

Anion Encapsulated Endohedral Fullerenes as Large Anions: A DFT Study

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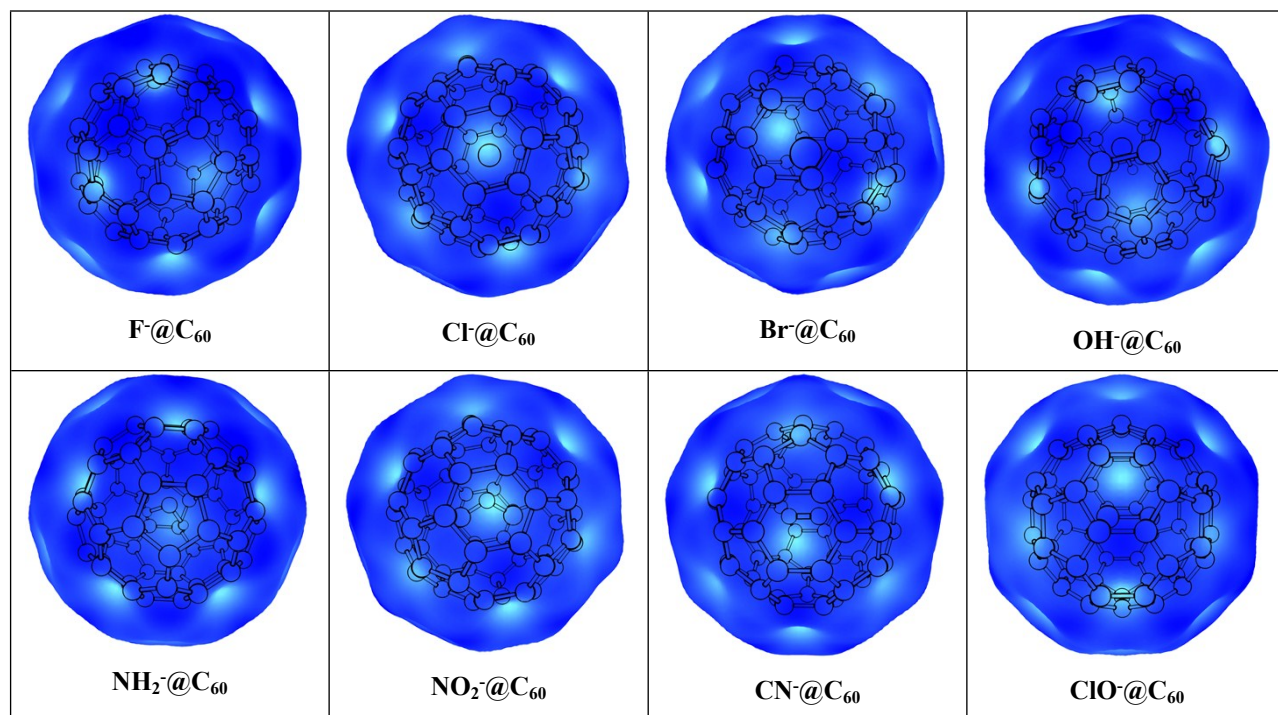
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Supporting Information

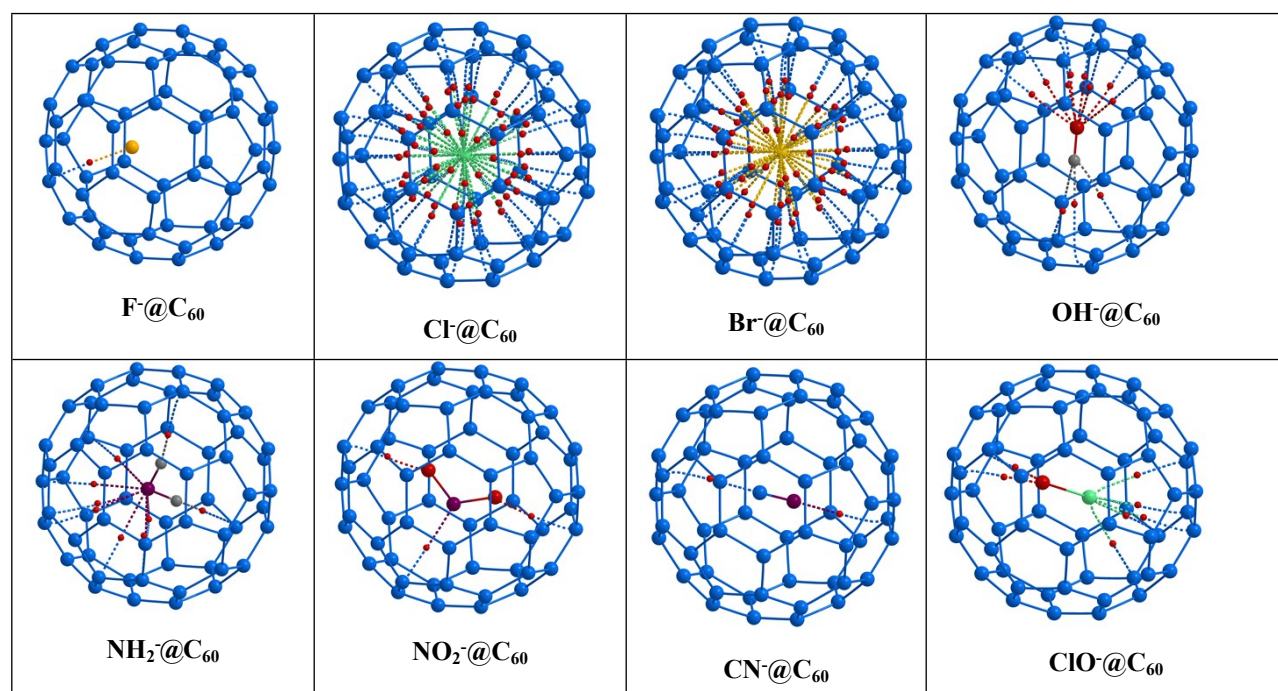
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- 1. Fig. S1** MESP of $X^{-}@C_{60}$ endohedral fullerene systems plotted at an isosurface value of 0.003 au. The color coding from blue to red indicates MESP values in the range -0.01 – +0.01 au.
- 2. Fig. S2** QTAIM graph of $X^{-}@C_{60}$ systems at M06L/6-311++G(d,p) level.
- 3.** Cartesian coordinates of optimized geometry of complexes at M06L/6-31G(d,p) level.

1. **Fig. S1** MESP of $X^-@C_{60}$ endohedral fullerene systems plotted at an isosurface value of 0.003 au. The color coding from blue to red indicates MESP values in the range -0.1 – +0.1 au.



2. **Fig. S2** QTAIM graph of $X^-@C_{60}$ systems at M06L/6-311++G(d,p) level.



3. Cartesian coordinates of optimized geometry of complexes at M06L/6-31G(d,p) level

C ₆₀				C ₆₀ ⁻			
SCF Energy = -2286.48157 au				SCF Energy = -2286.57586 au			
6	-3.123585000	-1.660360000	0.000000000	6	2.004284000	2.675056000	1.168352000
6	-3.236638000	-0.817302000	1.170013000	6	3.009591000	1.736903000	0.719221000
6	-2.239599000	-2.738980000	0.000000000	6	1.231159000	2.392955000	2.295746000
6	-2.461885000	-1.083923000	2.298505000	6	3.198159000	0.535838000	1.424663000
6	-1.840381000	0.003879000	3.021553000	6	3.386124000	-0.703530000	0.697179000
6	-3.418563000	0.545936000	0.722989000	6	3.009591000	1.736903000	-0.719221000
6	-2.820328000	1.594649000	1.420917000	6	3.198159000	0.535838000	-1.424663000
6	-2.016833000	1.318936000	2.591713000	6	3.386124000	-0.703530000	-0.697179000
6	-1.545131000	-2.203138000	-2.298697000	6	-0.780869000	3.259613000	1.169502000
6	-2.461885000	-1.083923000	-2.298505000	6	0.019791000	3.550231000	0.000000000
6	-1.435710000	-3.015864000	-1.170270000	6	-0.181505000	2.690138000	2.296645000
6	-3.236638000	-0.817302000	-1.170013000	6	1.385259000	3.263693000	0.000000000
6	-3.418563000	0.545936000	-0.722989000	6	2.004284000	2.675056000	-1.168352000
6	-1.840381000	0.003879000	-3.021553000	6	-0.780869000	3.259613000	-1.169502000
6	-2.016833000	1.318936000	-2.591713000	6	-0.181505000	2.690138000	-2.296645000
6	-2.820328000	1.594649000	-1.420917000	6	1.231159000	2.392955000	-2.295746000
6	1.011725000	-3.079130000	-1.421069000	6	-2.100188000	1.177345000	2.580995000
6	0.898357000	-2.236756000	-2.591595000	6	-2.721655000	1.766557000	1.421512000
6	-0.134050000	-3.461271000	-0.723259000	6	-0.852492000	1.627976000	3.018736000
6	-0.356558000	-1.805654000	-3.021380000	6	-2.073237000	2.795001000	0.720791000
6	-0.539312000	-0.442277000	-3.468361000	6	-2.073237000	2.795001000	-0.720791000
6	2.016830000	-1.318938000	-2.591695000	6	-3.386124000	0.703530000	0.697179000
6	1.840362000	-0.003888000	-3.021504000	6	-3.386124000	0.703530000	-0.697179000
6	0.539310000	0.442271000	-3.468356000	6	-2.721655000	1.766557000	-1.421512000
6	1.011725000	-3.079130000	1.421069000	6	-0.144832000	-0.689489000	3.477904000
6	2.199403000	-2.681993000	0.697380000	6	-1.429090000	-1.153818000	3.024460000
6	-0.134050000	-3.461271000	0.723259000	6	0.144832000	0.689489000	3.477904000
6	2.199403000	-2.681993000	-0.697380000	6	-2.398982000	-0.244193000	2.583513000
6	2.820333000	-1.594644000	-1.420911000	6	-3.198159000	-0.535838000	1.424663000
6	2.820333000	-1.594644000	1.420911000	6	-1.231159000	-2.392955000	2.295746000
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6	3.418591000	-0.545933000	-0.722989000	6	-3.009591000	-1.736903000	0.719221000
6	-1.545131000	-2.203138000	2.298697000	6	2.398982000	0.244193000	2.583513000
6	-0.356558000	-1.805654000	3.021380000	6	2.100188000	-1.177345000	2.580995000
6	-1.435710000	-3.015864000	1.170270000	6	1.429090000	1.153818000	3.024460000
6	0.898357000	-2.236756000	2.591595000	6	0.852492000	-1.627976000	3.018736000
6	2.016830000	-1.318938000	2.591695000	6	0.181505000	-2.690138000	2.296645000
6	-0.539312000	-0.442277000	3.468361000	6	2.721655000	-1.766557000	1.421512000
6	0.539310000	0.442271000	3.468356000	6	2.073237000	-2.795001000	0.720791000
6	1.840362000	-0.003888000	3.021504000	6	0.780869000	-3.259613000	1.169502000
6	3.123604000	1.660366000	0.000000000	6	-2.004284000	-2.675056000	-1.168352000
6	3.236644000	0.817305000	1.170009000	6	-1.385259000	-3.263693000	0.000000000
6	2.461880000	1.083920000	2.298494000	6	-0.019791000	-3.550231000	0.000000000
6	2.239596000	2.738967000	0.000000000	6	-1.231159000	-2.392955000	-2.295746000
6	1.545126000	2.203135000	-2.298689000	6	-2.398982000	-0.244193000	-2.583513000
6	2.461880000	1.083920000	-2.298494000	6	-3.198159000	-0.535838000	-1.424663000
6	3.236644000	0.817305000	-1.170009000	6	-3.009591000	-1.736903000	-0.719221000
6	1.435704000	3.015867000	-1.170269000	6	-1.429090000	-1.153818000	-3.024460000
6	-1.011727000	3.079136000	-1.421075000	6	0.144832000	0.689489000	-3.477904000
6	-0.898361000	2.236763000	-2.591606000	6	-0.852492000	1.627976000	-3.018736000

