Supplementary Information (SI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2025

Supporting information for

Coating the Fullerene. Evaluation of the Core-Shell Interaction Nature in a Saturated Exohedral Cuprofullerene

Raul Guajardo-Maturana,[a] Carlos Rivera,[b] Peter L. Rodríguez-Kessler[c] and Alvaro Muñoz-Castro[b*]

[a]*Universidad SEK, Facultad de Ciencias de la Salud, Instituto de Investigación Interdisciplinar en Ciencias Biomédicas SEK (I3CBSEK) Chile, Fernando Manterola 0789, Providencia, Santiago, Chile*

[b]*Facultad de Ingeniería, Arquitectura y Diseño, Universidad San Sebastián, Bellavista 7, Santiago, 8420524, Chile.*

[c]*Centro de Investigaciones en Óptica A.C., Loma del Bosque 115, Col. Lomas del Campestre, León, Guanajuato, 37150, Mexico.*

Figure 1. Optimized structure for the $[(C_2H_4)Cu(PhCH_2NH_2)_2]^+$ model.

Figure 2. Natural Orbitals for Chemical Valence extension of EDA (EDA-NOCV) for the C_{60}-$[Cu_{30}Cl_{36}(Cu(PhCH_2NH_2)_2)_6]^{6-}$ (**1**^{T}) interaction in **1**.

Table 1. Optimized coordinates for the studied species in a MultiXYZ format. Values in Angstrom (Å).

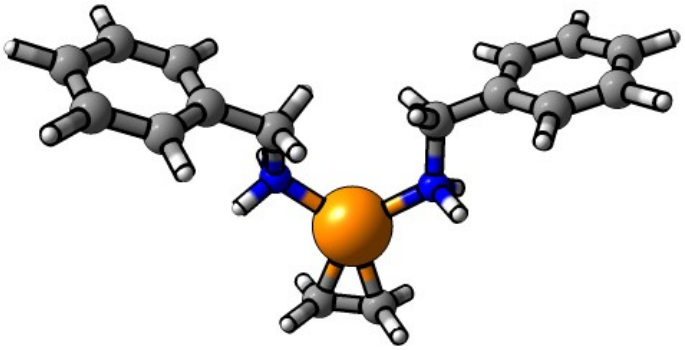

Figure 1. Optimized structure for the $[(C_2H_4)Cu(PhCH_2NH_2)_2]^+$ model.

