Binding of Cerium Monoxide to Annulenes and Buckybowls

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Electronic Supporting Information

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60.M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09 Revision-B.01, Gaussian, Inc., Wallingford CT, 2010.

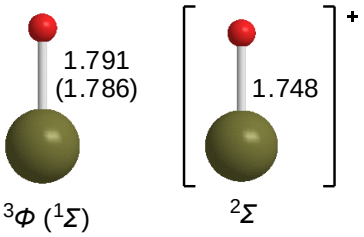

Figure S1. Equilibrium geometries of CeO and CeO^+ diatomics computed at the wB97XD/ANO-RCC(Ce) ∪ 6-31G**(O) level.

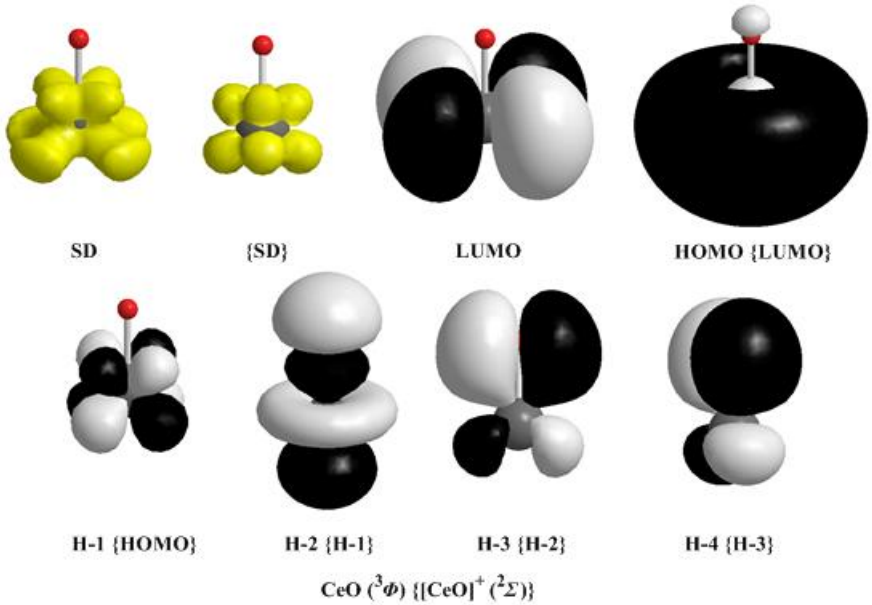

Figure S2. 3D plots of the frontier molecular orbitals of the CeO and CeO^+ molecules.

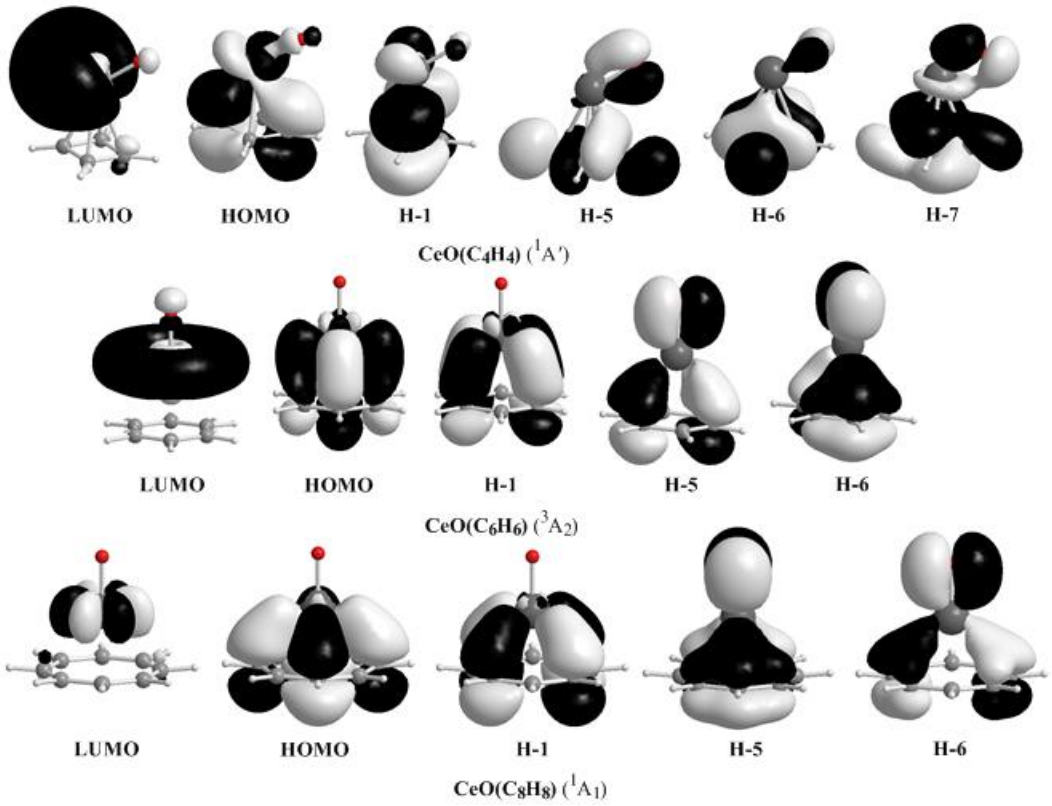

Figure S3. 3D plots of the bonding valence molecular orbitals of the CeO(annulene) adducts.