6	0.356557000	1.805645000	-3.021372000	6	-2.100188000	1.177345000	-2.580995000
6	0.134045000	3.461279000	-0.723261000	6	-0.144832000	-0.689489000	-3.477904000
6	-1.011727000	3.079136000	1.421075000	6	2.100188000	-1.177345000	-2.580995000
6	-2.199398000	2.681994000	0.697382000	6	2.398982000	0.244193000	-2.583513000
6	-2.199398000	2.681994000	-0.697382000	6	1.429090000	1.153818000	-3.024460000
6	0.134045000	3.461279000	0.723261000	6	0.852492000	-1.627976000	-3.018736000
6	1.545126000	2.203135000	2.298689000	6	0.780869000	-3.259613000	-1.169502000
6	0.356557000	1.805645000	3.021372000	6	2.073237000	-2.795001000	-0.720791000
6	-0.898361000	2.236763000	2.591606000	6	2.721655000	-1.766557000	-1.421512000
6	1.435704000	3.015867000	1.170269000	6	0.181505000	-2.690138000	-2.296645000
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6	-0.454348000	-0.511320000	3.461691000	6	-1.831232000	0.162313000	3.018266000
6	1.264076000	-2.036882000	2.589111000	6	-3.147690000	1.105224000	1.168645000
6	0.458297000	0.544145000	3.463222000	6	-2.125340000	-1.130289000	2.587687000
6	0.049714000	1.856544000	3.019636000	6	-1.095340000	-2.143623000	2.587769000
6	-1.810540000	-0.290504000	3.015610000	6	-0.496602000	0.488838000	3.464449000
6	-2.205705000	0.977512000	2.587358000	6	0.496650000	-0.488828000	3.464503000
6	-1.260853000	2.070290000	2.589291000	6	0.192293000	-1.828811000	3.018603000
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6	-0.900809000	-3.170607000	1.166851000	6	-1.156657000	3.130786000	1.169220000
6	1.526053000	-2.852839000	1.427747000	6	-2.958767000	1.934072000	0.000000000
6	-1.154163000	-2.415776000	2.308512000	6	-1.338635000	2.330534000	2.296440000
6	-2.241824000	-1.466786000	2.298816000	6	-0.192265000	1.828834000	3.018575000
6	-1.737695000	-3.035791000	0.000000000	6	0.178397000	3.457217000	0.722683000
6	-2.808525000	-2.146414000	0.000000000	6	1.284030000	2.972075000	1.419377000
6	-3.052016000	-1.335069000	1.169003000	6	1.095345000	2.143670000	2.587701000
6	2.619904000	-2.257554000	-0.698276000	6	-2.351934000	1.300306000	-2.296106000
6	1.526053000	-2.852839000	-1.427747000	6	-1.338635000	2.330534000	-2.296440000
6	2.619904000	-2.257554000	0.698276000	6	-3.147690000	1.105224000	-1.168645000
6	0.453432000	-3.389114000	-0.721192000	6	-1.156657000	3.130786000	-1.169220000
6	-0.900809000	-3.170607000	-1.166851000	6	0.178397000	3.457217000	-0.722683000
6	1.264076000	-2.036882000	-2.589111000	6	-0.192265000	1.828834000	-3.018575000
6	-0.046941000	-1.823444000	-3.020434000	6	1.095345000	2.143670000	-2.587701000
6	-1.154163000	-2.415776000	-2.308512000	6	1.284030000	2.972075000	-1.419377000
6	3.459521000	0.055889000	0.721881000	6	-2.950239000	-1.332712000	-1.419179000
6	3.459521000	0.055889000	-0.721881000	6	-2.125340000	-1.130289000	-2.587687000
6	3.044263000	-1.080286000	1.417292000	6	-3.452383000	-0.234624000	-0.722185000
6	3.044263000	-1.080286000	-1.417292000	6	-1.831232000	0.162313000	-3.018266000
6	2.206370000	-0.943754000	-2.585541000	6	-0.496602000	0.488838000	-3.464449000
6	3.053666000	1.368112000	-1.168628000	6	-1.095340000	-2.143623000	-2.587769000
6	2.244436000	1.500133000	-2.298128000	6	0.192293000	-1.828811000	-3.018603000
6	1.813887000	0.323751000	-3.017402000	6	0.496650000	-0.488828000	-3.464503000
6	1.813887000	0.323751000	3.017402000	6	-2.950239000	-1.332712000	1.419179000
6	2.244436000	1.500133000	2.298128000	6	-2.430617000	-2.471205000	0.697058000
6	2.206370000	-0.943754000	2.585541000	6	-3.452383000	-0.234624000	0.722185000
6	3.053666000	1.368112000	1.168628000	6	-2.430617000	-2.471205000	-0.697058000
6	2.802013000	2.180066000	0.000000000	6	-1.283920000	-2.971953000	-1.419311000
6	1.153629000	2.447923000	2.298743000	6	-1.283920000	-2.971953000	1.419311000
6	0.909055000	3.231399000	1.169287000	6	-0.178331000	-3.457121000	0.722721000
6	1.747582000	3.095302000	0.000000000	6	-0.178331000	-3.457121000	-0.722721000
6	0.049714000	1.856544000	-3.019636000	6	2.351955000	-1.300281000	-2.296009000
6	1.153629000	2.447923000	-2.298743000	6	1.338722000	-2.330564000	-2.296495000
6	0.909055000	3.231399000	-1.169287000	6	1.156729000	-3.130746000	-1.169210000

6	-1.260853000	2.070290000	-2.589291000	6	3.147749000	-1.105215000	-1.168593000
6	-1.810540000	-0.290504000	-3.015610000	6	2.950353000	1.332819000	-1.419226000
6	-0.454348000	-0.511320000	-3.461691000	6	2.125290000	1.130337000	-2.587546000
6	0.458297000	0.544145000	-3.463222000	6	1.831173000	-0.162259000	-3.018057000
6	-2.205705000	0.977512000	-2.587358000	6	3.452427000	0.234694000	-0.722229000
6	-3.455021000	-0.023079000	-0.722349000	6	2.950353000	1.332819000	1.419226000
6	-3.052016000	-1.335069000	-1.169003000	6	2.430660000	2.471288000	0.696984000
6	-2.241824000	-1.466786000	-2.298816000	6	2.430660000	2.471288000	-0.696984000
6	-3.043317000	1.113721000	-1.419170000	6	3.452427000	0.234694000	0.722229000
6	-2.616555000	2.290596000	0.697926000	6	2.351955000	-1.300281000	2.296009000
6	-3.043317000	1.113721000	1.419170000	6	1.831173000	-0.162259000	3.018057000
6	-3.455021000	-0.023079000	0.722349000	6	2.125290000	1.130337000	2.587546000
6	-2.616555000	2.290596000	-0.697926000	6	3.147749000	-1.105215000	1.168593000
6	-0.447771000	3.452059000	-0.722683000	6	1.981452000	-2.927713000	0.000000000
6	-0.447771000	3.452059000	0.722683000	6	1.156729000	-3.130746000	1.169210000
6	-1.514357000	2.882300000	1.421060000	6	1.338722000	-2.330564000	2.296495000
6	-1.514357000	2.882300000	-1.421060000	6	2.958978000	-1.934096000	0.000000000
9	-0.071695000	-0.751922000	0.000000000	17	-0.000515000	-0.000515000	0.000000000
Br@C₆₀				OH@C₆₀			
SCF Energy = -4860.66460 au				SCF Energy = -2362.39322 au			
6	0.238112000	3.452755000	0.722714000	6	3.227230000	-0.281956000	1.398474000
6	0.238112000	3.452755000	-0.722714000	6	2.378342000	-0.359521000	2.562589000
6	1.336492000	2.949861000	1.420726000	6	3.342538000	0.924032000	0.703067000
6	1.336492000	2.949861000	-1.420726000	6	1.681673000	0.762088000	3.009947000
6	1.133797000	2.126207000	-2.591283000	6	0.318837000	0.627965000	3.465575000
6	-1.102084000	3.149156000	-1.169283000	6	1.738871000	-1.653189000	2.564325000
6	-1.297995000	2.354129000	-2.298637000	6	0.426835000	-1.787386000	3.016115000
6	-0.160484000	1.833005000	-3.022307000	6	-0.298800000	-0.625833000	3.470001000
6	-0.160484000	1.833005000	3.022307000	6	3.211329000	-0.281843000	-1.433545000
6	-1.297995000	2.354129000	2.298637000	6	3.103154000	-1.527922000	-0.714854000
6	1.133797000	2.126207000	2.591283000	6	3.334314000	0.924053000	-0.739476000
6	-1.102084000	3.149156000	1.169283000	6	3.111615000	-1.528273000	0.681155000
6	-1.931012000	2.961709000	0.000000000	6	2.190864000	-2.375526000	1.400620000
6	-2.330146000	1.341688000	2.299045000	6	2.174494000	-2.375086000	-1.424099000
6	-3.130478000	1.161733000	1.170232000	6	1.298223000	-3.210422000	-0.728395000
6	-2.928831000	1.986964000	0.000000000	6	1.306452000	-3.210268000	0.714296000
6	1.829795000	-0.193636000	3.021340000	6	1.769486000	2.007295000	-2.308354000
6	0.488718000	-0.497265000	3.467307000	6	1.648425000	0.762550000	-3.028268000
6	2.147826000	1.094992000	2.590885000	6	2.591581000	2.079600000	-1.181860000
6	-0.488812000	0.497375000	3.467299000	6	2.349355000	-0.359207000	-2.588133000
6	-1.829897000	0.193701000	3.021321000	6	1.709660000	-1.652712000	-2.582691000
6	0.160383000	-1.832941000	3.022416000	6	0.280540000	0.628145000	-3.468429000
6	-1.133924000	-2.126126000	2.591404000	6	-0.337132000	-0.625665000	-3.466373000
6	-2.147952000	-1.094919000	2.590903000	6	0.393183000	-1.787585000	-3.020995000
6	3.458561000	0.173045000	0.723085000	6	0.892181000	3.412776000	-0.004636000
6	3.130394000	-1.161659000	1.170296000	6	0.041120000	3.336852000	-1.168853000
6	2.976102000	1.281140000	1.420232000	6	2.141616000	2.793787000	-0.011678000
6	2.330115000	-1.341643000	2.299155000	6	0.474423000	2.643140000	-2.300818000
6	1.297895000	-2.354024000	2.298679000	6	-0.446251000	1.790598000	-3.017542000
6	2.928604000	-1.986751000	0.000000000	6	-1.323812000	3.210275000	-0.715256000
6	1.930817000	-2.961430000	0.000000000	6	-2.213958000	2.383817000	-1.407992000
6	1.101952000	-3.148949000	1.169264000	6	-1.765011000	1.662547000	-2.576854000
6	2.474913000	2.428369000	-0.697596000	6	1.794711000	2.007002000	2.288739000
6	2.976102000	1.281140000	-1.420232000	6	0.499813000	2.643150000	2.296023000
6	2.474913000	2.428369000	0.697596000	6	2.604548000	2.079503000	1.153496000

