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4*f*-Electron Localization in Ce-Embedded Co_6Te_8 Clusters for Enhanced CO_2 Reduction Catalysis

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Part I. Electronic states searching for cage and M@cage (M=Ti, Zr, Hf, Ce and Th).

Table S1. Relative energies for intermediates of CO_2 reduction reaction with catalysts cage and M@cage (M=Ti, Zr, Hf, Ce and Th) in different electronic states at the PBE-D3 level. The lowest energy is used as the zero of the corresponding system in each intermediate.

ΔE (eV)	Electronic states	M@cage (I)	M@cage-CO_2 (II)	M@cage-COOH (III)	M@cage-CO (IV)	M@cage-CHO (V)	M@cage-OCH_2 (VI)	M@cage-OCH_3 (VII)	M@cage-CH_3OH
Cage	Singlet	0.14	0.15		**0.00**		**0.00**		0.15
	Doublet			**0.00**		**0.00**		**0.00**	
	Triplet	**0.00**	**0.00**		0.69		0.15		**0.00**
	Quartet			0.58		0.55		0.13	
Ti@cage	Singlet	**0.00**	**0.00**		**0.00**		**0.00**		**0.00**
	Doublet			**0.00**		**0.00**		**0.00**	
	Triplet	0.21	0.25		0.55		0.25		0.28
	Quartet			0.50		0.49		0.14	
Zr@cage	Singlet	**0.00**	**0.00**		**0.00**		**0.00**		**0.00**
	Doublet			**0.00**		**0.00**		**0.00**	
	Triplet	0.09	0.15		0.63		0.18		0.60
	Quartet			0.58		0.59		0.10	
Hf@cage	Singlet	**0.00**	**0.00**		**0.00**		**0.00**		**0.00**
	Doublet			**0.00**		**0.00**		**0.00**	
	Triplet	0.12	0.17		0.62		0.21		0.21
	Quartet			0.57		0.59		0.11	
Ce@cage	Singlet	**0.00**	**0.00**		**0.00**		0.05		**0.00**
	Doublet			**0.00**		**0.00**		**0.00**	
	Triplet	0.20	0.20		0.21		**0.00**		0.20
	Quartet			0.22		0.21		0.01	
Th@cage	Singlet	**0.00**	**0.00**		**0.00**		0.09		**0.00**
	Doublet			**0.00**		**0.00**		0.01	
	Triplet	0.05	0.03		0.42		**0.00**		0.04
	Quartet			0.39		0.01		**0.00**	

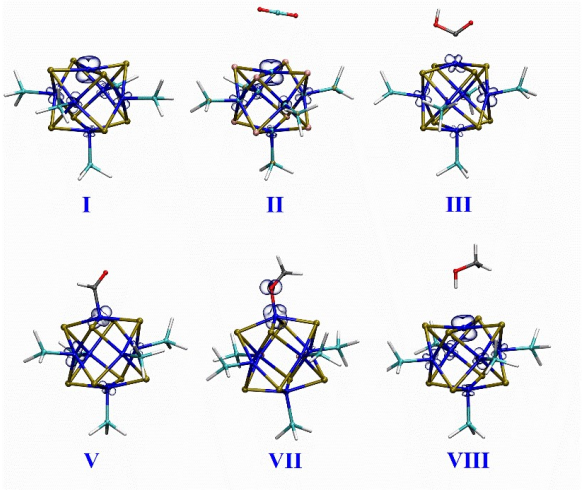

Figure S1. Spin population of the intermediates for CO_2RR on the hollowed cage catalyst.

Since the ground state of the hollow cage structure exhibits a spin magnetic moment (Triplet), its spin density distribution is presented in **Figure S1**. It is evident that the spin density is localized on the Co atom at the active site, and remains constant before and after the reaction circle. Therefore, the cage catalyst can participate in another CO_2RR.

Part II. Optimized geometries for $Co_6Te_8(PH_3)_5$ (abbreviated as cage) and M@cage (M=Ti, Zr, Hf, Ce and Th).

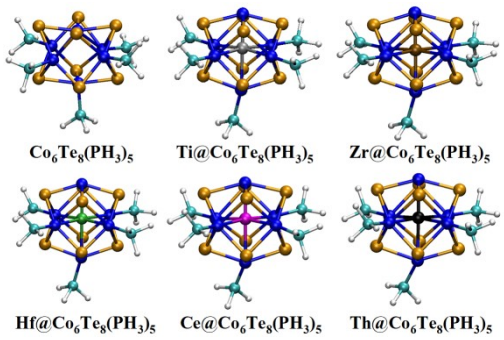

Figure S2. Structures of the ground-state catalysts cage and M@cage (M=Ti, Zr, Hf, Ce and Th) at PBE-D3 level. Silver, brown, green, magenta, black spheres represent the embedded Ti, Zr, Hf, Ce, Th atoms. The blue, yellow, cyan and white spheres are Co, Te, P and H atoms, respectively.

Table S2. Average bond lengths (Å) for cage and M@cage structures based on PBE-D3 functional.

Average nearest-neighbor distances of cage and M@cage			
structure	**Co-Co**	**Co-Te**	**Co-M**
cage	3.06	2.55	-
Ti@cage	3.58	2.58	2.53
Zr@cage	3.66	2.62	2.59
Hf@cage	3.67	2.61	2.59
Ce@cage	3.67	2.68	2.60
Th@cage	3.69	2.71	2.61

Part III. Reaction paths for two-electron-proton CO_2RR catalyzed by $Co_6Te_8(PH_3)_5$ (abbreviated as cage) and M@cage (M=Ti, Zr, Hf, Ce and Th).

A competing pathway of CO_2RR which produces formic acid through a two-electron-proton process has been revealed in the previous researches. (see Figure S3). In detail, the catalysts (I) engage with CO_2 (II) also at the uncapped Co atom for further reaction. The first electron-proton reaction could either happen on O atom (pathway A) or C atom (pathway B), as shown in **Figure S4**. In pathway A, result shows adsorption of *-OH and with CO dissociated and roams near the catalyst (III_A), whose energy is much higher than those of III; in pathway B, the intermediate is *-OCHO (III_B), which also has higher energy than III. For the second electron-proton reaction, both pathway A and B will lead to intermediate *-HCOOH (IV_A and IV_B). The energy of intermediate IV' is also higher than IV. Therefore, CO_2RR will tend to go through the six-electron pathway as shown above. Details energy diagram about the two-electron CO_2RR are included in SI.

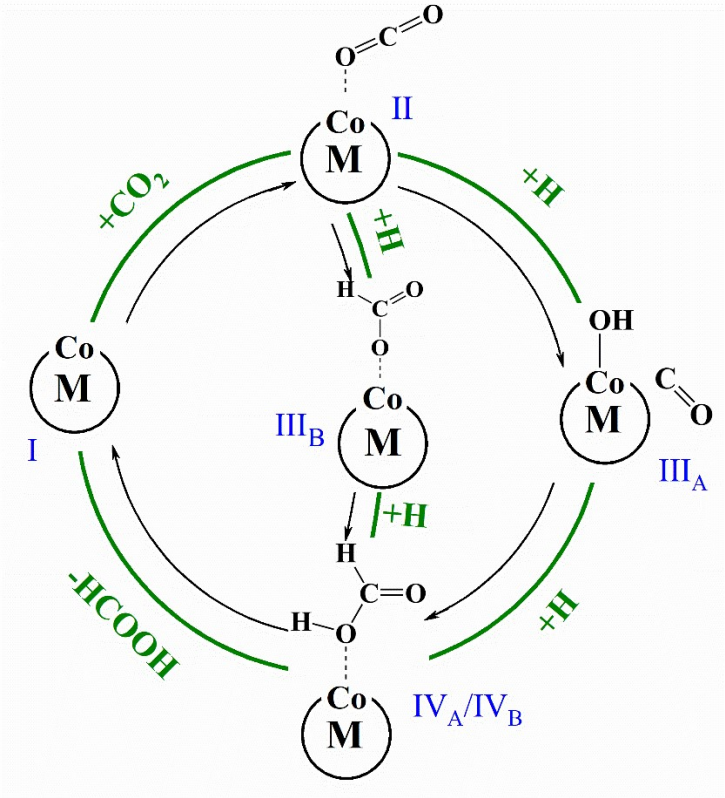

Figure S3. Scheme of the two-electron-proton CO_2RR circle producing formic acid.

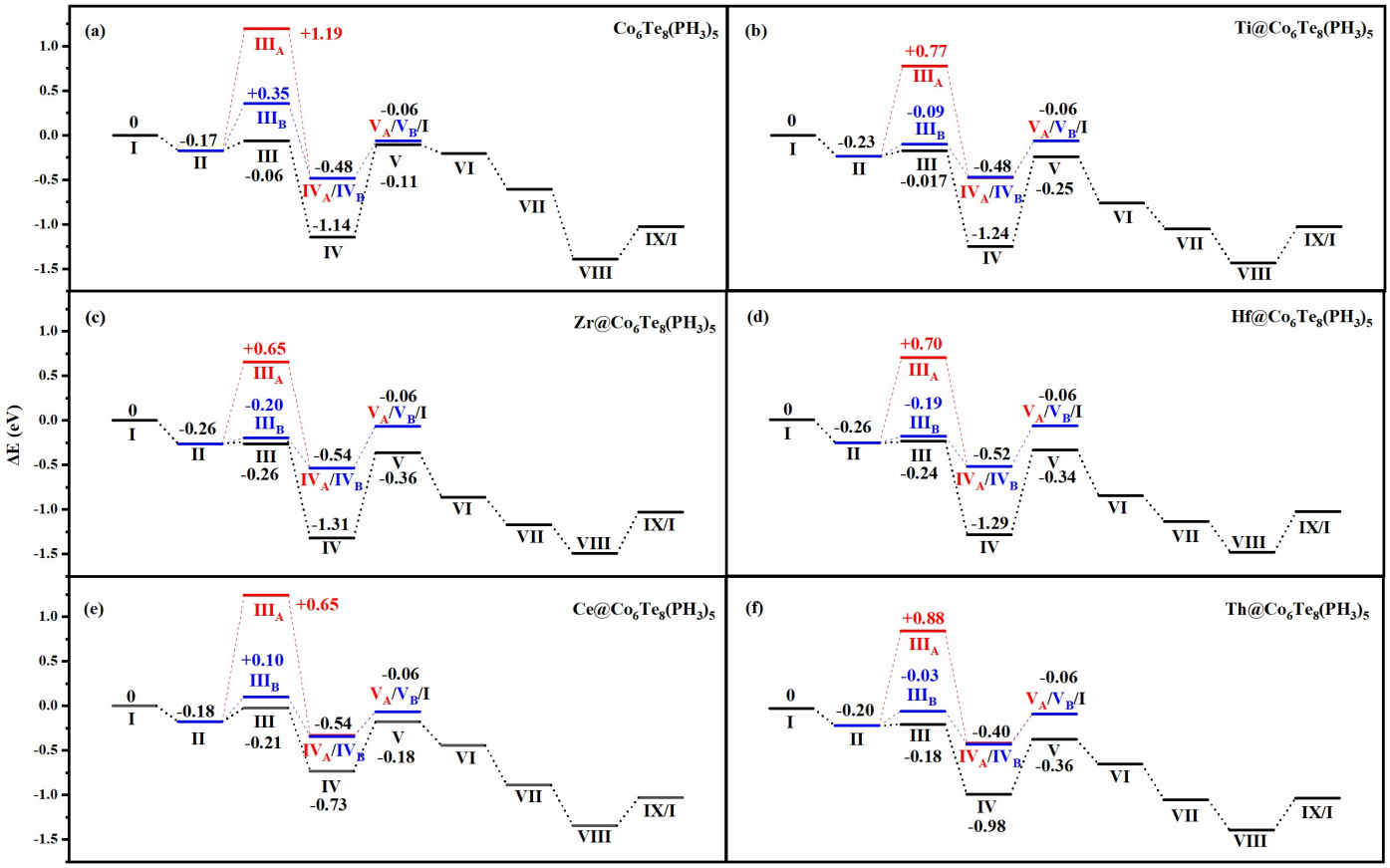

Figure S4. Comparison between two-electron reaction paths (blue and red) and six-electron reaction paths catalyzed by cage(a) M@cage, M=Ti(b), Zr(c), Hf(d), Ce(e) and Th(f). The intermediates are marked with Roman number and those colored blue and red are the two different pathways for the two-electron-proton CO_2RR. The intermediates III_A are M@cage-OH&CO, III_B are M@cage-OCHO. The intermediates IV_A and IV_B have same structures of M@cage-OHCHO. The V_A and V_B are the catalyst M@cage and the product HCOOH.

Part IV. Comparison of the calculated endothermic energy differences and previous experimental overpotentials of CO_2RR.

Table S3. The largest endothermic energy difference along the reaction path and over-potentials of CO_2 reaction reduction with different catalysts. The over-potential data in the lower part of this table is from references 1-4.

Catalyst	**cage**	**Ti@cage**	**Zr@cage**	**Hf@cage**	**Ce@cage**	**Th@cage**
Energy difference (eV)	-1.03	-1.00	-0.95	-0.95	-0.55	-0.62

Catalyst	**Electrolyte**	**Faradaic efficiency**	**Over-potential**
Partially oxidized Co/SL-NG*	0.1 M $KHCO_3$	71%	-0.90 V[ref 1]
CoPc/CNT**	0.1 M $NaHCO_3$	> 40.0 %	-0.94 V[ref 2]
CoPc***	0.5 M $KHCO_3$	0.3%	-0.88 V[ref 3]
Co-corrole	0.1 M $NaClO_4$	8%	-0.80 V[ref 4]

*NG: Single-Layer Nitrogen-Doped Graphene; **CNT: Carbon nanotube; ***Pc: Phthalocyanine

Part V. Comparison between the hybrid functional (PBE0) and the pure functional (PBE).

a. Comparison of optimized geometric parameters between the hybrid functional (PBE0) and the pure functional (PBE).

The geometries of the M@cage-CO (M=Ti, Zr, Hf, Ce and Th) systems were calculated using both PBE-D3 and PBE0-D3, and the resulting geometric parameters were compared (**Table S4 and S5**). Taking Ce@cage-CO as a typical example, the type of bond obtained by the two methods is similar, and the difference in bond lengths is on the order of around 10^{-2} Å, which is almost negligible. The distance between Ce and the active Co atom is greater than that between the Co atoms passivated by PH_3, which is again consistent with the PBE structure.

Table S4. Bond lengths comparison between M@cage-CO (M=Ti, Zr, Hf, Ce and Th) structures obtained based on PBE-D3 and PBE0-D3 functionals.

Bond length (Å)	Ti@cage-CO		Zr@cage-CO		Hf@cage-CO		Ce@cage-CO		Th@cage-CO	
	PBE	PBE0	PBE	PBE0	PBE	PBE0	PBE	PBE0	PBE	PBE0
C=O	1.16	1.14	1.16	1.14	1.16	1.14	1.16	1.14	1.16	1.14
Co-C	1.76	1.74	1.76	1.75	1.77	1.75	1.76	1.74	1.77	1.76
$M\text{-}Co_{active\text{-}site}$	2.63	2.51	2.66	2.57	2.66	2.58	2.74	2.63	2.71	2.61
$M\text{-}Co_{passivated}$	2.54	2.47	2.59	2.54	2.60	2.54	2.57	2.49	2.61	2.55
Co-Te	2.58	2.54	2.62	2.58	2.61	2.58	2.67	2.62	2.72	2.66
Co-P	2.16	2.15	2.17	2.15	2.17	2.15	2.20	2.17	2.18	2.16

b. Comparison of electronic structural properties between the hybrid functional (PBE0) and the pure functional (PBE).

To better verify the method, we analyzed the electronic structure of M@cage-CO (M=Ti, Zr, Hf, Ce and Th) at the PBE0-D3 level and compared the results with those obtained from PBE-D3. As expected, the HOMO-LUMO gaps are significantly larger with the PBE0 functional compared to the PBE functional. However, the trends observed for M@cage-CO structures are consistent between the two methods. The gap of Ce@cage-CO is the smallest, followed by that of Th@cage-CO (**Table S5**).

Table S5. The HOMO-LUMO gap (eV) for cage-CO and M@cage-CO structures.

Structures	PBE			PBE0		
	HOMO	LUMO	gap	HOMO	LUMO	gap
cage-CO	-4.12	-3.09	1.03	-4.95	-2.15	2.80
Ti@Cage-CO	-4.43	-3.39	1.04	-5.31	-2.79	2.55
Zr@Cage-CO	-4.55	-3.56	1.00	-5.32	-2.91	2.42
Hf@Cage-CO	-4.47	-3.47	1.00	-5.38	-2.93	2.47
Ce@Cage-CO	-4.35	-3.90	0.45	-5.29	-3.42	1.86
Th@Cage-CO	-4.61	-3.89	0.72	-5.39	-3.26	2.20

On the other hand, the MO energy levels differ between the PBE0 and PBE results. As a GGA functional, PBE utilizes the generalized gradient approximation to solve the exchange and correlation interaction of electrons, while hybrid functionals mixes HF and DFT exchange energies to improve the description of the electron interactions, particularly the exchange interaction. This mixture, along with the ratio of the components, can affect the ordering of MOs. According to the PBE0 results, the HOMO of the Ce@cage-CO structure is the antibonding MO between the 4*f*-electron of Ce and 3*d*-electron of Co (**Figure S10**). The antibonding interaction between localized 4*f*-electron and the 3*d*-electron rises the energy level of this MO to become the HOMO of the structure, thereby reducing the HOMO-LUMO gap. This phenomenon was not seen in other structures. This result qualitatively corresponds to the rise of 4f/5d-3d antibonding HOMO of Ce@cage-CO, which originates

from the localization of the 4f-electron, as discussed in the main text. Both GGA-PBE and hybrid-PBE0 calculation led to qualitatively similar conclusions, which verifies the reliability of the methodology.

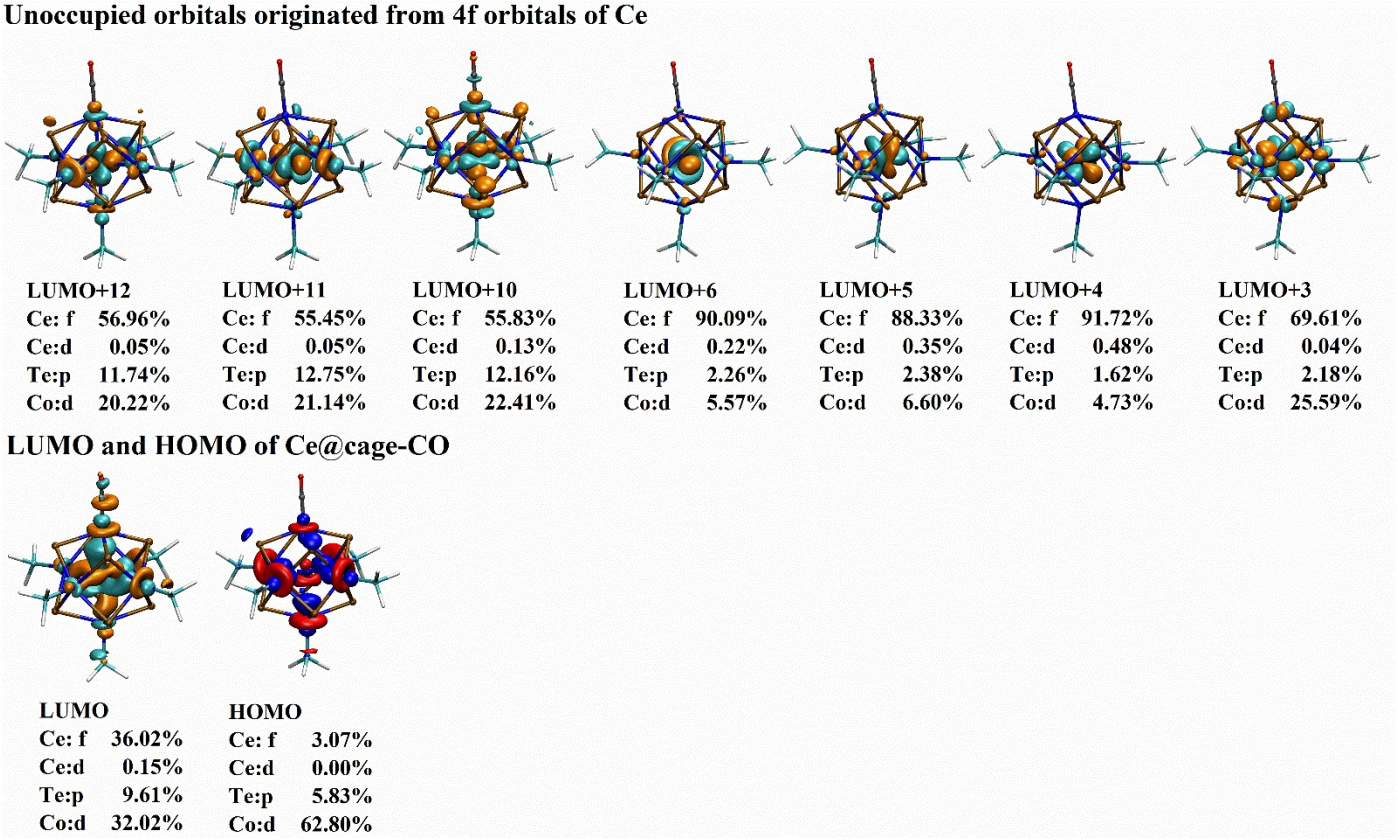

Figure S5. Molecular orbitals and orbital components of Ce@cage-CO obtained from hybrid PBE0-D3 calculation. The red and green (cyan and orange) bubbles are isosurfaces of the electronic density of occupied (unoccupied) orbitals with different electron orientation.

Part VI. Selected molecular orbitals (MOs) of cage-CO and M@cage-CO (M=Ti, Zr, Hf, Ce and Th).

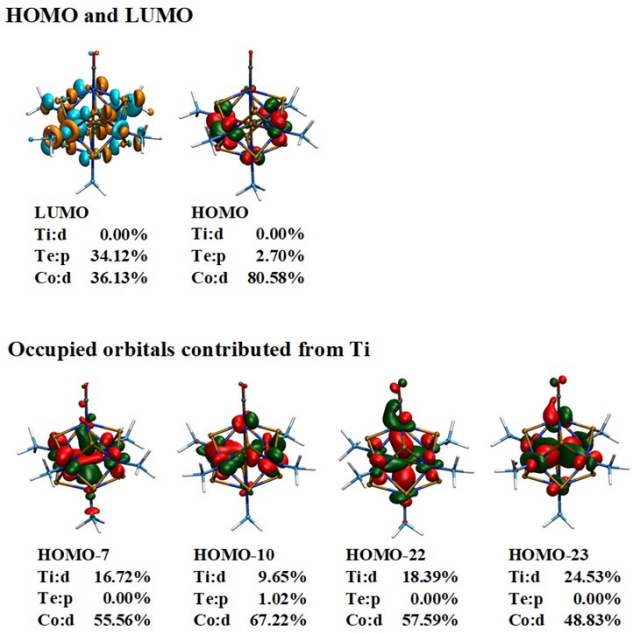

Figure S6. Molecular orbitals and orbital components of Ti@cage-CO. The red and green (cyan and orange) bubbles are isosurfaces of the electronic density of occupied (unoccupied) orbitals with different electron orientation.

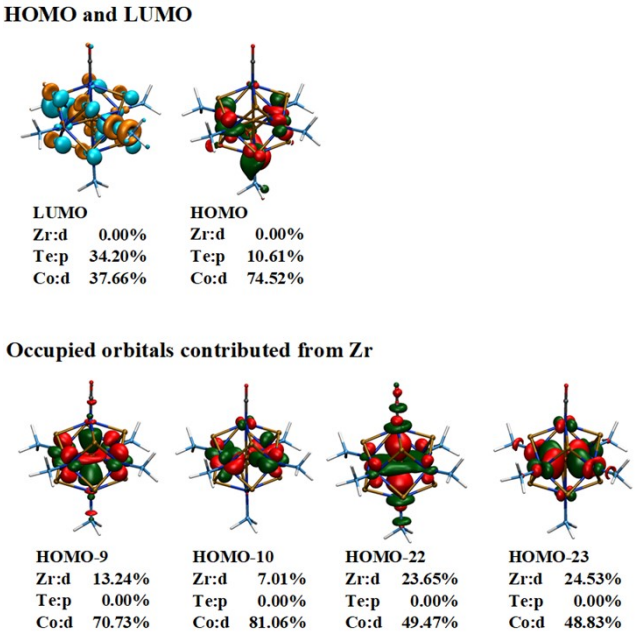

Figure S7. Molecular orbitals and orbital components of Zr@cage-CO. The red and green (cyan and orange) bubbles are isosurfaces of the electronic density of occupied (unoccupied) orbitals with different electron orientation.

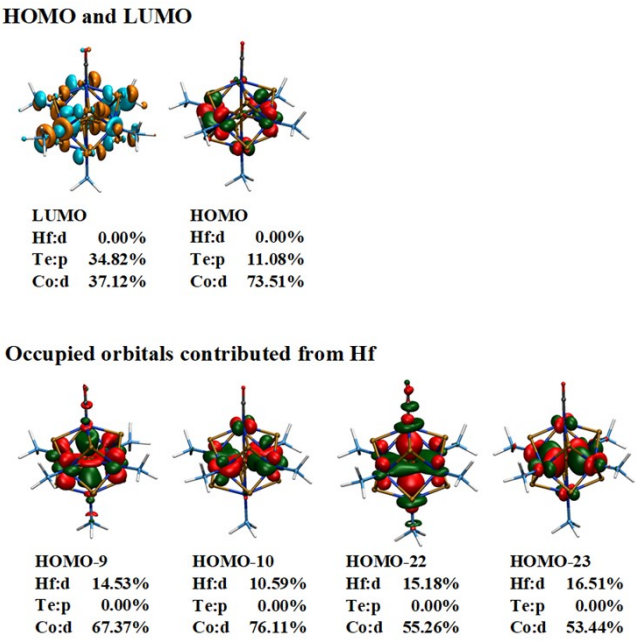

Figure S8. Molecular orbitals and orbital components of Hf@cage-CO. The red and green (cyan and orange) bubbles are isosurfaces of the electronic density of occupied (unoccupied) orbitals with different electron orientation.

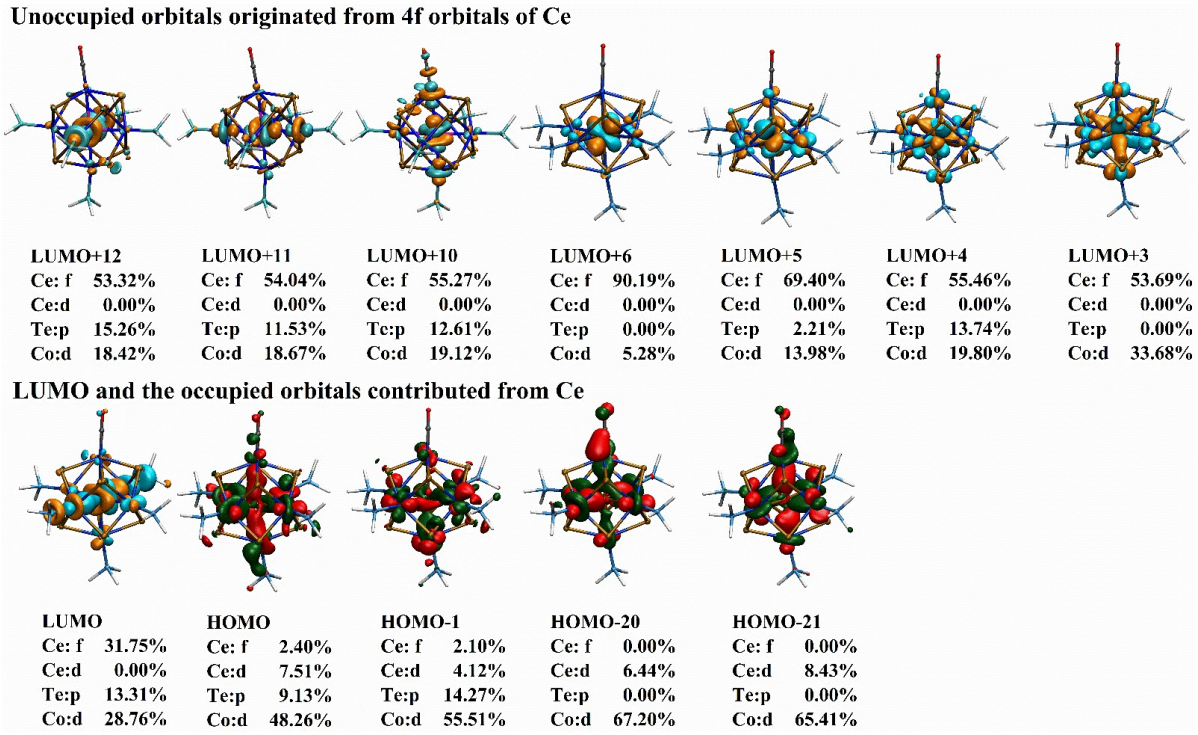

Figure S9. Molecular orbitals and orbital components of Ce@cage-CO. The red and green (cyan and orange) bubbles are isosurfaces of the electronic density of occupied (unoccupied) orbitals with different electron orientation.

