941898032	1.976302371	-3.831848410
C	-4.046388429	2.723760061	-3.826682636
C	-2.571283740	4.345022512	-2.705935370
C	-3.323229624	5.494090539	-2.971076421
C	-3.379035286	6.525709046	-2.038154122
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C	0.105047602	1.862530300	2.360074865
C	-0.877739128	2.872647467	2.188149015
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C	-3.109946394	3.791597207	2.676033534
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C	0.726387358	-0.404811869	3.151066664
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C	-2.315951817	-4.079278646	-1.879391536
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C	1.670391992	-3.427944091	-2.656056432
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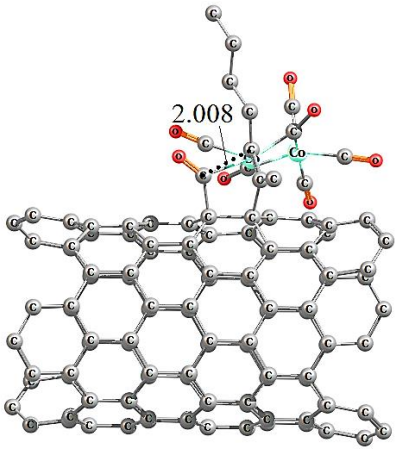

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C	4.984699308	-3.090313669	3.365029176
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H	-9.109653826	1.170331168	-1.336524922
H	-8.975629124	2.538111090	-3.404621948
H	-6.821811105	2.714598803	-4.623957553
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H	-2.988611823	7.112725149	0.002325581
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H	0.583527426	-8.775578857	2.546238958
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H	2.011193843	-6.811578891	-2.910295652
H	4.398884873	-6.153402585	-2.794736384
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H	4.656256172	-2.650094403	-0.271144381
H	6.060334170	-2.205841459	1.698532722
Co	4.091713045	2.057976285	-0.402540915
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O	7.387252350	2.697518841	-3.528155316
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H	5.919484900	7.403623942	0.672987773
H	7.547435294	7.465507084	1.392185330
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TS3*butyl,parallel*

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Co2C122H36O7

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C	-5.920056402	1.674375784	3.164168219
C	-6.902539477	2.638311652	3.404886110
C	-7.134898334	0.356392382	1.477498832
C	-7.421435760	0.023046099	-0.935895811
C	-8.532117894	0.847129345	-1.124003347
C	-8.622782491	1.644816495	-2.264505940
C	-6.417212044	0.943550833	-2.964312996
C	-7.539751903	1.757947196	-3.134498792
C	-4.699255995	2.603159273	-3.534898216
C	-3.138967028	4.286778660	-2.645130338
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C	-1.693413873	-0.369479445	-3.375211998
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C	-2.374987391	1.992821768	-3.199896632
C	-3.377916382	2.990302439	-3.276061609
C	-0.166159680	1.248432475	-2.393996687
C	-1.163448888	2.241307604	-2.472647505
C	-1.167753371	3.301438666	-1.539016011
C	-2.184618663	4.299736705	-1.597273535
C	0.694147261	2.261920566	-0.375565776
C	-0.315128551	3.224919045	-0.411554812
C	-0.835673794	3.792899790	0.819356216
C	1.425004388	2.086581817	0.932881725
C	3.256655918	-1.177188372	1.898630180
C	2.239030070	-0.192261956	1.851712869
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C	0.125619978	0.738689132	2.658465935
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C	-2.127546420	-3.578589657	2.602102473
C	-3.129598989	-2.587890835	2.568223140
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C	-2.138363979	-4.627416745	1.651840734
C	-2.943520738	-4.477990489	0.497892976
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C	-1.393761546	-5.997725325	-0.686036054
C	-2.389758629	-4.993357071	-0.725418667
C	-2.487865345	-4.134433060	-1.853527737
C	-3.495554098	-3.121972980	-1.892054524
C	-0.342723463	-5.031066765	-2.654324484
C	-1.350406640	-4.036634807	-2.699777606
C	-1.045546102	-2.725387011	-3.198046383
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C	0.318261526	-2.342900789	-3.180884416
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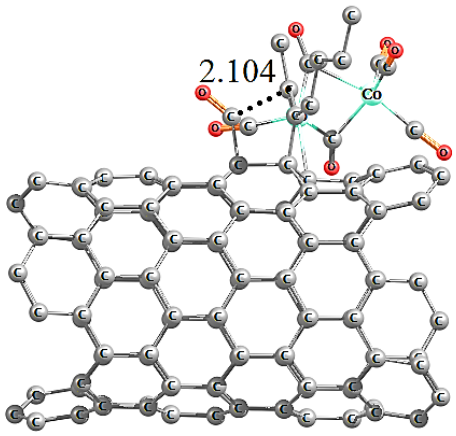

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C	3.178707977	-2.254972138	2.809502220
C	1.469084731	-3.927975931	3.453262180
C	0.654781461	-6.759702826	2.878438642
C	-0.151770354	-5.630918007	2.723440098
C	0.579826994	-7.802849737	1.955128123
C	-0.162923222	-7.657006606	0.784469780
C	-0.976588513	-6.535221280	0.610355667
C	-0.468997695	-6.081478023	-1.736947771
C	2.011964620	-5.646199297	-3.355870252
C	0.995437886	-4.710479899	-3.153581607
C	3.341626482	-5.231810677	-3.427145016
C	3.690375323	-3.911552340	-3.149589037
C	2.693452157	-2.954913783	-2.939913948
C	3.945680454	-1.549703530	-1.350062938
C	5.478764155	-1.856592903	1.221517735
H	-3.643696600	5.472777904	1.735477745
H	-4.952071296	5.417961963	3.618768582
H	-7.306404739	4.691720411	3.905402386
H	-7.954698176	2.357746384	3.371645007
H	-7.816212689	1.199149632	1.386509049
H	-9.313210383	0.885202388	-0.365288256
H	-9.512720737	2.251455467	-2.429082544
H	-7.555684157	2.498083750	-3.933772469
H	-5.478138257	3.357055827	-3.451115678
H	-4.650318239	5.452564983	-3.651676906
H	-4.538583258	7.329985263	-2.039936071
H	-3.265120537	7.070426199	0.075907760
H	6.400966140	-3.324283125	2.511205669
H	4.336117787	-3.805477061	3.780739676
H	2.240779463	-4.690253087	3.373585333
H	1.360882419	-6.812202425	3.706472438
H	1.177611538	-8.701111078	2.106495980
H	-0.088773525	-8.400525788	-0.008629282
H	0.371342458	-6.761883054	-1.620575339
H	1.764690013	-6.703697486	-3.444263182
H	4.122945360	-5.963071798	-3.631636935
H	4.738864112	-3.622793377	-3.086607804
H	4.634326522	-2.380638997	-1.226975510
H	6.330357630	-1.802714031	0.544644400
Co	4.292440375	2.244723876	-1.097542863
Co	6.595709801	1.220469635	-1.683481072
C	4.850875075	1.169427693	-2.615606728
C	3.110716059	3.202291682	-1.988074254
C	5.760046470	3.251541480	-1.320327551
C	7.210246251	1.283364000	-0.001136498
C	6.795037269	-0.501490913	-1.943678901
O	2.434490008	3.938433109	-2.574008003
O	4.387780510	0.678949080	-3.583191449
O	6.249487255	4.316268640	-1.382970242
O	7.533535916	1.305171566	1.114235004
O	6.986604160	-1.636681200	-2.113853912
C	3.683304093	1.879961071	1.682319353
C	4.299630484	2.761132307	0.802617258
C	2.309587922	3.310459175	1.206102182
O	2.153017466	4.455616781	1.432920392
C	3.949641407	1.578457328	3.129230216
H	4.260682574	0.517623152	3.142232244
H	2.986474396	1.582989449	3.676190544
C	5.009489839	2.336894250	3.920921485
H	5.944532237	2.382480137	3.341727988
H	4.690462504	3.369801972	4.127844809
C	5.274091923	1.621136576	5.244895484
H	4.331321969	1.547718699	5.814426028
H	5.590348816	0.584963287	5.031042465
C	6.336081889	2.321842640	6.084921394
H	7.290989100	2.378264275	5.539788481
H	6.028367118	3.349824775	6.331562873
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C	5.049940153	3.948637737	1.326056712
H	4.925402895	4.797324606	0.641486216
H	4.728761556	4.258286657	2.325191008
H	6.125894527	3.720212917	1.357473603
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O	8.457053600	2.327357484	-3.668762497