6	3.458561000	0.173045000	-0.723085000	6	0.054110000	3.337137000	1.168849000
6	3.130394000	-1.161659000	-1.170296000	6	-1.315659000	3.210308000	0.730285000
6	2.147826000	1.094992000	-2.590885000	6	-0.412740000	1.790782000	3.023212000
6	1.829795000	-0.193636000	-3.021340000	6	-1.736186000	1.662451000	2.596669000
6	2.330115000	-1.341643000	-2.299155000	6	-2.197923000	2.383693000	1.432745000
6	-0.238219000	-3.452473000	-0.722716000	6	-3.246575000	0.284633000	-1.403068000
6	1.101952000	-3.148949000	-1.169264000	6	-3.128384000	1.532012000	-0.681923000
6	1.297895000	-2.354024000	-2.298679000	6	-3.120532000	1.532032000	0.716881000
6	-1.336541000	-2.949462000	-1.420733000	6	-3.356017000	-0.921891000	-0.704290000
6	-2.475192000	-2.428457000	0.697596000	6	-1.813033000	-2.006197000	-2.289291000
6	-1.336541000	-2.949462000	1.420733000	6	-1.701022000	-0.758935000	-3.012303000
6	-0.238219000	-3.452473000	0.722716000	6	-2.403662000	0.365271000	-2.573973000
6	-2.475192000	-2.428457000	-0.697596000	6	-2.625447000	-2.083530000	-1.155057000
6	-3.458689000	-0.173001000	-0.723084000	6	-0.909729000	-3.411327000	0.005029000
6	-3.458689000	-0.173001000	0.723084000	6	-0.070897000	-3.334219000	-1.167873000
6	-2.976259000	-1.281110000	1.420226000	6	-0.517319000	-2.641536000	-2.295504000
6	-2.976259000	-1.281110000	-1.420226000	6	-2.163768000	-2.800023000	0.012108000
6	-1.829897000	0.193701000	-3.021321000	6	-1.787790000	-2.006391000	2.309637000
6	-2.330146000	1.341688000	-2.299045000	6	-0.491893000	-2.641457000	2.301095000
6	-3.130478000	1.161733000	-1.170232000	6	-0.057892000	-3.333765000	1.168660000
6	-2.147952000	-1.094919000	-2.590903000	6	-2.612486000	-2.083599000	1.184250000
6	0.160383000	-1.832941000	-3.022416000	6	-3.230698000	0.284644000	1.439134000
6	0.488718000	-0.497265000	-3.467307000	6	-2.374988000	0.365222000	2.600836000
6	-0.488812000	0.497375000	-3.467299000	6	-1.667715000	-0.759194000	3.031238000
6	-1.133924000	-2.126126000	-2.591404000	6	-3.347893000	-0.921845000	0.741556000
35	0.000627000	-0.000596000	0.000000000	8	0.491959000	-0.090228000	-0.010527000
NH₂@C₆₀				1	-0.421526000	0.235483000	-0.001111000
SCF Energy = -2342.49906 au				NO₂@C₆₀			
6	0.499315000	-2.521776000	-2.427385000	SCF Energy = -2491.74396 au			
6	-0.222227000	-3.228967000	-1.398854000	6	1.883902000	-2.767086000	1.165696000
6	1.821325000	-2.111029000	-2.207692000	6	1.247139000	-3.348346000	0.000000000
6	0.384417000	-3.508249000	-0.172712000	6	1.124677000	-2.448400000	2.290602000
6	-0.358002000	-3.368373000	1.057262000	6	-0.133955000	-3.598338000	0.000000000
6	-1.600809000	-2.790753000	-1.430924000	6	-0.921388000	-3.256120000	-1.173421000
6	-2.323027000	-2.659766000	-0.243419000	6	1.883902000	-2.767086000	-1.165696000
6	-1.699307000	-2.953332000	1.025125000	6	1.124677000	-2.448400000	-2.290602000
6	1.332613000	0.055345000	-3.264313000	6	-0.300959000	-2.697235000	-2.297186000
6	-0.026400000	-0.375545000	-3.504357000	6	2.387606000	-0.341373000	2.585504000
6	2.241655000	-0.799672000	-2.634331000	6	3.177988000	-0.667989000	1.424380000
6	-0.433390000	-1.641565000	-3.090779000	6	1.377545000	-1.213412000	3.003264000
6	-1.732495000	-1.809432000	-2.479041000	6	2.912766000	-1.849633000	0.721497000
6	-0.901263000	0.758745000	-3.328156000	6	2.912766000	-1.849633000	-0.721497000
6	-2.169642000	0.594266000	-2.757011000	6	3.420188000	0.561015000	0.696352000
6	-2.588420000	-0.715540000	-2.322946000	6	3.420188000	0.561015000	-0.696352000
6	3.091020000	1.094864000	-1.305233000	6	3.177988000	-0.667989000	-1.424380000
6	2.170362000	1.982842000	-1.977551000	6	-0.116401000	0.692484000	3.450306000
6	3.125986000	-0.262198000	-1.626445000	6	0.918964000	1.598436000	3.005019000
6	1.298076000	1.457583000	-2.934042000	6	0.109590000	-0.687290000	3.443328000
6	-0.081617000	1.890449000	-2.971402000	6	2.143687000	1.086112000	2.577181000
6	1.699111000	2.952168000	-1.018817000	6	2.778989000	1.647033000	1.408714000
6	0.358299000	3.365192000	-1.049713000	6	0.290659000	2.694170000	2.296621000
6	-0.539113000	2.825349000	-2.043505000	6	0.908006000	3.248471000	1.172168000
6	3.350201000	-0.838915000	0.756276000	6	2.173170000	2.704071000	0.721887000
6	3.317757000	0.566298000	1.087298000	6	-2.147591000	-1.089538000	2.573162000
				6	-2.375311000	0.341361000	2.570677000

6	3.252222000	-1.243575000	-0.575266000	6	-0.925122000	-1.598740000	3.003266000
6	3.186566000	1.514698000	0.072683000	6	-1.384253000	1.220730000	3.010563000
6	2.323958000	2.662074000	0.248960000	6	-1.137944000	2.455601000	2.295217000
6	2.585477000	0.717043000	2.323877000	6	-3.156198000	0.668275000	1.406925000
6	1.735306000	1.816284000	2.486382000	6	-2.934943000	1.868909000	0.721100000
6	1.605446000	2.801344000	1.440191000	6	-1.900374000	2.779120000	1.169980000
6	1.741728000	-3.066328000	0.062517000	6	-0.921388000	-3.256120000	1.173421000
6	1.838935000	-2.646866000	1.439367000	6	-2.190074000	-2.714244000	0.724058000
6	2.443523000	-2.385305000	-0.935145000	6	-0.300959000	-2.697235000	2.297186000
6	2.637046000	-1.554544000	1.789427000	6	-2.795661000	-1.659506000	1.415404000
6	2.166331000	-0.593415000	2.757990000	6	-3.412373000	-0.566472000	0.694263000
6	0.539882000	-2.830341000	2.053054000	6	-2.190074000	-2.714244000	-0.724058000
6	0.081354000	-1.896141000	2.985043000	6	-2.795661000	-1.659506000	-1.415404000
6	0.901173000	-0.761339000	3.339352000	6	-3.412373000	-0.566472000	-0.694263000
6	-0.498149000	2.529569000	2.436445000	6	-1.900374000	2.779120000	-1.169980000
6	0.434315000	1.644551000	3.097041000	6	-2.934943000	1.868909000	-0.721100000
6	0.026727000	0.375457000	3.511205000	6	-3.156198000	0.668275000	-1.406925000
6	-1.819184000	2.111490000	2.210989000	6	-1.137944000	2.455601000	-2.295217000
6	-1.741260000	3.066629000	-0.057957000	6	0.908006000	3.248471000	-1.172168000
6	-0.383437000	3.511628000	0.179407000	6	0.119921000	3.593177000	0.000000000
6	0.224690000	3.240978000	1.408837000	6	-1.261903000	3.357064000	0.000000000
6	-2.443884000	2.385851000	0.938353000	6	0.290659000	2.694170000	-2.296621000
6	-3.349298000	0.838833000	-0.754280000	6	2.143687000	1.086112000	-2.577181000
6	-2.637868000	1.554484000	-1.787553000	6	2.778989000	1.647033000	-1.408714000
6	-1.837481000	2.643906000	-1.433936000	6	2.173170000	2.704071000	-0.721887000
6	-3.254227000	1.244438000	0.577579000	6	0.918964000	1.598436000	-3.005019000
6	-3.091487000	-1.095151000	1.308582000	6	0.109590000	-0.687290000	-3.443328000
6	-3.186486000	-1.514024000	-0.069491000	6	1.377545000	-1.213412000	-3.003264000
6	-3.317310000	-0.565914000	-1.085225000	6	2.387606000	-0.341373000	-2.585504000
6	-3.125714000	0.262327000	1.628068000	6	-0.116401000	0.692484000	-3.450306000
6	-1.334039000	-0.057725000	3.274446000	6	-2.375311000	0.341361000	-2.570677000
6	-1.300777000	-1.461966000	2.947369000	6	-2.147591000	-1.089538000	-2.573162000
6	-2.171054000	-1.984185000	1.984006000	6	-0.925122000	-1.598740000	-3.003266000
6	-2.238516000	0.798530000	2.635832000	6	-1.384253000	1.220730000	-3.010563000
7	-0.002002000	-0.033030000	-0.264253000	7	0.513579000	-0.001864000	0.000000000
1	0.022338000	0.831702000	0.299666000	8	-0.153453000	1.046388000	0.000000000
1	-0.061916000	-0.728186000	0.497207000	8	-0.138047000	-1.060553000	0.000000000
CN@C ₆₀				ClO@C ₆₀			
SCF Energy = -2379.43586 au				SCF Energy = -2821.95225 au			
6	1.388524000	2.942565000	1.418569000	6	0.727416000	-2.618997000	2.317005000
6	0.256459000	3.482757000	0.698178000	6	1.168810000	-1.433567000	3.019034000
6	2.480915000	2.425123000	0.722408000	6	1.419290000	-3.030733000	1.172861000
6	0.256459000	3.482757000	-0.698178000	6	2.291756000	-0.723924000	2.587019000
6	-0.942637000	3.118106000	-1.421946000	6	2.293472000	0.722089000	2.589142000
6	-0.942637000	3.118106000	1.421946000	6	0.000756000	-0.703238000	3.455619000
6	-2.096930000	2.765994000	0.722699000	6	-0.000779000	0.694935000	3.456562000
6	-2.096930000	2.765994000	-0.722699000	6	1.165258000	1.424006000	3.013289000
6	2.627607000	0.533026000	2.290100000	6	-0.694564000	-3.494943000	0.000000000
6	1.496468000	1.067243000	3.011581000	6	-1.412642000	-3.033894000	1.172895000
6	3.108967000	1.199771000	1.166650000	6	0.702191000	-3.493348000	0.000000000
6	0.889612000	2.249960000	2.586977000	6	-0.721696000	-2.620641000	2.317061000
6	-0.551327000	2.356618000	2.587461000	6	-1.165689000	-1.436127000	3.019023000
6	0.693280000	-0.047780000	3.456681000	6	-2.581423000	-2.307444000	0.722560000
6	-0.694589000	0.055465000	3.456958000	6	-3.010115000	-1.174620000	1.416454000
6	-1.327049000	1.277059000	3.012989000	6	-2.290176000	-0.728991000	2.586999000