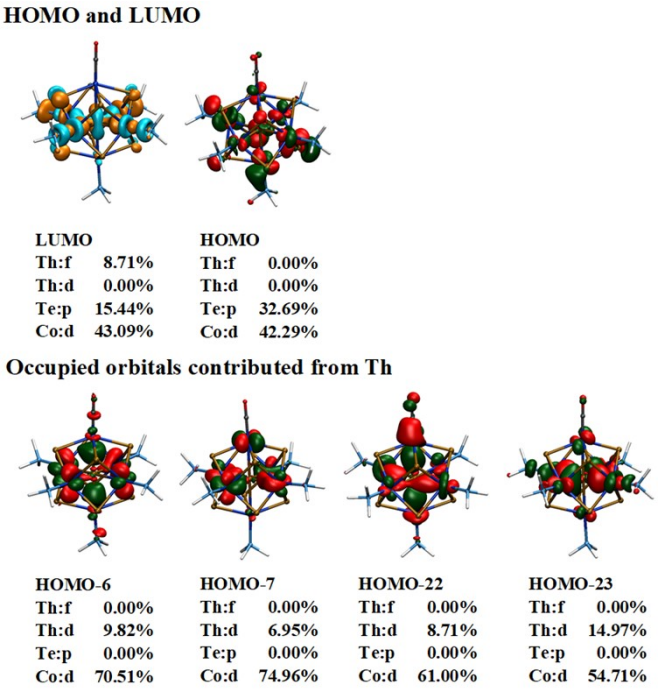

Figure S10. Molecular orbitals and orbital components of Th@cage-CO. The red and green (cyan and orange) bubbles are isosurfaces of the electronic density of occupied (unoccupied) orbitals with different electron orientation.

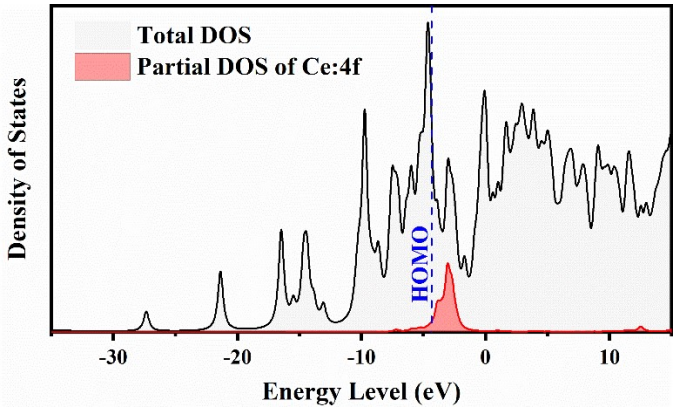

Figure S11. Density of state (DOS) plot of Ce@cage-CO structure, and the partial DOS for 4*f* shells of Ce atom.

Part VII. Selected bond lengths of M-Co-CO in the M@cage-CO (M=Ti, Zr, Hf, Ce and Th) structures.

Table S6. Bond lengths for cage-CO and M@cage-CO (M=Ti, Zr, Hf, Ce and Th) based on PBE-D3 functional.

Distances (Å) of M@cage-CO*			
structures	**Co-C**	**C=O**	**M-Co$_{(top)}$**
Ti@cage	1.76	1.16	2.63
Zr@cage	1.76	1.16	2.66
Hf@cage	1.77	1.16	2.66
Ce@cage	1.76	1.16	**2.74**
Th@cage	1.77	1.16	2.71

*The bond lengths of Co-C and M-Co are those between C/M atoms and the active site Co atoms.

Part VIII. Plots of EDA-NOCV in the M@cage-CO (M=Ti, Zr, Hf, Ce and Th) structures.

Table S7. EDA-NOCV results (eV) for the different forms of interacting fragments, taking CO as interacting fragments at the corresponding M@cage geometries.

Energy (eV)	Ti@cage-CO	Zr@cage-CO	Hf@cage-CO	Ce@cage-CO	Th@cage-CO
ΔE_{pauli}	7.31	7.09	7.14	7.91	7.24
[a]ΔE_{elect}	-5.33	-5.18	-5.21	-5.58	-5.20
[a]ΔE_{orb}	-4.25	-4.13	-4.12	-4.33	-4.10
[a]ΔE_{disper}	-0.09	-0.09	-0.09	-0.09	-0.10
ΔE_{int}	-2.36	-2.31	-2.28	-2.08	-2.17
[b]ΔE_{orb1}	-1.16 (27.24%) [CO{σ}→Co_{3d} & Ti_{3d}]	-1.11 (26.92%) [CO{σ}→Co_{3d} & Zr_{3d}]	-1.10 (26.68%) [CO{σ}→Co_{3d} & Hf_{3d}]	-1.38 (31.85%) [CO{σ} &Co_{3d} & Ce_{4f}→Co_{3d} & Ce_{4f}]	-1.16 (28.23%) [CO{σ} & Co_{3d}→Co_{3d} & Th_{5f}]
[b]ΔE_{orb2}	-1.26 (29.64%) [Co_{3d}→CO{π*}]	-1.21 (29.36%) [Co_{3d}→CO{π*}]	-1.22 (29.70%) [Co_{3d}→CO{π*}]	-1.26 (29.01%) [Co_{3d} & Ce_{4f}→CO{π*}]	-1.16 (28.37%) [Co_{3d}→CO{π*}]
[b]ΔE_{orb3}	-1.26 (29.64%) [Co_{3d}→CO{π*}]	-1.21 (29.38%) [Co_{3d}→CO{π*}]	-1.23 (29.72%) [Co_{3d}→CO{π*}]	-1.08 (24.97%) [Co_{3d} & Ce_{4f}→CO{π*}\	-1.15 (28.00%) [Co_{3d}→CO{π*}]
[b]ΔE_{orb4}	-0.57 (13.48%) [rest: polarization]	-0.60 (14.36%) [rest: polarization]	-0.57 (13.90%) [rest: polarization]	-0.61 (14.17%) [rest: polarization]	-0.63 (15.40%) [rest: polarization]

a: The value in parentheses gives the percentage contribution to the total attractive interactions ΔE_{elstat} + ΔE_{orb} + ΔE_{dis}; b: Values in parentheses give the percentage of each attractive term with respect to the △Eorb term.

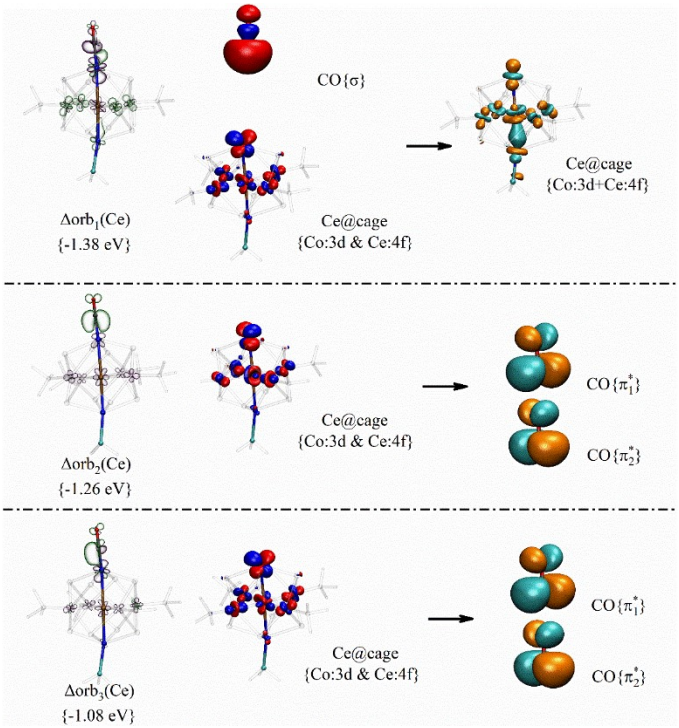

Figure S12. Plots of EDA–NOCV deformation densities Δρ (isovalue = 0.005) of the pairwise orbital interactions and the associated fragment molecular orbitals (isovalue = 0.05) for the different forms of interacting fragments in the Ce@cage-CO.

Energy values for each interaction are enclosed in brackets (eV). The charge flow direction is depicted from purple to green. The labels π* and σ represent π-antibonding and σ-bonding molecular orbitals, respectively.

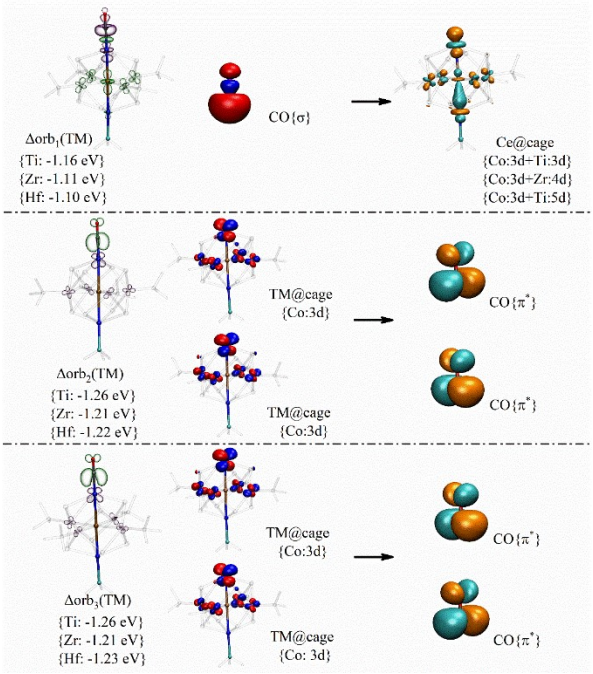

Figure S13. Plots of EDA-NOCV deformation densities Δρ (isovalue = 0.005) of the pairwise orbital interactions and the associated fragment molecular orbitals (isovalue = 0.05) for the different forms of interacting fragments in the Ti/Zr/Hf@cage-CO. Energy values for each interaction are enclosed in brackets (eV). The charge flow direction is depicted from purple to green. The labels π* and σ represent π-antibonding and σ-bonding molecular orbitals, respectively.

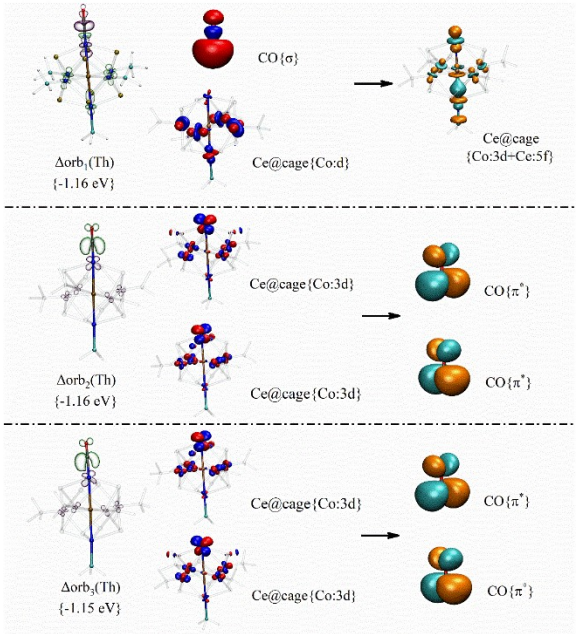

Figure S14. Plots of EDA–NOCV deformation densities Δρ (isovalue = 0.005) of the pairwise orbital interactions and the associated fragment molecular orbitals (isovalue = 0.05) for the different forms of interacting fragments in the Th@cage-CO.

Energy values for each interaction are enclosed in brackets (eV). The charge flow direction is depicted from purple to green. The labels π* and σ represent π-antibonding and σ-bonding molecular orbitals, respectively.

Part IX. Cartesian coordinates (Å) of the optimized PBE-D3/ZORA geometries for the intermediates in CO_2 reduction reaction with cage and M@cage-Ligands (M=Ti, Zr, Hf, Ce and Th) catalyst.

Table S8. Cartesian coordinates of cage.

	cage-singlet				cage-triplet		
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.624729	-1.770314	1.870531	**Te**	-1.731700	-1.724449	1.848569
Te	1.567521	1.934271	-1.841589	**Te**	1.727697	1.720725	-1.948911
Te	-1.819570	-1.888254	-1.648398	**Te**	-1.865243	-1.800616	-1.743867
Te	1.881022	1.733834	1.657222	**Te**	1.834673	1.804716	1.664035
Te	-1.636450	1.729462	1.881251	**Te**	-1.722075	1.845828	1.724089
Te	1.584824	-1.885298	-1.858238	**Te**	1.702173	-1.811622	-1.834913
Te	1.881767	-1.764130	1.591989	**Te**	1.796403	-1.744502	1.708086
Te	-1.818323	1.904980	-1.581372	**Te**	-1.837527	1.761729	-1.800618
Co	-2.241974	-0.023306	0.012851	**Co**	-2.252575	0.008777	0.000413
Co	2.228250	0.023575	-0.308089	**Co**	2.229328	0.004750	-0.134472
Co	-0.005394	-2.451514	0.039443	**Co**	-0.039151	-2.231893	-0.026198
Co	0.011465	2.455886	0.095746	**Co**	0.028157	2.239677	-0.131731
Co	0.102345	-0.011390	1.422628	**Co**	0.034256	0.047258	1.589747
Co	-0.134004	0.015316	-2.032916	**Co**	-0.091307	-0.042741	-2.259342
P	-0.119953	0.032577	-4.163003	**P**	-0.223701	0.012757	-4.370146
P	-0.081936	-4.576268	0.118903	**P**	-0.039100	-4.341544	-0.115872
P	0.069766	4.578760	0.244756	**P**	0.144943	4.351393	-0.047087
P	-4.362860	-0.023771	-0.080018	**P**	-4.357200	-0.096599	0.188777
P	4.322871	0.045320	-0.669582	**P**	4.341507	0.104598	-0.154872
H	1.272623	5.296183	-0.048103	**H**	1.339558	5.029941	-0.439264
H	-0.790416	5.395152	-0.557714	**H**	-0.760714	5.160315	-0.801661
H	-0.201381	5.244056	1.482291	**H**	-0.026557	5.026739	1.199048
H	-5.117411	1.033662	0.516045	**H**	-4.992451	0.276835	1.411087
H	-5.028256	-0.000669	-1.345330	**H**	-5.201759	0.663072	-0.678135
H	-5.119717	-1.099317	0.479120	**H**	-5.033509	-1.343809	0.026566
H	5.160028	-0.987122	-0.143968	**H**	5.103177	-0.379104	0.952556
H	4.824604	-0.004731	-2.007341	**H**	5.088430	-0.562128	-1.175270
H	5.128848	1.142732	-0.236450	**H**	5.000014	1.367461	-0.268040
H	0.550988	-5.314112	1.169680	**H**	1.047258	-5.089706	0.433271
H	-1.339228	-5.255248	0.197993	**H**	-1.089026	-5.096123	0.492474
H	0.443839	-5.362527	-0.956308	**H**	-0.071767	-5.004290	-1.381219
H	1.126453	0.069859	-4.858833	**H**	0.664239	-0.763276	-5.178506
H	-0.693847	-1.044258	-4.905874	**H**	-1.429653	-0.375370	-5.030584
H	-0.749506	1.091108	-4.887404	**H**	-0.044542	1.245705	-5.068088

Table S9. Cartesian coordinates of cage-CO_2.

cage-CO_2-singlet				cage-CO_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.687114	-1.715752	1.835174	**Te**	-1.797172	-1.752590	1.837854
Te	1.581295	1.844355	-1.832561	**Te**	1.743787	1.722616	-1.866132
Te	-1.852056	-1.902025	-1.578080	**Te**	-1.897748	-1.765452	-1.770190
Te	1.820267	1.790409	1.578506	**Te**	1.738251	1.807753	1.691601
Te	-1.692417	1.801462	1.836773	**Te**	-1.772910	1.832776	1.744077
Te	1.606398	-1.968058	-1.821488	**Te**	1.690680	-1.817455	-1.808948
Te	1.810367	-1.725556	1.717953	**Te**	1.706692	-1.786654	1.746881
Te	-1.789518	1.850930	-1.747690	**Te**	-1.887510	1.727199	-1.800957
Co	-2.270332	0.064023	-0.019015	**Co**	-2.313684	-0.002301	0.018240
Co	2.207310	-0.064304	-0.258401	**Co**	2.190241	-0.026153	-0.068722
Co	0.004071	-2.441779	0.083407	**Co**	-0.092461	-2.232572	-0.041048
Co	-0.064288	2.451785	0.011585	**Co**	-0.042286	2.227350	-0.126319
Co	0.047044	0.036031	1.426002	**Co**	-0.032953	0.025707	1.605336
Co	-0.107876	-0.076669	-2.054413	**Co**	-0.077598	-0.025048	-2.228653
P	-0.076781	-0.203442	-4.178277	**P**	-0.011440	0.032847	-4.344586
P	0.090900	-4.559026	0.249908	**P**	-0.140933	-4.341382	-0.161963
P	-0.147251	4.575222	0.115599	**P**	-0.021683	4.330592	-0.331100
P	-4.391102	0.192878	-0.042464	**P**	-4.418315	-0.077040	0.232314
P	4.314226	-0.114900	-0.535538	**P**	4.297301	-0.065347	0.122119
H	0.200144	5.266521	1.317688	**H**	1.092300	5.090914	0.141382
H	0.645712	5.386350	-0.758577	**H**	-0.089539	4.927081	-1.627812
H	-1.376646	5.273449	-0.107416	**H**	-1.041097	5.129762	0.272428
H	-5.161217	-0.510461	0.934360	**H**	-5.031082	0.182428	1.495160
H	-5.049636	1.451576	0.104596	**H**	-5.251249	0.791700	-0.538850
H	-5.134701	-0.244331	-1.183589	**H**	-5.130323	-1.282343	-0.051418
H	5.160643	0.778292	0.192005	**H**	4.906998	-0.020313	1.412054
H	5.058705	-1.303832	-0.263434	**H**	5.048998	-1.173860	-0.377035
H	4.882530	0.131402	-1.824800	**H**	5.096027	0.959221	-0.474236
H	1.314947	-5.260886	0.010478	**H**	0.893001	-5.123492	0.439876
H	-0.219293	-5.214643	1.482357	**H**	-1.243398	-5.074647	0.375914
H	-0.724675	-5.394271	-0.577995	**H**	-0.116808	-4.989011	-1.435109
H	1.147394	0.018341	-4.880840	**H**	1.205261	-0.251248	-5.036059
H	-0.431849	-1.415764	-4.842543	**H**	-0.848404	-0.824698	-5.123956
H	-0.888748	0.664065	-4.971848	**H**	-0.314951	1.240564	-5.043429
C	0.309275	0.197819	5.222343	**C**	0.571723	0.220084	5.402507
O	-0.846112	0.335889	5.360058	**O**	-0.520556	0.549844	5.668029
O	1.467680	0.061901	5.113718	**O**	1.670135	-0.109830	5.164292

Table S10. Cartesian coordinates of cage-COOH.

cage-COOH-doublet				cage-COOH-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.254182	-1.839592	1.976027	**Te**	-1.220839	-1.688653	2.212720
Te	1.718204	1.782111	-1.948455	**Te**	1.703026	1.857359	-1.909488
Te	-1.820204	-1.779656	-1.509668	**Te**	-1.607395	-1.966118	-1.771753
Te	2.042225	1.923542	1.514070	**Te**	2.081930	1.961912	1.508497
Te	-1.280603	1.802246	2.013113	**Te**	-1.745979	1.635877	1.788031
Te	1.754288	-1.724545	-1.981822	**Te**	1.816941	-1.779124	-1.846159
Te	2.105665	-1.881776	1.551787	**Te**	2.054519	-1.530015	1.746817
Te	-1.893419	1.737033	-1.524260	**Te**	-1.933748	1.546949	-1.582359
Co	-1.934702	-0.011607	0.345616	**Co**	-1.996152	-0.329807	0.155183
Co	2.257148	0.009632	-0.148699	**Co**	2.347831	0.082452	-0.208067
Co	0.193858	-2.290884	-0.072114	**Co**	0.154499	-2.120611	0.087436
Co	0.096784	2.301868	-0.076786	**Co**	0.001125	2.122863	-0.004422
Co	0.513500	-0.006204	2.131015	**Co**	0.349348	0.337472	2.210186
Co	-0.101032	0.011145	-2.133123	**Co**	-0.005623	0.009628	-2.147814
P	-0.470798	0.093386	-4.210400	**P**	-0.041016	0.194851	-4.256067
P	0.209354	-4.381170	-0.302164	**P**	0.063661	-4.363761	0.276812
P	-0.039748	4.389043	-0.273965	**P**	-0.123093	4.243022	0.151205
P	-3.963970	0.015655	0.932832	**P**	-4.047898	-0.882574	0.357489
P	4.377020	0.015288	-0.050078	**P**	4.443165	-0.068154	-0.433007
H	0.991934	5.223451	0.257597	**H**	0.879769	5.077316	-0.429915
H	-0.101394	4.999499	-1.563935	**H**	-1.254176	4.940329	-0.375391
H	-1.141614	5.097337	0.297350	**H**	-0.129680	4.857436	1.440012
H	-4.324406	-0.086649	2.309951	**H**	-4.823503	-0.376347	1.445910
H	-4.785479	1.143709	0.627217	**H**	-4.980690	-0.571728	-0.679712
H	-4.859633	-0.986770	0.447572	**H**	-4.417673	-2.253189	0.512330
H	5.040669	0.061957	1.211941	**H**	5.306845	0.750679	0.357881
H	5.122985	-1.070885	-0.600800	**H**	5.122734	-1.301953	-0.198431
H	5.111971	1.068159	-0.675263	**H**	5.048192	0.215928	-1.694916
H	-0.707168	-5.192797	0.435628	**H**	0.774081	-5.062982	1.307379
H	-0.034817	-4.972474	-1.579312	**H**	-1.193661	-5.005020	0.519155
H	1.387365	-5.129126	0.005862	**H**	0.455658	-5.231924	-0.795629
H	0.239789	-0.761671	-5.108677	**H**	1.138458	-0.052604	-5.021890
H	-1.777585	-0.175368	-4.719432	**H**	-0.924034	-0.618734	-5.031381
H	-0.258807	1.308206	-4.931893	**H**	-0.378086	1.441407	-4.864727
C	0.864233	0.008996	4.012495	**C**	0.548985	0.681927	4.075944
O	1.943143	0.145736	4.559089	**O**	0.930101	-0.119894	4.906001
O	-0.277734	-0.154075	4.785529	**O**	0.206907	1.970654	4.467277
H	0.052257	-0.122202	5.711101	**H**	0.359792	1.977679	5.437930

Table S11. Cartesian coordinates of cage-CO.

cage-CO-singlet				cage-CO-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.437825	-1.834061	1.826823	**Te**	-1.383151	-2.023007	1.795541
Te	1.754378	1.823725	-1.950229	**Te**	1.785165	2.084424	-1.627949
Te	-1.721292	-1.774786	-1.729956	**Te**	-1.672786	-1.534973	-2.058599
Te	2.046878	1.772749	1.573920	**Te**	1.997647	1.676187	1.842227
Te	-1.501143	1.715865	1.854233	**Te**	-1.551487	1.480905	2.058084
Te	1.764331	-1.699790	-2.029328	**Te**	1.829866	-1.468380	-2.080012
Te	2.091796	-1.774674	1.533208	**Te**	2.023565	-1.914982	1.397221
Te	-1.810657	1.780772	-1.626593	**Te**	-1.786050	1.902976	-1.431907
Co	-2.066413	-0.058170	0.115469	**Co**	-1.906201	-0.153335	0.106260
Co	2.364443	0.022875	-0.252507	**Co**	2.327497	0.099331	-0.130686
Co	0.185522	-2.222272	-0.099061	**Co**	0.082904	-2.147974	-0.300528
Co	0.126213	2.228902	-0.037341	**Co**	0.070296	2.226804	0.260157
Co	0.337181	-0.027593	2.171893	**Co**	0.344367	-0.193765	2.261899
Co	-0.053226	0.064675	-2.285807	**Co**	0.043346	0.357375	-2.245491
P	-0.307466	0.275973	-4.358967	**P**	0.113443	0.602791	-4.334837
P	0.282062	-4.320531	-0.038430	**P**	-0.100988	-4.390351	-0.592269
P	0.191224	4.325328	0.096393	**P**	-0.040872	4.337373	0.416951
P	-4.144441	-0.260998	0.350537	**P**	-3.997340	-0.534294	0.217317
P	4.461744	-0.082993	-0.354332	**P**	4.434147	0.037979	-0.133114
H	1.345556	5.042869	-0.343285	**H**	0.919582	5.065564	1.186465
H	-0.775732	5.125331	-0.587905	**H**	0.039345	5.150287	-0.755605
H	0.070433	4.963351	1.368395	**H**	-1.204364	4.957790	0.968052
H	-4.766836	0.139317	1.572532	**H**	-4.734856	-0.177208	1.387639
H	-5.042990	0.416562	-0.530008	**H**	-4.882418	0.053247	-0.738259
H	-4.760819	-1.546249	0.262129	**H**	-4.486326	-1.870196	0.105967
H	5.251717	0.219685	0.796019	**H**	5.157348	0.121167	1.095702
H	5.107886	-1.313954	-0.682087	**H**	5.121244	-1.099812	-0.654738
H	5.183081	0.735880	-1.277182	**H**	5.184173	1.028200	-0.840093
H	0.264989	-5.002475	1.216044	**H**	0.590222	-5.331164	0.242707
H	-0.724089	-5.111452	-0.674072	**H**	-1.381266	-5.021135	-0.472988
H	1.408053	-5.007843	-0.586600	**H**	0.243595	-5.020031	-1.833721
H	0.602893	-0.355565	-5.262698	**H**	-0.114655	-0.520585	-5.187312
H	-1.510475	-0.172770	-4.986674	**H**	-0.786067	1.499856	-4.990711
H	-0.276067	1.569264	-4.964867	**H**	1.305158	1.059665	-4.976321
C	0.461598	-0.018894	3.884166	**C**	0.556727	-0.350384	3.959711
O	0.545268	-0.013620	5.044599	**O**	0.697135	-0.466675	5.108202

Table S12. Cartesian coordinates of cage-CHO.

