

## Supplementary Information

### Computational Design of Valence Tautomeric Adducts of Co<sup>II</sup> Diketonates with Redox-Active *o*-Benzoquinone Ligands†

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### Absolute energies and optimized geometries at B3LYP\*/6-311++G(d,p)

#### 6 X=Y=O, BQ

E=-381.32057 a.u.

8	2.216387000	0.070998000	0.000000000
8	0.401067000	2.180678000	0.000000000
6	0.000000000	1.035048000	0.000000000
6	-1.431749000	0.686131000	0.000000000
6	-1.823525000	-0.604328000	0.000000000
6	-0.869961000	-1.712612000	0.000000000
6	0.464495000	-1.518080000	0.000000000
6	1.023862000	-0.154530000	0.000000000
1	-2.138280000	1.510826000	0.000000000
1	-2.882150000	-0.851119000	0.000000000
1	-1.271835000	-2.722564000	0.000000000
1	1.173903000	-2.340325000	0.000000000

#### 6 X=Y=O, SQ

E=-381.40166 a.u.

8	2.242101000	0.095903000	0.000000000
8	0.366381000	2.213987000	0.000000000
6	0.000000000	1.014200000	0.000000000
6	-1.399410000	0.642205000	0.000000000
6	-1.827327000	-0.668995000	0.000000000
6	-0.885185000	-1.733032000	0.000000000
6	0.468172000	-1.466747000	0.000000000
6	1.006787000	-0.122731000	0.000000000
1	-2.112451000	1.465460000	0.000000000
1	-2.892792000	-0.896600000	0.000000000
1	-1.239909000	-2.763122000	0.000000000
1	1.199078000	-2.274256000	0.000000000

#### 6 X=O,Y=NH, BQ

E=-361.44311 a.u.

7	1.879967000	1.234839000	0.000111000
8	1.618547000	-1.526848000	-0.000079000
6	0.622338000	-0.828660000	-0.000046000
6	-0.734672000	-1.405205000	0.000041000
6	-1.832531000	-0.620379000	0.000027000
6	-1.741739000	0.833705000	-0.000051000
6	-0.549078000	1.462914000	-0.000053000
6	0.710457000	0.709807000	-0.000006000
1	-0.796050000	-2.489073000	0.000235000
1	1.812229000	2.259476000	0.000106000
1	-2.822653000	-1.069243000	0.000189000
1	-2.664189000	1.407452000	0.000006000

1	-0.486131000	2.549204000	-0.000163000
<b>6 X=O,Y=NH SQ</b>			
E=-361.50894 a.u.			
7	0.422939000	2.244359000	0.000000000
8	2.250631000	0.091188000	0.000000000
6	1.015557000	-0.126266000	0.000000000
6	0.480415000	-1.470448000	0.000000000
6	-0.872559000	-1.753408000	0.000000000
6	-1.823290000	-0.701828000	0.000000000
6	-1.392177000	0.610216000	0.000000000
6	0.000000000	0.987437000	0.000000000
1	1.218130000	-2.271133000	0.000000000
1	-0.405798000	2.852830000	0.000000000
1	-1.213727000	-2.788247000	0.000000000
1	-2.888161000	-0.928900000	0.000000000
1	-2.123739000	1.421214000	0.000000000

**6 X=Y=NH, BQ**

E=-341.56193 a.u.

7	-1.388304000	0.084683000	-1.778645000
7	1.388304000	-0.084683000	-1.778645000
6	0.751482000	-0.113012000	-0.664327000
6	1.388304000	-0.318975000	0.643938000
6	0.706478000	-0.171993000	1.798682000
6	-0.706478000	0.171993000	1.798682000
6	-1.388304000	0.318975000	0.643938000
6	-0.751482000	0.113012000	-0.664327000
1	2.448672000	-0.561505000	0.646922000
1	-2.385802000	0.263405000	-1.619051000
1	1.209689000	-0.301496000	2.752883000
1	-1.209689000	0.301496000	2.752883000
1	-2.448672000	0.561505000	0.646922000
1	2.385802000	-0.263405000	-1.619051000

**6 X=Y=NH, SQ**

E=-341.61344 a.u.

7	1.807228000	1.410653000	-0.000454000
7	1.807229000	-1.410651000	0.000456000
6	0.660816000	-0.749569000	-0.000005000
6	-0.632250000	-1.392759000	-0.000366000
6	-1.833263000	-0.708163000	-0.000293000
6	-1.833264000	0.708162000	0.000295000
6	-0.632250000	1.392758000	0.000365000
6	0.660812000	0.749569000	-0.000004000
1	-0.633000000	-2.484150000	-0.000665000
1	1.585745000	2.413925000	-0.000623000

1	-2.775149000	-1.254763000	-0.000047000
1	-2.775151000	1.254761000	0.000055000
1	-0.633003000	2.484149000	0.000666000
1	1.585750000	-2.413924000	0.000644000

### **bis(malonate) Co<sup>II</sup>**

E=-1915.67069736 a.u.

6	0.002214000	0.000122000	3.215734000
6	0.000941000	-1.240524000	2.564685000
6	0.003201000	1.240855000	2.564854000
1	0.002685000	0.000053000	4.300355000
1	0.001111000	-2.140094000	3.196243000
1	0.004041000	2.140329000	3.196526000
6	1.241490000	0.000887000	-2.567928000
6	-1.239910000	0.002250000	-2.567103000
6	0.000595000	0.002161000	-3.218486000
1	2.140806000	0.001201000	-3.199815000
1	-2.139634000	0.002532000	-3.198438000
1	0.000228000	0.001893000	-4.303091000
8	-1.452400000	0.001070000	-1.312622000
8	1.454854000	-0.000095000	-1.313542000
8	0.002231000	1.453879000	1.310440000
8	-0.000205000	-1.453391000	1.310240000
27	0.001756000	0.000350000	-0.001357000

### **bis(acetylacetonate) Co<sup>II</sup>**

E=-2072.89123363 a.u.

27	0.000000000	0.000000000	0.000281000
8	1.320543000	1.017598000	-1.017942000
8	1.320543000	-1.017717000	1.018383000
6	2.585594000	-0.886587000	0.886424000
6	2.585594000	0.885976000	-0.886480000
6	3.225977000	-0.000500000	-0.000221000
1	4.309318000	-0.000814000	-0.000532000
6	3.418755000	-1.778282000	1.777152000
1	3.162951000	-1.581204000	2.823795000
1	4.491162000	-1.632367000	1.633654000
1	3.165501000	-2.824858000	1.576231000
6	3.418759000	1.777180000	-1.777693000
1	3.162105000	1.580438000	-2.824189000
1	4.491163000	1.630516000	-1.634932000
1	3.166371000	2.823903000	-1.576439000
8	-1.320543000	1.017717000	1.018383000
6	-2.585594000	0.886587000	0.886424000
6	-3.225977000	0.000500000	-0.000221000
6	-2.585594000	-0.885976000	-0.886480000

8	-1.320543000	-1.017598000	-1.017942000
6	-3.418759000	-1.777180000	-1.777693000
1	-3.166371000	-2.823903000	-1.576439000
1	-4.491163000	-1.630516000	-1.634932000
1	-3.162105000	-1.580438000	-2.824189000
1	-4.309318000	0.000814000	-0.000532000
6	-3.418755000	1.778282000	1.777152000
1	-4.491162000	1.632367000	1.633654000
1	-3.162951000	1.581204000	2.823795000
1	-3.165501000	2.824858000	1.576231000

**bis(hexafluoroacetylacetonate) Co<sup>II</sup>**

E=-3263.63635 a.u.

27	0.000000000	0.001337000	0.000296000
8	-1.335838000	-1.002032000	-1.013125000
8	-1.334490000	1.004020000	1.016228000
8	1.336187000	-1.013089000	1.002188000
8	1.334190000	1.016122000	-1.003881000
6	-2.585675000	-0.861401000	-0.869576000
6	-3.259809000	0.000546000	0.003255000
6	-2.584491000	0.862767000	0.874915000
6	2.585967000	-0.871063000	0.859652000
6	3.259851000	0.000748000	-0.003530000
6	2.584236000	0.873086000	-0.864821000
1	-4.339818000	0.000559000	0.004003000
1	4.339857000	0.000632000	-0.004753000
6	3.407877000	1.802455000	-1.784720000
9	3.116019000	3.089436000	-1.523779000
9	4.736283000	1.638184000	-1.624726000
9	3.113382000	1.557697000	-3.074228000
6	3.411442000	-1.802759000	1.775526000
9	4.739443000	-1.627136000	1.624428000
9	3.108056000	-1.573138000	3.065550000
9	3.130670000	-3.089398000	1.500122000
6	-3.408449000	1.780396000	1.806247000
9	-3.118391000	1.514679000	3.092725000
9	-3.112496000	3.070416000	1.566372000
9	-4.736797000	1.622107000	1.639845000
6	-3.410863000	-1.781391000	-1.797454000
9	-3.110376000	-1.531393000	-3.084469000
9	-3.126830000	-3.071376000	-1.542280000
9	-4.738947000	-1.610940000	-1.641278000

7

E= -2297.00361 a.u.

27	0.639002000	-0.000081000	-0.000598000
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8	0.635517000	1.676948000	1.134848000
8	2.003260000	0.880787000	-1.192547000
8	2.003899000	-0.879143000	1.192170000
8	0.637322000	-1.677235000	-1.135434000
6	1.456063000	2.638461000	1.071267000
6	2.458809000	2.823096000	0.111394000
6	2.649512000	1.943846000	-0.961714000
6	2.650180000	-1.942431000	0.962570000
6	2.459940000	-2.822622000	-0.109883000
6	1.457859000	-2.638709000	-1.070550000
1	3.086603000	3.704585000	0.178834000
1	3.087725000	-3.704202000	-0.176224000
1	3.431238000	-2.197213000	1.695884000
1	1.352282000	-3.413370000	-1.846223000
1	3.430930000	2.199199000	-1.694443000
1	1.349984000	3.412545000	1.847458000
8	-0.997996000	0.640047000	-1.139783000
8	-0.997621000	-0.641044000	1.139042000
6	-2.118154000	-0.377669000	0.650744000
6	-3.377465000	-0.738914000	1.244411000
6	-4.532472000	-0.369305000	0.621666000
6	-4.532675000	0.368926000	-0.620880000
6	-3.377865000	0.738308000	-1.244135000
6	-2.118377000	0.376760000	-0.651060000
1	-3.368471000	-1.290154000	2.178960000
1	-5.490502000	-0.629848000	1.062292000
1	-5.490844000	0.629695000	-1.061066000
1	-3.369180000	1.289588000	-2.178664000

## 8

E=-2297.02749 a.u.