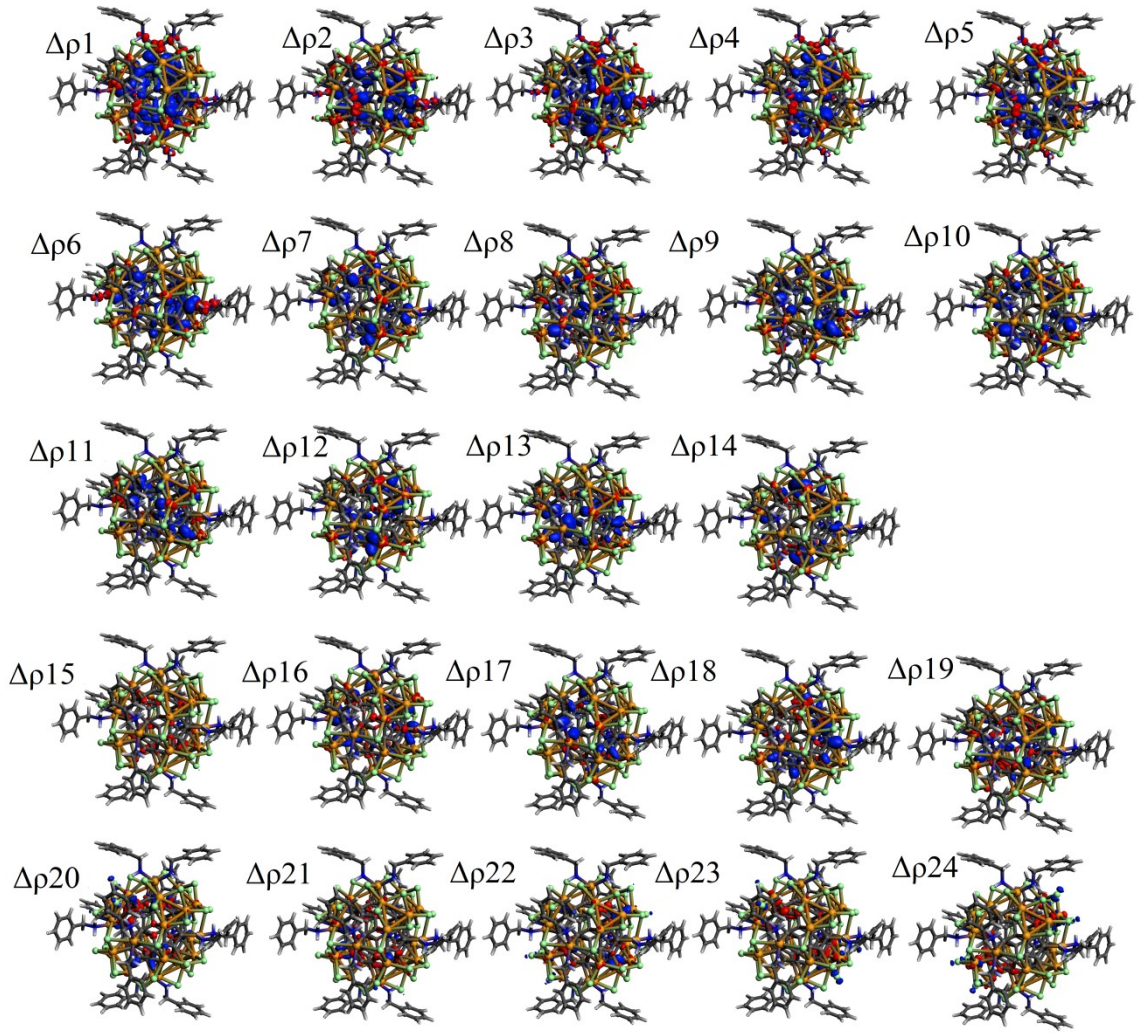

Figure 2. Natural Orbitals for Chemical Valence extension of EDA (EDA-NOCV) for the C_{60}-$[Cu_{30}Cl_{36}(Cu(PhCH_2NH_2)_2)_6]^{6-}$ (**1**^{T}) interaction in **1**, denoting the deformation densities ($\Delta\rho_n$) contributing to the ΔE_{orb} term. Charge flow from red to blue. Note that the color code is inversed in comparison to the electron density difference. Stabilization energy contribution per $\Delta\rho_n$ is given below (Values in kcal/mol).

Δρ1	-73.7	Δρ6	-54.1	Δρ11	-34.4	Δρ16	-24.3	Δρ21	-20.9
Δρ2	-73.9	Δρ7	-39.1	Δρ12	-33.8	Δρ17	-24.1	Δρ22	-20.8
Δρ3	-73.8	Δρ8	-39.0	Δρ13	-30.8	Δρ18	-24.4	Δρ23	-21.0
Δρ4	-54.0	Δρ9	-38.4	Δρ14	-30.5	Δρ19	-22.1	Δρ24	-17.1
Δρ5	-54.2	Δρ10	-34.7	Δρ15	-18.6	Δρ20	-22.0		

Table 1. Optimized coordinates for the studied species in a MultiXYZ format. Values in Angstrom (Å).