cage-CHO-doublet				cage-CHO-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.585539	-1.780621	1.809078	**Te**	-1.785473	-1.866846	1.642893
Te	1.721406	1.832630	-1.966553	**Te**	1.796609	2.023144	-1.866436
Te	-1.723929	-1.836189	-1.671791	**Te**	-1.682382	-1.668082	-1.712779
Te	2.051191	1.665865	1.621221	**Te**	1.947440	1.410923	1.838237
Te	-1.476262	1.605409	1.908875	**Te**	-1.303822	1.457977	2.092672
Te	1.838591	-1.775783	-1.958619	**Te**	1.675146	-1.731244	-1.951323
Te	2.258870	-1.715811	1.495112	**Te**	2.254776	-1.907095	1.324735
Te	-1.729395	1.773503	-1.696194	**Te**	-1.697535	2.028997	-1.608825
Co	-2.114041	-0.013348	0.044769	**Co**	-2.011896	0.164308	0.028191
Co	2.441760	0.059918	-0.321766	**Co**	2.299429	0.122948	-0.317652
Co	0.209631	-2.116822	0.014857	**Co**	0.114920	-2.357568	0.021010
Co	0.133205	2.131732	0.008665	**Co**	0.189291	2.131701	0.114533
Co	0.348190	-0.189266	2.123181	**Co**	0.305402	-0.529788	2.166355
Co	-0.002965	-0.049978	-2.217367	**Co**	0.014150	0.206061	-2.159371
P	-0.212845	-0.207935	-4.315171	**P**	-0.027531	0.310211	-4.292679
P	0.256116	-4.215848	0.328916	**P**	0.076526	-4.605635	0.108445
P	0.101857	4.218557	0.319730	**P**	0.178255	4.247549	0.357577
P	-4.207549	0.201400	0.062693	**P**	-4.109611	0.455683	0.094197
P	4.501005	0.308469	-0.672407	**P**	4.386949	0.359661	-0.587738
H	1.089840	5.050013	-0.293413	**H**	0.179575	5.103853	-0.785076
H	-1.037441	4.985373	-0.075810	**H**	-0.900712	4.890956	1.040623
H	0.220065	4.758448	1.635240	**H**	1.233487	4.908927	1.060235
H	-4.988049	-0.559305	0.987573	**H**	-4.903423	-0.340947	0.977148
H	-4.802828	1.468923	0.340359	**H**	-4.661993	1.719963	0.465748
H	-4.985051	-0.094178	-1.099789	**H**	-4.909895	0.263798	-1.074949
H	5.442007	-0.499519	0.040553	**H**	5.286498	-0.486748	0.130338
H	5.049053	0.099870	-1.975499	**H**	4.980836	0.188914	-1.875705
H	5.133957	1.564335	-0.425090	**H**	5.031090	1.595258	-0.274416
H	0.375881	-4.736507	1.651647	**H**	0.217366	-5.276132	1.366690
H	-0.846399	-5.027734	-0.077835	**H**	-1.067209	-5.363277	-0.308458
H	1.285962	-5.011108	-0.261138	**H**	1.038667	-5.420709	-0.575793
H	0.699361	0.461421	-5.188717	**H**	1.147662	0.021430	-5.053304
H	-0.146100	-1.485023	-4.948739	**H**	-0.918070	-0.509397	-5.054798
H	-1.412511	0.232905	-4.953084	**H**	-0.343836	1.542107	-4.943555
C	0.502386	-0.434460	3.996462	**C**	0.462588	-1.040409	3.963260
O	0.517957	0.431769	4.839251	**O**	0.624561	-0.324492	4.924206
H	0.584319	-1.510025	4.297781	**H**	0.393801	-2.152195	4.092418

Table S13. Cartesian coordinates of cage-OCH_2.

	cage-OCH_2-singlet				cage-OCH_2-triplet		
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.480228	-1.915613	1.835442	**Te**	-1.443736	-1.812190	1.743160
Te	1.813892	1.746980	-1.951221	**Te**	1.871923	1.711794	-1.881444
Te	-1.770377	-1.772490	-1.779634	**Te**	-1.698171	-1.847180	-1.767331
Te	2.104962	1.647040	1.649727	**Te**	1.922097	1.575346	1.672342
Te	-1.407033	1.619601	1.856996	**Te**	-1.450907	1.592381	1.878770
Te	1.750853	-1.782414	-2.002946	**Te**	1.883649	-1.837595	-1.954391
Te	2.052974	-1.925136	1.445711	**Te**	1.945805	-1.828581	1.654521
Te	-1.739246	1.759456	-1.588038	**Te**	-1.702521	1.731703	-1.759501
Co	-2.047903	-0.109169	0.124522	**Co**	-2.035214	-0.055763	0.002420
Co	2.371010	-0.044528	-0.228114	**Co**	2.376418	-0.101122	-0.176585
Co	0.093185	-2.289225	-0.123264	**Co**	0.188082	-2.302488	-0.134093
Co	0.224565	2.149041	-0.006144	**Co**	0.144251	2.114607	-0.065172
Co	0.379886	-0.174713	2.278355	**Co**	0.285634	-0.141249	2.750968
Co	-0.028083	0.015885	-2.286778	**Co**	0.064985	-0.059067	-2.252771
P	-0.207943	0.235111	-4.366752	**P**	-0.153316	0.022616	-4.357616
P	-0.090995	-4.379943	-0.163169	**P**	0.276304	-4.404756	-0.256420
P	0.369175	4.241593	0.132342	**P**	0.034199	4.219815	-0.053213
P	-4.125113	-0.223274	0.414132	**P**	-4.128729	0.106487	0.191124
P	4.468694	0.062689	-0.294719	**P**	4.480337	0.010768	-0.274745
H	1.611551	4.900175	-0.117682	**H**	0.252093	4.961382	-1.255347
H	-0.437176	5.076908	-0.701931	**H**	-1.177276	4.874750	0.327363
H	0.075968	4.897334	1.366724	**H**	0.907643	4.988911	0.776666
H	-4.690509	0.109090	1.682550	**H**	-4.800119	-0.484989	1.305883
H	-5.005445	0.575464	-0.380416	**H**	-4.747903	1.389937	0.288032
H	-4.815707	-1.461398	0.241736	**H**	-4.989763	-0.416563	-0.823068
H	5.246388	-0.325438	0.838554	**H**	5.289773	-0.742556	0.632345
H	5.194865	-0.693582	-1.266918	**H**	5.171569	-0.367638	-1.467445
H	5.121724	1.310932	-0.527892	**H**	5.146754	1.260987	-0.089355
H	0.487537	-5.170996	0.876528	**H**	1.488079	-5.095363	0.057227
H	-1.380038	-4.993447	-0.143518	**H**	-0.587863	-5.215234	0.544433
H	0.435079	-5.129090	-1.260873	**H**	0.024675	-5.068994	-1.496515
H	0.782192	-0.311796	-5.240079	**H**	0.535272	-0.900553	-5.206132
H	-1.347637	-0.289788	-5.050352	**H**	-1.441717	-0.136806	-4.951939
H	-0.246357	1.537212	-4.951856	**H**	0.210234	1.204697	-5.073745
O	0.144966	0.154011	4.179041	**O**	0.055168	0.142535	4.639859
C	1.066671	-0.760833	4.115902	**C**	0.975232	-0.779736	4.585434
H	2.121826	-0.477575	4.281924	**H**	2.030372	-0.504138	4.751532
H	0.805899	-1.807482	4.355716	**H**	0.703654	-1.828918	4.789915

Table S14. Cartesian coordinates of cage-OCH_3.

cage-OCH_3-doublet				cage-OCH_3-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.151776	-2.024034	1.814896	**Te**	-1.289761	-1.862896	1.727506
Te	1.593782	1.829986	-2.057419	**Te**	1.770373	1.884936	-1.949400
Te	-1.712664	-1.911746	-1.688473	**Te**	-1.714118	-1.764756	-1.852770
Te	2.053456	1.766333	1.504839	**Te**	2.011443	1.570536	1.606515
Te	-1.360217	1.540906	1.967017	**Te**	-1.375063	1.486492	1.906033
Te	1.864889	-1.700889	-2.146190	**Te**	1.798829	-1.643159	-2.205115
Te	2.257828	-1.807942	1.331484	**Te**	2.063640	-1.764212	1.427891
Te	-1.863187	1.594961	-1.593465	**Te**	-1.820058	1.814931	-1.590948
Co	-1.937441	-0.213331	0.205445	**Co**	-2.033824	-0.111917	0.040489
Co	2.359145	0.074521	-0.377192	**Co**	2.386795	0.002318	-0.368764
Co	0.322748	-2.348035	-0.234096	**Co**	0.235968	-2.217657	-0.292599
Co	0.072104	2.160453	-0.048159	**Co**	0.144280	2.150566	-0.026697
Co	0.550945	-0.163318	2.344082	**Co**	0.448511	-0.195710	2.778979
Co	-0.079643	-0.072968	-2.336610	**Co**	-0.048032	0.123858	-2.318668
P	-0.314083	-0.191845	-4.422009	**P**	-0.403612	0.338309	-4.394499
P	0.299375	-4.442064	-0.412047	**P**	0.431791	-4.316773	-0.397745
P	-0.077759	4.252042	0.122005	**P**	0.193742	4.261437	0.014893
P	-3.993089	-0.191195	0.646913	**P**	-4.119756	-0.343882	0.239072
P	4.434252	0.383889	-0.519928	**P**	4.480067	-0.095822	-0.599368
H	0.763957	5.106181	-0.654865	**H**	1.400184	4.953555	0.340512
H	-1.308278	4.916276	-0.170176	**H**	-0.116251	5.012549	-1.159377
H	0.158281	4.882090	1.380951	**H**	-0.656578	4.987314	0.905763
H	-4.455478	-0.550471	1.949685	**H**	-4.801481	0.217530	1.363833
H	-4.746074	1.017269	0.531907	**H**	-5.004242	0.158617	-0.764330
H	-4.895110	-1.022594	-0.087632	**H**	-4.696896	-1.646042	0.333042
H	5.291122	0.041100	0.570048	**H**	5.346980	0.582872	0.312858
H	5.187278	-0.273648	-1.541528	**H**	5.156181	-1.352816	-0.557186
H	4.960780	1.693162	-0.739611	**H**	5.094034	0.379470	-1.797982
H	1.266154	-5.230068	0.286297	**H**	-0.054590	-5.145364	0.661728
H	-0.849975	-5.186645	-0.006192	**H**	-0.165682	-5.045583	-1.471425
H	0.460159	-5.069019	-1.686018	**H**	1.724178	-4.920330	-0.490325
H	-0.368639	-1.461438	-5.073613	**H**	0.266415	-0.500752	-5.340081
H	-1.472635	0.365318	-5.045771	**H**	-1.718350	0.163042	-4.924283
H	0.650115	0.400988	-5.293186	**H**	-0.128638	1.575562	-5.054373
O	0.799221	-0.159110	4.119767	**O**	0.612321	-0.288226	4.586106
C	0.983718	-1.348423	4.859722	**C**	0.819873	-1.451704	5.347378
H	0.107067	-2.015354	4.790158	**H**	-0.059712	-2.120899	5.308784
H	1.867657	-1.913959	4.518346	**H**	1.695402	-2.024395	4.990024
H	1.130500	-1.064224	5.916092	**H**	0.995366	-1.174392	6.401498

Table S15. Cartesian coordinates of cage-CH_3OH.

cage-CH_3OH-singlet				cage-CH_3OH-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.222626	-1.673823	2.061385	**Te**	-1.219414	-1.692922	2.078083
Te	1.901900	1.771318	-1.902080	**Te**	1.810731	1.786140	-2.023330
Te	-1.781773	-1.709791	-1.346325	**Te**	-1.661742	-1.815507	-1.491901
Te	2.192292	1.886399	1.501090	**Te**	2.201401	1.931266	1.510005
Te	-1.296387	1.853982	2.001866	**Te**	-1.313893	1.867508	1.929121
Te	1.950040	-1.677215	-1.878737	**Te**	1.887236	-1.759556	-1.881086
Te	2.255218	-1.609020	1.661275	**Te**	2.276263	-1.631853	1.630853
Te	-1.884457	1.662852	-1.476087	**Te**	-1.746938	1.713931	-1.609739
Co	-2.169909	0.046220	0.453353	**Co**	-1.953603	0.000667	0.269038
Co	2.697754	0.064129	-0.191537	**Co**	2.515858	0.095341	-0.260408
Co	0.326730	-2.171255	-0.000434	**Co**	0.310218	-2.193811	0.067550
Co	0.163587	2.238650	-0.111146	**Co**	0.220582	2.289265	-0.101927
Co	0.436028	0.121126	1.521102	**Co**	0.467586	0.117137	1.624045
Co	0.029184	0.032960	-1.953223	**Co**	0.032883	-0.033143	-2.166077
P	-0.202787	0.112077	-4.072570	**P**	-0.237337	-0.012666	-4.264497
P	0.374378	-4.289531	-0.137075	**P**	0.230568	-4.307455	0.072319
P	0.002387	4.359300	-0.266511	**P**	0.154675	4.406378	-0.050497
P	-4.253296	0.051572	0.896957	**P**	-4.024448	-0.078361	0.704159
P	4.816427	-0.012279	-0.337978	**P**	4.627570	0.147991	-0.352006
H	0.261815	5.020749	-1.507924	**H**	1.036972	5.182987	-0.863517
H	-1.234655	5.017002	0.010311	**H**	-1.044201	5.102584	-0.394572
H	0.822925	5.201688	0.547295	**H**	0.404377	5.095849	1.173713
H	-4.712996	-0.021482	2.248996	**H**	-4.480988	0.051155	2.050022
H	-5.082715	1.152163	0.513246	**H**	-4.921280	0.875743	0.131291
H	-5.114302	-0.972836	0.387343	**H**	-4.788666	-1.241227	0.379577
H	5.647138	0.428359	0.740293	**H**	5.395429	0.191650	0.850349
H	5.488268	-1.257148	-0.548250	**H**	5.353293	-0.913697	-0.975192
H	5.505142	0.707666	-1.366918	**H**	5.297847	1.220442	-1.017171
H	1.572311	-5.010844	0.157395	**H**	1.065774	-5.059897	0.954621
H	-0.501770	-5.087312	0.662776	**H**	-0.990374	-4.980929	0.381523
H	0.098147	-4.938885	-1.380365	**H**	0.530396	-5.045991	-1.114117
H	0.847962	-0.302085	-4.945641	**H**	0.648811	-0.734789	-5.122038
H	-1.250205	-0.617291	-4.713071	**H**	-1.453518	-0.492146	-4.840653
H	-0.456746	1.368206	-4.701893	**H**	-0.191182	1.221013	-4.982649
C	1.098319	-0.929741	5.486364	**C**	1.003145	-0.866635	5.527525
H	2.113633	-1.186733	5.134093	**H**	1.842016	-1.412982	5.058284
H	1.095445	-0.955855	6.583767	**H**	1.144576	-0.880855	6.616477
H	0.400484	-1.703151	5.117508	**H**	0.068225	-1.405920	5.288438
O	0.705747	0.381430	5.100967	**O**	0.957275	0.497755	5.129234
H	0.650126	0.399878	4.121393	**H**	0.832640	0.516991	4.156161

Table S16. Cartesian coordinates of Ti@cage.

Ti@cage-singlet				Ti@cage-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.716161	-1.709045	1.835918	**Te**	-1.616307	-1.786405	1.795206
Te	1.718208	1.659749	-1.803185	**Te**	1.663797	1.710383	-1.859181
Te	-1.722885	-1.784571	-1.663220	**Te**	-1.813576	-1.717980	-1.702136
Te	1.787717	1.843330	1.588538	**Te**	1.773394	1.804071	1.649041
Te	-1.779423	1.828282	1.636788	**Te**	-1.630550	1.784492	1.785856
Te	1.663419	-1.752443	-1.722824	**Te**	1.674791	-1.706494	-1.848639
Te	1.769162	-1.683216	1.784098	**Te**	1.776678	-1.776793	1.655166
Te	-1.817450	1.647274	-1.731710	**Te**	-1.816198	1.700950	-1.708468
Co	-2.579490	-0.055916	0.025803	**Co**	-2.485322	-0.008131	0.122958
Co	2.553805	-0.023297	-0.051020	**Co**	2.490891	0.010494	-0.083615
Co	0.009024	-2.545631	0.097623	**Co**	0.006729	-2.544704	-0.062140
Co	-0.017824	2.562812	-0.167915	**Co**	0.000389	2.553328	-0.069611
Co	0.020530	0.129155	2.350861	**Co**	0.109690	0.011271	2.481511
Co	-0.059485	-0.041319	-2.578162	**Co**	-0.112346	-0.011622	-2.613124
P	-0.149904	0.456601	-4.636632	**P**	-0.228340	0.034349	-4.799254
P	0.035730	-4.697127	-0.024603	**P**	0.032261	-4.693029	-0.288896
P	0.006898	4.726038	-0.131361	**P**	-0.001674	4.715612	-0.172683
P	-4.727612	-0.262890	0.094622	**P**	-4.617716	-0.019651	0.469145
P	4.704662	-0.200454	-0.052658	**P**	4.643386	0.008750	0.089363
H	1.190311	5.464545	-0.450079	**H**	1.197656	5.442664	-0.454692
H	-0.865322	5.514855	-0.948219	**H**	-0.815617	5.429661	-1.108151
H	-0.269436	5.434431	1.080085	**H**	-0.374308	5.504089	0.961822
H	-5.488002	0.297813	1.169018	**H**	-5.154487	-0.045572	1.794278
H	-5.567860	0.247457	-0.946381	**H**	-5.449603	1.047053	0.003355
H	-5.349253	-1.550313	0.146863	**H**	-5.444625	-1.072329	-0.035644
H	5.348075	-1.476409	-0.120654	**H**	5.283692	-0.038221	1.367920
H	5.512859	0.411015	-1.063589	**H**	5.434488	-1.028566	-0.498179
H	5.478795	0.281746	1.049293	**H**	5.428639	1.091720	-0.419063
H	1.120461	-5.456153	0.518632	**H**	1.137632	-5.472861	0.176375
H	-0.998144	-5.480743	0.579225	**H**	-0.976416	-5.514704	0.307336
H	0.007558	-5.381408	-1.281178	**H**	-0.035256	-5.308168	-1.578266
H	0.864731	-0.016153	-5.527785	**H**	0.548382	-0.849818	-5.615739
H	-1.262823	0.043855	-5.435257	**H**	-1.460047	-0.204871	-5.488941
H	-0.132263	1.811733	-5.094343	**H**	0.103404	1.213744	-5.540683
Ti	-0.014597	0.026444	0.134696	**Ti**	0.000502	0.007333	-0.050942

Table S17. Cartesian coordinates of Ti@cage-CO_2.

Ti@cage-CO_2-singlet				Ti@cage-CO_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.906773	-1.755377	1.716007	**Te**	-1.362040	-1.826455	1.892814
Te	1.715435	1.661650	-1.645983	**Te**	1.707738	1.705603	-1.906448
Te	-1.762533	-1.746517	-1.726742	**Te**	-1.775405	-1.700837	-1.571462
Te	1.618764	1.760493	1.784496	**Te**	2.018733	1.754197	1.593703
Te	-1.904141	1.791981	1.645762	**Te**	-1.355609	1.763779	1.931522
Te	1.654544	-1.734173	-1.631679	**Te**	1.703582	-1.693037	-1.937630
Te	1.577543	-1.761319	1.855296	**Te**	2.012460	-1.821069	1.555024
Te	-1.782552	1.711880	-1.728062	**Te**	-1.771088	1.715649	-1.537980
Co	-2.668340	-0.020293	-0.064236	**Co**	-2.326743	-0.012808	0.316629
Co	2.463066	-0.048554	0.131744	**Co**	2.629430	-0.013892	-0.199094
Co	-0.096748	-2.578429	0.056489	**Co**	0.146503	-2.558326	-0.069282
Co	-0.063624	2.559102	-0.041279	**Co**	0.153838	2.534577	-0.015411
Co	-0.198453	0.036912	2.440285	**Co**	0.413671	-0.041206	2.523230
Co	-0.035493	-0.005132	-2.519806	**Co**	-0.126015	0.016350	-2.565796
P	-0.182493	0.261580	-4.619662	**P**	-0.358452	0.051493	-4.746330
P	-0.019339	-4.731422	-0.077862	**P**	0.172118	-4.698908	-0.369291
P	0.044859	4.716048	-0.110366	**P**	0.195955	4.687515	-0.225386
P	-4.826925	-0.099837	-0.056822	**P**	-4.429465	-0.004974	0.816542
P	4.618252	-0.170733	0.164831	**P**	4.787058	-0.021029	-0.155681
H	1.273731	5.403545	0.142134	**H**	1.367954	5.440924	0.099189
H	-0.277154	5.451767	-1.295541	**H**	-0.024662	5.319211	-1.489719
H	-0.745154	5.524331	0.767237	**H**	-0.709833	5.522301	0.502945
H	-5.575428	0.366852	1.069542	**H**	-4.870303	-0.023314	2.176872
H	-5.613576	0.586733	-1.036261	**H**	-5.280847	1.069503	0.407487
H	-5.523400	-1.343805	-0.175156	**H**	-5.298493	-1.051458	0.373050
H	5.374803	0.427562	1.221148	**H**	5.506333	-0.036342	1.080544
H	5.288295	-1.433676	0.215921	**H**	5.537397	-1.076479	-0.764172
H	5.420180	0.362018	-0.894967	**H**	5.542758	1.043860	-0.740753
H	1.140521	-5.456563	0.341504	**H**	1.325604	-5.479584	-0.042152
H	-0.956363	-5.550170	0.628790	**H**	-0.765346	-5.554367	0.291935
H	-0.158832	-5.415059	-1.327874	**H**	-0.014507	-5.269905	-1.667379
H	0.702679	-0.442786	-5.495795	**H**	0.518901	-0.680832	-5.609949
H	-1.383245	-0.061403	-5.327104	**H**	-1.561902	-0.392477	-5.383314
H	-0.001132	1.544941	-5.224848	**H**	-0.268754	1.274400	-5.486695
Ti	-0.110337	-0.004348	0.179726	**Ti**	0.144824	-0.009454	-0.016345
C	0.941645	0.079487	5.231766	**C**	-1.230273	0.038920	5.339066
O	-0.181351	0.083747	4.879854	**O**	-2.383034	0.171320	5.481322
O	2.041188	0.076516	5.624708	**O**	-0.069968	-0.095303	5.215591

Table S18. Cartesian coordinates of Ti@cage-COOH.

Ti@cage-COOH-doublet				Ti@cage-COOH-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.059229	-1.794819	1.987206	**Te**	-1.236102	-1.879643	2.222965
Te	1.651455	1.740677	-2.000731	**Te**	1.689783	1.807073	-1.833426
Te	-1.732452	-1.738913	-1.386807	**Te**	-1.573194	-1.959264	-1.773931
Te	2.196779	1.784186	1.459729	**Te**	2.035154	1.787440	1.564178
Te	-1.130573	1.754286	2.010711	**Te**	-1.541840	1.412801	1.862629
Te	1.699161	-1.641090	-2.028244	**Te**	1.779178	-1.771569	-1.811019
Te	2.253153	-1.712044	1.448602	**Te**	2.094901	-1.693100	1.610930
Te	-1.797913	1.719368	-1.356808	**Te**	-1.839599	1.423270	-1.476008
Co	-2.209406	-0.034586	0.519616	**Co**	-2.185100	-0.587529	0.261673
Co	2.736925	0.050675	-0.374834	**Co**	2.704929	0.028093	-0.212437
Co	0.323740	-2.532190	-0.038440	**Co**	0.028450	-2.484795	0.116413
Co	0.235854	2.557118	-0.005642	**Co**	-0.003833	2.414749	0.077091
Co	0.661081	0.011114	2.625335	**Co**	0.460656	0.051058	2.666026
Co	-0.213567	0.033421	-2.495616	**Co**	-0.008980	-0.062228	-2.513475
P	-0.737369	0.090460	-4.615759	**P**	-0.088891	0.184640	-4.688452
P	0.430398	-4.686626	-0.207034	**P**	-0.114874	-4.675847	0.240550
P	0.292098	4.712990	-0.148937	**P**	-0.213565	4.611594	0.271095
P	-4.305025	-0.087553	1.083952	**P**	-4.328630	-1.011306	0.403435
P	4.892949	0.067404	-0.424913	**P**	4.905373	0.012741	-0.414860
H	1.521408	5.434522	-0.026918	**H**	0.781989	5.503593	-0.241806
H	-0.150047	5.397071	-1.324745	**H**	-1.323080	5.325246	-0.287064
H	-0.438838	5.530972	0.769655	**H**	-0.296171	5.237041	1.555717
H	-4.702632	-0.102870	2.457618	**H**	-5.108874	-0.501549	1.488639
H	-5.205015	0.953067	0.691180	**H**	-5.230316	-0.593282	-0.624830
H	-5.156368	-1.164820	0.681628	**H**	-4.831846	-2.348576	0.490109
H	5.653186	0.109942	0.785434	**H**	5.713584	0.999591	0.235520
H	5.631390	-1.006277	-1.015346	**H**	5.695960	-1.101221	0.013583
H	5.615045	1.113733	-1.081125	**H**	5.549460	0.140888	-1.686920
H	-0.325881	-5.530928	0.666531	**H**	0.490329	-5.390345	1.321245
H	0.050602	-5.361156	-1.409908	**H**	-1.383214	-5.332532	0.336526
H	1.665013	-5.390296	-0.041257	**H**	0.399830	-5.520299	-0.793143
H	-0.189423	-0.845495	-5.550773	**H**	1.070681	-0.044205	-5.495102
H	-2.089291	-0.058878	-5.061439	**H**	-0.972256	-0.586728	-5.512047
H	-0.465143	1.245137	-5.417050	**H**	-0.416023	1.440490	-5.291547
Ti	0.239419	0.008600	-0.013003	**Ti**	0.270194	-0.003403	-0.011128
C	0.179539	0.008187	4.444263	**C**	0.559600	0.950059	4.315501
O	1.190158	0.152927	5.118590	**O**	0.887828	0.152479	5.182917
O	-1.057260	-0.129306	5.002507	**O**	0.327878	2.267483	4.584068
H	-0.919405	-0.078861	5.974713	**H**	0.485146	2.376240	5.548325

Table S19. Cartesian coordinates of Ti@cage-CO.

Ti@cage-CO-singlet				Ti@cage-CO-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.370924	-1.795821	1.803489	**Te**	-1.155747	-1.660775	2.216143
Te	1.700276	1.784304	-1.878066	**Te**	1.710876	1.818177	-1.986293
Te	-1.695553	-1.723810	-1.642629	**Te**	-1.715146	-1.764126	-1.724484
Te	2.013379	1.702650	1.563646	**Te**	2.169493	1.897897	1.343552
Te	-1.428576	1.653770	1.871710	**Te**	-1.338706	1.680028	1.856089
Te	1.733570	-1.662251	-1.971872	**Te**	1.660567	-1.749773	-1.898158
Te	2.050698	-1.736932	1.494715	**Te**	2.118672	-1.655908	1.459632
Te	-1.752492	1.735788	-1.545714	**Te**	-1.824216	1.602250	-1.504005
Co	-2.378889	-0.060146	0.204672	**Co**	-2.177103	-0.341748	0.319296
Co	2.693607	0.020604	-0.264717	**Co**	2.723561	0.030441	-0.370214
Co	0.200557	-2.549276	-0.089958	**Co**	-0.045112	-2.395621	0.070326
Co	0.131491	2.540327	0.029075	**Co**	0.093895	2.561358	-0.069706
Co	0.390278	-0.054114	2.548141	**Co**	0.638705	0.168585	2.526524
Co	-0.088815	0.066005	-2.583527	**Co**	-0.081478	0.031643	-2.570420
P	-0.320678	0.184864	-4.737158	**P**	-0.155145	0.182633	-4.735959
P	0.275821	-4.707547	-0.064691	**P**	-0.292402	-4.574224	0.189399
P	0.161683	4.699323	0.142071	**P**	-0.063564	4.761225	-0.049725
P	-4.526744	-0.173858	0.423553	**P**	-4.318918	-0.700545	0.637811
P	4.852919	-0.025143	-0.361309	**P**	4.914150	-0.017377	-0.611373
H	1.315251	5.445996	-0.254357	**H**	0.555644	5.573547	-1.053302
H	-0.776479	5.500250	-0.582436	**H**	-1.331512	5.423460	-0.114809
H	-0.015982	5.374463	1.390533	**H**	0.423268	5.531326	1.054501
H	-5.172506	0.208058	1.641409	**H**	-4.986024	-0.213211	1.805713
H	-5.402870	0.562587	-0.434650	**H**	-5.295916	-0.222346	-0.290861
H	-5.217284	-1.419257	0.287451	**H**	-4.851538	-2.026784	0.723611
H	5.643063	0.199287	0.809628	**H**	5.790207	0.143347	0.509418
H	5.552013	-1.202732	-0.774703	**H**	5.591727	-1.164615	-1.135106
H	5.588030	0.873315	-1.197998	**H**	5.599049	0.926395	-1.442407
H	0.317442	-5.426053	1.171729	**H**	0.376362	-5.338581	1.196566
H	-0.761600	-5.500409	-0.649457	**H**	-1.575287	-5.175746	0.393283
H	1.354526	-5.422905	-0.674754	**H**	0.082471	-5.421773	-0.900298
H	0.671838	-0.340871	-5.623262	**H**	1.006870	-0.055242	-5.535256
H	-1.431654	-0.418298	-5.407522	**H**	-1.027152	-0.641544	-5.517565
H	-0.434663	1.447325	-5.400922	**H**	-0.512907	1.407185	-5.383111
Ti	0.156252	-0.003509	-0.069361	**Ti**	0.266077	0.097257	-0.085891
C	0.504478	-0.070546	4.302561	**C**	0.967859	0.380135	4.239116
O	0.572565	-0.084512	5.463751	**O**	1.162444	0.523977	5.377034

Table S20. Cartesian coordinates of Ti@cage-CHO.