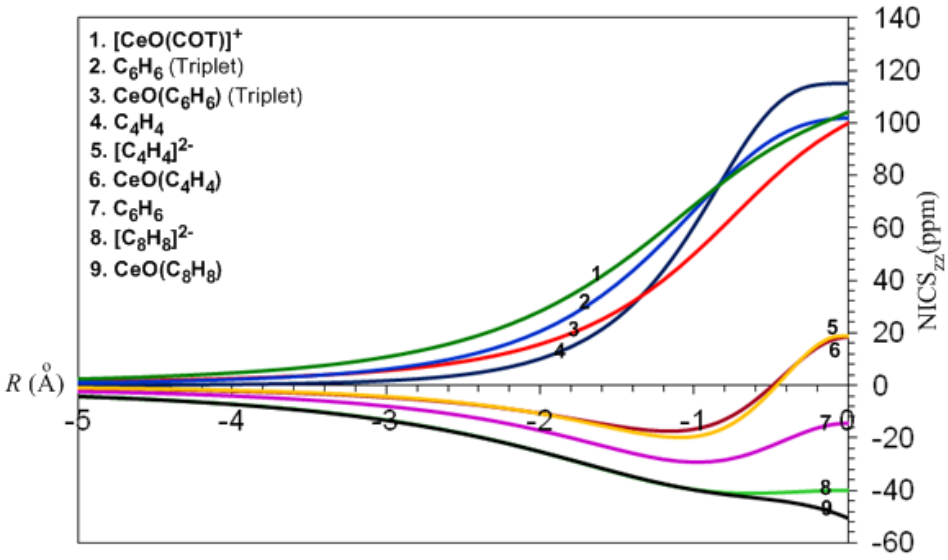

Figure S4. The $NICS_{zz}$-scan profiles of the CeO(annulene) adducts calculated at the B3LYP/ANO-RCC(Ln)∪6-31G**(O,C,H) level of theory.

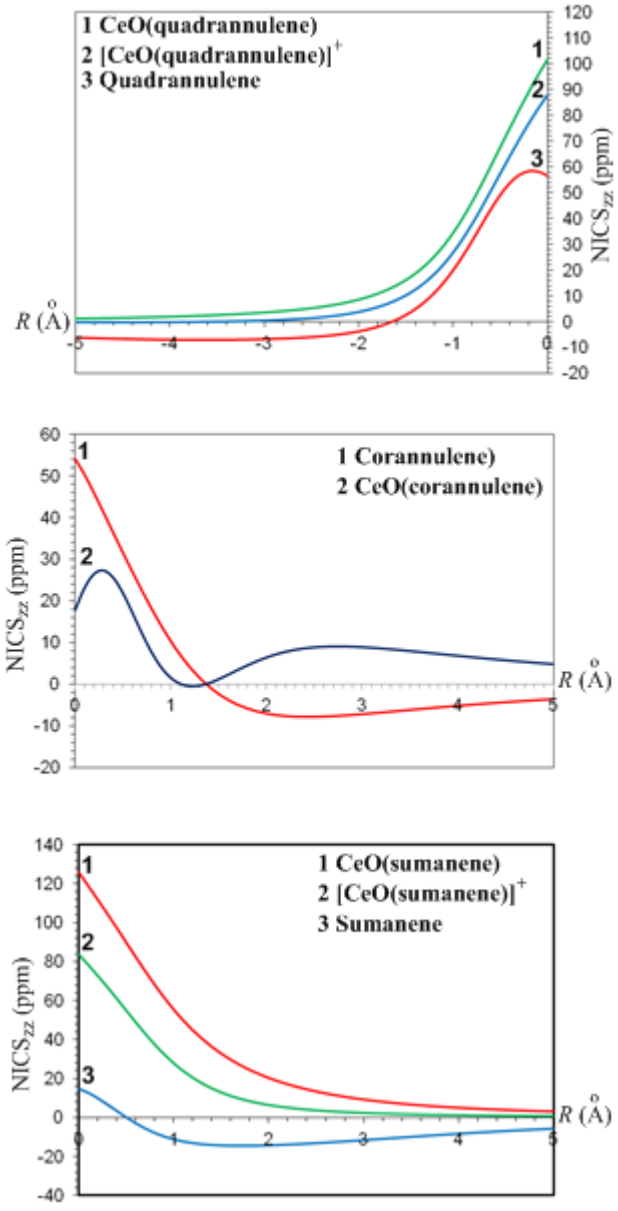

Figure S5. The $NICS_{zz}$-scan profiles of the buckybowls and their CeO(buckybowl) adducts calculated at the B3LYP/ANO-RCC(Ln) ∪ 6-31G**(O,C,H) level of theory.

Table S1. Selected electronic parameters for the CeO(annulene) adducts calculated at the wB97XD/ANO-RCC(Ce) ∪ 6-31G**(C,O,H) level of theory

Property	CeO(C_4H_4) ($^1A'$)	CeO(C_6H_6) ($^3A_2$)	CeO(C_8H_8) ($^1A_1$)	$[CeO(C_8H_8)]^+$ ($^2B_1$)
Q_{Ce} [a]	1.677	1.481	1.598	1.871
Q_{annul}	-0.847	-0.583	-0.846	-0.153
SD_{Ce} [b]		1.226		0.201
WBO(Ce-O) [c]	1.886	1.827	2.028	2.057
WBO(Ce-C)	0.413, 0.508	0.165	0.244	0.240
ω/cm^{-1} [d]	358.2	200.7	261.9	205.6
ω(Ce-O)/cm^{-1}	838.8	807.2	853.9	918.0
D_e/kcal mol^{-1}	58.3 (93.1) [e]	12.2 (46.9)	181.1 (215.9)	133.4
μ/Debye	4.98	2.29	0.06	2.29
Q_{zz}/Debye-Å [f]	-54.6	-89.8	-100.3	-85.0
ε_L-ε_H/(eV) [g]	6.743	5.994	7.393	7.014

[a] Natural atomic charge. [b] Mulliken atomic Spin Density (SD). [c] Wiberg Bond Order (WBO). [d] Binding energies (D_e) with respect to dissociation to annulenes and CeO($^3\Phi$). [d] Unscaled Ce-annulene harmonic vibrational frequencies. [e] Figures in parentheses are the binding energies with respect to dissociation to annulenes and CeO($^1\Sigma$). [f] Q_{zz} is the zz tensor of the quadrupole moment.). [g] $\varepsilon_L - \varepsilon_H$ is the HOMO-LUMO energy gap.