240
C_{60}-[$Cu_{30}Cl_{36}(Cu(PhCH_2NH_2)_2)_6]^{6-}$ (1)

Cu	1.138266000	5.233272000	-2.932913000
Cu	3.100866000	5.370858000	-0.219282000
Cu	3.963014000	3.602403000	-2.932913000
Cu	-1.909922000	0.000000000	6.157962000
Cu	0.954961000	1.654041000	6.157962000
Cu	0.954961000	-1.654041000	6.157962000
Cu	3.100866000	-5.370858000	-0.219282000
Cu	1.138266000	-5.233272000	-2.932913000
Cu	3.963014000	-3.602403000	-2.932913000
Cu	-5.101280000	-1.630869000	-2.932913000
Cu	-5.101280000	1.630869000	-2.932913000
Cu	-6.201732000	0.000000000	-0.219282000
N	0.677837000	6.296048000	-1.403007000
N	1.440475000	6.294427000	-0.279782000
N	4.730896000	4.394701000	-0.279782000
N	5.113619000	3.735048000	-1.403007000
N	2.882170000	3.633891000	-4.506848000
N	1.705957000	4.312978000	-4.506848000
N	-1.884952000	1.907234000	6.181338000
N	-0.709237000	2.586034000	6.181338000
N	2.594189000	0.678799000	6.181338000
N	2.594189000	-0.678799000	6.181338000
N	-0.709237000	-2.586034000	6.181338000
N	-1.884952000	-1.907234000	6.181338000
N	1.440475000	-6.294427000	-0.279782000
N	0.677837000	-6.296048000	-1.403007000
N	1.705957000	-4.312978000	-4.506848000
N	2.882170000	-3.633891000	-4.506848000
N	5.113619000	-3.735048000	-1.403007000
N	4.730896000	-4.394701000	-0.279782000
N	-4.588127000	-0.679087000	-4.506848000
N	-4.588127000	0.679087000	-4.506848000
N	-5.791456000	2.561000000	-1.403007000
N	-6.171371000	1.899725000	-0.279782000
N	-6.171371000	-1.899725000	-0.279782000
N	-5.791456000	-2.561000000	-1.403007000
C	-0.984399000	3.899166000	6.006159000
C	5.602131000	4.081680000	0.706123000
C	-3.974428000	0.000000000	-6.559554000
C	6.227417000	-3.028020000	-1.110723000
C	3.060504000	3.107420000	-5.739312000
C	3.060504000	-3.107420000	-5.739312000
C	-6.335905000	2.810748000	0.706123000
C	-5.736050000	-3.879091000	-1.110723000
C	-4.221357000	-1.096764000	-5.739312000
C	1.987214000	3.441955000	-6.559554000
C	-5.736050000	3.879091000	-1.110723000
C	6.576916000	-3.213800000	0.224232000
C	3.868976000	1.097069000	6.006159000
C	-0.505226000	-7.302677000	0.224232000
C	6.227417000	3.028020000	-1.110723000
C	4.718678000	0.000000000	5.889412000
C	-2.359339000	-4.086495000	5.889412000
C	1.160853000	4.204184000	-5.739312000
C	-4.221357000	1.096764000	-5.739312000
C	-0.491366000	-6.907111000	-1.110723000
C	1.987214000	-3.441955000	-6.559554000
C	1.160853000	-4.204184000	-5.739312000
C	-2.359339000	4.086495000	5.889412000
C	-2.884577000	-2.802097000	6.006159000
C	5.602131000	-4.081680000	0.706123000
C	-2.884577000	2.802097000	6.006159000

C	-0.984399000	-3.899166000	6.006159000
C	0.733773000	-6.892428000	0.706123000
C	-6.335905000	-2.810748000	0.706123000
C	-0.505226000	7.302677000	0.224232000
C	3.868976000	-1.097069000	6.006159000
C	0.733773000	6.892428000	0.706123000
C	-0.491366000	6.907111000	-1.110723000
C	6.576916000	3.213800000	0.224232000
C	-6.071691000	4.088876000	0.224232000
C	-6.071691000	-4.088876000	0.224232000
C	0.112288000	4.904629000	5.991818000
F	-0.380239000	6.151966000	5.782258000
F	0.801068000	4.913759000	7.171264000
F	1.021007000	4.635556000	5.010272000
C	-4.303677000	2.355070000	5.991818000
F	-5.137639000	3.405279000	5.782258000
F	-4.525013000	1.433560000	5.010272000
F	-4.655974000	1.763135000	7.171264000
C	-4.303677000	-2.355070000	5.991818000
F	-4.525013000	-1.433560000	5.010272000
F	-5.137639000	-3.405279000	5.782258000
F	-4.655974000	-1.763135000	7.171264000
C	0.112288000	-4.904629000	5.991818000
F	1.021007000	-4.635556000	5.010272000
F	0.801068000	-4.913759000	7.171264000
F	-0.380239000	-6.151966000	5.782258000
C	4.191389000	-2.549559000	5.991818000
F	3.854907000	-3.150625000	7.171264000
F	3.504005000	-3.201996000	5.010272000
F	5.517878000	-2.746686000	5.782258000
C	4.191389000	2.549559000	5.991818000
F	3.504005000	3.201996000	5.010272000
F	3.854907000	3.150625000	7.171264000
F	5.517878000	2.746686000	5.782258000
C	5.434184000	-4.656927000	2.066238000
F	6.362700000	-4.162943000	2.919921000
F	4.200448000	-4.372021000	2.571587000
F	5.550004000	-6.011708000	2.058039000
C	6.899721000	-2.230237000	-2.170169000
F	6.034289000	-1.341431000	-2.737081000
F	7.947566000	-1.535663000	-1.663095000
F	7.366299000	-3.019570000	-3.178626000
C	4.278936000	-2.318941000	-6.059895000
F	4.145663000	-1.695021000	-7.260054000
F	4.518287000	-1.371260000	-5.109302000
F	5.395282000	-3.106348000	-6.123632000
C	-0.131206000	-4.865138000	-6.059895000
F	-0.604900000	-4.437760000	-7.260054000
F	-0.007465000	-6.225625000	-6.123632000
F	-1.071598000	-4.598582000	-5.109302000
C	-1.518419000	-7.090452000	-2.170169000
F	-1.855431000	-5.896563000	-2.737081000
F	-1.068126000	-7.889187000	-3.178626000
F	-2.643860000	-7.650626000	-1.663095000
C	1.315925000	-7.034605000	2.066238000
F	1.686057000	-5.823705000	2.571587000
F	0.423864000	-7.591732000	2.919921000
F	2.431290000	-7.812299000	2.058039000
C	-5.381302000	-4.860216000	-2.170169000
F	-4.178858000	-4.555132000	-2.737081000
F	-5.303707000	-6.114963000	-1.663095000
F	-6.298174000	-4.869617000	-3.178626000
C	-6.750109000	-2.377678000	2.066238000
F	-7.981294000	-1.800591000	2.058039000
F	-6.786564000	-3.428789000	2.919921000
F	-5.886505000	-1.451684000	2.571587000
C	-6.750109000	2.377678000	2.066238000
F	-6.786564000	3.428789000	2.919921000