6	3.393649000	-0.949432000	0.000000000	6	0.727416000	-2.618997000	-2.317005000
6	2.898836000	-1.641993000	1.166031000	6	-0.721696000	-2.620641000	-2.317061000
6	3.497316000	0.442657000	0.000000000	6	1.419290000	-3.030733000	-1.172861000
6	2.521013000	-0.908977000	2.288799000	6	-1.412642000	-3.033894000	-1.172895000
6	1.325776000	-1.269066000	3.012034000	6	-2.581423000	-2.307444000	-0.722560000
6	2.098187000	-2.762694000	0.722910000	6	-1.165689000	-1.436127000	-3.019023000
6	0.942640000	-3.112803000	1.421427000	6	-2.290176000	-0.728991000	-2.586999000
6	0.550554000	-2.347394000	2.584467000	6	-3.010115000	-1.174620000	-1.416454000
6	2.627607000	0.533026000	-2.290100000	6	3.012585000	-1.167892000	-1.416442000
6	2.521013000	-0.908977000	-2.288799000	6	2.291756000	-0.723924000	-2.587019000
6	3.108967000	1.199771000	-1.166650000	6	2.586476000	-2.301715000	-0.722555000
6	2.898836000	-1.641993000	-1.166031000	6	1.168810000	-1.433567000	-3.019034000
6	2.098187000	-2.762694000	-0.722910000	6	0.000756000	-0.703238000	-3.455619000
6	1.325776000	-1.269066000	-3.012034000	6	2.293472000	0.722089000	-2.589142000
6	0.550554000	-2.347394000	-2.584467000	6	1.165258000	1.424006000	-3.013289000
6	0.942640000	-3.112803000	-1.421427000	6	-0.000779000	0.694935000	-3.456562000
6	1.388524000	2.942565000	-1.418569000	6	3.012585000	-1.167892000	1.416442000
6	0.889612000	2.249960000	-2.586977000	6	3.458586000	0.003721000	0.697264000
6	2.480915000	2.425123000	-0.722408000	6	2.586476000	-2.301715000	0.722555000
6	1.496468000	1.067243000	-3.011581000	6	3.458586000	0.003721000	-0.697264000
6	0.693280000	-0.047780000	-3.456681000	6	3.013987000	1.174333000	-1.419486000
6	-0.551327000	2.356618000	-2.587461000	6	3.013987000	1.174333000	1.419486000
6	-1.327049000	1.277059000	-3.012989000	6	2.586825000	2.309446000	0.723710000
6	-0.694589000	0.055465000	-3.456958000	6	2.586825000	2.309446000	-0.723710000
6	-1.389240000	-2.935334000	-1.417523000	6	-0.726629000	2.597555000	-2.292060000
6	-0.889884000	-2.240030000	-2.583703000	6	0.720889000	2.599144000	-2.292072000
6	-1.497807000	-1.059429000	-3.011592000	6	1.424845000	3.050530000	-1.170768000
6	-2.481725000	-2.417600000	-0.722266000	6	-1.431582000	3.047328000	-1.170748000
6	-1.389240000	-2.935334000	1.417523000	6	-3.016558000	1.167549000	-1.419512000
6	-0.257092000	-3.478131000	0.698083000	6	-2.295106000	0.717004000	-2.589190000
6	-0.257092000	-3.478131000	-0.698083000	6	-1.168407000	1.421449000	-3.013279000
6	-2.481725000	-2.417600000	0.722266000	6	-2.591779000	2.303488000	-0.723689000
6	-2.629838000	-0.525745000	2.291491000	6	-3.016558000	1.167549000	1.419512000
6	-1.497807000	-1.059429000	3.011592000	6	-3.458653000	-0.003995000	0.697271000
6	-0.889884000	-2.240030000	2.583703000	6	-3.458653000	-0.003995000	-0.697271000
6	-3.108762000	-1.191950000	1.166623000	6	-2.591779000	2.303488000	0.723689000
6	-3.397463000	0.957044000	0.000000000	6	-0.726629000	2.597555000	2.292060000
6	-2.901770000	1.649017000	1.166669000	6	-1.168407000	1.421449000	3.013279000
6	-2.523029000	0.916438000	2.289804000	6	-2.295106000	0.717004000	2.589190000
6	-3.498350000	-0.435266000	0.000000000	6	-1.431582000	3.047328000	1.170748000
6	-2.629838000	-0.525745000	-2.291491000	6	0.699351000	3.502968000	0.000000000
6	-2.523029000	0.916438000	-2.289804000	6	1.424845000	3.050530000	1.170768000
6	-2.901770000	1.649017000	-1.166669000	6	0.720889000	2.599144000	2.292072000
6	-3.108762000	-1.191950000	-1.166623000	6	-0.707118000	3.501431000	0.000000000
6	0.009458000	0.537748000	0.000000000	8	0.000643000	-1.097167000	0.000000000
7	0.018061000	-0.645582000	0.000000000	17	-0.000052000	0.548184000	0.000000000
C₇₀				Cl@C₇₀			
SCF Energy = -2667.66325 au				SCF Energy = -3128.03616 au			
6	-0.731296000	3.478329000	0.000000000	6	0.016385000	-2.289830000	-2.708687000
6	3.082105000	1.770367000	0.000000000	6	0.015900000	1.869818000	-3.015511000
6	2.636141000	-2.384182000	0.000000000	6	0.016561000	3.445351000	0.847127000
6	-1.452880000	-3.243872000	0.000000000	6	0.017674000	0.259945000	3.538246000
6	-3.534070000	0.379359000	0.000000000	6	0.017366000	-3.284729000	1.339590000
6	-3.082105000	1.770367000	0.000000000	6	0.017052000	-3.547789000	-0.097284000
6	0.731296000	3.478329000	0.000000000	6	0.016118000	-1.003893000	-3.400104000

6	3.534070000	0.379359000	0.000000000	6	0.015947000	2.926870000	-2.006855000
6	1.452880000	-3.243872000	0.000000000	6	0.017011000	2.811574000	2.163301000
6	-2.636141000	-2.384182000	0.000000000	6	0.017750000	-1.187803000	3.343254000
6	-0.722501000	0.994437000	3.954722000	6	-3.932137000	-1.106276000	-0.531334000
6	-0.722501000	0.994437000	-3.954722000	6	3.971812000	-1.106797000	-0.533254000
6	0.722501000	0.994437000	3.954722000	6	-3.933579000	0.164583000	-1.216462000
6	0.722501000	0.994437000	-3.954722000	6	3.970702000	0.165027000	-1.218347000
6	1.169031000	-0.379841000	3.954722000	6	-3.932955000	1.208555000	-0.219260000
6	1.169031000	-0.379841000	-3.954722000	6	3.971125000	1.209604000	-0.220657000
6	0.000000000	-1.229192000	3.954722000	6	-3.932079000	0.582477000	1.081957000
6	0.000000000	-1.229192000	-3.954722000	6	3.972701000	0.583816000	1.081606000
6	-1.169031000	-0.379841000	3.954722000	6	-3.932516000	-0.848289000	0.889253000
6	-1.169031000	-0.379841000	-3.954722000	6	3.972353000	-0.847927000	0.888156000
6	-1.416041000	1.949013000	3.207953000	6	-3.188591000	-2.169912000	-1.042890000
6	-1.416041000	1.949013000	-3.207953000	6	3.222863000	-2.168866000	-1.043879000
6	1.416041000	1.949013000	3.207953000	6	-3.189672000	0.322332000	-2.385866000
6	1.416041000	1.949013000	-3.207953000	6	3.221827000	0.322482000	-2.386145000
6	2.291202000	-0.744457000	3.207953000	6	-3.190027000	2.370199000	-0.430828000
6	2.291202000	-0.744457000	-3.207953000	6	3.221061000	2.368054000	-0.431498000
6	0.000000000	-2.409113000	3.207953000	6	-3.188892000	1.142399000	2.121092000
6	0.000000000	-2.409113000	-3.207953000	6	3.222496000	1.142428000	2.118231000
6	-2.291202000	-0.744457000	3.207953000	6	-3.189296000	-1.663811000	1.742599000
6	-2.291202000	-0.744457000	-3.207953000	6	3.222512000	-1.661399000	1.739470000
6	-0.694964000	2.926722000	2.433310000	6	-2.414533000	-1.998574000	-2.244845000
6	-0.694964000	2.926722000	-2.433310000	6	2.446635000	-1.998549000	-2.245916000
6	2.568722000	1.565357000	2.433310000	6	-2.415157000	1.518692000	-2.594351000
6	2.568722000	1.565357000	-2.433310000	6	2.446471000	1.519107000	-2.596331000
6	2.282522000	-1.959278000	2.433310000	6	-2.414215000	2.936993000	0.642336000
6	2.282522000	-1.959278000	-2.433310000	6	2.446479000	2.938483000	0.641474000
6	-1.158046000	-2.776257000	2.433310000	6	-2.413945000	0.296435000	2.991895000
6	-1.158046000	-2.776257000	-2.433310000	6	2.448099000	0.297360000	2.991721000
6	-2.998234000	0.243457000	2.433310000	6	-2.414250000	-2.753227000	1.207370000
6	-2.998234000	0.243457000	-2.433310000	6	2.447679000	-2.752710000	1.206323000
6	-2.568722000	1.565357000	2.433310000	6	-2.414218000	-3.001689000	-0.158703000
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6	0.694964000	2.926722000	2.433310000	6	-2.414750000	-0.775935000	-2.902804000
6	0.694964000	2.926722000	-2.433310000	6	2.446070000	-0.775656000	-2.904445000
6	2.998234000	0.243457000	2.433310000	6	-2.415542000	2.523331000	-1.635597000
6	2.998234000	0.243457000	-2.433310000	6	2.446086000	2.523072000	-1.636220000
6	1.158046000	-2.776257000	2.433310000	6	-2.413843000	2.335074000	1.893449000
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6	-2.282522000	-1.959278000	2.433310000	6	-2.413245000	-1.079312000	2.805746000
6	-2.282522000	-1.959278000	-2.433310000	6	2.447633000	-1.079133000	2.805686000
6	-1.409763000	3.158623000	1.203704000	6	-1.186847000	-2.737525000	-2.109612000
6	-1.409763000	3.158623000	-1.203704000	6	1.219366000	-2.739304000	-2.111069000
6	2.568388000	2.316832000	1.203704000	6	-1.187029000	1.160607000	-3.253556000
6	2.568388000	2.316832000	-1.203704000	6	1.218451000	1.161726000	-3.257867000
6	2.997114000	-1.726742000	1.203704000	6	-1.186160000	3.453553000	0.098493000
6	2.997114000	-1.726742000	-1.203704000	6	1.218515000	3.457937000	0.097906000
6	-0.716070000	-3.384018000	1.203704000	6	-1.185776000	0.973424000	3.315450000
6	-0.716070000	-3.384018000	-1.203704000	6	1.220465000	0.975244000	3.318862000
6	-3.439670000	-0.364696000	1.203704000	6	-1.185627000	-2.851883000	1.950181000
6	-3.439670000	-0.364696000	-1.203704000	6	1.220159000	-2.854392000	1.951878000
6	-2.568388000	2.316832000	1.203704000	6	-1.186847000	-3.357981000	-0.820376000
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6	1.409763000	3.158623000	1.203704000	6	-1.186790000	-0.257057000	-3.444223000