PD*methyl,parallel*

167
Co2C122H36O7

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C	-5.056333847	4.724449031	3.332552495
C	-6.417235078	4.426608025	3.402607748
C	-5.961318413	2.095527684	2.955843948
C	-6.874240451	3.137983755	3.137179473
C	-7.189509297	0.857532998	1.219591222
C	-7.386973336	0.516111425	-1.202584008
C	-8.418744530	1.422670601	-1.451272847
C	-8.396502774	2.204782890	-2.605846586
C	-6.228800888	1.315253258	-3.201329371
C	-7.273360784	2.214256822	-3.431031627
C	-4.359151567	2.817904701	-3.731217561
C	-2.706102663	4.382808928	-2.797058977
C	-3.425169112	5.563534855	-3.011562605
C	-3.348105932	6.604827955	-2.091516331
C	-1.947683908	5.267853044	-0.645110223
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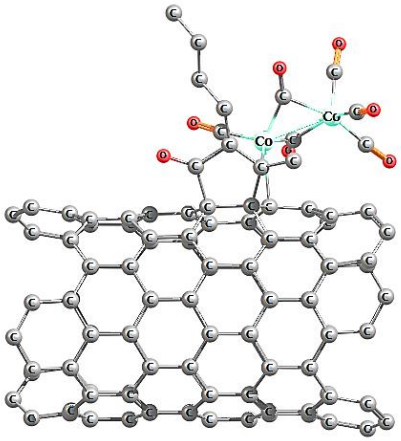

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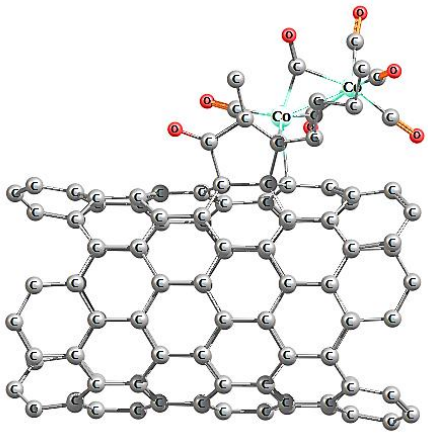

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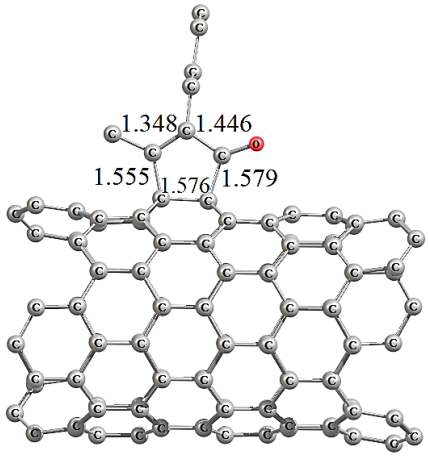
H	5.605921033	-3.764079713	-2.272118097
C	7.846386707	-1.735164796	2.185120672
O	8.619801802	-2.233277736	2.882405664

PK*methyl,parallel*

153
C116H36O

C	4.791526993	2.704536328	-0.788980966
C	4.813486513	1.294427384	-2.801050020
C	6.186359614	1.324058663	-3.050960524
C	6.832846284	0.190584311	-3.543815834
C	4.777522213	-1.074865318	-3.414724239
C	6.154189729	-1.021160636	-3.649630056
C	4.701984908	-3.275740455	-2.320293024
C	4.682651421	-4.401857453	-0.140385750
C	6.051952933	-4.650731670	-0.031373820
C	6.688853620	-4.518624987	1.202287365
C	4.638978604	-3.724809787	2.208628381
C	6.009723713	-3.981016462	2.294215311
C	4.600816991	-1.631320783	3.494851848
C	4.683266886	0.822196020	3.344281866
C	6.056533582	0.978228365	3.560456333
C	6.759498363	1.975868841	2.891036031
C	4.772407846	2.598083207	1.663794770
C	6.141986259	2.727617036	1.889712245
C	4.094804829	2.956178157	0.414011140
C	0.569879518	2.894251893	-0.846436578
C	1.989323449	2.838377990	-0.836875537
C	2.693155368	2.228855595	-1.905271994
C	4.116435393	2.216884908	-1.905771069
C	0.551549674	1.324752497	-2.691851047
C	1.961438300	1.310485153	-2.713581495
C	2.655291927	0.158867114	-3.177030334
C	4.080836436	0.139087055	-3.179431998
C	0.522496914	-1.013377967	-3.364683634
C	1.935502666	-1.040562478	-3.352426959
C	2.631665962	-2.267899457	-3.085096547
C	4.045841634	-2.294121782	-3.077899497
C	0.470577558	-3.249198113	-2.413076179
C	1.898902159	-3.270949195	-2.395309463
C	2.581604957	-4.023571636	-1.404615934
C	3.998268463	-4.042227044	-1.383138341
C	0.424186372	-4.321504318	-0.236176576
C	1.834787820	-4.318467899	-0.212350243
C	2.519310648	-4.133957302	1.014068074
C	3.944948066	-4.139114119	1.042758588
C	0.383244911	-3.632141102	2.092271829
C	1.793777366	-3.633498964	2.120792957
C	2.503817540	-2.749452092	3.003733434
C	3.917976620	-2.772706655	3.052958200
C	0.376176021	-1.564701455	3.370410644
C	1.800712375	-1.593337493	3.432707568
C	2.523145398	-0.379000573	3.558879518
C	3.937953121	-0.403688604	3.624843538
C	0.430215509	0.857392617	3.105072593
C	1.837061061	0.822318240	3.172992895
C	2.588252103	1.797145279	2.482725726
C	4.014878696	1.771968493	2.533367889
C	0.527040412	2.705387774	1.540730255
C	1.925680317	2.636550507	1.559891288
C	2.696561163	3.010635286	0.390829833
C	-0.088914296	3.482035261	0.394837522
C	-3.728073740	2.862918141	-0.891524348
C	-2.307301161	2.905450982	-0.858627266
C	-1.588021771	2.258705566	-1.846870434
C	-0.145738160	2.250140606	-1.843669249
C	-3.704004655	1.401006480	-2.826763975
C	-2.293196197	1.367015851	-2.734669542
C	-1.593972450	0.234443260	-3.220872235
C	-0.166278948	0.210926638	-3.196357665
C	-3.733176867	-0.943251126	-3.482112178
C	-2.314756258	-0.965949167	-3.423478646
C	-1.621256481	-2.184459605	-3.121309620
C	-0.212846737	-2.214476484	-3.106112157
C	-3.781931524	-3.145285115	-2.449967421
C	-2.355852699	-3.172331733	-2.423665242
C	-1.677781713	-3.962731068	-1.466110265
C	-0.265843991	-3.987445329	-1.448262174
C	-3.841209132	-4.295433696	-0.315181255
C	-2.426015302	-4.308364730	-0.287809994
C	-1.738018882	-4.159711191	0.946814209
C	-0.309326774	-4.167850655	0.972771260
C	-3.878975337	-3.589524356	2.012096157
C	-2.463374090	-3.606322812	2.036174005
C	-1.746201753	-2.675094743	2.860471596
C	-0.338951452	-2.701935904	2.908179506
C	-3.864025231	-1.478751640	3.221223010
C	-2.440083809	-1.499818397	3.236437885
C	-1.716503482	-0.292955882	3.354944472
C	-0.310734236	-0.324451340	3.410360369
C	-3.816581864	0.955616289	3.081712530
C	-2.402746354	0.927402284	3.046260667