F	-7.981294000	1.800591000	2.058039000
F	-5.886505000	1.451684000	2.571587000
C	-5.381302000	4.860216000	-2.170169000
F	-6.298174000	4.869617000	-3.178626000
F	-5.303707000	6.114963000	-1.663095000
F	-4.178858000	4.555132000	-2.737081000
C	-4.147730000	2.546197000	-6.059895000
F	-3.446690000	3.227322000	-5.109302000
F	-3.540763000	2.742739000	-7.260054000
F	-5.387817000	3.119278000	-6.123632000
C	-4.147730000	-2.546197000	-6.059895000
F	-3.540763000	-2.742739000	-7.260054000
F	-3.446690000	-3.227322000	-5.109302000
F	-5.387817000	-3.119278000	-6.123632000
C	-1.518419000	7.090452000	-2.170169000
F	-1.068126000	7.889187000	-3.178626000
F	-1.855431000	5.896563000	-2.737081000
F	-2.643860000	7.650626000	-1.663095000
C	1.315925000	7.034605000	2.066238000
F	2.431290000	7.812299000	2.058039000
F	0.423864000	7.591732000	2.919921000
F	1.686057000	5.823705000	2.571587000
C	5.434184000	4.656927000	2.066238000
F	5.550004000	6.011708000	2.058039000
F	4.200448000	4.372021000	2.571587000
F	6.362700000	4.162943000	2.919921000
C	6.899721000	2.230237000	-2.170169000
F	7.366299000	3.019570000	-3.178626000
F	7.947566000	1.535663000	-1.663095000
F	6.034289000	1.341431000	-2.737081000
C	4.278936000	2.318941000	-6.059895000
F	4.518287000	1.371260000	-5.109302000
F	4.145663000	1.695021000	-7.260054000
F	5.395282000	3.106348000	-6.123632000
C	-0.131206000	4.865138000	-6.059895000
F	-1.071598000	4.598582000	-5.109302000
F	-0.007465000	6.225625000	-6.123632000
F	-0.604900000	4.437760000	-7.260054000
H	5.791399000	0.000000000	5.751870000
H	-2.895700000	5.015499000	5.751870000
H	-2.895700000	-5.015499000	5.751870000
H	-1.290998000	-7.819470000	0.758847000
H	7.417358000	-2.791698000	0.758847000
H	1.819589000	-3.151621000	-7.587736000
H	-6.126360000	-5.027772000	0.758847000
H	-6.126360000	5.027772000	0.758847000
H	-3.639178000	0.000000000	-7.587736000
H	1.819589000	3.151621000	-7.587736000
H	7.417358000	2.791698000	0.758847000
H	-1.290998000	7.819470000	0.758847000
C	-3.084247000	0.731660000	-1.439785000
C	-2.177768000	1.430016000	-2.245831000
C	2.188502000	-1.428462000	2.588237000
C	3.095646000	-0.727131000	1.785496000
C	-0.918108000	3.044474000	1.785496000
C	0.142834000	2.609529000	2.588237000
C	-0.149547000	-2.601010000	-2.245831000
C	0.908487000	-3.036866000	-1.439785000
C	-2.331335000	-1.181067000	2.588237000
C	-2.177537000	-2.317342000	1.785496000
C	2.175760000	2.305206000	-1.439785000
C	2.327314000	1.170994000	-2.245831000
C	-3.322788000	1.176746000	-0.073045000
C	-3.084247000	-0.731660000	-1.439785000
C	-1.505257000	2.607181000	-1.727229000
C	-1.251448000	0.702309000	-3.099414000
C	1.245539000	-0.698587000	3.415056000
C	1.503835000	-2.604719000	2.072889000

```
C         3.095646000      0.727131000      1.785496000
C         3.356701000     -1.176027000      0.422271000
C        -2.177537000      2.317342000      1.785496000
C        -0.659881000      3.495002000      0.422271000
C        -0.017775000      1.427962000      3.415056000
C         1.503835000      2.604719000      2.072889000
C        -1.505257000     -2.607181000     -1.727229000
C         0.017507000     -1.434941000     -3.099414000
C         0.642302000     -3.465992000     -0.073045000
C         2.175760000     -2.305206000     -1.439785000
C        -3.007671000      0.000000000      2.072889000
C        -1.227764000     -0.729375000      3.415056000
C        -2.696820000     -2.318975000      0.422271000
C        -0.918108000     -3.044474000      1.785496000
C         0.908487000      3.036866000     -1.439785000
C         2.680486000      2.289246000     -0.073045000
C         1.233942000      0.732632000     -3.099414000
C         3.010514000      0.000000000     -1.727229000
C        -2.696820000      2.318975000      0.422271000
C        -2.177768000     -1.430016000     -2.245831000
C        -1.757633000      3.044310000     -0.421559000
C        -1.251448000     -0.702309000     -3.099414000
C         1.245539000      0.698587000      3.415056000
C         1.745671000     -3.023590000      0.764383000
C         2.188502000      1.428462000      2.588237000
C         2.680486000     -2.289246000     -0.073045000
C        -2.331335000      1.181067000      2.588237000
C         0.642302000      3.465992000     -0.073045000
C        -1.227764000      0.729375000      3.415056000
C         1.745671000      3.023590000      0.764383000
C        -1.757633000     -3.044310000     -0.421559000
C         1.233942000     -0.732632000     -3.099414000
C        -0.659881000     -3.495002000      0.422271000
C         2.327314000     -1.170994000     -2.245831000
C        -3.491341000      0.000000000      0.764383000
C        -0.017775000     -1.427962000      3.415056000
C        -3.322788000     -1.176746000     -0.073045000
C         0.142834000     -2.609529000      2.588237000
C        -0.149547000      2.601010000     -2.245831000
C         3.356701000      1.176027000      0.422271000
C         0.017507000      1.434941000     -3.099414000
C         3.515266000      0.000000000     -0.421559000
41
