

Understanding *exo*-selective Diels-Alder reactions involving Fischer-type carbene complexes

*Jorge Juan Cabrera-Trujillo and Israel Fernández**

† Departamento de Química Orgánica I and Centro de Innovación en Química Avanzada (ORFEO-CINQA), Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040-Madrid, Spain.

israel@quim.ucm.es

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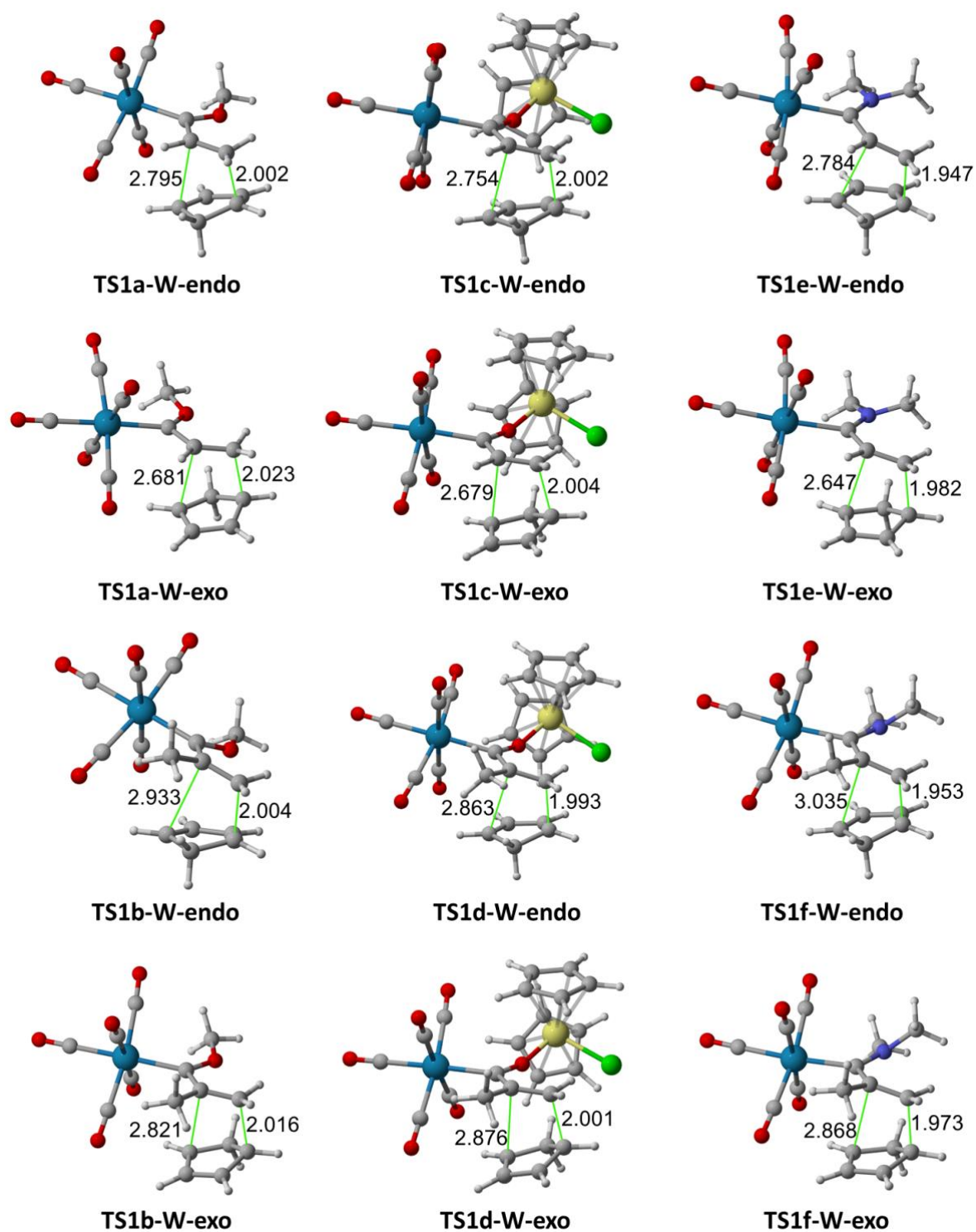


Figure S1. Fully optimized geometries of transition states associated with the Diels-Alder reaction between cyclopentadiene and Fischer carbene complexes **1[a-f]-W**. Bond distances are given in angstroms. All data have been computed at the B3LYP-D3/def2-SVP level.

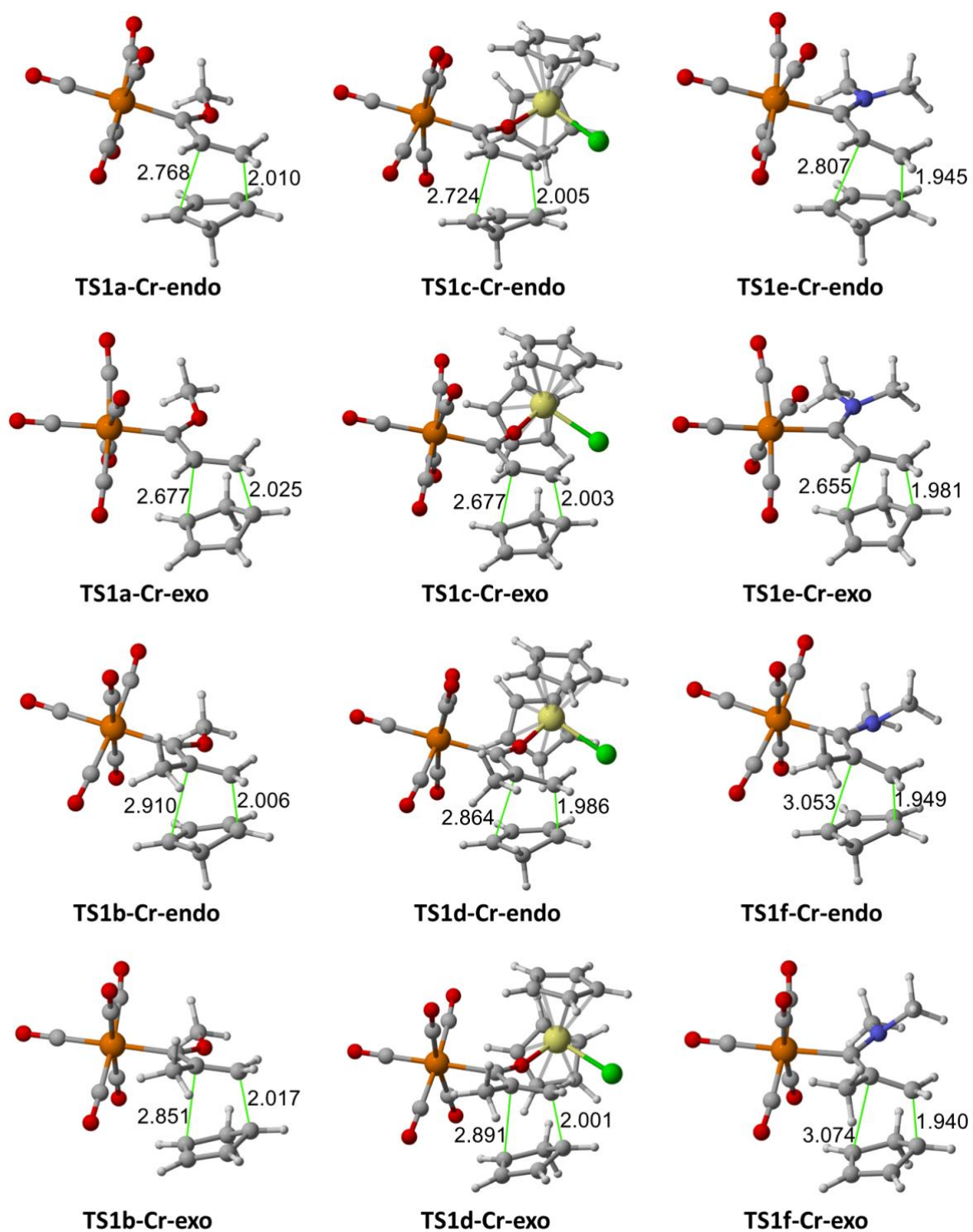


Figure S2. Fully optimized geometries of transition states associated with the Diels-Alder reaction between cyclopentadiene and Fischer carbene complexes **1[a-f]-Cr**. Bond distances are given in angstroms. All data have been computed at the B3LYP-D3/def2-SVP level.

Table S1. Computed HOMO-LUMO energies for all the species involved in the considered Diels-Alder cycloaddition reactions. All data have been computed at the B3LYP-D3/def2-SVP level.

| | HOMO / eV | LUMO / eV | gap / eV HOMO(diene)- LUMO(dienophile) |
|------------------------|-----------|-----------|----------------------------------------------|
| 1a-W | -5.84 | -3.07 | 2.95 |
| 1b-W | -5.79 | -2.91 | 3.11 |
| 1c-W | -5.63 | -3.02 | 3.00 |
| 1d-W | -5.57 | -3.02 | 3.00 |
| 1e-W | -5.39 | -2.25 | 3.77 |
| 1f-W | -5.35 | -2.17 | 3.85 |
| 1a-Cr | -6.07 | -2.69 | 3.33 |
| 1b-Cr | -6.04 | -2.23 | 3.79 |
| 1c-Cr | -5.88 | -2.81 | 3.21 |
| 1d-Cr | -5.85 | -2.80 | 3.22 |
| 1e-Cr | -5.68 | -1.63 | 4.39 |
| 1f-Cr | -5.65 | -1.42 | 4.60 |
| cyclopentadiene | -6.02 | -0.59 | |

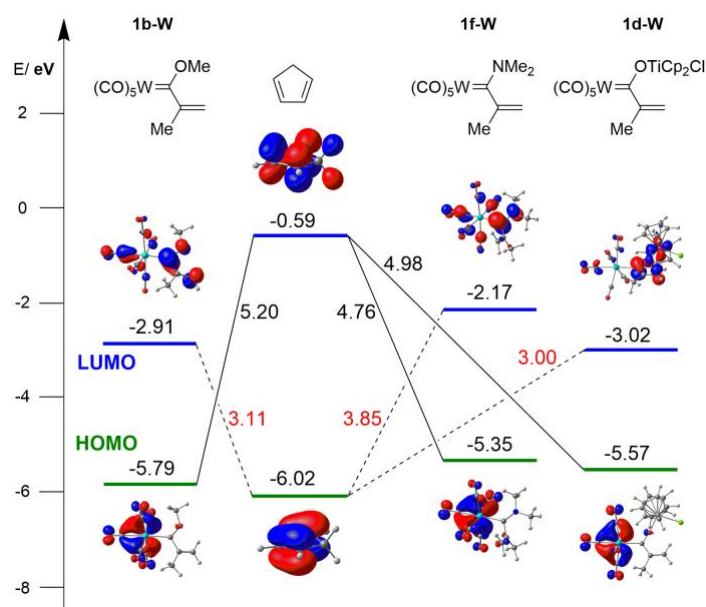


Figure S3. Computed Frontier Molecular Orbital diagram for the Diels-Alder cycloaddition reactions involving cyclopentadiene and carbene complexes **1b-W**, **1d-W** and **1f-W**.

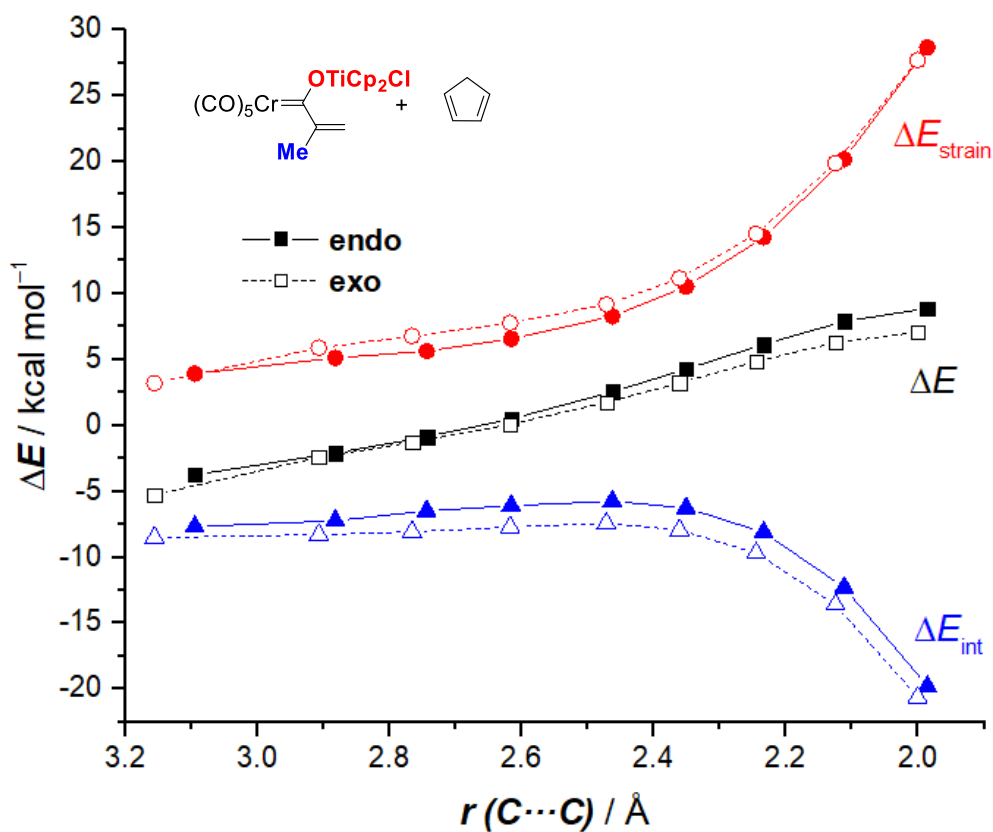


Figure S4. Comparative activation-strain diagrams of the Diels-Alder cycloaddition reactions between cyclopentadiene and Fischer carbene complex **1d-Cr** for the corresponding endo (solid lines) and exo (dashed lines) approaches along the reaction coordinate projected onto the forming C...C bond distance. All data have been computed at the PCM(CH_2Cl_2)-B3LYP-D3/def2-TZVPP//B3LYP-D3/def2-SVP level.

Cartesian coordinates (in Å) and total energies (in a.u., noncorrected ZVPE included) of all the stationary points discussed in the text. All calculations have been performed at the B3LYP-D3/def2-SVP level.

Cyclopentadiene: E= -193.876023

| | | | |
|---|--------------|--------------|--------------|
| C | 0.000000000 | 0.735087000 | -0.993010000 |
| C | 0.000000000 | -0.735087000 | -0.993010000 |
| C | 0.000000000 | -1.181368000 | 0.283835000 |
| C | 0.000000000 | 0.000000000 | 1.216150000 |
| C | 0.000000000 | 1.181368000 | 0.283835000 |
| H | 0.000000000 | 1.353978000 | -1.892651000 |
| H | 0.000000000 | -1.353978000 | -1.892651000 |
| H | 0.000000000 | -2.221152000 | 0.613909000 |
| H | -0.882300000 | 0.000000000 | 1.885347000 |
| H | 0.882300000 | 0.000000000 | 1.885347000 |
| H | 0.000000000 | 2.221152000 | 0.613909000 |

1a-W: E= -863.578005

| | | | |
|---|--------------|--------------|--------------|
| C | -2.620228000 | -1.161940000 | 0.000503000 |
| C | -3.966327000 | -1.200882000 | 0.000547000 |
| H | -4.499732000 | -2.154840000 | 0.000957000 |
| C | -1.809914000 | 0.067977000 | 0.000358000 |
| W | 0.384375000 | -0.056010000 | 0.000059000 |
| C | 0.255836000 | -1.555517000 | 1.471096000 |
| C | 2.466698000 | -0.350388000 | -0.000518000 |
| C | 0.253758000 | -1.554433000 | -1.472064000 |
| C | 0.686268000 | 1.433860000 | -1.446540000 |
| C | 0.685792000 | 1.433445000 | 1.447236000 |
| O | -2.605034000 | 1.130592000 | 0.000182000 |
| O | 0.885064000 | 2.258976000 | 2.230256000 |
| O | 0.200408000 | -2.386754000 | 2.267267000 |
| O | 0.197025000 | -2.385100000 | -2.268725000 |
| O | 3.609032000 | -0.514236000 | -0.000535000 |
| O | 0.886482000 | 2.259164000 | -2.229534000 |
| C | -2.086016000 | 2.453062000 | -0.000120000 |
| H | -4.560247000 | -0.284061000 | 0.000326000 |
| H | -1.476323000 | 2.632661000 | 0.896907000 |
| H | -1.475553000 | 2.632027000 | -0.896727000 |
| H | -2.954352000 | 3.124298000 | -0.000769000 |
| H | -2.056532000 | -2.097614000 | 0.000698000 |

1a-Cr: E= -1841.572533

| | | | |
|----|--------------|--------------|--------------|
| C | 2.303578000 | -1.246540000 | 0.000341000 |
| C | 3.647779000 | -1.299843000 | 0.000022000 |
| H | 4.170795000 | -2.259965000 | -0.000084000 |
| C | 1.496630000 | -0.000744000 | 0.000438000 |
| Cr | -0.555107000 | -0.068120000 | -0.000001000 |
| C | -0.442615000 | -1.409756000 | -1.356749000 |
| C | -2.447505000 | -0.264865000 | -0.000354000 |
| C | -0.443135000 | -1.408763000 | 1.357763000 |
| C | -0.715862000 | 1.263299000 | 1.350350000 |
| C | -0.715082000 | 1.262343000 | -1.351389000 |
| O | 2.328006000 | 1.022194000 | 0.000338000 |
| O | -0.854707000 | 2.054186000 | -2.173864000 |
| O | -0.391854000 | -2.216260000 | -2.171577000 |
| O | -0.392624000 | -2.214690000 | 2.173177000 |
| O | -3.590055000 | -0.386157000 | -0.000618000 |
| O | -0.856035000 | 2.055730000 | 2.172166000 |
| C | 1.927695000 | 2.390736000 | 0.000055000 |
| H | 4.254624000 | -0.391290000 | -0.000155000 |
| H | 1.344156000 | 2.629650000 | -0.898848000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 1.344222000 | 2.630008000 | 0.898905000 |
| H | 2.858318000 | 2.972467000 | -0.000093000 |
| H | 1.739704000 | -2.181209000 | 0.000454000 |

1b-W: E= -902.837723

| | | | |
|---|--------------|--------------|--------------|
| C | -2.815163000 | -0.403150000 | -0.075127000 |
| C | -3.957156000 | 0.034537000 | 0.495917000 |
| H | -4.810131000 | -0.636341000 | 0.629038000 |
| C | -1.653069000 | 0.530320000 | -0.182376000 |
| W | 0.464094000 | -0.075409000 | 0.018271000 |
| C | -0.110518000 | -1.441357000 | 1.506289000 |
| C | 2.436366000 | -0.744697000 | 0.286803000 |
| C | 0.299311000 | -1.574271000 | -1.444372000 |
| C | 1.215888000 | 1.250128000 | -1.422132000 |
| C | 0.872483000 | 1.369901000 | 1.483273000 |
| O | -2.134875000 | 1.759418000 | -0.325579000 |
| O | 1.138191000 | 2.159582000 | 2.283706000 |
| O | -0.409206000 | -2.205073000 | 2.317007000 |
| O | 0.243762000 | -2.409165000 | -2.237742000 |
| O | 3.519453000 | -1.114516000 | 0.437440000 |
| O | 1.673176000 | 1.974544000 | -2.198092000 |
| C | -1.317148000 | 2.921692000 | -0.365001000 |
| H | -4.057848000 | 1.056336000 | 0.864707000 |
| H | -0.740846000 | 3.030826000 | 0.564286000 |
| H | -0.630039000 | 2.885786000 | -1.221357000 |
| H | -2.004864000 | 3.769551000 | -0.478123000 |
| C | -2.695124000 | -1.820349000 | -0.578906000 |
| H | -1.929956000 | -2.394543000 | -0.038038000 |
| H | -3.652306000 | -2.349588000 | -0.469136000 |
| H | -2.416192000 | -1.836635000 | -1.643590000 |

1b-Cr: E= -1880.832875

| | | | |
|----|--------------|--------------|--------------|
| C | -2.499509000 | -0.362652000 | -0.084369000 |
| C | -3.486781000 | 0.014401000 | 0.750237000 |
| H | -4.345219000 | -0.636612000 | 0.938884000 |
| C | -1.300534000 | 0.527127000 | -0.211495000 |
| Cr | 0.638735000 | -0.135826000 | 0.045497000 |
| C | -0.021108000 | -1.509154000 | 1.196499000 |
| C | 2.381385000 | -0.815937000 | 0.365833000 |
| C | 0.471337000 | -1.266230000 | -1.483336000 |
| C | 1.438935000 | 1.171311000 | -1.079515000 |
| C | 0.799626000 | 1.021333000 | 1.545930000 |
| O | -1.760560000 | 1.749119000 | -0.369499000 |
| O | 0.901154000 | 1.718864000 | 2.454744000 |
| O | -0.374491000 | -2.345789000 | 1.898510000 |
| O | 0.401152000 | -1.936889000 | -2.412761000 |
| O | 3.436772000 | -1.226570000 | 0.562042000 |
| O | 1.996160000 | 1.921042000 | -1.751668000 |
| C | -0.951033000 | 2.924424000 | -0.455490000 |
| H | -3.445010000 | 0.959816000 | 1.295378000 |
| H | -0.251685000 | 2.994078000 | 0.387347000 |
| H | -0.397862000 | 2.934958000 | -1.403556000 |
| H | -1.653546000 | 3.766933000 | -0.428661000 |
| C | -2.552929000 | -1.666262000 | -0.843152000 |
| H | -1.828848000 | -2.403632000 | -0.467230000 |
| H | -3.555390000 | -2.110261000 | -0.761577000 |
| H | -2.329907000 | -1.513838000 | -1.910296000 |

1c-W: E= -2520.011961

| | | | |
|---|--------------|-------------|--------------|
| C | 0.379915000 | 2.563184000 | -0.883438000 |
| C | -0.676228000 | 3.335629000 | -1.202017000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -0.537514000 | 4.386915000 | -1.469548000 |
| C | 0.272341000 | 1.140787000 | -0.496818000 |
| W | 2.049237000 | -0.071230000 | 0.020101000 |
| C | 3.222333000 | 1.078958000 | -1.296795000 |
| C | 3.800104000 | -1.134994000 | 0.467363000 |
| C | 2.425215000 | 1.301798000 | 1.569853000 |
| C | 1.064007000 | -1.391965000 | 1.287495000 |
| C | 1.602163000 | -1.432067000 | -1.510563000 |
| O | -0.935004000 | 0.691124000 | -0.483982000 |
| O | 1.323961000 | -2.184675000 | -2.341998000 |
| O | 3.894364000 | 1.687256000 | -2.010013000 |
| O | 2.606333000 | 2.061101000 | 2.418909000 |
| O | 4.766205000 | -1.719654000 | 0.713126000 |
| O | 0.542557000 | -2.172943000 | 1.972258000 |
| H | -1.694081000 | 2.935242000 | -1.206523000 |
| Ti | -2.605981000 | -0.043175000 | -0.007251000 |
| C | -3.829097000 | 0.895405000 | 1.854268000 |
| C | -2.535534000 | 1.478604000 | 1.853455000 |
| C | -1.593683000 | 0.453233000 | 2.117527000 |
| C | -2.291568000 | -0.768985000 | 2.230379000 |
| C | -3.683882000 | -0.491893000 | 2.069077000 |
| H | -4.760431000 | 1.417354000 | 1.652810000 |
| H | -2.306554000 | 2.520939000 | 1.641481000 |
| H | -0.511992000 | 0.570621000 | 2.128062000 |
| H | -1.834570000 | -1.737734000 | 2.414055000 |
| H | -4.494768000 | -1.215585000 | 2.119099000 |
| C | -3.102068000 | -2.380189000 | -0.156750000 |
| C | -1.798028000 | -2.183714000 | -0.674995000 |
| C | -1.918302000 | -1.437124000 | -1.880408000 |
| C | -3.276454000 | -1.134239000 | -2.075488000 |
| C | -4.016308000 | -1.692766000 | -0.992705000 |
| H | -3.350669000 | -2.943717000 | 0.738980000 |
| H | -0.871556000 | -2.546780000 | -0.238322000 |
| H | -1.091194000 | -1.105044000 | -2.501514000 |
| H | -3.686256000 | -0.521331000 | -2.872966000 |
| H | -5.091612000 | -1.607326000 | -0.845900000 |
| Cl | -3.960420000 | 1.587634000 | -1.048522000 |
| H | 1.389473000 | 2.981875000 | -0.885858000 |

1c-Cr: E= -3498.009918

| | | | |
|----|--------------|--------------|--------------|
| C | 0.971631000 | 2.590973000 | 0.246688000 |
| C | -0.049375000 | 3.444875000 | 0.053213000 |
| H | 0.107542000 | 4.525476000 | 0.120486000 |
| C | 0.845854000 | 1.115822000 | 0.128702000 |
| Cr | 2.485416000 | -0.141104000 | 0.002933000 |
| C | 3.697761000 | 1.319332000 | -0.225395000 |
| C | 4.013199000 | -1.258402000 | -0.122941000 |
| C | 2.566436000 | 0.036059000 | 1.896770000 |
| C | 1.474640000 | -1.715664000 | 0.183505000 |
| C | 2.108799000 | -0.149077000 | -1.854734000 |
| O | -0.364256000 | 0.713766000 | 0.071169000 |
| O | 1.804163000 | -0.131787000 | -2.965603000 |
| O | 4.481425000 | 2.147034000 | -0.368200000 |
| O | 2.548500000 | 0.154208000 | 3.040763000 |
| O | 4.935407000 | -1.941444000 | -0.200471000 |
| O | 0.922171000 | -2.727703000 | 0.263254000 |
| H | -1.057298000 | 3.089353000 | -0.176052000 |
| Ti | -2.103909000 | -0.043263000 | 0.005607000 |
| C | -3.445162000 | -0.354322000 | 1.984272000 |
| C | -2.166035000 | 0.105217000 | 2.403380000 |
| C | -1.217920000 | -0.892763000 | 2.080324000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -1.888733000 | -1.942100000 | 1.411511000 |
| C | -3.277551000 | -1.611030000 | 1.367787000 |
| H | -4.376501000 | 0.198747000 | 2.069603000 |
| H | -1.954676000 | 1.073765000 | 2.851230000 |
| H | -0.146380000 | -0.829960000 | 2.249040000 |
| H | -1.416979000 | -2.840171000 | 1.022071000 |
| H | -4.069803000 | -2.220130000 | 0.937566000 |
| C | -2.531643000 | -1.832923000 | -1.514175000 |
| C | -1.283487000 | -1.276998000 | -1.872714000 |
| C | -1.513359000 | 0.044233000 | -2.352082000 |
| C | -2.893801000 | 0.303466000 | -2.271577000 |
| C | -3.529632000 | -0.841096000 | -1.716968000 |
| H | -2.693265000 | -2.839562000 | -1.136973000 |
| H | -0.320127000 | -1.772339000 | -1.800433000 |
| H | -0.743828000 | 0.739003000 | -2.679636000 |
| H | -3.382385000 | 1.241242000 | -2.517911000 |
| H | -4.594099000 | -0.940992000 | -1.511194000 |
| C1 | -3.329038000 | 1.982957000 | 0.131191000 |
| H | 1.968452000 | 2.977380000 | 0.467527000 |

1d-w: E= -2559.272855

| | | | |
|----|--------------|--------------|--------------|
| C | 0.322941000 | 2.646416000 | -0.559548000 |
| C | -0.815662000 | 3.331365000 | -0.808240000 |
| H | -0.788461000 | 4.417038000 | -0.940696000 |
| C | 0.266123000 | 1.164446000 | -0.358168000 |
| W | 1.991005000 | -0.206919000 | 0.027834000 |
| C | 3.369243000 | 0.897643000 | -1.109089000 |
| C | 3.612738000 | -1.491544000 | 0.348611000 |
| C | 2.438960000 | 0.882166000 | 1.765148000 |
| C | 0.921740000 | -1.612706000 | 1.120494000 |
| C | 1.452393000 | -1.267491000 | -1.696581000 |
| O | -0.929686000 | 0.679444000 | -0.422675000 |
| O | 1.130486000 | -1.855753000 | -2.637722000 |
| O | 4.177510000 | 1.446729000 | -1.724066000 |
| O | 2.662326000 | 1.490944000 | 2.720437000 |
| O | 4.507762000 | -2.202104000 | 0.523947000 |
| O | 0.383090000 | -2.459241000 | 1.707965000 |
| H | -1.785544000 | 2.841276000 | -0.893704000 |
| C | 1.643936000 | 3.370763000 | -0.477464000 |
| H | 2.252212000 | 3.197359000 | -1.377423000 |
| H | 1.483735000 | 4.455353000 | -0.392467000 |
| H | 2.242507000 | 3.046733000 | 0.384576000 |
| Ti | -2.630202000 | -0.061090000 | -0.010219000 |
| C | -3.843792000 | 0.748375000 | 1.919116000 |
| C | -2.539562000 | 1.305869000 | 1.965475000 |
| C | -1.617860000 | 0.245226000 | 2.148890000 |
| C | -2.338575000 | -0.968865000 | 2.163580000 |
| C | -3.724724000 | -0.653769000 | 2.023053000 |
| H | -4.765037000 | 1.300998000 | 1.758422000 |
| H | -2.289657000 | 2.357031000 | 1.836939000 |
| H | -0.534389000 | 0.340366000 | 2.171396000 |
| H | -1.900567000 | -1.956732000 | 2.273827000 |
| H | -4.547839000 | -1.365418000 | 2.011541000 |
| C | -3.102751000 | -2.383522000 | -0.337620000 |
| C | -1.841821000 | -2.115716000 | -0.921838000 |
| C | -2.052212000 | -1.261882000 | -2.041484000 |
| C | -3.426851000 | -0.981181000 | -2.124359000 |
| C | -4.082845000 | -1.645682000 | -1.049728000 |
| H | -3.282254000 | -3.030157000 | 0.517480000 |
| H | -0.884390000 | -2.495877000 | -0.579243000 |
| H | -1.273999000 | -0.857103000 | -2.682387000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -3.900066000 | -0.315149000 | -2.839505000 |
| H | -5.148131000 | -1.602161000 | -0.829902000 |
| Cl | -3.979323000 | 1.662521000 | -0.906960000 |