C	-1.675602802	1.951085618	2.373069380
C	-0.232540106	1.897583030	2.390477569
C	-3.770631415	2.817796361	1.515781280
C	-2.363745080	2.847477619	1.536012494
C	-1.662423223	3.568974494	0.366933631
C	-4.485031464	3.166101108	0.275191394
C	-6.489653226	3.197566479	-1.068430354
C	-5.805859215	2.612463883	-2.121858293
C	-4.425441941	2.361769933	-2.018741989
C	-4.391802808	0.274529798	-3.319879630
C	-5.839004062	-2.350952583	-3.442913374
C	-4.467888515	-2.186540227	-3.239317391
C	-6.527204971	-3.366467778	-2.778746409
C	-5.896770660	-4.115618240	-1.786883499
C	-4.524915764	-3.969387154	-1.567546828
C	-4.543247499	-4.073329537	0.878209839
C	-5.967421535	-2.665889925	3.109035295
C	-4.591371590	-2.646113044	2.875143262
C	-6.613425007	-1.519915892	3.571304535
C	-5.931827042	-0.307076621	3.658297978
C	-4.555150532	-0.259555611	3.426880786
C	-4.473282340	1.963337681	2.377884435
C	-5.847400682	3.383570753	0.166763626
H	5.866863549	2.551092899	-0.731753537
H	6.754881096	2.228516837	-2.837268885
H	7.896817624	0.234856391	-3.774540732
H	6.696053086	-1.932400811	-3.900406730
H	5.780423186	-3.194056351	-2.206447948
H	6.625606377	-4.920970718	-0.917346535
H	7.748633811	-4.755974101	1.290085530
H	6.550349454	-3.735853014	3.207752223
H	5.684100468	-1.617331093	3.402196767
H	6.577223555	0.304599796	4.240089286
H	7.820646630	2.116924354	3.094030043
H	6.732219962	3.399561789	1.267278216
H	-7.550789283	3.424231983	-1.167107160
H	-6.336319133	2.330923533	-3.030913540
H	-5.476041527	0.267041763	-3.242314902
H	-6.375004589	-1.668371682	-4.101469178
H	-7.588171838	-3.516864808	-2.975880582
H	-6.475108838	-4.796971655	-1.163598495
H	-5.619034456	-3.926448143	0.816009172
H	-6.537635694	-3.573095316	2.911710330
H	-7.679255308	-1.555752114	3.794546298
H	-6.474795199	0.608333165	3.890564188
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C	-1.932342912	5.100351666	0.382242850
C	-0.801064968	5.826575911	0.486987327
C	0.375295523	4.985709547	0.524924118
O	1.528795503	5.357207703	0.641598962
C	-0.639075518	7.308399820	0.520933608
H	0.289185629	7.530827485	1.071304608
H	-1.468814698	7.779228806	1.070386253
C	-0.537676592	7.890572090	-0.894401485
H	0.297506705	7.395506688	-1.420524312
H	-1.454321144	7.640994613	-1.458400473
C	-0.325285977	9.400654193	-0.889445973
H	-1.155760425	9.882670938	-0.343563255
H	0.594964589	9.632255038	-0.325683481
C	-0.228772577	9.979643742	-2.297660976
H	0.608848735	9.526286537	-2.849639219
H	-1.150300454	9.782311975	-2.867158341
H	-0.070933628	11.067619052	-2.274468979
C	-3.268304950	5.746688226	0.297599847
H	-3.797503444	5.464883387	-0.624449290
H	-3.905838282	5.467243189	1.149779160
H	-3.152177031	6.837243899	0.303667639

PK*butyl,parallel*

153
C116H36O

C	-3.630251571	4.147244476	1.177142871
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C	-5.386332498	3.180850182	3.402210223
C	-6.374105656	2.303815557	3.850073732
C	-4.872664334	0.428500573	3.582865168
C	-6.146570109	0.929709474	3.864304621
C	-5.559602834	-1.591965179	2.360526871
C	-5.944784270	-2.515368827	0.119847976
C	-7.318270507	-2.278907613	0.039573728
C	-7.885017895	-1.861285217	-1.164288660
C	-5.697780610	-1.745855486	-2.187736415
C	-7.074864890	-1.517413859	-2.244997100
C	-4.964926289	0.288245459	-3.355248714
C	-4.208832832	2.609891183	-3.062499710
C	-5.449607798	3.234807858	-3.226047512
C	-5.765841426	4.364875542	-2.477267392
C	-3.674212056	4.195743524	-1.277916631
C	-4.920488104	4.795580206	-1.453119819
C	-2.903036110	4.221803431	-0.031511173
C	0.405724276	2.894702172	1.112748732
C	-0.949044776	3.321124073	1.144263970
C	-1.806147102	2.921020213	2.199333703
C	-3.148640219	3.391305049	2.243755093
C	-0.090108113	1.298144677	2.865272709
C	-1.420796248	1.760165798	2.931305484
C	-2.459987726	0.884135879	3.350048167
C	-3.807431885	1.347557057	3.395781483
C	-0.850859950	-0.949863425	3.403532291
C	-2.188904387	-0.496747914	3.434057561
C	-3.263034545	-1.396117883	3.118030986
C	-4.601997329	-0.941756244	3.153200461
C	-1.570219678	-3.004744908	2.323594608
C	-2.921042629	-2.540725587	2.348741471
C	-3.827935053	-2.951886265	1.337684393
C	-5.166907808	-2.488740213	1.359219830
C	-1.910936476	-3.885792142	0.087898107
C	-3.237074320	-3.404518640	0.107973859
C	-3.830555242	-2.921888577	-1.084265999
C	-5.173664068	-2.443149656	-1.068955025
C	-1.661737809	-3.103911591	-2.198003788
C	-2.989475926	-2.627076004	-2.183118559
C	-3.366676890	-1.501588614	-2.993250767
C	-4.705240340	-1.042360337	-2.999638954
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C	-2.586454470	0.765910813	-3.414355559
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C	-0.193514577	1.191144465	-2.956396087
C	-1.529577234	1.637034048	-2.981616894
C	-1.899605851	2.759119976	-2.210519020
C	-3.250382679	3.221653172	-2.217932270
C	0.356146150	2.851330264	-1.281798520
C	-0.983369509	3.259737765	-1.260120081
C	-1.569705928	3.797014571	-0.049060478
C	1.212280034	3.302098179	-0.115422469
C	4.434536683	1.392236439	1.013340774
C	3.117003225	1.931810516	1.030633584
C	2.231235379	1.505450679	2.004780130
C	0.871730738	1.985698235	2.049219280
C	3.937174091	-0.080584113	2.872488821
C	2.598734019	0.371858970	2.818819021
C	1.561664894	-0.485074181	3.263518333
C	0.211043730	-0.022833966	3.282589016
C	3.175573744	-2.331774662	3.396112507
C	1.833721596	-1.868774535	3.377992521
C	0.764964766	-2.758606230	3.027723273
C	-0.569786386	-2.309484701	3.053948718
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C	1.114265509	-3.889280668	2.251934695
C	0.199616471	-4.339309093	1.270990323
C	-1.137075923	-3.884001742	1.295277718
C	2.111543312	-5.307042194	0.036413988
C	0.775424855	-4.839599657	0.052079349
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C	2.363783391	-4.507312822	-2.246819823
C	1.025968431	-4.043791000	-2.228118590
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C	3.051574616	-2.444756016	-3.338255679
C	1.705244408	-1.982025199	-3.308209271
C	1.432471979	-0.596699914	-3.336218277
C	0.098925273	-0.149173283	-3.350871764
C	3.832819205	-0.151298981	-3.066280242
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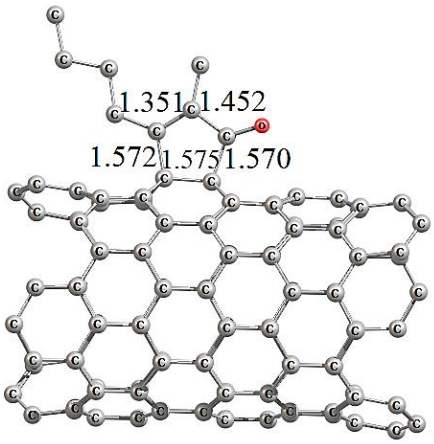