[(C2H4)Cu(PhCH2NH2)2]+ model
C         2.820966000      0.746270000      1.592366000
C         2.213245000      1.922319000      1.976623000
C         4.839994000      3.251414000      5.630016000
C         4.460993000      4.304675000      6.634073000
C         3.874501000      3.942807000      7.852381000
C         3.451317000      4.922527000      8.753707000
C         3.605469000      6.274378000      8.438013000
C         4.193973000      6.643900000      7.224977000
C         4.621935000      5.663819000      6.329145000
C         6.829564000      0.984033000      3.902961000
C         8.025686000      0.105374000      3.653475000
C         8.251164000     -1.025205000      4.450706000
C         9.319491000     -1.880550000      4.179538000
C        10.177552000     -1.609519000      3.110393000
C         9.962806000     -0.481731000      2.314586000
C         8.891095000      0.372145000      2.586045000
Cu        3.922532000      1.607895000      3.174197000
H         2.906777000      3.150803000      4.933767000
H         3.878638000      4.051777000      3.987867000
H         5.792634000      0.025725000      2.403774000
H         5.333250000     -0.435149000      3.896579000
H         4.885811000      2.264913000      6.113046000
H         5.822390000      3.462381000      5.185229000
H         3.748728000      2.885591000      8.097866000
```

```
H        2.998405000      4.629397000      9.702714000
H        3.272401000      7.041076000      9.139697000
H        4.322546000      7.699637000      6.978726000
H        5.086007000      5.957916000      5.384010000
H        6.979067000      1.971046000      3.449718000
H        6.665478000      1.125280000      4.977180000
H        7.585781000     -1.236721000      5.291175000
H        9.489093000     -2.756722000      4.808520000
H       11.015507000     -2.276619000      2.899867000
H       10.634218000     -0.263673000      1.482324000
H        8.726020000      1.255067000      1.963612000
N        3.847913000      3.167817000      4.515628000
N        5.577107000      0.395790000      3.339801000
H        3.509904000      0.724405000      0.743170000
H        2.474908000     -0.217561000      1.978335000
H        2.416311000      2.859722000      1.444648000
H        1.362463000      1.924579000      2.665546000
240
C60@[Cu3(3,5-(CF3)2Pz)3]4 (2)
Cu       1.138266000      5.233272000     -2.932913000
Cu       3.100866000      5.370858000     -0.219282000
Cu       3.963014000      3.602403000     -2.932913000
Cu      -1.909922000      0.000000000      6.157962000
Cu       0.954961000      1.654041000      6.157962000
Cu       0.954961000     -1.654041000      6.157962000
Cu       3.100866000     -5.370858000     -0.219282000
Cu       1.138266000     -5.233272000     -2.932913000
Cu       3.963014000     -3.602403000     -2.932913000
Cu      -5.101280000     -1.630869000     -2.932913000
Cu      -5.101280000      1.630869000     -2.932913000
Cu      -6.201732000      0.000000000     -0.219282000
N        0.677837000      6.296048000     -1.403007000
N        1.440475000      6.294427000     -0.279782000
N        4.730896000      4.394701000     -0.279782000
N        5.113619000      3.735048000     -1.403007000
N        2.882170000      3.633891000     -4.506848000
N        1.705957000      4.312978000     -4.506848000
N       -1.884952000      1.907234000      6.181338000
N       -0.709237000      2.586034000      6.181338000
N        2.594189000      0.678799000      6.181338000
N        2.594189000     -0.678799000      6.181338000
N       -0.709237000     -2.586034000      6.181338000
N       -1.884952000     -1.907234000      6.181338000
N        1.440475000     -6.294427000     -0.279782000
N        0.677837000     -6.296048000     -1.403007000
N        1.705957000     -4.312978000     -4.506848000
N        2.882170000     -3.633891000     -4.506848000
N        5.113619000     -3.735048000     -1.403007000
N        4.730896000     -4.394701000     -0.279782000
N       -4.588127000     -0.679087000     -4.506848000
N       -4.588127000      0.679087000     -4.506848000
N       -5.791456000      2.561000000     -1.403007000
N       -6.171371000      1.899725000     -0.279782000
N       -6.171371000     -1.899725000     -0.279782000
N       -5.791456000     -2.561000000     -1.403007000
C       -0.984399000      3.899166000      6.006159000
C        5.602131000      4.081680000      0.706123000
C       -3.974428000      0.000000000     -6.559554000
C        6.227417000     -3.028020000     -1.110723000
C        3.060504000      3.107420000     -5.739312000
C        3.060504000     -3.107420000     -5.739312000
C       -6.335905000      2.810748000      0.706123000
C       -5.736050000     -3.879091000     -1.110723000
C       -4.221357000     -1.096764000     -5.739312000
C        1.987214000      3.441955000     -6.559554000
C       -5.736050000      3.879091000     -1.110723000
C        6.576916000     -3.213800000      0.224232000
C        3.868976000      1.097069000      6.006159000
```