1d-Cr: E= -3537.271577

| | | | |
|----|--------------|--------------|--------------|
| C | 0.890227000 | 2.416173000 | -0.385505000 |
| C | 0.103740000 | 2.949199000 | -1.337860000 |
| H | 0.152233000 | 4.014203000 | -1.582585000 |
| C | 0.821157000 | 0.934680000 | -0.154354000 |
| Cr | 2.427835000 | -0.364337000 | 0.026237000 |
| C | 3.624957000 | 0.868925000 | -0.808128000 |
| C | 3.897884000 | -1.553294000 | 0.154345000 |
| C | 2.726799000 | 0.387368000 | 1.749586000 |
| C | 1.353698000 | -1.718674000 | 0.773752000 |
| C | 1.900486000 | -0.968283000 | -1.688105000 |
| O | -0.376714000 | 0.502489000 | -0.170123000 |
| O | 1.520123000 | -1.311334000 | -2.720263000 |
| O | 4.388542000 | 1.553549000 | -1.325635000 |
| O | 2.853850000 | 0.848379000 | 2.795990000 |
| O | 4.786822000 | -2.279092000 | 0.235223000 |
| O | 0.728092000 | -2.593134000 | 1.196193000 |
| H | -0.606572000 | 2.339331000 | -1.897583000 |
| C | 1.830904000 | 3.243038000 | 0.455216000 |
| H | 2.887701000 | 3.009318000 | 0.264903000 |
| H | 1.678890000 | 4.314043000 | 0.257663000 |
| H | 1.656584000 | 3.064654000 | 1.528466000 |
| Ti | -2.181436000 | -0.048141000 | 0.022950000 |
| C | -3.493106000 | 0.440394000 | 1.980584000 |
| C | -2.178567000 | 0.925655000 | 2.224408000 |
| C | -1.306336000 | -0.185245000 | 2.270861000 |
| C | -2.058712000 | -1.352575000 | 2.004535000 |
| C | -3.422301000 | -0.961699000 | 1.842760000 |
| H | -4.382400000 | 1.053642000 | 1.860682000 |
| H | -1.895014000 | 1.972533000 | 2.306465000 |
| H | -0.228865000 | -0.144682000 | 2.408449000 |
| H | -1.653755000 | -2.359748000 | 1.950353000 |
| H | -4.261788000 | -1.625832000 | 1.648384000 |
| C | -2.769362000 | -2.218350000 | -0.784659000 |
| C | -1.516759000 | -1.895258000 | -1.349398000 |
| C | -1.706000000 | -0.796802000 | -2.236506000 |
| C | -3.068674000 | -0.443384000 | -2.209145000 |
| C | -3.729315000 | -1.292629000 | -1.282043000 |
| H | -2.960285000 | -3.026626000 | -0.083220000 |
| H | -0.574010000 | -2.392488000 | -1.138266000 |
| H | -0.920055000 | -0.304636000 | -2.803963000 |
| H | -3.523613000 | 0.384753000 | -2.743945000 |
| H | -4.786542000 | -1.255489000 | -1.025055000 |
| Cl | -3.145235000 | 2.018703000 | -0.558735000 |

1e-W: E= -882.984537

| | | | |
|---|--------------|--------------|--------------|
| C | -2.110987000 | 1.585377000 | 0.380793000 |
| C | -2.810243000 | 2.317031000 | -0.499352000 |
| H | -3.004185000 | 3.377924000 | -0.323025000 |
| C | -1.665499000 | 0.183488000 | 0.154752000 |
| W | 0.558747000 | -0.003623000 | 0.002895000 |
| C | 0.613843000 | 1.819611000 | -1.037955000 |
| C | 2.646446000 | -0.072029000 | -0.057586000 |
| C | 0.734314000 | 1.046275000 | 1.809573000 |
| C | 0.594267000 | -1.827608000 | 1.030359000 |
| C | 0.541500000 | -1.039322000 | -1.818623000 |
| N | -2.619254000 | -0.743415000 | 0.063253000 |

| | | | |
|---|--------------|--------------|--------------|
| O | 0.547889000 | -1.625011000 | -2.816136000 |
| O | 0.646161000 | 2.825529000 | -1.602191000 |
| O | 0.832415000 | 1.640209000 | 2.795867000 |
| O | 3.802147000 | -0.114324000 | -0.087076000 |
| O | 0.631440000 | -2.843800000 | 1.582811000 |
| C | -2.313331000 | -2.139345000 | -0.245768000 |
| H | -1.722263000 | 2.061273000 | 1.287529000 |
| H | -3.167771000 | 1.892411000 | -1.442712000 |
| H | -1.410585000 | -2.204621000 | -0.859372000 |
| H | -2.153312000 | -2.714107000 | 0.680744000 |
| H | -3.155941000 | -2.582381000 | -0.796138000 |
| C | -4.039639000 | -0.531515000 | 0.364538000 |
| H | -4.377534000 | -1.322113000 | 1.053226000 |
| H | -4.201727000 | 0.445522000 | 0.827789000 |
| H | -4.643615000 | -0.594461000 | -0.555630000 |

1e-Cr: E= -1860.980702

| | | | |
|----|--------------|--------------|--------------|
| C | 1.758524000 | 1.593764000 | -0.442835000 |
| C | 2.432649000 | 2.378924000 | 0.411090000 |
| H | 2.587893000 | 3.439976000 | 0.200883000 |
| C | 1.340042000 | 0.202028000 | -0.158072000 |
| Cr | -0.775525000 | -0.022414000 | -0.001801000 |
| C | -0.907930000 | 1.721589000 | 0.768725000 |
| C | -2.650114000 | -0.172223000 | 0.097620000 |
| C | -0.911487000 | 0.729950000 | -1.743521000 |
| C | -0.727519000 | -1.750148000 | -0.787304000 |
| C | -0.589809000 | -0.740160000 | 1.748219000 |
| N | 2.316275000 | -0.686575000 | -0.050132000 |
| O | -0.476519000 | -1.170464000 | 2.809861000 |
| O | -1.025905000 | 2.763216000 | 1.237397000 |
| O | -0.991585000 | 1.191758000 | -2.794176000 |
| O | -3.795875000 | -0.272115000 | 0.159076000 |
| O | -0.738040000 | -2.793754000 | -1.274065000 |
| C | 2.096930000 | -2.081138000 | 0.347872000 |
| H | 1.354156000 | 2.030714000 | -1.363052000 |
| H | 2.801528000 | 2.001088000 | 1.369976000 |
| H | 1.192401000 | -2.178049000 | 0.950151000 |
| H | 2.008415000 | -2.724396000 | -0.541508000 |
| H | 2.956090000 | -2.420525000 | 0.944861000 |
| C | 3.731385000 | -0.443781000 | -0.385472000 |
| H | 4.088892000 | -1.272578000 | -1.016072000 |
| H | 3.851475000 | 0.500646000 | -0.922862000 |
| H | 4.345199000 | -0.414863000 | 0.529088000 |

1f-W: E= -922.250526

| | | | |
|---|--------------|--------------|--------------|
| C | -2.318259000 | 1.188697000 | 0.117140000 |
| C | -2.507533000 | 1.871393000 | 1.255998000 |
| H | -3.027526000 | 2.833255000 | 1.257230000 |
| C | -1.590594000 | -0.126480000 | 0.106159000 |
| W | 0.639609000 | 0.001426000 | -0.000963000 |
| C | 0.635918000 | 1.521096000 | 1.446870000 |
| C | 2.717676000 | 0.195371000 | -0.113020000 |
| C | 0.961517000 | -1.425913000 | 1.500199000 |
| C | 0.766608000 | -1.481737000 | -1.473392000 |
| C | 0.551842000 | 1.488282000 | -1.472650000 |
| N | -2.381101000 | -1.201557000 | 0.112008000 |
| O | 0.536210000 | 2.318635000 | -2.277382000 |
| O | 0.658103000 | 2.367920000 | 2.230572000 |
| O | 1.169089000 | -2.215987000 | 2.319484000 |
| O | 3.868308000 | 0.296136000 | -0.178722000 |
| O | 0.863486000 | -2.306425000 | -2.279677000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.840878000 | -2.554966000 | -0.015706000 |
| H | -2.128602000 | 1.502895000 | 2.212036000 |
| H | -1.657505000 | -2.797852000 | -1.074089000 |
| H | -0.894503000 | -2.640518000 | 0.527576000 |
| H | -2.557875000 | -3.278346000 | 0.395009000 |
| C | -2.810259000 | 1.672921000 | -1.227651000 |
| H | -3.432571000 | 0.911763000 | -1.727637000 |
| H | -3.404406000 | 2.592201000 | -1.121362000 |
| H | -1.968685000 | 1.883274000 | -1.903140000 |
| C | -3.845999000 | -1.163157000 | 0.157172000 |
| H | -4.204811000 | -1.821678000 | 0.963451000 |
| H | -4.203922000 | -0.148581000 | 0.353603000 |
| H | -4.264736000 | -1.526343000 | -0.796409000 |

1f-Cr: E= -1900.246576

| | | | |
|----|--------------|--------------|--------------|
| C | -1.962756000 | -1.204628000 | -0.131223000 |
| C | -2.123071000 | -1.923000000 | -1.252994000 |
| H | -2.622472000 | -2.895271000 | -1.227244000 |
| C | -1.250594000 | 0.109369000 | -0.090371000 |
| Cr | 0.874842000 | -0.000832000 | 0.019258000 |
| C | 0.858262000 | -0.769845000 | -1.722435000 |
| C | 2.748368000 | -0.151975000 | 0.130102000 |
| C | 1.157384000 | 1.687137000 | -0.798660000 |
| C | 0.773090000 | 0.768203000 | 1.753672000 |
| C | 0.783297000 | -1.751738000 | 0.773075000 |
| N | -2.054654000 | 1.161861000 | -0.076561000 |
| O | 0.798495000 | -2.811064000 | 1.218923000 |
| O | 0.855013000 | -1.226788000 | -2.777444000 |
| O | 1.400611000 | 2.690234000 | -1.310397000 |
| O | 3.894810000 | -0.235017000 | 0.204204000 |
| O | 0.682343000 | 1.235609000 | 2.801818000 |
| C | -1.580758000 | 2.539431000 | 0.103080000 |
| H | -1.749995000 | -1.577938000 | -2.219350000 |
| H | -2.376512000 | 3.130663000 | 0.577695000 |
| H | -0.697918000 | 2.566156000 | 0.745550000 |
| H | -1.334137000 | 2.994715000 | -0.868001000 |
| C | -2.464327000 | -1.669048000 | 1.219040000 |
| H | -3.244736000 | -0.992284000 | 1.607328000 |
| H | -2.884002000 | -2.683350000 | 1.156664000 |
| H | -1.653582000 | -1.675321000 | 1.963472000 |
| C | -3.513249000 | 1.110048000 | -0.276729000 |
| H | -3.795676000 | 1.848046000 | -1.043541000 |
| H | -3.823798000 | 0.116953000 | -0.614307000 |
| H | -4.034860000 | 1.367067000 | 0.659272000 |

RC1a-W-endo: E= -1057.467635

| | | | |
|---|--------------|--------------|--------------|
| C | 1.300935000 | -1.961441000 | 0.943006000 |
| C | 2.435840000 | -2.391090000 | 1.526744000 |
| H | 2.807913000 | -3.403853000 | 1.351736000 |
| C | 0.734724000 | -0.612358000 | 1.101526000 |
| W | -1.030089000 | -0.012530000 | -0.067811000 |
| C | -0.157480000 | -0.910943000 | -1.750086000 |
| C | -2.705394000 | 0.413988000 | -1.259973000 |
| C | -1.922273000 | -1.860321000 | 0.393745000 |
| C | -2.038009000 | 0.934703000 | 1.511449000 |
| C | -0.280478000 | 1.870826000 | -0.591224000 |
| O | 1.442291000 | 0.068600000 | 1.990401000 |
| O | 0.108366000 | 2.917612000 | -0.890160000 |
| O | 0.318610000 | -1.407522000 | -2.677292000 |
| O | -2.422490000 | -2.872029000 | 0.629458000 |
| O | -3.627580000 | 0.646322000 | -1.914953000 |

| | | | |
|---|--------------|--------------|--------------|
| O | -2.617002000 | 1.471773000 | 2.354545000 |
| C | 1.128207000 | 1.410928000 | 2.330789000 |
| H | 0.747842000 | -2.632985000 | 0.282301000 |
| H | 3.020403000 | -1.736139000 | 2.175127000 |
| H | 1.226783000 | 2.064787000 | 1.454199000 |
| H | 0.107145000 | 1.482434000 | 2.731650000 |
| H | 1.853328000 | 1.709056000 | 3.098777000 |
| C | 2.738959000 | 0.784302000 | -1.525742000 |
| C | 3.195607000 | 1.571059000 | -0.523714000 |
| C | 4.229243000 | 0.846397000 | 0.226713000 |
| C | 4.409383000 | -0.375059000 | -0.329141000 |
| C | 3.481982000 | -0.521741000 | -1.503067000 |
| H | 1.975550000 | 1.040375000 | -2.259082000 |
| H | 2.856074000 | 2.585182000 | -0.306021000 |
| H | 4.761313000 | 1.244726000 | 1.092945000 |
| H | 5.109254000 | -1.144603000 | -0.001477000 |
| H | 2.801944000 | -1.385096000 | -1.396361000 |
| H | 4.033970000 | -0.690262000 | -2.447928000 |

RC1a-W-exo: E= -1057.466828

| | | | |
|---|--------------|--------------|--------------|
| C | 4.695270000 | -1.142632000 | 0.040270000 |
| C | 3.472675000 | -1.559185000 | -0.652294000 |
| C | 2.924688000 | -0.486523000 | -1.272391000 |
| C | 4.892084000 | 0.183536000 | -0.156495000 |
| C | 3.786609000 | 0.718712000 | -1.025003000 |
| H | 5.334248000 | -1.808233000 | 0.624066000 |
| H | 3.064542000 | -2.570462000 | -0.645317000 |
| H | 2.000578000 | -0.467295000 | -1.848699000 |
| H | 5.717523000 | 0.785482000 | 0.225836000 |
| H | 3.224450000 | 1.528584000 | -0.526330000 |
| H | 4.174273000 | 1.149804000 | -1.968271000 |
| C | 1.596260000 | 0.106318000 | 1.729350000 |
| C | 2.695388000 | 0.614193000 | 2.320949000 |
| H | 3.307776000 | 0.000301000 | 2.984585000 |
| C | 0.711957000 | 0.840270000 | 0.815625000 |
| W | -1.089219000 | -0.115597000 | -0.006149000 |
| C | -0.034818000 | -1.912927000 | -0.255388000 |
| C | -0.692037000 | 0.456457000 | -1.980244000 |
| C | -1.571454000 | -0.745563000 | 1.945101000 |
| C | -2.779026000 | -1.150566000 | -0.702696000 |
| C | -2.333334000 | 1.563220000 | 0.153479000 |
| O | 0.513451000 | -2.918537000 | -0.394977000 |
| O | -3.708945000 | -1.719392000 | -1.083075000 |
| O | -3.051965000 | 2.466638000 | 0.213465000 |
| O | -1.835835000 | -1.104528000 | 3.007269000 |
| O | -0.474790000 | 0.764764000 | -3.073208000 |
| O | 1.182096000 | 2.070997000 | 0.625827000 |
| C | 0.526353000 | 3.008307000 | -0.217352000 |
| H | 1.319447000 | -0.932452000 | 1.918784000 |
| H | 3.006298000 | 1.647525000 | 2.156167000 |
| H | -0.468934000 | 3.257629000 | 0.176934000 |
| H | 1.156883000 | 3.906880000 | -0.223077000 |
| H | 0.429314000 | 2.615151000 | -1.239542000 |

RC1a-Cr-endo: E= -2035.461388

| | | | |
|----|--------------|--------------|--------------|
| C | 1.017324000 | 0.016690000 | 1.896843000 |
| C | 2.137551000 | 0.483659000 | 2.479568000 |
| H | 2.637325000 | -0.082880000 | 3.269731000 |
| C | 0.279375000 | 0.699655000 | 0.812414000 |
| Cr | -1.395192000 | -0.156050000 | -0.037661000 |
| C | -0.515579000 | -1.842053000 | 0.050175000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.927340000 | -1.031248000 | -0.739652000 |
| C | -2.058384000 | -0.393807000 | 1.739613000 |
| C | -2.334894000 | 1.494539000 | -0.168264000 |
| C | -0.688868000 | 0.070766000 | -1.784861000 |
| O | 0.877414000 | 1.848639000 | 0.570614000 |
| O | -0.254900000 | 0.183390000 | -2.845315000 |
| O | 0.005034000 | -2.866472000 | 0.086745000 |
| O | -2.454555000 | -0.543051000 | 2.806433000 |
| O | -3.853718000 | -1.562595000 | -1.165299000 |
| O | -2.948549000 | 2.462879000 | -0.263793000 |
| C | 0.456258000 | 2.786226000 | -0.413920000 |
| H | 0.609931000 | -0.941403000 | 2.223825000 |
| H | 2.581430000 | 1.433757000 | 2.180202000 |
| H | 0.266813000 | 2.298264000 | -1.377634000 |
| H | -0.449043000 | 3.310987000 | -0.078826000 |
| H | 1.280703000 | 3.503550000 | -0.516728000 |
| C | 2.588583000 | -1.048079000 | -1.222891000 |
| C | 2.858970000 | 0.259197000 | -1.446793000 |
| C | 3.912760000 | 0.698726000 | -0.526566000 |
| C | 4.285985000 | -0.342937000 | 0.255891000 |
| C | 3.482096000 | -1.554994000 | -0.126093000 |
| H | 1.854629000 | -1.660502000 | -1.745235000 |
| H | 2.371339000 | 0.891999000 | -2.189772000 |
| H | 4.321303000 | 1.710620000 | -0.488848000 |
| H | 5.052631000 | -0.334063000 | 1.031707000 |
| H | 2.900897000 | -1.961141000 | 0.721722000 |
| H | 4.127815000 | -2.384341000 | -0.474115000 |

RC1a-Cr-exo: E= -2035.460624

| | | | |
|----|--------------|--------------|--------------|
| C | 4.275614000 | -1.126135000 | 0.284287000 |
| C | 3.149025000 | -1.581408000 | -0.533775000 |
| C | 2.696887000 | -0.547985000 | -1.285375000 |
| C | 4.508143000 | 0.185690000 | 0.036156000 |
| C | 3.530670000 | 0.668527000 | -1.000244000 |
| H | 4.825794000 | -1.755898000 | 0.986299000 |
| H | 2.735290000 | -2.590475000 | -0.520015000 |
| H | 1.872691000 | -0.570153000 | -1.998255000 |
| H | 5.281825000 | 0.808611000 | 0.487011000 |
| H | 2.914707000 | 1.507958000 | -0.630182000 |
| H | 4.042743000 | 1.040052000 | -1.908846000 |
| C | 1.177486000 | 0.210208000 | 1.608711000 |
| C | 2.191198000 | 0.856988000 | 2.215033000 |
| H | 2.816511000 | 0.349844000 | 2.952828000 |
| C | 0.255249000 | 0.805578000 | 0.621904000 |
| Cr | -1.430194000 | -0.197402000 | -0.012816000 |
| C | -0.432338000 | -1.819842000 | -0.062414000 |
| C | -0.956673000 | 0.094775000 | -1.826399000 |
| C | -1.829577000 | -0.502035000 | 1.833134000 |
| C | -2.959001000 | -1.195437000 | -0.537334000 |
| C | -2.533860000 | 1.353509000 | 0.004231000 |
| O | 0.129617000 | -2.820886000 | -0.107729000 |
| O | -3.883984000 | -1.797391000 | -0.858732000 |
| O | -3.252425000 | 2.251977000 | 0.004178000 |
| O | -2.064634000 | -0.690642000 | 2.940148000 |
| O | -0.644531000 | 0.244178000 | -2.924854000 |
| O | 0.712135000 | 2.003877000 | 0.298709000 |
| C | 0.053171000 | 2.910501000 | -0.581583000 |
| H | 0.988010000 | -0.831529000 | 1.870313000 |
| H | 2.413104000 | 1.904195000 | 1.999406000 |
| H | -0.852403000 | 3.314204000 | -0.109051000 |
| H | 0.767272000 | 3.724788000 | -0.760644000 |

H -0.206267000 2.429528000 -1.533041000

RC1b-W-endo: E= -1096.726092

C -1.656856000 -1.155869000 -1.357573000
C -2.697331000 -1.019216000 -2.211726000
H -3.326259000 -1.877466000 -2.462268000
C -0.799217000 0.023224000 -1.039293000
W 1.129008000 -0.017557000 0.066854000
C 0.343948000 -1.267065000 1.551707000
C 2.936935000 -0.135828000 1.122478000
C 1.791947000 -1.672816000 -1.042909000
C 2.135775000 1.259848000 -1.257413000
C 0.653608000 1.639793000 1.249782000
O -1.374154000 1.099632000 -1.564150000
O 0.412774000 2.552946000 1.918922000
O -0.055719000 -1.944055000 2.398254000
O 2.184710000 -2.583106000 -1.632819000
O 3.932455000 -0.202005000 1.704414000
O 2.731375000 1.968367000 -1.949929000
C -0.843778000 2.411628000 -1.489951000
H -2.939184000 -0.066457000 -2.679821000
H -0.730582000 2.732535000 -0.445914000
H 0.125676000 2.477138000 -2.002719000
H -1.572712000 3.058020000 -1.995981000
C -3.072051000 -0.250210000 1.650471000
C -2.892789000 1.035595000 1.265672000
C -3.922964000 1.395604000 0.285542000
C -4.731545000 0.330161000 0.075292000
C -4.273557000 -0.811396000 0.942207000
H -2.464863000 -0.806846000 2.364320000
H -2.109703000 1.706278000 1.620383000
H -4.007431000 2.372228000 -0.194683000
H -5.590791000 0.284398000 -0.594844000
H -4.029757000 -1.713561000 0.352765000
H -5.058806000 -1.121265000 1.658969000
C -1.389746000 -2.500652000 -0.726354000
H -1.583175000 -2.474576000 0.354924000
H -2.049842000 -3.263740000 -1.163090000
H -0.354965000 -2.838542000 -0.864320000

RC1b-W-exo: E= -1096.727159

C 4.474783000 -1.373049000 0.056611000
C 3.285401000 -1.712482000 -0.736296000
C 2.900649000 -0.628206000 -1.450643000
C 4.815230000 -0.084675000 -0.179783000
C 3.846640000 0.506314000 -1.167174000
H 4.988520000 -2.063503000 0.728415000
H 2.791272000 -2.684984000 -0.727548000
H 2.053078000 -0.567802000 -2.132264000
H 5.650526000 0.462191000 0.259484000
H 3.322319000 1.386356000 -0.752958000
H 4.355716000 0.857278000 -2.085852000
C 1.510213000 0.973709000 1.675756000
C 2.118685000 2.065439000 2.188699000
H 2.712003000 1.994632000 3.104091000
C 0.664714000 1.115985000 0.454584000
W -1.105398000 -0.119994000 -0.017239000
C -0.091327000 -1.930358000 0.296491000
C -0.700182000 -0.266385000 -2.063109000
C -1.650027000 -0.061206000 2.012068000
C -2.799601000 -1.312528000 -0.354588000

| | | | |
|---|--------------|--------------|--------------|
| C | -2.342506000 | 1.523058000 | -0.423152000 |
| O | 0.421772000 | -2.950696000 | 0.456994000 |
| O | -3.733122000 | -1.966937000 | -0.537117000 |
| O | -3.059485000 | 2.396270000 | -0.667008000 |
| O | -1.961144000 | -0.049574000 | 3.122037000 |
| O | -0.492958000 | -0.366797000 | -3.197179000 |
| O | 1.123031000 | 2.157067000 | -0.238137000 |
| C | 0.513725000 | 2.643789000 | -1.425669000 |
| H | 2.019324000 | 3.049059000 | 1.727757000 |
| H | -0.510311000 | 2.990099000 | -1.230466000 |
| H | 1.133774000 | 3.486828000 | -1.756887000 |
| H | 0.498212000 | 1.868424000 | -2.202963000 |
| C | 1.664107000 | -0.372560000 | 2.335601000 |
| H | 2.328160000 | -0.298839000 | 3.207985000 |
| H | 0.703800000 | -0.785512000 | 2.673467000 |
| H | 2.105308000 | -1.090394000 | 1.630327000 |

RC1b-Cr-endo: E= -2074.722549

| | | | |
|----|--------------|--------------|--------------|
| C | -0.473198000 | -2.252500000 | -0.228848000 |
| C | -0.722321000 | -3.131193000 | -1.219771000 |
| H | -0.821415000 | -4.200676000 | -1.012959000 |
| C | -0.234907000 | -0.818510000 | -0.600073000 |
| Cr | 1.392405000 | 0.276962000 | 0.058547000 |
| C | 0.776112000 | 0.114269000 | 1.851166000 |
| C | 2.940651000 | 1.190112000 | 0.661994000 |
| C | 2.392882000 | -1.343708000 | 0.185292000 |
| C | 1.969506000 | 0.478511000 | -1.744320000 |
| C | 0.507473000 | 1.957867000 | 0.004274000 |
| O | -1.154473000 | -0.505264000 | -1.483772000 |
| O | 0.035200000 | 3.007265000 | 0.026417000 |
| O | 0.398119000 | 0.057586000 | 2.935433000 |
| O | 3.031018000 | -2.294180000 | 0.273110000 |
| O | 3.880092000 | 1.742813000 | 1.027574000 |
| O | 2.331619000 | 0.604673000 | -2.828507000 |
| C | -1.234353000 | 0.744665000 | -2.173222000 |
| H | -0.792583000 | -2.813403000 | -2.261973000 |
| H | -1.487700000 | 1.543087000 | -1.467737000 |
| H | -0.295246000 | 0.969216000 | -2.694166000 |
| H | -2.052397000 | 0.626942000 | -2.893623000 |
| C | -2.801601000 | 0.303459000 | 1.383988000 |
| C | -2.998248000 | 1.549860000 | 0.892114000 |
| C | -3.976891000 | 1.488452000 | -0.202370000 |
| C | -4.370747000 | 0.205229000 | -0.376599000 |
| C | -3.660747000 | -0.667366000 | 0.621109000 |
| H | -2.143463000 | 0.033300000 | 2.209548000 |
| H | -2.509895000 | 2.462434000 | 1.237970000 |
| H | -4.319115000 | 2.352098000 | -0.776349000 |
| H | -5.086369000 | -0.164666000 | -1.112120000 |
| H | -3.062342000 | -1.450079000 | 0.119043000 |
| H | -4.369052000 | -1.201546000 | 1.283257000 |
| C | -0.376882000 | -2.695999000 | 1.210347000 |
| H | -1.011356000 | -2.074421000 | 1.858652000 |
| H | -0.706515000 | -3.740281000 | 1.307172000 |
| H | 0.646748000 | -2.631120000 | 1.605633000 |

RC1b-Cr-exo: E= -2074.722461

| | | | |
|---|-------------|--------------|--------------|
| C | 2.763672000 | 0.580403000 | -1.545394000 |
| C | 2.946537000 | 1.761547000 | -0.689803000 |
| C | 3.725098000 | 1.429907000 | 0.366365000 |
| C | 3.433141000 | -0.465353000 | -1.006391000 |
| C | 4.092040000 | -0.025674000 | 0.270256000 |

| | | | |
|----|--------------|--------------|--------------|
| H | 2.175755000 | 0.567024000 | -2.464308000 |
| H | 2.506213000 | 2.740433000 | -0.886268000 |
| H | 4.041816000 | 2.090077000 | 1.175127000 |
| H | 3.491649000 | -1.479071000 | -1.403037000 |
| H | 3.696199000 | -0.599894000 | 1.130211000 |
| H | 5.186097000 | -0.190263000 | 0.263216000 |
| C | 0.706677000 | -2.157600000 | 0.280262000 |
| C | 1.077437000 | -2.999174000 | 1.266794000 |
| H | 1.286052000 | -4.052397000 | 1.057934000 |
| C | 0.318664000 | -0.757862000 | 0.652357000 |
| Cr | -1.366663000 | 0.213537000 | -0.072272000 |
| C | -0.739639000 | 0.039971000 | -1.861548000 |
| C | -0.572792000 | 1.940635000 | -0.055345000 |
| C | -2.255432000 | -1.473906000 | -0.150317000 |
| C | -2.951183000 | 1.011034000 | -0.737919000 |
| C | -2.028225000 | 0.450589000 | 1.695831000 |
| O | -0.382984000 | -0.008589000 | -2.953208000 |
| O | -3.913713000 | 1.493802000 | -1.141069000 |
| O | -2.465327000 | 0.601546000 | 2.749190000 |
| O | -2.824736000 | -2.469498000 | -0.203819000 |
| O | -0.152390000 | 3.011268000 | -0.102985000 |
| O | 1.156641000 | -0.370936000 | 1.588864000 |
| C | 1.057494000 | 0.845401000 | 2.333766000 |
| H | 1.143671000 | -2.672637000 | 2.306264000 |
| H | 0.114933000 | 0.882991000 | 2.894424000 |
| H | 1.905286000 | 0.828112000 | 3.029730000 |
| H | 1.153582000 | 1.711641000 | 1.671812000 |
| C | 0.598825000 | -2.633796000 | -1.147276000 |
| H | 1.063359000 | -3.625050000 | -1.249791000 |
| H | -0.444447000 | -2.720203000 | -1.482926000 |
| H | 1.105939000 | -1.943123000 | -1.833473000 |