Ti@cage-CHO-doublet				Ti@cage-CHO-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.436032	-1.602954	1.908439	**Te**	-1.492344	-1.665915	1.951976
Te	1.642849	1.790138	-1.948649	**Te**	1.594329	1.766574	-2.180464
Te	-1.695877	-1.757047	-1.516730	**Te**	-1.885063	-1.727737	-1.462128
Te	2.026231	1.836151	1.563415	**Te**	2.113700	1.763250	1.795922
Te	-1.456701	1.785308	1.874576	**Te**	-1.283373	1.819249	1.922158
Te	1.753931	-1.699564	-1.834680	**Te**	1.650392	-1.638232	-1.856100
Te	2.112662	-1.546373	1.590397	**Te**	2.089736	-1.592546	1.465521
Te	-1.711064	1.743326	-1.641501	**Te**	-1.687559	1.834941	-1.498215
Co	-2.376094	0.063950	0.195898	**Co**	-2.390272	0.132364	0.308341
Co	2.675061	0.139375	-0.260385	**Co**	2.504345	0.356973	-0.284305
Co	0.207711	-2.449628	0.113099	**Co**	0.122969	-2.472294	0.063651
Co	0.119342	2.568787	-0.013235	**Co**	0.469567	2.419553	-0.006506
Co	0.392309	0.067314	2.615510	**Co**	0.427899	-0.038995	2.617257
Co	-0.080007	-0.036442	-2.550938	**Co**	-0.223771	-0.013448	-2.529733
P	-0.264205	-0.243384	-4.721758	**P**	-0.569276	-0.330496	-4.671437
P	0.297190	-4.606349	0.304409	**P**	0.184781	-4.684105	0.147125
P	0.131861	4.712354	0.198454	**P**	0.773420	4.595355	0.018965
P	-4.535724	0.163722	0.201421	**P**	-4.586581	0.291894	0.484006
P	4.804243	0.299955	-0.589275	**P**	4.650950	0.639192	-0.584253
H	1.179051	5.506586	-0.366246	**H**	2.078406	5.166600	-0.120859
H	-0.941558	5.513213	-0.304566	**H**	0.144096	5.451763	-0.938539
H	0.171804	5.323581	1.490489	**H**	0.407134	5.369655	1.163878
H	-5.309686	-0.702667	1.037310	**H**	-5.351446	-0.739228	1.117479
H	-5.228185	1.361609	0.565100	**H**	-5.220192	1.368569	1.183362
H	-5.294959	-0.076872	-0.986946	**H**	-5.428577	0.381324	-0.669792
H	5.727727	-0.424960	0.228669	**H**	5.596423	0.109226	0.349000
H	5.400996	-0.072285	-1.834924	**H**	5.309551	0.137631	-1.750507
H	5.483033	1.554754	-0.483366	**H**	5.235356	1.943937	-0.647425
H	0.301453	-5.243659	1.585636	**H**	0.227188	-5.391179	1.392097
H	-0.713515	-5.447601	-0.259562	**H**	-0.864798	-5.483417	-0.410192
H	1.401565	-5.350882	-0.217823	**H**	1.245582	-5.437131	-0.452833
H	0.696995	0.333863	-5.612589	**H**	0.273114	0.248696	-5.675889
H	-0.269566	-1.526998	-5.355300	**H**	-0.562669	-1.643517	-5.239948
H	-1.406299	0.252539	-5.429232	**H**	-1.797661	0.068598	-5.289043
Ti	0.149394	0.046548	-0.021279	**Ti**	0.014812	-0.045800	0.010264
C	0.533601	-0.807909	4.253762	**C**	0.592446	-1.017171	4.193626
O	0.557438	0.060597	5.106575	**O**	0.620899	-0.194402	5.090784
H	0.594125	-1.890468	4.501527	**H**	0.657585	-2.112105	4.378456

Table S21. Cartesian coordinates of Ti@cage-OCH_2.

Ti@cage-OCH_2-singlet				Ti@cage-OCH_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.439150	-1.862629	1.769399	**Te**	-1.401572	-1.837556	1.770947
Te	1.757770	1.712016	-1.829791	**Te**	1.738424	1.739807	-1.865075
Te	-1.726513	-1.709922	-1.677898	**Te**	-1.682560	-1.722352	-1.723068
Te	2.036367	1.582640	1.633222	**Te**	2.006019	1.618019	1.610147
Te	-1.393291	1.596237	1.895378	**Te**	-1.435316	1.600749	1.892565
Te	1.718968	-1.721781	-1.919431	**Te**	1.751138	-1.707759	-1.976123
Te	1.981973	-1.857216	1.486076	**Te**	2.013435	-1.817051	1.515577
Te	-1.678409	1.727685	-1.500384	**Te**	-1.697909	1.718123	-1.598817
Co	-2.388609	-0.075139	0.201061	**Co**	-2.338993	-0.072349	0.163337
Co	2.709498	-0.051030	-0.216068	**Co**	2.670783	-0.039852	-0.221997
Co	0.109519	-2.625324	-0.122757	**Co**	0.166214	-2.565615	-0.112251
Co	0.214663	2.487016	0.082484	**Co**	0.152053	2.460111	0.054957
Co	0.368988	-0.178901	2.606282	**Co**	0.382117	-0.146683	2.739832
Co	-0.054348	0.037679	-2.564254	**Co**	-0.035639	0.039983	-2.612382
P	-0.248879	0.173832	-4.702675	**P**	-0.213348	0.125892	-4.815733
P	0.048183	-4.790639	-0.234498	**P**	0.117004	-4.725697	-0.209530
P	0.301717	4.648049	0.188856	**P**	0.124808	4.616511	0.226566
P	-4.540877	-0.081114	0.440606	**P**	-4.486532	-0.134908	0.397708
P	4.871114	-0.003729	-0.375218	**P**	4.831386	-0.030088	-0.351968
H	1.504670	5.358534	-0.118507	**H**	1.106611	5.432512	-0.419551
H	-0.549550	5.475861	-0.609369	**H**	-1.001141	5.384589	-0.208254
H	0.048263	5.335315	1.417220	**H**	0.239169	5.247719	1.505680
H	-5.137830	0.120481	1.724567	**H**	-5.083041	-0.145266	1.697904
H	-5.374818	0.857202	-0.246051	**H**	-5.323988	0.896639	-0.131949
H	-5.326091	-1.229009	0.104678	**H**	-5.261316	-1.220330	-0.119229
H	5.706685	-0.461754	0.692243	**H**	5.638722	-0.152044	0.822861
H	5.564256	-0.718320	-1.402917	**H**	5.542930	-1.013663	-1.108061
H	5.572439	1.226951	-0.573966	**H**	5.539307	1.091073	-0.887584
H	0.804824	-5.608212	0.663526	**H**	0.763253	-5.529549	0.783120
H	-1.177992	-5.507759	-0.065498	**H**	-1.123464	-5.438013	-0.175899
H	0.446256	-5.489150	-1.418132	**H**	0.650489	-5.436321	-1.330815
H	0.677226	-0.478794	-5.576754	**H**	0.639340	-0.634455	-5.680657
H	-1.422639	-0.288046	-5.377752	**H**	-1.425011	-0.241320	-5.486381
H	-0.196835	1.438324	-5.370075	**H**	-0.046841	1.355246	-5.532450
Ti	0.162915	-0.073736	0.017820	**Ti**	0.165260	-0.049498	-0.052136
O	0.146242	0.125047	4.533596	**O**	0.192143	0.183430	4.618969
C	1.055926	-0.790756	4.453464	**C**	1.128384	-0.724186	4.566237
H	2.119247	-0.522150	4.593877	**H**	2.180381	-0.423364	4.698878
H	0.791252	-1.846058	4.650204	**H**	0.880424	-1.770777	4.807192

Table S22. Cartesian coordinates of Ti@cage-OCH_3.

Ti@cage-OCH_3-doublet				Ti@cage-OCH_3-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.137129	-1.875126	1.809892	**Te**	-1.325271	-1.840241	1.740662
Te	1.537023	1.822295	-2.027072	**Te**	1.698066	1.792737	-1.965865
Te	-1.663168	-1.837190	-1.580477	**Te**	-1.658552	-1.739306	-1.730848
Te	2.011439	1.803983	1.447832	**Te**	2.024994	1.684089	1.525703
Te	-1.304118	1.582726	1.926873	**Te**	-1.389592	1.605867	1.847380
Te	1.812204	-1.619060	-2.060196	**Te**	1.751723	-1.645487	-2.075148
Te	2.249487	-1.668577	1.314863	**Te**	2.108424	-1.744664	1.410570
Te	-1.825883	1.599058	-1.554778	**Te**	-1.751004	1.714058	-1.615027
Co	-2.278196	-0.156131	0.292267	**Co**	-2.317429	-0.090495	0.157476
Co	2.702490	0.165412	-0.415074	**Co**	2.686274	0.038532	-0.333775
Co	0.353828	-2.576471	-0.138768	**Co**	0.248728	-2.537661	-0.161358
Co	0.046126	2.524594	-0.040755	**Co**	0.144156	2.490381	-0.014021
Co	0.619524	-0.088339	2.649453	**Co**	0.451868	-0.107556	2.721397
Co	-0.141676	-0.049957	-2.621618	**Co**	-0.078984	0.068155	-2.658385
P	-0.401935	-0.232565	-4.776031	**P**	-0.311922	0.216980	-4.850616
P	0.392755	-4.739074	-0.301478	**P**	0.357352	-4.702067	-0.108812
P	-0.103645	4.690091	0.104577	**P**	0.175328	4.652599	0.052349
P	-4.407376	-0.173449	0.683365	**P**	-4.464095	-0.124990	0.432143
P	4.845132	0.428491	-0.571631	**P**	4.844321	0.078354	-0.482004
H	0.746959	5.552898	-0.657133	**H**	1.355254	5.382590	-0.295384
H	-1.314991	5.377555	-0.224172	**H**	-0.712491	5.443461	-0.743703
H	0.099059	5.368358	1.348086	**H**	-0.067425	5.358023	1.272779
H	-4.927958	-0.562446	1.957878	**H**	-5.037952	-0.162239	1.741846
H	-5.195654	1.014787	0.572849	**H**	-5.291383	0.936846	-0.051342
H	-5.292709	-0.995814	-0.082691	**H**	-5.268514	-1.180356	-0.101727
H	5.700178	0.234000	0.558467	**H**	5.661124	0.186062	0.687381
H	5.625987	-0.361700	-1.473261	**H**	5.568792	-1.014104	-1.054903
H	5.414808	1.681798	-0.959420	**H**	5.525406	1.096228	-1.220953
H	1.269100	-5.536200	0.501886	**H**	0.432893	-5.407589	1.133723
H	-0.776210	-5.520619	-0.037461	**H**	-0.680683	-5.515080	-0.664086
H	0.711450	-5.393942	-1.533431	**H**	1.433029	-5.409369	-0.732031
H	-0.441073	-1.508229	-5.424372	**H**	0.646767	-0.348875	-5.753271
H	-1.566806	0.279994	-5.432054	**H**	-1.451207	-0.326406	-5.528309
H	0.531371	0.348561	-5.692793	**H**	-0.369352	1.484838	-5.515078
Ti	0.203504	-0.013126	-0.107753	**Ti**	0.182257	-0.026580	-0.119247
O	0.888012	-0.373822	4.415985	**O**	0.635072	-0.563949	4.463666
C	0.995224	-1.627174	5.047353	**C**	0.791271	-1.770154	5.154487
H	0.031494	-2.168106	5.038347	**H**	-0.065391	-2.447024	4.976744
H	1.746999	-2.274565	4.561703	**H**	1.709519	-2.298169	4.835881
H	1.296363	-1.472891	6.098465	**H**	0.860616	-1.577413	6.239426

Table S23. Cartesian coordinates of Ti@cage-CH_3OH.

Ti@cage-CH_3OH-singlet				Ti@cage-CH_3OH-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.424434	-2.022244	1.732046	**Te**	-1.150123	-2.032533	1.942333
Te	1.889597	1.753172	-1.514626	**Te**	1.794668	1.699278	-1.747569
Te	-1.583827	-1.650746	-1.618473	**Te**	-1.650505	-1.739251	-1.520553
Te	2.104020	1.478842	1.956929	**Te**	2.205334	1.558059	1.711224
Te	-1.374494	1.503585	2.106506	**Te**	-1.170015	1.522438	2.173003
Te	1.894266	-1.621270	-1.832932	**Te**	1.805203	-1.717129	-1.963478
Te	2.085682	-2.017010	1.585841	**Te**	2.212200	-2.011413	1.493535
Te	-1.533541	1.801639	-1.311019	**Te**	-1.663185	1.654308	-1.308968
Co	-2.308971	-0.068217	0.261765	**Co**	-2.169598	-0.161703	0.469954
Co	2.819246	-0.089130	0.020063	**Co**	2.776914	-0.115677	-0.179302
Co	0.260474	-2.649845	-0.152722	**Co**	0.291357	-2.668693	-0.095144
Co	0.297136	2.457832	0.376206	**Co**	0.273463	2.407706	0.229976
Co	0.362105	-0.356614	2.552530	**Co**	0.641362	-0.295979	2.642701
Co	0.098236	0.136186	-2.399627	**Co**	-0.026180	0.025143	-2.457273
P	-0.242047	0.098698	-4.496482	**P**	-0.260626	0.181378	-4.637655
P	0.364887	-4.795761	-0.387985	**P**	0.179062	-4.796712	-0.447900
P	0.395182	4.615896	0.369661	**P**	0.184637	4.571016	0.223175
P	-4.458934	0.013415	0.466887	**P**	-4.281839	-0.245041	0.919223
P	4.972551	-0.001637	-0.139357	**P**	4.934241	-0.115964	-0.222351
H	1.601931	5.307198	0.705427	**H**	0.692824	5.343085	-0.869060
H	0.134890	5.369288	-0.818659	**H**	-1.068315	5.257027	0.300804
H	-0.453401	5.397728	1.215767	**H**	0.825585	5.341244	1.244794
H	-5.091801	-0.374671	1.689529	**H**	-4.757875	-0.246576	2.268085
H	-5.175333	1.244311	0.329153	**H**	-5.176208	0.772045	0.457694
H	-5.328620	-0.743656	-0.381598	**H**	-5.086023	-1.346495	0.487315
H	5.813884	-0.752790	0.740823	**H**	5.702281	-0.130638	0.984056
H	5.650919	-0.388042	-1.338836	**H**	5.663314	-1.166438	-0.863967
H	5.676994	1.233282	0.020317	**H**	5.659186	0.954480	-0.835028
H	1.623170	-5.470428	-0.476818	**H**	1.140406	-5.693542	0.117953
H	-0.187309	-5.668942	0.601738	**H**	-0.967040	-5.552573	-0.046104
H	-0.225827	-5.468323	-1.505316	**H**	0.244792	-5.339967	-1.769534
H	-0.050009	-1.095808	-5.260091	**H**	0.816269	-0.127592	-5.529429
H	-1.520840	0.419029	-5.052052	**H**	-1.237694	-0.582880	-5.353677
H	0.514259	0.951423	-5.361288	**H**	-0.590104	1.424548	-5.267557
Ti	0.260031	-0.115400	0.269163	**Ti**	0.295986	-0.123820	0.092297
C	0.677266	-0.448064	5.216153	**C**	0.966703	-0.129639	5.278055
H	1.566955	-1.000375	4.875464	**H**	1.790513	-0.286147	4.536651
H	0.248053	-0.974464	6.078592	**H**	1.248542	-0.689288	6.179647
H	-0.140964	-0.490776	4.433102	**H**	0.027581	-0.583387	4.888722
O	0.959296	0.881940	5.613983	**O**	0.810935	1.230123	5.636549
H	1.290023	1.343351	4.819291	**H**	0.532673	1.699802	4.825856

Table S24. Cartesian coordinates of Zr@cage.

Zr@cage-singlet				Zr@cage-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.718390	-1.664080	1.901193	**Te**	-1.638919	-1.786523	1.843367
Te	1.751324	1.625188	-1.863216	**Te**	1.676876	1.744780	-1.853215
Te	-1.745493	-1.843690	-1.634434	**Te**	-1.852590	-1.709554	-1.687768
Te	1.803897	1.887352	1.581492	**Te**	1.805752	1.805112	1.686439
Te	-1.772595	1.884173	1.626627	**Te**	-1.634011	1.812059	1.848982
Te	1.694682	-1.821959	-1.686160	**Te**	1.668768	-1.715768	-1.858980
Te	1.775084	-1.649407	1.853519	**Te**	1.796123	-1.792256	1.679356
Te	-1.816816	1.626463	-1.791442	**Te**	-1.845512	1.752382	-1.679024
Co	-2.612286	-0.040353	0.025839	**Co**	-2.554139	0.016028	0.164995
Co	2.604501	-0.023328	-0.041512	**Co**	2.549672	0.007985	-0.079723
Co	0.005035	-2.589989	0.162122	**Co**	-0.007293	-2.579655	-0.038381
Co	-0.000851	2.601579	-0.232494	**Co**	0.006841	2.610184	-0.026918
Co	0.027260	0.195973	2.473630	**Co**	0.120610	0.008510	2.589774
Co	-0.044109	-0.128738	-2.622687	**Co**	-0.130207	0.020825	-2.630608
P	-0.192944	0.393559	-4.690779	**P**	-0.185254	0.007747	-4.832789
P	0.028945	-4.754397	0.070280	**P**	-0.016118	-4.737915	-0.258802
P	0.019551	4.775332	-0.239134	**P**	0.020742	4.771777	-0.225493
P	-4.771990	-0.223277	0.130415	**P**	-4.696567	-0.005330	0.485957
P	4.766933	-0.179279	-0.042473	**P**	4.708743	-0.008084	0.063586
H	1.193248	5.506562	-0.604278	**H**	1.178214	5.532619	0.130160
H	-0.875741	5.535949	-1.056158	**H**	-0.177916	5.403918	-1.492508
H	-0.232487	5.509688	0.961259	**H**	-0.911337	5.589178	0.487885
H	-5.509148	0.342946	1.216920	**H**	-5.252766	0.013898	1.802762
H	-5.614831	0.301830	-0.899956	**H**	-5.528619	1.033446	-0.037335
H	-5.404323	-1.504647	0.185300	**H**	-5.497221	-1.089335	0.007563
H	5.421194	-1.450555	-0.011385	**H**	5.369979	-0.043469	1.331014
H	5.552924	0.354143	-1.112572	**H**	5.475696	-1.060569	-0.527805
H	5.543837	0.403442	1.007071	**H**	5.488451	1.063267	-0.475335
H	1.116225	-5.504513	0.618638	**H**	1.050655	-5.538012	0.258872
H	-1.004729	-5.527712	0.685919	**H**	-1.069857	-5.533399	0.291178
H	-0.002919	-5.447269	-1.180320	**H**	-0.036733	-5.350497	-1.550248
H	0.782924	-0.107630	-5.609022	**H**	1.017910	-0.040010	-5.606403
H	-1.340590	0.016276	-5.456322	**H**	-0.848984	-1.030808	-5.560597
H	-0.147856	1.749851	-5.139608	**H**	-0.772195	1.082154	-5.574470
Zr	-0.005450	0.020559	0.075014	**Zr**	-0.004778	0.015358	-0.014200

Table S25. Cartesian coordinates of Zr@cage-CO_2.

Zr@cage-CO_2-singlet				Zr@cage-CO_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.917474	-1.718121	1.754812	**Te**	-1.386529	-1.813916	1.919385
Te	1.717969	1.706487	-1.689303	**Te**	1.741041	1.706341	-1.934972
Te	-1.791023	-1.752005	-1.734737	**Te**	-1.793936	-1.718623	-1.586751
Te	1.629444	1.804398	1.792734	**Te**	2.076698	1.747710	1.588122
Te	-1.908537	1.831257	1.674438	**Te**	-1.355084	1.793535	1.939756
Te	1.673834	-1.749630	-1.644059	**Te**	1.700908	-1.745909	-1.961594
Te	1.595194	-1.731565	1.868187	**Te**	2.036569	-1.840474	1.571360
Te	-1.791589	1.744466	-1.767911	**Te**	-1.761763	1.746860	-1.561583
Co	-2.707911	0.013799	-0.063669	**Co**	-2.379737	0.006981	0.311284
Co	2.506185	-0.011229	0.112996	**Co**	2.702367	-0.048037	-0.226382
Co	-0.105925	-2.594506	0.067377	**Co**	0.135161	-2.611178	-0.044495
Co	-0.066573	2.628320	-0.045891	**Co**	0.184440	2.580245	-0.013255
Co	-0.191064	0.076270	2.556101	**Co**	0.439680	-0.032582	2.598085
Co	-0.030761	-0.013073	-2.575920	**Co**	-0.125048	0.008991	-2.620089
P	-0.163475	0.179153	-4.703400	**P**	-0.366293	0.105574	-4.814925
P	-0.037143	-4.761890	0.000342	**P**	0.163878	-4.769514	-0.271422
P	0.019666	4.796312	-0.085524	**P**	0.183905	4.747241	-0.148729
P	-4.875698	-0.043979	-0.063968	**P**	-4.495702	-0.011829	0.780271
P	4.672972	-0.083513	0.152239	**P**	4.866876	-0.074467	-0.225823
H	1.243812	5.491177	0.166725	**H**	0.946547	5.546807	0.759709
H	-0.319405	5.536551	-1.261959	**H**	0.616401	5.427005	-1.329642
H	-0.774066	5.583122	0.806853	**H**	-1.031513	5.485197	-0.000253
H	-5.627061	0.487287	1.030387	**H**	-4.957082	0.012824	2.133090
H	-5.640731	0.601453	-1.086113	**H**	-5.359156	1.027736	0.312371
H	-5.580784	-1.286469	-0.127389	**H**	-5.329656	-1.095165	0.361484
H	5.407327	0.515418	1.222964	**H**	5.607572	-0.102193	0.996735
H	5.370153	-1.331908	0.183738	**H**	5.591726	-1.133929	-0.856132
H	5.459952	0.488552	-0.896458	**H**	5.614930	0.988650	-0.821862
H	1.119077	-5.476022	0.444938	**H**	1.344961	-5.522881	0.014652
H	-0.981623	-5.554685	0.724819	**H**	-0.723269	-5.607879	0.474218
H	-0.174345	-5.473060	-1.233282	**H**	-0.091182	-5.385056	-1.536576
H	0.696089	-0.588046	-5.550702	**H**	0.629078	-0.413736	-5.703676
H	-1.375405	-0.125424	-5.398123	**H**	-1.471512	-0.512946	-5.482579
H	0.066412	1.434133	-5.348771	**H**	-0.496031	1.361752	-5.488301
Zr	-0.104366	0.019585	0.107725	**Zr**	0.157162	-0.014556	-0.008011
C	0.972026	-0.201432	5.218186	**C**	-1.241381	0.070327	5.318695
O	-0.114341	0.130210	4.902735	**O**	-2.390235	0.203388	5.483008
O	2.031307	-0.523844	5.586078	**O**	-0.082672	-0.064748	5.172021

Table S26. Cartesian coordinates of Zr@cage-COOH.

Zr@cage-COOH-doublet				Zr@cage-COOH-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.071908	-1.827226	2.008216	**Te**	-1.243362	-1.860921	2.197798
Te	1.678634	1.760696	-2.022731	**Te**	1.739319	1.778927	-1.822033
Te	-1.739511	-1.757654	-1.402429	**Te**	-1.538309	-1.969922	-1.759606
Te	2.238628	1.798461	1.479966	**Te**	2.060638	1.784099	1.579140
Te	-1.132231	1.773950	2.041251	**Te**	-1.588832	1.468213	1.876859
Te	1.732794	-1.662586	-2.050409	**Te**	1.821534	-1.818211	-1.823697
Te	2.298341	-1.739606	1.456693	**Te**	2.120595	-1.734956	1.688683
Te	-1.796364	1.739737	-1.373527	**Te**	-1.845821	1.456250	-1.518880
Co	-2.244331	-0.031836	0.534788	**Co**	-2.289496	-0.550024	0.254157
Co	2.807600	0.052464	-0.385885	**Co**	2.762431	-0.028430	-0.169727
Co	0.339620	-2.581379	-0.033401	**Co**	0.073762	-2.611165	0.134515
Co	0.254406	2.602544	0.007654	**Co**	-0.011665	2.453317	0.079255
Co	0.667774	-0.002663	2.665750	**Co**	0.445927	0.088593	2.713146
Co	-0.204329	0.028764	-2.550611	**Co**	0.015751	-0.068521	-2.558007
P	-0.760873	0.057976	-4.674737	**P**	-0.138599	0.240522	-4.731799
P	0.425664	-4.742962	-0.208035	**P**	-0.092160	-4.816556	0.248775
P	0.296058	4.766673	-0.130128	**P**	-0.113670	4.662199	0.264117
P	-4.340693	-0.044416	1.111910	**P**	-4.423263	-1.017635	0.385322
P	4.971987	0.089185	-0.434422	**P**	4.952484	-0.044399	-0.371687
H	1.511673	5.500085	0.039676	**H**	0.901383	5.495512	-0.304523
H	-0.112609	5.444215	-1.320948	**H**	-1.212992	5.420474	-0.252021
H	-0.480225	5.569386	0.763608	**H**	-0.105707	5.298279	1.545546
H	-4.727505	-0.165963	2.482466	**H**	-5.204716	-0.535591	1.481364
H	-5.193500	1.065192	0.819226	**H**	-5.332633	-0.598654	-0.635152
H	-5.235320	-1.046147	0.620325	**H**	-4.901190	-2.364543	0.453347
H	5.731669	0.092961	0.776343	**H**	5.785461	0.688921	0.531453
H	5.714493	-0.955148	-1.068897	**H**	5.702057	-1.259981	-0.285304
H	5.677929	1.168288	-1.052478	**H**	5.596267	0.425965	-1.559308
H	-0.285995	-5.581585	0.706321	**H**	0.473104	-5.541858	1.344226
H	-0.022434	-5.410137	-1.390545	**H**	-1.364992	-5.469389	0.297699
H	1.666024	-5.447883	-0.110322	**H**	0.452032	-5.657384	-0.772658
H	-0.208712	-0.882182	-5.601600	**H**	0.944879	-0.104057	-5.600686
H	-2.115777	-0.116952	-5.099062	**H**	-1.148280	-0.402323	-5.518428
H	-0.514458	1.207349	-5.490189	**H**	-0.345110	1.540658	-5.290818
Zr	0.264976	0.007679	0.002728	**Zr**	0.234238	-0.063411	0.024308
C	0.123764	-0.020180	4.463658	**C**	0.515319	1.068564	4.320605
O	1.135077	0.104575	5.140461	**O**	0.731441	0.280191	5.230337
O	-1.118872	-0.137639	5.003270	**O**	0.353248	2.404807	4.528679
H	-0.996949	-0.096883	5.977989	**H**	0.453445	2.541585	5.496943

Table S27. Cartesian coordinates of Zr@cage-CO.