C	-0.505226000	-7.302677000	0.224232000
C	6.227417000	3.028020000	-1.110723000
C	4.718678000	0.000000000	5.889412000
C	-2.359339000	-4.086495000	5.889412000
C	1.160853000	4.204184000	-5.739312000
C	-4.221357000	1.096764000	-5.739312000
C	-0.491366000	-6.907111000	-1.110723000
C	1.987214000	-3.441955000	-6.559554000
C	1.160853000	-4.204184000	-5.739312000
C	-2.359339000	4.086495000	5.889412000
C	-2.884577000	-2.802097000	6.006159000
C	5.602131000	-4.081680000	0.706123000
C	-2.884577000	2.802097000	6.006159000
C	-0.984399000	-3.899166000	6.006159000
C	0.733773000	-6.892428000	0.706123000
C	-6.335905000	-2.810748000	0.706123000
C	-0.505226000	7.302677000	0.224232000
C	3.868976000	-1.097069000	6.006159000
C	0.733773000	6.892428000	0.706123000
C	-0.491366000	6.907111000	-1.110723000
C	6.576916000	3.213800000	0.224232000
C	-6.071691000	4.088876000	0.224232000
C	-6.071691000	-4.088876000	0.224232000
C	0.112288000	4.904629000	5.991818000
F	-0.380239000	6.151966000	5.782258000
F	0.801068000	4.913759000	7.171264000
F	1.021007000	4.635556000	5.010272000
C	-4.303677000	2.355070000	5.991818000
F	-5.137639000	3.405279000	5.782258000
F	-4.525013000	1.433560000	5.010272000
F	-4.655974000	1.763135000	7.171264000
C	-4.303677000	-2.355070000	5.991818000
F	-4.525013000	-1.433560000	5.010272000
F	-5.137639000	-3.405279000	5.782258000
F	-4.655974000	-1.763135000	7.171264000
C	0.112288000	-4.904629000	5.991818000
F	1.021007000	-4.635556000	5.010272000
F	0.801068000	-4.913759000	7.171264000
F	-0.380239000	-6.151966000	5.782258000
C	4.191389000	-2.549559000	5.991818000
F	3.854907000	-3.150625000	7.171264000
F	3.504005000	-3.201996000	5.010272000
F	5.517878000	-2.746686000	5.782258000
C	4.191389000	2.549559000	5.991818000
F	3.504005000	3.201996000	5.010272000
F	3.854907000	3.150625000	7.171264000
F	5.517878000	2.746686000	5.782258000
C	5.434184000	-4.656927000	2.066238000
F	6.362700000	-4.162943000	2.919921000
F	4.200448000	-4.372021000	2.571587000
F	5.550004000	-6.011708000	2.058039000
C	6.899721000	-2.230237000	-2.170169000
F	6.034289000	-1.341431000	-2.737081000
F	7.947566000	-1.535663000	-1.663095000
F	7.366299000	-3.019570000	-3.178626000
C	4.278936000	-2.318941000	-6.059895000
F	4.145663000	-1.695021000	-7.260054000
F	4.518287000	-1.371260000	-5.109302000
F	5.395282000	-3.106348000	-6.123632000
C	-0.131206000	-4.865138000	-6.059895000
F	-0.604900000	-4.437760000	-7.260054000
F	-0.007465000	-6.225625000	-6.123632000
F	-1.071598000	-4.598582000	-5.109302000
C	-1.518419000	-7.090452000	-2.170169000
F	-1.855431000	-5.896563000	-2.737081000
F	-1.068126000	-7.889187000	-3.178626000
F	-2.643860000	-7.650626000	-1.663095000
C	1.315925000	-7.034605000	2.066238000

