Dalton Transaction

Computational Supporting Information

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Improved Selectivity for Pb(II) by Sulfur, Selenium and Tellurium Analogues of 1,8-Anthraquinone-18-Crown-5: Synthesis, Spectroscopy, X-ray Crystallography and Computational Studies

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Table of atomic coordinates for 1

Atoms	X	Y	Z
O	-4.39212600	-0.00000500	-0.24921300
O	-2.93373700	2.62220400	-0.30143500
O	-2.93371100	-2.62219300	-0.30136500
O	0.32261300	-0.00001500	1.47902300
O	-0.11917200	-2.51784800	0.49368000
C	3.98011600	2.46522300	-0.48551100
H	5.03155300	2.42108600	-0.74570500
O	-0.11920600	2.51782800	0.49367300
C	1.30112000	-0.00000500	0.68578900
C	-2.33060100	3.47931500	0.71249800
H	-2.38017000	2.99357000	1.69838300
H	-2.86641200	4.44093400	0.76898200
O	5.33093200	0.00002200	-0.34386500
C	-4.36829500	-2.41066000	-0.09369700
H	-4.57566300	-2.21241700	0.96867900
H	-4.91762100	-3.31542100	-0.39702600
C	1.91112100	-3.70597100	-0.17823900
H	1.38485300	-4.65213300	-0.21469400
C	1.23061300	-2.51972700	0.18906100
C	-4.36832700	2.41066000	-0.09380500
H	-4.91765400	3.31539900	-0.39719900
H	-4.57572700	2.21246600	0.96857400
C	-2.33056200	-3.47934300	0.71252800
H	-2.86637600	-4.44096100	0.76898500
H	-2.38011600	-2.99363400	1.69843200
C	1.93466200	1.27846100	0.22455600
C	3.30932900	-1.27707600	-0.14087700
C	-4.81804000	-1.22304000	-0.92646100
H	-5.91624200	-1.23482900	-1.01955500
H	-4.38138700	-1.27669700	-1.93584800
C	1.23058800	2.51972500	0.18908900
C	3.30931900	1.27710100	-0.14084900
C	3.98013300	-2.46518400	-0.48557100
H	5.03156800	-2.42103300	-0.74577200
C	-0.89117500	3.76360200	0.33266500
H	-0.82711800	4.10572400	-0.70818700
H	-0.48602600	4.53487000	1.00043200
C	3.27595800	3.67703900	-0.49955400
H	3.77955300	4.60063300	-0.76894800
C	-0.89114200	-3.76362000	0.33266400
H	-0.48598100	-4.53490000	1.00040900
H	-0.82710300	-4.10572400	-0.70819500
C	3.27598600	-3.67700600	-0.49963400

H	3.77958700	-4.60058900	-0.76905400
C	-4.81802900	1.22299500	-0.92652800
H	-4.38134200	1.27661200	-1.93590200
H	-5.91622800	1.23477200	-1.01966400
C	1.93467500	-1.27845600	0.22453800
C	4.07554600	0.00001600	-0.19723300
C	1.91108800	3.70598300	-0.17817700
H	1.38481000	4.65214000	-0.21462200

Sum of electronic and zero-point energies: -1377.519140 Hartrees

Table of atomic coordinates for 1 with Pb(II)