Zr@cage-CO-singlet				Zr@cage-CO-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.391725	-1.825427	1.834480	**Te**	-1.168285	-1.625822	2.210074
Te	1.722351	1.807255	-1.876774	**Te**	1.752924	1.814063	-1.991032
Te	-1.714046	-1.745945	-1.652198	**Te**	-1.707454	-1.760109	-1.705813
Te	2.035213	1.719080	1.607434	**Te**	2.205243	1.905629	1.351080
Te	-1.447288	1.664435	1.917106	**Te**	-1.356202	1.741625	1.878478
Te	1.764335	-1.686092	-1.972051	**Te**	1.689875	-1.796363	-1.915279
Te	2.077877	-1.766579	1.524674	**Te**	2.150259	-1.681184	1.515310
Te	-1.767240	1.753624	-1.555335	**Te**	-1.827048	1.648301	-1.538372
Co	-2.422472	-0.062147	0.220097	**Co**	-2.274733	-0.292639	0.323475
Co	2.744471	0.024479	-0.249587	**Co**	2.784084	-0.013669	-0.366109
Co	0.202435	-2.601681	-0.081080	**Co**	-0.023905	-2.491083	0.090857
Co	0.129371	2.582005	0.055973	**Co**	0.098639	2.613120	-0.075770
Co	0.395174	-0.068040	2.609387	**Co**	0.648101	0.193537	2.575103
Co	-0.080081	0.060686	-2.611031	**Co**	-0.066509	0.024445	-2.604331
P	-0.289398	0.145206	-4.774810	**P**	-0.139612	0.190655	-4.773108
P	0.260017	-4.769194	-0.090335	**P**	-0.321012	-4.666783	0.221965
P	0.127798	4.747947	0.149991	**P**	-0.024486	4.815858	-0.076826
P	-4.579558	-0.138835	0.431956	**P**	-4.426149	-0.650723	0.618116
P	4.909195	0.013474	-0.387058	**P**	4.976915	-0.064175	-0.612268
H	1.217286	5.510944	-0.374432	**H**	0.581632	5.604721	-1.105811
H	-0.901542	5.518225	-0.476021	**H**	-1.286161	5.489063	-0.119635
H	0.070155	5.426232	1.407254	**H**	0.499180	5.589230	1.007274
H	-5.220433	0.305770	1.630320	**H**	-5.103873	-0.159092	1.777598
H	-5.437777	0.572361	-0.463488	**H**	-5.388703	-0.169614	-0.323756
H	-5.281670	-1.381378	0.346814	**H**	-4.962990	-1.975079	0.697212
H	5.716538	0.197048	0.778568	**H**	5.845660	0.370293	0.438207
H	5.612716	-1.133780	-0.869478	**H**	5.672804	-1.289194	-0.861321
H	5.608793	0.961845	-1.196947	**H**	5.636198	0.676451	-1.644582
H	0.175691	-5.509397	1.130038	**H**	0.325472	-5.435388	1.239855
H	-0.720845	-5.537383	-0.792331	**H**	-1.617571	-5.239146	0.419873
H	1.391506	-5.474510	-0.606674	**H**	0.045448	-5.526617	-0.860246
H	0.635807	-0.522696	-5.636904	**H**	1.033774	-0.000366	-5.567462
H	-1.465374	-0.341824	-5.426420	**H**	-0.980141	-0.663357	-5.555587
H	-0.251191	1.394019	-5.470006	**H**	-0.542764	1.405838	-5.408842
Zr	0.159620	-0.008536	-0.039343	**Zr**	0.248286	0.065596	-0.051170
C	0.520759	-0.095006	4.369108	**C**	0.970261	0.414090	4.297151
O	0.597560	-0.115261	5.528173	**O**	1.156867	0.558816	5.434764

Table S28. Cartesian coordinates of Zr@cage-CHO.

Zr@cage-CHO-doublet				Zr@cage-CHO-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.455011	-1.626182	1.935715	**Te**	-1.454620	-1.671205	1.895686
Te	1.672572	1.812344	-1.960218	**Te**	1.732614	1.850906	-1.925378
Te	-1.711739	-1.763667	-1.530622	**Te**	-1.610524	-1.807416	-1.544019
Te	2.042000	1.873797	1.583179	**Te**	2.006532	1.874111	1.640606
Te	-1.474983	1.820847	1.891836	**Te**	-1.466267	1.823418	1.890923
Te	1.781732	-1.704972	-1.844603	**Te**	1.865407	-1.741693	-1.812419
Te	2.136793	-1.567920	1.618692	**Te**	2.144432	-1.599904	1.646590
Te	-1.731575	1.761787	-1.657662	**Te**	-1.642828	1.795338	-1.675145
Co	-2.422976	0.068669	0.214924	**Co**	-2.354733	0.057216	0.171752
Co	2.731390	0.147935	-0.240337	**Co**	2.735469	0.149142	-0.192110
Co	0.211494	-2.496547	0.119342	**Co**	0.247612	-2.545450	0.104849
Co	0.118161	2.635219	-0.017452	**Co**	0.116420	2.672972	-0.020710
Co	0.394455	0.065411	2.660521	**Co**	0.369559	0.024438	2.659732
Co	-0.075933	-0.027997	-2.599418	**Co**	0.051092	-0.008146	-2.632396
P	-0.268432	-0.260423	-4.779404	**P**	-0.632830	-0.306362	-4.746214
P	0.292472	-4.661544	0.280376	**P**	0.376737	-4.767906	0.397404
P	0.121159	4.788919	0.175618	**P**	0.279034	4.918427	0.165871
P	-4.590589	0.165720	0.238442	**P**	-4.513596	0.208507	-0.023217
P	4.871397	0.300656	-0.556940	**P**	4.881079	0.379175	-0.452213
H	1.152421	5.581611	-0.417951	**H**	1.442734	5.630138	-0.265328
H	-0.969094	5.572455	-0.316044	**H**	-0.653449	5.798774	-0.470589
H	0.180725	5.409552	1.461737	**H**	0.206071	5.551990	1.445809
H	-5.348713	-0.652215	1.134106	**H**	-5.355812	-0.611282	0.791162
H	-5.276972	1.382821	0.540868	**H**	-5.198245	1.435692	0.238197
H	-5.359859	-0.145205	-0.925748	**H**	-5.178757	-0.070387	-1.256994
H	5.783081	-0.458468	0.241807	**H**	5.791609	-0.287867	0.425446
H	5.465668	-0.037398	-1.812768	**H**	5.529472	-0.016375	-1.663077
H	5.555709	1.547213	-0.408716	**H**	5.509462	1.660298	-0.365671
H	0.299364	-5.313015	1.553702	**H**	0.405592	-5.345899	1.706395
H	-0.725793	-5.486156	-0.292574	**H**	-0.630712	-5.652575	-0.106199
H	1.392828	-5.398669	-0.258643	**H**	1.478693	-5.534616	-0.101270
H	0.689006	0.309028	-5.678364	**H**	-0.020160	0.423038	-5.815513
H	-0.276890	-1.551179	-5.397055	**H**	-0.570634	-1.581281	-5.392294
H	-1.415518	0.228639	-5.482372	**H**	-1.977633	-0.020039	-5.132696
Zr	0.155304	0.061274	-0.000865	**Zr**	0.198521	0.056107	0.008741
C	0.537805	-0.845036	4.274305	**C**	0.487837	-0.953708	4.236204
O	0.560931	0.028040	5.121181	**O**	0.507684	-0.105580	5.108455
H	0.598709	-1.927720	4.517110	**H**	0.538240	-2.044371	4.445337

Table S29. Cartesian coordinates of Zr@cage-OCH_2.

Zr@cage-OCH_2-singlet				Zr@cage-OCH_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.465430	-1.883428	1.772435	**Te**	-1.429639	-1.892875	1.778776
Te	1.763451	1.740558	-1.859010	**Te**	1.743393	1.746280	-1.891785
Te	-1.756907	-1.713030	-1.706737	**Te**	-1.701983	-1.762006	-1.734299
Te	2.067485	1.608780	1.627994	**Te**	2.033202	1.637363	1.625598
Te	-1.409018	1.626731	1.923824	**Te**	-1.449016	1.612261	1.914195
Te	1.733042	-1.734142	-1.967138	**Te**	1.784526	-1.733202	-1.991271
Te	2.008466	-1.886078	1.481910	**Te**	2.057448	-1.858999	1.515454
Te	-1.712573	1.765822	-1.525248	**Te**	-1.721817	1.708091	-1.616888
Co	-2.438883	-0.058516	0.203615	**Co**	-2.395750	-0.089160	0.179345
Co	2.752554	-0.053952	-0.237039	**Co**	2.732733	-0.031967	-0.222065
Co	0.101932	-2.665625	-0.146758	**Co**	0.175219	-2.639606	-0.117371
Co	0.205640	2.541371	0.079704	**Co**	0.146804	2.498274	0.056076
Co	0.381340	-0.182294	2.627153	**Co**	0.393554	-0.171330	2.750232
Co	-0.071345	0.052790	-2.620277	**Co**	-0.041156	0.014670	-2.661854
P	-0.258277	0.174316	-4.769515	**P**	-0.212527	0.091122	-4.875756
P	0.042328	-4.838216	-0.258931	**P**	0.120780	-4.806125	-0.218669
P	0.297588	4.709920	0.192405	**P**	0.128965	4.662504	0.190956
P	-4.593978	-0.073910	0.488349	**P**	-4.543540	-0.042003	0.478481
P	4.925845	-0.026144	-0.329923	**P**	4.898493	0.052175	-0.335281
H	1.486339	5.418938	-0.166210	**H**	1.124289	5.454818	-0.461396
H	-0.592028	5.536001	-0.563610	**H**	-0.988764	5.422130	-0.274577
H	0.098640	5.386357	1.436129	**H**	0.231343	5.315584	1.458629
H	-5.157135	-0.027406	1.801398	**H**	-5.100593	-0.181461	1.787539
H	-5.423371	0.954776	-0.058526	**H**	-5.313158	1.106053	0.114321
H	-5.397522	-1.162843	0.027178	**H**	-5.403198	-0.997532	-0.148187
H	5.713688	-0.317320	0.827365	**H**	5.704967	-0.214937	0.815051
H	5.646909	-0.892372	-1.210952	**H**	5.631114	-0.795983	-1.223567
H	5.638134	1.160707	-0.689166	**H**	5.570838	1.258821	-0.703809
H	0.789641	-5.650646	0.650696	**H**	0.728481	-5.611397	0.795079
H	-1.187352	-5.551013	-0.103971	**H**	-1.124580	-5.507759	-0.230236
H	0.456185	-5.532746	-1.438568	**H**	0.691408	-5.512510	-1.323209
H	0.672039	-0.485545	-5.632042	**H**	0.654908	-0.661150	-5.731581
H	-1.431608	-0.292941	-5.440488	**H**	-1.416687	-0.295111	-5.547421
H	-0.204067	1.435885	-5.440488	**H**	-0.059348	1.320963	-5.592889
Zr	0.155577	-0.065085	-0.003015	**Zr**	0.165859	-0.071704	-0.033512
O	0.170341	0.106371	4.554793	**O**	0.178811	0.113762	4.631425
C	1.083464	-0.803142	4.469000	**C**	1.095892	-0.811248	4.578295
H	2.146840	-0.529531	4.599531	**H**	2.151535	-0.536180	4.736448
H	0.825154	-1.861694	4.656698	**H**	0.820319	-1.858920	4.782289

Table S30. Cartesian coordinates of Zr@cage-OCH_3.

Zr@cage-OCH_3-doublet				Zr@cage-OCH_3-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.239770	-1.898581	1.829337	**Te**	-1.357352	-1.869306	1.761563
Te	1.564487	1.822694	-2.021093	**Te**	1.703344	1.816157	-1.969915
Te	-1.702399	-1.846053	-1.594575	**Te**	-1.681295	-1.749213	-1.736315
Te	1.997803	1.847369	1.484728	**Te**	2.058142	1.723235	1.547167
Te	-1.398573	1.647642	1.920850	**Te**	-1.423246	1.644548	1.883527
Te	1.816848	-1.644072	-2.037821	**Te**	1.768668	-1.657500	-2.081660
Te	2.227412	-1.699188	1.383648	**Te**	2.145765	-1.771587	1.420577
Te	-1.852439	1.619495	-1.597108	**Te**	-1.767946	1.739542	-1.617519
Co	-2.374799	-0.143307	0.284809	**Co**	-2.376738	-0.083451	0.179974
Co	2.733188	0.149506	-0.361146	**Co**	2.741935	0.046961	-0.327162
Co	0.321694	-2.617533	-0.108968	**Co**	0.247144	-2.587785	-0.153691
Co	0.024416	2.580944	-0.048130	**Co**	0.139163	2.555684	0.012093
Co	0.536792	-0.062338	2.694620	**Co**	0.455137	-0.098163	2.742596
Co	-0.143556	-0.059480	-2.657512	**Co**	-0.085968	0.071305	-2.697399
P	-0.368584	-0.256271	-4.821974	**P**	-0.313330	0.183670	-4.902393
P	0.427593	-4.777545	-0.351327	**P**	0.346109	-4.757162	-0.106795
P	-0.122353	4.757850	0.060120	**P**	0.189125	4.726566	0.063898
P	-4.508534	-0.155470	0.694283	**P**	-4.531522	-0.131042	0.441082
P	4.886471	0.379181	-0.508371	**P**	4.904057	0.110439	-0.489747
H	0.746616	5.601360	-0.700937	**H**	1.369165	5.438184	-0.315844
H	-1.326449	5.437183	-0.305794	**H**	-0.710290	5.514611	-0.720202
H	0.057971	5.453895	1.296448	**H**	-0.021311	5.439616	1.285204
H	-5.008762	-0.379885	2.014602	**H**	-5.114912	-0.128391	1.746354
H	-5.318083	0.992214	0.427940	**H**	-5.364075	0.902045	-0.091146
H	-5.374326	-1.094219	0.050560	**H**	-5.310733	-1.217989	-0.063612
H	5.723212	0.241193	0.642713	**H**	5.725113	0.222647	0.674201
H	5.660818	-0.476764	-1.352625	**H**	5.630075	-0.972903	-1.073413
H	5.473032	1.600161	-0.965262	**H**	5.563729	1.138997	-1.229952
H	1.600797	-5.506806	0.019203	**H**	0.394458	-5.467214	1.133538
H	-0.493208	-5.647066	0.313881	**H**	-0.687856	-5.555155	-0.688529
H	0.287494	-5.387668	-1.637300	**H**	1.430628	-5.461474	-0.716466
H	-0.379925	-1.533561	-5.467178	**H**	0.572946	-0.513258	-5.784293
H	-1.530200	0.241873	-5.492999	**H**	-1.509509	-0.254254	-5.555456
H	0.572942	0.337488	-5.721060	**H**	-0.235837	1.427923	-5.606261
Zr	0.173896	-0.008252	-0.062288	**Zr**	0.178759	-0.016576	-0.082146
O	0.813525	-0.385680	4.452979	**O**	0.642526	-0.588441	4.472839
C	1.079271	-1.616582	5.077837	**C**	0.801158	-1.790793	5.168112
H	0.408610	-2.418850	4.721553	**H**	-0.041931	-2.479644	4.972322
H	2.119833	-1.941007	4.893687	**H**	1.733610	-2.304681	4.868659
H	0.939229	-1.503842	6.167388	**H**	0.845082	-1.596123	6.253931

Table S31. Cartesian coordinates of Zr@cage-CH_3OH.

Zr@cage-CH_3OH-singlet				Zr@cage-CH_3OH-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.362378	-2.018628	1.853580	**Te**	-1.236050	-2.048865	1.967398
Te	1.853745	1.810957	-1.555441	**Te**	1.796752	1.733752	-1.720899
Te	-1.606326	-1.697490	-1.585898	**Te**	-1.692914	-1.751724	-1.534000
Te	2.128282	1.551035	1.928143	**Te**	2.174470	1.589375	1.788255
Te	-1.386584	1.513304	2.158266	**Te**	-1.246187	1.533314	2.195363
Te	1.874830	-1.628480	-1.861397	**Te**	1.805746	-1.720259	-1.941174
Te	2.148809	-1.967168	1.616503	**Te**	2.176262	-2.014518	1.548561
Te	-1.627712	1.793125	-1.284909	**Te**	-1.707913	1.685842	-1.308582
Co	-2.353273	-0.114558	0.330471	**Co**	-2.275774	-0.160414	0.475779
Co	2.854992	-0.053942	-0.031378	**Co**	2.804176	-0.101616	-0.128443
Co	0.282714	-2.679445	-0.089853	**Co**	0.254024	-2.709288	-0.068758
Co	0.246540	2.519880	0.369292	**Co**	0.240440	2.465405	0.266421
Co	0.427392	-0.303955	2.686152	**Co**	0.580203	-0.299167	2.749088
Co	0.043029	0.149430	-2.426630	**Co**	-0.042176	0.043598	-2.475541
P	-0.269472	0.210345	-4.547443	**P**	-0.229116	0.220149	-4.673457
P	0.371225	-4.836005	-0.306243	**P**	0.210189	-4.850913	-0.411132
P	0.300019	4.690513	0.414383	**P**	0.162238	4.630896	0.157096
P	-4.520886	-0.185682	0.436981	**P**	-4.399214	-0.229312	0.904912
P	5.014637	-0.088383	-0.251423	**P**	4.970597	-0.120167	-0.169384
H	0.090811	5.457965	-0.774287	**H**	0.055054	5.301951	-1.100350
H	-0.611705	5.436183	1.225607	**H**	-0.879234	5.370556	0.799973
H	1.472731	5.394715	0.830905	**H**	1.234680	5.435875	0.654284
H	-5.246233	0.615500	1.373525	**H**	-4.889957	-0.221275	2.247677
H	-5.328582	0.154446	-0.693569	**H**	-5.278009	0.791618	0.424885
H	-5.204832	-1.405217	0.735709	**H**	-5.199307	-1.329382	0.465455
H	5.871297	0.500279	0.731017	**H**	5.735869	-0.156936	1.037667
H	5.725481	-1.326437	-0.335747	**H**	5.685855	-1.170386	-0.825202
H	5.656266	0.516235	-1.378001	**H**	5.701781	0.952001	-0.769923
H	1.623027	-5.527384	-0.300567	**H**	1.255391	-5.699653	0.071814
H	-0.269701	-5.697969	0.637823	**H**	-0.864591	-5.653918	0.083659
H	-0.144312	-5.492082	-1.468126	**H**	0.191195	-5.390080	-1.735165
H	-0.041212	-0.947377	-5.355093	**H**	0.901767	0.036421	-5.532095
H	-1.549866	0.524585	-5.101255	**H**	-1.103046	-0.623647	-5.432066
H	0.474211	1.115122	-5.368100	**H**	-0.661201	1.437554	-5.290621
Zr	0.258140	-0.087207	0.224351	**Zr**	0.259665	-0.120398	0.127083
C	0.789100	-0.358081	5.219802	**C**	0.949310	-0.192307	5.224140
H	1.661369	-0.898460	4.819405	**H**	1.739162	-0.553116	4.514907
H	0.394059	-0.926576	6.071646	**H**	0.986416	-0.861717	6.093288
H	-0.083962	-0.362310	4.484907	**H**	-0.066684	-0.326821	4.767034
O	1.090784	0.949838	5.667209	**O**	1.177659	1.126527	5.668671
H	1.414250	1.441980	4.888739	**H**	1.183171	1.693646	4.872433

Table S32. Cartesian coordinates of Hf@cage.

Hf@cage-singlet				Hf@cage-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.717339	-1.744202	1.857705	**Te**	-1.622413	-1.797566	1.823917
Te	1.745270	1.687998	-1.753780	**Te**	1.676015	1.721299	-1.875673
Te	-1.744073	-1.784574	-1.663971	**Te**	-1.810316	-1.755665	-1.703543
Te	1.776572	1.812330	1.694267	**Te**	1.808247	1.799006	1.655082
Te	-1.764704	1.800937	1.732610	**Te**	-1.640718	1.781504	1.809426
Te	1.706267	-1.760427	-1.707381	**Te**	1.689387	-1.742177	-1.854873
Te	1.764871	-1.724411	1.818081	**Te**	1.820582	-1.784169	1.667513
Te	-1.811794	1.679122	-1.702773	**Te**	-1.822985	1.708031	-1.718668
Co	-2.618154	-0.047509	0.057551	**Co**	-2.544896	-0.018799	0.123922
Co	2.605179	-0.023123	0.002662	**Co**	2.571306	0.008721	-0.100944
Co	0.008640	-2.610146	0.087207	**Co**	0.019992	-2.607671	-0.029087
Co	-0.014640	2.602300	-0.098920	**Co**	0.003435	2.589355	-0.048808
Co	0.020169	0.080893	2.530121	**Co**	0.128550	0.004957	2.562224
Co	-0.039164	-0.037903	-2.584822	**Co**	-0.109045	-0.023085	-2.659429
P	-0.140523	0.388309	-4.678912	**P**	-0.184970	0.054059	-4.861984
P	0.025983	-4.769738	-0.108497	**P**	-0.046351	-4.769796	-0.193727
P	-0.013889	4.773056	-0.179777	**P**	-0.004316	4.759684	-0.115040
P	-4.783854	-0.192743	0.122949	**P**	-4.691646	-0.002399	0.421019
P	4.771864	-0.148370	0.007664	**P**	4.734081	0.020959	0.022166
H	1.057791	5.537974	0.379288	**H**	1.063157	5.490465	-0.726345
H	-0.039626	5.473729	-1.427851	**H**	-1.053458	5.492101	-0.755889
H	-1.059148	5.540316	0.424412	**H**	-0.021032	5.528374	1.091710
H	-5.533106	0.365604	1.206037	**H**	-5.263584	-0.029782	1.731676
H	-5.600318	0.368213	-0.910411	**H**	-5.492875	1.081261	-0.058444
H	-5.444096	-1.461650	0.140633	**H**	-5.520021	-1.038316	-0.114602
H	5.443449	-1.411080	0.039812	**H**	5.405671	0.010493	1.284925
H	5.556910	0.392999	-1.059864	**H**	5.516383	-1.025692	-0.560074
H	5.543463	0.442572	1.057175	**H**	5.498631	1.095142	-0.532796
H	1.103471	-5.552924	0.413845	**H**	0.776907	-5.609239	0.622149
H	-1.016150	-5.571857	0.455074	**H**	-1.258528	-5.489564	0.048503
H	0.006831	-5.402866	-1.391064	**H**	0.260099	-5.432730	-1.423630
H	0.859286	-0.127706	-5.562699	**H**	0.892255	-0.439522	-5.666727
H	-1.264244	-0.035619	-5.456032	**H**	-1.214283	-0.603609	-5.610202
H	-0.108845	1.725636	-5.185028	**H**	-0.299970	1.300724	-5.557530
Hf	-0.008333	0.004910	0.105981	**Hf**	0.010723	-0.006311	-0.034928

Table S33. Cartesian coordinates of Hf@cage-CO_2.

Hf@cage-CO_2-singlet				Hf@cage-CO_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.910903	-1.751204	1.734385	**Te**	-1.464665	-1.886129	2.032540
Te	1.718654	1.696790	-1.665384	**Te**	1.788891	1.801603	-1.988440
Te	-1.791264	-1.751133	-1.747016	**Te**	-1.887235	-1.826148	-1.644149
Te	1.627693	1.751619	1.810439	**Te**	2.100784	1.807804	1.724601
Te	-1.895902	1.785218	1.692622	**Te**	-1.450618	1.838600	2.054275
Te	1.670135	-1.756700	-1.659119	**Te**	1.771605	-1.826248	-2.013124
Te	1.587756	-1.768826	1.851117	**Te**	2.083142	-1.885911	1.701227
Te	-1.785960	1.740418	-1.745152	**Te**	-1.872019	1.826378	-1.619661
Co	-2.708976	-0.003382	-0.061516	**Co**	-2.421237	-0.011648	0.322029
Co	2.510949	-0.043120	0.111022	**Co**	2.699513	-0.032010	-0.187203
Co	-0.107226	-2.621745	0.037718	**Co**	0.125434	-2.657842	-0.021718
Co	-0.061308	2.607019	-0.016599	**Co**	0.148906	2.621579	0.009835
Co	-0.188353	0.024510	2.566114	**Co**	0.408760	-0.037117	2.665002
Co	-0.030926	-0.005719	-2.573310	**Co**	-0.141784	-0.002924	-2.640914
P	-0.156533	0.183861	-4.703475	**P**	-0.379479	0.106524	-4.855107
P	-0.037441	-4.790933	-0.054525	**P**	0.222362	-4.814805	-0.321995
P	0.019836	4.777647	-0.048783	**P**	0.247130	4.791186	-0.216207
P	-4.880024	-0.059369	-0.061336	**P**	-4.552577	-0.021659	0.789298
P	4.680499	-0.121278	0.145777	**P**	4.879306	-0.048979	-0.199250
H	1.250583	5.476139	0.161317	**H**	1.457366	5.499908	0.055981
H	-0.362632	5.527436	-1.206311	**H**	-0.014230	5.412024	-1.475526
H	-0.739667	5.561913	0.875900	**H**	-0.606656	5.639868	0.554632
H	-5.629926	0.434578	1.052067	**H**	-5.005993	-0.016098	2.142960
H	-5.651947	0.620783	-1.056479	**H**	-5.394440	1.037670	0.330402
H	-5.590593	-1.297030	-0.163799	**H**	-5.382527	-1.095499	0.343060
H	5.424083	0.475110	1.212410	**H**	5.624165	-0.065761	1.018919
H	5.377456	-1.370417	0.176040	**H**	5.588497	-1.113770	-0.835525
H	5.470259	0.446026	-0.904294	**H**	5.603310	1.017811	-0.815222
H	1.122313	-5.512523	0.370666	**H**	1.432988	-5.531971	-0.075379
H	-0.972606	-5.597661	0.668076	**H**	-0.632023	-5.689702	0.418582
H	-0.184036	-5.492226	-1.293310	**H**	-0.039336	-5.389691	-1.602743
H	0.691218	-0.591115	-5.556963	**H**	0.478911	-0.630846	-5.730546
H	-1.370970	-0.104503	-5.402188	**H**	-1.599126	-0.281524	-5.493764
H	0.087163	1.435036	-5.352607	**H**	-0.248927	1.351205	-5.547128
Hf	-0.101613	-0.007135	0.103365	**Th**	0.134047	-0.016564	0.014086
C	0.950937	0.049405	5.248913	**C**	-1.270179	0.060066	5.394137
O	-0.175499	0.054616	4.900751	**O**	-2.418500	0.190585	5.563329
O	2.046891	0.045444	5.650663	**O**	-0.111450	-0.072419	5.245902

Table S34. Cartesian coordinates of Hf@cage-COOH.