F	1.686057000	-5.823705000	2.571587000
F	0.423864000	-7.591732000	2.919921000
F	2.431290000	-7.812299000	2.058039000
C	-5.381302000	-4.860216000	-2.170169000
F	-4.178858000	-4.555132000	-2.737081000
F	-5.303707000	-6.114963000	-1.663095000
F	-6.298174000	-4.869617000	-3.178626000
C	-6.750109000	-2.377678000	2.066238000
F	-7.981294000	-1.800591000	2.058039000
F	-6.786564000	-3.428789000	2.919921000
F	-5.886505000	-1.451684000	2.571587000
C	-6.750109000	2.377678000	2.066238000
F	-6.786564000	3.428789000	2.919921000
F	-7.981294000	1.800591000	2.058039000
F	-5.886505000	1.451684000	2.571587000
C	-5.381302000	4.860216000	-2.170169000
F	-6.298174000	4.869617000	-3.178626000
F	-5.303707000	6.114963000	-1.663095000
F	-4.178858000	4.555132000	-2.737081000
C	-4.147730000	2.546197000	-6.059895000
F	-3.446690000	3.227322000	-5.109302000
F	-3.540763000	2.742739000	-7.260054000
F	-5.387817000	3.119278000	-6.123632000
C	-4.147730000	-2.546197000	-6.059895000
F	-3.540763000	-2.742739000	-7.260054000
F	-3.446690000	-3.227322000	-5.109302000
F	-5.387817000	-3.119278000	-6.123632000
C	-1.518419000	7.090452000	-2.170169000
F	-1.068126000	7.889187000	-3.178626000
F	-1.855431000	5.896563000	-2.737081000
F	-2.643860000	7.650626000	-1.663095000
C	1.315925000	7.034605000	2.066238000
F	2.431290000	7.812299000	2.058039000
F	0.423864000	7.591732000	2.919921000
F	1.686057000	5.823705000	2.571587000
C	5.434184000	4.656927000	2.066238000
F	5.550004000	6.011708000	2.058039000
F	4.200448000	4.372021000	2.571587000
F	6.362700000	4.162943000	2.919921000
C	6.899721000	2.230237000	-2.170169000
F	7.366299000	3.019570000	-3.178626000
F	7.947566000	1.535663000	-1.663095000
F	6.034289000	1.341431000	-2.737081000
C	4.278936000	2.318941000	-6.059895000
F	4.518287000	1.371260000	-5.109302000
F	4.145663000	1.695021000	-7.260054000
F	5.395282000	3.106348000	-6.123632000
C	-0.131206000	4.865138000	-6.059895000
F	-1.071598000	4.598582000	-5.109302000
F	-0.007465000	6.225625000	-6.123632000
F	-0.604900000	4.437760000	-7.260054000
H	5.791399000	0.000000000	5.751870000
H	-2.895700000	5.015499000	5.751870000
H	-2.895700000	-5.015499000	5.751870000
H	-1.290998000	-7.819470000	0.758847000
H	7.417358000	-2.791698000	0.758847000
H	1.819589000	-3.151621000	-7.587736000
H	-6.126360000	-5.027772000	0.758847000
H	-6.126360000	5.027772000	0.758847000
H	-3.639178000	0.000000000	-7.587736000
H	1.819589000	3.151621000	-7.587736000
H	7.417358000	2.791698000	0.758847000
H	-1.290998000	7.819470000	0.758847000
C	-3.084247000	0.731660000	-1.439785000
C	-2.177768000	1.430016000	-2.245831000
C	2.188502000	-1.428462000	2.588237000
C	3.095646000	-0.727131000	1.785496000
C	-0.918108000	3.044474000	1.785496000