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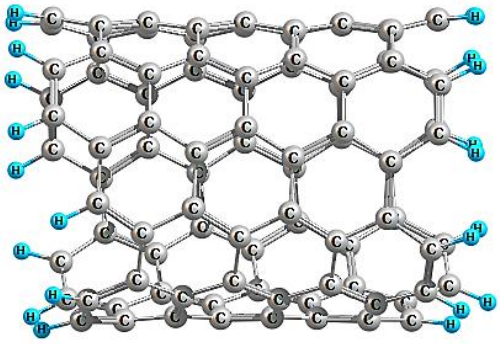
C	2.725233586	2.864723342	-0.128592186
C	5.239411222	1.485297168	-0.155832366
C	7.149391206	0.764004666	1.128839135
C	6.318079980	0.387722953	2.171154908
C	4.933156387	0.622944624	2.093470095
C	4.206867425	-1.400914933	3.283699684
C	4.678060744	-4.363077630	3.211188045
C	3.442380021	-3.731831900	3.059584840
C	4.975151089	-5.505087679	2.467151452
C	4.119448190	-5.929614309	1.452253873
C	2.876599309	-5.314273455	1.284092336
C	2.835975155	-5.258171344	-1.163237073
C	4.629524252	-4.276319261	-3.356993527
C	3.344312411	-3.807927185	-3.078549428
C	5.619667595	-3.389621565	-3.778603653
C	5.388025669	-2.015002517	-3.780104926
C	4.111787184	-1.520165929	-3.502074344
C	4.799678799	0.525316202	-2.326726922
C	6.595413818	1.222754509	-0.077145771
H	-4.694164502	4.371466366	1.145906443
H	-5.615868379	4.236139629	3.258560418
H	-7.357140444	2.690665653	4.116883195
H	-6.963276383	0.241473682	4.079095422
H	-6.547256589	-1.143016786	2.285179479
H	-7.940551083	-2.394771835	0.926356769
H	-8.963240047	-1.719889851	-1.232236336
H	-7.509365424	-1.046614391	-3.126179741
H	-5.978054739	0.661788001	-3.227517353
H	-6.174450924	2.823280604	-3.927510963
H	-6.717888727	4.869642140	-2.638387491
H	-5.241512873	5.585123272	-0.774239320
H	8.225756070	0.615486846	1.209347770
H	6.729899459	-0.104318593	3.051724855
H	5.223644350	-1.769258063	3.173698122
H	5.419593901	-3.946755180	3.892164051
H	5.923865490	-6.017892659	2.622444623
H	4.427009722	-6.723454356	0.772245664
H	3.898433545	-5.487469267	-1.125954509
H	4.861364579	-5.332887413	-3.226575286
H	6.607642066	-3.769359026	-4.037095713
H	6.206007200	-1.324120341	-3.980978598
H	5.782098321	0.071016214	-2.229648449
H	7.226822768	1.337284619	-0.958797947
C	3.493258161	4.234207780	-0.049299301
C	2.656824907	5.294800126	-0.074995681
C	1.270715001	4.870608517	-0.152914445
O	0.301898330	5.602546524	-0.243097940
C	4.980165024	4.289908556	0.046732016
H	5.399339370	3.817780579	-0.858972623
H	5.284583630	3.642917385	0.884825364
C	5.685137029	5.629185213	0.248985947
H	5.524355956	6.295076850	-0.610765572
H	5.291010936	6.136610824	1.142526306
C	7.184658083	5.394396505	0.424404435
H	7.343161696	4.707849157	1.274277548
H	7.573104834	4.874489366	-0.468901429
C	7.961486323	6.686833171	0.649075506
H	7.837771386	7.374093027	-0.202267408
H	7.606851504	7.205444819	1.553294551
H	9.036652127	6.491817013	0.772018257
C	2.901933823	6.771679240	-0.070881658
H	1.937392287	7.270027106	-0.236368194
H	3.302852588	7.113360934	0.892260340
H	3.592660605	7.076174145	-0.864944374

(6,5)-SWCNT



118
C96H22

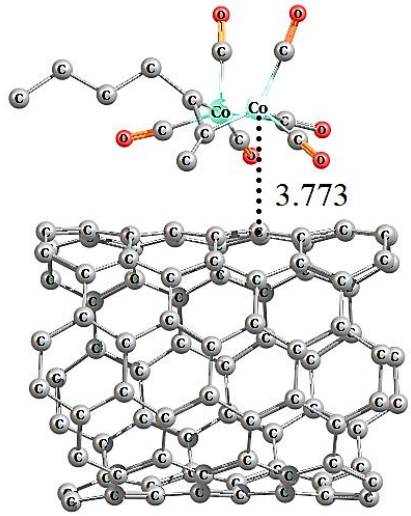
C	5.351096006	-1.854773955	-2.719919136
C	4.299923296	-2.501265755	-2.005477207
C	2.977566831	-2.292220643	-2.484268750
C	2.706123372	-1.182120720	-3.332366708
C	3.756351062	-0.284615909	-3.658927078
C	5.087150868	-0.773051285	-3.516604892
C	3.452396054	1.113701058	-3.725103460
C	2.110506415	1.526461759	-3.515756454
C	1.048365115	0.585092577	-3.657371523
C	1.350155940	-0.790553044	-3.539665047
C	4.459704248	2.112828652	-3.596451667
C	4.210128449	3.266376830	-2.900478884
C	2.935613449	3.496207071	-2.309061903
C	1.848530159	2.738513553	-2.816714048
C	0.528291484	2.982393049	-2.335354224
C	0.365585814	3.650734078	-1.101385873
C	1.531079216	4.015297919	-0.365743756
C	2.779634581	4.130359877	-1.031921098
C	-0.564444018	2.245351095	-2.865670327
C	-1.878905985	2.506509293	-2.395620354
C	-2.047792697	3.213602365	-1.183308400
C	-0.895788745	3.601640307	-0.448593845
C	-2.977457672	1.746879005	-2.894730601
C	-4.299851421	2.047425615	-2.467540910
C	-4.477547962	2.801318568	-1.266346206
C	-3.317430028	3.177815416	-0.537312441
C	-3.357162703	3.166633676	0.881160207
C	-4.564928951	2.812044958	1.547968502
C	-5.775726568	2.876846293	0.788148545
C	-5.729080777	2.859650054	-0.577198490
C	-2.705928109	0.489119364	-3.502666308
C	-3.756049550	-0.455847985	-3.642286986
C	-5.086923550	0.050984805	-3.600865133
C	-5.350977221	1.270562936	-3.037557059
C	-0.934701360	3.539386708	0.967645136
C	-2.139962694	3.136119159	1.608267519
C	1.497320606	3.906059242	1.053601165
C	0.288276796	3.485336596	1.682312232
C	0.362802059	2.673296605	2.837393871
C	-0.795146638	1.975667372	3.273311764
C	-2.076261712	2.367392292	2.798946742
C	3.894976092	4.526209205	-0.242112671
C	3.866336759	4.394494580	1.122863093
C	2.715804659	3.876781480	1.778837693
C	2.800154361	3.010339990	2.921879690
C	1.649602055	2.266374638	3.295290343
C	-0.298570889	1.012684709	-3.516049979
C	-1.349891661	0.064079216	-3.626892060
C	-1.048096255	-1.307101827	-3.465287102
C	0.298790843	-1.697486132	-3.240561642
C	0.564547831	-2.774375645	-2.355787121
C	1.878946014	-2.936074493	-1.842885231
C	-0.646160191	0.675874467	3.819462155
C	0.645922622	0.104902686	3.877385391
C	1.799496003	0.944269074	3.804579353
C	3.095969712	0.380315488	3.900285427
C	4.186420688	1.288302859	3.920977480
C	4.042925881	2.570943133	3.450763661
C	0.794982787	-1.278167219	3.603689896
C	-0.363032600	-2.049088990	3.316572825
C	-1.649835375	-1.558543813	3.683458767
C	-1.799729481	-0.161034809	3.916645061
C	-2.800349791	-2.362295193	3.466942269
C	-4.043181808	-1.825643503	3.896663401
C	-4.186696919	-0.474676750	4.099480922
C	-3.096207311	0.410609472	3.896905310
C	-3.452058813	-1.838887218	-3.426006424
C	-2.110251006	-2.200789615	-3.137404461
C	-1.848414855	-3.247628256	-2.209006122
C	-2.935553787	-3.888128047	-1.559726271
C	-4.209890481	-3.782052784	-2.185674504
C	-4.459307786	-2.791953266	-3.099391402
C	-0.528269419	-3.389883725	-1.688426178
C	-0.288426630	-3.076615219	2.348219357
C	-1.497446181	-3.615065785	1.816807550
C	-2.715935843	-3.440780308	2.521346431
C	0.934634310	-3.273106407	1.659131740
C	2.139852019	-2.749437440	2.205854896
C	2.076107741	-1.757242217	3.217865762
C	-1.531138011	-4.006908669	0.448235036
C	-2.779667585	-4.253253344	-0.181333763
C	-3.894965618	-4.482800312	0.671881872
C	-3.866396137	-4.079776159	1.982645641
C	0.895784166	-3.618304831	0.284191053
C	-0.365597027	-3.797257045	-0.345508304