Table S2. The NICS values (in ppm) calculated at the ring center, $NICS_{zz}(0)$, 1.0 Å below the ring center, $NICS_{zz}(-1)$ and 1.0 Å above the ring center $NICS_{zz}$ (1) for the CeO(annulene) adducts calculated at the GIAO/uB3LYP/ANO-RCC(Ce)∪6-31G**(O,C,H) level of theory

Adduct	$NICS_{zz}(0)$	$NICS_{zz}(-1)$	$NICS_{zz}(1)$
$CeO(C_4H_4)$	18.7	-19.7	0.6
C_4H_4	115.3	61.0	61.0
$[C_4H_4]^{2-}$	18.6	-16.7	-16.7
$CeO(C_6H_6)$	100.0	50.1	165.1
C_6H_6 (Triplet)	101.8	66.8	66.8
C_6H_6	-14.3	-29.3	-29.3
$CeO(C_8H_8)$	-50.5	-39.8	-123.5
$[CeO(C_8H_8)]^{+}$	104.3	68.8	166.0
$(C_8H_8)^{2-}$	-40.0	-39.7	-39.7

Table S3. Selected electronic parameters for the CeO(buckybowl)[a] adducts calculated at the wB97XD/ANO-RCC(Ce) ∪ 6-31G**(C,O,H) level of theory

Property	CeO(L) ($^3B_1$) [CeO(L)]$^+$ ($^2B_1$)	CeO(L′) (^3A)	CeO(L″) ($^3A'$) [CeO(L″)]$^+$ ($^2A'$)
Q_{Ce}[b]	1.754	1.772	1.677
	1.791		1.805
Q_{annul}	-0.767	-0.772	-0.689
	0.169		0.169
SD_{Ce}[c]	1.043	1.022	1.056
	1.019		1.021
WBO(Ce-O)[d]	1.707	1.691	1.712
	1.734		1.725
$WBO(Ce-C)_{tot}$	0.51	1.37	0.60
	0.38		0.36
ω/cm^{-1} [e]	282.0	195.8	115.1
	285.0		91.8
ω(Ce-O)/cm^{-1}	831.1	836.4	818.8
	865.7		867.0
D_e/kcal mol^{-1}	45.9	43.6	31.3
	56.4		52.8
μ/Debye	0.66	1.52	2.90
	0.18		1.39
Q_{zz}/Debye-Å[f]	-240.2	-138.3	-145.2
	-228.0		-115.1
ε_L-ε_H/(eV)[g]	4.516	4.553	4.790
	6.412		7.354

[a] L = Quadrannulene, L′ = Corannulene, L″ = Sumanene. [b] Natural atomic charge. [c] Mulliken atomic Spin Density (SD). [d] Wiberg Bond Order (WBO).[e] Unscaled Ce-annulene harmonic vibrational frequencies. [f] Q_{zz} is the zz tensor of the quadrupole moment.). [g] $\varepsilon_L - \varepsilon_H$ is the HOMO-LUMO energy gap.

Table S4. The NICS values (in ppm) calculated at the central ring center, $NICS_{zz}(0)$, 1.0 Å below the central ring center, $NICS_{zz}(-1)$ and 1.0 Å above the central ring center $NICS_{zz}$ (1) for the buckybowls and their CeO(buckybowl) adducts calculated at the GIAO/uPBE0/ANO-RCC(Ce)∪6-31G**(O,C,H) level of theory

Adduct	$NICS_{zz}(0)$	$NICS_{zz}(-1)$	$NICS_{zz}(1)$
Quadrannulene	56.4	20.0	12.3
CeO(quadrannulene)	101.9	150.1	34.5
$[CeO(quadrannulene)]^+$	87.9	121.9	26.9
Corannulene	54.3	10.4	12.9
CeO(corannulene)	6.9	61.6	-2.3
Sumanene	15.0	-11.1	-1.2
CeO(sumanene)	126.1	286.1	55.5
$[CeO(sumanene]^+$	83.8	240.2	27.9

Cartesian Coordinates of the Optimized Structures
and
Total electronic Energies (in Hartrees)

CeO ($^3\Phi$)
Ce,0,0.,0.,-0.2116002463
O,0,0.,0.,1.5790439563

Sum of electronic and zero-point Energies= -550.315458
Sum of electronic and thermal Energies= -550.313036
Sum of electronic and thermal Enthalpies= -550.312091
Sum of electronic and thermal Free Energies= -550.339635

CeO ($^2\Sigma$)
Ce,0,0.,0.,-0.2090088285
O,0,0.,0.,1.5764525385

Sum of electronic and zero-point Energies= -550.260065
Sum of electronic and thermal Energies= -550.257641
Sum of electronic and thermal Enthalpies= -550.256697
Sum of electronic and thermal Free Energies= -550.283199

CeO$^+$ ($^2\Sigma$)
Ce,0,0.,0.,0.1955001427
O,0,0.,0.,-1.5521001427

Sum of electronic and zero-point Energies= -550.133406
Sum of electronic and thermal Energies= -550.130998
Sum of electronic and thermal Enthalpies= -550.130054
Sum of electronic and thermal Free Energies= -550.157150

CeO(C_4H_4) ($^1A'$)
Ce,0,0.570050564,-0.2389121909,0.
H,0,-1.798894089,0.2445582137,-2.1018145431
O,0,1.8603412206,0.9919934984,0.
C,0,-1.6947346389,0.2191657472,-1.0239500326
C,0,-1.557433208,1.2150028996,0.
H,0,-1.3509694778,2.2787236856,0.
C,0,-1.6947346389,0.2191657472,1.0239500326
H,0,-1.798894089,0.2445582137,2.1018145431
C,0,-1.8581967289,-0.8082668524,0.
H,0,-2.2591300219,-1.8147972533,0.