C	0.142834000	2.609529000	2.588237000
C	-0.149547000	-2.601010000	-2.245831000
C	0.908487000	-3.036866000	-1.439785000
C	-2.331335000	-1.181067000	2.588237000
C	-2.177537000	-2.317342000	1.785496000
C	2.175760000	2.305206000	-1.439785000
C	2.327314000	1.170994000	-2.245831000
C	-3.322788000	1.176746000	-0.073045000
C	-3.084247000	-0.731660000	-1.439785000
C	-1.505257000	2.607181000	-1.727229000
C	-1.251448000	0.702309000	-3.099414000
C	1.245539000	-0.698587000	3.415056000
C	1.503835000	-2.604719000	2.072889000
C	3.095646000	0.727131000	1.785496000
C	3.356701000	-1.176027000	0.422271000
C	-2.177537000	2.317342000	1.785496000
C	-0.659881000	3.495002000	0.422271000
C	-0.017775000	1.427962000	3.415056000
C	1.503835000	2.604719000	2.072889000
C	-1.505257000	-2.607181000	-1.727229000
C	0.017507000	-1.434941000	-3.099414000
C	0.642302000	-3.465992000	-0.073045000
C	2.175760000	-2.305206000	-1.439785000
C	-3.007671000	0.000000000	2.072889000
C	-1.227764000	-0.729375000	3.415056000
C	-2.696820000	-2.318975000	0.422271000
C	-0.918108000	-3.044474000	1.785496000
C	0.908487000	3.036866000	-1.439785000
C	2.680486000	2.289246000	-0.073045000
C	1.233942000	0.732632000	-3.099414000
C	3.010514000	0.000000000	-1.727229000
C	-2.696820000	2.318975000	0.422271000
C	-2.177768000	-1.430016000	-2.245831000
C	-1.757633000	3.044310000	-0.421559000
C	-1.251448000	-0.702309000	-3.099414000
C	1.245539000	0.698587000	3.415056000
C	1.745671000	-3.023590000	0.764383000
C	2.188502000	1.428462000	2.588237000
C	2.680486000	-2.289246000	-0.073045000
C	-2.331335000	1.181067000	2.588237000
C	0.642302000	3.465992000	-0.073045000
C	-1.227764000	0.729375000	3.415056000
C	1.745671000	3.023590000	0.764383000
C	-1.757633000	-3.044310000	-0.421559000
C	1.233942000	-0.732632000	-3.099414000
C	-0.659881000	-3.495002000	0.422271000
C	2.327314000	-1.170994000	-2.245831000
C	-3.491341000	0.000000000	0.764383000
C	-0.017775000	-1.427962000	3.415056000
C	-3.322788000	-1.176746000	-0.073045000
C	0.142834000	-2.609529000	2.588237000
C	-0.149547000	2.601010000	-2.245831000
C	3.356701000	1.176027000	0.422271000
C	0.017507000	1.434941000	-3.099414000
C	3.515266000	0.000000000	-0.421559000