C	2.047812517	-3.385682010	-0.513401332
C	3.317445421	-3.221278232	0.112298127
C	3.357100362	-2.925508254	1.499686584
C	4.477605705	-2.998882837	-0.677455033
C	5.729139550	-2.917868096	0.009366848
C	5.775701079	-2.660292112	1.350313271
C	4.564854649	-2.444022088	2.081527067
C	-4.492824629	2.131059978	2.767875549
C	-3.254312599	1.709947904	3.278121263
C	3.254142509	-1.016904396	3.555241452
C	4.492655205	-1.531448229	3.139366391
H	-5.476092613	-2.654574050	-3.462029563
H	-5.918688669	-0.583268202	-3.901737351
H	-6.386740809	1.576155706	-2.903626352
H	-6.657392701	2.771187351	-1.138430844
H	-5.182750906	-0.076301870	4.283983181
H	-5.416032325	1.714440875	3.166195411
H	-4.929353403	-2.456651796	3.923952298
H	-4.780987195	-4.136222162	2.569950076
H	-4.832189662	-4.846501128	0.255384312
H	-5.034087024	-4.407590207	-1.847999189
H	-6.732876762	2.801994619	1.304830860
H	4.780943825	4.567539607	1.686899146
H	4.832256296	4.798699560	-0.723141299
H	5.034369303	3.946821177	-2.694995695
H	4.929119447	3.194545210	3.350766766
H	5.182458243	0.935197922	4.181931697
H	5.415790850	-1.042968767	3.445535189
H	6.732816713	-2.483220978	1.841501958
H	6.657473332	-2.944133865	-0.558193101
H	6.386825429	-2.127464238	-2.527470515
H	5.919057782	-0.212167150	-3.938431995
H	5.476625624	1.905130754	-3.923415492

RC*methyl*

151
Co2C109H34O6

C	1.591110962	5.202475889	1.289837852
C	0.994329536	4.153145759	2.050613640
C	1.344651985	2.824504293	1.685469474
C	1.890430353	2.571015518	0.392989008
C	2.030903461	3.647135516	-0.521908947
C	2.085750522	4.957119495	0.035976894
C	1.707764923	3.404772682	-1.896733820
C	1.329396751	2.092315461	-2.283532051
C	1.657476550	0.983948962	-1.449812973
C	1.926175020	1.227405682	-0.082110693
C	1.368963776	4.460819005	-2.789056644
C	0.383652758	4.290496511	-3.727416686
C	-0.303627518	3.049704520	-3.844969733
C	0.329813594	1.911155426	-3.281777368
C	-0.256311455	0.620872459	-3.443736278
C	-1.623936146	0.530152564	-3.787148157
C	-2.375334893	1.735152465	-3.916050356
C	-1.704324861	2.965659676	-4.145125736
C	0.392035413	-0.522097480	-2.902403984
C	-0.184056045	-1.807809853	-3.082799077
C	-1.541102032	-1.903117930	-3.467746619
C	-2.298189617	-0.710414055	-3.621898666
C	0.442587978	-2.954385535	-2.511527058
C	-0.105931810	-4.246803760	-2.736168771
C	-1.465032775	-4.349905214	-3.168747601
C	-2.213247738	-3.150508973	-3.314810669
C	-3.586394045	-3.142755969	-2.955834580
C	-4.199153909	-4.341330967	-2.489794422
C	-3.531326610	-5.573034597	-2.779553362
C	-2.202035908	-5.573211329	-3.096225857
C	1.361530615	-2.760282408	-1.441497956
C	1.693503995	-3.853705978	-0.600693185
C	1.464926223	-5.157991057	-1.123513384
C	0.594756096	-5.349111373	-2.164003900
C	-3.656482949	-0.704707948	-3.213952095
C	-4.230822953	-1.904282871	-2.706729862
C	-3.726139550	1.742933323	-3.464915502
C	-4.284178298	0.537609220	-2.945426975
C	-5.201224730	0.615036800	-1.871759174
C	-5.500725095	-0.556292359	-1.126821750
C	-5.193411419	-1.834183032	-1.666839799
C	-2.518465610	4.122896803	-4.294676867
C	-3.811747487	4.132421582	-3.837455513
C	-4.371374831	2.981709695	-3.217483006
C	-5.264668785	3.065548990	-2.095015340
C	-5.489513637	1.897268688	-1.320374665
C	1.338813939	-0.333962927	-1.865312322
C	1.646629399	-1.430508847	-1.016618216
C	1.865098737	-1.184709317	0.355973601
C	1.812168414	0.150079401	0.834455734
C	1.222028079	0.399866830	2.100506845
C	0.823373594	1.722560315	2.425703521
C	-5.695088963	-0.445216881	0.273356899
C	-5.548141027	0.821506842	0.883288531
C	-5.641781539	2.006840763	0.092051240
C	-5.533563595	3.280093274	0.703976786
C	-5.741667542	4.408229472	-0.131940291
C	-5.617532634	4.304497990	-1.495988250
C	-4.920552171	0.900631232	2.152391440
C	-4.497003005	-0.299271874	2.783704573
C	-5.036148025	-1.549645185	2.362020422
C	-5.627483743	-1.629891303	1.068151683
C	-4.674139524	-2.741209730	3.043803971
C	-5.287044333	-3.942000835	2.596223876
C	-5.835844121	-4.019061252	1.339174933
C	-5.813314798	-2.899639347	0.467236564
C	1.857130950	-3.603126733	0.800316487
C	1.727057066	-2.270834371	1.266999275
C	1.100210434	-2.021948607	2.521328979
C	0.586000210	-3.112579327	3.266890717
C	1.123698344	-4.397872769	2.971654285
C	1.750487409	-4.635004765	1.776012231
C	0.683641045	-0.693764348	2.829158824
C	-3.296375652	-0.303465323	3.531024446
C	-2.700324352	-1.553230982	3.876172960
C	-3.479707492	-2.738175332	3.843427451
C	-2.527165800	0.886299766	3.587539781
C	-3.132772684	2.131485041	3.256608713
C	-4.366478949	2.145657942	2.555930247
C	-1.279486640	-1.650544991	3.915767068
C	-0.660550757	-2.928924607	3.956187938
C	-1.480175815	-4.025954495	4.341451418
C	-2.847977838	-3.934869107	4.279234830
C	-1.112344444	0.785569642	3.580013519
C	-0.512324230	-0.502910277	3.558625221