27	0.623771000	-0.000048000	-0.000028000
8	0.539856000	1.459684000	1.226657000
8	1.968452000	0.747397000	-1.112303000
8	1.968469000	-0.746394000	1.113012000
8	0.541754000	-1.459849000	-1.226729000
6	1.260683000	2.495207000	1.120044000
6	2.209300000	2.774126000	0.132292000
6	2.489146000	1.885606000	-0.906866000
6	2.490763000	-1.883841000	0.907427000
6	2.212577000	-2.772372000	-0.132162000
6	1.263870000	-2.494470000	-1.120116000
1	2.745701000	3.714367000	0.174219000
1	2.750215000	-3.711904000	-0.174155000
1	3.246180000	-2.176566000	1.648242000
1	1.104642000	-3.244292000	-1.906356000

1	3.244575000	2.179039000	-1.647387000
1	1.100315000	3.244961000	1.906117000
8	-0.780236000	-0.829632000	1.007565000
8	-0.780453000	0.828407000	-1.008204000
6	-1.934434000	0.462446000	-0.564738000
6	-3.168990000	0.907765000	-1.105188000
6	-4.343430000	0.451994000	-0.551393000
6	-4.343309000	-0.453409000	0.551390000
6	-3.168749000	-0.909108000	1.104982000
6	-1.934306000	-0.463680000	0.564350000
1	-3.153501000	1.595019000	-1.944685000
1	-5.294261000	0.784793000	-0.956926000
1	-5.294052000	-0.786252000	0.957095000
1	-3.153072000	-1.596360000	1.944478000

**9**

E=-2454.22355 a.u.

27	0.205580000	0.000056000	0.000208000
8	0.221407000	1.816305000	0.857718000
8	1.553881000	0.707595000	-1.299059000
8	1.551862000	-0.707929000	1.301450000
8	0.222802000	-1.815717000	-0.858493000
6	1.024326000	2.784632000	0.669141000
6	2.017481000	2.820139000	-0.325321000
6	2.217217000	1.791585000	-1.263114000
6	2.216517000	-1.791084000	1.264613000
6	2.019128000	-2.818542000	0.325116000
6	1.026878000	-2.783153000	-0.670266000
1	2.640024000	3.703908000	-0.395552000
1	2.642748000	-3.701594000	0.394856000
8	-1.419240000	0.464159000	-1.221384000
8	-1.419289000	-0.465245000	1.221109000
6	-2.544516000	-0.277153000	0.695209000
6	-3.800786000	-0.548512000	1.333967000
6	-4.960638000	-0.275325000	0.665663000
6	-4.960616000	0.272896000	-0.666610000
6	-3.800742000	0.546478000	-1.334711000
6	-2.544489000	0.275618000	-0.695705000
1	-3.791043000	-0.956798000	2.339395000
1	-5.917102000	-0.470456000	1.142209000
1	-5.917064000	0.467689000	-1.143324000
1	-3.790957000	0.954766000	-2.340138000
6	0.853654000	-3.964603000	-1.598636000
1	-0.169174000	-4.346147000	-1.509797000
1	0.984349000	-3.629378000	-2.633084000
1	1.559503000	-4.770754000	-1.387225000

6	3.273333000	-1.945187000	2.335703000
1	3.816348000	-2.889240000	2.254165000
1	3.980756000	-1.111877000	2.267091000
1	2.797789000	-1.884291000	3.320457000
6	3.275093000	1.945308000	-2.333190000
1	3.982876000	1.112440000	-2.263085000
1	2.800637000	1.883293000	-3.318405000
1	3.817505000	2.889735000	-2.251932000
6	0.848645000	3.966910000	1.595984000
1	1.553487000	4.773830000	1.384141000
1	-0.174671000	4.346847000	1.505902000
1	0.979047000	3.633120000	2.630934000

## 10

E=-2454.24826 a.u.

27	7.772574000	-9.476508000	1.270509000
8	7.717633000	-7.584070000	1.448604000
8	9.646425000	-9.625155000	1.468486000
8	7.558851000	-9.587882000	3.145882000
8	7.727679000	-11.353116000	0.968257000
6	8.736553000	-6.846604000	1.641865000
6	10.062457000	-7.295383000	1.740076000
6	10.438850000	-8.641652000	1.643017000
6	7.437638000	-10.675582000	3.800026000
6	7.459283000	-11.965440000	3.252953000
6	7.602611000	-12.229699000	1.882186000
1	10.840002000	-6.558575000	1.896141000
1	7.351982000	-12.806514000	3.925987000
8	5.871281000	-9.432703000	0.980492000
8	7.918587000	-9.244357000	-0.633270000
6	6.751331000	-9.166653000	-1.171775000
6	6.530450000	-8.988616000	-2.563334000
6	5.238891000	-8.914647000	-3.033276000
6	4.121585000	-9.012370000	-2.152000000
6	4.290790000	-9.186997000	-0.797300000
6	5.606677000	-9.268601000	-0.269099000
1	7.390001000	-8.916629000	-3.221853000
1	5.059389000	-8.778624000	-4.095718000
1	3.119389000	-8.947393000	-2.565431000
1	3.450349000	-9.261899000	-0.114871000
6	7.613931000	-13.656790000	1.386563000
1	8.560285000	-13.850567000	0.870954000
1	7.489080000	-14.375939000	2.198318000
1	6.811448000	-13.791618000	0.654040000
6	7.254292000	-10.488840000	5.287973000
1	6.347718000	-9.901162000	5.466594000



1	7.177725000	-11.441258000	5.815826000
1	8.096815000	-9.916182000	5.689132000
6	11.895835000	-9.028538000	1.742283000
1	12.024983000	-9.753613000	2.552365000
1	12.199761000	-9.521997000	0.813094000
1	12.540175000	-8.165525000	1.920412000
6	8.427864000	-5.372984000	1.766939000
1	7.904697000	-5.034996000	0.866551000
1	7.750362000	-5.218774000	2.613282000
1	9.328865000	-4.773445000	1.910187000

## 11

E=-3644.98270 a.u.

27	0.001514000	0.521254000	-0.000063000
8	0.321325000	2.198746000	-1.275364000
8	-0.304903000	2.201893000	1.274607000
8	-1.934954000	0.548587000	-0.625794000
8	-0.553309000	-0.859799000	1.376490000
8	0.545802000	-0.865447000	-1.375239000
8	1.938557000	0.534906000	0.624798000
6	-0.177140000	3.309075000	0.740162000
6	-0.356334000	4.577778000	1.410406000
6	-0.162751000	5.718875000	0.703459000
6	0.211699000	5.716987000	-0.705036000
6	0.394664000	4.573976000	-1.411713000
6	0.203770000	3.307165000	-0.741146000
6	-2.840258000	-0.267895000	-0.312385000
6	-2.783899000	-1.292396000	0.639041000
6	-1.639590000	-1.491223000	1.423042000
6	1.627560000	-1.504544000	-1.422029000
6	2.773872000	-1.312917000	-0.639161000
6	2.837952000	-0.288102000	0.311435000
1	-0.632225000	4.573642000	2.459553000
1	-3.651339000	-1.914662000	0.799791000
1	3.636915000	-1.941220000	-0.800081000
1	-0.286193000	6.682065000	1.190051000
1	0.344117000	6.678881000	-1.191828000
1	0.670533000	4.567020000	-2.460851000
6	-4.163407000	-0.040526000	-1.078767000
9	-4.647475000	1.193819000	-0.814379000
9	-3.964252000	-0.127226000	-2.406641000
9	-5.122059000	-0.931381000	-0.748137000
6	-1.667293000	-2.590234000	2.510767000
9	-2.831814000	-3.274236000	2.533301000
9	-0.676163000	-3.478863000	2.305354000
9	-1.490815000	-2.046510000	3.731421000

6	4.163161000	-0.069359000	1.076769000
9	3.964478000	-0.154612000	2.404821000
9	5.115705000	-0.966498000	0.745487000
9	4.655121000	1.161748000	0.811881000
6	1.646277000	-2.605403000	-2.508077000
9	0.652737000	-3.490016000	-2.296412000
9	1.466165000	-2.063299000	-3.728819000
9	2.808091000	-3.293835000	-2.534711000

## 12

E=-3644.99359 a.u.

27	-0.000224000	0.458854000	-0.000494000
8	-1.758640000	0.523244000	-0.724733000
8	-0.401745000	-0.898731000	1.274639000
8	0.403315000	-0.897829000	-1.275886000
8	1.757876000	0.525510000	0.724175000
6	-2.712661000	-0.196885000	-0.322103000
6	-2.705029000	-1.158683000	0.690123000
6	-1.539130000	-1.428563000	1.408546000
6	1.541147000	-1.426970000	-1.408780000
6	2.706372000	-1.156094000	-0.689635000
6	2.712711000	-0.193962000	0.322275000
1	-3.610887000	-1.698985000	0.918866000
1	3.612763000	-1.695802000	-0.917676000
6	-4.026391000	0.083374000	-1.085433000
9	-5.036557000	-0.704661000	-0.665156000
9	-4.401232000	1.364255000	-0.905528000
9	-3.859769000	-0.124190000	-2.401711000
6	-1.567232000	-2.496857000	2.523561000
9	-2.770200000	-3.096990000	2.623750000
9	-0.649894000	-3.449688000	2.278201000
9	-1.284292000	-1.937357000	3.713078000
6	1.570652000	-2.495753000	-2.523286000
9	0.654846000	-3.449908000	-2.276957000
9	1.286429000	-1.937506000	-3.713009000
9	2.774510000	-3.094101000	-2.623475000
6	4.025884000	0.087837000	1.085984000
9	3.858694000	-0.117894000	2.402413000
9	5.036604000	-0.700339000	0.667319000
9	4.400271000	1.368682000	0.904414000
8	0.491105000	1.840462000	-1.202715000
8	-0.493528000	1.839654000	1.201973000
6	-0.276468000	3.001619000	0.674432000
6	-0.542179000	4.230017000	1.328158000
6	-0.271654000	5.402697000	0.661795000
6	0.265120000	5.403142000	-0.661848000

6	0.537009000	4.230900000	-1.328429000
6	0.272715000	3.002082000	-0.674929000
1	-0.947951000	4.213707000	2.333926000
1	-0.468392000	6.353697000	1.147082000
1	0.460750000	6.354468000	-1.146941000
1	0.942803000	4.215237000	-2.334197000

### 13

E=-3644.97636 a.u.

27	-0.003453000	0.548661000	-0.001033000
8	-0.361202000	2.067281000	1.254797000
8	0.324804000	2.075083000	-1.255435000
8	1.880454000	0.571540000	0.619944000
8	0.462729000	-0.845996000	-1.337808000
8	-0.444825000	-0.854213000	1.335764000
8	-1.887484000	0.537702000	-0.621675000
6	0.163755000	3.209748000	-0.718454000
6	0.322690000	4.457522000	-1.397340000
6	0.120557000	5.614318000	-0.697936000
6	-0.238468000	5.610311000	0.697647000
6	-0.413801000	4.448981000	1.396939000
6	-0.226252000	3.205257000	0.717867000
6	2.789294000	-0.229644000	0.275640000
6	2.724886000	-1.246059000	-0.681445000
6	1.559292000	-1.458973000	-1.425227000
6	-1.530935000	-1.485063000	1.424924000
6	-2.700144000	-1.293434000	0.680987000
6	-2.782290000	-0.278884000	-0.276884000
1	0.591951000	4.449275000	-2.447953000
1	3.595509000	-1.855999000	-0.869140000
1	-3.560192000	-1.917893000	0.869410000
1	0.231714000	6.571711000	-1.198019000
1	-0.371673000	6.564932000	1.197415000
1	-0.682956000	4.434145000	2.447571000
6	4.121394000	0.011672000	1.021475000
9	4.584979000	1.249812000	0.753143000
9	3.942203000	-0.085839000	2.349823000
9	5.078689000	-0.870365000	0.667096000
6	1.562179000	-2.554011000	-2.517224000
9	2.724726000	-3.237958000	-2.557870000
9	0.572810000	-3.438955000	-2.295864000
9	1.367700000	-2.003940000	-3.730575000
6	-4.118745000	-0.060109000	-1.021468000
9	-3.939633000	-0.154259000	-2.350217000
9	-5.061033000	-0.957815000	-0.666350000
9	-4.602425000	1.170272000	-0.752284000

6	-1.514945000	-2.577847000	2.518983000
9	-0.516705000	-3.451772000	2.293154000
9	-1.319513000	-2.023510000	3.730220000
9	-2.669322000	-3.274994000	2.567837000

#### 14

E=-2277.13620 a.u.