Sum of electronic and zero-point Energies= -704.972618
Sum of electronic and thermal Energies= -704.965657
Sum of electronic and thermal Enthalpies= -704.964713
Sum of electronic and thermal Free Energies= -705.005946

CeO(C_4H_4) ($^3B_1$) (NImag = -146.7, -89.1 cm^{-1})
Ce,0,-0.0000000004,0.,0.8140190177
H,0,-0.0000000014,2.0913215634,-2.0124096429
O,0,-0.0000000006,0.0000000002,2.6403540477
C,0,-0.0000000008,1.0474624415,-1.7311808624
C,0,-0.9944966442,-0.0000000009,-1.8693636724
H,0,-2.062446128,-0.0000000016,-2.0641328621
C,0,0.0000000005,-1.047462442,-1.7311808622
H,0,0.0000000012,-2.091321564,-2.0124096425
C,0,0.9944966439,0.0000000004,-1.8693636722
H,0,2.0624461278,0.000000001,-2.0641328617

Sum of electronic and zero-point Energies= -704.935721
Sum of electronic and thermal Energies= -704.929907
Sum of electronic and thermal Enthalpies= -704.928963
Sum of electronic and thermal Free Energies= -704.967160

$CeO(C_6H_6)$ ($^3A_2$)
Ce,0,0.,0.,0.7993615679
O,0,0.,0.,2.6133926113
H,0,2.1654337238,-1.2493242998,-1.5973672144
H,0,0.,2.500186069,-1.5980928772
C,0,0.,1.4163760976,-1.5541700551
C,0,1.2263957196,0.7082848716,-1.5538898633
H,0,2.1654337238,1.2493242998,-1.5973672144
C,0,1.2263957196,-0.7082848716,-1.5538898633
C,0,-1.2263957196,0.7082848716,-1.5538898633
H,0,-2.1654337238,1.2493242998,-1.5973672144
C,0,-1.2263957196,-0.7082848716,-1.5538898633
C,0,0.,-1.4163760976,-1.5541700551
H,0,-2.1654337238,-1.2493242998,-1.5973672144
H,0,0.,-2.500186069,-1.5980928772

Sum of electronic and zero-point Energies= -782.406395
Sum of electronic and thermal Energies= -782.398408
Sum of electronic and thermal Enthalpies= -782.397463
Sum of electronic and thermal Free Energies= -782.445166

$CeO(C_6H_6)$ (^1A) (NImag = -11.3 cm^{-1})
Ce,0,0.,0.,0.7508127212
O,0,0.,0.,2.5556550307
H,0,-2.1536583775,1.2715532199,-1.5799030212
H,0,0.,-2.4829394011,-1.7809546954
C,0,0.,-1.4046287375,-1.6443774448
C,0,-1.2168826538,-0.7386318673,-1.4646728427
H,0,-2.1536583775,-1.2715532199,-1.5799030212
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C,0,1.2168826538,-0.7386318673,-1.4646728427
H,0,2.1536583775,-1.2715532199,-1.5799030212
C,0,1.2168826538,0.7386318673,-1.4646728427
C,0,0.,1.4046287375,-1.6443774448
H,0,2.1536583775,1.2715532199,-1.5799030212
H,0,0.,2.4829394011,-1.7809546954

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Sum of electronic and thermal Energies= -782.397906
Sum of electronic and thermal Enthalpies= -782.396962
Sum of electronic and thermal Free Energies= -782.438109

$CeO(C_8H_8)$ ($^3A_2$)
Ce,0,0.,0.,0.7631
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H,0,-2.0702,-2.0702,-1.0797
O,0,0.,0.,2.5426
C,0,0.,1.8445,-1.1659
C,0,1.3042,1.3042,-1.1659
H,0,2.0702,2.0702,-1.0797
C,0,1.8445,0.,-1.1659
H,0,2.9277,0.,-1.0797
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H,0,2.0702,-2.0702,-1.0797

C,0,0.,-1.8445,-1.1659
H,0,0.,-2.9277,-1.0797
C,0,-1.3042,-1.3042,-1.1659
C,0,-1.8445,0.,-1.1659
H,0,-2.9277,0.,-1.0797
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H,0,-2.0702,2.0702,-1.0797

Sum of electronic and zero-point Energies= -859.801637
Sum of electronic and thermal Energies= -859.792721
Sum of electronic and thermal Enthalpies= -859.791777
Sum of electronic and thermal Free Energies= -859.835418

$CeO(C_8H_8)$ ($^3A'$) (NImag = -1261.5, -274.5, -19.9 cm^{-1})
Ce,0,0.0005141307,0.0000000005,1.1312802956
H,0,-0.0000908045,2.935739277,-1.1401943585
H,0,-2.0675601077,-2.0671368337,-1.1920958053
O,0,0.0005706272,0.000000001,2.9598101608
C,0,-0.0000704127,1.8499674006,-1.1489430857
C,0,1.2976702393,1.2977980264,-1.194663449
H,0,2.0674480741,2.06718529,-1.1918082334
C,0,1.8494032787,0.0000000006,-1.157558473
H,0,2.9352470117,0.0000000011,-1.1545964577
C,0,1.2976702404,-1.2977980256,-1.1946634483
H,0,2.0674480759,-2.0671852886,-1.1918082323
C,0,-0.0000704111,-1.8499674008,-1.1489430847
H,0,-0.000090802,-2.9357392773,-1.1401943569
C,0,-1.2977986153,-1.2977253126,-1.1948520043
C,0,-1.8495457385,-0.0000000009,-1.1579272527
H,0,-2.9353860714,-0.0000000014,-1.154994401
C,0,-1.2977986164,1.2977253112,-1.194852005
H,0,-2.0675601095,2.0671368316,-1.1920958064