6	1.409763000	3.158623000	-1.203704000	6	1.218532000	-0.256949000	-3.448905000
6	3.439670000	-0.364696000	1.203704000	6	-1.186719000	3.197706000	-1.308896000
6	3.439670000	-0.364696000	-1.203704000	6	1.218349000	3.201323000	-1.310441000
6	0.716070000	-3.384018000	1.203704000	6	-1.185836000	2.232611000	2.636952000
6	0.716070000	-3.384018000	-1.203704000	6	1.219838000	2.235067000	2.639350000
6	-2.997114000	-1.726742000	1.203704000	6	-1.185108000	-1.817294000	2.937953000
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C₈₄				17	-0.418353000	-0.004685000	-0.002094000
SCF Energy = -3201.28667 au				Cl@C₈₄			
6	-1.420042000	3.881899000	1.199251000	SCF Energy = -3661.65382 au			
6	-0.731523000	4.202751000	0.000000000	6	-2.966458000	-2.849873000	-1.198549000
6	-1.420042000	3.881899000	-1.199251000	6	-2.489158000	-3.438665000	0.000347000
6	-2.651802000	3.170742000	1.199251000	6	-2.966355000	-2.849842000	1.199263000
6	-3.273928000	2.734893000	0.000000000	6	-3.754787000	-1.666903000	-1.197710000
6	-2.651802000	3.170742000	-1.199251000	6	-4.117828000	-1.001590000	0.000402000
6	0.731523000	4.202751000	0.000000000	6	-3.754739000	-1.666896000	1.198491000
6	1.420042000	3.881899000	-1.199251000	6	-1.179810000	-4.088686000	0.000287000
6	-0.684316000	3.466794000	2.371700000	6	-0.419800000	-4.104719000	1.198358000
6	0.684316000	3.466794000	2.371700000	6	-2.122906000	-2.802154000	-2.368297000
6	1.420042000	3.881899000	1.199251000	6	-0.896132000	-3.409543000	-2.370315000
6	-3.344490000	1.140762000	2.371700000	6	-0.419956000	-4.104719000	-1.197887000
6	-2.660174000	2.326032000	2.371700000	6	-3.476861000	0.458052000	-2.368402000
6	-1.392341000	2.411605000	3.032706000	6	-3.387678000	-0.906541000	-2.368159000
6	-4.071844000	0.711157000	-1.199251000	6	-2.293265000	-1.545970000	-3.031932000
6	-4.005451000	1.467858000	0.000000000	6	-3.939533000	1.163918000	1.198465000
6	-4.071844000	0.711157000	1.199251000	6	-4.211880000	0.456966000	0.000383000
6	2.660174000	2.326032000	2.371700000	6	-3.939586000	1.163848000	-1.197756000
6	2.651802000	3.170742000	1.199251000	6	1.379411000	-3.260740000	-2.368813000
6	3.273928000	2.734893000	0.000000000	6	1.000562000	-4.016866000	-1.199131000
6	2.651802000	3.170742000	-1.199251000	6	1.751002000	-3.900447000	0.000120000
6	3.344490000	1.140762000	2.371700000	6	1.000735000	-4.016929000	1.199475000
6	3.344490000	-1.140762000	2.371700000	6	2.518626000	-2.500835000	-2.370375000
6	2.784682000	0.000000000	3.032706000	6	3.523852000	-0.455372000	-2.369240000
6	2.660174000	-2.326032000	2.371700000	6	2.518793000	-1.230467000	-3.029631000
6	-2.784682000	0.000000000	3.032706000	6	3.434725000	0.910477000	-2.369392000
6	-1.456736000	0.000000000	3.536701000	6	-2.474615000	1.234271000	-3.031585000
6	-0.728368000	1.261570000	3.536701000	6	-1.281155000	0.644984000	-3.521323000
6	0.728368000	1.261570000	3.536701000	6	-1.186398000	-0.806593000	-3.521559000
6	1.392341000	2.411605000	3.032706000	6	0.117721000	-1.450046000	-3.527070000
6	-0.728368000	-1.261570000	3.536701000	6	0.204908000	-2.776635000	-3.029655000
6	0.728368000	-1.261570000	3.536701000	6	-0.072069000	1.453329000	-3.527703000
6	1.456736000	0.000000000	3.536701000	6	1.232040000	0.809738000	-3.531171000
6	1.392341000	-2.411605000	3.032706000	6	1.326709000	-0.641803000	-3.530483000
6	4.071844000	0.711157000	1.199251000	6	2.337831000	1.548406000	-3.030898000
6	4.005451000	1.467858000	0.000000000	6	3.362874000	-2.439345000	-1.199919000
6	4.071844000	0.711157000	-1.199251000	6	2.968242000	-3.088254000	0.000038000
6	3.344490000	1.140762000	-2.371700000	6	3.363122000	-2.439353000	1.199929000
6	2.660174000	2.326032000	-2.371700000	6	2.518948000	-2.500773000	2.370452000
6	4.005451000	-1.467858000	0.000000000	6	1.379729000	-3.260698000	2.369060000
6	4.071844000	-0.711157000	-1.199251000	6	4.263658000	-0.454516000	-0.000096000
6	4.071844000	-0.711157000	1.199251000	6	3.991629000	-1.162153000	1.199743000
6	-0.684316000	3.466794000	-2.371700000	6	3.991402000	-1.162175000	-1.199862000
6	0.684316000	3.466794000	-2.371700000	6	-2.122620000	-2.802047000	2.368871000
6	1.392341000	2.411605000	-3.032706000	6	-0.895837000	-3.409422000	2.370771000
				6	0.205278000	-2.776506000	3.029968000

6	2.784682000	0.000000000	-3.032706000	6	2.519168000	-1.230344000	3.029616000
6	0.728368000	-1.261570000	-3.536701000	6	1.232461000	0.809884000	3.531190000
6	1.456736000	0.000000000	-3.536701000	6	1.327131000	-0.641656000	3.530547000
6	0.728368000	1.261570000	-3.536701000	6	0.118146000	-1.449921000	3.527434000
6	-1.392341000	-2.411605000	-3.032706000	6	-0.158546000	2.780061000	3.030377000
6	-0.728368000	-1.261570000	-3.536701000	6	-0.071645000	1.453488000	3.527963000
6	-1.456736000	0.000000000	-3.536701000	6	-1.280743000	0.645132000	3.521810000
6	-0.728368000	1.261570000	-3.536701000	6	-1.185981000	-0.806453000	3.522078000
6	-1.392341000	2.411605000	-3.032706000	6	-2.292874000	-1.545819000	3.032450000
6	2.660174000	-2.326032000	-2.371700000	6	3.435063000	0.910589000	2.369226000
6	3.344490000	-1.140762000	-2.371700000	6	3.524201000	-0.455275000	2.369129000
6	1.392341000	-2.411605000	-3.032706000	6	2.338194000	1.548540000	3.030766000
6	2.651802000	-3.170742000	1.199251000	6	3.805952000	1.671859000	-1.199939000
6	3.273928000	-2.734893000	0.000000000	6	4.168138000	1.005539000	-0.000123000
6	2.651802000	-3.170742000	-1.199251000	6	3.806170000	1.671949000	1.199712000
6	-2.660174000	2.326032000	-2.371700000	6	-3.387437000	-0.906452000	2.368843000
6	-3.344490000	1.140762000	-2.371700000	6	-3.476624000	0.458139000	2.369065000
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6	-2.651802000	-3.170742000	-1.199251000	6	-0.951103000	4.015213000	1.198315000
6	-2.660174000	-2.326032000	-2.371700000	6	-1.332663000	3.264288000	2.370803000
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6	-3.273928000	-2.734893000	0.000000000	6	-1.703034000	3.902453000	0.000150000
6	0.684316000	-3.466794000	-2.371700000	6	2.170980000	2.807518000	2.371205000
6	-1.420042000	-3.881899000	1.199251000	6	0.468334000	4.112476000	-1.199368000
6	-0.731523000	-4.202751000	0.000000000	6	1.226536000	4.091599000	-0.000024000
6	-1.420042000	-3.881899000	-1.199251000	6	0.468497000	4.112602000	1.199416000
6	-0.684316000	-3.466794000	-2.371700000	6	0.942758000	3.412595000	2.369246000
6	-0.684316000	-3.466794000	2.371700000	6	0.942435000	3.412451000	-2.369242000
6	0.684316000	-3.466794000	2.371700000	6	2.170624000	2.807345000	-2.371285000
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6	0.731523000	-4.202751000	0.000000000	6	2.537931000	3.444242000	-0.000078000
6	1.420042000	-3.881899000	-1.199251000	6	3.015163000	2.854876000	1.199817000
6	-3.344490000	-1.140762000	2.371700000	6	-2.470032000	2.501759000	-2.367820000
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6	-1.392341000	-2.411605000	3.032706000	6	-0.158934000	2.779960000	-3.030281000
6	-4.071844000	-0.711157000	-1.199251000	6	-3.312418000	2.439632000	1.199004000
6	-4.005451000	-1.467858000	0.000000000	6	-2.916011000	3.085829000	0.000249000
6	-4.071844000	-0.711157000	1.199251000	6	-3.312517000	2.439576000	-1.198441000
C₉₀				17	-0.711669000	-0.045855000	-0.003837000
SCF Energy = -3429.96528 au				CF@C₉₀			
6	-1.728686000	3.888230000	-1.674018000	6	1.728054000	3.883628000	1.671452000
6	-1.382706000	4.401173000	-0.391405000	6	1.382881000	4.398075000	0.390121000
6	-2.067800000	1.847635000	-3.661983000	6	2.067536000	1.846559000	3.659967000
6	-3.022111000	2.026059000	-2.687342000	6	3.020825000	2.024409000	2.686353000
6	-2.898697000	3.084147000	-1.724136000	6	2.895747000	3.079667000	1.721976000
6	-1.757600000	0.528932000	-4.107790000	6	1.756141000	0.529077000	4.104745000
6	-3.596175000	0.884000000	-2.047283000	6	3.589046000	0.882466000	2.044239000
6	-3.187987000	-0.424725000	-2.344069000	6	3.176922000	-0.422936000	2.337822000
6	-2.277171000	-0.621229000	-3.468783000	6	2.270587000	-0.618821000	3.462439000
6	-1.710315000	-2.847435000	-2.600550000	6	1.704346000	-2.840787000	2.594438000
6	-1.488302000	-1.838359000	-3.554390000	6	1.482002000	-1.834052000	3.546744000
6	-0.188813000	-1.818737000	-4.134645000	6	0.186615000	-1.816713000	4.130005000
6	-3.561234000	2.655792000	-0.533842000	6	3.555750000	2.651308000	0.532317000