Atoms	X	Y	Z
Pb	1.65493300	-0.00997100	-0.64044600
O	3.11089000	-0.00798000	1.21820400
O	2.06472600	-2.34033600	0.28445400
O	2.10335400	2.33162500	0.25697500
O	-0.31637600	0.00362000	0.34309300
O	-0.46471400	2.32249600	-1.03795100
C	-4.38439400	-2.48201100	0.50773500
H	-5.41308800	-2.48824700	0.85015400
O	-0.47517800	-2.30989900	-1.05165000
C	-1.58026600	0.00696200	0.11308800
C	1.29496400	-3.58477100	0.05880000
H	0.66371400	-3.77121600	0.93655900
H	2.00510900	-4.41195200	-0.06193000
O	-5.53081000	0.01269300	1.29958100
C	2.89462200	2.37696900	1.50630100
H	2.21140900	2.29065500	2.35896200
H	3.43656200	3.32820300	1.55984900
C	-2.40713200	3.68578200	-0.34567100
H	-1.95823600	4.61563200	-0.67492000
C	-1.70332900	2.46529400	-0.42432500
C	2.80293400	-2.37476600	1.56656300
H	3.31135000	-3.34017200	1.66910300
H	2.08782200	-2.24263100	2.38663200
C	1.33103900	3.57805600	0.05408700
H	2.03973200	4.40586000	-0.07231100
H	0.71526600	3.75798000	0.94423000
C	-2.32626500	-1.24945000	0.01912900
C	-3.68004200	1.29027500	0.44821500
C	3.88536000	1.23424900	1.46778400
C	-1.71562700	-2.44804900	-0.43930700
C	-3.68631000	-1.26815800	0.43959300
C	-4.37162400	2.50732000	0.52450000
H	-5.40012800	2.51692800	0.86740700
C	0.46091700	-3.43780900	-1.20119900
H	1.07798500	-3.17015500	-2.06157300
H	-0.05704300	-4.37374700	-1.42440400
C	-3.74204800	-3.67502200	0.12069000
H	-4.27740800	-4.61786800	0.17340700
C	0.47631100	3.44506400	-1.19342700
H	-0.03872400	4.38621500	-1.40086400
H	1.07875400	3.18021000	-2.06505500
C	-3.72296100	3.69934500	0.14472200
H	-4.25324700	4.64468400	0.20390300

C	3.83172600	-1.26581600	1.53773000
C	-2.32026200	1.26721100	0.02731400
C	-4.37873900	0.01165800	0.79090400
C	-2.42578700	-3.66520500	-0.36866000
H	-1.98155700	-4.59537300	-0.70340100
H	4.60095100	-1.43333800	0.77615900
H	4.29641900	-1.15988100	2.52307000
H	4.39097700	1.14276200	2.43403600
H	4.62516600	1.35252100	0.66856200

Sum of electronic and zero-point energies: -1380.763549 Hartrees

Table of atomic coordinates for 2

Atoms	X	Y	Z
S	4.121132000000	0.042669000000	-0.157696000000
O	2.721975000000	2.916753000000	0.861128000000
O	2.841112000000	-3.233756000000	-0.257173000000
O	-0.335193000000	-0.216567000000	-1.201640000000
O	0.006621000000	-2.610431000000	0.168665000000
C	-4.100658000000	2.507467000000	0.073692000000
H	-5.171619000000	2.509677000000	0.241906000000
O	0.075239000000	2.384574000000	-0.455562000000
C	-1.377756000000	-0.098920000000	-0.504045000000
C	2.335303000000	3.237958000000	-0.513877000000
H	2.502870000000	2.379081000000	-1.177967000000
H	2.926516000000	4.092274000000	-0.877000000000
O	-5.476349000000	0.054327000000	0.233359000000
C	4.247404000000	-2.832964000000	-0.271031000000
H	4.590318000000	-2.656731000000	-1.302340000000
H	4.789791000000	-3.700646000000	0.122735000000
C	-2.091348000000	-3.672527000000	0.700798000000
H	-1.536850000000	-4.588233000000	0.884611000000
C	-1.387203000000	-2.532702000000	0.263065000000
C	4.144391000000	2.622081000000	1.066129000000
H	4.455365000000	3.207137000000	1.940914000000
H	4.738673000000	2.954378000000	0.203198000000
C	1.984662000000	-2.576599000000	-1.249474000000
H	2.353928000000	-2.808795000000	-2.261894000000
H	1.980355000000	-1.491546000000	-1.105022000000
C	-2.021842000000	1.225307000000	-0.258744000000
C	-3.469913000000	-1.260245000000	0.296923000000
C	4.562211000000	-1.633994000000	0.635231000000
H	5.634885000000	-1.614648000000	0.857946000000
H	4.003046000000	-1.721341000000	1.572186000000
C	-1.298908000000	2.453282000000	-0.330007000000
C	-3.424462000000	1.277107000000	-0.021797000000
C	-4.168875000000	-2.409312000000	0.713957000000
H	-5.236876000000	-2.339546000000	0.889968000000
C	0.868563000000	3.626427000000	-0.515414000000
H	0.650699000000	4.259196000000	0.353810000000
H	0.617880000000	4.164861000000	-1.438402000000
C	-3.380301000000	3.705345000000	-0.044988000000
H	-3.893507000000	4.660084000000	0.021010000000
C	0.574933000000	-3.113172000000	-1.107359000000
H	-0.034772000000	-2.747363000000	-1.940123000000
H	0.566134000000	-4.210675000000	-1.086329000000
C	-3.479632000000	-3.616686000000	0.911480000000