Hf@cage-COOH-doublet				Hf@cage-COOH-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.068724	-1.820817	2.013830	**Te**	-1.257616	-1.860342	2.194748
Te	1.667734	1.751954	-2.015748	**Te**	1.735238	1.775849	-1.814934
Te	-1.745792	-1.752735	-1.385655	**Te**	-1.542919	-1.969925	-1.754942
Te	2.235681	1.795051	1.472863	**Te**	2.056199	1.777770	1.584936
Te	-1.128326	1.770678	2.042357	**Te**	-1.587568	1.475059	1.868677
Te	1.718854	-1.663982	-2.038807	**Te**	1.813267	-1.813645	-1.810473
Te	2.294861	-1.738011	1.454451	**Te**	2.106893	-1.731480	1.690637
Te	-1.799736	1.730149	-1.364596	**Te**	-1.836161	1.461380	-1.514738
Co	-2.253572	-0.031909	0.548568	**Co**	-2.291526	-0.540634	0.252143
Co	2.807441	0.046595	-0.388374	**Co**	2.765535	-0.023841	-0.162010
Co	0.331550	-2.587304	-0.024902	**Co**	0.066080	-2.607243	0.136886
Co	0.247095	2.604831	0.008223	**Co**	-0.007243	2.465592	0.080389
Co	0.678307	-0.000840	2.665716	**Co**	0.434856	0.085739	2.711795
Co	-0.215028	0.022311	-2.547618	**Co**	0.013824	-0.068649	-2.554569
P	-0.730716	0.046792	-4.680601	**P**	-0.150148	0.222731	-4.729890
P	0.415655	-4.747926	-0.220597	**P**	-0.096911	-4.814471	0.254180
P	0.283868	4.770233	-0.132037	**P**	-0.073203	4.674351	0.265189
P	-4.350451	-0.031632	1.130329	**P**	-4.424388	-1.012785	0.375207
P	4.972526	0.087533	-0.444338	**P**	4.953357	-0.049915	-0.376718
H	1.496622	5.509443	0.038753	**H**	0.962165	5.493490	-0.288257
H	-0.123880	5.449964	-1.322509	**H**	-1.151768	5.454916	-0.263018
H	-0.494313	5.575177	0.758978	**H**	-0.070633	5.310965	1.546969
H	-4.736475	-0.154808	2.501645	**H**	-5.212782	-0.534825	1.468629
H	-5.198344	1.085256	0.846996	**H**	-5.332600	-0.593782	-0.646960
H	-5.259728	-1.022172	0.640652	**H**	-4.903027	-2.359916	0.438775
H	5.738236	0.076710	0.763145	**H**	5.794672	0.661808	0.536739
H	5.718247	-0.946030	-1.094012	**H**	5.700025	-1.269005	-0.317943
H	5.678657	1.174806	-1.049263	**H**	5.598388	0.439768	-1.556667
H	-0.311509	-5.598113	0.671430	**H**	0.466945	-5.538717	1.351648
H	-0.015370	-5.403309	-1.416472	**H**	-1.368669	-5.470335	0.304295
H	1.651390	-5.460462	-0.112792	**H**	0.447348	-5.661734	-0.762769
H	-0.088480	-0.827353	-5.615034	**H**	0.885472	-0.219061	-5.613861
H	-2.058498	-0.227990	-5.139092	**H**	-1.221105	-0.344514	-5.493816
H	-0.563912	1.226288	-5.474650	**H**	-0.260107	1.527540	-5.306846
Hf	0.259890	0.006319	0.010539	**Hf**	0.229144	-0.061749	0.030341
C	0.136043	-0.016168	4.466546	**C**	0.500382	1.066415	4.321453
O	1.141284	0.117541	5.150827	**O**	0.714214	0.284307	5.237272
O	-1.108941	-0.141209	5.004361	**O**	0.339411	2.405107	4.525709
H	-0.987629	-0.095712	5.978828	**H**	0.439475	2.542927	5.493734

Table S35. Cartesian coordinates of Hf@cage-CO.

Hf@cage-CO-singlet				Hf@cage-CO-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.387613	-1.820920	1.829111	**Te**	-1.173583	-1.632624	2.204222
Te	1.718041	1.802355	-1.871127	**Te**	1.745245	1.791828	-1.998509
Te	-1.708983	-1.741125	-1.646778	**Te**	-1.719304	-1.766137	-1.700078
Te	2.031504	1.715717	1.601897	**Te**	2.198526	1.892600	1.341947
Te	-1.443668	1.661723	1.911133	**Te**	-1.347032	1.733189	1.869822
Te	1.759767	-1.681120	-1.966484	**Te**	1.679697	-1.803085	-1.911604
Te	2.073326	-1.761819	1.520154	**Te**	2.142974	-1.690169	1.498858
Te	-1.762305	1.749038	-1.549937	**Te**	-1.822533	1.637980	-1.539902
Co	-2.427995	-0.062493	0.221285	**Co**	-2.277160	-0.292580	0.324321
Co	2.750179	0.024700	-0.249855	**Co**	2.784954	-0.019559	-0.370189
Co	0.203312	-2.606991	-0.081508	**Co**	-0.027826	-2.499787	0.088686
Co	0.129598	2.588226	0.056889	**Co**	0.101891	2.610494	-0.082965
Co	0.395365	-0.066509	2.610407	**Co**	0.648342	0.181199	2.570209
Co	-0.081483	0.061136	-2.614287	**Co**	-0.074944	0.009871	-2.612455
P	-0.291072	0.142771	-4.780049	**P**	-0.154851	0.163673	-4.784275
P	0.260946	-4.775371	-0.091193	**P**	-0.336376	-4.674194	0.224740
P	0.128229	4.754878	0.152235	**P**	0.008403	4.813069	-0.091183
P	-4.585541	-0.139286	0.434365	**P**	-4.425235	-0.655716	0.636358
P	4.915641	0.013143	-0.386464	**P**	4.978804	-0.000973	-0.595150
H	1.213010	5.521168	-0.378377	**H**	0.603913	5.589086	-1.136953
H	-0.904733	5.527754	-0.465414	**H**	-1.241746	5.509851	-0.109029
H	0.078937	5.435154	1.409343	**H**	0.569604	5.584339	0.975996
H	-5.226910	0.297689	1.635829	**H**	-5.098021	-0.157457	1.796403
H	-5.446979	0.577393	-0.454118	**H**	-5.399348	-0.186654	-0.300388
H	-5.291057	-1.379940	0.342848	**H**	-4.959178	-1.980624	0.731581
H	5.724908	0.197736	0.778340	**H**	5.838233	0.072032	0.546977
H	5.621794	-1.133853	-0.866897	**H**	5.688983	-1.075854	-1.219864
H	5.618383	0.959749	-1.196383	**H**	5.644990	1.036154	-1.323806
H	0.160030	-5.517766	1.127038	**H**	0.298464	-5.446074	1.248147
H	-0.709731	-5.545421	-0.805951	**H**	-1.637188	-5.239399	0.418795
H	1.398555	-5.482859	-0.591661	**H**	0.028087	-5.544145	-0.850871
H	0.626849	-0.533879	-5.644000	**H**	1.011007	-0.039748	-5.587339
H	-1.470801	-0.335657	-5.432476	**H**	-1.005714	-0.685584	-5.561766
H	-0.243245	1.388408	-5.480970	**H**	-0.551000	1.378128	-5.427001
Hf	0.159834	-0.008303	-0.039837	**Hf**	0.241961	0.055366	-0.056109
C	0.520698	-0.092443	4.371051	**C**	0.974798	0.399455	4.292574
O	0.597240	-0.112056	5.530913	**O**	1.166187	0.552981	5.428874

Table S36. Cartesian coordinates of Hf@cage-CHO.

Hf@cage-CHO-doublet				Hf@cage-CHO-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.452703	-1.622550	1.931248	**Te**	-1.604191	-1.563019	1.841314
Te	1.670750	1.803666	-1.955318	**Te**	1.895731	1.798685	-1.831363
Te	-1.702579	-1.764318	-1.524632	**Te**	-1.473290	-1.850862	-1.586976
Te	2.038962	1.873587	1.580593	**Te**	1.879581	1.959364	1.713039
Te	-1.474160	1.819184	1.885228	**Te**	-1.617159	1.913243	1.685017
Te	1.780896	-1.705213	-1.834531	**Te**	1.996237	-1.796440	-1.574426
Te	2.133517	-1.562272	1.619605	**Te**	1.996283	-1.496631	1.887309
Te	-1.722480	1.753469	-1.656102	**Te**	-1.493777	1.750138	-1.860753
Co	-2.425548	0.066274	0.211852	**Co**	-2.367018	0.074870	-0.023936
Co	2.737312	0.146759	-0.238418	**Co**	2.752233	0.153658	0.026856
Co	0.215101	-2.504715	0.127094	**Co**	0.231212	-2.518255	0.237261
Co	0.119607	2.637194	-0.019325	**Co**	0.124959	2.687380	-0.111973
Co	0.391698	0.074681	2.656086	**Co**	0.151164	0.168387	2.677218
Co	-0.071337	-0.034445	-2.603139	**Co**	0.274361	-0.092837	-2.610991
P	-0.273021	-0.270261	-4.781143	**P**	-0.334225	-0.436531	-4.743488
P	0.295136	-4.672112	0.278720	**P**	0.369492	-4.729757	0.588688
P	0.118158	4.791253	0.181004	**P**	0.207275	4.937022	0.000257
P	-4.592831	0.183820	0.237593	**P**	-4.498198	0.174822	-0.441120
P	4.878120	0.309844	-0.553778	**P**	4.916323	0.290957	-0.133259
H	1.145896	5.591696	-0.409732	**H**	1.314002	5.695121	-0.500826
H	-0.973336	5.579500	-0.302127	**H**	-0.793686	5.758008	-0.612623
H	0.180339	5.407680	1.469641	**H**	0.160779	5.602163	1.265575
H	-5.360614	-0.604445	1.152402	**H**	-5.405987	-0.656171	0.288671
H	-5.267378	1.413981	0.515119	**H**	-5.236728	1.387049	-0.266374
H	-5.373074	-0.142903	-0.915693	**H**	-5.029611	-0.129564	-1.732991
H	5.796403	-0.437553	0.249608	**H**	5.759765	-0.633721	0.559708
H	5.479381	-0.031836	-1.806005	**H**	5.578982	0.165648	-1.394476
H	5.557822	1.560493	-0.413305	**H**	5.623728	1.463557	0.278796
H	0.300804	-5.332911	1.548026	**H**	0.068144	-5.318479	1.858943
H	-0.720684	-5.498376	-0.297839	**H**	-0.418672	-5.659425	-0.164340
H	1.395061	-5.410494	-0.261125	**H**	1.598837	-5.443028	0.414914
H	0.661215	0.320856	-5.691561	**H**	0.304960	0.271665	-5.813424
H	-0.254410	-1.560892	-5.400068	**H**	-0.252525	-1.723739	-5.364827
H	-1.436741	0.188135	-5.478597	**H**	-1.668589	-0.161215	-5.172810
Hf	0.157378	0.057461	0.003389	**Hf**	0.196736	0.079346	0.029234
C	0.534619	-0.853019	4.263568	**C**	0.145740	-0.755449	4.293814
O	0.561567	0.005848	5.125095	**O**	0.128306	0.112956	5.145927
H	0.592252	-1.939442	4.492269	**H**	0.159923	-1.841290	4.534138

Table S37. Cartesian coordinates of Hf@cage-OCH_2.

Hf@cage-OCH_2-singlet				Hf@cage-OCH_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.459604	-1.879658	1.772219	**Te**	-1.415114	-1.892830	1.782989
Te	1.760751	1.735303	-1.853673	**Te**	1.744337	1.742994	-1.874219
Te	-1.750007	-1.712617	-1.699025	**Te**	-1.691802	-1.755289	-1.721672
Te	2.062877	1.604179	1.628359	**Te**	2.037029	1.630896	1.629200
Te	-1.403338	1.622029	1.921629	**Te**	-1.437428	1.599612	1.927360
Te	1.732756	-1.729767	-1.955984	**Te**	1.787468	-1.731158	-1.978778
Te	2.005636	-1.881211	1.482882	**Te**	2.061506	-1.862949	1.513014
Te	-1.706383	1.758084	-1.517371	**Te**	-1.710530	1.705013	-1.601295
Co	-2.441187	-0.061648	0.207864	**Co**	-2.392528	-0.087753	0.190508
Co	2.757523	-0.052112	-0.233502	**Co**	2.744027	-0.035272	-0.215987
Co	0.102669	-2.669767	-0.143018	**Co**	0.178432	-2.648491	-0.114138
Co	0.208907	2.543878	0.081096	**Co**	0.148684	2.501449	0.071498
Co	0.382730	-0.182519	2.632848	**Co**	0.407210	-0.179748	2.754770
Co	-0.070792	0.050961	-2.620033	**Co**	-0.034958	0.015890	-2.654765
P	-0.262945	0.167226	-4.769178	**P**	-0.205843	0.090576	-4.867905
P	0.047166	-4.843806	-0.259987	**P**	0.100503	-4.814463	-0.255608
P	0.296651	4.713992	0.187337	**P**	0.091915	4.665816	0.228103
P	-4.599523	-0.073975	0.481249	**P**	-4.547068	-0.046370	0.445636
P	4.931965	-0.016361	-0.332380	**P**	4.910519	0.059337	-0.330787
H	1.487491	5.425758	-0.161068	**H**	0.919641	5.499404	-0.587594
H	-0.584379	5.541530	-0.578195	**H**	-1.115755	5.394100	-0.009627
H	0.085943	5.397271	1.426130	**H**	0.407670	5.318075	1.461146
H	-5.170311	-0.069086	1.792411	**H**	-5.147178	-0.414269	1.690588
H	-5.425167	0.975780	-0.031544	**H**	-5.282516	1.170109	0.289306
H	-5.410530	-1.141327	-0.017897	**H**	-5.414700	-0.840190	-0.369007
H	5.728188	-0.323738	0.815808	**H**	5.722153	-0.195629	0.819498
H	5.657525	-0.863297	-1.229493	**H**	5.651022	-0.789646	-1.212883
H	5.642478	1.177891	-0.672958	**H**	5.580263	1.265791	-0.706915
H	0.814679	-5.659911	0.630292	**H**	0.880299	-5.648595	0.606760
H	-1.175345	-5.565133	-0.082556	**H**	-1.126543	-5.522269	-0.059231
H	0.438622	-5.537103	-1.448673	**H**	0.457454	-5.492183	-1.463465
H	0.653403	-0.507384	-5.636135	**H**	0.669188	-0.649056	-5.727913
H	-1.443933	-0.286447	-5.437104	**H**	-1.404839	-0.309570	-5.542465
H	-0.195321	1.423871	-5.449491	**H**	-0.069057	1.321916	-5.586834
Hf	0.157507	-0.066621	0.002549	**Hf**	0.173203	-0.073674	-0.021554
O	0.166450	0.109016	4.562927	**O**	0.208219	0.116855	4.638922
C	1.078795	-0.801734	4.478291	**C**	1.129830	-0.803564	4.581705
H	2.142302	-0.529702	4.612424	**H**	2.185713	-0.521798	4.727487
H	0.818874	-1.860139	4.665514	**H**	0.862696	-1.851361	4.796719

Table S38. Cartesian coordinates of Hf@cage-OCH_3.

Hf@cage-OCH_3-doublet				Hf@cage-OCH_3-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.235306	-1.883786	1.830044	**Te**	-1.346000	-1.856820	1.767861
Te	1.556483	1.816459	-2.025464	**Te**	1.695114	1.813964	-1.971674
Te	-1.697226	-1.843981	-1.586341	**Te**	-1.673610	-1.749586	-1.724324
Te	1.995809	1.852519	1.470296	**Te**	2.064610	1.726418	1.531303
Te	-1.392537	1.649365	1.911521	**Te**	-1.419088	1.648475	1.875125
Te	1.815600	-1.644780	-2.029076	**Te**	1.755135	-1.654904	-2.080016
Te	2.228667	-1.685009	1.380047	**Te**	2.147534	-1.759499	1.418552
Te	-1.845048	1.612671	-1.598811	**Te**	-1.769601	1.732484	-1.610008
Co	-2.377721	-0.140769	0.284055	**Co**	-2.378821	-0.086941	0.185166
Co	2.738704	0.155175	-0.368498	**Co**	2.746267	0.046962	-0.337328
Co	0.323702	-2.615197	-0.100898	**Co**	0.251267	-2.590949	-0.143468
Co	0.023933	2.588159	-0.055786	**Co**	0.139033	2.561781	0.006648
Co	0.542362	-0.049990	2.690817	**Co**	0.463248	-0.079744	2.737378
Co	-0.143163	-0.065521	-2.662136	**Co**	-0.093421	0.071650	-2.699836
P	-0.362373	-0.294128	-4.822980	**P**	-0.309325	0.222822	-4.902432
P	0.402864	-4.779341	-0.318625	**P**	0.354382	-4.761572	-0.077058
P	-0.117387	4.767757	0.052149	**P**	0.191156	4.733724	0.063446
P	-4.513932	-0.144763	0.686905	**P**	-4.533915	-0.159579	0.448247
P	4.893528	0.382198	-0.518685	**P**	4.908881	0.071902	-0.524391
H	0.758745	5.612661	-0.700243	**H**	1.371762	5.447716	-0.312295
H	-1.315048	5.456890	-0.319191	**H**	-0.704924	5.528476	-0.718962
H	0.057462	5.463948	1.289881	**H**	-0.019551	5.447390	1.285028
H	-5.019863	-0.376141	2.004574	**H**	-5.119741	-0.122457	1.752585
H	-5.321916	1.006731	0.429315	**H**	-5.386915	0.840098	-0.116182
H	-5.386501	-1.074232	0.037526	**H**	-5.299516	-1.274058	-0.017070
H	5.732456	0.247722	0.631940	**H**	5.745538	0.215180	0.627099
H	5.671135	-0.475897	-1.358798	**H**	5.615845	-1.044494	-1.071496
H	5.485229	1.600233	-0.978762	**H**	5.581994	1.059980	-1.309668
H	1.474796	-5.547194	0.237453	**H**	0.451921	-5.458380	1.168637
H	-0.640009	-5.616662	0.189703	**H**	-0.698822	-5.572327	-0.605982
H	0.451954	-5.397683	-1.607886	**H**	1.414000	-5.477146	-0.718084
H	-0.381262	-1.581126	-5.449505	**H**	0.616493	-0.409049	-5.794760
H	-1.517348	0.200221	-5.509434	**H**	-1.477039	-0.251997	-5.583357
H	0.585148	0.276496	-5.731682	**H**	-0.282448	1.486784	-5.576014
Hf	0.176178	-0.006391	-0.061895	**Hf**	0.182594	-0.014120	-0.078028
O	0.821768	-0.374623	4.451780	**O**	0.644420	-0.569284	4.471130
C	1.087568	-1.606147	5.074002	**C**	0.777817	-1.775059	5.165147
H	0.442766	-2.417267	4.690780	**H**	-0.081170	-2.445036	4.972667
H	2.138866	-1.911503	4.919676	**H**	1.697188	-2.310627	4.863134
H	0.912904	-1.507046	6.159955	**H**	0.829696	-1.582153	6.250994

Table S39. Cartesian coordinates of Hf@cage-CH_3OH.

Hf@cage-CH_3OH-singlet				Hf@cage-CH_3OH-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.409264	-2.019819	1.775750	**Te**	-1.166775	-2.042306	1.968609
Te	1.896764	1.781881	-1.547969	**Te**	1.797570	1.718426	-1.755366
Te	-1.597320	-1.673098	-1.635106	**Te**	-1.676137	-1.753132	-1.509180
Te	2.119877	1.488568	1.952516	**Te**	2.227996	1.568975	1.729631
Te	-1.373069	1.502089	2.128067	**Te**	-1.179338	1.533908	2.211578
Te	1.897403	-1.644140	-1.864413	**Te**	1.807438	-1.728226	-1.969590
Te	2.106611	-2.008004	1.598556	**Te**	2.240656	-2.018625	1.514183
Te	-1.564746	1.811758	-1.325984	**Te**	-1.688327	1.674528	-1.288565
Co	-2.348110	-0.081415	0.275678	**Co**	-2.240226	-0.161719	0.503930
Co	2.865377	-0.084378	-0.007967	**Co**	2.843331	-0.109845	-0.184310
Co	0.261878	-2.691818	-0.141377	**Co**	0.292790	-2.719121	-0.075162
Co	0.286990	2.505090	0.368627	**Co**	0.277622	2.459893	0.253925
Co	0.385607	-0.358963	2.669094	**Co**	0.659199	-0.303940	2.719972
Co	0.087772	0.142303	-2.455797	**Co**	-0.048366	0.033724	-2.487592
P	-0.230099	0.147359	-4.577330	**P**	-0.255408	0.203398	-4.683723
P	0.325920	-4.851318	-0.352238	**P**	0.215549	-4.862782	-0.410775
P	0.380515	4.675713	0.393575	**P**	0.210253	4.628572	0.167198
P	-4.510650	-0.035114	0.467948	**P**	-4.361516	-0.208319	0.958173
P	5.032838	-0.026982	-0.149412	**P**	5.008798	-0.113808	-0.236128
H	1.587637	5.365816	0.729581	**H**	0.202772	5.319061	-1.085309
H	0.111882	5.440033	-0.785449	**H**	-0.883527	5.357834	0.731133
H	-0.464275	5.447780	1.252278	**H**	1.233414	5.433800	0.761240
H	-5.149288	-0.448773	1.678949	**H**	-4.835741	-0.270765	2.306061
H	-5.244750	1.185985	0.337951	**H**	-5.223602	0.860343	0.556515
H	-5.358577	-0.795044	-0.399106	**H**	-5.199514	-1.258171	0.466298
H	5.857882	-0.697735	0.807558	**H**	5.780889	-0.151056	0.967206
H	5.721771	-0.528533	-1.298970	**H**	5.731422	-1.155881	-0.897850
H	5.745424	1.212507	-0.096706	**H**	5.734895	0.964395	-0.833465
H	1.565412	-5.564205	-0.311242	**H**	1.245777	-5.726239	0.079256
H	-0.351081	-5.701938	0.577431	**H**	-0.871457	-5.652575	0.079598
H	-0.168242	-5.509410	-1.523240	**H**	0.195953	-5.409415	-1.732315
H	-0.057063	-1.038898	-5.357882	**H**	0.870515	0.030833	-5.551609
H	-1.494602	0.505692	-5.141797	**H**	-1.125918	-0.646762	-5.440425
H	0.553448	0.994463	-5.423149	**H**	-0.702284	1.416953	-5.299518
Hf	0.264564	-0.101408	0.198916	**Hf**	0.297459	-0.128893	0.117745
C	0.711642	-0.436494	5.222559	**C**	0.944104	-0.168625	5.251223
H	1.612775	-0.939859	4.838346	**H**	1.810670	-0.199446	4.540748
H	0.325881	-1.018791	6.069467	**H**	1.229661	-0.783204	6.114861
H	-0.144225	-0.478984	4.470234	**H**	0.056293	-0.666366	4.786399
O	0.951092	0.884323	5.672778	**O**	0.660900	1.136501	5.709595
H	1.269101	1.386361	4.898333	**H**	0.342911	1.640683	4.934854

Table S40. Cartesian coordinates of Ce@cage.

Ce@cage-singlet				Ce@cage-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.779109	-1.675478	2.020830	**Te**	-1.548104	-1.768376	2.087672
Te	1.816712	1.632634	-1.934903	**Te**	1.628567	1.657673	-2.078424
Te	-1.811410	-1.929036	-1.664113	**Te**	-1.942955	-1.972242	-1.497959
Te	1.865981	2.003977	1.530910	**Te**	1.827678	2.008797	1.554232
Te	-1.894568	1.959217	1.602038	**Te**	-1.638468	1.919660	1.820524
Te	1.779719	-1.903218	-1.743137	**Te**	1.716003	-1.943317	-1.821078
Te	1.844652	-1.658643	1.935672	**Te**	1.901092	-1.743145	1.821998
Te	-1.967939	1.560964	-1.918521	**Te**	-2.014525	1.565586	-1.772475
Co	-2.640223	-0.074600	0.025294	**Co**	-2.531157	-0.066485	0.274784
Co	2.605082	-0.022462	-0.089886	**Co**	2.559656	0.009648	-0.156467
Co	0.058771	-2.604831	0.196111	**Co**	0.049508	-2.646942	0.154666
Co	-0.063780	2.568446	-0.401720	**Co**	-0.070440	2.566241	-0.246471
Co	0.023781	0.251423	2.394959	**Co**	0.222639	0.164721	2.582990
Co	-0.084314	-0.230832	-2.690806	**Co**	-0.226597	-0.326690	-2.646249
P	0.087587	0.751103	-4.587690	**P**	-0.181078	0.025974	-4.846122
P	-0.044871	-4.767696	-0.003280	**P**	0.077818	-4.787579	-0.245878
P	-0.096520	4.767673	-0.419541	**P**	-0.133495	4.740911	-0.634159
P	-4.801431	-0.388427	0.155753	**P**	-4.663631	-0.014148	0.779818
P	4.755112	-0.336666	0.135255	**P**	4.721631	0.116549	0.150215
H	0.958537	5.523127	-1.022723	**H**	0.981806	5.580171	-0.320817
H	-1.159970	5.500573	-1.035607	**H**	-0.322722	5.256505	-1.954175
H	-0.111546	5.505695	0.803952	**H**	-1.113192	5.582965	-0.019245
H	-5.551390	0.116672	1.263018	**H**	-5.120284	-0.036893	2.133540
H	-5.678631	0.117841	-0.855205	**H**	-5.472940	1.091377	0.371903
H	-5.367214	-1.700680	0.187429	**H**	-5.553610	-1.030518	0.309306
H	5.331959	-1.642623	0.077146	**H**	5.300641	0.198101	1.453287
H	5.674518	0.267582	-0.781031	**H**	5.568332	-0.934091	-0.324106
H	5.440699	0.072077	1.320464	**H**	5.476893	1.190191	-0.416437
H	0.954876	-5.592444	0.602554	**H**	1.209435	-5.579510	0.125212
H	-1.167704	-5.498447	0.496578	**H**	-0.905827	-5.649584	0.334141
H	-0.010261	-5.408407	-1.280571	**H**	-0.035982	-5.306124	-1.572036
H	1.247157	0.578187	-5.406822	**H**	0.997389	-0.228247	-5.616529
H	-0.873625	0.351824	-5.571707	**H**	-1.072050	-0.678686	-5.720048
H	-0.045480	2.159952	-4.774611	**H**	-0.433074	1.316965	-5.404678
Ce	-0.021142	0.015570	0.095198	**Ce**	0.015058	-0.009414	0.000352

Table S41. Cartesian coordinates of Ce@cage-CO_2.