RC1c-W-endo: E= -2713.905352

| | | | |
|---|--------------|--------------|--------------|
| C | 0.355446000 | 1.512228000 | 1.805131000 |
| C | -0.705009000 | 2.178074000 | 2.305525000 |
| H | -0.578644000 | 2.900766000 | 3.115801000 |
| C | 0.265011000 | 0.514464000 | 0.728273000 |
| W | 2.058707000 | -0.555362000 | -0.015596000 |
| C | 3.243362000 | 1.099297000 | 0.504182000 |
| C | 3.799828000 | -1.533302000 | -0.643290000 |
| C | 2.292175000 | -1.335255000 | 1.923696000 |
| C | 0.984755000 | -2.220804000 | -0.647132000 |
| C | 1.848592000 | 0.255165000 | -1.932676000 |
| O | -0.934697000 | 0.300849000 | 0.299552000 |
| O | 1.710338000 | 0.714727000 | -2.984858000 |
| O | 3.899376000 | 2.011099000 | 0.773072000 |
| O | 2.403181000 | -1.756419000 | 2.992377000 |
| O | 4.761793000 | -2.077159000 | -0.984459000 |
| O | 0.403171000 | -3.159836000 | -1.009900000 |
| H | -1.713470000 | 2.017409000 | 1.919747000 |
| C | 1.041402000 | 3.504384000 | -0.865452000 |
| C | -0.172207000 | 3.068656000 | -1.279014000 |
| C | -1.219737000 | 3.726509000 | -0.494953000 |
| C | -0.642246000 | 4.575989000 | 0.390096000 |
| C | 0.851543000 | 4.519965000 | 0.225915000 |
| H | 2.011247000 | 3.198020000 | -1.256436000 |
| H | -0.343801000 | 2.334330000 | -2.065255000 |
| H | -2.287926000 | 3.521494000 | -0.580421000 |
| H | -1.157335000 | 5.207672000 | 1.114731000 |
| H | 1.364104000 | 4.221247000 | 1.159051000 |
| H | 1.278143000 | 5.503517000 | -0.050361000 |

| | | | |
|----|--------------|--------------|--------------|
| Ti | -2.611201000 | -0.510634000 | -0.012562000 |
| C | -3.756016000 | -1.361443000 | 1.941853000 |
| C | -2.407708000 | -1.128907000 | 2.304267000 |
| C | -1.593466000 | -2.018737000 | 1.555850000 |
| C | -2.430166000 | -2.775614000 | 0.708247000 |
| C | -3.776116000 | -2.361247000 | 0.941531000 |
| H | -4.618506000 | -0.819600000 | 2.319600000 |
| H | -2.051884000 | -0.371902000 | 2.999761000 |
| H | -0.506104000 | -2.046352000 | 1.569489000 |
| H | -2.095955000 | -3.544531000 | 0.017370000 |
| H | -4.667201000 | -2.769253000 | 0.470729000 |
| C | -2.251469000 | -1.647404000 | -2.073544000 |
| C | -1.697333000 | -0.355344000 | -2.236094000 |
| C | -2.742543000 | 0.587768000 | -2.140996000 |
| C | -3.964371000 | -0.125664000 | -1.973462000 |
| C | -3.664636000 | -1.501693000 | -1.939936000 |
| H | -1.692546000 | -2.578205000 | -2.094901000 |
| H | -0.637786000 | -0.135438000 | -2.311137000 |
| H | -2.639932000 | 1.668870000 | -2.155384000 |
| H | -4.946154000 | 0.322896000 | -1.844638000 |
| H | -4.382235000 | -2.311832000 | -1.838035000 |
| Cl | -3.911000000 | 1.352339000 | 0.670633000 |
| H | 1.355219000 | 1.693274000 | 2.205621000 |

RC1c-W-exo: E= -2713.905922

| | | | |
|----|--------------|--------------|--------------|
| C | -0.047860000 | 4.958562000 | 0.375428000 |
| C | 0.936065000 | 4.185319000 | -0.385727000 |
| C | 0.291551000 | 3.251933000 | -1.128394000 |
| C | -1.291533000 | 4.495913000 | 0.097213000 |
| C | -1.187300000 | 3.376498000 | -0.899483000 |
| H | 0.199053000 | 5.768190000 | 1.065104000 |
| H | 2.016521000 | 4.328340000 | -0.336839000 |
| H | 0.754354000 | 2.521031000 | -1.790678000 |
| H | -2.235115000 | 4.855414000 | 0.509053000 |
| H | -1.641721000 | 2.448742000 | -0.512394000 |
| H | -1.732732000 | 3.608594000 | -1.835082000 |
| C | 0.334710000 | 1.622124000 | 1.714677000 |
| C | -0.748300000 | 2.205262000 | 2.266609000 |
| H | -0.636565000 | 2.980538000 | 3.027789000 |
| C | 0.272686000 | 0.548616000 | 0.710608000 |
| W | 2.083634000 | -0.505522000 | -0.000656000 |
| C | 2.522939000 | -0.887442000 | 2.022405000 |
| C | 3.122652000 | 1.322624000 | 0.074296000 |
| C | 1.182792000 | -2.362837000 | -0.255847000 |
| C | 3.879784000 | -1.406050000 | -0.594250000 |
| C | 1.614927000 | -0.149032000 | -2.005062000 |
| O | 2.745143000 | -1.096271000 | 3.134671000 |
| O | 4.874471000 | -1.899221000 | -0.916671000 |
| O | 1.334620000 | 0.052127000 | -3.109937000 |
| O | 0.693672000 | -3.400310000 | -0.443816000 |
| O | 3.708188000 | 2.316569000 | 0.093614000 |
| O | -0.922835000 | 0.258770000 | 0.316484000 |
| H | -1.761721000 | 1.927007000 | 1.967841000 |
| Ti | -2.561507000 | -0.608999000 | -0.002762000 |
| Cl | -3.947075000 | 1.201756000 | 0.635871000 |
| C | -3.609544000 | -2.548583000 | 0.895976000 |
| C | -3.778955000 | -1.535966000 | 1.865142000 |
| C | -2.495478000 | -1.162937000 | 2.340216000 |
| C | -1.534744000 | -1.978357000 | 1.692392000 |
| C | -2.211459000 | -2.822219000 | 0.785042000 |
| H | -4.408680000 | -3.043184000 | 0.347815000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.720601000 | -1.075513000 | 2.151296000 |
| H | -2.282402000 | -0.364122000 | 3.047226000 |
| H | -0.455239000 | -1.899105000 | 1.804009000 |
| H | -1.735406000 | -3.549368000 | 0.131955000 |
| C | -1.859143000 | 0.025664000 | -2.240996000 |
| C | -3.222710000 | 0.347135000 | -2.139349000 |
| C | -3.950272000 | -0.860942000 | -1.931100000 |
| C | -3.021918000 | -1.929917000 | -1.948969000 |
| C | -1.722054000 | -1.382063000 | -2.088565000 |
| H | -1.040134000 | 0.729549000 | -2.346298000 |
| H | -3.646879000 | 1.346799000 | -2.152653000 |
| H | -5.027227000 | -0.939526000 | -1.792584000 |
| H | -3.257903000 | -2.986397000 | -1.850317000 |
| H | -0.787752000 | -1.936665000 | -2.089024000 |
| H | 1.337599000 | 1.923266000 | 2.024986000 |

RC1c-Cr-endo: E= -3691.901356

| | | | |
|----|--------------|--------------|--------------|
| C | 1.011460000 | 1.267210000 | 1.699424000 |
| C | 0.031732000 | 2.023796000 | 2.233262000 |
| H | 0.252899000 | 2.736933000 | 3.031687000 |
| C | 0.799810000 | 0.249359000 | 0.650568000 |
| Cr | 2.338077000 | -0.969425000 | -0.043752000 |
| C | 3.622699000 | 0.356711000 | 0.434502000 |
| C | 3.767184000 | -2.074791000 | -0.612669000 |
| C | 2.350189000 | -1.689737000 | 1.720134000 |
| C | 1.138257000 | -2.303964000 | -0.615612000 |
| C | 2.176785000 | -0.123092000 | -1.726323000 |
| O | -0.417372000 | 0.154619000 | 0.254957000 |
| O | 2.058289000 | 0.409263000 | -2.741951000 |
| O | 4.415980000 | 1.150200000 | 0.685163000 |
| O | 2.311811000 | -2.109579000 | 2.790122000 |
| O | 4.632039000 | -2.751108000 | -0.957559000 |
| O | 0.439690000 | -3.147170000 | -0.984407000 |
| H | -1.002660000 | 1.950672000 | 1.893494000 |
| C | 1.814153000 | 3.247098000 | -0.854832000 |
| C | 0.545978000 | 2.989584000 | -1.255756000 |
| C | -0.389884000 | 3.757623000 | -0.432941000 |
| C | 0.310562000 | 4.492073000 | 0.466726000 |
| C | 1.780428000 | 4.246793000 | 0.266483000 |
| H | 2.727269000 | 2.824454000 | -1.272918000 |
| H | 0.264338000 | 2.307844000 | -2.057639000 |
| H | -1.476642000 | 3.702165000 | -0.507089000 |
| H | -0.103429000 | 5.165790000 | 1.217839000 |
| H | 2.270954000 | 3.860231000 | 1.178793000 |
| H | 2.323691000 | 5.174971000 | 0.003173000 |
| Ti | -2.218620000 | -0.364084000 | -0.017980000 |
| C | -3.449407000 | -1.003917000 | 1.967790000 |
| C | -2.073956000 | -1.024400000 | 2.300763000 |
| C | -1.453836000 | -2.042883000 | 1.531858000 |
| C | -2.430430000 | -2.624212000 | 0.696167000 |
| C | -3.673227000 | -1.973807000 | 0.964054000 |
| H | -4.190756000 | -0.318095000 | 2.367162000 |
| H | -1.570617000 | -0.353736000 | 2.993824000 |
| H | -0.397950000 | -2.295038000 | 1.550656000 |
| H | -2.257723000 | -3.431554000 | -0.010817000 |
| H | -4.634295000 | -2.204059000 | 0.510799000 |
| C | -2.048347000 | -1.490952000 | -2.109309000 |
| C | -1.390473000 | -0.248383000 | -2.287631000 |
| C | -2.340793000 | 0.779993000 | -2.132055000 |
| C | -3.612516000 | 0.174201000 | -1.907173000 |
| C | -3.434583000 | -1.223104000 | -1.913061000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -1.575803000 | -2.467963000 | -2.157338000 |
| H | -0.325814000 | -0.114252000 | -2.445631000 |
| H | -2.143003000 | 1.848212000 | -2.144414000 |
| H | -4.542926000 | 0.705718000 | -1.723441000 |
| H | -4.214773000 | -1.969310000 | -1.787258000 |
| Cl | -3.210281000 | 1.680028000 | 0.697809000 |
| H | 2.033570000 | 1.375594000 | 2.065187000 |

RC1c-Cr-exo: E= -3691.902808

| | | | |
|----|--------------|--------------|--------------|
| C | -1.189030000 | 4.692482000 | -0.494981000 |
| C | -1.996441000 | 3.844645000 | 0.384662000 |
| C | -1.174151000 | 3.096878000 | 1.161697000 |
| C | 0.125166000 | 4.458815000 | -0.257416000 |
| C | 0.251794000 | 3.428102000 | 0.827562000 |
| H | -1.597257000 | 5.387490000 | -1.231523000 |
| H | -3.087241000 | 3.814191000 | 0.393087000 |
| H | -1.478114000 | 2.382097000 | 1.925957000 |
| H | 0.977174000 | 4.922722000 | -0.755416000 |
| H | 0.825118000 | 2.552072000 | 0.478246000 |
| H | 0.806196000 | 3.816234000 | 1.704087000 |
| C | -1.036889000 | 1.324851000 | -1.635231000 |
| C | -0.054896000 | 2.013669000 | -2.248605000 |
| H | -0.295024000 | 2.768907000 | -3.000363000 |
| C | -0.813941000 | 0.242155000 | -0.654662000 |
| Cr | -2.345276000 | -0.981755000 | 0.026405000 |
| C | -2.591047000 | -1.454322000 | -1.807533000 |
| C | -3.567869000 | 0.479590000 | -0.121230000 |
| C | -1.196704000 | -2.448554000 | 0.289334000 |
| C | -3.795800000 | -2.061694000 | 0.594183000 |
| C | -1.935728000 | -0.416153000 | 1.779519000 |
| O | -2.695978000 | -1.731135000 | -2.917734000 |
| O | -4.674898000 | -2.718765000 | 0.939418000 |
| O | -1.656806000 | -0.056643000 | 2.839360000 |
| O | -0.522060000 | -3.361996000 | 0.503628000 |
| O | -4.323637000 | 1.342939000 | -0.175518000 |
| O | 0.412191000 | 0.103806000 | -0.303001000 |
| H | 0.998781000 | 1.850158000 | -2.013850000 |
| Ti | 2.206997000 | -0.392212000 | 0.015628000 |
| Cl | 3.191287000 | 1.650001000 | -0.700851000 |
| C | 2.276984000 | -2.640366000 | -0.742197000 |
| C | 3.609784000 | -2.131175000 | -0.811781000 |
| C | 3.637242000 | -1.114053000 | -1.788735000 |
| C | 2.326937000 | -0.980486000 | -2.321377000 |
| C | 1.501818000 | -1.943933000 | -1.696319000 |
| H | 1.908927000 | -3.429399000 | -0.091762000 |
| H | 4.459343000 | -2.469447000 | -0.222485000 |
| H | 4.493920000 | -0.498312000 | -2.049123000 |
| H | 2.007900000 | -0.243034000 | -3.054302000 |
| H | 0.436647000 | -2.075070000 | -1.867710000 |
| C | 2.849487000 | 0.710710000 | 2.092255000 |
| C | 3.666585000 | -0.438075000 | 1.901846000 |
| C | 2.830135000 | -1.581134000 | 1.998371000 |
| C | 1.498655000 | -1.137537000 | 2.170664000 |
| C | 1.518582000 | 0.283694000 | 2.246487000 |
| H | 3.188904000 | 1.741417000 | 2.054935000 |
| H | 4.742633000 | -0.434956000 | 1.736331000 |
| H | 3.150241000 | -2.618121000 | 1.935739000 |
| H | 0.618714000 | -1.770260000 | 2.243018000 |
| H | 0.645809000 | 0.919299000 | 2.358076000 |
| H | -2.076389000 | 1.530480000 | -1.894315000 |

RC1d-W-endo: E= -2753.165434

| | | | |
|----|--------------|--------------|--------------|
| C | 0.276115000 | 1.664805000 | 1.694209000 |
| C | -0.876794000 | 2.287910000 | 2.032493000 |
| H | -0.880054000 | 3.070346000 | 2.796347000 |
| C | 0.255684000 | 0.580631000 | 0.672333000 |
| W | 2.019419000 | -0.590371000 | -0.066312000 |
| C | 3.414018000 | 0.958282000 | 0.161290000 |
| C | 3.645783000 | -1.713114000 | -0.748108000 |
| C | 2.347055000 | -1.258390000 | 1.895990000 |
| C | 0.897459000 | -2.282096000 | -0.514986000 |
| C | 1.710070000 | 0.122763000 | -2.007291000 |
| O | -0.929193000 | 0.300296000 | 0.231724000 |
| O | 1.530058000 | 0.521447000 | -3.078015000 |
| O | 4.223843000 | 1.779420000 | 0.238970000 |
| O | 2.514702000 | -1.618568000 | 2.980667000 |
| O | 4.542909000 | -2.340090000 | -1.122708000 |
| O | 0.327087000 | -3.256162000 | -0.794847000 |
| H | -1.829616000 | 2.045353000 | 1.566056000 |
| C | 0.889844000 | 3.510832000 | -1.055774000 |
| C | -0.263116000 | 2.969262000 | -1.515697000 |
| C | -1.402727000 | 3.637223000 | -0.882917000 |
| C | -0.943212000 | 4.598155000 | -0.045063000 |
| C | 0.560102000 | 4.616959000 | -0.092350000 |
| H | 1.902663000 | 3.218659000 | -1.333909000 |
| H | -0.333048000 | 2.154611000 | -2.235386000 |
| H | -2.449283000 | 3.364573000 | -1.025925000 |
| H | -1.546314000 | 5.263131000 | 0.574208000 |
| H | 1.007827000 | 4.454415000 | 0.904760000 |
| H | 0.951757000 | 5.591855000 | -0.442090000 |
| C | 1.570238000 | 2.047558000 | 2.369030000 |
| H | 2.122637000 | 1.169483000 | 2.730932000 |
| H | 2.238869000 | 2.590380000 | 1.686794000 |
| H | 1.374084000 | 2.702036000 | 3.231012000 |
| Ti | -2.606139000 | -0.574565000 | 0.019388000 |
| C | -3.731097000 | -1.256732000 | 2.052389000 |
| C | -2.393286000 | -0.938741000 | 2.389345000 |
| C | -1.544965000 | -1.872485000 | 1.739590000 |
| C | -2.350258000 | -2.744501000 | 0.976470000 |
| C | -3.710942000 | -2.356823000 | 1.164472000 |
| H | -4.613794000 | -0.709759000 | 2.371264000 |
| H | -2.067613000 | -0.101307000 | 3.002232000 |
| H | -0.457473000 | -1.857267000 | 1.752832000 |
| H | -1.985379000 | -3.570169000 | 0.372572000 |
| H | -4.583675000 | -2.846105000 | 0.739383000 |
| C | -2.339901000 | -1.949808000 | -1.906270000 |
| C | -1.718479000 | -0.715919000 | -2.207475000 |
| C | -2.711783000 | 0.288518000 | -2.215013000 |
| C | -3.967494000 | -0.335512000 | -1.971983000 |
| C | -3.741625000 | -1.712572000 | -1.780023000 |
| H | -1.833943000 | -2.907430000 | -1.835668000 |
| H | -0.650725000 | -0.560303000 | -2.311028000 |
| H | -2.549831000 | 1.353513000 | -2.352619000 |
| H | -4.923551000 | 0.174940000 | -1.894708000 |
| H | -4.502738000 | -2.464422000 | -1.587874000 |
| Cl | -3.964245000 | 1.307257000 | 0.523358000 |

RC1d-W-exo: E= -2753.167689

| | | | |
|---|--------------|-------------|--------------|
| C | 0.207289000 | 4.856702000 | 0.047390000 |
| C | 1.065833000 | 3.986825000 | -0.760990000 |
| C | 0.294085000 | 3.098410000 | -1.433734000 |
| C | -1.087536000 | 4.500630000 | -0.137273000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -1.149854000 | 3.358637000 | -1.112611000 |
| H | 0.570395000 | 5.653567000 | 0.699354000 |
| H | 2.155041000 | 4.043913000 | -0.799836000 |
| H | 0.646330000 | 2.330421000 | -2.120453000 |
| H | -1.965338000 | 4.950568000 | 0.327601000 |
| H | -1.662771000 | 2.480909000 | -0.683815000 |
| H | -1.727500000 | 3.628229000 | -2.018533000 |
| C | 0.295338000 | 1.690601000 | 1.682190000 |
| C | -0.862721000 | 2.256217000 | 2.095725000 |
| H | -0.847856000 | 3.060957000 | 2.834791000 |
| C | 0.265720000 | 0.573347000 | 0.696195000 |
| W | 2.008802000 | -0.614078000 | -0.046391000 |
| C | 2.529244000 | -1.044919000 | 1.942784000 |
| C | 3.226741000 | 1.094426000 | -0.158081000 |
| C | 1.010015000 | -2.429313000 | -0.199622000 |
| C | 3.691661000 | -1.661114000 | -0.715453000 |
| C | 1.469508000 | -0.268310000 | -2.033344000 |
| O | 2.804522000 | -1.295462000 | 3.035631000 |
| O | 4.625686000 | -2.237028000 | -1.081085000 |
| O | 1.165117000 | -0.085390000 | -3.135443000 |
| O | 0.488451000 | -3.458991000 | -0.340827000 |
| O | 3.928901000 | 2.004129000 | -0.269819000 |
| O | -0.924715000 | 0.276819000 | 0.279131000 |
| H | -1.835984000 | 1.949992000 | 1.714947000 |
| C | 1.607212000 | 2.195340000 | 2.227037000 |
| H | 2.277527000 | 1.382812000 | 2.536444000 |
| H | 2.139004000 | 2.790380000 | 1.471585000 |
| H | 1.436926000 | 2.844950000 | 3.097472000 |
| Ti | -2.600557000 | -0.563718000 | 0.021671000 |
| Cl | -3.960298000 | 1.308801000 | 0.541950000 |
| C | -3.704481000 | -2.404909000 | 1.050289000 |
| C | -3.831788000 | -1.329025000 | 1.955348000 |
| C | -2.532612000 | -0.968761000 | 2.395913000 |
| C | -1.604952000 | -1.853783000 | 1.792795000 |
| C | -2.317477000 | -2.731327000 | 0.947098000 |
| H | -4.523720000 | -2.905258000 | 0.538151000 |
| H | -4.755615000 | -0.821819000 | 2.219356000 |
| H | -2.285907000 | -0.136446000 | 3.051262000 |
| H | -0.522552000 | -1.802848000 | 1.889379000 |
| H | -1.871442000 | -3.514184000 | 0.339788000 |
| C | -3.075947000 | -2.009454000 | -1.831514000 |
| C | -1.795073000 | -1.440567000 | -2.035283000 |
| C | -1.969942000 | -0.047178000 | -2.265217000 |
| C | -3.339864000 | 0.244738000 | -2.159028000 |
| C | -4.031167000 | -0.963472000 | -1.858599000 |
| H | -3.283681000 | -3.063229000 | -1.664658000 |
| H | -0.849432000 | -1.973784000 | -2.024942000 |
| H | -1.173048000 | 0.668999000 | -2.434287000 |
| H | -3.790508000 | 1.230143000 | -2.229345000 |
| H | -5.102996000 | -1.059328000 | -1.694048000 |

RCld-Cr-endo: E= -3731.158806

| | | | |
|----|--------------|--------------|--------------|
| C | 0.952736000 | 1.368149000 | 1.652544000 |
| C | -0.107311000 | 2.122237000 | 2.024323000 |
| H | 0.003986000 | 2.892146000 | 2.793019000 |
| C | 0.772626000 | 0.292565000 | 0.622510000 |
| Cr | 2.253863000 | -1.029267000 | -0.123893000 |
| C | 3.713523000 | 0.176738000 | 0.091986000 |
| C | 3.551095000 | -2.247695000 | -0.748293000 |
| C | 2.380856000 | -1.668447000 | 1.662258000 |
| C | 0.999910000 | -2.369929000 | -0.541680000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 2.010560000 | -0.240703000 | -1.823030000 |
| O | -0.442552000 | 0.167881000 | 0.225588000 |
| O | 1.873096000 | 0.253727000 | -2.855263000 |
| O | 4.654187000 | 0.838225000 | 0.117538000 |
| O | 2.418262000 | -2.049237000 | 2.747583000 |
| O | 4.337976000 | -2.998616000 | -1.126057000 |
| O | 0.309048000 | -3.250463000 | -0.830162000 |
| H | -1.095528000 | 2.007579000 | 1.584774000 |
| C | 1.682794000 | 3.233913000 | -1.074119000 |
| C | 0.438422000 | 2.894732000 | -1.487837000 |
| C | -0.551305000 | 3.696347000 | -0.765038000 |
| C | 0.091844000 | 4.535274000 | 0.082862000 |
| C | 1.575697000 | 4.331664000 | -0.052927000 |
| H | 2.623518000 | 2.810344000 | -1.426360000 |
| H | 0.207783000 | 2.136026000 | -2.234490000 |
| H | -1.632609000 | 3.591381000 | -0.860798000 |
| H | -0.369731000 | 5.253421000 | 0.761661000 |
| H | 2.050937000 | 4.065717000 | 0.908228000 |
| H | 2.087892000 | 5.252357000 | -0.394434000 |
| C | 2.292557000 | 1.602016000 | 2.309410000 |
| H | 3.020247000 | 2.039749000 | 1.613406000 |
| H | 2.181202000 | 2.301453000 | 3.150963000 |
| H | 2.736045000 | 0.677368000 | 2.704009000 |
| Ti | -2.255235000 | -0.393553000 | 0.012662000 |
| C | -3.461668000 | -0.915943000 | 2.049649000 |
| C | -2.084203000 | -0.875763000 | 2.372885000 |
| C | -1.442723000 | -1.932884000 | 1.677747000 |
| C | -2.407879000 | -2.600116000 | 0.894404000 |
| C | -3.665552000 | -1.963865000 | 1.123288000 |
| H | -4.218883000 | -0.222498000 | 2.403441000 |
| H | -1.594229000 | -0.143641000 | 3.011051000 |
| H | -0.380622000 | -2.156317000 | 1.708899000 |
| H | -2.216188000 | -3.453300000 | 0.249239000 |
| H | -4.623290000 | -2.254630000 | 0.699533000 |
| C | -2.160597000 | -1.677068000 | -1.989586000 |
| C | -1.481775000 | -0.466300000 | -2.271159000 |
| C | -2.407630000 | 0.591755000 | -2.176053000 |
| C | -3.686895000 | 0.031471000 | -1.888849000 |
| C | -3.537125000 | -1.364784000 | -1.788970000 |
| H | -1.711728000 | -2.665458000 | -1.979343000 |
| H | -0.420478000 | -0.366304000 | -2.463861000 |
| H | -2.187871000 | 1.650924000 | -2.275371000 |
| H | -4.603376000 | 0.593894000 | -1.730896000 |
| H | -4.330918000 | -2.081631000 | -1.596336000 |
| Cl | -3.294798000 | 1.671745000 | 0.593928000 |

RC1d-Cr-exo: E= -3731.161383

| | | | |
|---|--------------|-------------|--------------|
| C | 1.484027000 | 4.518711000 | 0.135144000 |
| C | 2.079543000 | 3.563366000 | -0.803492000 |
| C | 1.092030000 | 2.920935000 | -1.473450000 |
| C | 0.133848000 | 4.458379000 | 0.034591000 |
| C | -0.237483000 | 3.444224000 | -1.010803000 |
| H | 2.052720000 | 5.160536000 | 0.810796000 |
| H | 3.150919000 | 3.397188000 | -0.929746000 |
| H | 1.225548000 | 2.168870000 | -2.250040000 |
| H | -0.593535000 | 5.038324000 | 0.603571000 |
| H | -0.894474000 | 2.657412000 | -0.600622000 |
| H | -0.808777000 | 3.903806000 | -1.841007000 |
| C | 0.999175000 | 1.360453000 | 1.636248000 |
| C | -0.055324000 | 2.063843000 | 2.108528000 |
| H | 0.097685000 | 2.844062000 | 2.858392000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 0.774711000 | 0.257325000 | 0.643108000 |
| Cr | 2.202164000 | -1.116631000 | -0.092786000 |
| C | 2.525952000 | -1.578400000 | 1.728946000 |
| C | 3.583854000 | 0.200065000 | -0.164904000 |
| C | 0.970660000 | -2.528123000 | -0.249483000 |
| C | 3.511310000 | -2.334574000 | -0.696649000 |
| C | 1.740434000 | -0.593337000 | -1.845066000 |
| O | 2.681004000 | -1.871893000 | 2.829682000 |
| O | 4.310214000 | -3.079454000 | -1.060323000 |
| O | 1.456995000 | -0.278472000 | -2.917650000 |
| O | 0.277707000 | -3.437669000 | -0.420022000 |
| O | 4.456465000 | 0.934521000 | -0.306158000 |
| O | -0.451415000 | 0.151001000 | 0.273927000 |
| H | -1.076012000 | 1.904139000 | 1.766658000 |
| C | 2.380536000 | 1.689302000 | 2.145235000 |
| H | 2.937951000 | 0.802644000 | 2.474048000 |
| H | 2.978510000 | 2.188460000 | 1.370928000 |
| H | 2.312879000 | 2.378190000 | 2.999243000 |
| Ti | -2.272430000 | -0.326854000 | 0.010083000 |
| Cl | -3.235947000 | 1.765311000 | 0.614779000 |
| C | -3.710327000 | -1.965182000 | 0.971455000 |
| C | -3.674262000 | -0.899709000 | 1.895041000 |
| C | -2.345149000 | -0.783914000 | 2.381453000 |
| C | -1.571523000 | -1.806172000 | 1.783520000 |
| C | -2.398700000 | -2.524905000 | 0.892162000 |
| H | -4.588117000 | -2.302823000 | 0.424634000 |
| H | -4.502084000 | -0.243061000 | 2.147839000 |
| H | -1.978761000 | -0.022826000 | 3.066569000 |
| H | -0.507149000 | -1.965515000 | 1.933466000 |
| H | -2.079357000 | -3.361152000 | 0.276415000 |
| C | -2.983659000 | -1.610384000 | -1.885026000 |
| C | -1.648244000 | -1.207912000 | -2.116809000 |
| C | -1.639101000 | 0.207334000 | -2.269802000 |
| C | -2.956317000 | 0.671606000 | -2.109406000 |
| C | -3.792289000 | -0.445107000 | -1.833016000 |
| H | -3.324007000 | -2.634691000 | -1.756130000 |
| H | -0.787544000 | -1.866019000 | -2.183314000 |
| H | -0.758040000 | 0.818291000 | -2.435383000 |
| H | -3.273045000 | 1.709865000 | -2.125191000 |
| H | -4.862644000 | -0.407251000 | -1.638141000 |

RC1e-W-endo: E= -1076.874615

| | | | |
|---|--------------|--------------|--------------|
| C | 1.030922000 | 0.553047000 | 2.060981000 |
| C | 2.275759000 | 0.126397000 | 2.327029000 |
| H | 2.510918000 | -0.324669000 | 3.294675000 |
| C | 0.541825000 | 1.031374000 | 0.741097000 |
| W | -1.215758000 | -0.144030000 | -0.027644000 |
| C | -0.206672000 | -1.880724000 | 0.565795000 |
| C | -2.891520000 | -1.265527000 | -0.566864000 |
| C | -2.110215000 | -0.001197000 | 1.863917000 |
| C | -2.194587000 | 1.602457000 | -0.650237000 |
| C | -0.573791000 | -0.427757000 | -1.991198000 |
| N | 1.187322000 | 2.054436000 | 0.185663000 |
| O | -0.241932000 | -0.589724000 | -3.090113000 |
| O | 0.369147000 | -2.827863000 | 0.893788000 |
| O | -2.618422000 | 0.052988000 | 2.900192000 |
| O | -3.822925000 | -1.884917000 | -0.862726000 |
| O | -2.727927000 | 2.563191000 | -1.009889000 |
| C | 0.868938000 | 2.538316000 | -1.155610000 |
| H | 0.258121000 | 0.430085000 | 2.825314000 |
| H | 3.080998000 | 0.173384000 | 1.590184000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 0.411017000 | 1.743145000 | -1.749049000 |
| H | 0.170279000 | 3.389025000 | -1.102246000 |
| H | 1.793340000 | 2.869637000 | -1.650380000 |
| C | 2.924964000 | -0.760696000 | -1.097013000 |
| C | 3.861833000 | 0.213872000 | -1.177373000 |
| C | 5.053228000 | -0.194871000 | -0.419522000 |
| C | 4.839162000 | -1.419895000 | 0.117570000 |
| C | 3.469157000 | -1.895988000 | -0.277333000 |
| H | 1.927178000 | -0.749792000 | -1.529200000 |
| H | 3.765727000 | 1.155287000 | -1.722323000 |
| H | 5.961620000 | 0.402856000 | -0.319782000 |
| H | 5.537017000 | -1.995865000 | 0.726617000 |
| H | 2.824134000 | -2.132735000 | 0.588706000 |
| H | 3.515231000 | -2.832296000 | -0.866961000 |
| C | 2.233096000 | 2.854616000 | 0.832871000 |
| H | 2.221330000 | 2.714348000 | 1.917309000 |
| H | 3.224792000 | 2.568748000 | 0.446868000 |
| H | 2.056988000 | 3.916082000 | 0.601590000 |