H	-4.012716000000	-4.503134000000	1.241765000000
C	4.392343000000	1.142992000000	1.369994000000
H	3.715058000000	0.799313000000	2.157880000000
H	5.428626000000	1.007062000000	1.700361000000
C	-2.073170000000	-1.310306000000	0.036763000000
C	-4.215537000000	0.022412000000	0.155175000000
C	-1.990125000000	3.684439000000	-0.233789000000
H	-1.453625000000	4.623344000000	-0.302387000000

Sum of electronic and zero-point energies: -1312.410418 Hartrees

Table of atomic coordinates for 2 with Pb(II)

Atoms	X	Y	Z
Pb	1.448433000000	-0.014036000000	-0.698047000000
S	2.918252000000	-0.125670000000	1.761941000000
O	2.004344000000	-2.539739000000	0.052314000000
O	2.273939000000	2.366474000000	0.046273000000
O	-0.427652000000	-0.070505000000	0.373100000000
O	-0.393237000000	2.258268000000	-0.921277000000
C	-4.631090000000	-2.302581000000	0.559302000000
H	-5.660409000000	-2.255009000000	0.896591000000
O	-0.714686000000	-2.334076000000	-0.989332000000
C	-1.695386000000	0.017147000000	0.167173000000
C	1.110624000000	-3.711927000000	-0.097786000000
H	0.574954000000	-3.866808000000	0.847602000000
H	1.727081000000	-4.594715000000	-0.312557000000
O	-5.641751000000	0.267368000000	1.323569000000
C	3.263134000000	2.583533000000	1.128057000000
H	2.724393000000	2.876133000000	2.038160000000
H	3.933837000000	3.399065000000	0.829901000000
C	-2.266945000000	3.740134000000	-0.272195000000
H	-1.755507000000	4.644303000000	-0.579523000000
C	-1.641575000000	2.478374000000	-0.347027000000
C	3.054318000000	-2.831962000000	1.056345000000
H	3.651070000000	-3.681932000000	0.701365000000
H	2.569346000000	-3.106469000000	2.001942000000
C	1.525677000000	3.612068000000	-0.236250000000
H	2.233357000000	4.381496000000	-0.570105000000
H	1.036287000000	3.943923000000	0.687752000000
C	-2.508456000000	-1.189279000000	0.077959000000
C	-3.704638000000	1.428431000000	0.496680000000
C	4.086199000000	1.323668000000	1.343524000000
H	4.758162000000	1.456831000000	2.193162000000
H	4.664847000000	1.054694000000	0.456563000000
C	-1.958091000000	-2.418395000000	-0.381833000000
C	-3.868727000000	-1.128810000000	0.491493000000
C	-4.317608000000	2.686573000000	0.566894000000
H	-5.346937000000	2.763178000000	0.898449000000
C	0.146988000000	-3.499605000000	-1.251274000000
H	0.678688000000	-3.249820000000	-2.172625000000
H	-0.437169000000	-4.407569000000	-1.420553000000
C	-4.049606000000	-3.529747000000	0.177591000000
H	-4.635013000000	-4.442256000000	0.233106000000
C	0.514190000000	3.346687000000	-1.336573000000
H	-0.029388000000	4.259292000000	-1.588093000000
H	0.997017000000	2.970285000000	-2.241776000000

C	-3.587027000000	3.834365000000	0.199033000000
H	-4.054285000000	4.812393000000	0.257560000000
C	3.967089000000	-1.629491000000	1.232202000000
H	4.497440000000	-1.373441000000	0.311706000000
H	4.688335000000	-1.821595000000	2.028559000000
C	-2.344526000000	1.320957000000	0.090367000000
C	-4.485394000000	0.192977000000	0.831018000000
C	-2.733698000000	-3.595231000000	-0.309290000000
H	-2.339985000000	-4.549920000000	-0.638005000000