Sum of electronic and zero-point Energies= -859.766472
Sum of electronic and thermal Energies= -859.758275
Sum of electronic and thermal Enthalpies= -859.757331
Sum of electronic and thermal Free Energies= -859.801774

$[CeO(C_8H_8)]^+$ ($^2B_1$)
Ce,0,-0.0000000003,-0.0000000007,-0.855870627
H,0,-2.0726277188,-2.072627714,1.1457091694
H,0,0.0000000034,2.9272164893,1.2347335483
O,0,-0.0000000003,-0.0000000007,-2.5929940756
C,0,-1.3057299932,-1.3057299903,1.182287301
C,0,-0.0000000026,-1.8404122071,1.2480266188
H,0,-0.0000000039,-2.9272164907,1.2347335483
C,0,1.3057299893,-1.3057299936,1.182287301
H,0,2.072627713,-2.0726277192,1.1457091694
C,0,1.8404122061,-0.000000003,1.2480266188
H,0,2.9272164897,-0.0000000043,1.2347335483
C,0,1.3057299926,1.3057299889,1.182287301
H,0,2.0726277182,2.0726277126,1.1457091694
C,0,0.000000002,1.8404122057,1.2480266188
C,0,-1.3057299899,1.3057299922,1.182287301
H,0,-2.0726277136,2.0726277178,1.1457091694
C,0,-1.8404122067,0.0000000016,1.2480266188
H,0,-2.9272164903,0.000000003,1.2347335483

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Sum of electronic and thermal Energies= -859.533459

Sum of electronic and thermal Enthalpies= -859.532515
Sum of electronic and thermal Free Energies= -859.581658

Quadrannulene ($^1A_1$)
C,0,-0.7267296028,-0.7267296028,-1.6399823092
C,0,0.7267296028,-0.7267296028,-1.6399823092
C,0,0.7267296028,0.7267296028,-1.6399823092
C,0,-0.7267296028,0.7267296028,-1.6399823092
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C,0,2.6261863599,0.7252355035,-0.2281987846
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C,0,-3.7398920935,1.3812576375,0.3183975227
C,0,-4.8146836282,0.6961625095,0.8551596234
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H,0,-3.7828999597,-2.4614004072,0.2952686479
H,0,2.4614004072,3.7828999597,0.2952686479
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H,0,-1.2465250479,5.658152742,1.2589908404
H,0,-2.4614004072,3.7828999597,0.2952686479
H,0,3.7828999597,-2.4614004072,0.2952686479
H,0,5.658152742,-1.2465250479,1.2589908404
H,0,5.658152742,1.2465250479,1.2589908404
H,0,3.7828999597,2.4614004072,0.2952686479
H,0,-2.4614004072,-3.7828999597,0.2952686479
H,0,-1.2465250479,-5.658152742,1.2589908404
H,0,1.2465250479,-5.658152742,1.2589908404
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Sum of electronic and zero-point Energies= -1228.186507
Sum of electronic and thermal Energies= -1228.167094
Sum of electronic and thermal Enthalpies= -1228.166150
Sum of electronic and thermal Free Energies= -1228.232057

CeO(quadrannulene) ($^3B_1$)
C,0,-0.7182067345,0.7249520641,-2.0862189663

C,0,-0.7182067344,-0.7249520643,-2.0862189663
C,0,0.7182067345,-0.7249520642,-2.0862189663
C,0,0.7182067344,0.7249520642,-2.0862189663
C,0,0.729344818,2.5461610791,-0.5080327255
C,0,-0.7293448183,2.546161079,-0.5080327255
C,0,-1.4641511646,1.4476105204,-1.1864856814
C,0,2.6841761947,-0.7253419977,-0.7195671976
C,0,2.6841761946,0.725341998,-0.7195671976
C,0,1.4641511644,1.4476105205,-1.1864856814
C,0,-0.729344818,-2.5461610792,-0.5080327255
C,0,0.7293448182,-2.5461610791,-0.5080327255
C,0,1.4641511646,-1.4476105205,-1.1864856814
C,0,-2.6841761947,0.7253419977,-0.7195671976
C,0,-2.6841761946,-0.725341998,-0.7195671976
C,0,-1.4641511644,-1.4476105206,-1.1864856814
C,0,1.3820984152,3.5175728657,0.2679868861
C,0,0.6937462521,4.4562902379,1.02585265
C,0,-0.6937462526,4.4562902378,1.02585265
C,0,-1.3820984156,3.5175728655,0.2679868861
C,0,3.838937071,-1.3837026963,-0.2799729208
C,0,4.9515626708,-0.6936731253,0.188541146
C,0,4.9515626707,0.6936731258,0.188541146
C,0,3.8389370709,1.3837026967,-0.2799729208
C,0,-1.3820984152,-3.5175728658,0.2679868861
C,0,-0.6937462521,-4.456290238,1.02585265
C,0,0.6937462526,-4.4562902379,1.02585265
C,0,1.3820984156,-3.5175728656,0.2679868861
C,0,-3.8389370711,1.3837026963,-0.2799729208
C,0,-4.9515626708,0.6936731252,0.188541146
C,0,-4.9515626707,-0.6936731259,0.188541146
C,0,-3.8389370709,-1.3837026968,-0.2799729208
H,0,2.4624637619,3.5343600919,0.2911928159
H,0,1.2466845819,5.1802368492,1.6149808337
H,0,-1.2466845825,5.180236849,1.6149808337
H,0,-2.4624637623,3.5343600916,0.2911928159
H,0,3.8916205587,-2.4627618918,-0.3492040041
H,0,5.8240957663,-1.2438378494,0.5252324792
H,0,5.8240957662,1.24383785,0.5252324792
H,0,3.8916205585,2.4627618922,-0.3492040041
H,0,-2.4624637619,-3.534360092,0.2911928159
H,0,-1.246684582,-5.1802368493,1.6149808337
H,0,1.2466845825,-5.1802368491,1.6149808337
H,0,2.4624637623,-3.5343600917,0.2911928159
H,0,-3.8916205588,2.4627618918,-0.3492040041
H,0,-5.8240957663,1.2438378493,0.5252324792
H,0,-5.8240957662,-1.2438378501,0.5252324792
H,0,-3.8916205585,-2.4627618923,-0.3492040041
Ce,0,0.,0.,1.1211991871
O,0,0.,0.,2.9340827695