RC1e-W-exo: E= -1076.877106

| | | | |
|---|--------------|--------------|--------------|
| C | 4.854224000 | -0.057269000 | -0.515208000 |
| C | 4.809936000 | -1.335385000 | 0.209279000 |
| C | 3.647121000 | -1.968058000 | -0.077376000 |
| C | 3.717833000 | 0.082984000 | -1.240411000 |
| C | 2.848142000 | -1.121733000 | -1.024056000 |
| H | 5.684844000 | 0.650634000 | -0.473359000 |
| H | 5.596057000 | -1.698272000 | 0.874125000 |
| H | 3.305780000 | -2.926336000 | 0.315271000 |
| H | 3.461284000 | 0.911032000 | -1.901947000 |
| H | 1.863458000 | -0.848714000 | -0.600200000 |
| H | 2.608961000 | -1.642793000 | -1.970014000 |
| C | 0.980964000 | 0.669015000 | 2.083336000 |
| C | 2.208993000 | 0.213122000 | 2.375572000 |
| H | 2.430260000 | -0.198716000 | 3.363542000 |
| C | 0.527886000 | 1.082758000 | 0.729716000 |
| W | -1.191227000 | -0.140216000 | -0.025245000 |
| C | -0.280432000 | -1.836749000 | 0.804442000 |
| C | -0.411437000 | -0.599428000 | -1.906117000 |
| C | -2.189284000 | 0.207495000 | 1.787086000 |
| C | -2.849717000 | -1.291033000 | -0.556179000 |
| C | -2.141004000 | 1.519878000 | -0.881528000 |
| O | 0.240096000 | -2.764381000 | 1.254217000 |
| O | -3.773385000 | -1.923551000 | -0.847897000 |
| O | -2.673661000 | 2.422610000 | -1.370071000 |
| O | -2.753710000 | 0.379279000 | 2.779971000 |
| O | 0.005748000 | -0.855441000 | -2.956644000 |
| N | 1.200227000 | 2.068194000 | 0.136847000 |
| C | 0.914133000 | 2.480545000 | -1.235797000 |
| H | 0.196169000 | 0.613520000 | 2.843807000 |
| H | 3.009847000 | 0.185371000 | 1.632951000 |
| H | 0.164497000 | 3.288125000 | -1.247994000 |
| H | 1.837829000 | 2.848140000 | -1.704524000 |
| H | 0.529743000 | 1.636167000 | -1.814322000 |
| C | 2.231690000 | 2.898241000 | 0.771449000 |
| H | 2.198871000 | 2.799927000 | 1.860025000 |
| H | 3.229954000 | 2.596852000 | 0.415284000 |
| H | 2.056630000 | 3.949285000 | 0.495668000 |

RC1e-Cr-endo: E= -2054.870391

| | | | |
|---|-------------|-------------|-------------|
| C | 0.420158000 | 0.646560000 | 2.068506000 |
| C | 1.593584000 | 0.122427000 | 2.454525000 |

| | | | |
|----|--------------|--------------|--------------|
| H | 1.738789000 | -0.222953000 | 3.481479000 |
| C | 0.048961000 | 0.970513000 | 0.671995000 |
| Cr | -1.572573000 | -0.223082000 | -0.068470000 |
| C | -0.833217000 | -1.725099000 | 0.841649000 |
| C | -3.020688000 | -1.274469000 | -0.650169000 |
| C | -2.567719000 | 0.248889000 | 1.486552000 |
| C | -2.309918000 | 1.284230000 | -0.962450000 |
| C | -0.592825000 | -0.737183000 | -1.604435000 |
| N | 0.748131000 | 1.930772000 | 0.090056000 |
| O | -0.005766000 | -1.073729000 | -2.538339000 |
| O | -0.384231000 | -2.642310000 | 1.369424000 |
| O | -3.178199000 | 0.519012000 | 2.422822000 |
| O | -3.906529000 | -1.915377000 | -1.012714000 |
| O | -2.772364000 | 2.190599000 | -1.500151000 |
| C | 0.589474000 | 2.313057000 | -1.314966000 |
| H | -0.394579000 | 0.716677000 | 2.797421000 |
| H | 2.424673000 | -0.024454000 | 1.759177000 |
| H | 0.113901000 | 1.515521000 | -1.885700000 |
| H | -0.022012000 | 3.225938000 | -1.392498000 |
| H | 1.582462000 | 2.512442000 | -1.742876000 |
| C | 2.988346000 | -0.322820000 | -1.344939000 |
| C | 4.097427000 | 0.285551000 | -0.860565000 |
| C | 4.700880000 | -0.562741000 | 0.177815000 |
| C | 3.960735000 | -1.688074000 | 0.316910000 |
| C | 2.801787000 | -1.635770000 | -0.638046000 |
| H | 2.330521000 | 0.032225000 | -2.136725000 |
| H | 4.505096000 | 1.243661000 | -1.190986000 |
| H | 5.604962000 | -0.311665000 | 0.736071000 |
| H | 4.146351000 | -2.510957000 | 1.008179000 |
| H | 1.830674000 | -1.695521000 | -0.112384000 |
| H | 2.799973000 | -2.484932000 | -1.347599000 |
| C | 1.754313000 | 2.778821000 | 0.754303000 |
| H | 1.664674000 | 2.717383000 | 1.841993000 |
| H | 2.764709000 | 2.456427000 | 0.458020000 |
| H | 1.603592000 | 3.819857000 | 0.430867000 |

RC1e-Cr-exo: E= -2054.868808

| | | | |
|----|--------------|--------------|--------------|
| C | 4.726571000 | -0.537477000 | 0.175122000 |
| C | 3.931061000 | -1.764299000 | 0.322654000 |
| C | 2.882252000 | -1.719957000 | -0.531553000 |
| C | 4.160365000 | 0.252047000 | -0.769168000 |
| C | 2.934624000 | -0.433441000 | -1.306117000 |
| H | 5.632048000 | -0.314226000 | 0.743199000 |
| H | 4.157184000 | -2.569881000 | 1.023425000 |
| H | 2.099317000 | -2.469145000 | -0.648053000 |
| H | 4.527108000 | 1.219746000 | -1.115399000 |
| H | 2.019847000 | 0.162867000 | -1.147321000 |
| H | 2.982561000 | -0.605538000 | -2.397739000 |
| C | 0.447009000 | 0.767433000 | 2.012784000 |
| C | 1.670278000 | 0.330272000 | 2.348283000 |
| H | 1.885522000 | 0.001017000 | 3.368184000 |
| C | -0.001597000 | 1.052644000 | 0.630690000 |
| Cr | -1.551591000 | -0.258139000 | -0.048597000 |
| C | -0.655359000 | -1.704941000 | 0.817269000 |
| C | -0.608618000 | -0.720314000 | -1.624776000 |
| C | -2.514722000 | 0.133523000 | 1.548178000 |
| C | -2.944917000 | -1.412463000 | -0.566620000 |
| C | -2.428809000 | 1.189195000 | -0.912133000 |
| O | -0.118062000 | -2.593057000 | 1.308870000 |
| O | -3.799329000 | -2.114371000 | -0.889353000 |
| O | -2.971705000 | 2.060385000 | -1.433078000 |

| | | | |
|---|--------------|--------------|--------------|
| O | -3.106456000 | 0.352419000 | 2.509515000 |
| O | -0.044198000 | -1.037398000 | -2.579066000 |
| N | 0.612109000 | 2.053809000 | 0.016028000 |
| C | 0.373759000 | 2.412224000 | -1.385266000 |
| H | -0.339416000 | 0.784252000 | 2.774965000 |
| H | 2.474271000 | 0.232039000 | 1.614598000 |
| H | -0.315655000 | 3.268915000 | -1.447113000 |
| H | 1.330343000 | 2.693275000 | -1.850153000 |
| H | -0.051189000 | 1.572737000 | -1.936270000 |
| C | 1.587819000 | 2.969204000 | 0.637716000 |
| H | 1.525202000 | 2.927802000 | 1.728409000 |
| H | 2.610024000 | 2.695845000 | 0.330215000 |
| H | 1.375945000 | 3.993246000 | 0.295685000 |

RC1f-W-endo: E= -1116.140918

| | | | |
|---|--------------|--------------|--------------|
| C | 0.881855000 | 1.872199000 | 1.251555000 |
| C | 1.787340000 | 1.255070000 | 2.023311000 |
| H | 2.063569000 | 1.663189000 | 2.999302000 |
| C | 0.459550000 | 1.328948000 | -0.083493000 |
| W | -1.126032000 | -0.249044000 | -0.006571000 |
| C | 0.015442000 | -1.319768000 | 1.385576000 |
| C | -2.543912000 | -1.775089000 | 0.131783000 |
| C | -2.066474000 | 0.690557000 | 1.612710000 |
| C | -2.418184000 | 0.741834000 | -1.325994000 |
| C | -0.248914000 | -1.306869000 | -1.580776000 |
| N | 1.065662000 | 1.888951000 | -1.130099000 |
| O | 0.224816000 | -1.903730000 | -2.453002000 |
| O | 0.613840000 | -1.920486000 | 2.171004000 |
| O | -2.596429000 | 1.185046000 | 2.513397000 |
| O | -3.328987000 | -2.622864000 | 0.200574000 |
| O | -3.140590000 | 1.271012000 | -2.058691000 |
| C | 0.690389000 | 1.600148000 | -2.511415000 |
| H | 2.279143000 | 0.338059000 | 1.698911000 |
| H | -0.320522000 | 1.187788000 | -2.552066000 |
| H | 0.725280000 | 2.530447000 | -3.098288000 |
| H | 1.389340000 | 0.876646000 | -2.959349000 |
| C | 2.858199000 | -2.003114000 | -0.342444000 |
| C | 3.187563000 | -0.952443000 | -1.128906000 |
| C | 4.272377000 | -0.193257000 | -0.492685000 |
| C | 4.600911000 | -0.782222000 | 0.681474000 |
| C | 3.732035000 | -1.994419000 | 0.879532000 |
| H | 2.088135000 | -2.746952000 | -0.543310000 |
| H | 2.726542000 | -0.711662000 | -2.086970000 |
| H | 4.736336000 | 0.701483000 | -0.913141000 |
| H | 5.370125000 | -0.456929000 | 1.382903000 |
| H | 3.134330000 | -1.951095000 | 1.809294000 |
| H | 4.333169000 | -2.920853000 | 0.959460000 |
| C | 0.206233000 | 3.167669000 | 1.638319000 |
| H | -0.888476000 | 3.059204000 | 1.641753000 |
| H | 0.525982000 | 3.496650000 | 2.637778000 |
| H | 0.443903000 | 3.968410000 | 0.916972000 |
| C | 2.190143000 | 2.824522000 | -1.038282000 |
| H | 2.599815000 | 2.838923000 | -0.024112000 |
| H | 2.981388000 | 2.499797000 | -1.731284000 |
| H | 1.870146000 | 3.839040000 | -1.328737000 |

RC1f-W-exo: E= -1116.144822

| | | | |
|---|-------------|--------------|--------------|
| C | 4.681387000 | -1.461556000 | -0.306654000 |
| C | 4.864954000 | -0.128107000 | 0.284345000 |
| C | 3.850310000 | 0.121048000 | 1.146714000 |
| C | 3.558097000 | -2.022629000 | 0.201391000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.925969000 | -1.062458000 | 1.168343000 |
| H | 5.354660000 | -1.913709000 | -1.037647000 |
| H | 5.697367000 | 0.541776000 | 0.057591000 |
| H | 3.702558000 | 1.024306000 | 1.739872000 |
| H | 3.137163000 | -2.996777000 | -0.046890000 |
| H | 1.899065000 | -0.793325000 | 0.857996000 |
| H | 2.811259000 | -1.492150000 | 2.181536000 |
| C | 0.350465000 | 2.448544000 | 0.490999000 |
| C | 0.780049000 | 2.484431000 | 1.761112000 |
| H | 0.665471000 | 3.388127000 | 2.365616000 |
| C | 0.457929000 | 1.216649000 | -0.360917000 |
| W | -1.137858000 | -0.305188000 | -0.001549000 |
| C | -0.519330000 | -0.503931000 | 1.989115000 |
| C | -0.020221000 | -1.975326000 | -0.562009000 |
| C | -2.454530000 | 1.204503000 | 0.619799000 |
| C | -2.683262000 | -1.649376000 | 0.403565000 |
| C | -1.863241000 | -0.130358000 | -1.963149000 |
| O | -0.172511000 | -0.613695000 | 3.086189000 |
| O | -3.540996000 | -2.394784000 | 0.621082000 |
| O | -2.266743000 | -0.042102000 | -3.042428000 |
| O | -3.208566000 | 2.004705000 | 0.974388000 |
| O | 0.568345000 | -2.925467000 | -0.869695000 |
| N | 1.451822000 | 1.226993000 | -1.244207000 |
| C | 2.493653000 | 2.256233000 | -1.319093000 |
| H | 1.236619000 | 1.616056000 | 2.239097000 |
| H | 2.371751000 | 2.853187000 | -2.237929000 |
| H | 2.455956000 | 2.910043000 | -0.442780000 |
| H | 3.475631000 | 1.762354000 | -1.337956000 |
| C | -0.307501000 | 3.625690000 | -0.192190000 |
| H | -1.310760000 | 3.352041000 | -0.553014000 |
| H | -0.405934000 | 4.479097000 | 0.494126000 |
| H | 0.269289000 | 3.951219000 | -1.074156000 |
| C | 1.643282000 | 0.150293000 | -2.216870000 |
| H | 0.680027000 | -0.294211000 | -2.483559000 |
| H | 2.111843000 | 0.562268000 | -3.121900000 |
| H | 2.302503000 | -0.626463000 | -1.799252000 |

RC1f-Cr-exo: E= -2094.130614

| | | | |
|----|--------------|--------------|--------------|
| C | 4.749069000 | -0.165700000 | 0.519685000 |
| C | 3.746285000 | -1.203099000 | 0.798196000 |
| C | 3.137260000 | -1.552596000 | -0.357965000 |
| C | 4.741658000 | 0.121097000 | -0.803437000 |
| C | 3.713327000 | -0.741275000 | -1.484065000 |
| H | 5.390424000 | 0.294764000 | 1.274220000 |
| H | 3.520778000 | -1.606734000 | 1.786203000 |
| H | 2.342308000 | -2.287243000 | -0.480411000 |
| H | 5.374479000 | 0.845316000 | -1.318475000 |
| H | 2.931696000 | -0.151634000 | -1.999601000 |
| H | 4.160138000 | -1.379434000 | -2.270704000 |
| C | 0.430715000 | 1.585919000 | 1.269043000 |
| C | 1.763439000 | 1.533436000 | 1.118141000 |
| H | 2.434834000 | 1.635200000 | 1.974969000 |
| C | -0.450626000 | 1.329145000 | 0.089829000 |
| Cr | -1.338315000 | -0.611434000 | -0.012240000 |
| C | -0.047566000 | -1.285168000 | 1.227046000 |
| C | -0.179085000 | -0.932782000 | -1.475896000 |
| C | -2.488776000 | -0.105973000 | 1.415900000 |
| C | -2.027249000 | -2.361461000 | -0.052362000 |
| C | -2.751776000 | -0.146977000 | -1.184702000 |
| O | 0.673242000 | -1.763906000 | 1.982710000 |
| O | -2.443119000 | -3.435376000 | -0.084872000 |

| | | | |
|---|--------------|--------------|--------------|
| O | -3.650600000 | 0.054944000 | -1.877366000 |
| O | -3.203927000 | 0.205010000 | 2.261739000 |
| O | 0.519769000 | -1.080359000 | -2.380758000 |
| N | -0.535081000 | 2.346726000 | -0.751862000 |
| C | -0.008780000 | 3.701346000 | -0.497443000 |
| H | 2.234468000 | 1.328618000 | 0.154236000 |
| H | -0.790746000 | 4.434102000 | -0.749960000 |
| H | 0.280122000 | 3.822464000 | 0.549573000 |
| H | 0.872047000 | 3.896414000 | -1.129570000 |
| C | -0.228210000 | 1.819723000 | 2.608114000 |
| H | -0.623672000 | 0.883826000 | 3.031141000 |
| H | 0.495843000 | 2.234469000 | 3.324340000 |
| H | -1.080529000 | 2.513967000 | 2.526684000 |
| C | -1.214810000 | 2.266781000 | -2.050413000 |
| H | -1.106429000 | 1.269564000 | -2.482856000 |
| H | -2.284864000 | 2.501942000 | -1.947334000 |
| H | -0.757938000 | 2.994740000 | -2.735311000 |

TS1a-W-endo: E= -1057.447557

| | | | |
|---|--------------|--------------|--------------|
| C | 1.814095000 | -0.368289000 | 1.358727000 |
| C | 3.078766000 | 0.002382000 | 1.861959000 |
| H | 3.572148000 | -0.703682000 | 2.536245000 |
| C | 0.906813000 | 0.550376000 | 0.751159000 |
| W | -1.100479000 | -0.095057000 | -0.005987000 |
| C | -0.328067000 | -1.989213000 | -0.417199000 |
| C | -2.932792000 | -0.794018000 | -0.722780000 |
| C | -1.559322000 | -0.769229000 | 1.934154000 |
| C | -2.100983000 | 1.709789000 | 0.338487000 |
| C | -0.527647000 | 0.538890000 | -1.911829000 |
| O | 1.471012000 | 1.768993000 | 0.697722000 |
| O | -0.155306000 | 0.890171000 | -2.952314000 |
| O | 0.100398000 | -3.040406000 | -0.652611000 |
| O | -1.790647000 | -1.151892000 | 2.997310000 |
| O | -3.947337000 | -1.180641000 | -1.124499000 |
| O | -2.689832000 | 2.693595000 | 0.501029000 |
| C | 0.795067000 | 2.893547000 | 0.157882000 |
| H | 1.483777000 | -1.403046000 | 1.444772000 |
| H | 3.240082000 | 1.052128000 | 2.110797000 |
| H | 0.382511000 | 2.676470000 | -0.837708000 |
| H | -0.020975000 | 3.212277000 | 0.822576000 |
| H | 1.542365000 | 3.695446000 | 0.086060000 |
| C | 2.860959000 | -1.012081000 | -1.151679000 |
| C | 3.046491000 | 0.327444000 | -1.424474000 |
| C | 4.030490000 | 0.842308000 | -0.548376000 |
| C | 4.409135000 | -0.158821000 | 0.374018000 |
| C | 3.941073000 | -1.476245000 | -0.226251000 |
| H | 2.135964000 | -1.670714000 | -1.628043000 |
| H | 2.466245000 | 0.908551000 | -2.141782000 |
| H | 4.362993000 | 1.880771000 | -0.515738000 |
| H | 5.339783000 | -0.087443000 | 0.943790000 |
| H | 3.647976000 | -2.261154000 | 0.483364000 |
| H | 4.771819000 | -1.884976000 | -0.837211000 |

TS1a-W-exo: E= -1057.445949

| | | | |
|---|-------------|--------------|--------------|
| C | 4.561832000 | -1.111027000 | 0.172562000 |
| C | 3.515368000 | -1.604858000 | -0.634672000 |
| C | 2.853746000 | -0.533215000 | -1.214643000 |
| C | 4.493696000 | 0.301987000 | 0.208162000 |
| C | 3.651974000 | 0.707694000 | -0.988186000 |
| H | 5.225803000 | -1.721631000 | 0.787258000 |
| H | 3.211726000 | -2.648271000 | -0.723000000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.973776000 | -0.589747000 | -1.854928000 |
| H | 5.328270000 | 0.914440000 | 0.560268000 |
| H | 3.067778000 | 1.629037000 | -0.881803000 |
| H | 4.336097000 | 0.843915000 | -1.850665000 |
| C | 1.883965000 | 0.133340000 | 1.194638000 |
| C | 3.114852000 | 0.658318000 | 1.645192000 |
| H | 3.610274000 | 0.145515000 | 2.472185000 |
| C | 0.839731000 | 0.866129000 | 0.547449000 |
| W | -1.091278000 | -0.134584000 | 0.015493000 |
| C | -0.062273000 | -1.906035000 | -0.392946000 |
| C | -0.915706000 | 0.436759000 | -1.989042000 |
| C | -1.251908000 | -0.745223000 | 2.022291000 |
| C | -2.847160000 | -1.169261000 | -0.441467000 |
| C | -2.326344000 | 1.516321000 | 0.375635000 |
| O | 0.501244000 | -2.892011000 | -0.622555000 |
| O | -3.820165000 | -1.742322000 | -0.695434000 |
| O | -3.045113000 | 2.406674000 | 0.550231000 |
| O | -1.325708000 | -1.093173000 | 3.119428000 |
| O | -0.803971000 | 0.752437000 | -3.097808000 |
| O | 1.208105000 | 2.142502000 | 0.344576000 |
| C | 0.330557000 | 3.096896000 | -0.234511000 |
| H | 1.656238000 | -0.908148000 | 1.418826000 |
| H | 3.224712000 | 1.745454000 | 1.657398000 |
| H | -0.471873000 | 3.363547000 | 0.468809000 |
| H | 0.939365000 | 3.986314000 | -0.446342000 |
| H | -0.116712000 | 2.718958000 | -1.164804000 |

TS1a-Cr-endo: E= -2035.443149

| | | | |
|----|--------------|--------------|--------------|
| C | 1.391661000 | -0.326315000 | 1.324788000 |
| C | 2.621968000 | 0.119223000 | 1.850148000 |
| H | 3.113866000 | -0.525788000 | 2.584182000 |
| C | 0.459000000 | 0.522708000 | 0.644341000 |
| Cr | -1.429314000 | -0.159532000 | -0.017155000 |
| C | -0.697005000 | -1.880251000 | -0.296535000 |
| C | -3.086765000 | -0.849210000 | -0.593639000 |
| C | -1.750495000 | -0.595897000 | 1.813672000 |
| C | -2.325742000 | 1.498656000 | 0.231095000 |
| C | -0.881135000 | 0.310660000 | -1.761790000 |
| O | 1.013257000 | 1.734797000 | 0.521942000 |
| O | -0.478984000 | 0.587560000 | -2.808151000 |
| O | -0.270379000 | -2.934377000 | -0.487468000 |
| O | -1.912784000 | -0.859239000 | 2.919827000 |
| O | -4.096865000 | -1.270622000 | -0.953177000 |
| O | -2.943790000 | 2.461541000 | 0.363711000 |
| C | 0.378212000 | 2.847001000 | -0.090963000 |
| H | 1.100972000 | -1.364977000 | 1.476756000 |
| H | 2.745982000 | 1.187172000 | 2.034108000 |
| H | -0.027186000 | 2.593388000 | -1.079528000 |
| H | -0.428157000 | 3.234691000 | 0.546987000 |
| H | 1.155515000 | 3.615778000 | -0.199742000 |
| C | 2.523688000 | -1.072598000 | -1.088458000 |
| C | 2.705058000 | 0.248969000 | -1.444020000 |
| C | 3.652034000 | 0.832053000 | -0.571255000 |
| C | 4.017140000 | -0.103769000 | 0.421110000 |
| C | 3.586848000 | -1.462238000 | -0.109412000 |
| H | 1.828279000 | -1.772874000 | -1.549524000 |
| H | 2.141058000 | 0.774251000 | -2.215111000 |
| H | 3.968284000 | 1.876003000 | -0.592928000 |
| H | 4.925349000 | 0.019063000 | 1.017534000 |
| H | 3.290365000 | -2.209686000 | 0.637927000 |
| H | 4.438780000 | -1.889497000 | -0.676889000 |

TS1a-Cr-exo: E= -2035.440570

| | | | |
|----|--------------|--------------|--------------|
| C | 4.193076000 | -1.053293000 | 0.278457000 |
| C | 3.192027000 | -1.612669000 | -0.540921000 |
| C | 2.516133000 | -0.587173000 | -1.187239000 |
| C | 4.081900000 | 0.356751000 | 0.251698000 |
| C | 3.268021000 | 0.686407000 | -0.985000000 |
| H | 4.854893000 | -1.616962000 | 0.938689000 |
| H | 2.929199000 | -2.669253000 | -0.598625000 |
| H | 1.686747000 | -0.705655000 | -1.883629000 |
| H | 4.883187000 | 1.010535000 | 0.606507000 |
| H | 2.652463000 | 1.592119000 | -0.935412000 |
| H | 3.974521000 | 0.808853000 | -1.831279000 |
| C | 1.450031000 | 0.124143000 | 1.163102000 |
| C | 2.641666000 | 0.721342000 | 1.628241000 |
| H | 3.133427000 | 0.265951000 | 2.490505000 |
| C | 0.378582000 | 0.785439000 | 0.473707000 |
| Cr | -1.423475000 | -0.219368000 | 0.011869000 |
| C | -0.454879000 | -1.831011000 | -0.224380000 |
| C | -1.102005000 | 0.188424000 | -1.806460000 |
| C | -1.552263000 | -0.579189000 | 1.882305000 |
| C | -2.992543000 | -1.187865000 | -0.383255000 |
| C | -2.541020000 | 1.302722000 | 0.238042000 |
| O | 0.107036000 | -2.824540000 | -0.383083000 |
| O | -3.949921000 | -1.778892000 | -0.630414000 |
| O | -3.285295000 | 2.171835000 | 0.368138000 |
| O | -1.602678000 | -0.795524000 | 3.009207000 |
| O | -0.849349000 | 0.422522000 | -2.907568000 |
| O | 0.732875000 | 2.049481000 | 0.212530000 |
| C | -0.113613000 | 3.005312000 | -0.411754000 |
| H | 1.269559000 | -0.914602000 | 1.434858000 |
| H | 2.710852000 | 1.811374000 | 1.594684000 |
| H | -0.908793000 | 3.327897000 | 0.274928000 |
| H | 0.527287000 | 3.865004000 | -0.650942000 |
| H | -0.561973000 | 2.614479000 | -1.334868000 |

TS1b-W-endo: E= -1096.707069

| | | | |
|---|--------------|--------------|--------------|
| C | -1.869669000 | -0.745130000 | -1.209001000 |
| C | -3.141503000 | -0.360263000 | -1.706865000 |
| H | -3.759696000 | -1.153794000 | -2.137879000 |
| C | -0.911811000 | 0.271130000 | -0.863550000 |
| W | 1.133075000 | -0.043060000 | 0.039269000 |
| C | 0.445303000 | -1.521564000 | 1.338291000 |
| C | 3.013989000 | -0.365031000 | 0.882165000 |
| C | 1.597783000 | -1.498211000 | -1.401875000 |
| C | 2.074585000 | 1.428336000 | -1.116348000 |
| C | 0.720873000 | 1.333686000 | 1.551847000 |
| O | -1.467340000 | 1.474776000 | -1.130097000 |
| O | 0.473820000 | 2.083368000 | 2.402449000 |
| O | 0.080062000 | -2.328586000 | 2.087579000 |
| O | 1.870438000 | -2.313009000 | -2.173736000 |
| O | 4.057959000 | -0.542411000 | 1.350427000 |
| O | 2.640627000 | 2.239451000 | -1.717855000 |
| C | -0.792434000 | 2.711395000 | -0.985700000 |
| H | -3.232636000 | 0.600549000 | -2.211043000 |
| H | -0.384881000 | 2.842628000 | 0.025304000 |
| H | 0.023037000 | 2.799621000 | -1.717464000 |
| H | -1.542415000 | 3.489615000 | -1.184142000 |
| C | -2.851098000 | -0.495599000 | 1.543552000 |
| C | -2.852497000 | 0.873465000 | 1.405324000 |
| C | -3.802553000 | 1.237140000 | 0.417596000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.346918000 | 0.070531000 | -0.164509000 |
| C | -4.006646000 | -1.067908000 | 0.786349000 |
| H | -2.186715000 | -1.077002000 | 2.182269000 |
| H | -2.174916000 | 1.558888000 | 1.915287000 |
| H | -4.009797000 | 2.256040000 | 0.088776000 |
| H | -5.297532000 | 0.095907000 | -0.704287000 |
| H | -3.828415000 | -2.050294000 | 0.330605000 |
| H | -4.857875000 | -1.194071000 | 1.486316000 |
| C | -1.530646000 | -2.214790000 | -1.152905000 |
| H | -1.040116000 | -2.516727000 | -0.221134000 |
| H | -2.432926000 | -2.831809000 | -1.279848000 |
| H | -0.847752000 | -2.484915000 | -1.975064000 |

TS1b-W-exo: E= -1096.706850

| | | | |
|---|--------------|--------------|--------------|
| C | 4.462465000 | -0.987667000 | -0.258179000 |
| C | 3.380885000 | -1.312589000 | -1.110881000 |
| C | 2.713103000 | -0.150889000 | -1.450919000 |
| C | 4.412162000 | 0.393709000 | 0.049046000 |
| C | 3.521809000 | 1.022351000 | -1.010495000 |
| H | 5.152609000 | -1.706124000 | 0.187561000 |
| H | 3.068007000 | -2.318629000 | -1.391755000 |
| H | 1.807980000 | -0.078668000 | -2.052113000 |
| H | 5.278390000 | 0.923326000 | 0.455178000 |
| H | 2.938749000 | 1.896419000 | -0.699001000 |
| H | 4.168393000 | 1.340096000 | -1.853698000 |
| C | 1.925916000 | -0.043821000 | 1.255813000 |
| C | 3.158312000 | 0.556988000 | 1.619483000 |
| H | 3.772027000 | 0.025662000 | 2.351592000 |
| C | 0.833827000 | 0.721492000 | 0.701773000 |
| W | -1.137359000 | -0.104125000 | -0.028698000 |
| C | -0.207108000 | -1.710340000 | -0.981540000 |
| C | -1.002483000 | 0.946693000 | -1.829556000 |
| C | -1.346861000 | -1.211950000 | 1.744061000 |
| C | -2.939906000 | -0.922522000 | -0.685430000 |
| C | -2.317020000 | 1.421753000 | 0.785814000 |
| O | 0.299002000 | -2.599393000 | -1.527025000 |
| O | -3.941592000 | -1.376539000 | -1.047289000 |
| O | -3.016553000 | 2.246039000 | 1.199589000 |
| O | -1.470594000 | -1.836874000 | 2.706742000 |
| O | -0.930397000 | 1.518624000 | -2.835295000 |
| O | 1.176051000 | 2.029348000 | 0.690149000 |
| C | 0.301501000 | 3.072628000 | 0.296909000 |
| H | 3.202343000 | 1.643433000 | 1.701421000 |
| H | -0.528304000 | 3.177312000 | 1.010076000 |
| H | 0.904316000 | 3.991261000 | 0.305858000 |
| H | -0.105286000 | 2.910133000 | -0.710414000 |
| C | 1.805526000 | -1.506556000 | 1.583276000 |
| H | 2.786592000 | -2.001470000 | 1.486282000 |
| H | 1.484779000 | -1.638850000 | 2.630994000 |
| H | 1.093823000 | -2.043962000 | 0.951628000 |