27	0.623940000	-0.018248000	0.051340000
7	-1.004496000	-0.637901000	1.127387000
8	-1.049221000	0.557698000	-1.180489000
8	0.584369000	1.727355000	1.123876000
8	2.018319000	0.846250000	-1.150247000
8	1.967407000	-0.896339000	1.300566000
8	0.746986000	-1.687293000	-1.142123000
6	-2.159327000	0.296208000	-0.681849000
6	-3.421928000	0.622084000	-1.301830000
6	-4.584887000	0.282165000	-0.681713000
6	-4.607650000	-0.397244000	0.594571000
6	-3.459847000	-0.732387000	1.240907000
6	-2.188117000	-0.403668000	0.644758000
6	1.379594000	2.707051000	1.010313000
6	2.382687000	2.873324000	0.049494000
6	2.618800000	1.942753000	-0.972947000
6	2.754627000	-1.841830000	0.991330000
6	2.705635000	-2.634576000	-0.159144000
6	1.693242000	-2.521558000	-1.126678000
1	-3.399884000	1.130530000	-2.259879000
1	-0.984761000	-1.102097000	2.036365000
1	2.979078000	3.778863000	0.074631000
1	3.448882000	-3.415286000	-0.279998000
1	-5.535235000	0.522875000	-1.149992000
1	-5.570389000	-0.638441000	1.034839000
1	-3.476089000	-1.241804000	2.200698000
1	3.545272000	-2.068165000	1.724936000
1	1.707940000	-3.253522000	-1.951319000
1	3.401059000	2.191143000	-1.708939000
1	1.249379000	3.518615000	1.744838000

#### 15

E=-2277.15655 a.u.

27	0.622544000	-0.013185000	0.035438000
7	-0.787395000	-0.843249000	1.006141000
8	-0.797134000	0.764267000	-0.986140000
8	0.510882000	1.456278000	1.257459000
8	1.947776000	0.788579000	-1.095001000
8	2.001110000	-0.722425000	1.155690000

8	0.625366000	-1.470522000	-1.211409000
6	-1.964184000	0.388116000	-0.568246000
6	-3.180919000	0.814906000	-1.148777000
6	-4.377950000	0.373524000	-0.619254000
6	-4.416845000	-0.500647000	0.501481000
6	-3.255451000	-0.941330000	1.093960000
6	-2.002308000	-0.514806000	0.572579000
6	1.159911000	2.534920000	1.106248000
6	2.062559000	2.857114000	0.091348000
6	2.392989000	1.961731000	-0.929817000
6	2.640628000	-1.786084000	0.885311000
6	2.444754000	-2.643836000	-0.196590000
6	1.451142000	-2.425381000	-1.159274000
1	-3.143453000	1.484747000	-2.001482000
1	-0.701555000	-1.422669000	1.836153000
1	2.532040000	3.833455000	0.102530000
1	3.077389000	-3.518414000	-0.290397000
1	-5.313062000	0.701149000	-1.064041000
1	-5.378001000	-0.822686000	0.890307000
1	-3.277852000	-1.610395000	1.950090000
1	3.427896000	-2.040777000	1.607555000
1	1.353176000	-3.160471000	-1.969868000
1	3.123698000	2.287715000	-1.682556000
1	0.972817000	3.288305000	1.883282000

## 16

E=-2434.35434 a.u.

27	0.167426000	-0.029949000	0.071867000
7	-1.448409000	-0.510321000	1.220807000
8	-1.495557000	0.263376000	-1.257392000
8	0.070405000	1.860666000	0.815781000
8	1.532875000	0.687037000	-1.237370000
8	1.503736000	-0.644599000	1.461741000
8	0.385839000	-1.862743000	-0.792565000
6	-2.608298000	0.057240000	-0.729626000
6	-3.868680000	0.234059000	-1.406325000
6	-5.033193000	-0.033263000	-0.749685000
6	-5.053702000	-0.487409000	0.619506000
6	-3.902266000	-0.670441000	1.322673000
6	-2.634961000	-0.404644000	0.692210000
6	0.815160000	2.861528000	0.563946000
6	1.817972000	2.895453000	-0.418887000
6	2.109371000	1.816179000	-1.275460000
6	2.368862000	-1.572623000	1.339592000
6	2.371411000	-2.541326000	0.323469000
6	1.372226000	-2.649089000	-0.666358000

1	-3.847908000	0.573916000	-2.436471000
1	-1.426813000	-0.812242000	2.195237000
1	2.378103000	3.814022000	-0.546143000
1	3.159226000	-3.285152000	0.332582000
1	-5.982417000	0.095082000	-1.262533000
1	-6.013868000	-0.682786000	1.087382000
1	-3.916327000	-1.010674000	2.354837000
6	3.173866000	1.975904000	-2.340660000
1	3.635810000	2.965786000	-2.327827000
1	3.946390000	1.213162000	-2.195140000
1	2.726076000	1.797958000	-3.324256000
6	0.554170000	4.093369000	1.405436000
1	1.203188000	4.930653000	1.138502000
1	-0.492167000	4.395580000	1.288545000
1	0.702771000	3.844165000	2.461808000
6	3.443790000	-1.605290000	2.405460000
1	4.146320000	-2.430294000	2.267718000
1	3.992071000	-0.657003000	2.391607000
1	2.974169000	-1.690551000	3.391399000
6	1.434739000	-3.789401000	-1.660897000
1	1.534274000	-3.374351000	-2.669909000
1	2.266024000	-4.471537000	-1.468662000
1	0.492262000	-4.346246000	-1.632655000

## 17

E=-2434.37650 a.u.

27	-0.220602000	-0.018742000	-0.053308000
7	1.174853000	-0.721417000	-1.143121000
8	1.219247000	0.511639000	1.101880000
8	-0.039996000	1.633611000	-0.989191000
8	-1.522054000	0.633800000	1.181705000
8	-1.599364000	-0.475820000	-1.285352000
8	-0.302247000	-1.667382000	0.908123000
6	2.375166000	0.172337000	0.629701000
6	3.601371000	0.445545000	1.280620000
6	4.788434000	0.057549000	0.689629000
6	4.808894000	-0.610674000	-0.564767000
6	3.638513000	-0.897717000	-1.230495000
6	2.394737000	-0.520322000	-0.651368000
6	-0.640929000	2.712877000	-0.677072000
6	-1.545237000	2.874086000	0.381891000
6	-1.931764000	1.836478000	1.244161000
6	-2.313158000	-1.532336000	-1.218185000
6	-2.158993000	-2.563833000	-0.284213000
6	-1.168200000	-2.575516000	0.714253000
1	3.578441000	0.958433000	2.236629000

1	1.080589000	-1.150743000	-2.058966000
1	-1.974489000	3.855389000	0.539786000
1	-2.834916000	-3.407766000	-0.339817000
1	5.729411000	0.267879000	1.189805000
1	5.762153000	-0.897070000	-0.998602000
1	3.646896000	-1.409060000	-2.189641000
6	-0.308140000	3.888698000	-1.566799000
1	0.769704000	4.077735000	-1.527546000
1	-0.557185000	3.638582000	-2.603319000
1	-0.845132000	4.792808000	-1.273364000
6	-2.913485000	2.111481000	2.359797000
1	-3.759882000	1.421809000	2.278895000
1	-2.425795000	1.915627000	3.320756000
1	-3.279093000	3.140124000	2.344569000
6	-3.399890000	-1.618076000	-2.265187000
1	-2.959017000	-1.502252000	-3.260502000
1	-3.946857000	-2.561669000	-2.217046000
1	-4.100424000	-0.787935000	-2.123686000
6	-1.075488000	-3.746980000	1.664853000
1	-1.812229000	-4.520481000	1.439613000
1	-0.069123000	-4.175133000	1.616775000
1	-1.226428000	-3.388679000	2.688595000

## 18

E=-3625.11931 a.u.

27	0.218978000	0.557352000	0.083878000
7	0.706033000	2.169914000	1.294686000
8	1.115635000	1.970026000	-1.273646000
8	2.035398000	-0.266296000	0.579910000
8	0.045759000	-0.955314000	-1.284189000
8	-0.817564000	-0.466032000	1.519300000
8	-1.598622000	1.286453000	-0.548621000
6	1.511931000	3.014797000	-0.741301000
6	2.170768000	4.087752000	-1.454656000
6	2.567338000	5.193346000	-0.775573000
6	2.359564000	5.348094000	0.654758000
6	1.751569000	4.391010000	1.395518000
6	1.295598000	3.179898000	0.747028000
6	2.494063000	-1.380489000	0.213977000
6	1.947259000	-2.279803000	-0.706251000
6	0.764491000	-1.977859000	-1.397619000
6	-2.050859000	-0.723452000	1.505765000
6	-3.031830000	-0.196236000	0.659680000
6	-2.722183000	0.792837000	-0.286042000
1	2.323998000	3.968554000	-2.521746000
1	0.559558000	2.242116000	2.303418000

1	2.462383000	-3.205314000	-0.915375000
1	-4.056098000	-0.518261000	0.772434000
1	3.060824000	6.002530000	-1.306409000
1	2.707561000	6.261741000	1.126719000
1	1.597478000	4.506947000	2.464626000
6	3.852373000	-1.724242000	0.866601000
9	4.793961000	-0.837373000	0.469421000
9	3.768764000	-1.655100000	2.209049000
9	4.298156000	-2.957417000	0.547357000
6	0.255056000	-2.977689000	-2.462731000
9	0.978520000	-4.118628000	-2.500916000
9	-1.025276000	-3.315552000	-2.218868000
9	0.309897000	-2.420963000	-3.690277000
6	-3.877970000	1.421811000	-1.099886000
9	-3.644017000	1.315663000	-2.419549000
9	-5.074151000	0.848042000	-0.847224000
9	-3.990009000	2.737358000	-0.805092000
6	-2.480820000	-1.725186000	2.601828000
9	-1.810147000	-2.885631000	2.470582000
9	-2.204593000	-1.224938000	3.826084000
9	-3.800358000	-2.009290000	2.568346000

## 19

E=-3625.12493 a.u.