6	-3.182611000	3.143385000	0.738511000	6	3.178133000	3.139155000	-0.738538000
6	-2.096451000	4.061316000	0.786362000	6	2.096472000	4.060133000	-0.787370000
6	-3.384217000	2.283620000	1.844546000	6	3.379715000	2.280719000	-1.843025000
6	-3.941290000	1.275687000	-0.714482000	6	3.932266000	1.272494000	0.712639000
6	-2.589004000	-2.622380000	-1.470966000	6	2.583649000	-2.618067000	1.468143000
6	-3.244204000	-1.403041000	-1.261815000	6	3.231262000	-1.399193000	1.257512000
6	-3.526085000	-1.018474000	0.110263000	6	3.513633000	-1.015877000	-0.110209000
6	-3.918543000	0.362354000	0.356888000	6	3.906400000	0.360852000	-0.356436000
6	-3.758976000	0.921161000	1.648084000	6	3.751880000	0.919094000	-1.645963000
6	-2.533683000	2.326098000	2.997329000	6	2.532761000	2.325124000	-2.996112000
6	-1.378277000	3.158197000	3.009342000	6	1.378845000	3.157533000	-3.007609000
6	-1.166697000	4.012846000	1.898831000	6	1.168813000	4.014625000	-1.899649000
6	-0.217569000	2.669017000	3.672929000	6	0.219165000	2.669052000	-3.671165000
6	-2.490311000	1.022536000	3.579932000	6	2.489056000	1.022132000	-3.577224000
6	-1.111592000	-0.849980000	4.243786000	6	1.108634000	-0.849063000	-4.235794000
6	-1.340402000	0.557708000	4.265856000	6	1.338356000	0.557196000	-4.257664000
6	-0.212113000	1.411552000	4.342530000	6	0.213090000	1.410805000	-4.337345000
6	-2.150284000	-3.432920000	-0.396436000	6	2.144728000	-3.427374000	0.396322000
6	-2.277171000	-3.025024000	0.939426000	6	2.264886000	-3.014903000	-0.935127000
6	-3.021677000	-1.814021000	1.208182000	6	3.010384000	-1.807939000	-1.204243000
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6	-3.233071000	0.144771000	2.722241000	6	3.227586000	0.144637000	-2.717841000
6	-1.885039000	-1.709213000	3.423852000	6	1.878995000	-1.706634000	-3.416276000
6	1.078963000	2.843402000	3.089301000	6	-1.073940000	2.839488000	-3.083750000
6	1.266111000	3.529416000	1.884328000	6	-1.257574000	3.521135000	-1.878590000
6	0.143181000	4.253509000	1.391271000	6	-0.140155000	4.253524000	-1.390638000
6	0.001985000	4.536014000	-0.003966000	6	0.000000000	4.534077000	0.003531000
6	0.999115000	4.174649000	-0.871292000	6	-0.994412000	4.167087000	0.868829000
6	1.885039000	1.709213000	3.423852000	6	-1.878995000	1.706634000	-3.416276000
6	3.233071000	-0.144771000	2.722241000	6	-3.227586000	-0.144637000	-2.717841000
6	2.861551000	1.194345000	2.523261000	6	-2.852057000	1.190865000	-2.515635000
6	3.021677000	1.814021000	1.208182000	6	-3.010384000	1.807939000	-1.204243000
6	2.277171000	3.025024000	0.939426000	6	-2.264886000	3.014903000	-0.935127000
6	2.150284000	3.432920000	-0.396436000	6	-2.144728000	3.427374000	0.396322000
6	0.212113000	-1.411552000	4.342530000	6	-0.213090000	-1.410805000	-4.337345000
6	1.340402000	-0.557708000	4.265856000	6	-1.338356000	-0.557196000	-4.257664000
6	1.111592000	0.849980000	4.243786000	6	-1.108634000	0.849063000	-4.235794000
6	2.490311000	-1.022536000	3.579932000	6	-2.489056000	-1.022132000	-3.577224000
6	-0.866346000	2.649963000	-3.646806000	6	0.867973000	2.648988000	3.645788000
6	-0.658175000	3.612238000	-2.633514000	6	0.659462000	3.607980000	2.630879000
6	0.696004000	3.761598000	-2.206972000	6	-0.692543000	3.755657000	2.203107000
6	1.710315000	2.847435000	-2.600550000	6	-1.704346000	2.840787000	2.594438000
6	1.488302000	1.838359000	-3.554390000	6	-1.482002000	1.834052000	3.546744000
6	0.188813000	1.818737000	-4.134645000	6	-0.186615000	1.816713000	4.130005000
6	0.385994000	-0.565161000	-4.540565000	6	-0.385774000	-0.564395000	4.536331000
6	-0.385994000	0.565161000	-4.540565000	6	0.385774000	0.564395000	4.536331000
6	3.596175000	-0.884000000	-2.047283000	6	-3.589046000	-0.882466000	2.044239000
6	3.187987000	0.424725000	-2.344069000	6	-3.176922000	0.422936000	2.337822000
6	2.277171000	0.621229000	-3.468783000	6	-2.270587000	0.618821000	3.462439000
6	1.757600000	-0.528932000	-4.107790000	6	-1.756141000	-0.529077000	4.104745000
6	3.758976000	-0.921161000	1.648084000	6	-3.751880000	-0.919094000	-1.645963000
6	3.918543000	-0.362354000	0.356888000	6	-3.906400000	-0.360852000	-0.356436000
6	3.526085000	1.018474000	0.110263000	6	-3.513633000	1.015877000	-0.110209000
6	3.244204000	1.403041000	-1.261815000	6	-3.231262000	1.399193000	1.257512000
6	2.589004000	2.622380000	-1.470966000	6	-2.583649000	2.618067000	1.468143000
6	3.941290000	-1.275687000	-0.714482000	6	-3.932266000	-1.272494000	0.712639000

6	2.898697000	-3.084147000	-1.724136000	6	-2.895747000	-3.079667000	1.721976000
6	3.022111000	-2.026059000	-2.687342000	6	-3.020825000	-2.024409000	2.686353000
6	2.067800000	-1.847635000	-3.661983000	6	-2.067536000	-1.846559000	3.659967000
6	1.382706000	-4.401173000	-0.391405000	6	-1.382881000	-4.398075000	0.390121000
6	1.728686000	-3.888230000	-1.674018000	6	-1.728054000	-3.883628000	1.671452000
6	3.384217000	-2.283620000	1.844546000	6	-3.379715000	-2.280719000	-1.843025000
6	2.096451000	-4.061316000	0.786362000	6	-2.096472000	-4.060133000	-0.787370000
6	3.182611000	-3.143385000	0.738511000	6	-3.178133000	-3.139155000	-0.738538000
6	3.561234000	-2.655792000	-0.533842000	6	-3.555750000	-2.651308000	0.532317000
6	0.217569000	-2.669017000	3.672929000	6	-0.219165000	-2.669052000	-3.671165000
6	1.166697000	-4.012846000	1.898831000	6	-1.168813000	-4.014625000	-1.899649000
6	1.378277000	-3.158197000	3.009342000	6	-1.378845000	-3.157533000	-3.007609000
6	2.533683000	-2.326098000	2.997329000	6	-2.532761000	-2.325124000	-2.996112000
6	-0.999115000	-4.174649000	-0.871292000	6	0.994412000	-4.167087000	0.868829000
6	-0.001985000	-4.536014000	-0.003966000	6	0.000000000	-4.534077000	0.003531000
6	-0.143181000	-4.253509000	1.391271000	6	0.140155000	-4.253524000	-1.390638000
6	-1.266111000	-3.529416000	1.884328000	6	1.257574000	-3.521135000	-1.878590000
6	-1.078963000	-2.843402000	3.089301000	6	1.073940000	-2.839488000	-3.087500000
6	0.866346000	-2.6449963000	-3.646806000	6	-0.867973000	-2.648988000	3.645788000
6	0.658175000	-3.612238000	-2.633514000	6	-0.659462000	-3.607980000	2.630879000
6	-0.696004000	-3.761598000	-2.206972000	6	0.692543000	-3.755657000	2.203107000
17	0.000000000	0.000000000	0.000356000	17	0.000000000	0.000000000	0.000356000
F@C₆₀K⁺				Cl@C₆₀K⁺			
SCF Energy = -2986.30201 au				SCF Energy = -3346.71819 au			
6	-2.947424000	-0.801889000	-1.147316000	6	1.317820000	3.121524000	0.425862000
6	-2.925620000	0.639071000	-1.279125000	6	-0.030373000	3.527427000	0.104923000
6	-2.952907000	-1.386743000	0.130802000	6	2.123651000	2.540865000	-0.552811000
6	-2.914999000	1.454184000	-0.139591000	6	-0.527785000	3.320920000	-1.180475000
6	-2.081904000	2.631538000	-0.091299000	6	-1.878210000	2.842555000	-1.365636000
6	-2.095933000	0.974007000	-2.411850000	6	-0.862426000	3.257276000	1.254645000
6	-1.283956000	2.107124000	-2.360664000	6	-2.162137000	2.790446000	1.075704000
6	-1.276559000	2.949212000	-1.185651000	6	-2.679268000	2.580631000	-0.256836000
6	-1.318755000	-3.031558000	-0.597792000	6	2.949461000	0.902772000	1.096723000
6	-1.316764000	-2.438936000	-1.913677000	6	2.124513000	1.514787000	2.111499000
6	-2.151753000	-2.552560000	0.410127000	6	2.948373000	1.406142000	-0.210685000
6	-2.137822000	-1.353947000	-2.206934000	6	1.318259000	2.601334000	1.774909000
6	-1.603270000	-0.257633000	-2.978659000	6	-0.028948000	2.686898000	2.287500000
6	0.025966000	-2.513529000	-2.434543000	6	1.611703000	0.463869000	2.959517000
6	0.529364000	-1.467967000	-3.202854000	6	0.307202000	0.541204000	3.443548000
6	-0.297545000	-0.314516000	-3.467683000	6	-0.525559000	1.671559000	3.103637000
6	-0.310955000	-2.825984000	2.028462000	6	2.945279000	-0.888938000	-1.120936000
6	0.520580000	-3.383722000	0.988103000	6	2.945982000	-1.410560000	0.232097000
6	-1.613699000	-2.414678000	1.743263000	6	2.945593000	0.494695000	-1.338904000
6	0.022200000	-3.475517000	-0.307097000	6	2.946807000	-0.529523000	1.321694000
6	0.853493000	-3.151911000	-1.440468000	6	2.121900000	-0.797955000	2.475857000
6	1.872440000	-2.922738000	1.194688000	6	2.116755000	-2.592105000	0.254597000
6	2.675435000	-2.596509000	0.101734000	6	1.310505000	-2.841314000	1.364116000
6	2.161250000	-2.721395000	-1.241747000	6	1.313077000	-1.933691000	2.488914000
6	-1.296492000	-0.401615000	3.125738000	6	1.309831000	0.235749000	-3.144186000
6	0.046818000	-0.830846000	3.424100000	6	1.308415000	-1.192459000	-2.919154000
6	-2.110042000	-1.182437000	2.304309000	6	2.119663000	1.069670000	-2.374101000
6	0.529312000	-2.020642000	2.880161000	6	2.116389000	-1.751151000	-1.930063000
6	1.878358000	-2.080427000	2.366272000	6	1.602828000	-2.799693000	-1.079224000
6	0.890775000	0.340645000	3.473358000	6	-0.040418000	-1.672439000	-3.106993000
6	2.191045000	0.282537000	2.976503000	6	-0.537044000	-2.683226000	-2.285227000