Sum of electronic and zero-point energies: -1315.647218 Hartrees

Table of atomic coordinates for 3

Atoms	X	Y	Z
Se	3.489143000000	-0.013258000000	-1.452087000000
O	2.552340000000	-2.699891000000	0.276215000000
O	2.517025000000	2.718982000000	0.231882000000
O	-1.008289000000	-0.004537000000	1.802508000000
O	-0.375573000000	2.488721000000	0.867245000000
C	-4.244992000000	-2.483952000000	-0.761546000000
H	-5.238642000000	-2.450064000000	-1.193867000000
O	-0.355952000000	-2.488510000000	0.857353000000
C	-1.819834000000	-0.005377000000	0.839446000000
C	1.834044000000	-3.347990000000	1.370384000000
H	1.756805000000	-2.673065000000	2.235539000000
H	2.369400000000	-4.258912000000	1.681143000000
O	-5.606383000000	-0.016707000000	-0.877313000000
C	3.805204000000	2.139669000000	0.611015000000
H	3.657048000000	1.369428000000	1.383329000000
H	4.453855000000	2.929274000000	1.028505000000
C	-2.285322000000	3.704580000000	-0.067462000000
H	-1.765004000000	4.652380000000	0.005260000000
C	-1.666163000000	2.510511000000	0.372293000000
C	3.809165000000	-2.080348000000	0.695552000000
H	4.461337000000	-2.844799000000	1.152480000000
H	3.609878000000	-1.301877000000	1.447933000000
C	1.819560000000	3.356507000000	1.345346000000
H	2.356218000000	4.268824000000	1.650148000000
H	1.764868000000	2.676093000000	2.208014000000
C	-2.354353000000	-1.282641000000	0.269554000000
C	-3.661539000000	1.269548000000	-0.306945000000
C	4.458992000000	1.559837000000	-0.638718000000
H	5.478160000000	1.228172000000	-0.415896000000
H	4.505139000000	2.319164000000	-1.425757000000
C	-1.643276000000	-2.516632000000	0.354439000000
C	-3.648032000000	-1.288067000000	-0.319891000000
C	-4.271612000000	2.463980000000	-0.734498000000
H	-5.266046000000	2.424730000000	-1.164546000000
C	0.448258000000	-3.723690000000	0.881503000000
H	0.504392000000	-4.156716000000	-0.125235000000
H	-0.013623000000	-4.444638000000	1.568162000000
C	-3.543346000000	-3.692251000000	-0.642283000000
H	-3.993548000000	-4.621498000000	-0.978644000000
C	0.422168000000	3.728139000000	0.887484000000
H	-0.030614000000	4.440076000000	1.589412000000
H	0.456907000000	4.170376000000	-0.116136000000
C	-3.581743000000	3.677883000000	-0.604208000000

H	-4.042511000000	4.606231000000	-0.928513000000
C	4.497630000000	-1.505772000000	-0.537733000000
H	4.626575000000	-2.285808000000	-1.294494000000
H	5.483858000000	-1.111238000000	-0.272622000000
C	-2.366514000000	1.271048000000	0.279278000000
C	-4.397932000000	-0.012152000000	-0.507470000000
C	-2.248922000000	-3.711936000000	-0.100585000000
H	-1.719325000000	-4.655168000000	-0.036098000000

Sum of electronic and zero-point energies: -1311.541685 Hartrees

Table of atomic coordinates for 3 with Pb(II)