TS1b-Cr-endo: E= -2074.699885

| | | | |
|----|--------------|--------------|--------------|
| C | -1.451446000 | -0.768409000 | -1.157041000 |
| C | -2.693239000 | -0.361710000 | -1.711766000 |
| H | -3.304801000 | -1.143586000 | -2.172769000 |
| C | -0.475100000 | 0.232317000 | -0.785565000 |
| Cr | 1.465640000 | -0.071540000 | 0.084054000 |
| C | 0.799527000 | -1.396944000 | 1.254988000 |
| C | 3.162763000 | -0.362382000 | 0.837161000 |
| C | 1.830963000 | -1.349760000 | -1.283651000 |
| C | 2.282561000 | 1.264296000 | -0.996418000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.1030129000 | 1.160012000 | 1.446747000 |
| O | -1.023347000 | 1.428276000 | -1.063621000 |
| O | 0.741951000 | 1.870537000 | 2.310333000 |
| O | 0.434838000 | -2.168981000 | 2.031263000 |
| O | 2.082625000 | -2.114255000 | -2.104415000 |
| O | 4.202694000 | -0.538428000 | 1.301885000 |
| O | 2.854402000 | 2.045344000 | -1.620237000 |
| C | -0.397172000 | 2.692418000 | -0.928450000 |
| H | -2.752522000 | 0.601983000 | -2.214786000 |
| H | 0.029895000 | 2.843870000 | 0.070317000 |
| H | 0.387510000 | 2.822471000 | -1.686350000 |
| H | -1.188277000 | 3.435765000 | -1.100325000 |
| C | -2.514945000 | -0.468367000 | 1.535298000 |
| C | -2.534733000 | 0.901074000 | 1.392172000 |
| C | -3.452766000 | 1.244556000 | 0.369393000 |
| C | -3.964556000 | 0.067530000 | -0.220154000 |
| C | -3.644481000 | -1.058264000 | 0.751738000 |
| H | -1.869707000 | -1.035166000 | 2.205911000 |
| H | -1.886760000 | 1.599574000 | 1.922344000 |
| H | -3.659019000 | 2.258253000 | 0.023604000 |
| H | -4.895324000 | 0.077595000 | -0.793921000 |
| H | -3.449082000 | -2.044561000 | 0.312742000 |
| H | -4.513501000 | -1.180192000 | 1.430236000 |
| C | -1.166302000 | -2.252021000 | -1.096100000 |
| H | -0.732574000 | -2.586421000 | -0.147640000 |
| H | -2.087178000 | -2.830498000 | -1.264437000 |
| H | -0.466531000 | -2.548155000 | -1.894023000 |

TS1b-Cr-exo: E= -2074.698955

| | | | |
|----|--------------|--------------|--------------|
| C | -4.128110000 | -0.936372000 | 0.125185000 |
| C | -3.109075000 | -1.358484000 | 1.010847000 |
| C | -2.412362000 | -0.251410000 | 1.457868000 |
| C | -4.005420000 | 0.456266000 | -0.093249000 |
| C | -3.141613000 | 0.981682000 | 1.040540000 |
| H | -4.825013000 | -1.595705000 | -0.395176000 |
| H | -2.862152000 | -2.393194000 | 1.250177000 |
| H | -1.564734000 | -0.261358000 | 2.141736000 |
| H | -4.826898000 | 1.047882000 | -0.506538000 |
| H | -2.503199000 | 1.841127000 | 0.805498000 |
| H | -3.814470000 | 1.287957000 | 1.867255000 |
| C | -1.489284000 | -0.020413000 | -1.229318000 |
| C | -2.683024000 | 0.648000000 | -1.603969000 |
| H | -3.291680000 | 0.180662000 | -2.382769000 |
| C | -0.377513000 | 0.678083000 | -0.613935000 |
| Cr | 1.476121000 | -0.172236000 | 0.056085000 |
| C | 0.570700000 | -1.652560000 | 0.815310000 |
| C | 1.233741000 | 0.674958000 | 1.728451000 |
| C | 1.625821000 | -1.023028000 | -1.645502000 |
| C | 3.083690000 | -0.957515000 | 0.633518000 |
| C | 2.536852000 | 1.257998000 | -0.612056000 |
| O | 0.060520000 | -2.544462000 | 1.338502000 |
| O | 4.068402000 | -1.439461000 | 0.988916000 |
| O | 3.254572000 | 2.073027000 | -0.995396000 |
| O | 1.728610000 | -1.529975000 | -2.671542000 |
| O | 1.059951000 | 1.148040000 | 2.766532000 |
| O | -0.705400000 | 1.979352000 | -0.528914000 |
| C | 0.144303000 | 3.032372000 | -0.103601000 |
| H | -2.687543000 | 1.738025000 | -1.627721000 |
| H | 0.931732000 | 3.222797000 | -0.845932000 |
| H | -0.498677000 | 3.920529000 | -0.028701000 |
| H | 0.601086000 | 2.834117000 | 0.874057000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.432728000 | -1.467397000 | -1.639337000 |
| H | -2.437285000 | -1.918646000 | -1.563832000 |
| H | -1.127037000 | -1.555471000 | -2.696052000 |
| H | -0.750141000 | -2.080328000 | -1.047333000 |

TS1c-W-endo: E= -2713.888502

| | | | |
|----|--------------|--------------|--------------|
| C | -0.311923000 | 1.839866000 | -1.431268000 |
| C | 0.825884000 | 2.588600000 | -1.801290000 |
| H | 0.728029000 | 3.241584000 | -2.673862000 |
| C | -0.260167000 | 0.690802000 | -0.584805000 |
| W | -2.089012000 | -0.480322000 | 0.006459000 |
| C | -3.291970000 | 1.193502000 | -0.360391000 |
| C | -3.816960000 | -1.509834000 | 0.554483000 |
| C | -2.300877000 | -1.039978000 | -2.007579000 |
| C | -1.065859000 | -2.230781000 | 0.468138000 |
| C | -1.825200000 | 0.211640000 | 1.955699000 |
| O | 0.939812000 | 0.383772000 | -0.157938000 |
| O | -1.640356000 | 0.631753000 | 3.021199000 |
| O | -3.959821000 | 2.122016000 | -0.541180000 |
| O | -2.393904000 | -1.331728000 | -3.121335000 |
| O | -4.777729000 | -2.080947000 | 0.859328000 |
| O | -0.525899000 | -3.226928000 | 0.734522000 |
| H | 1.810776000 | 2.133365000 | -1.679274000 |
| C | -0.833626000 | 3.416087000 | 0.765665000 |
| C | 0.299915000 | 2.952955000 | 1.403842000 |
| C | 1.440646000 | 3.395259000 | 0.695911000 |
| C | 1.030014000 | 4.073097000 | -0.473057000 |
| C | -0.433421000 | 4.426980000 | -0.262848000 |
| H | -1.862883000 | 3.196464000 | 1.047554000 |
| H | 0.300541000 | 2.280807000 | 2.261354000 |
| H | 2.474477000 | 3.130719000 | 0.916413000 |
| H | 1.711990000 | 4.729155000 | -1.020254000 |
| H | -1.064544000 | 4.466476000 | -1.160146000 |
| H | -0.473285000 | 5.431365000 | 0.206306000 |
| Ti | 2.544907000 | -0.573598000 | -0.006212000 |
| C | 3.622625000 | -1.236626000 | -2.074010000 |
| C | 2.286836000 | -0.878833000 | -2.379731000 |
| C | 1.427856000 | -1.805960000 | -1.737478000 |
| C | 2.224843000 | -2.714129000 | -1.007939000 |
| C | 3.591117000 | -2.355953000 | -1.211451000 |
| H | 4.512997000 | -0.703948000 | -2.395496000 |
| H | 1.970839000 | -0.022408000 | -2.971217000 |
| H | 0.341630000 | -1.766918000 | -1.734516000 |
| H | 1.849176000 | -3.544935000 | -0.417619000 |
| H | 4.459363000 | -2.871937000 | -0.809267000 |
| C | 2.207572000 | -1.984935000 | 1.887942000 |
| C | 1.652381000 | -0.729410000 | 2.228475000 |
| C | 2.698072000 | 0.218954000 | 2.259387000 |
| C | 3.918856000 | -0.461324000 | 1.987973000 |
| C | 3.619858000 | -1.819169000 | 1.762090000 |
| H | 1.648064000 | -2.910100000 | 1.788529000 |
| H | 0.592909000 | -0.521612000 | 2.339200000 |
| H | 2.593180000 | 1.286072000 | 2.433011000 |
| H | 4.899769000 | 0.001150000 | 1.917591000 |
| H | 4.338560000 | -2.604341000 | 1.541922000 |
| Cl | 3.981411000 | 1.274651000 | -0.487898000 |
| H | -1.292298000 | 2.114604000 | -1.820614000 |

TS1c-W-exo: E= -2713.886948

| | | | |
|---|--------------|-------------|--------------|
| C | -0.167185000 | 4.865209000 | -0.330253000 |
| C | -1.181127000 | 4.240086000 | 0.425764000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -0.631618000 | 3.163337000 | 1.106114000 |
| C | 1.023445000 | 4.105633000 | -0.228977000 |
| C | 0.855498000 | 3.230159000 | 0.997233000 |
| H | -0.314332000 | 5.714334000 | -1.000374000 |
| H | -2.240311000 | 4.499592000 | 0.413967000 |
| H | -1.172582000 | 2.464822000 | 1.743461000 |
| H | 2.001579000 | 4.498581000 | -0.516873000 |
| H | 1.387313000 | 2.273841000 | 0.973825000 |
| H | 1.242811000 | 3.797674000 | 1.868156000 |
| C | -0.340387000 | 1.894389000 | -1.234951000 |
| C | 0.763857000 | 2.688011000 | -1.622154000 |
| H | 0.637708000 | 3.326441000 | -2.499837000 |
| C | -0.271424000 | 0.671604000 | -0.498987000 |
| W | -2.066845000 | -0.573889000 | -0.010666000 |
| C | -2.444167000 | -0.692123000 | -2.074166000 |
| C | -3.220252000 | 1.172491000 | 0.107891000 |
| C | -1.078396000 | -2.402443000 | -0.023431000 |
| C | -3.788458000 | -1.652324000 | 0.464959000 |
| C | -1.550475000 | -0.366380000 | 2.000452000 |
| O | -2.618195000 | -0.740344000 | -3.214761000 |
| O | -4.746295000 | -2.247759000 | 0.729145000 |
| O | -1.222477000 | -0.219964000 | 3.103267000 |
| O | -0.545679000 | -3.436269000 | 0.003010000 |
| O | -3.854523000 | 2.137171000 | 0.189279000 |
| O | 0.922282000 | 0.311886000 | -0.096877000 |
| H | 1.763690000 | 2.261815000 | -1.505539000 |
| Ti | 2.581866000 | -0.528555000 | -0.003918000 |
| Cl | 3.877096000 | 1.454897000 | -0.288614000 |
| C | 3.673774000 | -2.221276000 | -1.280198000 |
| C | 3.816048000 | -1.026637000 | -2.016375000 |
| C | 2.520864000 | -0.596359000 | -2.411139000 |
| C | 1.582860000 | -1.548406000 | -1.947492000 |
| C | 2.282372000 | -2.541490000 | -1.226189000 |
| H | 4.483947000 | -2.795608000 | -0.835757000 |
| H | 4.744947000 | -0.493179000 | -2.199490000 |
| H | 2.287829000 | 0.323093000 | -2.943129000 |
| H | 0.500928000 | -1.476235000 | -2.039225000 |
| H | 1.823253000 | -3.395900000 | -0.735563000 |
| C | 2.027093000 | -0.299196000 | 2.365543000 |
| C | 3.406183000 | -0.052261000 | 2.248379000 |
| C | 4.031077000 | -1.236349000 | 1.763988000 |
| C | 3.026106000 | -2.227810000 | 1.630666000 |
| C | 1.780647000 | -1.639160000 | 1.959155000 |
| H | 1.262791000 | 0.415586000 | 2.657333000 |
| H | 3.905205000 | 0.894422000 | 2.433064000 |
| H | 5.092707000 | -1.356994000 | 1.555015000 |
| H | 3.178168000 | -3.257112000 | 1.316214000 |
| H | 0.808220000 | -2.121436000 | 1.908458000 |
| H | -1.337900000 | 2.179037000 | -1.571233000 |

TS1c-Cr-endo: E= -3691.885046

| | | | |
|----|--------------|--------------|--------------|
| C | -0.983127000 | 1.588634000 | -1.369613000 |
| C | 0.059907000 | 2.442988000 | -1.788742000 |
| H | -0.127501000 | 3.047994000 | -2.681274000 |
| C | -0.806136000 | 0.439359000 | -0.533156000 |
| Cr | -2.400987000 | -0.853244000 | 0.026253000 |
| C | -3.661517000 | 0.516913000 | -0.351288000 |
| C | -3.848180000 | -1.965758000 | 0.490217000 |
| C | -2.372892000 | -1.376615000 | -1.802735000 |
| C | -1.260463000 | -2.277374000 | 0.493352000 |
| C | -2.191477000 | -0.130315000 | 1.749712000 |

| | | | |
|----|--------------|--------------|--------------|
| O | 0.415845000 | 0.244716000 | -0.130147000 |
| O | -2.017247000 | 0.351470000 | 2.785834000 |
| O | -4.440960000 | 1.343114000 | -0.542885000 |
| O | -2.302098000 | -1.664295000 | -2.914745000 |
| O | -4.732793000 | -2.646992000 | 0.776116000 |
| O | -0.616182000 | -3.186730000 | 0.801240000 |
| H | 1.092439000 | 2.108529000 | -1.676771000 |
| C | -1.611555000 | 3.135834000 | 0.782172000 |
| C | -0.406759000 | 2.864929000 | 1.404085000 |
| C | 0.638874000 | 3.439237000 | 0.648819000 |
| C | 0.106919000 | 4.003430000 | -0.531376000 |
| C | -1.384144000 | 4.160684000 | -0.285105000 |
| H | -2.593055000 | 2.796894000 | 1.111770000 |
| H | -0.287924000 | 2.237215000 | 2.286320000 |
| H | 1.704188000 | 3.340197000 | 0.853618000 |
| H | 0.675237000 | 4.724140000 | -1.125058000 |
| H | -2.040011000 | 4.088300000 | -1.162009000 |
| H | -1.546802000 | 5.162579000 | 0.162318000 |
| Ti | 2.161720000 | -0.430768000 | 0.000682000 |
| C | 3.256219000 | -0.883410000 | -2.122305000 |
| C | 1.863073000 | -0.842958000 | -2.363828000 |
| C | 1.267126000 | -1.922411000 | -1.662435000 |
| C | 2.281373000 | -2.608589000 | -0.961780000 |
| C | 3.519522000 | -1.955171000 | -1.238050000 |
| H | 3.988563000 | -0.174984000 | -2.497476000 |
| H | 1.331391000 | -0.099050000 | -2.953242000 |
| H | 0.207491000 | -2.153297000 | -1.639328000 |
| H | 2.135467000 | -3.486652000 | -0.338159000 |
| H | 4.500587000 | -2.244951000 | -0.869110000 |
| C | 2.002178000 | -1.805571000 | 1.940873000 |
| C | 1.392767000 | -0.576402000 | 2.292140000 |
| C | 2.375572000 | 0.431486000 | 2.240220000 |
| C | 3.621210000 | -0.181947000 | 1.912114000 |
| C | 3.393603000 | -1.560593000 | 1.743468000 |
| H | 1.494829000 | -2.763717000 | 1.879747000 |
| H | 0.335636000 | -0.426860000 | 2.485993000 |
| H | 2.214988000 | 1.495207000 | 2.392016000 |
| H | 4.565599000 | 0.337967000 | 1.772800000 |
| H | 4.142967000 | -2.308689000 | 1.497189000 |
| Cl | 3.311489000 | 1.609444000 | -0.512867000 |
| H | -1.988626000 | 1.764832000 | -1.749526000 |

TS1c-Cr-exo: E= -3691.884127

| | | | |
|----|--------------|--------------|--------------|
| C | 1.268686000 | 4.580786000 | 0.400073000 |
| C | 2.171125000 | 3.860241000 | -0.408675000 |
| C | 1.469388000 | 2.887030000 | -1.106427000 |
| C | -0.012465000 | 3.985274000 | 0.312535000 |
| C | 0.006990000 | 3.139088000 | -0.943881000 |
| H | 1.542802000 | 5.379795000 | 1.091693000 |
| H | 3.254133000 | 3.987873000 | -0.425567000 |
| H | 1.896004000 | 2.172897000 | -1.809804000 |
| H | -0.924220000 | 4.487466000 | 0.644623000 |
| H | -0.643131000 | 2.259387000 | -0.930915000 |
| H | -0.331189000 | 3.780397000 | -1.783467000 |
| C | 1.081850000 | 1.585975000 | 1.200451000 |
| C | 0.107130000 | 2.503640000 | 1.654393000 |
| H | 0.349844000 | 3.093625000 | 2.541612000 |
| C | 0.819602000 | 0.375577000 | 0.480101000 |
| Cr | 2.315587000 | -1.042360000 | 0.001699000 |
| C | 2.501743000 | -1.243308000 | 1.886538000 |
| C | 3.613496000 | 0.348797000 | -0.024220000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 1.108659000 | -2.484588000 | -0.048885000 |
| C | 3.690743000 | -2.258224000 | -0.428159000 |
| C | 1.885645000 | -0.633989000 | -1.783743000 |
| O | 2.556936000 | -1.338839000 | 3.031526000 |
| O | 4.529659000 | -3.001552000 | -0.695944000 |
| O | 1.577416000 | -0.324595000 | -2.853759000 |
| O | 0.408585000 | -3.402218000 | -0.118808000 |
| O | 4.406490000 | 1.182179000 | -0.068091000 |
| O | -0.419468000 | 0.191937000 | 0.127863000 |
| H | -0.944088000 | 2.219036000 | 1.568755000 |
| Ti | -2.207141000 | -0.329726000 | -0.011171000 |
| Cl | -3.133069000 | 1.852775000 | 0.331484000 |
| C | -3.612046000 | -1.849624000 | 1.183236000 |
| C | -3.597124000 | -0.657811000 | 1.935106000 |
| C | -2.269244000 | -0.446622000 | 2.398710000 |
| C | -1.475455000 | -1.528960000 | 1.957718000 |
| C | -2.287716000 | -2.384711000 | 1.178860000 |
| H | -4.481231000 | -2.282447000 | 0.692850000 |
| H | -4.436534000 | 0.015269000 | 2.087071000 |
| H | -1.921112000 | 0.413313000 | 2.966073000 |
| H | -0.407358000 | -1.643011000 | 2.124284000 |
| H | -1.950068000 | -3.294007000 | 0.688429000 |
| C | -1.652088000 | -0.076887000 | -2.377519000 |
| C | -2.984324000 | 0.351189000 | -2.229790000 |
| C | -3.759803000 | -0.752488000 | -1.780539000 |
| C | -2.898653000 | -1.879214000 | -1.704247000 |
| C | -1.590995000 | -1.456024000 | -2.037588000 |
| H | -0.799689000 | 0.534693000 | -2.659230000 |
| H | -3.349540000 | 1.364062000 | -2.369927000 |
| H | -4.825332000 | -0.734867000 | -1.558332000 |
| H | -3.187367000 | -2.890739000 | -1.430338000 |
| H | -0.699988000 | -2.077134000 | -2.041617000 |
| H | 2.115460000 | 1.741657000 | 1.506981000 |

TS1d-W-endo: E= -2753.147568

| | | | |
|---|--------------|--------------|--------------|
| C | 0.238790000 | 1.902444000 | 1.358344000 |
| C | -0.955978000 | 2.652292000 | 1.525188000 |
| H | -0.969864000 | 3.366160000 | 2.354796000 |
| C | 0.239226000 | 0.726298000 | 0.532549000 |
| W | 2.027732000 | -0.549181000 | -0.039922000 |
| C | 3.400333000 | 1.025987000 | -0.007895000 |
| C | 3.655889000 | -1.714045000 | -0.614061000 |
| C | 2.381174000 | -0.976566000 | 1.981704000 |
| C | 0.949076000 | -2.311476000 | -0.264038000 |
| C | 1.667731000 | -0.042891000 | -2.029116000 |
| O | -0.945368000 | 0.399265000 | 0.049153000 |
| O | 1.453026000 | 0.257948000 | -3.128806000 |
| O | 4.195352000 | 1.869111000 | -0.040527000 |
| O | 2.564238000 | -1.209406000 | 3.099797000 |
| O | 4.560133000 | -2.364318000 | -0.934070000 |
| O | 0.404289000 | -3.328098000 | -0.420990000 |
| H | -1.915841000 | 2.174481000 | 1.335587000 |
| C | 0.831565000 | 3.302099000 | -1.067526000 |
| C | -0.274971000 | 2.775651000 | -1.699562000 |
| C | -1.442256000 | 3.244673000 | -1.053919000 |
| C | -1.076357000 | 4.013210000 | 0.074529000 |
| C | 0.388606000 | 4.369987000 | -0.118439000 |
| H | 1.871560000 | 3.069357000 | -1.295903000 |
| H | -0.244869000 | 2.048510000 | -2.509503000 |
| H | -2.465190000 | 2.948102000 | -1.283052000 |
| H | -1.782298000 | 4.706522000 | 0.539037000 |

| | | | |
|----|--------------|--------------|--------------|
| H | 0.992452000 | 4.482374000 | 0.789989000 |
| H | 0.431942000 | 5.343082000 | -0.649186000 |
| C | 1.470896000 | 2.301138000 | 2.139590000 |
| H | 1.851446000 | 1.455426000 | 2.731586000 |
| H | 2.302581000 | 2.641984000 | 1.509368000 |
| H | 1.235971000 | 3.112320000 | 2.845022000 |
| Ti | -2.563504000 | -0.568759000 | 0.034741000 |
| C | -3.680251000 | -1.012655000 | 2.142977000 |
| C | -2.365588000 | -0.569613000 | 2.436841000 |
| C | -1.457736000 | -1.536928000 | 1.941599000 |
| C | -2.201439000 | -2.556111000 | 1.307164000 |
| C | -3.584495000 | -2.229484000 | 1.433344000 |
| H | -4.597535000 | -0.477423000 | 2.371179000 |
| H | -2.097662000 | 0.362960000 | 2.927642000 |
| H | -0.373440000 | -1.463038000 | 1.964641000 |
| H | -1.779805000 | -3.440533000 | 0.839718000 |
| H | -4.420554000 | -2.827488000 | 1.079879000 |
| C | -2.357943000 | -2.253038000 | -1.647717000 |
| C | -1.683124000 | -1.109989000 | -2.132504000 |
| C | -2.635748000 | -0.081915000 | -2.317148000 |
| C | -3.916174000 | -0.606558000 | -1.992630000 |
| C | -3.748766000 | -1.941120000 | -1.572598000 |
| H | -1.889767000 | -3.206033000 | -1.421589000 |
| H | -0.608478000 | -1.013436000 | -2.238417000 |
| H | -2.427263000 | 0.937908000 | -2.627708000 |
| H | -4.851681000 | -0.054608000 | -2.011994000 |
| H | -4.542487000 | -2.617859000 | -1.266546000 |
| Cl | -4.016613000 | 1.316407000 | 0.298170000 |

TS1d-W-exo: E= -2753.149724

| | | | |
|---|--------------|--------------|--------------|
| C | 0.315593000 | 4.741457000 | -0.016805000 |
| C | 1.285374000 | 4.026609000 | -0.762052000 |
| C | 0.668571000 | 2.970258000 | -1.403257000 |
| C | -0.922349000 | 4.059509000 | -0.089531000 |
| C | -0.810098000 | 3.109462000 | -1.268595000 |
| H | 0.516498000 | 5.616267000 | 0.604313000 |
| H | 2.357636000 | 4.224988000 | -0.770011000 |
| H | 1.163522000 | 2.217753000 | -2.015447000 |
| H | -1.870806000 | 4.542606000 | 0.158066000 |
| H | -1.375872000 | 2.176258000 | -1.180895000 |
| H | -1.198080000 | 3.636110000 | -2.164334000 |
| C | 0.280868000 | 1.912694000 | 1.243355000 |
| C | -0.872793000 | 2.723154000 | 1.398657000 |
| H | -0.868710000 | 3.423977000 | 2.238859000 |
| C | 0.261214000 | 0.688878000 | 0.487492000 |
| W | 1.994756000 | -0.670583000 | -0.018862000 |
| C | 2.514963000 | -0.726333000 | 2.014090000 |
| C | 3.239065000 | 0.960004000 | -0.435829000 |
| C | 0.941569000 | -2.451187000 | 0.186985000 |
| C | 3.614413000 | -1.879746000 | -0.522205000 |
| C | 1.387551000 | -0.591323000 | -2.010243000 |
| O | 2.780748000 | -0.750682000 | 3.138383000 |
| O | 4.517660000 | -2.550257000 | -0.801050000 |
| O | 1.037320000 | -0.526962000 | -3.114506000 |
| O | 0.388662000 | -3.472642000 | 0.253232000 |
| O | 3.926664000 | 1.853903000 | -0.699794000 |
| O | -0.924685000 | 0.329321000 | 0.029527000 |
| H | -1.852466000 | 2.306079000 | 1.164514000 |
| C | 1.510072000 | 2.390797000 | 1.963478000 |
| H | 1.413659000 | 2.205488000 | 3.047379000 |
| H | 2.433626000 | 1.912030000 | 1.627430000 |

| | | | |
|----|--------------|--------------|--------------|
| H | 1.625554000 | 3.482857000 | 1.840412000 |
| Ti | -2.603732000 | -0.496553000 | 0.021839000 |
| Cl | -3.893000000 | 1.516260000 | 0.101839000 |
| C | -3.733949000 | -2.028570000 | 1.464258000 |
| C | -3.846185000 | -0.764079000 | 2.078400000 |
| C | -2.540218000 | -0.326433000 | 2.425713000 |
| C | -1.625293000 | -1.340273000 | 2.056117000 |
| C | -2.351184000 | -2.385043000 | 1.441665000 |
| H | -4.557905000 | -2.626784000 | 1.081109000 |
| H | -4.761985000 | -0.194062000 | 2.209534000 |
| H | -2.285113000 | 0.633340000 | 2.868166000 |
| H | -0.541290000 | -1.282527000 | 2.134455000 |
| H | -1.914719000 | -3.296196000 | 1.041859000 |
| C | -3.066119000 | -2.350825000 | -1.431860000 |
| C | -1.837437000 | -1.781253000 | -1.844120000 |
| C | -2.110892000 | -0.488392000 | -2.368067000 |
| C | -3.492009000 | -0.252038000 | -2.249598000 |
| C | -4.088782000 | -1.390425000 | -1.640153000 |
| H | -3.197271000 | -3.347654000 | -1.019169000 |
| H | -0.859380000 | -2.247688000 | -1.773684000 |
| H | -1.365397000 | 0.204642000 | -2.746521000 |
| H | -4.009015000 | 0.664227000 | -2.518018000 |
| H | -5.143947000 | -1.503651000 | -1.397623000 |

TS1d-Cr-endo: E= -3731.140349

| | | | |
|----|--------------|--------------|--------------|
| C | 0.917211000 | 1.644312000 | 1.334109000 |
| C | -0.181508000 | 2.523445000 | 1.539893000 |
| H | -0.101798000 | 3.207977000 | 2.390463000 |
| C | 0.763492000 | 0.474027000 | 0.503997000 |
| Cr | 2.290652000 | -0.951537000 | -0.082354000 |
| C | 3.695728000 | 0.323423000 | -0.021109000 |
| C | 3.608517000 | -2.188994000 | -0.583961000 |
| C | 2.447792000 | -1.375014000 | 1.763874000 |
| C | 1.061473000 | -2.356869000 | -0.326230000 |
| C | 1.984381000 | -0.371694000 | -1.844165000 |
| O | -0.454227000 | 0.289651000 | 0.055433000 |
| O | 1.794168000 | 0.005369000 | -2.919635000 |
| O | 4.592258000 | 1.045291000 | -0.082791000 |
| O | 2.504633000 | -1.631837000 | 2.885046000 |
| O | 4.416665000 | -2.952323000 | -0.890674000 |
| O | 0.386789000 | -3.276628000 | -0.514589000 |
| H | -1.194097000 | 2.168343000 | 1.359570000 |
| C | 1.598535000 | 3.026176000 | -1.080243000 |
| C | 0.414011000 | 2.668833000 | -1.691329000 |
| C | -0.661649000 | 3.264898000 | -0.996019000 |
| C | -0.167256000 | 3.936962000 | 0.144957000 |
| C | 1.324166000 | 4.111229000 | -0.087857000 |
| H | 2.594589000 | 2.682630000 | -1.359860000 |
| H | 0.325256000 | 1.972860000 | -2.523724000 |
| H | -1.720194000 | 3.116123000 | -1.203858000 |
| H | -0.763419000 | 4.700137000 | 0.651897000 |
| H | 1.964784000 | 4.120657000 | 0.801796000 |
| H | 1.473260000 | 5.086165000 | -0.595633000 |
| C | 2.192091000 | 1.909497000 | 2.108680000 |
| H | 3.041485000 | 2.214898000 | 1.483529000 |
| H | 2.028356000 | 2.708651000 | 2.847226000 |
| H | 2.514783000 | 1.019845000 | 2.668212000 |
| Ti | -2.205848000 | -0.413237000 | 0.030031000 |
| C | -3.368677000 | -0.721612000 | 2.141161000 |
| C | -1.997287000 | -0.511307000 | 2.434097000 |
| C | -1.267238000 | -1.603098000 | 1.906202000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -2.171535000 | -2.465696000 | 1.249138000 |
| C | -3.480303000 | -1.917731000 | 1.400185000 |
| H | -4.183416000 | -0.049542000 | 2.394304000 |
| H | -1.574546000 | 0.348402000 | 2.948462000 |
| H | -0.190114000 | -1.724425000 | 1.954008000 |
| H | -1.905491000 | -3.392357000 | 0.749058000 |
| H | -4.407508000 | -2.357331000 | 1.042616000 |
| C | -2.238015000 | -2.029577000 | -1.731549000 |
| C | -1.491946000 | -0.931751000 | -2.219725000 |
| C | -2.351756000 | 0.184089000 | -2.300474000 |
| C | -3.656730000 | -0.238255000 | -1.918144000 |
| C | -3.589833000 | -1.600642000 | -1.571763000 |
| H | -1.847880000 | -3.029049000 | -1.566039000 |
| H | -0.429472000 | -0.933067000 | -2.433396000 |
| H | -2.069229000 | 1.192728000 | -2.588478000 |
| H | -4.536688000 | 0.396062000 | -1.858842000 |
| H | -4.423633000 | -2.219251000 | -1.251146000 |
| Cl | -3.368606000 | 1.666679000 | 0.365938000 |