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C	-2.351165370	3.315461062	3.285595574
C	-0.172287379	4.356031880	2.853977246
C	-0.805092444	5.632360892	2.975055794
C	-2.165318454	5.735654489	3.060552394
C	-2.980996447	4.561819372	3.004240821
C	-5.211378898	-4.257925333	-1.527290141
C	-5.547250107	-3.022517416	-0.950935799
C	-4.830486764	3.365725797	1.966851394
C	-4.240279712	4.565688688	2.394002221
H	2.035339853	-5.654569777	1.523183304
H	1.881557993	-6.026303890	-0.616533153
H	0.339418011	-6.365567152	-2.457146525
H	-1.677618368	-6.523252315	-3.179363105
H	-6.165106033	-4.988787745	0.969969524
H	-5.534878204	-5.184314704	-1.056296765
H	-5.196753299	-4.852989672	3.184656570
H	-3.441557238	-4.832755536	4.440943356
H	-1.029146329	-4.994551120	4.547700124
H	0.928052689	-5.234598714	3.640035103
H	-4.055344455	-6.514335623	-2.612077861
H	-4.362031678	5.071516039	-3.835260085
H	-2.078663972	5.055745404	-4.641677016
H	0.044375981	5.153751753	-4.296897222
H	-5.645256605	5.212281061	-2.095616170
H	-5.866835269	5.395676872	0.308900966
H	-4.618771182	5.518275591	2.028072122
H	-2.642704349	6.715508599	3.033438728
H	-0.211180562	6.539308752	2.878708506
H	1.526637094	6.231606422	1.638265800
H	2.394976741	5.798450460	-0.581439270
H	1.782518238	5.455789639	-2.636564020
Co	5.249374782	-0.416447718	-1.183081370
Co	5.523894923	-1.139671474	1.276895816
C	6.931560806	-0.583027863	-1.804518395
C	4.734221349	1.228961358	-1.598650255
C	4.649463628	-2.053856774	2.511428057
C	4.971357179	-2.130484341	-0.271825367
C	7.121626611	-1.923317482	1.280844004
O	4.513597440	2.295969060	-1.996275460
O	7.949086905	-0.676702655	-2.345526959
O	4.104190204	-2.584733413	3.382627025
O	4.659323211	-3.243035350	-0.498245458
O	8.197444780	-2.332919503	1.390475072
C	4.866984355	0.524852373	1.703574569
C	5.775404076	0.705062991	0.743051455
C	4.293549826	-1.130934272	-2.462657514
O	3.746971730	-1.594924592	-3.370722102
C	6.732948797	1.845304635	0.532117278
H	7.184536263	1.802628260	-0.467412061
H	7.562297739	1.727706398	1.252813563
C	6.024173092	3.192006704	0.741681242
H	5.007726510	3.133730982	0.320469085
H	5.898381135	3.378854049	1.821349378
C	6.748067674	4.365322028	0.094537119
H	7.767210453	4.454611072	0.508429809
H	6.860090179	4.158435360	-0.983581739
C	5.983387502	5.671552908	0.288321205
H	4.970876684	5.583501868	-0.135076032
H	5.874914526	5.910667253	1.357786678
H	6.489494182	6.516203825	-0.201472180
C	4.190859654	1.234550297	2.797520475
H	3.645763477	2.122394818	2.445440494
H	3.520857873	0.589918702	3.379438689
H	4.980346284	1.595339275	3.482420465

TS1'*methyl,oblique*

151
Co2C109H34O6

C	1.430067769	5.369581958	1.079685997
C	0.953514227	4.271605608	1.861891869
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C	1.885916243	2.773711247	0.149286043
C	1.852470367	3.855749332	-0.767474599
C	1.849737032	5.166943099	-0.206813457
C	1.419480218	3.586663824	-2.105579449
C	1.063660696	2.254235184	-2.432131822
C	1.535644069	1.172083552	-1.625870227
C	2.000996848	1.437160679	-0.328289024
C	0.939737921	4.615786077	-2.966840481
C	-0.123939900	4.387230070	-3.800762570
C	-0.751291617	3.110494302	-3.848909711
C	-0.011391445	2.013787137	-3.332371428
C	-0.531361823	0.693108938	-3.450463944
C	-1.906031699	0.514627665	-3.709804537
C	-2.738766466	1.668782200	-3.787628597
C	-2.161537953	2.939999479	-4.047752637
C	0.225371500	-0.407452621	-2.959806153
C	-0.279785508	-1.728149866	-3.118651140
C	-1.646316908	-1.910223879	-3.416315106
C	-2.488248383	-0.768730318	-3.515499835
C	0.462439543	-2.833425250	-2.613757108
C	-0.012937786	-4.159612509	-2.815314393
C	-1.390160261	-4.348691944	-3.147587042
C	-2.223683157	-3.200562852	-3.235549857
C	-3.570612702	-3.284362652	-2.796817459
C	-4.072813099	-4.522261230	-2.302291069
C	-3.343115661	-5.706811623	-2.637829805
C	-2.038741272	-5.618408857	-3.034624213
C	1.457690983	-2.587480073	-1.631872354
C	1.956119443	-3.665477899	-0.859297314
C	1.768614772	-4.977521516	-1.380913952
C	0.813324252	-5.217459058	-2.332968472
C	-3.816762621	-0.854392020	-3.033498882
C	-4.280433780	-2.091986245	-2.502796745
C	-4.059002256	1.586003243	-3.260517971
C	-4.507187928	0.344442197	-2.719681736
C	-5.359178086	0.357337424	-1.591264662
C	-5.530259781	-0.833488632	-0.836022704
C	-5.178144137	-2.088012302	-1.404982437
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C	1.710543422	-1.242796741	-1.216927598
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C	1.421262331	0.546252299	1.865120062
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C	-5.982454840	4.011529407	-1.157766326
C	-4.779590804	0.648534634	2.393892589
C	-4.224905667	-0.523735645	2.971969431
C	-4.718763282	-1.805404263	2.589849101
C	-5.417513007	-1.919339741	1.353488441
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C	2.088609204	-2.087937692	1.004834420
C	1.505297124	-1.876229713	2.291334419
C	1.102167092	-2.990695056	3.057696214
C	1.710905536	-4.242193892	2.736562925
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C	-2.956079408	-2.896891714	3.909636491
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C	-4.267969337	1.924731247	2.752077037
C	-0.834050519	-1.667039337	3.804197486
C	-0.124352368	-2.896899551	3.806566731
C	-0.838338486	-4.047681769	4.233179671
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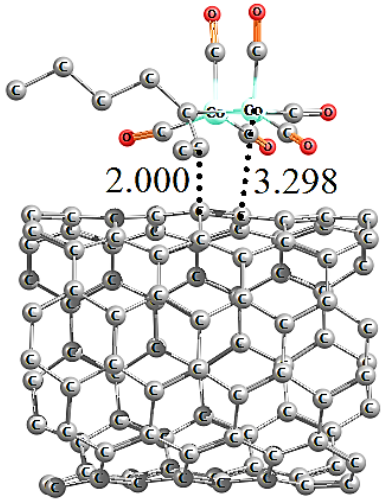

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H	2.299273264	-5.817818826	-0.936682336
H	0.603327371	-6.245215474	-2.622597338
H	-1.458639399	-6.531494799	-3.153939356
H	-5.746286080	-5.305141064	1.275156847
H	-5.258903996	-5.454940141	-0.794780992
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H	-2.786088872	6.589368186	3.083341348
H	-0.367750418	6.565307303	2.752381328
H	1.321287265	6.388748103	1.446001930
H	2.059242921	6.029218035	-0.837428520
H	1.319512867	5.630573687	-2.864062226
Co	5.076690103	-0.363547816	-1.282364880
Co	5.252872263	-0.968031273	1.139303396
C	6.807278501	-0.342386912	-1.751919021
C	4.417088489	1.006963538	-2.140215214
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CP5*methyl,oblique*

151
Co2C109H34O6

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C	1.199931532	3.668680566	-2.432106072
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C	-3.382145123	-3.561732926	-2.687922853
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C	-5.220319625	-2.195094533	1.435640586
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C	1.823488213	-1.617692801	2.108979927
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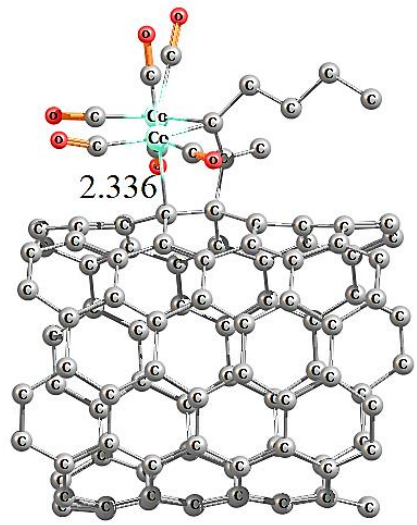