Atoms	X	Y	Z
Pb	-1.246019000000	-0.048562000000	-0.847309000000
Se	-2.827856000000	-0.125670000000	1.650643000000
O	-2.231308000000	2.347794000000	-0.269582000000
O	-1.727977000000	-2.592789000000	-0.102646000000
O	0.598610000000	-0.099629000000	0.283346000000
O	1.034904000000	-2.322569000000	-1.092984000000
C	4.357687000000	2.807271000000	0.721184000000
H	5.368416000000	2.916967000000	1.097642000000
O	0.517082000000	2.258463000000	-0.939119000000
C	1.869314000000	0.043815000000	0.143328000000
C	-1.483037000000	3.600689000000	-0.510097000000
H	-1.103113000000	3.972463000000	0.449684000000
H	-2.162210000000	4.344658000000	-0.945946000000
O	5.750477000000	0.427734000000	1.475073000000
C	-2.806200000000	-2.935724000000	0.856457000000
H	-2.347738000000	-3.196095000000	1.819332000000
H	-3.343409000000	-3.812474000000	0.471807000000
C	3.073704000000	-3.513797000000	-0.353745000000
H	2.733189000000	-4.474931000000	-0.720930000000
C	2.253713000000	-2.367966000000	-0.433891000000
C	-3.357651000000	2.574990000000	0.663605000000
H	-4.048169000000	3.295104000000	0.205946000000
H	-2.960013000000	3.004714000000	1.592016000000
C	-0.779597000000	-3.727455000000	-0.209420000000
H	-1.353652000000	-4.640099000000	-0.416929000000
H	-0.259491000000	-3.839730000000	0.750606000000
C	2.465886000000	1.374443000000	0.126166000000
C	4.073034000000	-1.020746000000	0.540716000000
C	-3.789583000000	-1.784739000000	1.001467000000
H	-4.543473000000	-2.034278000000	1.750550000000
H	-4.282167000000	-1.544388000000	0.056064000000
C	1.733371000000	2.513273000000	-0.312839000000
C	3.801363000000	1.527303000000	0.594624000000
C	4.879546000000	-2.164269000000	0.617093000000
H	5.891706000000	-2.082547000000	0.997060000000
C	-0.355333000000	3.318256000000	-1.486140000000
H	-0.736992000000	2.903610000000	-2.422711000000
H	0.201946000000	4.229158000000	-1.712593000000
C	3.594185000000	3.933226000000	0.353352000000
H	4.015228000000	4.928070000000	0.459594000000
C	0.201856000000	-3.509338000000	-1.347059000000
H	0.808016000000	-4.408436000000	-1.486497000000
H	-0.315854000000	-3.288689000000	-2.283442000000

C	4.365475000000	-3.405653000000	0.187198000000
H	4.986215000000	-4.294241000000	0.246901000000
C	-4.100140000000	1.271824000000	0.920901000000
H	-4.551871000000	0.872136000000	0.009638000000
H	-4.875090000000	1.427309000000	1.673791000000
C	2.734683000000	-1.127278000000	0.069446000000
C	4.619070000000	0.317038000000	0.933557000000
C	2.299487000000	3.797475000000	-0.175088000000
H	1.759892000000	4.688774000000	-0.471707000000

Sum of electronic and zero-point energies: -1314.769372 Hartrees

Table of atomic coordinates for 6

Atom	X	Y	Z
Te	4.100705000000	-0.621360000000	-0.154258000000
O	2.528858000000	2.570919000000	-0.106351000000
O	1.109157000000	-2.586036000000	1.413969000000
O	-1.124980000000	0.174787000000	-1.579809000000
O	-0.835501000000	-2.438466000000	-0.753781000000
C	-4.550225000000	2.615011000000	0.801318000000
H	-5.601513000000	2.620085000000	1.066092000000
O	-0.476668000000	2.500427000000	-0.285388000000
C	-2.091649000000	0.153327000000	-0.773134000000
C	1.670850000000	3.475411000000	-0.868921000000
H	1.479941000000	3.062660000000	-1.870675000000
H	2.171397000000	4.451023000000	-0.982396000000
O	-6.118189000000	0.343076000000	0.226960000000
C	2.300613000000	-2.026775000000	2.054851000000
H	3.136037000000	-2.741678000000	1.996789000000
H	2.008691000000	-1.933640000000	3.107097000000
C	-2.985921000000	-3.570705000000	-0.449914000000
H	-2.523977000000	-4.546516000000	-0.552627000000
C	-2.205830000000	-2.397226000000	-0.574721000000
C	3.871591000000	2.482347000000	-0.688280000000
H	4.352460000000	3.474259000000	-0.619986000000
H	3.801146000000	2.209390000000	-1.752432000000
C	1.294061000000	-3.175047000000	0.089685000000
H	1.981195000000	-4.034014000000	0.147817000000
H	1.698307000000	-2.439371000000	-0.619129000000
C	-2.616151000000	1.397789000000	-0.127868000000
C	-4.212248000000	-1.061484000000	-0.172350000000
C	2.697176000000	-0.631049000000	1.532705000000
H	3.213362000000	-0.081135000000	2.327539000000
H	1.805168000000	-0.070923000000	1.240595000000
C	-1.811597000000	2.557956000000	0.077931000000
C	-3.986318000000	1.448533000000	0.252435000000
C	-4.981236000000	-2.234152000000	-0.045804000000
H	-6.038417000000	-2.151624000000	0.180475000000
C	0.361588000000	3.705450000000	-0.140047000000
H	0.533928000000	3.909396000000	0.924210000000
H	-0.149204000000	4.560207000000	-0.601189000000
C	-3.741299000000	3.741282000000	1.010181000000
H	-4.160011000000	4.641797000000	1.449526000000
C	-0.071449000000	-3.646323000000	-0.379813000000
H	0.015791000000	-4.297616000000	-1.257253000000
H	-0.575411000000	-4.181107000000	0.433458000000
C	-4.365392000000	-3.484853000000	-0.203372000000