27	-0.068684000	0.484932000	-0.066724000
8	-1.827640000	0.202924000	-0.744461000
8	-0.192823000	-0.917476000	1.247135000
8	0.557288000	-0.798185000	-1.348907000
8	1.670601000	0.837939000	0.643196000
6	-2.633594000	-0.653312000	-0.284299000
6	-2.439888000	-1.561163000	0.756357000
6	-1.220605000	-1.619377000	1.437485000
6	1.753231000	-1.200878000	-1.419007000
6	2.847763000	-0.787035000	-0.660697000
6	2.710885000	0.214653000	0.306832000
1	-3.237508000	-2.233900000	1.031829000
1	3.815758000	-1.232247000	-0.833311000
6	-3.992797000	-0.628652000	-1.017525000
9	-4.842364000	-1.566863000	-0.552907000
9	-4.582221000	0.572159000	-0.863707000
9	-3.821131000	-0.844066000	-2.333951000
6	-1.040619000	-2.653986000	2.570505000
9	-2.131183000	-3.431361000	2.731107000
9	0.003422000	-3.460655000	2.301767000
9	-0.800826000	-2.033616000	3.738777000
6	1.961344000	-2.257907000	-2.524850000



9	1.038346000	-3.228383000	-2.434894000
9	1.844550000	-1.678956000	-3.738739000
9	3.178157000	-2.833674000	-2.460542000
6	3.959998000	0.680429000	1.089297000
9	3.780373000	0.508972000	2.408197000
9	5.068929000	0.001751000	0.729056000
9	4.186902000	1.988167000	0.860776000
7	0.100388000	1.954758000	-1.245856000
8	-0.764677000	1.758833000	1.147609000
6	-0.791108000	2.958227000	0.642971000
6	-1.252622000	4.091558000	1.345421000
6	-1.265863000	5.316364000	0.707681000
6	-0.827924000	5.460577000	-0.638800000
6	-0.366377000	4.380145000	-1.353020000
6	-0.326639000	3.105104000	-0.725011000
1	-1.590124000	3.972297000	2.369255000
1	0.372765000	1.918458000	-2.224100000
1	-1.621228000	6.192641000	1.241297000
1	-0.859379000	6.440989000	-1.103403000
1	-0.028195000	4.483249000	-2.380131000

## 20

E=-3625.10976 a.u.

27	0.214431000	0.588398000	0.086923000
7	0.451880000	2.056957000	1.201264000
8	1.174317000	1.709924000	-1.180621000
8	2.051721000	-0.278722000	0.710011000
8	-0.004153000	-0.836134000	-1.175303000
8	-0.684071000	-0.433800000	1.461470000
8	-1.690187000	1.254865000	-0.626475000
6	1.513534000	2.829776000	-0.694481000
6	2.235663000	3.840907000	-1.399745000
6	2.545328000	4.998732000	-0.742783000
6	2.168708000	5.232470000	0.629343000
6	1.475487000	4.303297000	1.348019000
6	1.122661000	3.074391000	0.704871000
6	2.539691000	-1.311697000	0.207025000
6	2.003889000	-2.104638000	-0.824882000
6	0.784210000	-1.796363000	-1.419240000
6	-1.921865000	-0.712825000	1.511047000
6	-2.965589000	-0.246510000	0.721385000
6	-2.763423000	0.723316000	-0.284042000
1	2.517771000	3.660124000	-2.431035000
1	0.147132000	2.112477000	2.173536000
1	2.543219000	-2.978583000	-1.157077000
1	-3.963468000	-0.614631000	0.906031000

1	3.095823000	5.777606000	-1.262088000
1	2.449252000	6.174444000	1.089592000
1	1.189090000	4.474651000	2.381397000
6	3.904025000	-1.722406000	0.815639000
9	4.393881000	-2.865621000	0.289915000
9	4.818614000	-0.751571000	0.598817000
9	3.796759000	-1.896528000	2.145707000
6	0.249517000	-2.712963000	-2.541396000
9	1.064348000	-3.760001000	-2.789174000
9	-0.959518000	-3.206096000	-2.209661000
9	0.114798000	-2.020559000	-3.688935000
6	-2.244588000	-1.689458000	2.663035000
9	-1.478712000	-2.791617000	2.584575000
9	-1.995883000	-1.096661000	3.853244000
9	-3.534184000	-2.084239000	2.668945000
6	-4.001797000	1.244753000	-1.058047000
9	-3.848794000	1.055199000	-2.379880000
9	-5.150610000	0.639102000	-0.685559000
9	-4.154685000	2.570024000	-0.843544000

## 21

E=-3625.11015 a.u.

27	0.227127000	0.480666000	0.047660000
8	1.938207000	-0.230517000	0.675906000
8	0.037332000	-0.962850000	-1.238036000
8	-0.841608000	-0.595284000	1.523076000
8	-1.485495000	1.189192000	-0.630856000
6	2.474184000	-1.302881000	0.280336000
6	2.020242000	-2.182269000	-0.705347000
6	0.829998000	-1.927734000	-1.396382000
6	-2.080732000	-0.768044000	1.489243000
6	-3.014081000	-0.180207000	0.616205000
6	-2.636524000	0.753496000	-0.350163000
1	2.597135000	-3.063576000	-0.941742000
1	-4.057261000	-0.442427000	0.709155000
6	3.801050000	-1.611574000	1.005665000
9	4.390060000	-2.740358000	0.560051000
9	4.678994000	-0.599787000	0.831600000
9	3.594868000	-1.751523000	2.329090000
6	0.392310000	-2.896621000	-2.516722000
9	1.205223000	-3.971475000	-2.615672000
9	-0.855837000	-3.346876000	-2.292100000
9	0.400604000	-2.269027000	-3.708168000
6	-2.605929000	-1.734148000	2.580087000
9	-2.014297000	-2.938359000	2.471632000
9	-2.323126000	-1.244039000	3.807955000

9	-3.941932000	-1.928559000	2.521414000
6	-3.741737000	1.410618000	-1.208547000
9	-3.494584000	1.237530000	-2.518969000
9	-4.971381000	0.913818000	-0.954300000
9	-3.787900000	2.742269000	-0.970817000
7	0.484700000	2.046648000	1.164668000
8	1.339143000	1.882806000	-1.313817000
6	1.588102000	2.935559000	-0.719823000
6	2.313218000	4.048713000	-1.303190000
6	2.540765000	5.163207000	-0.565467000
6	2.080539000	5.294926000	0.806665000
6	1.397533000	4.304162000	1.428913000
6	1.116491000	3.081151000	0.710615000
1	2.655281000	3.945018000	-2.327773000
1	0.164050000	2.106795000	2.133926000
1	3.085118000	5.996505000	-0.999881000
1	2.296725000	6.219130000	1.334040000
1	1.054143000	4.404612000	2.454616000

## 22

E=-2257.26601 a.u.

27	-0.624133000	-0.000022000	-0.000041000
7	0.808621000	0.777238000	0.987481000
7	0.808658000	-0.777213000	-0.987551000
8	-0.595512000	-1.469313000	1.239939000
8	-1.981381000	-0.762156000	-1.142051000
8	-1.981444000	0.762044000	1.141954000
8	-0.595513000	1.469445000	-1.239865000
6	2.031513000	-0.428766000	-0.588766000
6	3.270536000	-0.809067000	-1.169002000
6	4.452006000	-0.400885000	-0.586410000
6	4.451984000	0.400919000	0.586477000
6	3.270491000	0.809087000	1.169032000
6	2.031491000	0.428791000	0.588745000
6	-1.347742000	-2.481154000	1.137436000
6	-2.296157000	-2.749812000	0.144576000
6	-2.544505000	-1.875235000	-0.915502000
6	-2.544618000	1.875114000	0.915479000
6	-2.296264000	2.749797000	-0.144505000
6	-1.347773000	2.481257000	-1.137325000
1	3.271487000	-1.430793000	-2.060251000
1	0.707910000	1.298714000	1.852637000
1	-2.861897000	-3.672205000	0.202997000
1	-2.862035000	3.672173000	-0.202872000
1	5.399514000	-0.699051000	-1.025073000
1	5.399475000	0.699094000	1.025171000

1	3.271407000	1.430809000	2.060285000
1	-3.308062000	2.165272000	1.650835000
1	-1.221084000	3.225715000	-1.935497000
1	-3.307901000	-2.165503000	-1.650864000
1	-1.221103000	-3.225525000	1.935696000
1	0.707979000	-1.298710000	-1.852697000

## 23

E=-2257.28289 a.u.

27	-0.601517000	-0.000053000	-0.000346000
7	1.037781000	-0.498041000	-1.188445000
7	1.037585000	0.497586000	1.188447000
8	-0.694140000	1.764425000	-1.093060000
8	-1.984760000	0.828943000	1.271704000
8	-1.983162000	-0.829919000	-1.273147000
8	-0.695501000	-1.763365000	1.094433000
6	2.216365000	0.273560000	0.694460000
6	3.487850000	0.501994000	1.343456000
6	4.645083000	0.250982000	0.678378000
6	4.645196000	-0.251332000	-0.677806000
6	3.488073000	-0.502358000	-1.343075000
6	2.216487000	-0.273922000	-0.694296000
6	-1.599308000	2.641063000	-1.004825000
6	-2.608026000	2.726644000	-0.033918000
6	-2.714438000	1.836381000	1.042245000
6	-2.713445000	-1.836879000	-1.043285000
6	-2.608535000	-2.725922000	0.033990000
6	-1.600901000	-2.639692000	1.006032000
1	3.491160000	0.882954000	2.360934000
1	1.027409000	-0.844705000	-2.147910000
1	-3.308837000	3.552818000	-0.091157000
1	-3.309721000	-3.551772000	0.091346000
1	5.599860000	0.429548000	1.164027000
1	5.600055000	-0.429891000	-1.163298000
1	3.491556000	-0.883319000	-2.360552000
1	-3.504871000	-2.041010000	-1.784255000
1	-1.581217000	-3.435115000	1.770721000
1	-3.506630000	2.039925000	1.782569000
1	-1.578324000	3.437286000	-1.768640000
1	1.027078000	0.844118000	2.147960000

## 24

E=-2257.26081 a.u.

27	0.555428000	0.000124000	0.000998000
7	-0.968554000	0.582657000	-1.120493000
7	-0.969065000	-0.580959000	1.121430000

8	0.683593000	-1.776975000	-1.142216000
8	1.921928000	-0.753933000	1.242362000
8	1.926036000	0.748803000	-1.238032000
8	0.685910000	1.777179000	1.142955000
6	-2.167617000	-0.321719000	0.665088000
6	-3.425725000	-0.602539000	1.299849000
6	-4.587657000	-0.302217000	0.653082000
6	-4.587385000	0.300771000	-0.655383000
6	-3.424948000	0.602984000	-1.300544000
6	-2.167270000	0.323764000	-0.664666000
6	1.594309000	-2.634440000	-1.015180000
6	2.583237000	-2.681902000	-0.014744000
6	2.660836000	-1.765960000	1.035555000
6	2.662146000	1.763799000	-1.035208000
6	2.581539000	2.684315000	0.010505000
6	1.594062000	2.636776000	1.012086000
1	-3.428603000	-1.061959000	2.284048000
1	-0.916350000	0.992291000	-2.052382000
1	3.300526000	-3.495277000	-0.038693000
1	3.295918000	3.500336000	0.030749000
1	-5.541200000	-0.520431000	1.124031000
1	-5.540743000	0.517017000	-1.127657000
1	-3.427440000	1.062144000	-2.285165000
1	3.445524000	1.932118000	-1.791428000
1	1.609097000	3.451547000	1.757772000
1	3.443621000	-1.936314000	1.791635000
1	1.610406000	-3.447324000	-1.762533000
1	-0.916882000	-0.991766000	2.052917000

## 25

E=-2414.48273 a.u.