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H	-0.729648607	6.671039958	2.399951909
H	0.879293174	6.590902551	1.012901348
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Co	4.813184542	-0.765385209	-0.988792863
Co	5.369253339	-0.406207000	1.526471310
C	6.585031142	-0.756002341	-1.216393602
C	4.289617437	-0.057786551	-2.524192046
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C	6.992624933	0.251769388	1.836038423
O	4.024055802	0.361579842	-3.565312099
O	7.726737149	-0.730754151	-1.375103851
O	3.932903712	-0.286681462	4.059960978
O	5.800423563	-3.291874420	1.527843016
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C	4.993199731	0.924621789	-0.003493730
C	4.842653996	-2.553115966	-1.368797989
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H	3.806359664	3.324787934	1.343779632
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(8,0)-SWCNT

118
C96H22

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C	2.742383015	-3.202722823	-1.757838861
C	4.062235399	-3.529657970	-1.970357896
C	4.991710396	-3.551753221	-0.883028717
C	6.365706278	-3.816333384	-1.035137119
C	3.162894337	-2.947776829	0.629257439
C	4.550095433	-3.032661899	0.369651377
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C	6.833371133	-2.767447369	1.104952379
C	3.565358125	-1.304325373	2.357603017
C	4.958396593	-1.375389396	2.099146598
C	5.712404002	-0.197769151	2.142306270
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C	5.077877201	1.054154329	2.117730430
C	5.710867319	2.074664949	1.276712809
C	7.087091662	2.228457775	1.106795543
C	3.444674498	2.728228141	0.570679091
C	4.840583838	2.634492637	0.305680382
C	5.350845552	2.912367489	-0.991064395
C	6.734659221	3.049663727	-1.143969901
C	3.028001964	2.742092410	-1.807865066
C	4.408207344	2.688141469	-2.079367965
C	4.824221807	2.017460864	-3.251793501
C	2.606892897	1.071361097	-3.526319517
C	3.955179106	1.168872262	-3.915945470
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C	-1.147590716	3.024760063	-1.046716414
C	0.233355089	2.920413290	-1.294512401
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C	-1.552812261	1.246681040	-2.655158341
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C	-2.287001703	-2.188804310	-1.820741908
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C	-4.246208462	-2.934373628	-0.509849614
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C	-3.765911551	-2.707440703	1.872085745
C	-2.891863965	-2.075111998	2.774441719
C	-1.502117840	-2.129039318	2.528606433
C	-4.741488612	-0.890736206	4.041501187
C	-3.429128726	-0.969543849	3.568904849
C	-2.650807409	0.217286721	3.536237905
C	-1.245712639	0.148982736	3.313020787
C	-4.622187504	1.528428215	4.032125968
C	-3.311406518	1.474059287	3.557225507
C	-2.675305041	2.503822647	2.729893676
C	-1.283427509	2.422516085	2.485432248
C	-3.490267860	3.170686770	1.803993168
C	-3.009420752	3.465818399	0.516074333
C	-1.618992369	3.363122810	0.268476493
C	-5.331046496	3.455447025	-0.497212064
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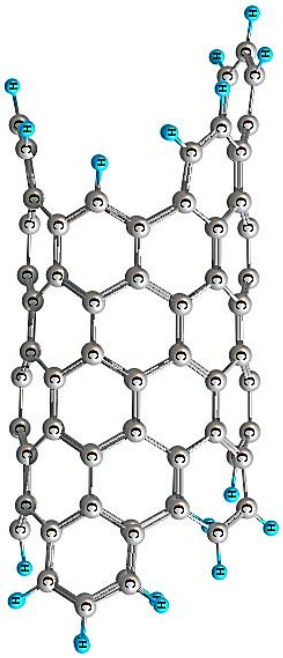
C	-3.462732482	2.391608350	-1.601253994



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C	-6.208854792	2.608257557	-1.153769448
C	-7.926457638	0.205926234	-1.779255451
H	6.728871562	-4.252988934	-1.965516900
H	8.312059887	-3.722545962	-0.136456895
H	7.568246967	-2.402274245	1.821667930
H	7.772377605	1.864655839	1.871896022
H	8.656186752	2.948533401	-0.181507303
H	7.149291284	3.331238244	-2.111009859
H	3.572701083	-1.367237957	-3.432390867
H	4.452803886	-3.608953394	-2.985589471
H	6.745713107	-0.245469536	1.806828848
H	5.880402098	2.000296708	-3.515979723
H	4.342565998	0.498055253	-4.682531492
H	-4.832530300	-2.530601756	1.992823199
H	-4.567499713	3.100864840	1.937045148
H	-9.662978645	-1.001066443	-1.380087256
H	-8.365655435	-2.983592702	-0.653881940
H	-6.082930005	-3.716028022	0.269034861
H	-5.337584933	-1.797330737	4.139835159
H	-6.305927852	0.400570766	4.759349070
H	-5.128056928	2.489506236	4.119374025
H	-5.722192036	4.205651585	0.189951949
H	-7.277286072	2.722705972	-0.978217823
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RC*methyl*

151
Co2C109H34O6

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C	-1.467528339	-8.120977020	0.270505371
C	0.422986677	-5.265425046	-1.160133058
C	-0.609337989	-6.207880185	-0.948521392
C	-1.755906212	-6.211297982	-1.784022011
C	-2.637560609	-7.285748830	-1.687499828
C	-1.014223350	-3.988827846	-2.628711004
C	-2.062054608	-4.921115937	-2.412507249
C	-3.374570457	-4.447548595	-2.300605956
C	-2.573557442	-2.156150369	-2.286952879
C	-3.625044017	-3.081813401	-2.090881510
C	-4.692135745	-2.762121818	-1.134728222
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C	-5.930716052	-2.931366008	1.374960356
C	-2.741307566	-1.030704050	2.076619130
C	-3.794397067	-1.936077726	2.306203778
C	-3.635211087	-2.877412274	3.349926446
C	-1.276540069	-2.325005398	3.530098566
C	-2.383939576	-3.113691237	3.895214374
C	0.099030016	-2.811064764	3.433741177
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C	3.165074352	-3.619065222	0.755003037
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C	-1.617311924	0.618073153	0.623252915
C	-2.633878626	-0.332140935	0.822821509
C	0.358263107	1.814448889	1.469361483
C	-0.653693951	0.859847071	1.660816160
C	-0.484868462	-0.183210349	2.610153233
C	-1.530491723	-1.124157410	2.824937705
C	1.866600225	0.452348529	2.804930397
C	0.836445109	-0.482943262	3.035316516
C	1.141258499	-1.879241056	3.205652214
C	3.228193185	0.006823360	2.717142618
C	6.526114829	1.423553604	1.658815585
C	5.477671852	0.502896690	1.898518932
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C	5.693289608	-1.492922053	-1.021375320
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C	4.555874665	-0.622692008	-3.001409414
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C	5.224259452	1.596423492	-4.027802919
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C	2.928249937	1.131267809	-3.420984233
C	1.868775652	0.194776674	-3.247822188
C	3.669666603	3.419831047	-3.671317189
C	2.691496430	2.521024970	-3.244118115
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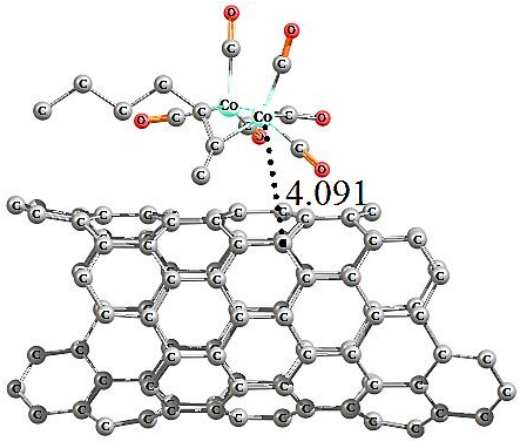