H	-4.949679000000	-4.396517000000	-0.121210000000
C	4.705251000000	1.462212000000	0.081576000000
H	4.698635000000	1.681274000000	1.155278000000
H	5.742750000000	1.505698000000	-0.268975000000
C	-2.827697000000	-1.118396000000	-0.484564000000
C	-4.865469000000	0.252462000000	0.088680000000
C	-2.382449000000	3.714233000000	0.662775000000
H	-1.775882000000	4.591379000000	0.853489000000

Sum of electronic and zero-point energies: -1310.359451 Hartrees

Table of atomic coordinates for 6 with Pb(II)

Atoms	X	Y	Z
Pb	-1.011669000000	-0.054213000000	-0.934985000000
Te	-2.898990000000	-0.094362000000	1.545396000000
O	-2.105593000000	2.366852000000	-0.579265000000
O	-1.539567000000	-2.607685000000	-0.292492000000
O	0.799459000000	-0.106488000000	0.261992000000
O	1.287474000000	-2.308801000000	-1.123613000000
C	4.535392000000	2.819524000000	0.820583000000
H	5.539276000000	2.929051000000	1.214935000000
O	0.711503000000	2.276974000000	-0.886094000000
C	2.072226000000	0.048616000000	0.163528000000
C	-1.330552000000	3.614682000000	-0.742507000000
H	-1.075359000000	4.003637000000	0.251161000000
H	-1.945075000000	4.352105000000	-1.275221000000
O	5.921994000000	0.442513000000	1.585342000000
C	-2.720211000000	-3.011169000000	0.512928000000
H	-2.371438000000	-3.328977000000	1.504400000000
H	-3.189832000000	-3.869071000000	0.013229000000
C	3.315462000000	-3.494463000000	-0.347685000000
H	2.990992000000	-4.453557000000	-0.733985000000
C	2.489678000000	-2.353273000000	-0.434776000000
C	-3.378250000000	2.622357000000	0.132945000000
H	-4.002058000000	3.265666000000	-0.501968000000
H	-3.153188000000	3.157171000000	1.065014000000
C	-0.562196000000	-3.722781000000	-0.332584000000
H	-1.104614000000	-4.649669000000	-0.560885000000
H	-0.093761000000	-3.814194000000	0.655603000000
C	2.658554000000	1.384005000000	0.181385000000
C	4.274704000000	-1.006205000000	0.599850000000
C	-3.740293000000	-1.884291000000	0.613614000000
H	-4.575573000000	-2.212329000000	1.236969000000
H	-4.125770000000	-1.597165000000	-0.369290000000
C	1.927339000000	2.524827000000	-0.256857000000
C	3.985058000000	1.539126000000	0.674963000000
C	5.087757000000	-2.144918000000	0.681900000000
H	6.090261000000	-2.060262000000	1.086027000000
C	-0.088137000000	3.321209000000	-1.562827000000
H	-0.347567000000	2.890635000000	-2.533922000000
H	0.488455000000	4.232756000000	-1.729392000000
C	3.774958000000	3.945759000000	0.447884000000
H	4.190561000000	4.941229000000	0.568755000000
C	0.474323000000	-3.499387000000	-1.419409000000
H	1.091676000000	-4.395050000000	-1.527062000000
H	0.001479000000	-3.282133000000	-2.379981000000