Sum of electronic and zero-point Energies= -1778.575146
Sum of electronic and thermal Energies= -1778.550626
Sum of electronic and thermal Enthalpies= -1778.549682
Sum of electronic and thermal Free Energies= -1778.631684

[CeO(quadrannulene)]$^{+}$ ($^{2}B_{1}$)
C,0,-0.7249575128,0.7300874776,-2.1028437863
C,0,-0.7249575128,-0.7300874776,-2.1028437863
C,0,0.7249575128,-0.7300874776,-2.1028437863
C,0,0.7249575128,0.7300874776,-2.1028437863

C,0,0.7286286643,2.5715220359,-0.583550388
C,0,-0.7286286643,2.5715220359,-0.583550388
C,0,-1.4613651005,1.4504232369,-1.2186588759
C,0,2.6684280988,-0.7267347001,-0.7381331042
C,0,2.6684280988,0.7267347001,-0.7381331042
C,0,1.4613651005,1.4504232369,-1.2186588759
C,0,-0.7286286643,-2.5715220359,-0.583550388
C,0,0.7286286643,-2.5715220359,-0.583550388
C,0,1.4613651005,-1.4504232369,-1.2186588759
C,0,-2.6684280988,0.7267347001,-0.7381331042
C,0,-2.6684280988,-0.7267347001,-0.7381331042
C,0,-1.4613651005,-1.4504232369,-1.2186588759
C,0,1.3858961183,3.5837784996,0.1408219725
C,0,0.6972919285,4.5601106799,0.8347534416
C,0,-0.6972919285,4.5601106799,0.8347534416
C,0,-1.3858961183,3.5837784996,0.1408219725
C,0,3.8171378672,-1.3869366613,-0.273965983
C,0,4.9205340976,-0.6966616456,0.1954774444
C,0,4.9205340976,0.6966616456,0.1954774444
C,0,3.8171378672,1.3869366613,-0.273965983
C,0,-1.3858961183,-3.5837784996,0.1408219725
C,0,-0.6972919285,-4.5601106799,0.8347534416
C,0,0.6972919285,-4.5601106799,0.8347534416
C,0,1.3858961183,-3.5837784996,0.1408219725
C,0,-3.8171378672,1.3869366613,-0.273965983
C,0,-4.9205340976,0.6966616456,0.1954774444
C,0,-4.9205340976,-0.6966616456,0.1954774444
C,0,-3.8171378672,-1.3869366613,-0.273965983
H,0,2.465312119,3.6165485634,0.1490631146
H,0,1.2451125424,5.3250005087,1.3736462789
H,0,-1.2451125424,5.3250005087,1.3736462789
H,0,-2.465312119,3.6165485634,0.1490631146
H,0,3.875209348,-2.4648960159,-0.3402939051
H,0,5.793794697,-1.243612834,0.533184537
H,0,5.793794697,1.243612834,0.533184537
H,0,3.875209348,2.4648960159,-0.3402939051
H,0,-2.465312119,-3.6165485634,0.1490631146
H,0,-1.2451125424,-5.3250005087,1.3736462789
H,0,1.2451125424,-5.3250005087,1.3736462789
H,0,2.465312119,-3.6165485634,0.1490631146
H,0,-3.875209348,2.4648960159,-0.3402939051
H,0,-5.793794697,1.243612834,0.533184537
H,0,-5.793794697,-1.243612834,0.533184537
H,0,-3.875209348,-2.4648960159,-0.3402939051
Ce,0,0.,0.,1.1488349581
O,0,0.,0.,2.9388414451

Sum of electronic and zero-point Energies= -1778.409764
Sum of electronic and thermal Energies= -1778.386014
Sum of electronic and thermal Enthalpies= -1778.385070
Sum of electronic and thermal Free Energies= -1778.463992

Corannulene ($^1A_1$)
C,0,1.1446633139,-0.3719236572,0.6162568002
C,0,0.0000000001,-1.2035702351,0.6162568002
C,0,-1.1446633138,-0.3719236574,0.6162568002
C,0,-0.7074408337,0.9737087721,0.6162568002
C,0,0.7074408335,0.9737087722,0.6162568002
C,0,-3.2373917819,0.3256369724,-0.2578497158
C,0,-2.81050958,1.6394452981,-0.2578497158