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C	7.678926911	0.987366670	0.939641820
C	4.896721267	2.946660151	-4.137719528
C	4.635236200	4.544504148	1.629370099
C	7.495350627	3.620649676	1.927159364
H	-1.418778976	-8.814601262	1.110013043
H	-3.134847112	-9.107995454	-0.651776759
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H	-6.249416259	-4.093029622	-1.807054623
H	-7.465780149	-4.044927111	0.358694662
H	-6.363490611	-3.092240525	2.361602027
H	-0.573745695	-4.813690068	3.061484612
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H	6.431513416	0.087588767	-2.251895244
H	2.800027082	4.362064913	-1.384231481
H	9.576146911	3.779533168	1.400426995
H	9.696234095	1.525630378	0.377324320
H	8.264159363	-0.317688904	-0.692904828
H	6.238092264	1.259755816	-4.241906468
H	5.640535866	3.652239330	-4.506537000
H	3.485459218	4.491791182	-3.607493663
H	3.184967884	5.685093257	0.538346264
H	5.403051980	5.304820266	1.495375071
H	7.426650256	4.662245386	2.237155243
Co	-3.675091656	3.182498242	-1.314468652
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C	-4.820751832	4.418223563	-1.951125854
C	-4.630896750	1.691487600	-1.395695252
C	-1.358449045	4.585615430	1.770261039
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O	-2.107775299	2.398957476	-3.630513257
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H	-8.217992437	2.026254960	2.129370808
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C	-3.137767731	2.120639034	3.049792159
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TS1'*methyl,parallel*

151
Co2C109H34O6

C	-2.805360221	7.710150167	0.881973017
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C	0.875042570	5.335115566	-1.176513409
C	-0.060521908	6.340392657	-1.257657270
C	-0.842787872	6.699221964	-0.113684905
C	-1.861202046	7.669677405	-0.135903446
C	0.364804641	5.007960138	1.181059670
C	-0.762903644	5.846665922	1.026958908
C	-1.864506171	5.732667550	1.913538866
C	-2.851048374	6.715953424	1.867017392
C	-0.874061928	3.585894202	2.692879906
C	-2.013909159	4.415272695	2.541292218
C	-3.278157029	3.817354804	2.499337072
C	-2.267780207	1.611871371	2.409534942
C	-3.411331145	2.434344626	2.294001982
C	-4.513061239	2.007926912	1.430924263
C	-5.739946041	2.672203557	1.334718902
C	-3.034868741	0.232031869	0.551935221
C	-4.130754500	1.128600731	0.383397734
C	-4.710031206	1.340847527	-0.900212370
C	-5.921922685	2.025150870	-0.984331043
C	-2.620442130	0.409078053	-1.831448764
C	-3.759417363	1.203560310	-2.006415948
C	-3.734349832	2.189492571	-3.019844074
C	-1.351040587	1.879703040	-3.307826808
C	-2.541264022	2.558933252	-3.615938263
C	-0.024579158	2.489363019	-3.311762334
C	3.477221753	1.373318960	-2.518387198
C	2.338986204	2.217076686	-2.695693938
C	2.298038262	3.485057065	-2.052485479
C	1.164390726	4.323508428	-2.211656757
C	4.265041659	2.817303072	-0.725427458
C	3.137024188	3.616164633	-0.884321078
C	2.446053633	4.102576005	0.280402025
C	1.292972616	4.894130171	0.128619316
C	3.832050007	2.604252024	1.649019281
C	2.666297566	3.408072831	1.493848711
C	1.540088755	3.214851459	2.351273839
C	0.402784981	4.024077696	2.211407510
C	2.562193625	1.099648351	3.068776176
C	1.421078707	1.919638077	2.954788739
C	0.120375782	1.343781862	2.958347362
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C	1.164300400	-0.877706032	2.797670955
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C	-0.727641632	-1.408690288	0.813013360
C	-1.251644604	-1.146597777	-0.466962020
C	-2.501547661	-0.451995551	-0.634810041
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C	-0.331620033	-1.274330343	-1.549292977
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C	3.393584373	-0.019751260	-2.817954249
C	6.878941202	-1.108394843	-1.991424685
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C	5.674605059	0.965119157	-1.528192527
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C	6.613472873	1.214256896	-0.465566977
C	5.939016886	1.726514161	0.740994751
C	4.781485693	2.529645060	0.592063903
C	6.077975417	0.951533166	1.901050278
C	4.994649714	0.759457926	2.776097312
C	3.849388708	1.574858332	2.633220344
C	5.922871624	-1.374035525	3.776540378
C	4.854845954	-0.555877927	3.401884690
C	3.563647097	-1.136218861	3.289177633
C	2.411365688	-0.307796533	3.159286096
C	4.534740830	-3.340727020	3.516603481
C	3.453466791	-2.543446974	3.136646482
C	2.363690045	-2.975904455	2.258116378
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C	2.702121304	-3.852018514	1.212420859
C	2.140741182	-3.677788068	-0.062809434
C	1.010576769	-2.833569179	-0.199103730
C	4.117238971	-4.740275862	-1.237186597
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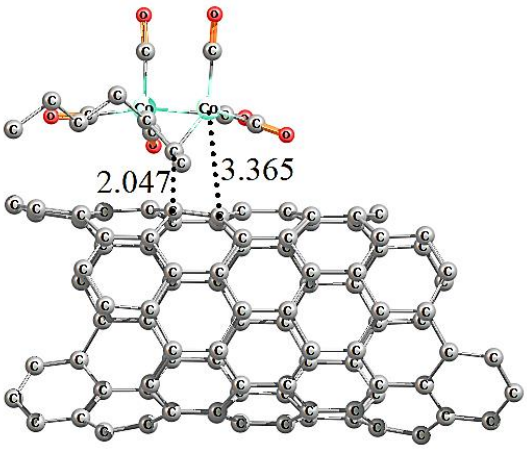

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C	5.309305149	-4.397205675	-1.853994863
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H	-3.679063146	6.691147788	2.574631904
H	-6.092211896	3.279271597	2.168704792
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H	-6.412443178	2.146053894	-1.949714255
H	-0.844078169	4.433530418	-2.927159594
H	-0.345831457	6.749776708	-2.227581578
H	-4.127504260	4.448187400	2.249588152
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H	-2.509552266	3.440553219	-4.255857106
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H	3.654739116	-4.372747934	1.279413728
H	10.152374997	-3.159125862	-1.941639138
H	10.118979606	-0.904751066	-0.912884653
H	8.585774024	0.792154889	0.257197510
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Co	-5.038641005	-2.027003005	1.432690108
Co	-3.530526816	-3.545338026	0.146032990
C	-6.043584228	-3.324176700	2.167990311
C	-6.285438002	-0.846622773	1.160757830
C	-2.104964692	-4.223426547	-0.619031181
C	-2.917981845	-3.301807538	1.804581150
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O	-1.178972973	-4.648133251	-1.168298850
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CP5*methyl,parallel*

151
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C	5.087723245	-1.164128302	-0.846882942
C	6.314533790	-1.789775255	-1.000374868
C	3.041639703	-0.017542945	-1.646260178
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C	-1.775053700	-3.443092347	-2.340662205
C	-0.586146400	-4.174168714	-2.590694864
C	-3.815242151	-3.107015673	-0.992551481
C	-2.639915867	-3.810831833	-1.241851226
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C	-0.744250913	-5.132644135	-0.387840560
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C	-1.112373703	-3.799757621	2.037133715
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C	-2.255779690	-1.854558860	3.012459232
C	-1.064747999	-2.579631119	2.787250086
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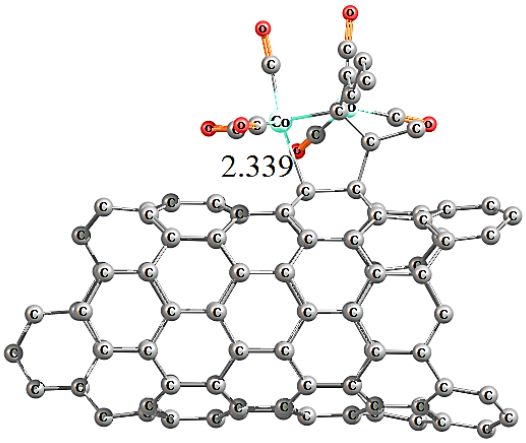

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Co	2.148312832	3.851848371	-0.049114132
Co	3.917958447	3.306599841	-1.873823619
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