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

Supporting Information

Of

Beryllium Carbonyl $Be(CO)_n$ (n = 1-4) Complex: A p-Orbital Analogy of Dewar-Chatt-Duncanson Model‡

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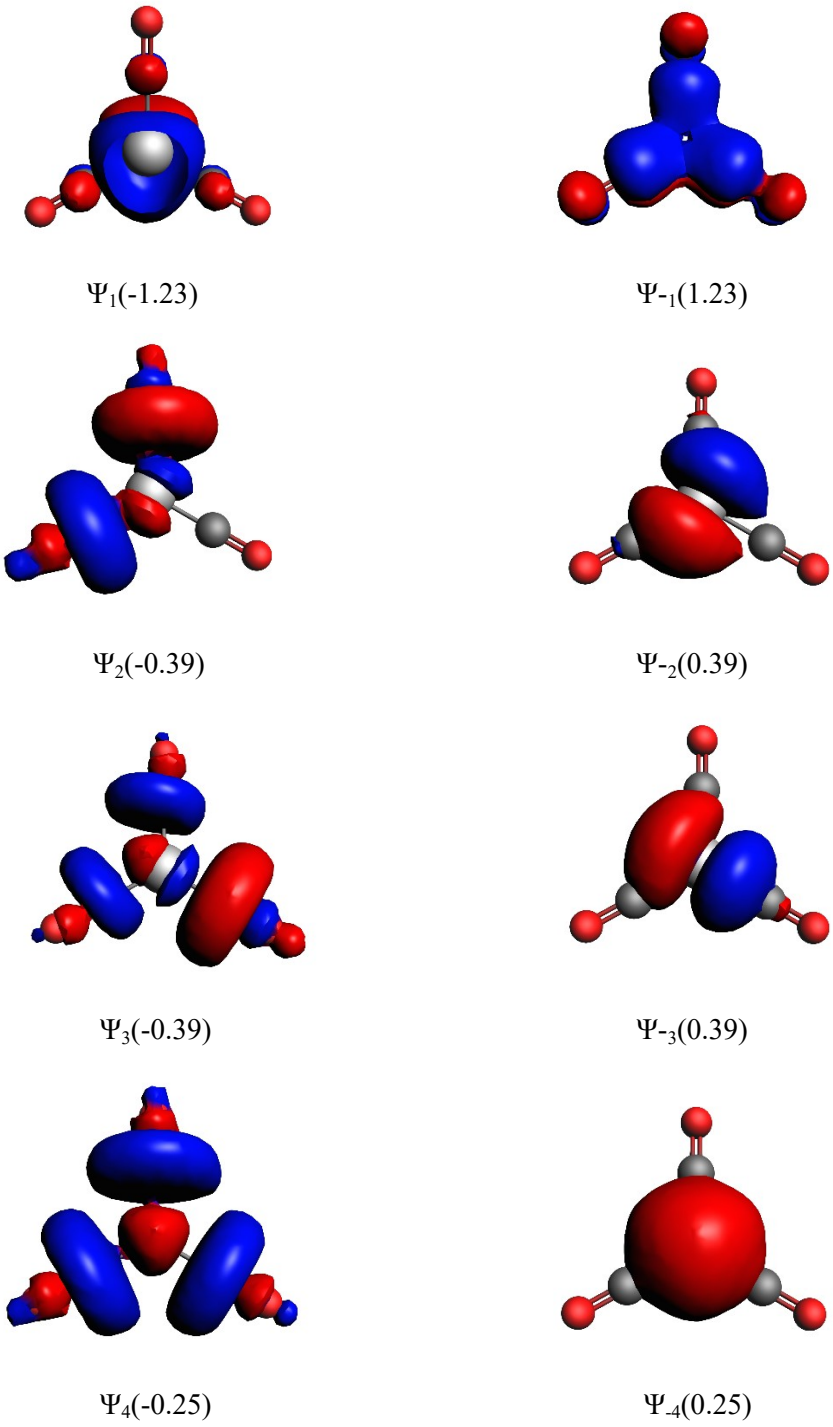
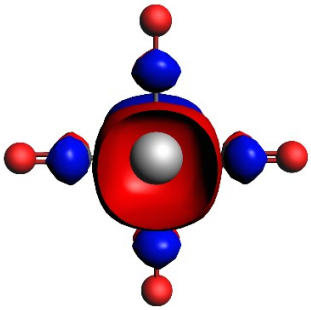
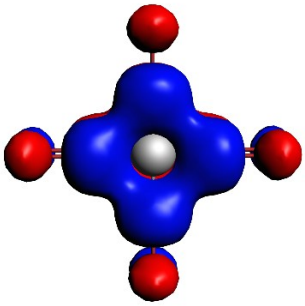


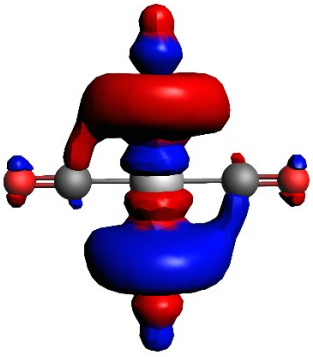
Fig. S1. Plots of important NOCV pair of orbitals Ψ_{-n}/Ψ_n in **$Be(CO)_3$** with their eigenvalues in parenthesis.