Ce@cage-CO_2-singlet				Ce@cage-CO_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-2.033999	-1.789819	1.726748	**Te**	-1.411797	-1.900353	2.005884
Te	1.890858	1.623312	-1.821804	**Te**	1.755604	1.690794	-2.039349
Te	-1.744270	-1.939573	-1.895242	**Te**	-1.887276	-1.892927	-1.585407
Te	1.656676	1.870681	1.803283	**Te**	2.048334	1.818944	1.610504
Te	-2.071209	1.957357	1.510720	**Te**	-1.427584	1.799620	1.944592
Te	1.769321	-1.869908	-1.622968	**Te**	1.758477	-1.914873	-1.988328
Te	1.543768	-1.743581	2.019854	**Te**	2.033208	-1.926079	1.667768
Te	-1.818607	1.760566	-1.949827	**Te**	-1.873465	1.676399	-1.634210
Co	-2.718355	-0.032345	-0.309597	**Co**	-2.389032	-0.081144	0.311112
Co	2.489799	-0.045405	0.158742	**Co**	2.688717	-0.082365	-0.231007
Co	-0.117249	-2.613679	0.089769	**Co**	0.109880	-2.699222	-0.007589
Co	-0.041377	2.604120	-0.267625	**Co**	0.117925	2.528474	-0.104966
Co	-0.317717	0.141097	2.395549	**Co**	0.423428	-0.036346	2.589861
Co	0.105878	-0.179773	-2.684962	**Co**	-0.140651	-0.201960	-2.667545
P	-0.504534	0.521373	-4.613568	**P**	-0.407710	0.236866	-4.831648
P	0.122865	-4.775723	-0.001780	**P**	0.153664	-4.820054	-0.505862
P	0.275474	4.775576	-0.150578	**P**	0.184461	4.724550	-0.321656
P	-4.887251	-0.320266	-0.168154	**P**	-4.504474	-0.126841	0.879640
P	4.653275	-0.319477	0.238102	**P**	4.864797	-0.099865	-0.004629
H	1.581724	5.340609	-0.275026	**H**	1.380845	5.457476	-0.044508
H	-0.353028	5.671220	-1.074400	**H**	-0.072294	5.356004	-1.578944
H	-0.085667	5.508336	1.021888	**H**	-0.678167	5.578715	0.436248
H	-5.598170	0.000824	1.028590	**H**	-4.921039	-0.057827	2.244728
H	-5.779759	0.365978	-1.053328	**H**	-5.397921	0.882849	0.403231
H	-5.477124	-1.610040	-0.343138	**H**	-5.333493	-1.237224	0.530096
H	5.417519	0.275083	1.290032	**H**	5.495938	-0.075728	1.276779
H	5.242517	-1.617531	0.346870	**H**	5.645255	-1.175200	-0.533252
H	5.496622	0.128350	-0.827156	**H**	5.647597	0.951285	-0.576332
H	1.344935	-5.407029	0.388466	**H**	1.309966	-5.615474	-0.230754
H	-0.733313	-5.623887	0.769118	**H**	-0.790682	-5.717429	0.086957
H	-0.023778	-5.495476	-1.228920	**H**	-0.026357	-5.279749	-1.846874
H	0.208351	-0.156920	-5.656944	**H**	0.530412	-0.249197	-5.797829
H	-1.813783	0.348665	-5.158442	**H**	-1.572343	-0.190339	-5.546033
H	-0.297265	1.849311	-5.096908	**H**	-0.429422	1.577863	-5.326089
Ce	-0.131862	0.021635	0.078919	**Ce**	0.151000	-0.061448	-0.011556
C	0.887157	0.274183	5.470404	**C**	-1.047820	0.404809	5.502827
O	-0.232092	0.281139	5.117490	**O**	-2.122870	0.729887	5.825199
O	1.995785	0.268565	5.843016	**O**	0.037008	0.074654	5.196136

Table S42. Cartesian coordinates of Ce@cage-COOH.

Ce@cage-COOH-doublet				Ce@cage-COOH-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.047462	-1.924049	2.118925	**Te**	-1.229481	-1.901477	2.282540
Te	1.753018	1.745792	-2.109896	**Te**	1.798491	1.802250	-1.919220
Te	-1.720341	-1.973195	-1.423942	**Te**	-1.577100	-2.050461	-1.763282
Te	2.280026	1.872104	1.502005	**Te**	2.115399	1.833454	1.658968
Te	-1.158608	1.837776	2.077094	**Te**	-1.667514	1.445547	1.950686
Te	1.848817	-1.757465	-2.064088	**Te**	1.848499	-1.941796	-1.872680
Te	2.378941	-1.747442	1.567369	**Te**	2.142945	-1.781977	1.808857
Te	-1.840713	1.739657	-1.422874	**Te**	-1.989893	1.390959	-1.550222
Co	-2.216363	-0.088209	0.540006	**Co**	-2.279138	-0.626330	0.292018
Co	2.813074	0.057142	-0.381368	**Co**	2.773436	-0.037290	-0.163641
Co	0.409440	-2.622692	0.032910	**Co**	0.070849	-2.601196	0.160172
Co	0.248403	2.567346	-0.044988	**Co**	-0.041589	2.381895	0.054363
Co	0.680333	0.024778	2.691105	**Co**	0.440539	0.096423	2.759413
Co	-0.126169	-0.134574	-2.610027	**Co**	-0.009368	-0.153173	-2.639216
P	-1.076082	0.298973	-4.558499	**P**	-0.144254	0.495804	-4.751429
P	0.700885	-4.765926	-0.264549	**P**	-0.036933	-4.826493	0.293346
P	0.386060	4.744741	-0.260782	**P**	-0.163243	4.634834	0.156991
P	-4.380418	-0.160207	1.020112	**P**	-4.401882	-1.161770	0.465817
P	4.994325	0.022490	-0.288853	**P**	4.980564	-0.153894	-0.401396
H	1.641667	5.426039	-0.213517	**H**	0.876805	5.450995	-0.387831
H	-0.093970	5.415301	-1.428832	**H**	-1.236663	5.378931	-0.428428
H	-0.274985	5.598652	0.677102	**H**	-0.212053	5.304748	1.419453
H	-4.834554	-0.223465	2.374003	**H**	-5.174298	-0.667551	1.562236
H	-5.257251	0.898689	0.627207	**H**	-5.333441	-0.783420	-0.550020
H	-5.214330	-1.218024	0.541135	**H**	-4.855600	-2.514582	0.574319
H	5.684036	0.116990	0.958315	**H**	5.850104	0.606320	0.442685
H	5.738706	-1.092245	-0.787186	**H**	5.698099	-1.383661	-0.263924
H	5.757440	1.028083	-0.961680	**H**	5.605337	0.233121	-1.628024
H	0.038964	-5.684854	0.609270	**H**	0.583415	-5.523723	1.376658
H	0.317537	-5.413190	-1.479180	**H**	-1.284067	-5.523984	0.381855
H	1.989657	-5.377836	-0.174593	**H**	0.507626	-5.653931	-0.737882
H	-0.641791	-0.429275	-5.714296	**H**	0.949425	0.288888	-5.650699
H	-2.474550	0.112645	-4.785223	**H**	-1.147885	-0.024355	-5.633068
H	-1.002532	1.590436	-5.166592	**H**	-0.352620	1.865682	-5.101791
Ce	0.257338	-0.027398	0.026548	**Ce**	0.264030	-0.041463	0.039173
C	0.038326	0.033540	4.452571	**C**	0.477193	1.149728	4.314206
O	1.021998	0.068198	5.178496	**O**	0.691953	0.407676	5.262534
O	-1.233291	0.004214	4.934938	**O**	0.300691	2.493787	4.463408
H	-1.151065	0.015608	5.913796	**H**	0.396134	2.670630	5.424995

Table S43. Cartesian coordinates of Ce@cage-CO.

Ce@cage-CO-singlet				Ce@cage-CO-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.446628	-1.773708	1.966016	**Te**	-1.141308	-1.637200	2.280739
Te	1.788766	1.893057	-1.917866	**Te**	1.777023	1.867547	-2.101476
Te	-1.775090	-1.842180	-1.674084	**Te**	-1.713710	-1.796863	-1.776491
Te	2.074756	1.810432	1.636138	**Te**	2.260777	1.969019	1.436178
Te	-1.555048	1.783681	1.926836	**Te**	-1.400019	1.758534	1.985897
Te	1.792129	-1.761738	-1.997381	**Te**	1.713876	-1.859460	-2.026567
Te	2.063083	-1.708631	1.682298	**Te**	2.210000	-1.719320	1.611969
Te	-1.889080	1.846038	-1.577634	**Te**	-1.915550	1.650122	-1.636091
Co	-2.442000	-0.039204	0.224761	**Co**	-2.267731	-0.355884	0.322759
Co	2.708336	0.033279	-0.218705	**Co**	2.769566	-0.016857	-0.356133
Co	0.189092	-2.552159	0.001687	**Co**	-0.044293	-2.498967	0.095848
Co	0.112517	2.606471	0.045158	**Co**	0.070510	2.591768	-0.066093
Co	0.344057	0.079314	2.648073	**Co**	0.676372	0.213154	2.626942
Co	-0.104802	0.045617	-2.611478	**Co**	-0.070642	0.017266	-2.660139
P	-0.381110	0.412192	-4.781223	**P**	-0.088761	0.295213	-4.832455
P	0.414315	-4.733611	0.033888	**P**	-0.350171	-4.685072	0.261538
P	0.207316	4.785930	0.223519	**P**	-0.101152	4.826980	-0.064487
P	-4.593036	-0.449514	0.268171	**P**	-4.418821	-0.753523	0.652427
P	4.860722	-0.289489	-0.467788	**P**	4.989706	-0.085337	-0.661849
H	1.331849	5.518331	-0.266423	**H**	0.479674	5.625790	-1.099372
H	-0.787578	5.606819	-0.392019	**H**	-1.373266	5.480704	-0.086649
H	0.158873	5.427276	1.499895	**H**	0.428396	5.599878	1.015746
H	-5.419679	0.176293	1.253182	**H**	-5.084122	-0.244892	1.811044
H	-5.423642	-0.131155	-0.849884	**H**	-5.397600	-0.298711	-0.284820
H	-5.104916	-1.768509	0.460862	**H**	-4.942875	-2.080744	0.765181
H	5.783514	0.302947	0.449947	**H**	5.885138	0.404945	0.339575
H	5.434579	-1.596927	-0.430037	**H**	5.681691	-1.319921	-0.868946
H	5.536905	0.134677	-1.653976	**H**	5.612457	0.603553	-1.749585
H	-0.095247	-5.521846	1.111844	**H**	0.301370	-5.436047	1.288515
H	-0.139502	-5.536028	-1.010919	**H**	-1.643910	-5.260984	0.470064
H	1.707544	-5.340752	0.011006	**H**	0.017910	-5.558237	-0.808919
H	0.512604	-0.165875	-5.736983	**H**	1.084988	0.089796	-5.622095
H	-1.579489	0.015778	-5.451519	**H**	-0.956024	-0.485041	-5.662739
H	-0.342341	1.729411	-5.332589	**H**	-0.431423	1.554168	-5.415507
Ce	0.125854	0.021252	-0.085138	**Ce**	0.273603	0.088890	-0.071044
C	0.467534	0.245776	4.399590	**C**	1.009260	0.459175	4.345608
O	0.568872	0.357679	5.551849	**O**	1.203086	0.617486	5.480498

Table S44. Cartesian coordinates of Ce@cage-CHO.

Ce@cage-CHO-doublet				Ce@cage-CHO-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.521177	-1.610965	2.047617	**Te**	-1.509410	-1.643371	1.917939
Te	1.643685	1.914984	-2.042340	**Te**	1.738322	1.926373	-2.001243
Te	-1.912872	-1.747062	-1.523764	**Te**	-1.820472	-1.753417	-1.671244
Te	2.122598	1.942157	1.566754	**Te**	2.215024	1.871300	1.582179
Te	-1.485005	1.906412	1.988538	**Te**	-1.434634	1.877234	1.930245
Te	1.784826	-1.726293	-1.911452	**Te**	1.767880	-1.796446	-1.953977
Te	2.215947	-1.575857	1.637825	**Te**	2.213698	-1.691084	1.564992
Te	-1.835572	1.885107	-1.647426	**Te**	-1.767451	1.926440	-1.706398
Co	-2.460610	0.130798	0.282625	**Co**	-2.373441	0.125597	0.159657
Co	2.703335	0.163738	-0.313469	**Co**	2.738907	0.080944	-0.310988
Co	0.179613	-2.466291	0.125405	**Co**	0.185109	-2.593464	-0.019650
Co	0.114511	2.662762	-0.027525	**Co**	0.250729	2.768977	-0.054652
Co	0.425997	0.107871	2.654953	**Co**	0.454584	0.025618	2.589664
Co	-0.245760	0.062483	-2.631736	**Co**	-0.158827	0.074872	-2.679903
P	-0.058821	-0.595862	-4.730246	**P**	0.295197	-0.157141	-4.843547
P	0.243434	-4.681939	0.172470	**P**	-0.085193	-4.735025	0.583404
P	0.045504	4.803822	0.387714	**P**	-0.096218	4.897534	0.574720
P	-4.628396	0.371947	0.227815	**P**	-4.571933	0.173418	0.187412
P	4.851160	0.382417	-0.694911	**P**	4.817488	0.237368	-0.980163
H	0.961593	5.693169	-0.257379	**H**	0.601273	5.977569	-0.061400
H	-1.130244	5.571670	0.118156	**H**	-1.386693	5.509444	0.509663
H	0.252035	5.303031	1.709812	**H**	0.188260	5.316374	1.910430
H	-5.442161	-0.469604	1.049759	**H**	-5.318486	-0.838915	0.868459
H	-5.262358	1.598912	0.596542	**H**	-5.283544	1.279313	0.748112
H	-5.377783	0.176851	-0.973257	**H**	-5.326878	0.115894	-1.024267
H	5.786655	-0.400431	0.051211	**H**	5.790133	-0.670912	-0.455829
H	5.419616	0.103313	-1.976767	**H**	5.192681	0.085587	-2.349839
H	5.526302	1.628376	-0.509544	**H**	5.578860	1.424645	-0.748765
H	0.065515	-5.418262	1.386153	**H**	0.212593	-5.188762	1.905910
H	-0.668130	-5.468399	-0.599462	**H**	-1.354334	-5.390533	0.499286
H	1.417961	-5.383654	-0.242016	**H**	0.646321	-5.770872	-0.083993
H	1.128584	-0.367369	-5.493498	**H**	1.610237	0.044317	-5.365099
H	-0.215758	-1.963081	-5.115063	**H**	0.059330	-1.387262	-5.535274
H	-0.962578	-0.063844	-5.707308	**H**	-0.366609	0.674838	-5.804361
Ce	0.129462	0.063820	0.019043	**Ce**	0.180417	0.072928	-0.024887
C	0.578801	-0.875538	4.230193	**C**	0.563400	-0.979896	4.154593
O	0.612310	-0.050589	5.121739	**O**	0.601356	-0.172025	5.060818
H	0.638880	-1.970972	4.408540	**H**	0.593422	-2.079830	4.313697

Table S45. Cartesian coordinates of Ce@cage-OCH_2.

Ce@cage-OCH_2-singlet				Ce@cage-OCH_2-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.493322	-1.867326	1.898041	**Te**	-1.535040	-1.895734	1.802004
Te	1.897015	1.624247	-2.007037	**Te**	1.773725	1.824786	-1.961794
Te	-1.788731	-1.850636	-1.761124	**Te**	-1.799396	-1.781522	-1.790870
Te	2.177745	1.715009	1.481200	**Te**	2.048402	1.725260	1.640842
Te	-1.472256	1.728285	1.830550	**Te**	-1.538630	1.726339	1.887588
Te	1.746096	-1.951695	-1.994669	**Te**	1.817080	-1.768885	-2.018751
Te	2.018468	-1.930511	1.620372	**Te**	2.032844	-1.862615	1.605314
Te	-1.784554	1.683726	-1.705911	**Te**	-1.793300	1.785470	-1.722336
Co	-2.424774	-0.103427	0.131263	**Co**	-2.440954	-0.053503	0.116534
Co	2.757903	-0.173227	-0.261898	**Co**	2.695788	-0.020118	-0.203445
Co	0.065455	-2.695013	-0.042155	**Co**	0.131718	-2.604809	-0.095996
Co	0.207643	2.487246	-0.167569	**Co**	0.127463	2.538144	-0.016196
Co	0.379615	-0.052911	2.616900	**Co**	0.319661	-0.098611	2.768778
Co	-0.039320	-0.106482	-2.695208	**Co**	-0.051471	0.026644	-2.680808
P	-0.142888	0.656918	-4.712085	**P**	-0.068022	-0.102534	-4.888037
P	-0.090858	-4.887023	-0.147767	**P**	0.222807	-4.768426	-0.450800
P	0.127826	4.675260	0.059357	**P**	0.081864	4.715169	0.278425
P	-4.569925	-0.286304	0.525244	**P**	-4.564710	0.043755	0.645084
P	4.947418	-0.442759	-0.313409	**P**	4.886737	-0.088796	-0.336839
H	0.980591	5.532671	-0.705388	**H**	1.033900	5.570288	-0.358392
H	-1.075339	5.401975	-0.201395	**H**	-1.070548	5.474548	-0.092433
H	0.396751	5.293991	1.318547	**H**	0.221316	5.284608	1.581259
H	-5.119831	0.045702	1.801668	**H**	-4.995911	-0.057141	2.003018
H	-5.499198	0.484961	-0.241416	**H**	-5.334552	1.205156	0.327442
H	-5.265153	-1.527534	0.387671	**H**	-5.497408	-0.904640	0.119399
H	5.741001	-0.211769	0.852917	**H**	5.698466	0.065367	0.830430
H	5.543264	-1.700451	-0.638803	**H**	5.557772	-1.253101	-0.825351
H	5.766606	0.330814	-1.194814	**H**	5.611755	0.845219	-1.141704
H	0.685062	-5.714021	0.724112	**H**	1.397783	-5.512671	-0.118565
H	-1.329799	-5.561654	0.084932	**H**	-0.700558	-5.662341	0.178315
H	0.230694	-5.600191	-1.344276	**H**	0.075335	-5.307150	-1.766003
H	0.868194	0.309417	-5.662295	**H**	1.111470	0.164366	-5.653851
H	-1.259947	0.303618	-5.532954	**H**	-0.389133	-1.326371	-5.557583
H	-0.164477	2.052717	-5.011969	**H**	-0.933650	0.717500	-5.680792
Ce	0.180778	-0.093542	-0.030275	**Ce**	0.129332	-0.034570	-0.051095
O	0.336682	0.472816	4.515615	**O**	0.072425	0.221257	4.640426
C	1.235102	-0.453220	4.477722	**C**	0.986234	-0.709852	4.615235
H	2.306633	-0.182495	4.483399	**H**	2.040163	-0.436819	4.788123
H	0.986958	-1.475480	4.815470	**H**	0.702366	-1.751963	4.835994

Table S46. Cartesian coordinates of Ce@cage-OCH_3.

Ce@cage-OCH_3-doublet				Ce@cage-OCH_3-quartet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.262406	-1.915145	1.896286	**Te**	-1.387028	-1.953760	1.755090
Te	1.580774	1.893985	-2.139284	**Te**	1.760017	1.883058	-2.011160
Te	-1.763637	-1.877763	-1.621449	**Te**	-1.698439	-1.812491	-1.793780
Te	2.049635	1.957099	1.470074	**Te**	2.112045	1.762895	1.627820
Te	-1.424883	1.739498	1.940932	**Te**	-1.422780	1.664417	1.964460
Te	1.868418	-1.651660	-2.103086	**Te**	1.866096	-1.694621	-2.140900
Te	2.319763	-1.687195	1.417605	**Te**	2.258798	-1.823963	1.417840
Te	-1.929190	1.671502	-1.669540	**Te**	-1.804485	1.782185	-1.654190
Co	-2.365147	-0.132872	0.286201	**Co**	-2.347008	-0.095666	0.166000
Co	2.732757	0.183279	-0.399774	**Co**	2.772753	0.066018	-0.323110
Co	0.347901	-2.578897	-0.074184	**Co**	0.291943	-2.591709	-0.188870
Co	0.018979	2.598693	-0.110291	**Co**	0.142531	2.546826	0.043130
Co	0.563128	0.023692	2.737840	**Co**	0.494987	-0.127539	2.772100
Co	-0.170595	-0.025247	-2.700718	**Co**	-0.057375	0.065495	-2.708410
P	-0.352881	-0.468734	-4.850130	**P**	-0.350388	0.149865	-4.902100
P	0.458327	-4.743648	-0.460595	**P**	0.406627	-4.782988	0.005540
P	-0.128548	4.803550	0.019009	**P**	0.176315	4.747069	-0.103460
P	-4.484910	-0.076823	0.847796	**P**	-4.490130	0.002370	0.599610
P	4.906326	0.463963	-0.449888	**P**	4.951380	0.277985	-0.451450
H	0.763655	5.650584	-0.710200	**H**	1.392816	5.479507	0.060260
H	-1.320339	5.489673	-0.372761	**H**	-0.227655	5.407095	-1.305200
H	0.020502	5.486864	1.266263	**H**	-0.601325	5.563656	0.777370
H	-4.897989	-0.226679	2.207153	**H**	-4.991841	-0.230840	1.917060
H	-5.294890	1.067543	0.572425	**H**	-5.243306	1.193502	0.363410
H	-5.396990	-1.037533	0.308528	**H**	-5.395107	-0.882202	-0.065680
H	5.690763	0.391064	0.742153	**H**	5.775890	0.105553	0.703190
H	5.728873	-0.414737	-1.222200	**H**	5.707891	-0.584834	-1.304330
H	5.487871	1.676122	-0.934286	**H**	5.563372	1.492738	-0.890340
H	1.634657	-5.487770	-0.132313	**H**	0.513787	-5.414741	1.283370
H	-0.460817	-5.650740	0.154540	**H**	-0.650546	-5.616065	-0.477950
H	0.318959	-5.274701	-1.779818	**H**	1.465254	-5.521897	-0.609080
H	-0.379807	-1.805852	-5.356729	**H**	0.319454	-0.755370	-5.785010
H	-1.489914	-0.018486	-5.593985	**H**	-1.644326	-0.027609	-5.485770
H	0.621391	0.009110	-5.782759	**H**	-0.028598	1.328059	-5.648310
Ce	0.180915	0.009743	-0.073898	**Ce**	0.212311	-0.018236	-0.084190
O	0.822797	-0.470865	4.459181	**O**	0.633170	-0.750231	4.465750
C	0.981017	-1.720235	5.073705	**C**	0.641719	-2.028460	5.034370
H	0.109911	-2.375793	4.890465	**H**	-0.354796	-2.502832	4.967060
H	1.880784	-2.243576	4.701461	**H**	1.366268	-2.692564	4.527410
H	1.086829	-1.580984	6.163993	**H**	0.921693	-1.959652	6.100170

Table S47. Cartesian coordinates of Ce@cage-CH_3OH.

Ce@cage-CH_3OH-singlet				Ce@cage-CH_3OH-triplet			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.546332	-2.161482	1.592076	**Te**	-1.184583	-2.110532	2.043247
Te	2.006558	1.907902	-1.523635	**Te**	1.791203	1.777947	-1.859418
Te	-1.634913	-1.652410	-1.815505	**Te**	-1.773369	-1.825573	-1.540186
Te	2.116580	1.489609	2.101232	**Te**	2.249664	1.648054	1.742481
Te	-1.496116	1.535238	2.142433	**Te**	-1.203410	1.568422	2.261817
Te	2.049766	-1.557260	-2.021305	**Te**	1.801638	-1.833893	-2.075508
Te	2.126462	-2.144399	1.544127	**Te**	2.259485	-2.120130	1.527551
Te	-1.562823	1.997063	-1.433803	**Te**	-1.792258	1.690996	-1.328776
Co	-2.348473	-0.034504	0.075002	**Co**	-2.231498	-0.185841	0.517855
Co	2.855455	-0.075330	0.023213	**Co**	2.822078	-0.126582	-0.253849
Co	0.273445	-2.638854	-0.388489	**Co**	0.272197	-2.761010	-0.094758
Co	0.271072	2.511215	0.417931	**Co**	0.253561	2.461407	0.204512
Co	0.290362	-0.440118	2.491016	**Co**	0.685450	-0.308130	2.683465
Co	0.215624	0.332295	-2.560836	**Co**	-0.106446	-0.010652	-2.507068
P	-0.547899	-0.188151	-4.491276	**P**	-0.154887	0.288737	-4.706233
P	0.516681	-4.809304	-0.609751	**P**	0.076521	-4.893737	-0.525680
P	0.511623	4.677077	0.376681	**P**	0.063119	4.641181	0.054462
P	-4.501983	0.123889	0.447110	**P**	-4.373704	-0.271014	1.001644
P	5.031919	0.096910	-0.015871	**P**	4.992125	-0.131780	-0.019391
H	1.752126	5.294995	0.725221	**H**	0.001688	5.295695	-1.214484
H	0.301447	5.431271	-0.819099	**H**	-1.053029	5.330140	0.623045
H	-0.308669	5.493473	1.217238	**H**	1.061672	5.501836	0.609986
H	-5.061831	-0.234033	1.711444	**H**	-4.843962	-0.284064	2.351500
H	-5.184321	1.374450	0.335149	**H**	-5.263396	0.753410	0.549580
H	-5.436255	-0.621725	-0.340082	**H**	-5.177430	-1.367065	0.558422
H	5.825391	-0.505803	1.008884	**H**	5.615404	-0.203689	1.263141
H	5.789770	-0.418894	-1.113834	**H**	5.779637	-1.157345	-0.630170
H	5.683130	1.368455	0.022914	**H**	5.765528	0.969261	-0.503211
H	1.812335	-5.400029	-0.727585	**H**	1.081571	-5.813283	-0.088697
H	0.042616	-5.704777	0.398247	**H**	-1.034871	-5.651657	-0.041775
H	-0.061259	-5.517750	-1.711912	**H**	0.008912	-5.381432	-1.867252
H	-0.399453	-1.471011	-5.101454	**H**	1.027543	0.165850	-5.501163
H	-1.895916	0.036920	-4.907574	**H**	-0.972836	-0.527774	-5.552480
H	0.083847	0.573345	-5.528573	**H**	-0.571627	1.533707	-5.274977
Ce	0.252911	-0.092561	0.184119	**Ce**	0.296057	-0.147457	0.109266
C	0.637553	-0.455380	5.467775	**C**	1.102745	-0.136177	5.294272
H	1.433710	-1.138052	5.123354	**H**	1.854283	-0.335084	4.485368
H	0.231566	-0.838515	6.413115	**H**	1.439108	-0.708540	6.168702
H	-0.197478	-0.474535	4.725801	**H**	0.112610	-0.539185	4.991859
O	1.109141	0.864036	5.707500	**O**	1.053098	1.230563	5.657648
H	1.423326	1.209335	4.848057	**H**	0.731110	1.717024	4.874306

Table S48. Cartesian coordinates of Th@cage.

	Th@cage				Th@cage		
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.771725	-1.664872	2.032493	**Te**	-1.750518	-1.794706	2.001472
Te	1.859732	1.620186	-2.034980	**Te**	1.740469	1.747100	-1.968412
Te	-1.818558	-2.009592	-1.706414	**Te**	-1.951032	-1.881957	-1.706912
Te	1.851342	2.034633	1.549469	**Te**	1.868360	1.874648	1.747768
Te	-1.848884	2.005005	1.600607	**Te**	-1.713213	1.892756	1.886210
Te	1.797725	-1.974335	-1.753838	**Te**	1.715310	-1.906556	-1.857236
Te	1.840058	-1.636929	1.986766	**Te**	1.816734	-1.807304	1.860945
Te	-1.946911	1.597635	-1.967333	**Te**	-1.909270	1.775301	-1.820821
Co	-2.644814	-0.067893	-0.031815	**Co**	-2.591872	0.003071	0.139115
Co	2.635769	-0.024316	-0.096608	**Co**	2.549110	-0.025465	-0.066971
Co	0.025182	-2.598775	0.197365	**Co**	-0.055730	-2.648162	0.075364
Co	-0.024905	2.577920	-0.418262	**Co**	0.014149	2.625271	-0.091914
Co	0.022270	0.282300	2.450532	**Co**	0.086007	0.065803	2.641351
Co	-0.036863	-0.254049	-2.696595	**Co**	-0.136230	-0.119142	-2.671159
P	-0.140369	0.699545	-4.613467	**P**	-0.167804	0.062074	-4.891454
P	0.036148	-4.771509	0.174302	**P**	0.025623	-4.807984	-0.183147
P	-0.037973	4.767467	-0.466119	**P**	0.043501	4.813846	-0.150118
P	-4.797595	-0.363947	0.155918	**P**	-4.754247	-0.011107	0.416445
P	4.791808	-0.304657	0.052885	**P**	4.730100	0.006297	-0.013881
H	1.032818	5.501067	-1.065286	**H**	1.245796	5.513390	-0.476986
H	-1.092327	5.488648	-1.108355	**H**	-0.803834	5.545619	-1.038062
H	-0.067020	5.511455	0.752027	**H**	-0.263236	5.577098	1.018469
H	-5.511006	0.161014	1.276789	**H**	-5.334008	0.165713	1.709375
H	-5.688941	0.139475	-0.843246	**H**	-5.577357	0.941230	-0.259824
H	-5.361770	-1.674506	0.215655	**H**	-5.512464	-1.166205	0.054827
H	5.369868	-1.610529	0.057818	**H**	5.438541	-0.159186	1.214998
H	5.665506	0.245086	-0.937423	**H**	5.490432	-0.940950	-0.767142
H	5.512157	0.186795	1.184295	**H**	5.438083	1.166315	-0.452762
H	1.107645	-5.495594	0.782595	**H**	1.163139	-5.553375	0.254116
H	-1.024585	-5.505593	0.789115	**H**	-0.957913	-5.644930	0.429417
H	0.035744	-5.494081	-1.057611	**H**	-0.055640	-5.394335	-1.482491
H	0.885556	0.367996	-5.554549	**H**	0.924159	-0.408484	-5.686911
H	-1.260083	0.416862	-5.457041	**H**	-1.191742	-0.567368	-5.667867
H	-0.116936	2.112166	-4.805301	**H**	-0.268139	1.337030	-5.529667
Th	-0.004054	0.005969	0.016897	**Th**	-0.021249	-0.005302	-0.004852

Table S49. Cartesian coordinates of Th@cage-CO_2.