TS1d-Cr-exo: E= -3731.143323

| | | | |
|----|--------------|--------------|--------------|
| C | 1.437628000 | 4.413779000 | 0.039691000 |
| C | 2.284802000 | 3.594318000 | -0.745218000 |
| C | 1.516360000 | 2.657446000 | -1.408511000 |
| C | 0.115562000 | 3.916109000 | -0.028336000 |
| C | 0.074240000 | 2.994661000 | -1.233050000 |
| H | 1.770017000 | 5.232244000 | 0.680903000 |
| H | 3.373704000 | 3.647302000 | -0.771748000 |
| H | 1.889809000 | 1.882734000 | -2.076438000 |
| H | -0.752714000 | 4.517914000 | 0.250811000 |
| H | -0.613310000 | 2.146612000 | -1.155618000 |
| H | -0.258110000 | 3.594057000 | -2.105096000 |
| C | 1.016359000 | 1.581275000 | 1.227251000 |
| C | 0.002713000 | 2.552436000 | 1.431308000 |
| H | 0.132946000 | 3.226991000 | 2.283039000 |
| C | 0.778955000 | 0.377355000 | 0.467762000 |
| Cr | 2.176224000 | -1.180990000 | -0.046157000 |
| C | 2.552893000 | -1.284230000 | 1.818214000 |
| C | 3.550285000 | 0.085006000 | -0.392445000 |
| C | 0.904884000 | -2.559091000 | 0.122642000 |
| C | 3.417665000 | -2.518161000 | -0.492808000 |
| C | 1.628732000 | -0.888869000 | -1.820820000 |
| O | 2.730200000 | -1.335450000 | 2.953709000 |
| O | 4.180241000 | -3.338771000 | -0.766023000 |
| O | 1.295572000 | -0.654800000 | -2.901985000 |
| O | 0.180987000 | -3.459651000 | 0.169157000 |
| O | 4.389992000 | 0.819832000 | -0.679491000 |
| O | -0.455125000 | 0.228454000 | 0.048996000 |
| H | -1.034784000 | 2.298155000 | 1.216850000 |
| C | 2.312559000 | 1.864479000 | 1.936638000 |
| H | 2.216016000 | 1.636846000 | 3.012438000 |
| H | 3.168451000 | 1.302189000 | 1.558198000 |
| H | 2.555660000 | 2.939785000 | 1.863897000 |
| Ti | -2.262214000 | -0.267379000 | 0.010297000 |
| Cl | -3.153582000 | 1.960080000 | 0.118958000 |
| C | -3.678736000 | -1.598680000 | 1.405689000 |
| C | -3.607230000 | -0.332667000 | 2.020426000 |
| C | -2.261412000 | -0.115157000 | 2.424265000 |
| C | -1.512010000 | -1.263079000 | 2.083178000 |
| C | -2.371990000 | -2.173176000 | 1.426802000 |
| H | -4.573547000 | -2.055319000 | 0.988772000 |
| H | -4.421871000 | 0.379688000 | 2.118408000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.871729000 | 0.789648000 | 2.884002000 |
| H | -0.442892000 | -1.392083000 | 2.232262000 |
| H | -2.075940000 | -3.141266000 | 1.032999000 |
| C | -3.026734000 | -1.990991000 | -1.475646000 |
| C | -1.738186000 | -1.601890000 | -1.909215000 |
| C | -1.823010000 | -0.266375000 | -2.388653000 |
| C | -3.152718000 | 0.168520000 | -2.233128000 |
| C | -3.899796000 | -0.882917000 | -1.637870000 |
| H | -3.294092000 | -2.967925000 | -1.081067000 |
| H | -0.846407000 | -2.220262000 | -1.886288000 |
| H | -0.989809000 | 0.316858000 | -2.769269000 |
| H | -3.531734000 | 1.158451000 | -2.467471000 |
| H | -4.955256000 | -0.845361000 | -1.374571000 |

TS1e-W-endo: E= -1076.837512

| | | | |
|---|--------------|--------------|--------------|
| C | 1.763218000 | -0.051110000 | 1.326785000 |
| C | 3.133370000 | 0.095008000 | 1.670926000 |
| H | 3.465990000 | -0.540489000 | 2.498010000 |
| C | 0.909301000 | 0.744819000 | 0.478013000 |
| W | -1.149720000 | -0.122073000 | 0.010113000 |
| C | -0.536445000 | -2.078639000 | 0.373879000 |
| C | -3.049752000 | -0.906572000 | -0.310790000 |
| C | -1.533963000 | 0.070806000 | 2.067743000 |
| C | -2.062783000 | 1.728056000 | -0.327055000 |
| C | -0.636070000 | -0.342696000 | -1.997786000 |
| N | 1.355480000 | 1.964546000 | 0.066132000 |
| O | -0.289225000 | -0.457783000 | -3.099828000 |
| O | -0.205759000 | -3.173100000 | 0.578641000 |
| O | -1.723828000 | 0.165400000 | 3.203015000 |
| O | -4.110594000 | -1.338162000 | -0.492137000 |
| O | -2.618192000 | 2.726626000 | -0.523249000 |
| C | 0.780380000 | 2.658599000 | -1.079475000 |
| H | 1.283403000 | -0.944674000 | 1.724991000 |
| H | 3.618446000 | 1.067225000 | 1.691163000 |
| H | 0.301874000 | 1.949217000 | -1.759545000 |
| H | 0.034118000 | 3.411480000 | -0.774471000 |
| H | 1.588283000 | 3.175353000 | -1.623411000 |
| C | 2.433539000 | -1.511523000 | -0.946160000 |
| C | 2.909269000 | -0.364912000 | -1.556647000 |
| C | 4.049553000 | 0.083129000 | -0.859754000 |
| C | 4.240118000 | -0.723050000 | 0.294006000 |
| C | 3.446472000 | -1.996195000 | 0.037769000 |
| H | 1.541965000 | -2.063077000 | -1.235163000 |
| H | 2.429402000 | 0.141422000 | -2.394557000 |
| H | 4.623805000 | 0.980566000 | -1.097050000 |
| H | 5.209163000 | -0.755901000 | 0.801134000 |
| H | 3.037612000 | -2.509578000 | 0.917390000 |
| H | 4.118494000 | -2.712505000 | -0.478179000 |
| C | 2.243606000 | 2.834732000 | 0.838491000 |
| H | 2.232633000 | 2.557333000 | 1.898404000 |
| H | 3.281787000 | 2.831990000 | 0.465325000 |
| H | 1.865858000 | 3.866632000 | 0.763439000 |

TS1e-W-exo: E= -1076.836761

| | | | |
|---|-------------|--------------|--------------|
| C | 4.263854000 | -1.655568000 | 0.222512000 |
| C | 3.101731000 | -2.092433000 | -0.438718000 |
| C | 2.555859000 | -1.023377000 | -1.137613000 |
| C | 4.397937000 | -0.253748000 | 0.047606000 |
| C | 3.554156000 | 0.087330000 | -1.169782000 |
| H | 4.875688000 | -2.262472000 | 0.892436000 |
| H | 2.643276000 | -3.076532000 | -0.345531000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.631020000 | -1.036812000 | -1.711934000 |
| H | 5.343955000 | 0.257646000 | 0.248309000 |
| H | 3.127836000 | 1.097539000 | -1.208461000 |
| H | 4.191342000 | -0.037392000 | -2.068533000 |
| C | 1.858339000 | 0.210893000 | 1.097913000 |
| C | 3.206889000 | 0.505507000 | 1.438625000 |
| H | 3.598709000 | -0.015056000 | 2.315522000 |
| C | 0.857841000 | 0.919083000 | 0.324706000 |
| W | -1.128936000 | -0.169297000 | 0.027803000 |
| C | -0.285215000 | -2.073101000 | 0.083943000 |
| C | -0.996134000 | -0.201641000 | -2.055111000 |
| C | -1.254690000 | -0.201500000 | 2.125531000 |
| C | -2.970394000 | -1.130873000 | -0.081882000 |
| C | -2.249145000 | 1.597233000 | -0.002516000 |
| O | 0.145269000 | -3.150898000 | 0.117131000 |
| O | -4.000165000 | -1.659982000 | -0.143373000 |
| O | -2.916106000 | 2.544636000 | -0.027810000 |
| O | -1.315437000 | -0.234478000 | 3.278331000 |
| O | -0.904971000 | -0.219831000 | -3.211416000 |
| N | 1.102090000 | 2.194641000 | -0.083586000 |
| C | 0.331858000 | 2.836015000 | -1.143888000 |
| H | 1.489429000 | -0.727073000 | 1.512079000 |
| H | 3.602655000 | 1.514234000 | 1.350658000 |
| H | -0.445689000 | 3.505277000 | -0.739687000 |
| H | 1.014488000 | 3.436679000 | -1.767579000 |
| H | -0.146239000 | 2.084510000 | -1.776986000 |
| C | 1.993054000 | 3.138273000 | 0.590879000 |
| H | 2.102796000 | 2.877152000 | 1.649736000 |
| H | 2.991689000 | 3.199236000 | 0.123109000 |
| H | 1.541289000 | 4.140400000 | 0.538376000 |

TS1e-Cr-endo: E= -2054.830520

| | | | |
|----|--------------|--------------|--------------|
| C | 1.352831000 | -0.034690000 | 1.309386000 |
| C | 2.708293000 | 0.195325000 | 1.667910000 |
| H | 3.061121000 | -0.392842000 | 2.521473000 |
| C | 0.475200000 | 0.676795000 | 0.411128000 |
| Cr | -1.491776000 | -0.214010000 | 0.016036000 |
| C | -0.856223000 | -1.952863000 | 0.392506000 |
| C | -3.189863000 | -0.974739000 | -0.211155000 |
| C | -1.738708000 | 0.095011000 | 1.878451000 |
| C | -2.328774000 | 1.453089000 | -0.343834000 |
| C | -0.969642000 | -0.460624000 | -1.779445000 |
| N | 0.867559000 | 1.902169000 | -0.019261000 |
| O | -0.572766000 | -0.614498000 | -2.853905000 |
| O | -0.502332000 | -3.030048000 | 0.609263000 |
| O | -1.858814000 | 0.283082000 | 3.006945000 |
| O | -4.233852000 | -1.443649000 | -0.358226000 |
| O | -2.914195000 | 2.423788000 | -0.552142000 |
| C | 0.334307000 | 2.530834000 | -1.224220000 |
| H | 0.923146000 | -0.940237000 | 1.735561000 |
| H | 3.142156000 | 1.191488000 | 1.661165000 |
| H | -0.100650000 | 1.787392000 | -1.894130000 |
| H | -0.427926000 | 3.291716000 | -0.988130000 |
| H | 1.162548000 | 3.028811000 | -1.755363000 |
| C | 2.164905000 | -1.549417000 | -0.909386000 |
| C | 2.583655000 | -0.397102000 | -1.550112000 |
| C | 3.675724000 | 0.146301000 | -0.843711000 |
| C | 3.886769000 | -0.603959000 | 0.343188000 |
| C | 3.178287000 | -1.931425000 | 0.118462000 |
| H | 1.321380000 | -2.171005000 | -1.201843000 |
| H | 2.094337000 | 0.047098000 | -2.417093000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 4.198984000 | 1.068983000 | -1.101424000 |
| H | 4.844519000 | -0.560175000 | 0.870570000 |
| H | 2.777134000 | -2.433294000 | 1.008176000 |
| H | 3.906492000 | -2.624617000 | -0.350872000 |
| C | 1.692281000 | 2.846398000 | 0.743799000 |
| H | 1.671114000 | 2.602778000 | 1.811602000 |
| H | 2.736983000 | 2.889492000 | 0.392664000 |
| H | 1.259750000 | 3.852471000 | 0.624333000 |

TS1e-Cr-exo: E= -2054.828864

| | | | |
|----|--------------|--------------|--------------|
| C | 3.955816000 | -1.554576000 | 0.283605000 |
| C | 2.840667000 | -2.040500000 | -0.420836000 |
| C | 2.277143000 | -0.996923000 | -1.145118000 |
| C | 4.036737000 | -0.148555000 | 0.111443000 |
| C | 3.226233000 | 0.156586000 | -1.136375000 |
| H | 4.567636000 | -2.135106000 | 0.976505000 |
| H | 2.425667000 | -3.045435000 | -0.347026000 |
| H | 1.401030000 | -1.064194000 | -1.786951000 |
| H | 4.951392000 | 0.403367000 | 0.346807000 |
| H | 2.756770000 | 1.146826000 | -1.191563000 |
| H | 3.901933000 | 0.062059000 | -2.010403000 |
| C | 1.446064000 | 0.191674000 | 1.078976000 |
| C | 2.766387000 | 0.562195000 | 1.455691000 |
| H | 3.160783000 | 0.069823000 | 2.347900000 |
| C | 0.420894000 | 0.824776000 | 0.272161000 |
| Cr | -1.469903000 | -0.289419000 | 0.037281000 |
| C | -0.603041000 | -1.967484000 | 0.150322000 |
| C | -1.234806000 | -0.353697000 | -1.836769000 |
| C | -1.516879000 | -0.180256000 | 1.938161000 |
| C | -3.090137000 | -1.225960000 | -0.032983000 |
| C | -2.514495000 | 1.295648000 | -0.044339000 |
| O | -0.133334000 | -3.019434000 | 0.211393000 |
| O | -4.088708000 | -1.802145000 | -0.082926000 |
| O | -3.213369000 | 2.211301000 | -0.076503000 |
| O | -1.532293000 | -0.116439000 | 3.086457000 |
| O | -1.042828000 | -0.407451000 | -2.974178000 |
| N | 0.600928000 | 2.105405000 | -0.129848000 |
| C | -0.145704000 | 2.707272000 | -1.232994000 |
| H | 1.132792000 | -0.764996000 | 1.494055000 |
| H | 3.115477000 | 1.588214000 | 1.368500000 |
| H | -0.943779000 | 3.375224000 | -0.869768000 |
| H | 0.550313000 | 3.304574000 | -1.845435000 |
| H | -0.584695000 | 1.939238000 | -1.870870000 |
| C | 1.436170000 | 3.104462000 | 0.545352000 |
| H | 1.542604000 | 2.862707000 | 1.608801000 |
| H | 2.436789000 | 3.210087000 | 0.090442000 |
| H | 0.934431000 | 4.081217000 | 0.471473000 |

TS1f-W-endo: E= -1116.092481

| | | | |
|---|--------------|--------------|--------------|
| C | 1.845412000 | -0.037475000 | 1.390816000 |
| C | 3.234770000 | 0.276165000 | 1.449930000 |
| H | 3.799212000 | -0.236445000 | 2.235284000 |
| C | 0.918314000 | 0.680867000 | 0.538847000 |
| W | -1.160656000 | -0.093429000 | -0.026066000 |
| C | -0.691456000 | -2.119559000 | -0.072900000 |
| C | -3.111286000 | -0.695979000 | -0.427642000 |
| C | -1.620128000 | -0.217243000 | 2.019280000 |
| C | -1.953498000 | 1.843656000 | -0.063101000 |
| C | -0.775664000 | -0.070574000 | -2.072445000 |
| N | 1.371790000 | 1.918259000 | 0.118316000 |
| O | -0.541394000 | -0.069479000 | -3.209920000 |

| | | | |
|---|--------------|--------------|--------------|
| O | -0.466765000 | -3.258706000 | -0.127911000 |
| O | -1.889193000 | -0.302674000 | 3.140091000 |
| O | -4.201202000 | -1.023257000 | -0.649498000 |
| O | -2.455942000 | 2.887377000 | -0.103218000 |
| C | 0.882130000 | 2.577971000 | -1.084192000 |
| H | 3.592883000 | 1.288899000 | 1.297992000 |
| H | 0.591457000 | 1.847807000 | -1.841324000 |
| H | 0.024078000 | 3.240217000 | -0.881806000 |
| H | 1.695394000 | 3.198677000 | -1.495404000 |
| C | 2.448077000 | -1.592231000 | -1.145426000 |
| C | 2.648241000 | -0.391136000 | -1.787951000 |
| C | 3.752060000 | 0.271811000 | -1.199208000 |
| C | 4.199686000 | -0.467927000 | -0.076037000 |
| C | 3.588785000 | -1.854168000 | -0.218647000 |
| H | 1.641745000 | -2.298573000 | -1.336657000 |
| H | 2.022166000 | 0.003933000 | -2.587378000 |
| H | 4.139080000 | 1.245887000 | -1.502459000 |
| H | 5.218113000 | -0.344106000 | 0.303606000 |
| H | 3.320425000 | -2.367606000 | 0.713786000 |
| H | 4.326645000 | -2.500503000 | -0.736972000 |
| C | 1.385720000 | -1.191393000 | 2.252109000 |
| H | 0.761149000 | -1.912914000 | 1.715079000 |
| H | 2.241096000 | -1.731706000 | 2.684639000 |
| H | 0.782414000 | -0.825393000 | 3.099308000 |
| C | 1.961522000 | 2.900600000 | 1.033248000 |
| H | 2.021583000 | 2.506418000 | 2.052654000 |
| H | 2.961699000 | 3.235251000 | 0.707222000 |
| H | 1.306739000 | 3.789659000 | 1.056668000 |

TS1f-W-exo: E= -1116.095039

| | | | |
|---|--------------|--------------|--------------|
| C | 4.227551000 | -1.505436000 | 0.026177000 |
| C | 3.046645000 | -2.044187000 | -0.536815000 |
| C | 2.439941000 | -1.078521000 | -1.314887000 |
| C | 4.306469000 | -0.127240000 | -0.295747000 |
| C | 3.366914000 | 0.078890000 | -1.475203000 |
| H | 4.905692000 | -2.032712000 | 0.699262000 |
| H | 2.631364000 | -3.030714000 | -0.330807000 |
| H | 1.488202000 | -1.172883000 | -1.832530000 |
| H | 5.254343000 | 0.414684000 | -0.227242000 |
| H | 2.873685000 | 1.058067000 | -1.537721000 |
| H | 3.950631000 | -0.055447000 | -2.408170000 |
| C | 1.939605000 | 0.349515000 | 1.121102000 |
| C | 3.274001000 | 0.843464000 | 1.076385000 |
| H | 3.911160000 | 0.616966000 | 1.936058000 |
| C | 0.837297000 | 0.899018000 | 0.342974000 |
| W | -1.156768000 | -0.171094000 | -0.005315000 |
| C | -0.374369000 | -2.099504000 | -0.057956000 |
| C | -1.053223000 | -0.132022000 | -2.088811000 |
| C | -1.386475000 | -0.254389000 | 2.081219000 |
| C | -3.024439000 | -1.072190000 | -0.169161000 |
| C | -2.217995000 | 1.631973000 | 0.007725000 |
| O | 0.028300000 | -3.188140000 | -0.097263000 |
| O | -4.068286000 | -1.568823000 | -0.257283000 |
| O | -2.862590000 | 2.595094000 | 0.003592000 |
| O | -1.522963000 | -0.310572000 | 3.227015000 |
| O | -0.998002000 | -0.111485000 | -3.247489000 |
| N | 1.026455000 | 2.197692000 | -0.085717000 |
| C | 1.580107000 | 3.260725000 | 0.755117000 |
| H | 3.483628000 | 1.820954000 | 0.648353000 |
| H | 0.819066000 | 4.055252000 | 0.854750000 |
| H | 1.814120000 | 2.888177000 | 1.757770000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.483116000 | 3.722998000 | 0.318698000 |
| C | 1.753681000 | -0.800731000 | 2.074463000 |
| H | 0.911668000 | -1.447980000 | 1.818801000 |
| H | 2.663734000 | -1.424087000 | 2.111950000 |
| H | 1.581912000 | -0.426663000 | 3.099367000 |
| C | 0.357643000 | 2.754673000 | -1.253108000 |
| H | 0.074813000 | 1.964407000 | -1.952648000 |
| H | -0.541413000 | 3.335741000 | -0.987973000 |
| H | 1.058155000 | 3.437569000 | -1.763964000 |

TS1f-Cr-endo: E= -2094.082755

| | | | |
|----|--------------|--------------|--------------|
| C | 1.448128000 | 0.038648000 | 1.376152000 |
| C | 2.822488000 | 0.420353000 | 1.433314000 |
| H | 3.394694000 | -0.012431000 | 2.260100000 |
| C | 0.507193000 | 0.644644000 | 0.451461000 |
| Cr | -1.508119000 | -0.172701000 | -0.041141000 |
| C | -0.973147000 | -1.982232000 | 0.049934000 |
| C | -3.248172000 | -0.792835000 | -0.329410000 |
| C | -1.828509000 | -0.071427000 | 1.831628000 |
| C | -2.227909000 | 1.577521000 | -0.207419000 |
| C | -1.094267000 | -0.290177000 | -1.878084000 |
| N | 0.894838000 | 1.875409000 | -0.016018000 |
| O | -0.823983000 | -0.409316000 | -2.995187000 |
| O | -0.711575000 | -3.106884000 | 0.028004000 |
| O | -2.048309000 | -0.000724000 | 2.959176000 |
| O | -4.322064000 | -1.175905000 | -0.508078000 |
| O | -2.745597000 | 2.602863000 | -0.301918000 |
| C | 0.453856000 | 2.438149000 | -1.287701000 |
| H | 3.138768000 | 1.436620000 | 1.224300000 |
| H | 0.172004000 | 1.653902000 | -1.989585000 |
| H | -0.391926000 | 3.134487000 | -1.166271000 |
| H | 1.293123000 | 3.004113000 | -1.724863000 |
| C | 2.196610000 | -1.643403000 | -1.058987000 |
| C | 2.358032000 | -0.475026000 | -1.769655000 |
| C | 3.411280000 | 0.276356000 | -1.195514000 |
| C | 3.858889000 | -0.369200000 | -0.015727000 |
| C | 3.319996000 | -1.790348000 | -0.086716000 |
| H | 1.431382000 | -2.399149000 | -1.230110000 |
| H | 1.736881000 | -0.162146000 | -2.608277000 |
| H | 3.759062000 | 1.248570000 | -1.548324000 |
| H | 4.859755000 | -0.174057000 | 0.380448000 |
| H | 3.048440000 | -2.256561000 | 0.869346000 |
| H | 4.104151000 | -2.429695000 | -0.542079000 |
| C | 1.047356000 | -1.073590000 | 2.321205000 |
| H | 0.443683000 | -1.857875000 | 1.854907000 |
| H | 1.933169000 | -1.550275000 | 2.767740000 |
| H | 0.452800000 | -0.674349000 | 3.159493000 |
| C | 1.453692000 | 2.937737000 | 0.830676000 |
| H | 1.494287000 | 2.626521000 | 1.879442000 |
| H | 2.455402000 | 3.264796000 | 0.501965000 |
| H | 0.784434000 | 3.813204000 | 0.764375000 |

TS1f-Cr-exo: E= -2094.085040

| | | | |
|---|-------------|--------------|--------------|
| C | 3.928138000 | -1.309030000 | 0.198351000 |
| C | 2.862323000 | -2.033740000 | -0.393824000 |
| C | 2.228497000 | -1.233476000 | -1.315744000 |
| C | 3.887432000 | 0.033754000 | -0.256878000 |
| C | 3.008056000 | 0.026041000 | -1.501149000 |
| H | 4.614845000 | -1.695754000 | 0.953131000 |
| H | 2.550863000 | -3.041908000 | -0.120381000 |
| H | 1.358310000 | -1.505489000 | -1.909501000 |

| | | | |
|----|--------------|--------------|--------------|
| H | 4.787126000 | 0.655520000 | -0.220297000 |
| H | 2.393492000 | 0.923114000 | -1.661226000 |
| H | 3.664636000 | -0.080550000 | -2.388247000 |
| C | 1.488035000 | 0.498470000 | 1.114126000 |
| C | 2.790744000 | 1.058198000 | 0.973141000 |
| H | 3.450555000 | 0.988050000 | 1.843544000 |
| C | 0.359807000 | 0.889247000 | 0.280572000 |
| Cr | -1.479752000 | -0.315880000 | -0.003329000 |
| C | -0.577056000 | -1.965102000 | 0.238151000 |
| C | -1.126080000 | -0.479911000 | -1.849410000 |
| C | -1.693964000 | -0.037510000 | 1.867066000 |
| C | -3.053465000 | -1.322725000 | -0.106053000 |
| C | -2.591054000 | 1.196556000 | -0.281546000 |
| O | -0.098626000 | -3.009155000 | 0.341691000 |
| O | -4.021674000 | -1.947343000 | -0.169712000 |
| O | -3.348749000 | 2.051078000 | -0.439347000 |
| O | -1.828924000 | 0.154651000 | 2.993657000 |
| O | -0.874399000 | -0.593840000 | -2.971127000 |
| N | 0.433501000 | 2.171337000 | -0.190655000 |
| C | 0.932524000 | 3.318083000 | 0.578944000 |
| H | 2.918635000 | 1.992727000 | 0.430671000 |
| H | 0.126846000 | 4.071629000 | 0.627739000 |
| H | 1.188698000 | 3.023412000 | 1.601912000 |
| H | 1.806245000 | 3.802648000 | 0.109490000 |
| C | 1.425617000 | -0.564046000 | 2.175053000 |
| H | 0.487749000 | -1.119972000 | 2.208974000 |
| H | 2.250670000 | -1.290768000 | 2.030373000 |
| H | 1.585448000 | -0.116202000 | 3.171565000 |
| C | -0.230394000 | 2.631024000 | -1.405477000 |
| H | -0.471076000 | 1.794797000 | -2.063580000 |
| H | -1.149469000 | 3.199695000 | -1.188829000 |
| H | 0.459990000 | 3.302685000 | -1.944114000 |

2a-W-endo: E= -1057.484770

| | | | |
|---|--------------|--------------|--------------|
| C | 2.064663000 | -0.452555000 | 0.493821000 |
| C | 3.220909000 | -0.105873000 | 1.485382000 |
| H | 3.219311000 | -0.806373000 | 2.334136000 |
| C | 0.946679000 | 0.547501000 | 0.334886000 |
| W | -1.127584000 | -0.103626000 | -0.004496000 |
| C | -0.429169000 | -1.711772000 | -1.155943000 |
| C | -3.062543000 | -0.872670000 | -0.275849000 |
| C | -0.949158000 | -1.300769000 | 1.715817000 |
| C | -2.030426000 | 1.439635000 | 1.088063000 |
| C | -1.391378000 | 1.056815000 | -1.732294000 |
| O | 1.449982000 | 1.763916000 | 0.404843000 |
| O | -1.552569000 | 1.701121000 | -2.677666000 |
| O | -0.063602000 | -2.607561000 | -1.786529000 |
| O | -0.840000000 | -1.968360000 | 2.649343000 |
| O | -4.126203000 | -1.296742000 | -0.423896000 |
| O | -2.565664000 | 2.284808000 | 1.667812000 |
| C | 0.658009000 | 2.935820000 | 0.237666000 |
| H | 1.610990000 | -1.414512000 | 0.763845000 |
| H | 3.140007000 | 0.913484000 | 1.883161000 |
| H | 0.047230000 | 2.872075000 | -0.673222000 |
| H | 0.003122000 | 3.075936000 | 1.109124000 |
| H | 1.364662000 | 3.772193000 | 0.164476000 |
| C | 2.862046000 | -0.707973000 | -0.869765000 |
| C | 3.521790000 | 0.593596000 | -1.281673000 |
| C | 4.510638000 | 0.837911000 | -0.405833000 |
| C | 4.510039000 | -0.292209000 | 0.609560000 |
| C | 4.075346000 | -1.469590000 | -0.290255000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 2.255192000 | -1.217620000 | -1.626670000 |
| H | 3.165676000 | 1.249024000 | -2.077881000 |
| H | 5.126065000 | 1.737315000 | -0.340036000 |
| H | 5.430363000 | -0.417768000 | 1.196247000 |
| H | 3.799567000 | -2.379167000 | 0.267807000 |
| H | 4.818810000 | -1.720951000 | -1.060993000 |

2a-W-exo: E= -1057.485172

| | | | |
|---|--------------|--------------|--------------|
| C | 4.732552000 | -1.076681000 | 0.168084000 |
| C | 3.747489000 | -1.511972000 | -0.634867000 |
| C | 2.839189000 | -0.327335000 | -0.911957000 |
| C | 4.489199000 | 0.403630000 | 0.430987000 |
| C | 3.861720000 | 0.827032000 | -0.914823000 |
| H | 5.509114000 | -1.677576000 | 0.645610000 |
| H | 3.534490000 | -2.536952000 | -0.943447000 |
| H | 2.156737000 | -0.416657000 | -1.765960000 |
| H | 5.353090000 | 0.980986000 | 0.788107000 |
| H | 3.403024000 | 1.825691000 | -0.893219000 |
| H | 4.564338000 | 0.756274000 | -1.758536000 |
| C | 2.083525000 | -0.072697000 | 0.478907000 |
| C | 3.234915000 | 0.499060000 | 1.365140000 |
| H | 3.356619000 | -0.080563000 | 2.290784000 |
| C | 0.861936000 | 0.788019000 | 0.257700000 |
| W | -1.118781000 | -0.139794000 | 0.013336000 |
| C | -0.193578000 | -1.770670000 | -0.927958000 |
| C | -1.479995000 | 0.773634000 | -1.840654000 |
| C | -0.825481000 | -1.094003000 | 1.865729000 |
| C | -2.938898000 | -1.167571000 | -0.183937000 |
| C | -2.222398000 | 1.398265000 | 0.910705000 |
| O | 0.311210000 | -2.676005000 | -1.436655000 |
| O | -3.939626000 | -1.733165000 | -0.291681000 |
| O | -2.866218000 | 2.234404000 | 1.383298000 |
| O | -0.651678000 | -1.627302000 | 2.872531000 |
| O | -1.691370000 | 1.281916000 | -2.856316000 |
| O | 1.223322000 | 2.055017000 | 0.172349000 |
| C | 0.286548000 | 3.097909000 | -0.087318000 |
| H | 1.737398000 | -1.040696000 | 0.857436000 |
| H | 3.042628000 | 1.545704000 | 1.637909000 |
| H | -0.373787000 | 3.234931000 | 0.780360000 |
| H | 0.878903000 | 4.006566000 | -0.253389000 |
| H | -0.318216000 | 2.868388000 | -0.975129000 |

2a-Cr-endo: E= -2035.480289

| | | | |
|----|--------------|--------------|--------------|
| C | -1.625773000 | -0.467970000 | -0.576757000 |
| C | -2.800844000 | -0.022944000 | -1.505189000 |
| H | -2.845094000 | -0.667549000 | -2.396164000 |
| C | -0.479543000 | 0.489364000 | -0.343176000 |
| Cr | 1.444333000 | -0.158127000 | 0.015411000 |
| C | 0.796486000 | -1.774492000 | 0.785351000 |
| C | 3.190197000 | -0.837524000 | 0.321048000 |
| C | 1.351852000 | -0.954079000 | -1.715524000 |
| C | 2.296297000 | 1.362693000 | -0.742192000 |
| C | 1.376404000 | 0.674418000 | 1.722841000 |
| O | -0.969586000 | 1.703524000 | -0.382206000 |
| O | 1.305979000 | 1.180624000 | 2.753732000 |
| O | 0.463838000 | -2.769899000 | 1.254791000 |
| O | 1.264288000 | -1.430402000 | -2.756836000 |
| O | 4.248231000 | -1.246382000 | 0.507643000 |
| O | 2.889239000 | 2.240101000 | -1.193380000 |
| C | -0.235189000 | 2.900573000 | -0.120959000 |
| H | -1.205721000 | -1.416477000 | -0.932504000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.704093000 | 1.016660000 | -1.841583000 |
| H | 0.365553000 | 2.811040000 | 0.792606000 |
| H | 0.413097000 | 3.138076000 | -0.974485000 |
| H | -0.989584000 | 3.688000000 | 0.001981000 |
| C | -2.395876000 | -0.807660000 | 0.788729000 |
| C | -3.003814000 | 0.477545000 | 1.316945000 |
| C | -4.006005000 | 0.817018000 | 0.489411000 |
| C | -4.070100000 | -0.233151000 | -0.606885000 |
| C | -3.647457000 | -1.486745000 | 0.188886000 |
| H | -1.791893000 | -1.393634000 | 1.489691000 |
| H | -2.605290000 | 1.059942000 | 2.149367000 |
| H | -4.594849000 | 1.736270000 | 0.509646000 |
| H | -5.010552000 | -0.286508000 | -1.172263000 |
| H | -3.415301000 | -2.359507000 | -0.442750000 |
| H | -4.375982000 | -1.774056000 | 0.961465000 |