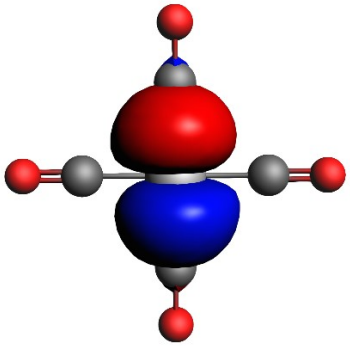
$\Psi_1(-1.24)$



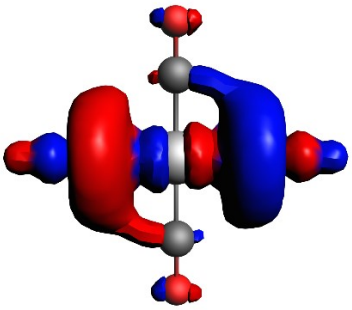
$\Psi_{-1}(1.24)$



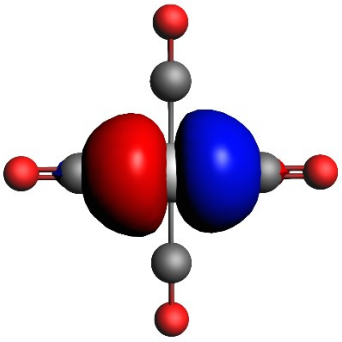
$\Psi_2(-0.36)$



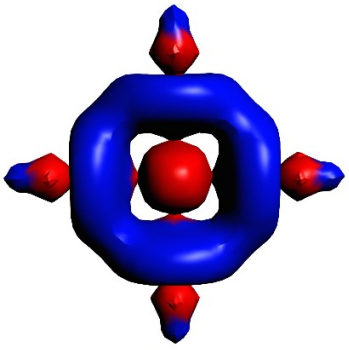
$\Psi_{-2}(0.36)$



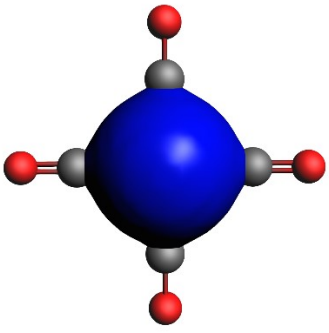
$\Psi_3(-0.36)$



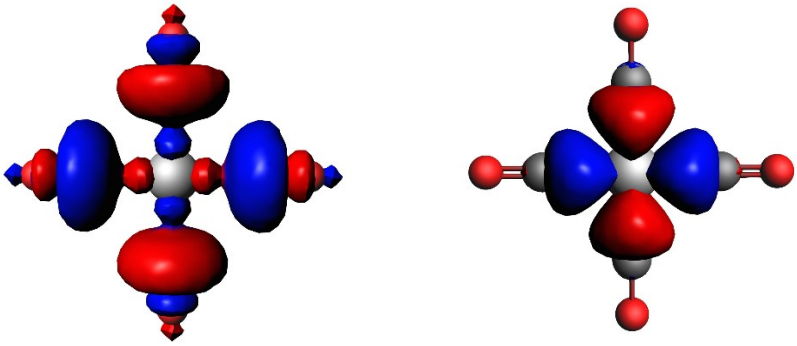
$\Psi_{-3}(0.36)$



$\Psi_4(-0.28)$



$\Psi_{-4}(0.28)$



Ψ_5(-0.14) Ψ_{-5}(0.14)

Fig. S2. Plots of important NOCV pair of orbitals Ψ_{-n}/Ψ_n in **$Be(CO)_4$** with their eigenvalues in parenthesis.

Cartesian coordinates of the TPSSh/def2-TZVP optimized geometries of the molecules.

BeCO (triplet)

4	0.000000000	0.000000000	1.816393000
6	0.000000000	0.000000000	0.142988000
8	0.000000000	0.000000000	-1.015437000

$Be(CO)_2$ (triplet)

4	0.000000000	0.000586000	0.000050000
6	-1.608751000	-0.000070000	0.000031000
8	-2.763409000	-0.000155000	-0.000023000
6	1.608751000	0.000316000	-0.000052000
8	2.763409000	-0.000323000	0.000013000

$Be(CO)_3$ (singlet)

4	-0.001095000	0.000055000	-0.000134000
6	-1.655956000	0.033774000	-0.000047000
8	-2.801053000	0.057078000	0.000059000
6	0.856719000	1.415724000	-0.000062000
8	1.450688000	2.395025000	0.000065000
6	0.798225000	-1.449443000	-0.000041000
8	1.351671000	-2.452171000	0.000056000

$Be(CO)_3$ (triplet)

4	-0.138554000	-0.000329000	0.000086000
6	-1.846243000	-0.001039000	0.000008000
8	-2.985066131	0.069683835	-0.000017422
6	0.748573000	-1.445909000	0.000077000
8	1.450334971	-2.367970008	-0.000065513
6	0.746806000	1.446159000	0.000074000
8	1.445143937	2.370822599	-0.000075254

$Be(CO)_4$ (singlet)

4	-0.000082000	0.000406000	-0.000026000
6	1.782436000	0.322000000	0.000412000
8	2.906882000	0.524944000	0.000920000
6	0.321941000	-1.782018000	-0.000433000
8	0.525444000	-2.906368000	-0.000898000
6	-0.322015000	1.782411000	-0.000432000
6	-1.782450000	-0.321965000	0.000411000
8	-2.906723000	-0.525871000	0.000919000
8	-0.525497000	2.906772000	-0.000896000

$Be(CO)_4$ (triplet)

4	-0.000423000	0.000210000	-0.000022000
6	-1.706290000	0.126331000	0.499123000
8	-2.762056000	0.204266000	0.946320000
6	0.126518000	1.705631000	-0.499507000
8	0.205378000	2.761457000	-0.946409000
6	-0.126175000	-1.705338000	-0.499696000
6	1.705389000	-0.126373000	0.499710000
8	2.761058000	-0.204801000	0.947088000
8	-0.203750000	-2.761215000	-0.946711000