C	4.593017000000	-3.384485000000	0.225714000000
H	5.218186000000	-4.269667000000	0.289794000000
C	-4.117892000000	1.316844000000	0.401398000000
H	-4.410228000000	0.818304000000	-0.527233000000
H	-5.015301000000	1.523666000000	0.989236000000
C	2.948862000000	-1.115504000000	0.095492000000
C	4.802981000000	0.330424000000	1.018517000000
C	2.489151000000	3.809397000000	-0.100762000000
H	1.949458000000	4.701456000000	-0.394735000000

Sum of electronic and zero-point energies: -1313.593304 Hartrees

Table of atomic coordinates for 6 with Mg(II)

Atoms	X	Y	Z
Mg	0.951058000000	1.035173000000	-0.058493000000
Te	3.630027000000	-0.274949000000	-0.302183000000
O	2.179542000000	2.674679000000	0.026463000000
O	2.123109000000	-2.676532000000	-0.141798000000
O	-0.651117000000	-0.048628000000	-0.139414000000
O	-0.717182000000	-2.664551000000	-0.307258000000
C	-4.742553000000	2.533834000000	0.211032000000
H	-5.824529000000	2.507510000000	0.261584000000
O	-0.511457000000	2.609087000000	-0.104987000000
C	-1.927524000000	-0.023918000000	-0.098666000000
C	1.538067000000	3.817264000000	-0.656719000000
H	1.545030000000	3.623005000000	-1.734929000000
H	2.094096000000	4.736221000000	-0.446926000000
O	-6.101232000000	0.119560000000	0.024988000000
C	2.996910000000	-2.929659000000	1.009956000000
H	3.843885000000	-3.554278000000	0.694291000000
H	2.449521000000	-3.443433000000	1.811604000000
C	-2.875272000000	-3.740018000000	0.017515000000
H	-2.415944000000	-4.719823000000	0.040979000000
C	-2.074309000000	-2.576126000000	-0.121219000000
C	3.663635000000	2.779621000000	0.135724000000
H	3.874283000000	3.662399000000	0.749899000000
H	4.061423000000	2.936776000000	-0.874127000000
C	1.388067000000	-3.784828000000	-0.731502000000
H	1.937037000000	-4.731077000000	-0.620467000000
H	1.308934000000	-3.547414000000	-1.797064000000
C	-2.614990000000	1.290385000000	-0.005146000000
C	-4.122720000000	-1.228261000000	0.000194000000
C	3.461871000000	-1.545407000000	1.477575000000
H	4.439939000000	-1.587782000000	1.962696000000
H	2.737594000000	-1.073242000000	2.145161000000
C	-1.920909000000	2.542975000000	0.038549000000
C	-4.039208000000	1.328786000000	0.073240000000
C	-4.895992000000	-2.391222000000	0.087738000000
H	-5.974131000000	-2.303572000000	0.152107000000
C	0.130045000000	3.965777000000	-0.107936000000
H	0.126249000000	4.332298000000	0.921882000000
H	-0.428427000000	4.635317000000	-0.765291000000
C	-4.037234000000	3.739775000000	0.301911000000
H	-4.562987000000	4.679205000000	0.436287000000
C	-0.009823000000	-3.955873000000	-0.144584000000
H	-0.516587000000	-4.749511000000	-0.705942000000
H	0.004239000000	-4.207223000000	0.922452000000

C	-4.264960000000	-3.647885000000	0.112860000000
H	-4.855393000000	-4.554052000000	0.204231000000
C	4.240342000000	1.523694000000	0.786797000000
H	3.894432000000	1.418108000000	1.820042000000
H	5.331125000000	1.595762000000	0.785086000000
C	-2.695104000000	-1.278215000000	-0.090942000000
C	-4.840329000000	0.073031000000	0.029561000000
C	-2.639153000000	3.742825000000	0.220667000000
H	-2.130359000000	4.691818000000	0.308310000000

Sum of electronic and zero-point energies: -1311.046571 Hartrees