27	0.118614000	-0.000179000	0.000087000
7	-1.515492000	-0.255727000	1.260541000
7	-1.515508000	0.253659000	-1.260891000
8	0.231578000	1.933736000	0.706858000
8	1.485239000	0.579680000	-1.403349000
8	1.484419000	-0.579252000	1.404424000
8	0.234488000	-1.933662000	-0.707856000
6	-2.697586000	0.134652000	-0.732772000
6	-3.967385000	0.239585000	-1.412049000
6	-5.127008000	0.117917000	-0.712312000
6	-5.127007000	-0.120774000	0.711848000
6	-3.967376000	-0.242177000	1.411622000
6	-2.697586000	-0.136930000	0.732389000
6	1.157671000	2.776367000	0.500909000
6	2.174575000	2.649998000	-0.465777000

6	2.267301000	1.580823000	-1.374771000
6	2.267990000	-1.579258000	1.375754000
6	2.177520000	-2.647911000	0.465973000
6	1.161522000	-2.775131000	-0.501617000
1	-3.970672000	0.423226000	-2.482986000
1	-1.503641000	-0.416132000	2.267693000
1	2.900395000	3.450713000	-0.546032000
1	2.904376000	-3.447679000	0.546304000
1	-6.081130000	0.202392000	-1.224138000
1	-6.081128000	-0.205454000	1.223644000
1	-3.970656000	-0.425802000	2.482562000
1	-1.503651000	0.413884000	-2.268070000
6	3.356528000	-1.590764000	2.430262000
1	2.897222000	-1.552757000	3.424153000
1	3.998234000	-2.472492000	2.364195000
1	3.968501000	-0.688453000	2.324191000
6	1.128422000	-4.014111000	-1.374983000
1	1.918780000	-4.726191000	-1.126138000
1	0.153923000	-4.503421000	-1.272028000
1	1.230802000	-3.714502000	-2.423857000
6	3.356706000	1.593212000	-2.428382000
1	3.970175000	0.692084000	-2.320905000
1	2.898310000	1.553423000	-3.422621000
1	3.996806000	2.476127000	-2.362613000
6	1.122193000	4.015707000	1.373660000
1	0.146914000	4.503338000	1.270149000
1	1.224718000	3.716773000	2.422716000
1	1.911456000	4.728981000	1.124761000

## 26

E=-2414.50216 a.u.

27	0.212114000	-0.000107000	0.000476000
7	-1.225419000	0.580464000	-1.113959000
7	-1.224982000	-0.583506000	1.113942000
8	0.189245000	-1.670007000	-0.936930000
8	1.561559000	-0.551074000	1.255177000
8	1.561277000	0.552942000	-1.253657000
8	0.185323000	1.669446000	0.937749000
6	-2.447370000	-0.317562000	0.656927000
6	-3.687421000	-0.588472000	1.294482000
6	-4.869913000	-0.292953000	0.648215000
6	-4.870078000	0.285168000	-0.649137000
6	-3.687839000	0.582219000	-1.295129000
6	-2.447624000	0.312966000	-0.657220000
6	0.941244000	-2.661603000	-0.678614000
6	1.897035000	-2.726186000	0.348971000

6	2.152035000	-1.679994000	1.247002000
6	2.147548000	1.684082000	-1.246839000
6	1.888532000	2.730515000	-0.350137000
6	0.933487000	2.663612000	0.677857000
1	-3.688610000	-1.039096000	2.283531000
1	-1.128645000	0.943162000	-2.057085000
1	2.470416000	-3.638765000	0.452967000
1	2.458782000	3.644929000	-0.455296000
1	-5.817118000	-0.508472000	1.133633000
1	-5.817448000	0.499493000	-1.134841000
1	-3.689436000	1.032762000	-2.284209000
1	-1.127964000	-0.945886000	2.057215000
6	0.742714000	-3.850530000	-1.591887000
1	-0.301840000	-4.174729000	-1.541298000
1	0.938612000	-3.546874000	-2.625545000
1	1.394989000	-4.686404000	-1.330994000
6	3.204744000	-1.850466000	2.319161000
1	3.980554000	-1.088676000	2.187032000
1	2.753480000	-1.683998000	3.302886000
1	3.664366000	-2.840625000	2.294770000
6	3.200623000	1.856696000	-2.318328000
1	2.751134000	1.685361000	-3.301995000
1	3.655562000	2.849019000	-2.296053000
1	3.979866000	1.098928000	-2.183287000
6	0.731422000	3.852491000	1.590385000
1	1.381318000	4.690101000	1.329274000
1	-0.314123000	4.173597000	1.539264000
1	0.927774000	3.550030000	2.624348000

## 27

E=-3605.25250 a.u.

27	0.277005000	0.586075000	-0.015893000
7	0.795456000	2.167291000	1.251565000
7	1.086494000	2.012004000	-1.316447000
8	2.058601000	-0.309710000	0.568641000
8	0.142134000	-0.929739000	-1.407520000
8	-0.742309000	-0.486976000	1.421739000
8	-1.589632000	1.286192000	-0.604868000
6	1.477117000	3.126325000	-0.790133000
6	2.016661000	4.273489000	-1.491224000
6	2.432398000	5.356196000	-0.791206000
6	2.346478000	5.409389000	0.656784000
6	1.835280000	4.383861000	1.379323000
6	1.349172000	3.198709000	0.703085000
6	2.445026000	-1.469883000	0.283384000
6	1.887045000	-2.368465000	-0.635989000

6	0.789513000	-2.007159000	-1.427312000
6	-1.975068000	-0.730868000	1.459596000
6	-2.987422000	-0.184892000	0.660698000
6	-2.705254000	0.800328000	-0.295402000
1	2.087430000	4.235252000	-2.574343000
1	0.732675000	2.197040000	2.270060000
1	2.340356000	-3.339277000	-0.769316000
1	-4.009836000	-0.495827000	0.814323000
1	2.846310000	6.213488000	-1.313400000
1	2.702461000	6.303088000	1.160320000
1	1.767596000	4.429400000	2.462356000
6	3.733153000	-1.890179000	1.030140000
9	4.775015000	-1.131924000	0.614395000
9	3.601090000	-1.707769000	2.357005000
9	4.068183000	-3.182219000	0.825836000
6	0.297348000	-3.002552000	-2.503863000
9	0.924567000	-4.197643000	-2.446328000
9	-1.023095000	-3.228803000	-2.375071000
9	0.509899000	-2.493561000	-3.738532000
6	-3.886276000	1.434341000	-1.067922000
9	-3.707226000	1.312773000	-2.397206000
9	-5.079490000	0.879903000	-0.763966000
9	-3.970603000	2.754726000	-0.785267000
6	-2.370411000	-1.736592000	2.565977000
9	-1.691463000	-2.890884000	2.422639000
9	-2.071625000	-1.231443000	3.783432000
9	-3.687880000	-2.034863000	2.564528000
1	1.142409000	1.969204000	-2.334722000

## 28

E=-3605.25353 a.u.

27	0.233109000	0.474785000	-0.012444000
8	1.905309000	-0.149212000	0.679536000
8	0.024000000	-1.024984000	-1.221787000
8	-0.600197000	-0.554572000	1.402126000
8	-1.433014000	1.113470000	-0.705708000
6	2.450931000	-1.234903000	0.347539000
6	2.015049000	-2.181991000	-0.583814000
6	0.830169000	-1.992040000	-1.297650000
6	-1.846892000	-0.663716000	1.559304000
6	-2.863562000	-0.070303000	0.808367000
6	-2.562988000	0.774399000	-0.264234000
1	2.604869000	-3.069702000	-0.754242000
1	-3.895401000	-0.261308000	1.060956000
6	3.781156000	-1.478469000	1.095584000
9	4.327650000	-2.673349000	0.790424000



9	4.675931000	-0.523909000	0.773834000
9	3.589240000	-1.440566000	2.424923000
6	0.397043000	-3.052763000	-2.332505000
9	1.246097000	-4.098469000	-2.385312000
9	-0.825230000	-3.528616000	-2.033748000
9	0.343188000	-2.505244000	-3.563218000
6	-2.222976000	-1.567194000	2.753414000
9	-1.681485000	-2.789605000	2.607070000
9	-1.754247000	-1.036936000	3.901096000
9	-3.555914000	-1.718601000	2.885701000
6	-3.722443000	1.429218000	-1.048617000
9	-3.630171000	1.138872000	-2.357344000
9	-4.930685000	1.013034000	-0.616799000
9	-3.676984000	2.768811000	-0.912255000
7	0.415530000	2.027006000	1.060734000
7	1.129961000	1.540200000	-1.298661000
6	1.407929000	2.786151000	-0.906132000
6	1.996423000	3.820221000	-1.679066000
6	2.296640000	5.023776000	-1.079894000
6	2.019928000	5.250012000	0.296899000
6	1.422424000	4.281079000	1.072698000
6	1.070381000	3.038631000	0.484881000
1	2.222671000	3.642195000	-2.726421000
1	0.256966000	2.051551000	2.063749000
1	2.759552000	5.813724000	-1.663090000
1	2.279114000	6.207406000	0.738087000
1	1.196576000	4.460155000	2.119959000
1	1.202544000	1.307836000	-2.284828000

## 29

E=-3605.24947 a.u.

27	0.303228000	0.649308000	-0.016544000
7	0.557962000	2.113784000	1.154486000
7	1.202178000	1.807351000	-1.213478000
8	2.108083000	-0.314781000	0.687482000
8	0.124970000	-0.756088000	-1.338001000
8	-0.600177000	-0.410932000	1.330319000
8	-1.631191000	1.314515000	-0.717531000
6	1.545054000	2.984055000	-0.749895000
6	2.200300000	4.054509000	-1.444719000
6	2.498110000	5.194797000	-0.761232000
6	2.169700000	5.352894000	0.635792000
6	1.537394000	4.373242000	1.340495000
6	1.187985000	3.155002000	0.668468000
6	2.461552000	-1.451417000	0.323070000
6	1.876283000	-2.263663000	-0.671658000

6	0.784057000	-1.836361000	-1.418337000
6	-1.842593000	-0.639979000	1.436431000
6	-2.903437000	-0.126436000	0.698270000
6	-2.706723000	0.825183000	-0.324873000
1	2.452233000	3.936208000	-2.494200000
1	0.300512000	2.134445000	2.140788000
1	2.299395000	-3.235814000	-0.875582000
1	-3.905819000	-0.454150000	0.929045000
1	2.998532000	6.013212000	-1.269355000
1	2.436735000	6.283699000	1.126418000
1	1.287562000	4.496096000	2.389963000
6	3.734542000	-1.980319000	1.033728000
9	4.820082000	-1.302727000	0.589088000
9	3.655600000	-1.800061000	2.362398000
9	3.959518000	-3.293157000	0.808987000
6	0.257880000	-2.749859000	-2.546542000
9	0.907606000	-3.930694000	-2.613986000
9	-1.051064000	-3.013137000	-2.376076000
9	0.403249000	-2.139152000	-3.744103000
6	-3.955766000	1.378562000	-1.058618000
9	-3.859019000	1.167886000	-2.384389000
9	-5.111521000	0.818993000	-0.638536000
9	-4.056446000	2.711696000	-0.859191000
6	-2.151366000	-1.621073000	2.588213000
9	-1.477117000	-2.774660000	2.426139000
9	-1.771733000	-1.083952000	3.769699000
9	-3.462873000	-1.923409000	2.685040000
1	1.385826000	1.614229000	-2.197577000

### 30

E=-3605.24546 a.u.