2a-Cr-exo: E= -2035.480768

| | | | |
|----|--------------|--------------|--------------|
| C | 4.335788000 | -1.042108000 | 0.229254000 |
| C | 3.374324000 | -1.528842000 | -0.572516000 |
| C | 2.435490000 | -0.379420000 | -0.896016000 |
| C | 4.046681000 | 0.437396000 | 0.445936000 |
| C | 3.425607000 | 0.802886000 | -0.918979000 |
| H | 5.122547000 | -1.606603000 | 0.733704000 |
| H | 3.194834000 | -2.568125000 | -0.852977000 |
| H | 1.776717000 | -0.513532000 | -1.762543000 |
| H | 4.888931000 | 1.049483000 | 0.796893000 |
| H | 2.940889000 | 1.789130000 | -0.933449000 |
| H | 4.140808000 | 0.726282000 | -1.751552000 |
| C | 1.654291000 | -0.112526000 | 0.480179000 |
| C | 2.777194000 | 0.523747000 | 1.360328000 |
| H | 2.903910000 | -0.023204000 | 2.305118000 |
| C | 0.400442000 | 0.692135000 | 0.210521000 |
| Cr | -1.438668000 | -0.215909000 | 0.014893000 |
| C | -0.578674000 | -1.740539000 | -0.741501000 |
| C | -1.651162000 | 0.508035000 | -1.730012000 |
| C | -1.151689000 | -0.913341000 | 1.768731000 |
| C | -3.083683000 | -1.153517000 | -0.130233000 |
| C | -2.417283000 | 1.230972000 | 0.765399000 |
| O | -0.086136000 | -2.672450000 | -1.199310000 |
| O | -4.079805000 | -1.720153000 | -0.218779000 |
| O | -3.067043000 | 2.065150000 | 1.219862000 |
| O | -0.962685000 | -1.330006000 | 2.821678000 |
| O | -1.776252000 | 0.940601000 | -2.788812000 |
| O | 0.747720000 | 1.951559000 | 0.085643000 |
| C | -0.147873000 | 3.018635000 | -0.236927000 |
| H | 1.348762000 | -1.081054000 | 0.886844000 |
| H | 2.552099000 | 1.572164000 | 1.599007000 |
| H | -0.785523000 | 3.248466000 | 0.626608000 |
| H | 0.489617000 | 3.881857000 | -0.466507000 |
| H | -0.768677000 | 2.768247000 | -1.105843000 |

2b-W-endo: E= -1096.740324

| | | | |
|---|--------------|--------------|--------------|
| C | -2.109292000 | -0.509993000 | -0.707387000 |
| C | -3.425244000 | 0.068950000 | -1.346890000 |
| H | -3.789755000 | -0.613425000 | -2.129453000 |
| C | -0.922259000 | 0.461332000 | -0.640987000 |
| W | 1.133928000 | -0.059630000 | 0.044948000 |
| C | 0.533172000 | -1.744639000 | 1.123078000 |
| C | 3.044652000 | -0.542814000 | 0.754603000 |
| C | 1.480658000 | -1.286956000 | -1.628068000 |
| C | 2.129071000 | 1.505113000 | -0.921895000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 0.786855000 | 1.136715000 | 1.729494000 |
| O | -1.356766000 | 1.662435000 | -0.953399000 |
| O | 0.571600000 | 1.799060000 | 2.652021000 |
| O | 0.264947000 | -2.695942000 | 1.724249000 |
| O | 1.666750000 | -1.966912000 | -2.539513000 |
| O | 4.097970000 | -0.802548000 | 1.150841000 |
| O | 2.744487000 | 2.350783000 | -1.418010000 |
| C | -0.586848000 | 2.858716000 | -0.875694000 |
| H | -3.289871000 | 1.054317000 | -1.803060000 |
| H | -0.083721000 | 2.941105000 | 0.096600000 |
| H | 0.156116000 | 2.885527000 | -1.683580000 |
| H | -1.303545000 | 3.680130000 | -1.002228000 |
| C | -2.607112000 | -0.771486000 | 0.804348000 |
| C | -2.841522000 | 0.590248000 | 1.438189000 |
| C | -3.929893000 | 1.116654000 | 0.854645000 |
| C | -4.442630000 | 0.102666000 | -0.158040000 |
| C | -4.066856000 | -1.210316000 | 0.558777000 |
| H | -1.957746000 | -1.460487000 | 1.351683000 |
| H | -2.158089000 | 1.076634000 | 2.135739000 |
| H | -4.328038000 | 2.124526000 | 0.987791000 |
| H | -5.487696000 | 0.223732000 | -0.475354000 |
| H | -4.173896000 | -2.108389000 | -0.067889000 |
| H | -4.612323000 | -1.361475000 | 1.502059000 |
| C | -1.704613000 | -1.826154000 | -1.391963000 |
| H | -0.890270000 | -2.334770000 | -0.863008000 |
| H | -2.557548000 | -2.517367000 | -1.432521000 |
| H | -1.375069000 | -1.640634000 | -2.425701000 |

2b-W-exo: E= -1096.739449

| | | | |
|---|--------------|--------------|--------------|
| C | -4.807027000 | -0.783159000 | 0.181043000 |
| C | -3.752139000 | -1.460789000 | 0.662408000 |
| C | -2.616143000 | -0.466859000 | 0.824366000 |
| C | -4.377886000 | 0.667925000 | 0.011847000 |
| C | -3.405225000 | 0.802746000 | 1.203732000 |
| H | -5.768174000 | -1.193572000 | -0.135416000 |
| H | -3.661116000 | -2.537147000 | 0.814669000 |
| H | -1.796269000 | -0.765460000 | 1.484691000 |
| H | -5.188844000 | 1.405571000 | -0.062687000 |
| H | -2.808853000 | 1.726218000 | 1.188090000 |
| H | -3.903660000 | 0.705353000 | 2.179286000 |
| C | -2.118419000 | -0.084012000 | -0.665881000 |
| C | -3.372693000 | 0.709753000 | -1.187556000 |
| H | -3.791925000 | 0.236270000 | -2.086514000 |
| C | -0.836414000 | 0.742986000 | -0.480454000 |
| W | 1.160131000 | -0.105962000 | 0.036403000 |
| C | 0.356838000 | -1.864385000 | 0.831002000 |
| C | 0.999743000 | 0.833337000 | 1.904929000 |
| C | 1.339324000 | -1.058818000 | -1.830236000 |
| C | 3.005146000 | -0.925461000 | 0.593385000 |
| C | 2.322839000 | 1.473543000 | -0.685616000 |
| O | -0.040063000 | -2.858739000 | 1.267967000 |
| O | 4.023745000 | -1.372075000 | 0.905038000 |
| O | 3.027587000 | 2.315882000 | -1.052023000 |
| O | 1.435185000 | -1.586168000 | -2.850156000 |
| O | 0.901869000 | 1.362074000 | 2.927112000 |
| O | -1.141798000 | 2.022585000 | -0.570392000 |
| C | -0.221262000 | 3.091965000 | -0.367349000 |
| H | -3.126626000 | 1.746299000 | -1.441889000 |
| H | 0.495254000 | 3.134701000 | -1.198077000 |
| H | -0.827397000 | 4.006717000 | -0.349322000 |
| H | 0.317848000 | 2.973047000 | 0.581776000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.856366000 | -1.311595000 | -1.550914000 |
| H | -1.122658000 | -2.001585000 | -1.119018000 |
| H | -2.792394000 | -1.867272000 | -1.697623000 |
| H | -1.489003000 | -0.999458000 | -2.540376000 |

2b-Cr-endo: E= -2074.734017

| | | | |
|----|--------------|--------------|--------------|
| C | -1.702443000 | -0.521009000 | -0.681964000 |
| C | -2.987733000 | 0.099300000 | -1.351833000 |
| H | -3.346080000 | -0.563409000 | -2.153726000 |
| C | -0.482986000 | 0.415892000 | -0.573252000 |
| Cr | 1.447340000 | -0.100430000 | 0.080802000 |
| C | 0.873455000 | -1.661194000 | 0.999211000 |
| C | 3.162020000 | -0.571021000 | 0.722494000 |
| C | 1.688014000 | -1.101220000 | -1.527458000 |
| C | 2.360287000 | 1.337227000 | -0.761685000 |
| C | 1.073115000 | 0.938035000 | 1.622636000 |
| O | -0.898817000 | 1.616126000 | -0.874522000 |
| O | 0.8111168000 | 1.567630000 | 2.550659000 |
| O | 0.639855000 | -2.623896000 | 1.584570000 |
| O | 1.847317000 | -1.686905000 | -2.501998000 |
| O | 4.203883000 | -0.851353000 | 1.120739000 |
| O | 3.026929000 | 2.147740000 | -1.236032000 |
| C | -0.166642000 | 2.838247000 | -0.775252000 |
| H | -2.817749000 | 1.086836000 | -1.791479000 |
| H | 0.345755000 | 2.919346000 | 0.190723000 |
| H | 0.555937000 | 2.915393000 | -1.597179000 |
| H | -0.918283000 | 3.632671000 | -0.867217000 |
| C | -2.250826000 | -0.775151000 | 0.816009000 |
| C | -2.479467000 | 0.586926000 | 1.453938000 |
| C | -3.539375000 | 1.138546000 | 0.842097000 |
| C | -4.039779000 | 0.143678000 | -0.194747000 |
| C | -3.712396000 | -1.181008000 | 0.523647000 |
| H | -1.640576000 | -1.485199000 | 1.381621000 |
| H | -1.815158000 | 1.054941000 | 2.181685000 |
| H | -3.924107000 | 2.151758000 | 0.974649000 |
| H | -5.072283000 | 0.287678000 | -0.542310000 |
| H | -3.820937000 | -2.073588000 | -0.110183000 |
| H | -4.287648000 | -1.325417000 | 1.450209000 |
| C | -1.339242000 | -1.848615000 | -1.369926000 |
| H | -0.580568000 | -2.419265000 | -0.823318000 |
| H | -2.228692000 | -2.487524000 | -1.454666000 |
| H | -0.964458000 | -1.670419000 | -2.388880000 |

2b-Cr-exo: E= -2074.732618

| | | | |
|----|--------------|--------------|--------------|
| C | -4.434346000 | -0.725467000 | 0.128675000 |
| C | -3.413303000 | -1.449528000 | 0.614406000 |
| C | -2.245781000 | -0.500232000 | 0.824310000 |
| C | -3.951233000 | 0.712631000 | 0.001299000 |
| C | -3.001354000 | 0.786654000 | 1.215721000 |
| H | -5.402358000 | -1.095108000 | -0.215776000 |
| H | -3.363029000 | -2.531636000 | 0.743061000 |
| H | -1.466335000 | -0.849532000 | 1.508039000 |
| H | -4.734103000 | 1.480139000 | -0.073084000 |
| H | -2.375296000 | 1.689928000 | 1.237146000 |
| H | -3.523986000 | 0.682628000 | 2.177881000 |
| C | -1.702245000 | -0.107467000 | -0.649510000 |
| C | -2.919934000 | 0.744695000 | -1.175420000 |
| H | -3.338539000 | 0.307843000 | -2.093031000 |
| C | -0.386593000 | 0.665736000 | -0.422555000 |
| Cr | 1.479265000 | -0.170624000 | 0.061364000 |
| C | 0.719465000 | -1.791403000 | 0.705202000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.242821000 | 0.624272000 | 1.770017000 |
| C | 1.597584000 | -0.897654000 | -1.700260000 |
| C | 3.129039000 | -0.940053000 | 0.570905000 |
| C | 2.545361000 | 1.277764000 | -0.546184000 |
| O | 0.358096000 | -2.803156000 | 1.116014000 |
| O | 4.132591000 | -1.403158000 | 0.888882000 |
| O | 3.296783000 | 2.078540000 | -0.894002000 |
| O | 1.687621000 | -1.319697000 | -2.764111000 |
| O | 1.070707000 | 1.114825000 | 2.796613000 |
| O | -0.670886000 | 1.942695000 | -0.474304000 |
| C | 0.216382000 | 3.037076000 | -0.232240000 |
| H | -2.634749000 | 1.777656000 | -1.401488000 |
| H | 0.919116000 | 3.145268000 | -1.067571000 |
| H | -0.428079000 | 3.923679000 | -0.174185000 |
| H | 0.763146000 | 2.910497000 | 0.710090000 |
| C | -1.489627000 | -1.324620000 | -1.563215000 |
| H | -0.811021000 | -2.074571000 | -1.142873000 |
| H | -2.454570000 | -1.817303000 | -1.742313000 |
| H | -1.089273000 | -1.009310000 | -2.538282000 |

2c-W-endo: E= -2713.926484

| | | | |
|----|--------------|--------------|--------------|
| C | -0.370187000 | 2.177804000 | -0.892871000 |
| C | 0.897845000 | 2.830167000 | -1.513912000 |
| H | 0.695047000 | 3.153969000 | -2.546405000 |
| C | -0.269354000 | 0.739816000 | -0.421391000 |
| W | -2.098176000 | -0.453629000 | 0.015538000 |
| C | -3.357247000 | 1.165710000 | -0.424719000 |
| C | -3.831461000 | -1.540282000 | 0.448360000 |
| C | -2.209349000 | -1.005538000 | -2.007954000 |
| C | -1.075641000 | -2.205519000 | 0.466135000 |
| C | -1.964701000 | 0.234378000 | 1.989660000 |
| O | 0.925648000 | 0.333155000 | -0.247026000 |
| O | -1.848202000 | 0.644799000 | 3.064463000 |
| O | -4.079919000 | 2.036580000 | -0.658375000 |
| O | -2.242655000 | -1.293054000 | -3.125875000 |
| O | -4.787423000 | -2.144219000 | 0.690396000 |
| O | -0.556750000 | -3.218204000 | 0.710156000 |
| H | 1.763297000 | 2.159097000 | -1.524263000 |
| C | -0.696435000 | 3.152383000 | 0.328423000 |
| C | 0.434881000 | 2.992675000 | 1.327546000 |
| C | 1.533717000 | 3.533426000 | 0.774898000 |
| C | 1.141646000 | 4.073065000 | -0.592120000 |
| C | -0.316887000 | 4.502457000 | -0.315102000 |
| H | -1.715241000 | 3.032749000 | 0.713703000 |
| H | 0.357170000 | 2.424349000 | 2.255862000 |
| H | 2.558498000 | 3.488413000 | 1.146085000 |
| H | 1.818188000 | 4.822243000 | -1.024863000 |
| H | -0.891966000 | 4.733799000 | -1.226525000 |
| H | -0.396714000 | 5.339265000 | 0.394965000 |
| Ti | 2.561787000 | -0.628203000 | -0.014206000 |
| C | 3.693929000 | -1.341560000 | -2.024639000 |
| C | 2.389415000 | -0.922466000 | -2.384441000 |
| C | 1.462268000 | -1.813909000 | -1.784076000 |
| C | 2.185617000 | -2.754664000 | -1.020864000 |
| C | 3.574834000 | -2.457344000 | -1.164625000 |
| H | 4.619559000 | -0.847773000 | -2.306742000 |
| H | 2.143056000 | -0.048051000 | -2.983153000 |
| H | 0.379109000 | -1.729115000 | -1.822319000 |
| H | 1.747937000 | -3.565477000 | -0.445815000 |
| H | 4.400089000 | -3.014318000 | -0.727819000 |
| C | 2.132144000 | -2.005428000 | 1.877800000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 1.571342000 | -0.739444000 | 2.163224000 |
| C | 2.622696000 | 0.206031000 | 2.222594000 |
| C | 3.846706000 | -0.486631000 | 2.020879000 |
| C | 3.548026000 | -1.847718000 | 1.799480000 |
| H | 1.574381000 | -2.930552000 | 1.772974000 |
| H | 0.508925000 | -0.521528000 | 2.224087000 |
| H | 2.513825000 | 1.279045000 | 2.349083000 |
| H | 4.832849000 | -0.031713000 | 1.982930000 |
| H | 4.271190000 | -2.640868000 | 1.626368000 |
| Cl | 4.000121000 | 1.191939000 | -0.459705000 |
| H | -1.223949000 | 2.225634000 | -1.584096000 |

2c-W-exo: E= -2713.925281

| | | | |
|----|--------------|--------------|--------------|
| C | -0.064651000 | 5.015048000 | -0.314643000 |
| C | -1.074366000 | 4.389688000 | 0.313591000 |
| C | -0.560530000 | 3.026376000 | 0.741863000 |
| C | 1.130303000 | 4.072307000 | -0.313716000 |
| C | 0.919688000 | 3.349893000 | 1.034424000 |
| H | -0.107233000 | 5.972701000 | -0.837688000 |
| H | -2.113325000 | 4.712519000 | 0.401039000 |
| H | -1.139843000 | 2.496629000 | 1.508731000 |
| H | 2.115629000 | 4.524195000 | -0.487984000 |
| H | 1.564215000 | 2.467129000 | 1.141116000 |
| H | 1.039035000 | 4.013519000 | 1.903897000 |
| C | -0.412998000 | 2.195802000 | -0.613465000 |
| C | 0.789400000 | 2.905335000 | -1.301477000 |
| H | 0.527004000 | 3.268653000 | -2.305258000 |
| C | -0.266781000 | 0.722679000 | -0.275431000 |
| W | -2.059283000 | -0.569090000 | -0.016285000 |
| C | -3.313282000 | 1.116505000 | -0.054036000 |
| C | -1.967552000 | -0.346034000 | 2.066241000 |
| C | -2.173070000 | -0.696641000 | -2.110148000 |
| C | -3.776275000 | -1.747285000 | 0.176751000 |
| C | -0.979308000 | -2.339442000 | 0.100177000 |
| O | -4.019750000 | 2.030179000 | -0.058819000 |
| O | -4.723716000 | -2.402022000 | 0.281033000 |
| O | -0.409036000 | -3.350673000 | 0.179359000 |
| O | -2.213101000 | -0.752184000 | -3.262672000 |
| O | -1.890880000 | -0.202825000 | 3.210449000 |
| O | 0.938654000 | 0.338218000 | -0.110687000 |
| H | 1.654377000 | 2.235888000 | -1.382929000 |
| Ti | 2.610819000 | -0.570529000 | 0.010666000 |
| Cl | 3.940182000 | 1.373970000 | -0.123030000 |
| C | 3.718805000 | -2.184198000 | -1.356917000 |
| C | 3.841425000 | -0.946632000 | -2.028717000 |
| C | 2.540676000 | -0.508475000 | -2.383261000 |
| C | 1.615767000 | -1.499956000 | -1.966996000 |
| C | 2.334266000 | -2.529344000 | -1.321671000 |
| H | 4.539940000 | -2.784161000 | -0.972509000 |
| H | 4.762930000 | -0.393968000 | -2.189932000 |
| H | 2.295015000 | 0.438839000 | -2.858102000 |
| H | 0.532553000 | -1.436562000 | -2.044050000 |
| H | 1.897100000 | -3.428747000 | -0.898787000 |
| C | 3.655609000 | -1.953160000 | 1.663177000 |
| C | 2.261714000 | -2.262164000 | 1.647257000 |
| C | 1.561442000 | -1.120254000 | 2.095028000 |
| C | 2.504650000 | -0.096465000 | 2.356057000 |
| C | 3.800491000 | -0.622641000 | 2.112463000 |
| H | 4.465620000 | -2.631789000 | 1.407458000 |
| H | 1.806155000 | -3.209326000 | 1.374863000 |
| H | 0.480999000 | -1.017750000 | 2.126741000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.278896000 | 0.922370000 | 2.661472000 |
| H | 4.734073000 | -0.073326000 | 2.199397000 |
| H | -1.337225000 | 2.298787000 | -1.194118000 |

2c-Cr-endo: E= -3691.924143

| | | | |
|----|--------------|--------------|--------------|
| C | -1.092458000 | 1.913596000 | -0.846546000 |
| C | 0.076718000 | 2.704188000 | -1.502087000 |
| H | -0.185727000 | 2.985544000 | -2.533701000 |
| C | -0.832901000 | 0.495419000 | -0.370300000 |
| Cr | -2.397521000 | -0.828550000 | 0.024436000 |
| C | -3.739710000 | 0.480152000 | -0.333771000 |
| C | -3.816839000 | -2.028967000 | 0.377697000 |
| C | -2.309225000 | -1.225065000 | -1.828990000 |
| C | -1.237439000 | -2.259599000 | 0.410769000 |
| C | -2.275245000 | -0.196926000 | 1.803985000 |
| O | 0.392316000 | 0.218190000 | -0.207968000 |
| O | -2.147683000 | 0.228011000 | 2.868325000 |
| O | -4.596280000 | 1.220634000 | -0.532136000 |
| O | -2.205851000 | -1.432594000 | -2.957065000 |
| O | -4.672130000 | -2.767109000 | 0.596572000 |
| O | -0.591558000 | -3.187968000 | 0.649340000 |
| H | 1.016883000 | 2.145017000 | -1.524056000 |
| C | -1.504423000 | 2.861238000 | 0.371966000 |
| C | -0.340802000 | 2.857488000 | 1.346625000 |
| C | 0.671111000 | 3.520302000 | 0.762097000 |
| C | 0.188582000 | 3.982543000 | -0.604212000 |
| C | -1.304508000 | 4.236319000 | -0.300374000 |
| H | -2.494457000 | 2.637721000 | 0.784226000 |
| H | -0.328855000 | 2.302041000 | 2.285733000 |
| H | 1.699438000 | 3.611480000 | 1.113476000 |
| H | 0.760434000 | 4.800013000 | -1.063565000 |
| H | -1.923621000 | 4.380476000 | -1.200802000 |
| H | -1.470753000 | 5.068551000 | 0.400079000 |
| Ti | 2.180644000 | -0.460299000 | -0.008395000 |
| C | 3.435184000 | -0.981480000 | -2.007270000 |
| C | 2.088057000 | -0.759326000 | -2.389206000 |
| C | 1.297146000 | -1.785179000 | -1.812945000 |
| C | 2.137429000 | -2.609297000 | -1.035055000 |
| C | 3.469553000 | -2.109678000 | -1.158263000 |
| H | 4.281932000 | -0.354132000 | -2.270853000 |
| H | 1.724385000 | 0.068827000 | -2.993659000 |
| H | 0.221409000 | -1.887200000 | -1.909933000 |
| H | 1.816617000 | -3.479415000 | -0.469075000 |
| H | 4.362509000 | -2.542689000 | -0.715020000 |
| C | 1.991420000 | -1.871800000 | 1.899936000 |
| C | 1.293561000 | -0.682430000 | 2.213634000 |
| C | 2.219657000 | 0.384754000 | 2.227442000 |
| C | 3.511493000 | -0.153685000 | 1.973888000 |
| C | 3.373180000 | -1.542535000 | 1.771674000 |
| H | 1.547765000 | -2.859124000 | 1.814611000 |
| H | 0.221582000 | -0.595608000 | 2.355428000 |
| H | 1.983677000 | 1.436363000 | 2.361089000 |
| H | 4.432068000 | 0.418415000 | 1.894850000 |
| H | 4.180893000 | -2.242629000 | 1.575439000 |
| Cl | 3.320578000 | 1.566875000 | -0.467314000 |
| H | -1.957421000 | 1.867757000 | -1.522408000 |

2c-Cr-exo: E= -3691.923321

| | | | |
|---|--------------|-------------|--------------|
| C | -1.171727000 | 4.706152000 | -0.334772000 |
| C | -2.076247000 | 3.959302000 | 0.320107000 |
| C | -1.383221000 | 2.672341000 | 0.732958000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 0.130565000 | 3.919282000 | -0.373174000 |
| C | 0.052339000 | 3.179949000 | 0.979403000 |
| H | -1.349362000 | 5.650449000 | -0.853633000 |
| H | -3.144211000 | 4.149716000 | 0.440237000 |
| H | -1.866668000 | 2.091824000 | 1.528160000 |
| H | 1.047195000 | 4.487623000 | -0.577550000 |
| H | 0.803995000 | 2.385356000 | 1.072532000 |
| H | 0.112221000 | 3.856850000 | 1.844885000 |
| C | -1.178319000 | 1.862919000 | -0.630571000 |
| C | -0.100733000 | 2.721648000 | -1.356320000 |
| H | -0.448355000 | 3.055604000 | -2.344280000 |
| C | -0.838569000 | 0.417083000 | -0.304074000 |
| Cr | -2.318437000 | -1.013513000 | -0.018956000 |
| C | -3.675510000 | 0.328320000 | 0.103126000 |
| C | -1.949535000 | -0.797355000 | 1.821766000 |
| C | -2.425523000 | -1.020767000 | -1.918728000 |
| C | -3.703017000 | -2.281940000 | 0.228388000 |
| C | -1.129938000 | -2.467617000 | -0.064759000 |
| O | -4.526114000 | 1.094647000 | 0.200242000 |
| O | -4.538286000 | -3.058499000 | 0.380504000 |
| O | -0.457858000 | -3.408388000 | -0.056512000 |
| O | -2.424883000 | -0.999207000 | -3.069085000 |
| O | -1.664984000 | -0.626454000 | 2.926271000 |
| O | 0.401463000 | 0.193453000 | -0.163408000 |
| H | 0.836818000 | 2.168276000 | -1.483232000 |
| Ti | 2.223393000 | -0.351262000 | 0.008524000 |
| Cl | 3.200993000 | 1.786504000 | -0.268022000 |
| C | 3.610818000 | -1.866916000 | -1.194655000 |
| C | 3.624914000 | -0.662256000 | -1.928088000 |
| C | 2.306086000 | -0.416875000 | -2.396038000 |
| C | 1.489481000 | -1.496885000 | -1.985889000 |
| C | 2.278768000 | -2.382739000 | -1.219005000 |
| H | 4.468447000 | -2.324746000 | -0.706251000 |
| H | 4.477806000 | -0.002308000 | -2.060334000 |
| H | 1.979694000 | 0.462324000 | -2.947055000 |
| H | 0.422807000 | -1.593001000 | -2.170103000 |
| H | 1.922140000 | -3.296858000 | -0.751725000 |
| C | 2.852729000 | -1.936830000 | 1.678744000 |
| C | 1.528770000 | -1.535872000 | 1.965818000 |
| C | 1.560131000 | -0.162886000 | 2.342133000 |
| C | 2.892142000 | 0.281897000 | 2.263267000 |
| C | 3.696597000 | -0.801617000 | 1.814913000 |
| H | 3.164838000 | -2.937815000 | 1.392043000 |
| H | 0.646612000 | -2.167468000 | 1.920035000 |
| H | 0.694247000 | 0.436751000 | 2.609114000 |
| H | 3.238497000 | 1.295065000 | 2.443738000 |
| H | 4.769862000 | -0.766721000 | 1.635420000 |
| H | -2.126344000 | 1.856111000 | -1.179611000 |

2d-W-endo: E= -2753.182162

| | | | |
|---|--------------|--------------|--------------|
| C | 0.339633000 | 2.252805000 | 0.819434000 |
| C | -1.043475000 | 2.897695000 | 1.164228000 |
| H | -0.998779000 | 3.377410000 | 2.153967000 |
| C | 0.267527000 | 0.778204000 | 0.371384000 |
| W | 2.041707000 | -0.539550000 | -0.039535000 |
| C | 3.400453000 | 1.042940000 | -0.229048000 |
| C | 3.699175000 | -1.726748000 | -0.494498000 |
| C | 2.405636000 | -0.690606000 | 2.021653000 |
| C | 1.045753000 | -2.358910000 | 0.023198000 |
| C | 1.552676000 | -0.317258000 | -2.059474000 |
| O | -0.916474000 | 0.346790000 | 0.184799000 |

| | | | |
|----|--------------|--------------|--------------|
| O | 1.239803000 | -0.178825000 | -3.165169000 |
| O | 4.199627000 | 1.870614000 | -0.345759000 |
| O | 2.569832000 | -0.764119000 | 3.162199000 |
| O | 4.616710000 | -2.383132000 | -0.749500000 |
| O | 0.562216000 | -3.417732000 | 0.019656000 |
| H | -1.868838000 | 2.184232000 | 1.176448000 |
| C | 0.793165000 | 3.147622000 | -0.433034000 |
| C | -0.136920000 | 2.789954000 | -1.583037000 |
| C | -1.352414000 | 3.271269000 | -1.276069000 |
| C | -1.235600000 | 3.987699000 | 0.061233000 |
| C | 0.209354000 | 4.522548000 | -0.039317000 |
| H | 1.867311000 | 3.091669000 | -0.636608000 |
| H | 0.141399000 | 2.157153000 | -2.426522000 |
| H | -2.290519000 | 3.099341000 | -1.805336000 |
| H | -2.031634000 | 4.709446000 | 0.288671000 |
| H | 0.599807000 | 4.929722000 | 0.906009000 |
| H | 0.344572000 | 5.268107000 | -0.837183000 |
| C | 1.315402000 | 2.392344000 | 2.000662000 |
| H | 2.329462000 | 2.061735000 | 1.747875000 |
| H | 1.375458000 | 3.440959000 | 2.324949000 |
| H | 0.973215000 | 1.796977000 | 2.861875000 |
| Ti | -2.578025000 | -0.607050000 | 0.045519000 |
| C | -3.792146000 | -1.123308000 | 2.065956000 |
| C | -2.529052000 | -0.598828000 | 2.444362000 |
| C | -1.530466000 | -1.508299000 | 2.013313000 |
| C | -2.165124000 | -2.565281000 | 1.326209000 |
| C | -3.572591000 | -2.325475000 | 1.359360000 |
| H | -4.753335000 | -0.645013000 | 2.231983000 |
| H | -2.359932000 | 0.353150000 | 2.943216000 |
| H | -0.454515000 | -1.369283000 | 2.099943000 |
| H | -1.655277000 | -3.408262000 | 0.869475000 |
| H | -4.342322000 | -2.964101000 | 0.930737000 |
| C | -2.797716000 | -2.370813000 | -1.553941000 |
| C | -1.635782000 | -1.639867000 | -1.886099000 |
| C | -2.038609000 | -0.337568000 | -2.295625000 |
| C | -3.440639000 | -0.266476000 | -2.205158000 |
| C | -3.917454000 | -1.508800000 | -1.705921000 |
| H | -2.825931000 | -3.407828000 | -1.229933000 |
| H | -0.615126000 | -2.002959000 | -1.834851000 |
| H | -1.372441000 | 0.471477000 | -2.577722000 |
| H | -4.049291000 | 0.608530000 | -2.410183000 |
| H | -4.958102000 | -1.758443000 | -1.506024000 |
| Cl | -4.037844000 | 1.237056000 | 0.255584000 |