C,0,-1.4557018006,2.0036016384,0.0924931709
C,0,-0.6907099125,3.1795699077,-0.2578497158
C,0,0.6907099119,3.1795699078,-0.2578497158
C,0,1.4557018002,2.0036016387,0.0924931709
C,0,2.8105095796,1.6394452987,-0.2578497158
C,0,3.2373917818,0.325636973,-0.2578497158
C,0,2.3553749906,-0.7653077273,0.0924931709
C,0,2.4277003584,-2.1663369919,-0.2578497158
C,0,1.3101082442,-2.978315192,-0.2578497158
C,0,0.0000000003,-2.4765878275,0.0924931709
C,0,-1.3101082436,-2.9783151923,-0.2578497158
C,0,-2.427700358,-2.1663369924,-0.2578497158
C,0,-2.3553749904,-0.7653077278,0.0924931709
H,0,-4.2392823054,0.1062753971,-0.6169062181
H,0,-3.4921185413,2.4058090144,-0.6169062181
H,0,-1.2089363664,4.064637964,-0.6169062181
H,0,1.2089363655,4.0646379643,-0.6169062181
H,0,3.4921185407,2.4058090151,-0.6169062181
H,0,4.2392823054,0.106275398,-0.6169062181
H,0,3.3671843173,-2.5777662237,-0.6169062181
H,0,1.4110841871,-3.9989561576,-0.6169062181
H,0,-1.4110841863,-3.9989561579,-0.6169062181
H,0,-3.3671843167,-2.5777662244,-0.6169062181

Sum of electronic and zero-point Energies= -767.666487
Sum of electronic and thermal Energies= -767.655154
Sum of electronic and thermal Enthalpies= -767.654210
Sum of electronic and thermal Free Energies= -767.701588

CeO(corannulene) (^{3}A)
C,0,1.2763200656,-1.2711270828,-0.7033399129
C,0,1.2763200656,-1.2711270831,0.7033399125
C,0,1.4329409512,0.0750944288,1.1403885493
C,0,1.5608012859,0.9076493514,0.0000000002
C,0,1.4329409512,0.0750944293,-1.1403885493
C,0,0.6481664471,1.9577217484,2.4135660667
C,0,0.7424696652,2.7658489375,1.2893676862
C,0,1.1164607454,2.2549873178,0.0000000004
C,0,0.7424696652,2.765848938,-1.2893676852
C,0,0.6481664471,1.9577217493,-2.413566066
C,0,0.8733144705,0.5170450745,-2.3457736237
C,0,0.332518396,-0.4945995658,-3.187769354
C,0,0.2040441255,-1.8341386233,-2.7575143643
C,0,0.6019147812,-2.2386581639,-1.4648805505
C,0,0.1444593338,-3.3852158773,-0.6858414357
C,0,0.1444593338,-3.3852158775,0.6858414344
C,0,0.6019147812,-2.2386581644,1.4648805497
C,0,0.2040441255,-1.8341386244,2.7575143636
C,0,0.332518396,-0.494599567,3.1877693538
C,0,0.8733144705,0.5170450737,2.3457736239
H,0,0.2737943574,2.3900415674,3.3363570235
H,0,0.4307245368,3.8035689264,1.3760150808
H,0,0.4307245368,3.8035689269,-1.3760150794
H,0,0.2737943574,2.3900415686,-3.3363570226
H,0,-0.1017201159,-0.2142880748,-4.1429838425
H,0,-0.3187020975,-2.5335825376,-3.4042499674
H,0,-0.2895292545,-4.2351899558,-1.2063432782
H,0,-0.2895292545,-4.2351899562,1.2063432766
H,0,-0.3187020975,-2.5335825388,3.4042499664
H,0,-0.1017201159,-0.2142880763,4.1429838424

Ce,0,-1.2790974442,0.4234413775,0.0000000001
O,0,-2.8930596894,1.2588683789,0.0000000002

Sum of electronic and zero-point Energies= -1318.051415
Sum of electronic and thermal Energies= -1318.035587
Sum of electronic and thermal Enthalpies= -1318.034643
Sum of electronic and thermal Free Energies= -1318.097471

Sumanene ($^1A_1$)
C,0,1.4068025255,0.0156581109,-1.2861693863
C,0,0.7169615839,1.2104976709,-1.2861693863
C,0,-0.7169615839,1.2104976709,-1.2861693863
C,0,-1.4068025255,0.0156581109,-1.2861693863
C,0,-0.6898409416,-1.2261557796,-1.2861693863
C,0,0.6898409416,-1.2261557796,-1.2861693863
C,0,-1.4341062328,-2.2233529631,-0.6588528386
C,0,-0.7125631999,-3.3006458553,-0.1446172518
C,0,0.7125631999,-3.3006458553,-0.1446172518
C,0,1.4341062328,-2.2233529631,-0.6588528386
C,0,2.6425332647,-0.1302959467,-0.6588528386
C,0,3.2147247601,1.0332250958,-0.1446172518
C,0,2.5021615603,2.2674207616,-0.1446172518
C,0,1.2084270318,2.353648912,-0.6588528386
C,0,-1.2084270318,2.353648912,-0.6588528386
C,0,-2.5021615603,2.2674207616,-0.1446172518
C,0,-3.2147247601,1.0332250958,-0.1446172518
C,0,-2.6425332647,-0.1302959467,-0.6588528386
C,0,0.,3.2870155951,-0.4027437466
C,0,2.8466390074,-1.6435077965,-0.4027437466
C,0,-2.8466390074,-1.6435077965,-0.4027437466
H,0,-1.2162308731,-4.1035383445,0.3868242691
H,0,1.2162308731,-4.1035383445,0.3868242691
H,0,4.161883889,0.9984823403,0.3868242691
H,0,2.9456530158,3.1050560064,0.3868242691
H,0,-2.9456530158,3.1050560064,0.3868242691
H,0,-4.161883889,0.9984823403,0.3868242691
H,0,0.,4.1550827835,-1.0731517117
H,0,0.,3.669800445,0.6218705161
H,0,3.5984072447,-2.0775413907,-1.0731517117
H,0,3.1781404115,-1.8349002214,0.6218705161
H,0,-3.1781404115,-1.8349002214,0.6218705161
H,0,-3.5984072447,-2.0775413907,-1.0731517117