27	0.058876000	0.691083000	-0.002209000
7	-0.016404000	2.221487000	1.233925000
7	0.437285000	2.168063000	-1.248224000
8	2.089779000	0.358459000	0.532553000
8	0.280692000	-0.731332000	-1.376772000
8	-0.432838000	-0.642978000	1.387721000
8	-1.995949000	0.733530000	-0.556513000
6	0.455182000	3.368336000	-0.742152000
6	0.671741000	4.610381000	-1.437889000
6	0.711664000	5.769594000	-0.729815000
6	0.532622000	5.791762000	0.705331000
6	0.308155000	4.656180000	1.417584000
6	0.234464000	3.394971000	0.725605000
6	2.773811000	-0.617412000	0.158046000
6	2.435031000	-1.603578000	-0.787187000

6	1.229078000	-1.558846000	-1.485201000
6	-1.528419000	-1.259588000	1.517660000
6	-2.722134000	-1.079890000	0.819987000
6	-2.858004000	-0.078793000	-0.160854000
1	0.812561000	4.595126000	-2.514327000
1	-0.137430000	2.180273000	2.245846000
1	3.138537000	-2.393385000	-1.003339000
1	-3.568982000	-1.706215000	1.055657000
1	0.887395000	6.710960000	-1.241911000
1	0.578797000	6.749069000	1.215491000
1	0.172022000	4.677788000	2.494375000
6	4.181581000	-0.678887000	0.802358000
9	4.949323000	0.328727000	0.323745000
9	4.106252000	-0.536710000	2.136618000
9	4.830014000	-1.835566000	0.548144000
6	0.972423000	-2.618831000	-2.579471000
9	1.950665000	-3.546127000	-2.655361000
9	-0.186565000	-3.266761000	-2.355555000
9	0.884376000	-2.024006000	-3.790614000
6	-4.241937000	0.099111000	-0.836411000
9	-4.130535000	0.029360000	-2.175444000
9	-5.144021000	-0.829553000	-0.451715000
9	-4.755306000	1.312144000	-0.529010000
6	-1.476864000	-2.329700000	2.631079000
9	-0.511145000	-3.233746000	2.374495000
9	-1.196316000	-1.753525000	3.820515000
9	-2.638406000	-3.003058000	2.771897000
1	0.552425000	2.099383000	-2.259415000

### 32

E=-3959.35280 a.u.

27	0.601813000	0.053855000	-0.161841000
8	-1.125763000	-0.441550000	1.006394000
8	-1.058045000	0.550962000	-1.403116000
8	0.545728000	1.877996000	0.757465000
8	2.038610000	0.803573000	-1.393591000
8	1.944044000	-0.696948000	1.176536000
8	0.608021000	-1.781775000	-1.064083000
6	-2.183496000	0.366874000	-0.925475000
6	-3.413180000	0.666999000	-1.601672000
6	-4.596977000	0.407935000	-0.982888000
6	-4.609366000	-0.171317000	0.371454000
6	-3.521070000	-0.499851000	1.118370000
6	-2.225180000	-0.231197000	0.489629000
6	1.378182000	2.810334000	0.613747000
6	2.437007000	2.891110000	-0.297858000

6	2.664967000	1.882527000	-1.244987000
6	2.585681000	-1.772850000	1.074306000
6	2.430664000	-2.783038000	0.115162000
6	1.433453000	-2.709342000	-0.864988000
1	-3.340591000	1.086918000	-2.597000000
1	3.067096000	3.767758000	-0.299315000
1	3.063515000	-3.656457000	0.161291000
1	-5.588866000	-0.344845000	0.798803000
6	1.125782000	4.007247000	1.559034000
9	-0.070479000	4.575691000	1.279632000
9	1.095150000	3.604017000	2.842918000
9	2.064596000	4.971819000	1.455299000
6	3.801050000	2.082805000	-2.275590000
9	4.482882000	3.234963000	-2.089305000
9	4.686926000	1.070316000	-2.203050000
9	3.300640000	2.105859000	-3.527568000
6	1.251097000	-3.909145000	-1.823041000
9	1.329022000	-3.511928000	-3.106117000
9	2.172339000	-4.879045000	-1.637645000
9	0.032725000	-4.469175000	-1.639565000
6	3.643911000	-1.967495000	2.185441000
9	4.524602000	-0.948410000	2.182926000
9	3.050840000	-1.998341000	3.397280000
9	4.346005000	-3.114106000	2.048394000
6	-3.588240000	-1.100950000	2.526270000
6	-2.892732000	-0.146174000	3.530070000
6	-2.877770000	-2.478458000	2.533659000
1	-3.350566000	-3.169326000	1.826833000
1	-1.820179000	-2.390250000	2.280147000
1	-2.950501000	-2.918934000	3.533801000
1	-1.837316000	-0.002771000	3.292887000
1	-2.959878000	-0.569163000	4.538136000
1	-3.382503000	0.833728000	3.543965000
6	-5.043687000	-1.306398000	2.982327000
1	-5.588052000	-1.997155000	2.328340000
1	-5.044817000	-1.739861000	3.986866000
1	-5.597432000	-0.362141000	3.033995000
6	-5.951572000	0.689170000	-1.633871000
6	-6.746409000	-0.637093000	-1.740809000
6	-5.807455000	1.285061000	-3.045220000
1	-5.275225000	2.241791000	-3.033401000
1	-5.283482000	0.604967000	-3.724678000
1	-6.801257000	1.467968000	-3.464975000
1	-6.214734000	-1.364421000	-2.362766000
1	-7.719132000	-0.441402000	-2.203870000
1	-6.933712000	-1.096419000	-0.765685000

6	-6.733261000	1.698496000	-0.753766000
1	-6.191295000	2.645784000	-0.667627000
1	-7.705648000	1.904226000	-1.213482000
1	-6.920771000	1.321418000	0.255998000

### 33

E=-3959.35675 a.u.

27	0.598991000	0.081482000	-0.121676000
8	0.519976000	1.629093000	0.984286000
8	1.979445000	0.761287000	-1.251637000
8	1.936209000	-0.606087000	1.059859000
8	0.556749000	-1.467749000	-1.229212000
6	1.231464000	2.655522000	0.808397000
6	2.199183000	2.882555000	-0.172195000
6	2.492909000	1.906261000	-1.126186000
6	2.468406000	-1.743067000	0.937660000
6	2.220336000	-2.710057000	-0.038294000
6	1.277498000	-2.485511000	-1.044117000
1	2.729572000	3.822287000	-0.190156000
1	2.763093000	-3.642624000	-0.015371000
6	0.934244000	3.762994000	1.843444000
9	1.693588000	4.860404000	1.648775000
9	-0.356915000	4.137426000	1.764221000
9	1.165264000	3.317105000	3.090051000
6	3.570165000	2.195488000	-2.194529000
9	4.153377000	3.398848000	-2.018469000
9	4.535444000	1.259373000	-2.149693000
9	3.025088000	2.177613000	-3.423747000
6	3.509731000	-2.034527000	2.040273000
9	4.469420000	-1.091841000	2.038103000
9	2.920929000	-2.030921000	3.250048000
9	4.106738000	-3.232525000	1.875462000
6	1.024409000	-3.587174000	-2.097364000
9	1.279925000	-3.125758000	-3.332856000
9	1.796057000	-4.674460000	-1.893028000
9	-0.262262000	-3.982874000	-2.054346000
8	-0.800579000	-0.660738000	0.908142000
8	-0.755295000	0.830508000	-1.197757000
6	-1.933058000	0.509137000	-0.752872000
6	-3.128225000	0.936658000	-1.367652000
6	-4.336995000	0.550660000	-0.828091000
6	-4.341492000	-0.275195000	0.351083000
6	-3.214753000	-0.726938000	1.007124000
6	-1.963814000	-0.326501000	0.434931000
1	-3.047252000	1.557509000	-2.250883000
1	-5.307678000	-0.557396000	0.748616000

6	-3.262981000	-1.593158000	2.274275000
6	-2.568567000	-0.843038000	3.438059000
6	-2.542513000	-2.939435000	2.016368000
1	-3.018051000	-3.486484000	1.194695000
1	-1.490041000	-2.789696000	1.768804000
1	-2.596194000	-3.565015000	2.914464000
1	-1.521161000	-0.632212000	3.214171000
1	-2.608173000	-1.453825000	4.347162000
1	-3.074816000	0.105878000	3.647082000
6	-4.710451000	-1.901931000	2.699921000
1	-5.254821000	-2.464302000	1.932969000
1	-4.694921000	-2.515199000	3.606490000
1	-5.275222000	-0.991943000	2.931165000
6	-5.683304000	0.967978000	-1.433936000
6	-6.500706000	1.752591000	-0.378240000
6	-6.466600000	-0.299611000	-1.855683000
1	-5.912398000	-0.870583000	-2.607962000
1	-6.666186000	-0.962658000	-1.008404000
1	-7.431844000	-0.013527000	-2.288379000
1	-6.714812000	1.152050000	0.510996000
1	-7.459959000	2.063017000	-0.807206000
1	-5.964781000	2.651868000	-0.056944000
6	-5.510767000	1.864282000	-2.673844000
1	-4.965213000	1.353214000	-3.474010000
1	-6.495310000	2.135901000	-3.068168000
1	-4.983210000	2.793791000	-2.435213000

### 34

E=-3939.48714 a.u.