6	2.691628000	-0.949310000	2.411901000	6	0.297000000	-3.254424000	-1.253428000
6	-2.919921000	0.852568000	1.178337000	6	0.304659000	2.711248000	-2.191460000
6	-2.088337000	1.659873000	2.039312000	6	-0.531562000	1.852493000	-2.997863000
6	-2.932548000	-0.542295000	1.307367000	6	1.610185000	2.330130000	-1.886116000
6	-1.285695000	1.037861000	2.993851000	6	-0.038245000	0.637545000	-3.469117000
6	0.066804000	1.497666000	3.208305000	6	-0.872768000	-0.541323000	-3.445915000
6	-1.567427000	2.755246000	1.252759000	6	-1.881007000	1.935952000	-2.489153000
6	-0.258504000	3.193436000	1.454555000	6	-2.684772000	0.798272000	-2.463887000
6	0.571574000	2.555184000	2.450863000	6	-2.171159000	-0.461935000	-2.949219000
6	3.543613000	0.822341000	1.147038000	6	-1.885561000	-3.122416000	-0.427016000
6	2.715896000	1.378378000	2.193770000	6	-1.886050000	-2.602854000	-1.774497000
6	1.920943000	2.494895000	1.935290000	6	-2.686966000	-1.510592000	-2.099751000
6	3.548397000	1.402550000	-0.122048000	6	-2.685884000	-2.529715000	0.547039000
6	3.520830000	-0.823763000	-1.166895000	6	-0.870035000	-2.713051000	2.193511000
6	3.516533000	-1.424934000	0.147639000	6	-0.038107000	-3.323767000	1.182591000
6	3.527848000	-0.615321000	1.282684000	6	-0.535543000	-3.523355000	-0.103909000
6	3.536607000	0.564297000	-1.298318000	6	-2.169331000	-2.321785000	1.879898000
6	1.892419000	0.427024000	-3.119447000	6	-1.877879000	-0.234383000	3.146314000
6	1.882643000	-1.010633000	-2.988802000	6	-0.527902000	-0.637240000	3.465662000
6	2.681655000	-1.624917000	-2.026395000	6	-0.034474000	-1.854811000	3.001173000
6	2.705501000	1.201854000	-2.293315000	6	-2.681985000	-1.061223000	2.365076000
6	0.904026000	2.852669000	-2.021815000	6	-3.514982000	0.884559000	1.115935000
6	0.061919000	2.049984000	-2.878515000	6	-2.678556000	1.741068000	1.923965000
6	0.545076000	0.856216000	-3.414637000	6	-1.876183000	1.192210000	2.921306000
6	2.202544000	2.435494000	-1.733096000	6	-3.516090000	-0.491591000	1.332755000
6	1.923582000	3.093749000	0.619952000	6	-3.519917000	-0.898576000	-1.090955000
6	0.576572000	3.524433000	0.322090000	6	-3.517599000	0.527700000	-1.315259000
6	0.076044000	3.409665000	-0.975466000	6	-3.515287000	1.403512000	-0.231661000
6	2.722954000	2.558551000	-0.389980000	6	-3.518965000	-1.399206000	0.209392000
9	-0.148342000	-0.670926000	-0.181660000	17	-0.264849000	-0.001165000	-0.002355000
19	-5.564620000	0.038844000	0.004686000	19	5.596906000	-0.002024000	0.000236000
Br@C₆₀K⁺				OH@C₆₀K⁺			
SCF Energy = -5460.52339 au				SCF Energy = -2962.25460 au			
6	-3.484957000	-1.099937000	-0.976922000	6	1.301534000	-3.070767000	0.711032000
6	-3.525121000	0.297379000	-1.342432000	6	-0.047283000	-3.321622000	1.157076000
6	-3.465861000	-1.467996000	0.368014000	6	2.114759000	-2.182220000	1.416585000
6	-3.546113000	1.277927000	-0.351930000	6	-0.546159000	-2.681826000	2.290686000
6	-2.746630000	2.472548000	-0.500398000	6	-1.895489000	-2.168087000	2.295589000
6	-2.704404000	0.476037000	-2.518247000	6	-0.882397000	-3.472758000	-0.010548000
6	-1.935211000	1.629928000	-2.663635000	6	-2.185726000	-2.982217000	-0.006641000
6	-1.955749000	2.645630000	-1.635737000	6	-2.702610000	-2.315108000	1.166352000
6	-1.782217000	-3.199494000	-0.103812000	6	2.931558000	-1.239899000	-0.704609000
6	-1.802988000	-2.817318000	-1.498114000	6	2.106351000	-2.170719000	-1.434416000
6	-2.596394000	-2.534289000	0.811908000	6	2.953209000	-1.252779000	0.698895000
6	-2.637723000	-1.785261000	-1.926123000	6	1.298161000	-3.066403000	-0.733460000
6	-2.155321000	-0.811523000	-2.879637000	6	-0.050425000	-3.315814000	-1.179007000
6	-0.452326000	-2.906024000	-2.004979000	6	1.578707000	-1.485129000	-2.590562000
6	0.011606000	-1.968385000	-2.927561000	6	0.279544000	-1.734485000	-3.029011000
6	-0.854792000	-0.901476000	-3.372463000	6	-0.551917000	-2.668461000	-2.308902000
6	-0.771035000	-2.497493000	2.460373000	6	2.944297000	1.228770000	0.724491000
6	0.075470000	-3.183890000	1.510774000	6	2.948026000	1.239472000	-0.722955000
6	-2.082053000	-2.176808000	2.114337000	6	2.930387000	0.006440000	1.413145000
6	-0.419279000	-3.525290000	0.250948000	6	2.912569000	0.020321000	-1.412797000
6	0.401486000	-3.347431000	-0.925666000	6	2.082419000	-0.134478000	-2.581079000
6	1.409334000	-2.644483000	1.634342000	6	2.107371000	2.327561000	-1.165855000

6	2.204351000	-2.483987000	0.498538000	6	1.298097000	2.174742000	-2.294743000
6	1.694001000	-2.838199000	-0.805949000	6	1.293057000	0.925547000	-3.022591000
6	-1.850344000	0.036132000	3.163779000	6	1.300263000	0.902203000	3.020700000
6	-0.487111000	-0.292770000	3.514165000	6	1.302047000	2.158343000	2.305450000
6	-2.633030000	-0.889760000	2.475243000	6	2.096875000	-0.153338000	2.578748000
6	0.040927000	-1.536856000	3.172601000	6	2.106198000	2.315270000	1.174975000
6	1.389465000	-1.627130000	2.662800000	6	1.590292000	2.990818000	0.007684000
6	0.312487000	0.902208000	3.369387000	6	-0.044913000	2.676176000	2.311471000
6	1.619325000	0.816786000	2.889475000	6	-0.545413000	3.328574000	1.182068000
6	2.163660000	-0.472553000	2.530622000	6	0.287317000	3.488855000	0.011937000
6	-3.527648000	0.897080000	1.041800000	6	0.288526000	-1.752317000	3.014130000
6	-2.713082000	1.854650000	1.754225000	6	-0.542940000	-0.662348000	3.467078000
6	-3.487289000	-0.451495000	1.395523000	6	1.588529000	-1.503050000	2.577465000
6	-1.891651000	1.432706000	2.797525000	6	-0.045274000	0.643046000	3.471351000
6	-0.554805000	1.967403000	2.922690000	6	-0.878459000	1.738602000	3.030754000
6	-2.230909000	2.828462000	0.802008000	6	-1.892617000	-0.918577000	3.022472000
6	-0.944205000	3.349704000	0.925671000	6	-2.694651000	0.138403000	2.591447000
6	-0.090516000	2.910301000	2.006007000	6	-2.180297000	1.489569000	2.597596000
6	2.937558000	1.106254000	0.980824000	6	-1.897638000	3.077607000	-0.709912000
6	2.099645000	1.793596000	1.936503000	6	-1.896092000	3.074187000	0.736114000
6	1.258926000	2.816528000	1.497759000	6	-2.700570000	2.169887000	1.431795000
6	2.920183000	1.476145000	-0.371202000	6	-2.704689000	2.178901000	-1.409457000
6	2.973776000	-0.899002000	-1.046447000	6	-0.886182000	1.757203000	-3.014482000
6	2.988255000	-1.280801000	0.352718000	6	-0.050208000	2.688686000	-2.290099000
6	2.973905000	-0.296531000	1.348585000	6	-0.548103000	3.333687000	-1.156874000
6	2.939772000	0.456587000	-1.402465000	6	-2.186555000	1.506061000	-2.579964000
6	1.305773000	-0.033199000	-3.161843000	6	-1.899186000	-0.897359000	-3.020591000
6	1.346514000	-1.431980000	-2.796617000	6	-0.551357000	-0.638173000	-3.468071000
6	2.173265000	-1.865178000	-1.760900000	6	-0.053795000	0.667440000	-3.467921000
6	2.093628000	0.900531000	-2.484834000	6	-2.702265000	0.155402000	-2.582886000
6	0.228488000	2.495839000	-2.457183000	6	-3.538853000	-1.217622000	-0.722746000
6	-0.583658000	1.534904000	-3.168285000	6	-2.703776000	-2.305645000	-1.173774000
6	-0.055178000	0.293540000	-3.518192000	6	-1.899647000	-2.152011000	-2.303629000
6	1.546297000	2.186725000	-2.121331000	6	-3.538016000	-0.005592000	-1.415563000
6	1.238310000	3.198264000	0.102721000	6	-3.535100000	1.239127000	0.707291000
6	-0.123273000	3.529239000	-0.250453000	6	-3.531922000	-0.015677000	1.424056000
6	-0.618961000	3.179918000	-1.507404000	6	-3.537049000	-1.222889000	0.723400000
6	2.058071000	2.546653000	-0.818274000	6	-3.538857000	1.244304000	-0.689590000
35	-0.269385000	-0.001123000	0.001224000	8	0.231922000	-0.225864000	-0.055722000
19	5.645295000	-0.011530000	0.000008000	1	-0.374967000	0.501686000	0.150262000
				19	5.589348000	0.012538000	-0.003109000
NH₂@C₆₀K⁺				NO₂@C₆₀K⁺			
SCF Energy = -2942.36181 au				SCF Energy = -3091.60534 au			
6	-1.310894000	-1.329848000	-2.861386000	6	0.177257000	-2.795826000	-2.136463000
6	0.035137000	-1.147134000	-3.340522000	6	1.023700000	-3.296099000	-1.075731000
6	-2.123378000	-0.222175000	-2.594023000	6	0.646813000	-1.806745000	-2.997602000
6	0.545881000	0.142543000	-3.534346000	6	2.318419000	-2.790552000	-0.909701000
6	1.894941000	0.456355000	-3.128294000	6	2.811180000	-2.493490000	0.424705000
6	0.866853000	-2.159564000	-2.729598000	6	0.175859000	-3.524936000	0.074391000
6	2.170076000	-1.856849000	-2.340157000	6	0.644903000	-3.237960000	1.351944000
6	2.701615000	-0.526089000	-2.544120000	6	1.983834000	-2.714736000	1.532603000
6	-2.950649000	-1.306712000	-0.537087000	6	-1.545570000	-0.666069000	-2.943030000
6	-2.115839000	-2.450855000	-0.818159000	6	-2.035263000	-1.694486000	-2.057853000
6	-2.961209000	-0.210259000	-1.422729000	6	-0.228295000	-0.722758000	-3.395930000
6	-1.310428000	-2.456564000	-1.953717000	6	-1.182191000	-2.724838000	-1.647781000