Sum of electronic and zero-point Energies= -806.921799
Sum of electronic and thermal Energies= -806.909545
Sum of electronic and thermal Enthalpies= -806.908601
Sum of electronic and thermal Free Energies= -806.958238

CeO(sumanene) ($^3A'$)
C,0,0.0599578034,1.4337042434,-1.4732628467
C,0,-1.1545829872,0.7041116315,-1.5129402189
C,0,-1.1545829872,-0.7041116315,-1.5129402189
C,0,0.0599578034,-1.4337042434,-1.4732628467
C,0,1.3096045566,-0.6923645135,-1.4337606079
C,0,1.3096045566,0.6923645135,-1.4337606079
C,0,2.2870902526,-1.4205367776,-0.7402953642
C,0,3.3357625698,-0.7111116104,-0.1599470151
C,0,3.3357625698,0.7111116104,-0.1599470151
C,0,2.2870902526,1.4205367776,-0.7402953642
C,0,0.2036542798,2.5996279946,-0.7278547904

C,0,-0.9264698484,3.1240284617,-0.0640423395
C,0,-2.1527623582,2.3871864277,-0.0780673541
C,0,-2.2859871204,1.186425226,-0.7609191445
C,0,-2.2859871204,-1.186425226,-0.7609191445
C,0,-2.1527623582,-2.3871864277,-0.0780673541
C,0,-0.9264698484,-3.1240284617,-0.0640423395
C,0,0.2036542798,-2.5996279946,-0.7278547904
C,0,-3.2563167452,0.,-0.5995352985
C,0,1.7092882457,2.8225439756,-0.4787616904
C,0,1.7092882457,-2.8225439756,-0.4787616904
H,0,4.1003963015,-1.2247204188,0.4162256834
H,0,4.1003963015,1.2247204188,0.4162256834
H,0,-0.8589904383,4.0203418289,0.5426700621
H,0,-2.9596030531,2.7346831217,0.5625116443
H,0,-2.9596030531,-2.7346831217,0.5625116443
H,0,-0.8589904383,-4.0203418289,0.5426700621
H,0,-4.0005831176,0.,-1.4100081413
H,0,-3.7996244614,0.,0.3498660592
H,0,2.1247933229,3.5707997799,-1.1653228731
H,0,1.9143763752,3.1707456896,0.5379673751
H,0,1.9143763752,-3.1707456896,0.5379673751
H,0,2.1247933229,-3.5707997799,-1.1653228731
Ce,0,-0.4086808068,0.,1.2169308338
O,0,-1.0254561334,0.,2.9324324032

Sum of electronic and zero-point Energies= -1357.287074
Sum of electronic and thermal Energies= -1357.270583
Sum of electronic and thermal Enthalpies= -1357.269639
Sum of electronic and thermal Free Energies= -1357.332910

[CeO(sumanene)]$^{+}$ (^{2}A′)

C,0,-1.4137755264,-0.0168341273,-1.4420790726
C,0,-0.7215001746,-1.216398198,-1.44240022
C,0,0.7215001746,-1.216398198,-1.44240022
C,0,1.4137755264,-0.0168341273,-1.4420790726
C,0,0.6925207766,1.2330988053,-1.4430465981
C,0,-0.6925207767,1.2330988052,-1.4430465981
C,0,1.4327947075,2.2094388757,-0.7553815141
C,0,0.7142587083,3.2464007044,-0.1617802255
C,0,-0.7142587083,3.2464007044,-0.1617802255
C,0,-1.4327947075,2.2094388757,-0.7553815141
C,0,-2.6298071145,0.1360332423,-0.7551956232
C,0,-3.169047079,-1.0048990132,-0.1624400159
C,0,-2.4548241342,-2.2419930823,-0.1623001524
C,0,-1.1971475607,-2.345731976,-0.755123939
C,0,1.1971475607,-2.345731976,-0.755123939
C,0,2.4548241343,-2.2419930822,-0.1623001524
C,0,3.169047079,-1.0048990131,-0.1624400159
C,0,2.6298071144,0.1360332424,-0.7551956232
C,0,0.,-3.2950415569,-0.5364642942
C,0,-2.8534711554,1.6474041775,-0.5367295319
C,0,2.8534711553,1.6474041776,-0.5367295319
H,0,1.2216819909,4.0123100979,0.4165895628
H,0,-1.221681991,4.0123100978,0.4165895628
H,0,-4.0865819533,-0.9487046034,0.4151204024
H,0,-2.8650539544,-3.0646382484,0.4152505103
H,0,2.8650539545,-3.0646382484,0.4152505103
H,0,4.0865819533,-0.9487046033,0.4151204024
H,0,0.,-4.1107053844,-1.2690779572
H,0,0.,-3.7539786023,0.4556481984

H,0,-3.5596466513,2.0554703937,-1.2693886475
H,0,-3.2509211231,1.8769293469,0.4553692049
H,0,3.2509211231,1.876929347,0.4553692049
H,0,3.5596466513,2.0554703938,-1.2693886475
Ce,0,0.,0.0019317267,1.3583963317
O,0,0.,0.0022210432,3.1480693442

Sum of electronic and zero-point Energies= -1357.139423
Sum of electronic and thermal Energies= -1357.123178
Sum of electronic and thermal Enthalpies= -1357.122234
Sum of electronic and thermal Free Energies= -1357.186494