27	-0.550087000	-0.036929000	-0.248275000
7	1.079697000	-0.386119000	-1.487082000
8	1.164187000	0.237471000	1.022070000
8	-0.539571000	1.916484000	-0.926592000
8	-1.912193000	0.592621000	1.152077000
8	-1.995175000	-0.641421000	-1.568420000
8	-0.642866000	-1.940101000	0.551215000
6	2.266373000	0.062585000	0.488263000
6	3.550694000	0.169108000	1.184193000
6	4.661437000	-0.021553000	0.419619000
6	4.687342000	-0.328096000	-1.015111000
6	3.514254000	-0.455054000	-1.686660000
6	2.266864000	-0.283111000	-0.988312000
6	-1.330929000	2.837703000	-0.600299000
6	-2.322449000	2.818713000	0.387140000
6	-2.517233000	1.691325000	1.198077000
6	-2.742117000	-1.647427000	-1.448831000

6	-2.639470000	-2.695182000	-0.526639000
6	-1.572657000	-2.765532000	0.381672000
1	-2.924471000	3.699782000	0.550765000
1	-3.366213000	-3.493273000	-0.551144000
1	5.627014000	0.056835000	0.903541000
1	3.475219000	-0.688385000	-2.744868000
6	-1.113185000	4.143880000	-1.398922000
9	0.124028000	4.636930000	-1.158984000
9	-1.210103000	3.915585000	-2.723157000
9	-2.000584000	5.112437000	-1.085993000
6	-3.579435000	1.765405000	2.320434000
9	-4.253842000	2.936866000	2.331919000
9	-4.484718000	0.777292000	2.180328000
9	-2.996482000	1.622594000	3.529159000
6	-1.447586000	-4.025739000	1.270434000
9	-1.319070000	-3.689547000	2.566246000
9	-2.507386000	-4.856497000	1.165412000
9	-0.346110000	-4.730345000	0.917952000
6	-3.868430000	-1.705728000	-2.506585000
9	-4.581537000	-0.564811000	-2.507471000
9	-3.337774000	-1.860988000	-3.741237000
9	-4.730084000	-2.726813000	-2.306566000
6	3.587409000	0.475205000	2.686435000
6	2.822927000	-0.631015000	3.457422000
6	2.930420000	1.852985000	2.954098000
1	3.457548000	2.650293000	2.418257000
1	1.881467000	1.865552000	2.654824000
1	2.980627000	2.077754000	4.024856000
1	1.772552000	-0.678629000	3.166752000
1	2.870113000	-0.423387000	4.531826000
1	3.276523000	-1.613403000	3.285072000
6	6.056541000	-0.494138000	-1.679369000
6	6.855955000	0.824292000	-1.526484000
6	5.939617000	-0.819211000	-3.178854000
1	5.406566000	-1.759980000	-3.352502000
1	5.430354000	-0.022748000	-3.731755000
1	6.940935000	-0.925993000	-3.607245000
1	6.337201000	1.656828000	-2.012945000
1	7.838924000	0.714844000	-1.997103000
1	7.021496000	1.094388000	-0.479233000
6	5.031560000	0.520546000	3.218485000
1	5.625249000	1.307995000	2.740058000
1	5.009937000	0.736136000	4.290892000
1	5.550171000	-0.436409000	3.089467000
6	6.822139000	-1.650209000	-0.987860000
1	6.991547000	-1.463639000	0.076792000

1	6.277570000	-2.595277000	-1.083508000
1	7.802833000	-1.774309000	-1.459312000
1	1.048972000	-0.598319000	-2.485832000

### 35

E=-3939.48630 a.u.

27	-0.582113000	-0.095984000	-0.206826000
8	-0.500835000	1.513714000	-1.227125000
8	-1.891706000	0.591861000	1.035794000
8	-2.001471000	-0.671234000	-1.367257000
8	-0.597729000	-1.694974000	0.843126000
6	-1.150616000	2.560314000	-0.952144000
6	-2.048053000	2.780517000	0.092929000
6	-2.348142000	1.764433000	1.005267000
6	-2.644733000	-1.747789000	-1.215215000
6	-2.454096000	-2.736865000	-0.250576000
6	-1.432483000	-2.625445000	0.699057000
1	-2.524473000	3.743899000	0.191479000
1	-3.094501000	-3.605562000	-0.243737000
6	-0.869822000	3.702097000	-1.953727000
9	-1.511454000	4.841996000	-1.625144000
9	0.447709000	3.971717000	-2.001360000
9	-1.268421000	3.347340000	-3.189544000
6	-3.350829000	2.051345000	2.144788000
9	-3.910875000	3.274286000	2.039139000
9	-4.342615000	1.142453000	2.137822000
9	-2.730752000	1.985125000	3.337809000
6	-3.755254000	-1.931365000	-2.271736000
9	-4.627717000	-0.909399000	-2.219554000
9	-3.218749000	-1.961179000	-3.507857000
9	-4.446593000	-3.075387000	-2.096492000
6	-1.226515000	-3.771000000	1.715980000
9	-1.242666000	-3.299360000	2.971940000
9	-2.180971000	-4.719165000	1.615841000
9	-0.034871000	-4.365464000	1.504606000
7	0.790813000	-0.800685000	-1.289451000
8	0.836308000	0.525292000	0.872149000
6	2.012904000	0.187369000	0.414392000
6	3.242873000	0.499341000	1.066536000
6	4.395712000	0.102355000	0.409554000
6	4.433309000	-0.585199000	-0.849871000
6	3.241835000	-0.897419000	-1.463034000
6	2.019829000	-0.537040000	-0.839231000
1	5.345961000	0.327233000	0.877210000
1	3.202051000	-1.424620000	-2.409764000
6	5.799294000	-0.948416000	-1.451943000



6	6.621323000	0.343668000	-1.677138000
6	5.665874000	-1.674402000	-2.802887000
1	5.120897000	-2.619519000	-2.705645000
1	5.156621000	-1.056071000	-3.549917000
1	6.661725000	-1.908003000	-3.193073000
1	6.107000000	1.018915000	-2.369194000
1	7.599158000	0.096203000	-2.105865000
1	6.796371000	0.888402000	-0.744626000
6	3.256389000	1.231418000	2.418136000
6	2.486540000	0.391632000	3.467039000
6	2.588669000	2.620412000	2.267814000
1	3.122629000	3.232318000	1.532131000
1	1.547408000	2.531015000	1.953018000
1	2.612420000	3.148688000	3.227832000
1	1.448485000	0.230814000	3.170407000
1	2.491625000	0.909645000	4.432976000
1	2.961634000	-0.585924000	3.605780000
6	4.688971000	1.447479000	2.939749000
1	5.285620000	2.069863000	2.263498000
1	4.645218000	1.962251000	3.904929000
1	5.216522000	0.500222000	3.097928000
6	6.558751000	-1.879148000	-0.475656000
1	6.727172000	-1.405868000	0.496279000
1	6.001479000	-2.806485000	-0.305843000
1	7.538253000	-2.141070000	-0.891728000
1	0.676955000	-1.213673000	-2.210467000

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E=-3919.61375 a.u.

27	-0.517391000	-0.003335000	-0.180828000
7	1.098731000	-0.138563000	-1.485392000
7	1.156454000	0.111129000	1.061360000
8	-0.631442000	2.012171000	-0.715201000
8	-1.891278000	0.468768000	1.296607000
8	-1.981504000	-0.465619000	-1.563834000
8	-0.628374000	-2.011031000	0.386382000
6	2.328103000	0.016339000	0.525870000
6	3.637198000	-0.013843000	1.195755000
6	4.727839000	-0.030784000	0.382544000
6	4.712085000	-0.036906000	-1.080430000
6	3.518210000	-0.051622000	-1.724964000
6	2.286761000	-0.062635000	-0.977616000
6	-1.484952000	2.848454000	-0.333652000
6	-2.467536000	2.698812000	0.655659000
6	-2.571376000	1.519971000	1.404646000
6	-2.708637000	-1.489859000	-1.590255000

6	-2.593691000	-2.652687000	-0.817484000
6	-1.540801000	-2.820938000	0.092556000
1	-3.130492000	3.523144000	0.871467000
1	-3.304422000	-3.453375000	-0.957025000
1	5.706601000	-0.038553000	0.842964000
1	3.445721000	-0.070215000	-2.806601000
6	-1.367542000	4.216139000	-1.048036000
9	-0.169688000	4.783425000	-0.772119000
9	-1.448675000	4.067492000	-2.384122000
9	-2.323376000	5.095888000	-0.676965000
6	-3.616584000	1.461987000	2.543335000
9	-4.364591000	2.583534000	2.636609000
9	-4.458733000	0.426006000	2.364168000
9	-3.000103000	1.289102000	3.734499000
6	-1.411238000	-4.182445000	0.816209000
9	-1.289618000	-4.011369000	2.146539000
9	-2.463838000	-5.001995000	0.604871000
9	-0.302707000	-4.831352000	0.385993000
6	-3.828627000	-1.423141000	-2.655150000
9	-4.562515000	-0.304550000	-2.506815000
9	-3.289976000	-1.400213000	-3.895812000
9	-4.674664000	-2.475908000	-2.603055000
6	3.757311000	-0.014760000	2.731944000
6	3.046212000	-1.259324000	3.325881000
6	3.172226000	1.294392000	3.325595000
1	3.703167000	2.167134000	2.931248000
1	2.109026000	1.442528000	3.121524000
1	3.294799000	1.288414000	4.413624000
1	1.978890000	-1.315313000	3.099638000
1	3.149469000	-1.254681000	4.416088000
1	3.503705000	-2.179552000	2.948261000
6	6.059886000	-0.034691000	-1.809524000
6	6.849807000	1.236534000	-1.409480000
6	5.891494000	-0.040020000	-3.338745000
1	5.362615000	-0.933097000	-3.687932000
1	5.351516000	0.844439000	-3.692864000
1	6.876760000	-0.035544000	-3.815126000
1	6.304659000	2.143092000	-1.692095000
1	7.816192000	1.246896000	-1.924746000
1	7.049886000	1.283050000	-0.334696000
6	5.230036000	-0.085695000	3.184415000
1	5.807251000	0.783174000	2.850723000
1	5.266991000	-0.100971000	4.277901000
1	5.726331000	-0.994270000	2.827500000
6	6.862938000	-1.295154000	-1.402553000
1	7.060749000	-1.336331000	-0.327194000

1	6.328767000	-2.208742000	-1.683589000
1	7.830846000	-1.296531000	-1.915171000
1	1.071242000	-0.156355000	-2.505380000
1	1.135389000	0.130179000	2.077181000

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E=-3919.60975 a.u.

27	0.583594000	0.053956000	-0.137417000
8	0.562431000	-1.608489000	-1.087928000
8	1.924933000	-0.543852000	1.140379000
8	1.990502000	0.598826000	-1.363044000
8	0.592543000	1.715242000	0.817137000
6	1.313015000	-2.585524000	-0.826474000
6	2.266015000	-2.708921000	0.188639000
6	2.486477000	-1.671498000	1.097640000
6	2.581851000	1.710565000	-1.309380000
6	2.361085000	2.761096000	-0.415562000
6	1.378147000	2.669168000	0.573797000
1	2.834085000	-3.622502000	0.275180000
1	2.956959000	3.657848000	-0.490193000
6	1.082736000	-3.777326000	-1.782602000
9	1.933963000	-4.796939000	-1.545587000
9	-0.171710000	-4.250251000	-1.640464000
9	1.242543000	-3.396787000	-3.061499000
6	3.520838000	-1.872376000	2.226378000
9	4.162498000	-3.055116000	2.134596000
9	4.447054000	-0.897790000	2.198210000
9	2.908364000	-1.831334000	3.427761000
6	3.664422000	1.869462000	-2.398947000
9	4.582025000	0.890797000	-2.297726000
9	3.105693000	1.792472000	-3.623630000
9	4.310132000	3.050820000	-2.316959000
6	1.155502000	3.871357000	1.518525000
9	1.228116000	3.484993000	2.803609000
9	2.066097000	4.848492000	1.328792000
9	-0.065564000	4.404247000	1.310629000
7	-0.808375000	0.667715000	-1.256162000
7	-0.862379000	-0.508047000	0.944415000
6	-2.086463000	-0.196530000	0.497962000
6	-3.356028000	-0.391976000	1.144373000
6	-4.476994000	-0.099092000	0.390070000
6	-4.458718000	0.384298000	-0.958386000
6	-3.239523000	0.617174000	-1.556095000
6	-2.045365000	0.380839000	-0.834499000
1	-5.448210000	-0.250976000	0.841633000
1	-3.160816000	1.003988000	-2.565921000