Th@cage-CO_2				Th@cage-CO_2			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-2.044324	-1.775055	1.800936	**Te**	-1.464665	-1.886129	2.032540
Te	1.886885	1.634655	-1.876751	**Te**	1.788891	1.801603	-1.988440
Te	-1.822495	-1.971810	-1.903989	**Te**	-1.887235	-1.826148	-1.644149
Te	1.640875	1.892286	1.795265	**Te**	2.100784	1.807804	1.724601
Te	-2.039056	1.924311	1.567992	**Te**	-1.450618	1.838600	2.054275
Te	1.788015	-1.943645	-1.695132	**Te**	1.771605	-1.826248	-2.013124
Te	1.575415	-1.769563	2.048226	**Te**	2.083142	-1.885911	1.701227
Te	-1.865020	1.727473	-1.979076	**Te**	-1.872019	1.826378	-1.619661
Co	-2.730796	-0.052823	-0.238721	**Co**	-2.421237	-0.011648	0.322029
Co	2.512749	-0.073318	0.111970	**Co**	2.699513	-0.032010	-0.187203
Co	-0.122260	-2.652999	0.086246	**Co**	0.125434	-2.657842	-0.021718
Co	-0.057199	2.575527	-0.270585	**Co**	0.148906	2.621579	0.009835
Co	-0.287009	0.129949	2.480277	**Co**	0.408760	-0.037117	2.665002
Co	0.058578	-0.188747	-2.685467	**Co**	-0.141784	-0.002924	-2.640914
P	-0.369250	0.536724	-4.654125	**P**	-0.379479	0.106524	-4.855107
P	0.069432	-4.818839	0.051302	**P**	0.222362	-4.814805	-0.321995
P	0.191325	4.748207	-0.240832	**P**	0.247130	4.791186	-0.216207
P	-4.900090	-0.281175	-0.118048	**P**	-4.552577	-0.021659	0.789298
P	4.671815	-0.286547	0.290488	**P**	4.879306	-0.048979	-0.199250
H	1.489723	5.335858	-0.326620	**H**	1.457366	5.499908	0.055981
H	-0.417786	5.580069	-1.232402	**H**	-0.014230	5.412024	-1.475526
H	-0.248524	5.508956	0.885326	**H**	-0.606656	5.639868	0.554632
H	-5.608185	0.126655	1.052993	**H**	-5.005993	-0.016098	2.142960
H	-5.756752	0.379742	-1.053927	**H**	-5.394440	1.037670	0.330402
H	-5.512893	-1.566185	-0.229790	**H**	-5.382527	-1.095499	0.343060
H	5.352820	0.230053	1.435081	**H**	5.624165	-0.065761	1.018919
H	5.289576	-1.574404	0.310162	**H**	5.588497	-1.113770	-0.835525
H	5.545176	0.287468	-0.685190	**H**	5.603310	1.017811	-0.815222
H	1.288694	-5.451508	0.442348	**H**	1.432988	-5.531971	-0.075379
H	-0.793450	-5.623951	0.857525	**H**	-0.632023	-5.689702	0.418582
H	-0.108656	-5.556299	-1.159568	**H**	-0.039336	-5.389691	-1.602743
H	0.436407	-0.080320	-5.665355	**H**	0.478911	-0.630846	-5.730546
H	-1.634256	0.352055	-5.289271	**H**	-1.599126	-0.281524	-5.493764
H	-0.164765	1.890071	-5.056998	**H**	-0.248927	1.351205	-5.547128
Th	-0.115471	-0.029554	0.021308	**Th**	0.134047	-0.016564	0.014086
C	0.905836	0.294021	5.400162	**C**	-1.270179	0.060066	5.394137
O	-0.209042	0.298673	5.028084	**O**	-2.418500	0.190585	5.563329
O	2.006076	0.291538	5.793353	**O**	-0.111450	-0.072419	5.245902

Table 50. Cartesian coordinates of Th@cage-COOH.

Th@cage-COOH				Th@cage-COOH			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.127277	-1.916136	2.116586	**Te**	-1.273166	-1.930472	2.291074
Te	1.787648	1.825669	-2.126577	**Te**	1.753499	1.804570	-1.918166
Te	-1.778935	-1.866917	-1.479045	**Te**	-1.610489	-2.086671	-1.748953
Te	2.337813	1.884651	1.588108	**Te**	2.093137	1.848328	1.650785
Te	-1.203583	1.861028	2.125145	**Te**	-1.683226	1.531327	1.983749
Te	1.848402	-1.741226	-2.137996	**Te**	1.846568	-1.937071	-1.901050
Te	2.404152	-1.799238	1.580215	**Te**	2.175194	-1.783108	1.818191
Te	-1.846224	1.810581	-1.457292	**Te**	-2.006542	1.478646	-1.582880
Co	-2.236500	-0.045281	0.524757	**Co**	-2.365877	-0.560790	0.305803
Co	2.846459	0.058572	-0.361806	**Co**	2.757851	-0.041692	-0.169048
Co	0.376552	-2.615120	-0.006591	**Co**	0.091353	-2.692161	0.178349
Co	0.281314	2.630301	0.005716	**Co**	-0.072151	2.447594	0.056656
Co	0.638715	0.007912	2.752455	**Co**	0.425181	0.099764	2.775223
Co	-0.137793	-0.001220	-2.619051	**Co**	-0.065673	-0.136851	-2.631045
P	-0.949370	0.118952	-4.678125	**P**	-0.099374	0.438367	-4.775043
P	0.562440	-4.775135	-0.226505	**P**	0.055112	-4.947063	0.311629
P	0.436113	4.800002	-0.141731	**P**	-0.142161	4.713726	0.127496
P	-4.360523	-0.115173	1.057143	**P**	-4.487167	-1.074107	0.463371
P	5.021701	0.083532	-0.402561	**P**	4.938363	-0.147057	-0.399773
H	1.708001	5.443743	-0.230425	**H**	0.900644	5.497550	-0.458719
H	-0.174991	5.511391	-1.219342	**H**	-1.214326	5.468714	-0.446605
H	-0.082943	5.623113	0.905468	**H**	-0.145592	5.409932	1.376928
H	-4.766345	-0.109141	2.426258	**H**	-5.250292	-0.577737	1.563966
H	-5.253613	0.910773	0.620135	**H**	-5.401810	-0.676191	-0.558496
H	-5.173276	-1.217906	0.652905	**H**	-4.937728	-2.426894	0.557816
H	5.773788	0.096637	0.810428	**H**	5.786521	0.562261	0.505791
H	5.744751	-0.974616	-1.033851	**H**	5.645524	-1.386539	-0.331237
H	5.713651	1.159921	-1.038083	**H**	5.564439	0.319968	-1.596306
H	-0.079061	-5.640345	0.713286	**H**	0.676435	-5.623232	1.407702
H	0.088780	-5.436779	-1.400067	**H**	-1.174733	-5.674959	0.386140
H	1.837549	-5.417630	-0.187792	**H**	0.634603	-5.767911	-0.706448
H	-0.506630	-0.796577	-5.685467	**H**	1.048475	0.240446	-5.604588
H	-2.344033	-0.029362	-4.950788	**H**	-1.036848	-0.151776	-5.683689
H	-0.773872	1.298115	-5.468644	**H**	-0.337540	1.786908	-5.180476
Th	0.288923	0.006036	0.034172	**Th**	0.196312	-0.075128	0.049935
C	-0.033004	-0.005531	4.503311	**C**	0.486689	1.138481	4.338049
O	0.936855	0.006288	5.247298	**O**	0.686461	0.367491	5.264898
O	-1.314509	-0.025286	4.954706	**O**	0.340024	2.479638	4.508444
H	-1.256607	-0.029451	5.935588	**H**	0.436827	2.642842	5.472464

Table S51. Cartesian coordinates of Th@cage-CO.

Th@cage-CO				Th@cage-CO			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.457318	-1.902212	1.929504	**Te**	-1.173634	-1.687987	2.272405
Te	1.803916	1.894476	-1.999914	**Te**	1.783371	1.903903	-2.091897
Te	-1.807563	-1.834577	-1.750966	**Te**	-1.769114	-1.830357	-1.737533
Te	2.131632	1.806943	1.674622	**Te**	2.276829	1.968780	1.428861
Te	-1.520267	1.755305	2.000558	**Te**	-1.406537	1.759073	2.013559
Te	1.841754	-1.772444	-2.094478	**Te**	1.771270	-1.892055	-2.021712
Te	2.172326	-1.843053	1.600965	**Te**	2.269194	-1.755481	1.566213
Te	-1.867011	1.843871	-1.654161	**Te**	-1.955738	1.691300	-1.600041
Co	-2.436281	-0.062618	0.220794	**Co**	-2.311956	-0.317642	0.348346
Co	2.764323	0.017517	-0.263935	**Co**	2.812633	-0.013493	-0.391149
Co	0.209185	-2.615632	-0.081800	**Co**	0.012010	-2.536420	0.087800
Co	0.135364	2.601511	0.041971	**Co**	0.058035	2.618179	-0.049698
Co	0.399967	-0.052097	2.639839	**Co**	0.688273	0.161305	2.615894
Co	-0.090562	0.064101	-2.663622	**Co**	-0.089408	-0.007966	-2.668597
P	-0.326780	0.197865	-4.830249	**P**	-0.085614	0.233404	-4.838680
P	0.277157	-4.793625	-0.064905	**P**	-0.314399	-4.705053	0.227312
P	0.150470	4.777815	0.151132	**P**	-0.133624	4.820261	-0.010144
P	-4.601010	-0.185744	0.443376	**P**	-4.508287	-0.649637	0.659934
P	4.941797	-0.028330	-0.368118	**P**	5.048600	-0.037668	-0.686508
H	1.252685	5.524193	-0.365799	**H**	0.422010	5.624949	-1.052475
H	-0.876275	5.543268	-0.481626	**H**	-1.416145	5.449859	-0.001668
H	0.087628	5.435960	1.416887	**H**	0.412077	5.577643	1.071439
H	-5.231826	0.256697	1.645928	**H**	-5.175702	-0.129617	1.812687
H	-5.462839	0.509342	-0.458926	**H**	-5.463911	-0.169745	-0.288570
H	-5.267128	-1.446430	0.365443	**H**	-5.063226	-1.964469	0.761811
H	5.721343	0.161704	0.812983	**H**	5.932584	0.452140	0.325507
H	5.624430	-1.194942	-0.828230	**H**	5.753982	-1.262405	-0.902638
H	5.649532	0.907309	-1.183276	**H**	5.670664	0.670233	-1.762777
H	0.194955	-5.506938	1.169371	**H**	0.349270	-5.463916	1.238976
H	-0.708638	-5.557596	-0.761313	**H**	-1.611878	-5.266519	0.438998
H	1.414849	-5.487961	-0.578089	**H**	0.043865	-5.550161	-0.866818
H	0.588872	-0.463653	-5.705025	**H**	1.111030	0.079023	-5.602621
H	-1.518166	-0.270981	-5.463751	**H**	-0.898845	-0.614140	-5.655093
H	-0.285881	1.464633	-5.488260	**H**	-0.493763	1.462716	-5.439974
Th	0.161907	-0.005319	-0.062708	**Th**	0.265424	0.064413	-0.070100
C	0.491821	-0.056146	4.407986	**C**	1.045627	0.391971	4.338098
O	0.545656	-0.061288	5.566864	**O**	1.249058	0.546509	5.469922

Table S52. Cartesian coordinates of Th@cage-CHO.

Th@cage-CHO				Th@cage-CHO			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.517889	-1.694018	2.040682	**Te**	-1.517889	-1.694018	2.040682
Te	1.736535	1.935161	-2.053297	**Te**	1.736535	1.935161	-2.053297
Te	-1.815312	-1.799788	-1.602662	**Te**	-1.815312	-1.799788	-1.602662
Te	2.140649	1.967980	1.666432	**Te**	2.140649	1.967980	1.666432
Te	-1.542709	1.912948	2.007519	**Te**	-1.542709	1.912948	2.007519
Te	1.843389	-1.744829	-1.944780	**Te**	1.843389	-1.744829	-1.944780
Te	2.228089	-1.637024	1.694388	**Te**	2.228089	-1.637024	1.694388
Te	-1.828026	1.884971	-1.722775	**Te**	-1.828026	1.884971	-1.722775
Co	-2.458108	0.095017	0.228897	**Co**	-2.458108	0.095017	0.228897
Co	2.762676	0.168897	-0.254691	**Co**	2.762676	0.168897	-0.254691
Co	0.206959	-2.488511	0.115471	**Co**	0.206959	-2.488511	0.115471
Co	0.119715	2.678320	0.001248	**Co**	0.119715	2.678320	0.001248
Co	0.413474	0.053284	2.725690	**Co**	0.413474	0.053284	2.725690
Co	-0.099623	0.046234	-2.656083	**Co**	-0.099623	0.046234	-2.656083
P	-0.254456	-0.392841	-4.826337	**P**	-0.254456	-0.392841	-4.826337
P	0.285082	-4.672163	0.241865	**P**	0.285082	-4.672163	0.241865
P	0.110628	4.835031	0.272158	**P**	0.110628	4.835031	0.272158
P	-4.633225	0.227374	0.215273	**P**	-4.633225	0.227374	0.215273
P	4.908165	0.344500	-0.597009	**P**	4.908165	0.344500	-0.597009
H	1.127522	5.640158	-0.326686	**H**	1.127522	5.640158	-0.326686
H	-1.002724	5.611464	-0.173213	**H**	-1.002724	5.611464	-0.173213
H	0.197471	5.401106	1.579266	**H**	0.197471	5.401106	1.579266
H	-5.397594	-0.609297	1.086336	**H**	-5.397594	-0.609297	1.086336
H	-5.299069	1.447952	0.541386	**H**	-5.299069	1.447952	0.541386
H	-5.381239	-0.049660	-0.969029	**H**	-5.381239	-0.049660	-0.969029
H	5.816176	-0.433258	0.186015	**H**	5.816176	-0.433258	0.186015
H	5.480306	0.025743	-1.866349	**H**	5.480306	0.025743	-1.866349
H	5.583080	1.592031	-0.429644	**H**	5.583080	1.592031	-0.429644
H	0.286975	-5.335891	1.507135	**H**	0.286975	-5.335891	1.507135
H	-0.738486	-5.472056	-0.352809	**H**	-0.738486	-5.472056	-0.352809
H	1.389493	-5.389109	-0.311954	**H**	1.389493	-5.389109	-0.311954
H	0.756208	0.046925	-5.738666	**H**	0.756208	0.046925	-5.738666
H	-0.321108	-1.731510	-5.321741	**H**	-0.321108	-1.731510	-5.321741
H	-1.360748	0.098024	-5.590078	**H**	-1.360748	0.098024	-5.590078
Th	0.156128	0.084961	0.024122	**Th**	0.156128	0.084961	0.024122
C	0.552603	-0.915241	4.307808	**C**	0.552603	-0.915241	4.307808
O	0.581163	-0.085622	5.193976	**O**	0.581163	-0.085622	5.193976
H	0.608930	-2.009636	4.487839	**H**	0.608930	-2.009636	4.487839

Table S53. Cartesian coordinates of Th@cage-OCH_2.

Th@cage-OCH_2				Th@cage-OCH_2			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.546180	-2.015676	1.864030	**Te**	-1.469129	-1.918710	1.904112
Te	1.847354	1.747861	-2.005135	**Te**	1.852787	1.832743	-1.992921
Te	-1.858000	-1.878339	-1.808349	**Te**	-1.775903	-1.828534	-1.808611
Te	2.160123	1.685355	1.633066	**Te**	2.131901	1.725484	1.699688
Te	-1.485563	1.654799	1.983263	**Te**	-1.507406	1.712592	1.993967
Te	1.800182	-1.916774	-2.091682	**Te**	1.872345	-1.828542	-2.067290
Te	2.088209	-1.987272	1.577421	**Te**	2.138289	-1.910034	1.635068
Te	-1.833698	1.762617	-1.681711	**Te**	-1.782449	1.815612	-1.712121
Co	-2.467822	-0.125393	0.171268	**Co**	-2.403379	-0.063929	0.176778
Co	2.767902	-0.102744	-0.273009	**Co**	2.773892	-0.047002	-0.217446
Co	0.089897	-2.737600	-0.143908	**Co**	0.185366	-2.649376	-0.084438
Co	0.172684	2.502795	-0.022812	**Co**	0.173004	2.544680	0.036784
Co	0.376665	-0.184464	2.623398	**Co**	0.406768	-0.120235	2.810784
Co	-0.064800	-0.050444	-2.693811	**Co**	-0.017092	0.019613	-2.717901
P	-0.159976	0.320097	-4.813348	**P**	-0.202190	0.111623	-4.941125
P	0.009251	-4.917852	-0.244037	**P**	0.073543	-4.824748	-0.224310
P	0.176145	4.676498	0.156108	**P**	0.071931	4.713684	0.249279
P	-4.602606	0.028536	0.596954	**P**	-4.569946	-0.114707	0.408842
P	4.955448	-0.089124	-0.319786	**P**	4.951307	-0.040713	-0.336064
H	1.235281	5.450545	-0.411642	**H**	0.908523	5.563637	-0.538616
H	-0.895116	5.459735	-0.376311	**H**	-1.150782	5.407669	-0.002090
H	0.200127	5.295208	1.443542	**H**	0.352203	5.328433	1.507603
H	-5.086917	-0.094960	1.934117	**H**	-5.157412	-0.128840	1.710528
H	-5.316758	1.224133	0.278410	**H**	-5.375629	0.937766	-0.122605
H	-5.535671	-0.877378	0.003459	**H**	-5.336702	-1.193565	-0.127264
H	5.711095	-0.268255	0.878949	**H**	5.739554	-0.141256	0.850987
H	5.682363	-1.037875	-1.103516	**H**	5.643972	-1.047584	-1.075066
H	5.662973	1.064514	-0.777452	**H**	5.644981	1.075602	-0.894986
H	0.773238	-5.712027	0.665700	**H**	0.832404	-5.648989	0.662949
H	-1.225872	-5.610503	-0.059178	**H**	-1.170445	-5.503503	-0.048275
H	0.402484	-5.611778	-1.428977	**H**	0.451094	-5.493393	-1.428493
H	0.918211	-0.077841	-5.661773	**H**	0.685360	-0.610116	-5.800548
H	-1.209156	-0.262877	-5.588412	**H**	-1.399952	-0.301793	-5.605384
H	-0.291357	1.645799	-5.326162	**H**	-0.084005	1.354991	-5.638272
Th	0.150719	-0.115423	-0.034183	**Th**	0.183948	-0.050544	-0.039546
O	0.231509	0.148744	4.564366	**O**	0.213818	0.195619	4.703531
C	1.138824	-0.760285	4.484267	**C**	1.129723	-0.724660	4.659368
H	2.206632	-0.485228	4.564624	**H**	2.188785	-0.445943	4.788215
H	0.885305	-1.815419	4.694816	**H**	0.860048	-1.771329	4.877460

Table S54. Cartesian coordinates of Th@cage-OCH_3.

	Th@cage-OCH_3				Th@cage-OCH_3		
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.274977	-1.935940	1.971757	**Te**	-1.375193	-1.932990	1.867961
Te	1.624731	1.920959	-2.153225	**Te**	1.730972	2.002829	-2.037939
Te	-1.802531	-1.910116	-1.653471	**Te**	-1.739028	-1.803904	-1.797420
Te	2.111231	1.940599	1.542443	**Te**	2.124931	1.865583	1.669982
Te	-1.442194	1.737684	2.033281	**Te**	-1.489130	1.713666	2.043577
Te	1.860870	-1.711383	-2.151994	**Te**	1.877479	-1.640316	-2.183860
Te	2.345584	-1.729990	1.472160	**Te**	2.292868	-1.764492	1.487598
Te	-1.969036	1.718035	-1.662362	**Te**	-1.879374	1.867723	-1.636911
Co	-2.387221	-0.134653	0.321980	**Co**	-2.385551	-0.091362	0.210019
Co	2.761227	0.149308	-0.386261	**Co**	2.777354	0.138414	-0.329721
Co	0.332614	-2.611651	-0.067560	**Co**	0.306148	-2.559889	-0.148885
Co	0.037879	2.615106	-0.059017	**Co**	0.112223	2.636713	0.076770
Co	0.578317	0.012987	2.772905	**Co**	0.490753	-0.035780	2.823493
Co	-0.186468	-0.026944	-2.728827	**Co**	-0.100835	0.151976	-2.738357
P	-0.392514	-0.260260	-4.924813	**P**	-0.470344	0.050438	-4.937279
P	0.440200	-4.774552	-0.340661	**P**	0.485463	-4.733771	-0.067245
P	-0.092900	4.796640	0.059235	**P**	0.172455	4.818503	0.145266
P	-4.522300	-0.135164	0.775431	**P**	-4.556098	-0.253361	0.345278
P	4.923727	0.396000	-0.531453	**P**	4.947707	0.210175	-0.525741
H	0.799282	5.620937	-0.692785	**H**	1.394588	5.513723	-0.102404
H	-1.290986	5.474972	-0.321215	**H**	-0.636517	5.598913	-0.736376
H	0.081276	5.473277	1.305141	**H**	-0.170755	5.518639	1.342257
H	-4.985313	-0.342869	2.110136	**H**	-5.269571	0.305316	1.449638
H	-5.328178	1.011777	0.502768	**H**	-5.390010	0.290064	-0.678565
H	-5.385390	-1.089520	0.154277	**H**	-5.171785	-1.540699	0.388318
H	5.752718	0.259832	0.623353	**H**	5.771046	0.417387	0.623011
H	5.685871	-0.464827	-1.379706	**H**	5.659436	-0.918774	-1.033429
H	5.492364	1.621737	-0.993146	**H**	5.579896	1.185612	-1.355623
H	1.636917	-5.485623	-0.019168	**H**	0.510768	-5.421504	1.184140
H	-0.453634	-5.643323	0.357927	**H**	-0.502464	-5.560475	-0.685271
H	0.251882	-5.359051	-1.629486	**H**	1.621007	-5.389872	-0.632904
H	-0.437913	-1.548002	-5.544726	**H**	-0.111004	-1.107617	-5.695779
H	-1.529845	0.267204	-5.614490	**H**	-1.792051	0.158888	-5.473011
H	0.581598	0.288986	-5.816596	**H**	0.120692	0.992424	-5.839003
Th	0.181991	0.001093	-0.061055	**Th**	0.191591	0.038649	-0.060856
O	0.849179	-0.479574	4.496790	**O**	0.688123	-0.600290	4.539498
C	1.015492	-1.741068	5.084372	**C**	0.787783	-1.854040	5.149390
H	0.156279	-2.404516	4.874594	**H**	-0.101413	-2.476365	4.934757
CH	1.927304	-2.243917	4.712614	**H**	1.677442	-2.404447	4.789485
H	1.104858	-1.624165	6.178575	**H**	0.872383	-1.735662	6.243863

Table S55. Cartesian coordinates of Th@cage-CH_3OH.

Th@cage-CH_3OH				Th@cage-CH_3OH			
Atoms	**x**	**y**	**z**	**Atoms**	**x**	**y**	**z**
Te	-1.535530	-2.119037	1.679069	**Te**	-1.222396	-2.104114	2.090049
Te	2.062300	1.953919	-1.592086	**Te**	1.868375	1.810953	-1.835332
Te	-1.642282	-1.672455	-1.852556	**Te**	-1.780294	-1.837070	-1.581798
Te	2.151237	1.512613	2.126083	**Te**	2.294779	1.624434	1.834422
Te	-1.486907	1.557636	2.170680	**Te**	-1.238067	1.601602	2.326312
Te	2.073773	-1.599618	-2.061659	**Te**	1.871745	-1.821011	-2.057493
Te	2.139853	-2.128360	1.604556	**Te**	2.303361	-2.089870	1.615081
Te	-1.569352	2.034836	-1.484139	**Te**	-1.793520	1.772759	-1.344475
Co	-2.349537	-0.015457	0.078195	**Co**	-2.261791	-0.162601	0.515356
Co	2.894256	-0.064063	0.004404	**Co**	2.847679	-0.118342	-0.172704
Co	0.279008	-2.652592	-0.355153	**Co**	0.283672	-2.759621	-0.068866
Co	0.307886	2.551179	0.388723	**Co**	0.275768	2.500101	0.255748
Co	0.306151	-0.412277	2.578935	**Co**	0.649549	-0.302435	2.772163
Co	0.212218	0.302765	-2.557163	**Co**	-0.064087	0.031799	-2.522851
P	-0.523767	-0.103771	-4.528970	**P**	-0.219381	0.249252	-4.739457
P	0.512366	-4.821306	-0.496076	**P**	0.166578	-4.902292	-0.454791
P	0.493136	4.720164	0.419487	**P**	0.192722	4.673468	0.094865
P	-4.504147	0.116494	0.413492	**P**	-4.393042	-0.271944	0.973489
P	5.069390	0.060953	0.004068	**P**	5.026527	-0.124555	-0.199356
H	1.721566	5.347218	0.791129	**H**	0.135918	5.313520	-1.180237
H	0.272037	5.493032	-0.760837	**H**	-0.883470	5.405447	0.684484
H	-0.348959	5.492543	1.277927	**H**	1.243983	5.482092	0.627698
H	-5.060211	-0.205965	1.687943	**H**	-4.861592	-0.231927	2.321584
H	-5.195673	1.355617	0.250632	**H**	-5.289212	0.716220	0.461573
H	-5.414447	-0.672943	-0.356655	**H**	-5.157918	-1.408427	0.569909
H	5.822967	-0.515695	1.071710	**H**	5.775554	-0.149516	1.015918
H	5.832753	-0.513682	-1.058492	**H**	5.739857	-1.177224	-0.850635
H	5.733759	1.325528	0.007591	**H**	5.739276	0.955515	-0.805513
H	1.796993	-5.407627	-0.706776	**H**	1.200053	-5.774767	0.007765
H	0.140054	-5.655060	0.602218	**H**	-0.926652	-5.675823	0.042590
H	-0.169082	-5.577045	-1.501096	**H**	0.121078	-5.408463	-1.789174
H	-0.375678	-1.370106	-5.170471	**H**	0.932232	0.092916	-5.572666
H	-1.875823	0.133389	-4.919361	**H**	-1.072100	-0.592379	-5.522243
H	0.101307	0.689772	-5.544035	**H**	-0.654094	1.476453	-5.331869
Th	0.274136	-0.062751	0.121399	**Th**	0.286424	-0.128818	0.118774
C	0.602547	-0.549389	5.321870	**C**	0.965619	-0.156790	5.312464
H	1.457804	-1.155763	4.981046	**H**	1.796508	-0.260642	4.565610
H	0.143983	-1.043201	6.188540	**H**	1.254380	-0.770323	6.175611
H	-0.200569	-0.546321	4.528723	**H**	0.027508	-0.597955	4.900361
O	0.966384	0.762174	5.712734	**O**	0.797646	1.174806	5.752747
H	1.344798	1.197255	4.923425	**H**	0.481525	1.688176	4.983937

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