6	0.034163000	-2.973065000	-1.874463000	6	-1.185987000	-3.179741000	-0.278174000
6	-1.599085000	-2.949591000	0.433256000	6	-2.898973000	-1.061982000	-1.088274000
6	-0.303416000	-3.463141000	0.509221000	6	-2.898961000	-1.505075000	0.240425000
6	0.529457000	-3.474343000	-0.669183000	6	-2.051035000	-2.603396000	0.658751000
6	-2.923490000	1.334866000	0.512296000	6	0.001150000	1.707885000	-3.083838000
6	-2.958970000	0.206969000	1.424782000	6	-1.359060000	1.772410000	-2.602452000
6	-2.923507000	1.131615000	-0.871259000	6	0.556624000	0.482315000	-3.467496000
6	-2.951213000	-1.097986000	0.890866000	6	-2.117319000	0.601261000	-2.536783000
6	-2.115130000	-2.112902000	1.488848000	6	-2.958097000	0.362940000	-1.388450000
6	-2.120654000	0.531912000	2.550881000	6	-1.422468000	2.750866000	-1.532309000
6	-1.309401000	-0.452297000	3.127798000	6	-2.251993000	2.540463000	-0.423249000
6	-1.308865000	-1.791822000	2.578519000	6	-3.020355000	1.309227000	-0.350989000
6	-1.294167000	2.957698000	-1.161506000	6	2.680237000	1.034927000	-2.373895000
6	-1.293383000	3.167231000	0.266047000	6	2.095226000	2.293332000	-1.958606000
6	-2.087015000	1.949340000	-1.715563000	6	1.917871000	0.140202000	-3.116297000
6	-2.087145000	2.360949000	1.086904000	6	0.788879000	2.634748000	-2.312706000
6	-1.585631000	1.859946000	2.342719000	6	-0.084151000	3.280117000	-1.353927000
6	0.056130000	3.475981000	0.672410000	6	2.579334000	2.588044000	-0.636202000
6	0.550848000	2.978994000	1.880201000	6	1.744582000	3.217364000	0.288531000
6	-0.282968000	2.165426000	2.737151000	6	0.385796000	3.567096000	-0.072198000
6	-0.284428000	1.286442000	-3.239721000	6	2.800409000	-1.754058000	-1.803636000
6	0.549172000	2.311737000	-2.653403000	6	3.587874000	-0.817809000	-1.025807000
6	-1.587176000	1.108506000	-2.775395000	6	1.980222000	-1.277999000	-2.831780000
6	0.055208000	3.136564000	-1.640889000	6	3.536181000	0.551158000	-1.314402000
6	0.891096000	3.458263000	-0.506872000	6	3.464079000	1.513001000	-0.237576000
6	1.897576000	1.797741000	-2.583789000	6	3.595127000	-1.274027000	0.350398000
6	2.703765000	2.111501000	-1.489895000	6	3.531475000	-0.335979000	1.387018000
6	2.187947000	2.951893000	-0.432511000	6	3.461612000	1.078267000	1.083597000
6	1.895934000	1.335431000	2.866073000	6	0.384400000	2.828691000	2.141770000
6	1.898000000	2.464232000	1.959890000	6	1.744406000	2.764256000	1.656039000
6	2.703175000	2.449442000	0.821570000	6	2.582686000	1.713155000	2.040727000
6	2.700890000	0.226142000	2.586760000	6	-0.082334000	1.835152000	3.001326000
6	0.868552000	-1.284488000	3.238342000	6	-2.232783000	1.790777000	1.806270000
6	0.036967000	-0.138801000	3.534830000	6	-1.760207000	2.833258000	0.913365000
6	0.547737000	1.153162000	3.348417000	6	-0.461907000	3.331760000	1.078785000
6	2.170817000	-1.106975000	2.775284000	6	-1.410429000	1.300023000	2.824445000
6	1.879976000	-2.950456000	1.162112000	6	-2.115208000	-1.023731000	2.386682000
6	0.530249000	-3.135798000	1.640826000	6	-2.942367000	-0.526555000	1.311919000
6	0.035743000	-2.309494000	2.652436000	6	-3.005198000	0.849194000	1.026380000
6	2.678725000	-1.948196000	1.715579000	6	-1.354328000	-0.118835000	3.124114000
6	3.517921000	-1.333021000	-0.509141000	6	0.553793000	-1.670276000	3.076022000
6	2.678059000	-2.358267000	-1.084283000	6	-0.236060000	-2.601359000	2.309270000
6	1.879159000	-3.159727000	-0.265992000	6	-1.562790000	-2.300662000	1.982895000
6	3.518604000	-1.131326000	0.870048000	6	0.002155000	-0.453915000	3.488677000
6	3.539272000	1.304763000	0.537582000	6	2.097386000	0.690470000	2.932579000
6	3.539904000	1.096016000	-0.889650000	6	2.678841000	-0.573848000	2.527885000
6	3.534458000	-0.202452000	-1.411305000	6	1.917770000	-1.739636000	2.598515000
6	3.533732000	0.210749000	1.409461000	6	0.789428000	0.752305000	3.407487000
7	-0.081614000	-0.133821000	-0.044129000	7	-0.074271000	-0.343258000	0.174419000
1	0.390366000	0.188350000	0.816687000	8	-0.401763000	0.844071000	-0.010591000
1	0.677281000	0.037212000	-0.724555000	8	1.096850000	-0.636558000	-0.118746000
19	-5.574449000	0.011469000	-0.001902000	19	-5.581993000	-0.222159000	-0.033290000
CN ⁻ @C ₆₀ K ⁺				ClO ⁻ @C ₆₀ K ⁺			
SCF Energy = -2979.29839 au				SCF Energy = -3421.81579 au			
6	3.540575000	0.374886000	-1.368609000	6	2.979836000	-1.281943000	0.731368000

6	3.546258000	-1.017369000	-0.980147000	6	2.104717000	-2.345508000	1.176502000
6	3.534933000	1.371448000	-0.394078000	6	2.964737000	-0.054285000	1.417876000
6	3.548244000	-1.364467000	0.371160000	6	1.289817000	-2.166694000	2.296548000
6	2.707660000	-2.445903000	0.836590000	6	-0.067855000	-2.664146000	2.304420000
6	2.707222000	-1.741286000	-1.909028000	6	1.569553000	-3.008314000	0.010512000
6	1.903333000	-2.787229000	-1.459008000	6	0.253067000	-3.476872000	0.013037000
6	1.903139000	-3.146177000	-0.060768000	6	-0.581115000	-3.306351000	1.179230000
6	1.885319000	2.664741000	-1.685511000	6	2.995185000	1.202593000	-0.708108000
6	1.890023000	1.632674000	-2.694998000	6	2.962903000	-0.065202000	-1.420980000
6	2.692004000	2.535596000	-0.556439000	6	2.996504000	1.208213000	0.695609000
6	2.700271000	0.509249000	-2.537988000	6	2.978602000	-1.287433000	-0.725075000
6	2.185384000	-0.798917000	-2.872654000	6	2.103212000	-2.354504000	-1.161113000
6	0.537259000	1.488793000	-3.185504000	6	2.134502000	0.108550000	-2.594383000
6	0.043421000	0.229573000	-3.510971000	6	1.303942000	-0.934539000	-3.007603000
6	0.882097000	-0.934146000	-3.349139000	6	1.287069000	-2.184384000	-2.281743000
6	0.865992000	3.373801000	0.864222000	6	1.383928000	3.076243000	0.712176000
6	0.030970000	3.508291000	-0.305777000	6	1.382909000	3.070587000	-0.737059000
6	2.170242000	2.896129000	0.741894000	6	2.169760000	2.157415000	1.415036000
6	0.531138000	3.155113000	-1.555660000	6	2.167640000	2.146311000	-1.433657000
6	-0.302988000	2.431884000	-2.485459000	6	1.642532000	1.467233000	-2.597910000
6	-1.319554000	3.144627000	0.059746000	6	0.031344000	3.327904000	-1.180330000
6	-2.130593000	2.456945000	-0.842704000	6	-0.482850000	2.672240000	-2.299959000
6	-1.610931000	2.089937000	-2.139209000	6	0.336085000	1.724204000	-3.017062000
6	1.885512000	1.526038000	2.758182000	6	0.339852000	1.747185000	3.003339000
6	0.531427000	2.018550000	2.881014000	6	-0.479991000	2.689656000	2.279890000
6	2.691964000	1.955474000	1.706261000	6	1.645900000	1.487116000	2.585018000
6	0.030407000	2.928946000	1.954568000	6	0.032834000	3.336676000	1.154742000
6	-1.319708000	2.785524000	1.458813000	6	-0.804193000	3.494992000	-0.012949000
6	-0.302227000	0.936814000	3.347680000	6	-1.839845000	2.196904000	2.286531000
6	-1.610034000	0.803600000	2.880030000	6	-2.644648000	2.352630000	1.159469000
6	-2.130064000	1.748110000	1.919131000	6	-2.116427000	3.017102000	-0.010414000
6	3.541643000	-0.330375000	1.381752000	6	1.307819000	-0.911588000	3.013414000
6	2.700653000	-0.774384000	2.471098000	6	-0.037715000	-0.637496000	3.460790000
6	3.535557000	1.012567000	1.005669000	6	2.137760000	0.128335000	2.591115000
6	1.889522000	0.136037000	3.146920000	6	-0.514392000	0.671649000	3.452809000
6	0.537011000	-0.226593000	3.507940000	6	-1.862901000	0.946768000	3.012067000
6	2.185706000	-2.081684000	2.133930000	6	-0.891863000	-1.719351000	3.023264000
6	0.882549000	-2.430084000	2.487206000	6	-2.194888000	-1.456810000	2.595484000
6	0.043018000	-1.487197000	3.188149000	6	-2.690284000	-0.096771000	2.589561000
6	-2.960091000	-0.373803000	1.376205000	6	-3.504402000	1.266545000	-0.726648000
6	-2.123138000	-0.505023000	2.548415000	6	-3.503345000	1.271958000	0.720746000
6	-1.307677000	-1.627000000	2.693107000	6	-3.537794000	0.066100000	1.427513000
6	-2.956205000	-1.376604000	0.396210000	6	-3.539761000	0.055269000	-1.424029000
6	-2.960852000	0.334714000	-1.388194000	6	-1.866832000	0.923882000	-3.017511000
6	-2.966361000	1.373592000	-0.373013000	6	-1.842785000	2.179569000	-2.301417000
6	-2.965203000	1.024991000	0.985974000	6	-2.646259000	2.343919000	-1.174638000
6	-2.957033000	-1.016175000	-1.010491000	6	-2.693789000	-0.116429000	-2.586029000
6	-1.302865000	-1.522195000	-2.753138000	6	-0.895554000	-1.742388000	-3.009265000
6	-1.306758000	-0.131738000	-3.142851000	6	-0.041979000	-0.663876000	-3.455824000
6	-2.123519000	0.783124000	-2.478684000	6	-0.518724000	0.645283000	-3.457515000
6	-2.115528000	-1.962146000	-1.709438000	6	-2.198070000	-1.476430000	-2.582017000
6	-0.286010000	-3.366784000	-0.862666000	6	-1.934535000	-3.044743000	-0.710642000
6	0.550296000	-2.922081000	-1.951719000	6	-0.582519000	-3.315204000	-1.153528000
6	0.049098000	-2.016016000	-2.881864000	6	-0.070648000	-2.681810000	-2.284312000
6	-1.595588000	-2.899990000	-0.743100000	6	-2.738821000	-2.146415000	-1.416381000
6	-1.303261000	-2.659661000	1.682913000	6	-3.563006000	-1.192306000	0.708482000

6	0.049077000	-3.153323000	1.557020000	6	-2.737118000	-2.135710000	1.435664000
6	0.549674000	-3.501263000	0.306107000	6	-1.933722000	-3.039346000	0.735811000
6	-2.115404000	-2.542676000	0.555444000	6	-3.563733000	-1.197579000	-0.695225000
6	0.781803000	-0.076909000	-0.005786000	8	0.776181000	0.350953000	0.002046000
7	-0.395638000	0.041104000	-0.002296000	17	-0.790624000	-0.159697000	-0.001372000
19	-5.591758000	-0.019114000	-0.001919000	19	5.629120000	-0.092862000	-0.001117000