6	-5.796296000	0.628343000	-1.673899000
6	-6.592876000	-0.697647000	-1.739157000
6	-5.602559000	1.141692000	-3.112465000
1	-5.073227000	2.100358000	-3.136175000
1	-5.049121000	0.426003000	-3.729805000
1	-6.579897000	1.295073000	-3.581698000
1	-6.036538000	-1.460883000	-2.293471000
1	-7.550217000	-0.536696000	-2.247835000
1	-6.809079000	-1.096921000	-0.743610000
6	-3.462632000	-0.920589000	2.588443000
6	-2.736873000	0.038071000	3.566943000
6	-2.873963000	-2.351202000	2.685370000
1	-3.431193000	-3.038471000	2.040100000
1	-1.823901000	-2.410682000	2.388739000
1	-2.949236000	-2.717012000	3.715481000
1	-1.674494000	0.171952000	3.347567000
1	-2.815033000	-0.344138000	4.590855000
1	-3.196650000	1.031461000	3.540649000
6	-4.927685000	-1.009252000	3.063153000
1	-5.514498000	-1.709168000	2.459258000
1	-4.948804000	-1.370632000	4.096419000
1	-5.423764000	-0.033211000	3.045547000
6	-6.616478000	1.683235000	-0.892397000
1	-6.835745000	1.360072000	0.129720000
1	-6.076654000	2.634468000	-0.835735000
1	-7.573133000	1.863778000	-1.395975000
1	-0.677880000	0.913987000	-2.233183000
1	-0.736698000	-0.768645000	1.914419000

### **3,5-di-(*tert*-butyl)-*o*-benzoquinone**

E=-695.68550 a.u.

8	-2.316578000	1.934643000	0.000497000
8	-0.037002000	3.434212000	-0.000311000
6	0.059501000	2.221310000	-0.000097000
6	1.342617000	1.524309000	0.000007000
6	1.405573000	0.172633000	0.000031000
6	0.162084000	-0.619025000	-0.000033000
6	-1.100599000	-0.127589000	0.000008000
6	-1.248341000	1.356588000	0.000128000
1	2.222540000	2.157141000	0.000014000
1	0.290619000	-1.694756000	-0.000107000
6	-2.354917000	-1.010956000	-0.000052000
6	-3.197608000	-0.717123000	-1.266955000
6	-3.197300000	-0.717808000	1.267215000
1	-2.619658000	-0.921822000	2.175980000
1	-3.533566000	0.319640000	1.293536000

1	-4.080703000	-1.366349000	1.278907000
1	-3.533886000	0.320340000	-1.292637000
1	-4.081016000	-1.365654000	-1.278783000
1	-2.620190000	-0.920646000	-2.175972000
6	-2.000911000	-2.509838000	-0.000498000
1	-1.430264000	-2.800061000	0.889119000
1	-2.925304000	-3.096119000	-0.000562000
1	-1.430442000	-2.799572000	-0.890388000
6	2.726974000	-0.603762000	0.000037000
6	3.950158000	0.330022000	0.000287000
6	2.794704000	-1.493805000	-1.266185000
1	1.977561000	-2.219830000	-1.311650000
1	2.756451000	-0.884301000	-2.175080000
1	3.735411000	-2.055130000	-1.272860000
1	3.973259000	0.970946000	-0.887079000
1	4.866701000	-0.268595000	0.000120000
1	3.973267000	0.970484000	0.887990000
6	2.794561000	-1.494234000	1.265972000
1	1.977155000	-2.219958000	1.311356000
1	3.735046000	-2.055933000	1.272339000
1	2.756689000	-0.885001000	2.175068000

### **3,5-di-(*tert*-butyl)-*o*-benzoquinone imine**

E=-675.80613 a.u.

7	-0.109235000	3.472931000	-0.036478000
8	-2.336923000	1.912103000	0.052267000
6	-1.253530000	1.358060000	0.017169000
6	-1.097852000	-0.126519000	-0.001152000
6	0.161747000	-0.628564000	-0.005303000
6	1.401977000	0.156861000	0.000773000
6	1.320411000	1.505930000	0.000808000
6	0.035977000	2.197621000	-0.006837000
1	0.282984000	-1.705371000	-0.012343000
1	2.207617000	2.132274000	0.000748000
6	-2.354152000	-1.009083000	-0.006552000
6	-3.207447000	-0.694629000	-1.261313000
6	-3.186913000	-0.742272000	1.272846000
1	-2.601476000	-0.965343000	2.172241000
1	-3.520894000	0.294743000	1.322544000
1	-4.070388000	-1.391156000	1.278430000
1	-3.542055000	0.343475000	-1.267242000
1	-4.091346000	-1.342686000	-1.276722000
1	-2.636936000	-0.884209000	-2.177844000
6	2.729169000	-0.611234000	0.003496000
6	2.799387000	-1.505418000	1.265941000
6	3.946371000	0.330596000	0.012010000

1	3.970324000	0.973110000	-0.874566000
1	3.961088000	0.968860000	0.901860000
1	4.867536000	-0.261046000	0.015266000
1	2.755283000	-0.899489000	2.177099000
1	3.741484000	-2.064760000	1.274427000
1	1.983403000	-2.233108000	1.305808000
6	-2.002713000	-2.508637000	-0.037747000
1	-1.427912000	-2.817463000	0.842945000
1	-2.928483000	-3.092844000	-0.043827000
1	-1.437502000	-2.782325000	-0.936109000
6	2.810337000	-1.497017000	-1.264145000
1	1.994749000	-2.224445000	-1.316029000
1	2.774236000	-0.885094000	-2.171640000
1	3.752465000	-2.056353000	-1.268098000
1	0.809233000	3.931713000	-0.049696000

### **3,5-di-(*tert*-butyl)-*o*-benzoquinone diimine**

E=-655.91799 a.u.

7	-2.174540000	2.018564000	0.764472000
7	-0.141689000	3.397462000	-0.517049000
6	0.024439000	2.186727000	-0.122260000
6	1.316204000	1.510640000	-0.023207000
6	1.395228000	0.160826000	0.006625000
6	0.152069000	-0.614752000	-0.057293000
6	-1.099802000	-0.096769000	0.010407000
6	-1.200513000	1.373897000	0.235903000
1	2.200606000	2.139668000	-0.049470000
1	-2.958854000	1.399215000	0.970764000
1	0.264151000	-1.686656000	-0.163646000
1	0.770046000	3.837224000	-0.688638000
6	-2.356595000	-0.985881000	-0.091078000
6	-2.008462000	-2.393795000	-0.619134000
6	-3.369600000	-0.370382000	-1.089069000
1	-3.713617000	0.624257000	-0.798311000
1	-2.922970000	-0.284257000	-2.085482000
1	-4.249287000	-1.018381000	-1.169672000
1	-1.498172000	-2.349525000	-1.586898000
1	-2.932438000	-2.965531000	-0.753697000
1	-1.380835000	-2.956621000	0.079594000
6	-3.016168000	-1.182590000	1.300185000
1	-3.388504000	-0.255881000	1.744617000
1	-3.868808000	-1.865573000	1.211104000
1	-2.302789000	-1.621000000	2.005837000
6	2.719571000	-0.611608000	0.051681000
6	3.936030000	0.326670000	0.141578000
6	2.863984000	-1.471405000	-1.227732000

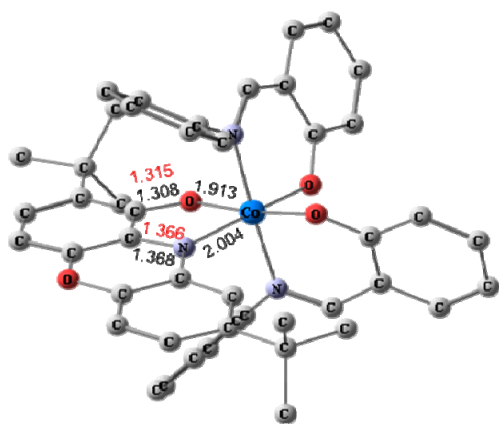
1	2.053644000	-2.199150000	-1.333627000
1	2.869685000	-0.841311000	-2.123445000
1	3.806569000	-2.029555000	-1.198300000
1	4.014772000	0.976630000	-0.736276000
1	4.854682000	-0.266791000	0.194996000
1	3.896470000	0.957969000	1.035591000
6	2.725702000	-1.532844000	1.296236000
1	1.904498000	-2.255741000	1.279491000
1	3.663777000	-2.097648000	1.339712000
1	2.638452000	-0.945938000	2.216741000

**Table S1.** Total and relative energies of the low- and high-spin electromeric forms of adducts of Co(acac)<sub>2</sub> and Co(hfacac)<sub>2</sub> with o-benzoquinone.

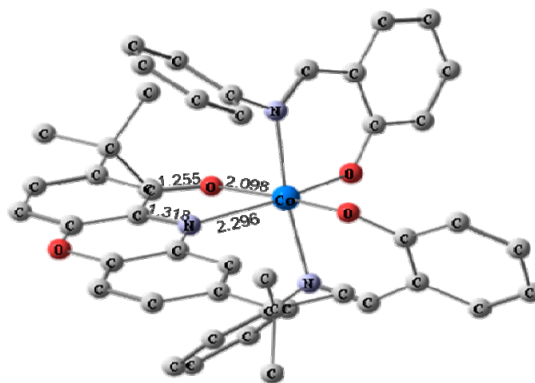
Functional	Structure	S	E, a.u.	$\Delta E$ , kcal•mol <sup>-1</sup>
B3LYP*	<b>9</b>	3/2	-2454.223550	15.5
	<b>10</b>	1/2	-2454.248260	0.0
	<b>11</b>	3/2	-3644.982700	6.8
	<b>12</b>	1/2	-3644.993590	0.0
B3LYP	<b>9</b>	3/2	-2455.039992	12.1
	<b>10</b>	1/2	-2455.059262	0.0
	<b>11</b>	3/2	-3646.292543	0.7
	<b>12</b>	1/2	-3646.293601	0.0
B3P86	<b>9</b>	3/2	-2458.502297	15.8
	<b>10</b>	1/2	-2458.527408	0.0
	<b>11</b>	3/2	-3651.390401	6.2
	<b>12</b>	1/2	-3651.400311	0.0
BLYP	<b>9</b>	3/2	-2454.769850	20.4
	<b>10</b>	1/2	-2454.802413	0.0
	<b>11</b>	3/2	-3646.042097	14.2
	<b>12</b>	1/2	-3646.064747	0.0
OPBE	<b>9</b>	3/2	-2454.789177	11.5
	<b>10</b>	1/2	-2454.807554	0.0
	<b>11</b>	3/2	-3645.413810	6.7
	<b>12</b>	1/2	-3645.424460	0.0



**Figure S1.** Electromeric forms of adduct **3** (the calculations have been carried out for model compounds stripped of two the bulky *tert*-butyl groups in positions 4,4'). The hydrogen atoms are omitted.



**S1**,  $_{LS}Co^{III}$



**S2**,  $_{HS}Co^{II}$

$\Delta E = 11.1$  kcal/mol,  $E_{stab} = 0.8$  kcal/mol