2d-W-exo: E= -2753.181328

| | | | |
|---|--------------|--------------|--------------|
| C | -0.922224000 | 4.988509000 | -0.148430000 |
| C | -1.967838000 | 4.194695000 | -0.427707000 |
| C | -1.667200000 | 2.825736000 | 0.160084000 |
| C | 0.091557000 | 4.147843000 | 0.615659000 |
| C | -0.859300000 | 3.227911000 | 1.412827000 |
| H | -0.759300000 | 6.014377000 | -0.485211000 |
| H | -2.838090000 | 4.429670000 | -1.042582000 |
| H | -2.535758000 | 2.183492000 | 0.319384000 |
| H | 0.851062000 | 4.702574000 | 1.184078000 |
| H | -0.351236000 | 2.376680000 | 1.897159000 |
| H | -1.465831000 | 3.759139000 | 2.160588000 |
| C | -0.519433000 | 2.162688000 | -0.709675000 |
| C | 0.684903000 | 3.119922000 | -0.396432000 |
| H | 1.072356000 | 3.602116000 | -1.304934000 |
| C | -0.273199000 | 0.695219000 | -0.287157000 |
| W | -1.865270000 | -0.846946000 | 0.062397000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -3.380285000 | 0.266340000 | -0.863421000 |
| C | -2.226765000 | 0.020496000 | 1.938013000 |
| C | -1.386245000 | -1.663555000 | -1.804811000 |
| C | -3.368845000 | -2.270055000 | 0.341169000 |
| C | -0.657607000 | -2.284437000 | 0.942773000 |
| O | -4.251084000 | 0.831286000 | -1.372145000 |
| O | -4.199927000 | -3.059597000 | 0.494557000 |
| O | -0.047076000 | -3.155980000 | 1.415116000 |
| O | -1.087862000 | -2.105679000 | -2.830934000 |
| O | -2.387063000 | 0.514240000 | 2.969566000 |
| O | 0.962439000 | 0.391053000 | -0.249074000 |
| H | 1.526121000 | 2.581098000 | 0.047152000 |
| C | -0.821994000 | 2.093307000 | -2.218923000 |
| H | -1.699751000 | 1.467853000 | -2.432631000 |
| H | -1.003488000 | 3.105598000 | -2.608987000 |
| H | 0.041075000 | 1.671615000 | -2.758888000 |
| Ti | 2.736682000 | -0.280147000 | -0.010959000 |
| Cl | 3.917630000 | 1.650386000 | -0.654796000 |
| C | 4.226866000 | -1.504440000 | -1.403347000 |
| C | 3.398076000 | -0.769240000 | -2.298464000 |
| C | 2.078186000 | -1.228677000 | -2.150273000 |
| C | 2.072889000 | -2.256821000 | -1.165975000 |
| C | 3.408963000 | -2.453545000 | -0.739901000 |
| H | 5.297401000 | -1.361815000 | -1.266367000 |
| H | 3.722423000 | 0.050986000 | -2.931980000 |
| H | 1.201528000 | -0.837980000 | -2.659154000 |
| H | 1.201065000 | -2.801590000 | -0.816370000 |
| H | 3.742337000 | -3.193292000 | -0.016392000 |
| C | 3.940673000 | -1.097625000 | 1.870137000 |
| C | 2.590547000 | -1.551336000 | 1.984637000 |
| C | 1.771158000 | -0.419247000 | 2.184333000 |
| C | 2.596827000 | 0.733045000 | 2.164080000 |
| C | 3.939879000 | 0.307960000 | 2.001818000 |
| H | 4.820146000 | -1.722337000 | 1.727870000 |
| H | 2.238342000 | -2.577820000 | 1.933438000 |
| H | 0.684533000 | -0.424334000 | 2.235649000 |
| H | 2.259332000 | 1.765234000 | 2.229343000 |
| H | 4.806061000 | 0.958657000 | 1.921332000 |

2d-Cr-endo: E= -3731.177111

| | | | |
|----|--------------|--------------|--------------|
| C | 1.051178000 | 1.981315000 | 0.795364000 |
| C | -0.239107000 | 2.780903000 | 1.183020000 |
| H | -0.117859000 | 3.231288000 | 2.180014000 |
| C | 0.802059000 | 0.519471000 | 0.341062000 |
| Cr | 2.298725000 | -0.931023000 | -0.072776000 |
| C | 3.718566000 | 0.331603000 | -0.230765000 |
| C | 3.625712000 | -2.207414000 | -0.476532000 |
| C | 2.533504000 | -1.087811000 | 1.808199000 |
| C | 1.134298000 | -2.402417000 | 0.005601000 |
| C | 1.841969000 | -0.637968000 | -1.882311000 |
| O | -0.420293000 | 0.232969000 | 0.179829000 |
| O | 1.528185000 | -0.443951000 | -2.974901000 |
| O | 4.640575000 | 1.006500000 | -0.362078000 |
| O | 2.620225000 | -1.198876000 | 2.950180000 |
| O | 4.432028000 | -2.990118000 | -0.727193000 |
| O | 0.518132000 | -3.380897000 | 0.024931000 |
| H | -1.143054000 | 2.172209000 | 1.201649000 |
| C | 1.571715000 | 2.834980000 | -0.460644000 |
| C | 0.574050000 | 2.620257000 | -1.589761000 |
| C | -0.563678000 | 3.241923000 | -1.240369000 |
| C | -0.324733000 | 3.908358000 | 0.106312000 |

| | | | |
|----|--------------|--------------|--------------|
| C | 1.171354000 | 4.264059000 | -0.027630000 |
| H | 2.626284000 | 2.660561000 | -0.698213000 |
| H | 0.750084000 | 1.982556000 | -2.456384000 |
| H | -1.527319000 | 3.206921000 | -1.749438000 |
| H | -1.019860000 | 4.717065000 | 0.369086000 |
| H | 1.635672000 | 4.602383000 | 0.911067000 |
| H | 1.375844000 | 5.001788000 | -0.818044000 |
| C | 2.057608000 | 2.018682000 | 1.959875000 |
| H | 3.039929000 | 1.615249000 | 1.692745000 |
| H | 2.207516000 | 3.055292000 | 2.292628000 |
| H | 1.680202000 | 1.448699000 | 2.822634000 |
| Ti | -2.225057000 | -0.433976000 | 0.038009000 |
| C | -3.552864000 | -0.741493000 | 2.028605000 |
| C | -2.235616000 | -0.413209000 | 2.444396000 |
| C | -1.377764000 | -1.467976000 | 2.048942000 |
| C | -2.144233000 | -2.421307000 | 1.343947000 |
| C | -3.499132000 | -1.970495000 | 1.337436000 |
| H | -4.434053000 | -0.120989000 | 2.164770000 |
| H | -1.937682000 | 0.503011000 | 2.949611000 |
| H | -0.302363000 | -1.505753000 | 2.201275000 |
| H | -1.757166000 | -3.336267000 | 0.904482000 |
| H | -4.345316000 | -2.488027000 | 0.890424000 |
| C | -2.748107000 | -2.135362000 | -1.558895000 |
| C | -1.492661000 | -1.598040000 | -1.917005000 |
| C | -1.690277000 | -0.246019000 | -2.316010000 |
| C | -3.061656000 | 0.045301000 | -2.199825000 |
| C | -3.719807000 | -1.105727000 | -1.690102000 |
| H | -2.932944000 | -3.155416000 | -1.231867000 |
| H | -0.547681000 | -2.129506000 | -1.907860000 |
| H | -0.909563000 | 0.444769000 | -2.616477000 |
| H | -3.528372000 | 1.005225000 | -2.395965000 |
| H | -4.782566000 | -1.185650000 | -1.468213000 |
| Cl | -3.376056000 | 1.628936000 | 0.239346000 |

2d-Cr-exo: E= -3731.176468

| | | | |
|----|--------------|--------------|--------------|
| C | -2.170913000 | 4.454356000 | -0.203275000 |
| C | -3.042161000 | 3.480941000 | -0.509876000 |
| C | -2.548733000 | 2.202780000 | 0.150969000 |
| C | -1.082871000 | 3.829154000 | 0.657729000 |
| C | -1.909591000 | 2.780759000 | 1.432634000 |
| H | -2.166372000 | 5.481852000 | -0.572809000 |
| H | -3.896947000 | 3.540622000 | -1.185596000 |
| H | -3.306503000 | 1.429833000 | 0.286249000 |
| H | -0.470987000 | 4.526226000 | 1.247379000 |
| H | -1.292057000 | 2.051502000 | 1.982709000 |
| H | -2.649828000 | 3.217922000 | 2.118490000 |
| C | -1.251306000 | 1.730522000 | -0.630593000 |
| C | -0.251357000 | 2.884588000 | -0.259458000 |
| H | 0.147179000 | 3.392809000 | -1.148156000 |
| C | -0.768397000 | 0.319735000 | -0.199102000 |
| Cr | -1.967496000 | -1.398530000 | 0.097173000 |
| C | -3.525479000 | -0.664744000 | -0.725363000 |
| C | -2.400951000 | -0.663165000 | 1.798460000 |
| C | -1.373904000 | -1.917812000 | -1.620420000 |
| C | -3.025638000 | -2.938530000 | 0.354338000 |
| C | -0.584973000 | -2.403128000 | 0.878988000 |
| O | -4.499934000 | -0.326773000 | -1.233731000 |
| O | -3.665797000 | -3.882062000 | 0.513621000 |
| O | 0.196391000 | -3.117860000 | 1.343634000 |
| O | -0.990249000 | -2.201650000 | -2.669745000 |
| O | -2.616998000 | -0.208518000 | 2.832926000 |

| | | | |
|----|--------------|--------------|--------------|
| O | 0.492843000 | 0.233373000 | -0.147858000 |
| H | 0.615245000 | 2.500869000 | 0.282983000 |
| C | -1.435798000 | 1.612248000 | -2.157946000 |
| H | -2.187366000 | 0.860495000 | -2.436145000 |
| H | -1.749633000 | 2.583753000 | -2.566131000 |
| H | -0.480336000 | 1.341413000 | -2.634513000 |
| Ti | 2.396542000 | -0.004566000 | -0.012058000 |
| Cl | 3.063701000 | 2.150166000 | -0.701224000 |
| C | 4.099801000 | -0.961324000 | -1.369418000 |
| C | 3.219558000 | -0.324371000 | -2.285665000 |
| C | 1.966077000 | -0.956820000 | -2.203574000 |
| C | 2.067424000 | -2.017161000 | -1.257410000 |
| C | 3.392398000 | -2.038692000 | -0.770106000 |
| H | 5.136277000 | -0.684092000 | -1.184891000 |
| H | 3.454747000 | 0.548099000 | -2.887231000 |
| H | 1.065581000 | -0.676196000 | -2.742662000 |
| H | 1.272960000 | -2.697832000 | -0.969379000 |
| H | 3.793511000 | -2.750762000 | -0.053397000 |
| C | 3.844255000 | -0.588923000 | 1.786483000 |
| C | 2.595688000 | -1.249164000 | 1.999321000 |
| C | 1.624781000 | -0.257109000 | 2.261560000 |
| C | 2.249441000 | 1.009326000 | 2.170329000 |
| C | 3.628314000 | 0.800110000 | 1.901725000 |
| H | 4.798464000 | -1.069889000 | 1.582063000 |
| H | 2.409162000 | -2.319201000 | 1.979510000 |
| H | 0.565729000 | -0.434369000 | 2.430735000 |
| H | 1.760443000 | 1.976361000 | 2.263320000 |
| H | 4.369772000 | 1.579375000 | 1.748658000 |

2e-W-endo: E= -1076.878268

| | | | |
|---|--------------|--------------|--------------|
| C | -1.959520000 | -0.335192000 | -0.364915000 |
| C | -3.089814000 | -0.303408000 | -1.452320000 |
| H | -2.808327000 | -0.961646000 | -2.287764000 |
| C | -0.882904000 | 0.735753000 | -0.162078000 |
| W | 1.204537000 | -0.142512000 | 0.002406000 |
| C | 0.483106000 | -1.803192000 | 1.051785000 |
| C | 3.068795000 | -1.076075000 | 0.067982000 |
| C | 0.850205000 | -1.100532000 | -1.831593000 |
| C | 2.203888000 | 1.392927000 | -1.007062000 |
| C | 1.649082000 | 0.771336000 | 1.833113000 |
| N | -1.200261000 | 2.029055000 | -0.089740000 |
| O | 1.917049000 | 1.283427000 | 2.835863000 |
| O | 0.114473000 | -2.741642000 | 1.620639000 |
| O | 0.649250000 | -1.643994000 | -2.831506000 |
| O | 4.104453000 | -1.592288000 | 0.103407000 |
| O | 2.807412000 | 2.224300000 | -1.541967000 |
| C | -0.167073000 | 3.046875000 | 0.133810000 |
| H | -1.378211000 | -1.227199000 | -0.611444000 |
| H | -3.303757000 | 0.678796000 | -1.891404000 |
| H | 0.552525000 | 2.710735000 | 0.886039000 |
| H | 0.372918000 | 3.259570000 | -0.800730000 |
| H | -0.639780000 | 3.973033000 | 0.486329000 |
| C | -2.751524000 | -0.794123000 | 0.938909000 |
| C | -3.817405000 | 0.227900000 | 1.282537000 |
| C | -4.762808000 | 0.161670000 | 0.328412000 |
| C | -4.323550000 | -0.894389000 | -0.674594000 |
| C | -3.627767000 | -1.888680000 | 0.283306000 |
| H | -2.082167000 | -1.099089000 | 1.750813000 |
| H | -3.758146000 | 0.942416000 | 2.105742000 |
| H | -5.631927000 | 0.813011000 | 0.212403000 |
| H | -5.109422000 | -1.291864000 | -1.331049000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.046634000 | -2.676076000 | -0.222192000 |
| H | -4.327807000 | -2.350077000 | 0.994776000 |
| C | -2.506280000 | 2.660129000 | -0.305901000 |
| H | -2.434959000 | 3.358074000 | -1.157033000 |
| H | -3.288135000 | 1.933119000 | -0.493534000 |
| H | -2.789787000 | 3.235288000 | 0.589374000 |

2e-W-exo: E= -1076.874821

| | | | |
|---|--------------|--------------|--------------|
| C | 4.246129000 | -1.741224000 | 0.172715000 |
| C | 3.306805000 | -1.791009000 | -0.786278000 |
| C | 2.832959000 | -0.363237000 | -1.024681000 |
| C | 4.427361000 | -0.278884000 | 0.563670000 |
| C | 4.162438000 | 0.388506000 | -0.805108000 |
| H | 4.727950000 | -2.584893000 | 0.670431000 |
| H | 2.839030000 | -2.672853000 | -1.226007000 |
| H | 2.273574000 | -0.178220000 | -1.949807000 |
| H | 5.368963000 | -0.028557000 | 1.071901000 |
| H | 4.079989000 | 1.481487000 | -0.774442000 |
| H | 4.917441000 | 0.116887000 | -1.557179000 |
| C | 2.003199000 | -0.030600000 | 0.304796000 |
| C | 3.145362000 | 0.145722000 | 1.364725000 |
| H | 2.967422000 | -0.506869000 | 2.231089000 |
| C | 0.815943000 | 0.918152000 | 0.091368000 |
| W | -1.164450000 | -0.185104000 | 0.017690000 |
| C | -0.279449000 | -1.753924000 | -1.050436000 |
| C | -1.847153000 | 0.592425000 | -1.802065000 |
| C | -0.639487000 | -1.045408000 | 1.860467000 |
| C | -2.904838000 | -1.333589000 | 0.080065000 |
| C | -2.257655000 | 1.287571000 | 1.024872000 |
| O | 0.187602000 | -2.637060000 | -1.635066000 |
| O | -3.871263000 | -1.969808000 | 0.118432000 |
| O | -2.903147000 | 2.088395000 | 1.556874000 |
| O | -0.353985000 | -1.537417000 | 2.866064000 |
| O | -2.257880000 | 1.024697000 | -2.794471000 |
| N | 0.990613000 | 2.232263000 | -0.062915000 |
| C | -0.136788000 | 3.117247000 | -0.375418000 |
| H | 1.523448000 | -0.973050000 | 0.569049000 |
| H | 3.248789000 | 1.162304000 | 1.765115000 |
| H | -0.668043000 | 3.407136000 | 0.543951000 |
| H | 0.240662000 | 4.025113000 | -0.865898000 |
| H | -0.842106000 | 2.621956000 | -1.047953000 |
| C | 2.218688000 | 3.012879000 | 0.106877000 |
| H | 2.017643000 | 3.852519000 | 0.791362000 |
| H | 3.027692000 | 2.421386000 | 0.523292000 |
| H | 2.540841000 | 3.429282000 | -0.861619000 |

2e-Cr-endo: E= -2054.870647

| | | | |
|----|--------------|--------------|--------------|
| C | 1.538115000 | -0.372047000 | 0.356559000 |
| C | 2.653993000 | -0.326409000 | 1.461720000 |
| H | 2.373621000 | -1.003852000 | 2.282139000 |
| C | 0.434640000 | 0.662399000 | 0.125844000 |
| Cr | -1.559867000 | -0.228052000 | -0.006483000 |
| C | -0.850526000 | -1.749114000 | -0.901843000 |
| C | -3.233554000 | -1.077648000 | -0.045448000 |
| C | -1.171556000 | -0.994752000 | 1.692546000 |
| C | -2.410982000 | 1.210045000 | 0.898136000 |
| C | -1.869160000 | 0.548502000 | -1.713011000 |
| N | 0.730041000 | 1.951536000 | 0.048440000 |
| O | -2.057705000 | 1.002779000 | -2.754299000 |
| O | -0.468904000 | -2.690163000 | -1.444688000 |
| O | -0.926888000 | -1.458784000 | 2.716633000 |

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|---|--------------|--------------|--------------|
| O | -4.262225000 | -1.597351000 | -0.069779000 |
| O | -2.981888000 | 2.039418000 | 1.457553000 |
| C | -0.282280000 | 2.977495000 | -0.249210000 |
| H | 0.983203000 | -1.280811000 | 0.589036000 |
| H | 2.841081000 | 0.651424000 | 1.922277000 |
| H | -1.080923000 | 2.574398000 | -0.870943000 |
| H | -0.713667000 | 3.370368000 | 0.683828000 |
| H | 0.197654000 | 3.806063000 | -0.788821000 |
| C | 2.362930000 | -0.796688000 | -0.940657000 |
| C | 3.408468000 | 0.255854000 | -1.254716000 |
| C | 4.340864000 | 0.201008000 | -0.287544000 |
| C | 3.912768000 | -0.877875000 | 0.695808000 |
| C | 3.256055000 | -1.876864000 | -0.283914000 |
| H | 1.719341000 | -1.111101000 | -1.769750000 |
| H | 3.344682000 | 0.978945000 | -2.070037000 |
| H | 5.190783000 | 0.873094000 | -0.149505000 |
| H | 4.698504000 | -1.264146000 | 1.359271000 |
| H | 2.686782000 | -2.684494000 | 0.202451000 |
| H | 3.978317000 | -2.311832000 | -0.990015000 |
| C | 2.019990000 | 2.618978000 | 0.297523000 |
| H | 1.873758000 | 3.392140000 | 1.069542000 |
| H | 2.789686000 | 1.926571000 | 0.616972000 |
| H | 2.366004000 | 3.111234000 | -0.624051000 |

2e-Cr-exo: E= -2054.867190

| | | | |
|----|--------------|--------------|--------------|
| C | 3.910839000 | -1.685891000 | 0.197730000 |
| C | 2.982125000 | -1.776909000 | -0.768440000 |
| C | 2.450743000 | -0.370681000 | -1.014758000 |
| C | 4.027893000 | -0.216703000 | 0.586303000 |
| C | 3.747088000 | 0.435394000 | -0.786006000 |
| H | 4.422627000 | -2.507813000 | 0.701942000 |
| H | 2.555792000 | -2.679320000 | -1.208241000 |
| H | 1.899867000 | -0.211924000 | -1.950022000 |
| H | 4.954555000 | 0.073665000 | 1.100900000 |
| H | 3.620972000 | 1.523634000 | -0.758356000 |
| H | 4.518251000 | 0.192127000 | -1.531493000 |
| C | 1.594465000 | -0.068037000 | 0.307542000 |
| C | 2.723029000 | 0.156437000 | 1.376055000 |
| H | 2.563327000 | -0.504309000 | 2.239830000 |
| C | 0.369256000 | 0.823196000 | 0.067571000 |
| Cr | -1.504516000 | -0.298167000 | 0.026703000 |
| C | -0.635454000 | -1.718362000 | -0.895520000 |
| C | -2.019740000 | 0.369343000 | -1.675217000 |
| C | -0.966854000 | -0.987207000 | 1.720837000 |
| C | -3.059500000 | -1.349157000 | 0.093776000 |
| C | -2.457432000 | 1.070124000 | 0.938200000 |
| O | -0.147424000 | -2.593034000 | -1.463297000 |
| O | -4.014308000 | -1.993544000 | 0.136756000 |
| O | -3.071027000 | 1.865669000 | 1.501263000 |
| O | -0.644155000 | -1.406720000 | 2.742006000 |
| O | -2.346733000 | 0.744560000 | -2.714054000 |
| N | 0.505873000 | 2.132639000 | -0.092141000 |
| C | -0.618302000 | 3.011489000 | -0.451740000 |
| H | 1.157472000 | -1.027442000 | 0.573205000 |
| H | 2.785279000 | 1.174732000 | 1.780488000 |
| H | -1.065039000 | 3.450361000 | 0.453473000 |
| H | -0.243802000 | 3.825739000 | -1.088927000 |
| H | -1.384386000 | 2.466220000 | -1.000568000 |
| C | 1.709573000 | 2.961863000 | 0.084333000 |
| H | 1.451562000 | 3.828865000 | 0.712446000 |
| H | 2.517476000 | 2.421006000 | 0.565840000 |

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|---|-------------|-------------|--------------|
| H | 2.056109000 | 3.337129000 | -0.891797000 |
|---|-------------|-------------|--------------|

2f-W-endo: E= -1116.123557

| | | | |
|---|--------------|--------------|--------------|
| C | 2.082686000 | -0.076352000 | 0.755016000 |
| C | 3.567106000 | 0.458164000 | 0.927454000 |
| H | 3.894006000 | 0.267515000 | 1.959668000 |
| C | 0.888031000 | 0.822710000 | 0.316587000 |
| W | -1.182264000 | -0.135565000 | -0.010023000 |
| C | -0.749914000 | -2.052924000 | 0.678474000 |
| C | -3.055456000 | -0.978556000 | -0.350210000 |
| C | -1.732198000 | 0.492228000 | 1.915066000 |
| C | -2.067850000 | 1.506492000 | -0.939646000 |
| C | -0.608359000 | -0.754933000 | -1.923755000 |
| N | 1.086479000 | 2.139518000 | 0.152433000 |
| O | -0.297014000 | -1.099474000 | -2.983155000 |
| O | -0.571467000 | -3.146526000 | 1.019618000 |
| O | -2.018404000 | 0.850310000 | 2.975719000 |
| O | -4.102004000 | -1.438628000 | -0.532960000 |
| O | -2.638632000 | 2.360001000 | -1.480032000 |
| C | 0.022686000 | 3.130174000 | 0.342881000 |
| H | 3.726624000 | 1.521957000 | 0.762313000 |
| H | -0.412293000 | 3.458263000 | -0.612676000 |
| H | -0.765687000 | 2.731813000 | 0.985644000 |
| H | 0.471507000 | 4.007094000 | 0.837038000 |
| C | 2.329659000 | -1.274821000 | -0.257708000 |
| C | 2.704477000 | -0.631399000 | -1.590403000 |
| C | 3.943540000 | -0.130052000 | -1.458133000 |
| C | 4.405888000 | -0.433785000 | -0.040558000 |
| C | 3.714711000 | -1.795931000 | 0.181516000 |
| H | 1.511634000 | -1.998298000 | -0.289113000 |
| H | 2.043727000 | -0.545276000 | -2.451820000 |
| H | 4.501737000 | 0.456083000 | -2.191442000 |
| H | 5.488788000 | -0.380315000 | 0.137850000 |
| H | 3.758438000 | -2.157767000 | 1.219790000 |
| H | 4.090400000 | -2.582658000 | -0.488829000 |
| C | 1.651804000 | -0.555195000 | 2.173095000 |
| H | 0.675379000 | -1.045572000 | 2.181971000 |
| H | 2.391552000 | -1.257890000 | 2.581125000 |
| H | 1.596439000 | 0.307337000 | 2.856553000 |
| C | 2.277708000 | 2.794360000 | -0.408526000 |
| H | 2.855403000 | 3.341632000 | 0.353119000 |
| H | 2.908056000 | 2.078432000 | -0.937379000 |
| H | 1.919543000 | 3.526261000 | -1.149531000 |

2f-W-exo: E= -1116.120803

| | | | |
|---|--------------|--------------|--------------|
| C | 4.596597000 | -1.291446000 | 0.047735000 |
| C | 3.427312000 | -1.948524000 | 0.088378000 |
| C | 2.361451000 | -1.018126000 | -0.462580000 |
| C | 4.307760000 | 0.102695000 | -0.497720000 |
| C | 3.184842000 | -0.233350000 | -1.503356000 |
| H | 5.561929000 | -1.624053000 | 0.434776000 |
| H | 3.226931000 | -2.934286000 | 0.510688000 |
| H | 1.461508000 | -1.513736000 | -0.827109000 |
| H | 5.173547000 | 0.666771000 | -0.871840000 |
| H | 2.651266000 | 0.641495000 | -1.909419000 |
| H | 3.524864000 | -0.860341000 | -2.339971000 |
| C | 2.082217000 | 0.133467000 | 0.601487000 |
| C | 3.503340000 | 0.830608000 | 0.630362000 |
| H | 3.980207000 | 0.666620000 | 1.606303000 |
| C | 0.778827000 | 0.930759000 | 0.275345000 |
| W | -1.187668000 | -0.198273000 | -0.021369000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.479595000 | -2.081671000 | 0.526746000 |
| C | -0.539333000 | -0.451615000 | -1.999631000 |
| C | -1.764232000 | 0.184235000 | 1.958226000 |
| C | -2.928791000 | -1.268017000 | -0.429888000 |
| C | -2.332450000 | 1.396000000 | -0.719942000 |
| O | -0.140072000 | -3.155375000 | 0.800599000 |
| O | -3.898155000 | -1.859417000 | -0.654590000 |
| O | -3.038787000 | 2.224803000 | -1.121060000 |
| O | -2.063043000 | 0.425733000 | 3.047892000 |
| O | -0.157226000 | -0.571417000 | -3.083787000 |
| N | 0.831802000 | 2.273371000 | 0.187914000 |
| C | 1.876050000 | 3.088327000 | -0.449535000 |
| H | 3.491777000 | 1.909272000 | 0.491770000 |
| H | 1.363004000 | 3.804219000 | -1.111406000 |
| H | 2.466946000 | 3.667196000 | 0.278241000 |
| H | 2.533600000 | 2.484382000 | -1.076123000 |
| C | 1.809042000 | -0.377985000 | 2.042538000 |
| H | 0.888656000 | -0.964031000 | 2.125464000 |
| H | 2.653036000 | -1.000821000 | 2.373398000 |
| H | 1.724114000 | 0.476218000 | 2.733374000 |
| C | -0.302710000 | 3.127734000 | 0.551960000 |
| H | -0.863111000 | 3.475666000 | -0.328570000 |
| H | -0.978804000 | 2.600171000 | 1.229239000 |
| H | 0.101686000 | 4.010691000 | 1.073894000 |

2f-Cr-endo: E= -2094.114296

| | | | |
|----|--------------|--------------|--------------|
| C | 1.703618000 | -0.153229000 | 0.737669000 |
| C | 3.160717000 | 0.432144000 | 1.001981000 |
| H | 3.459224000 | 0.193717000 | 2.032621000 |
| C | 0.481406000 | 0.733218000 | 0.367598000 |
| Cr | -1.527867000 | -0.214284000 | -0.033423000 |
| C | -1.037796000 | -2.001767000 | 0.371128000 |
| C | -3.174784000 | -1.027102000 | -0.379699000 |
| C | -1.933046000 | 0.172766000 | 1.788571000 |
| C | -2.447253000 | 1.313031000 | -0.668171000 |
| C | -0.908483000 | -0.450216000 | -1.804786000 |
| N | 0.648508000 | 2.044317000 | 0.224301000 |
| O | -0.556023000 | -0.580179000 | -2.894252000 |
| O | -0.885183000 | -3.130764000 | 0.546720000 |
| O | -2.135106000 | 0.434974000 | 2.889959000 |
| O | -4.192997000 | -1.528891000 | -0.581432000 |
| O | -3.124781000 | 2.133021000 | -1.115179000 |
| C | -0.433422000 | 3.014901000 | 0.444639000 |
| H | 3.279344000 | 1.510076000 | 0.906788000 |
| H | -0.873979000 | 3.361134000 | -0.501589000 |
| H | -1.209414000 | 2.594238000 | 1.085489000 |
| H | 0.005534000 | 3.884813000 | 0.958437000 |
| C | 2.039172000 | -1.248004000 | -0.367402000 |
| C | 2.449772000 | -0.488820000 | -1.626125000 |
| C | 3.664819000 | 0.036960000 | -1.399820000 |
| C | 4.073273000 | -0.358874000 | 0.011592000 |
| C | 3.423274000 | -1.755765000 | 0.093359000 |
| H | 1.258333000 | -2.001169000 | -0.498458000 |
| H | 1.819314000 | -0.349309000 | -2.503304000 |
| H | 4.233668000 | 0.696145000 | -2.059313000 |
| H | 5.144689000 | -0.284660000 | 0.244112000 |
| H | 3.435932000 | -2.200732000 | 1.099283000 |
| H | 3.856531000 | -2.471709000 | -0.620362000 |
| C | 1.273277000 | -0.787458000 | 2.093791000 |
| H | 0.375032000 | -1.402624000 | 2.017996000 |
| H | 2.079077000 | -1.416884000 | 2.494760000 |

| | | | |
|---|-------------|-------------|--------------|
| H | 1.074596000 | 0.004730000 | 2.833493000 |
| C | 1.833590000 | 2.765292000 | -0.283197000 |
| H | 2.363887000 | 3.310132000 | 0.513104000 |
| H | 2.507009000 | 2.092408000 | -0.813517000 |
| H | 1.464387000 | 3.504530000 | -1.010809000 |

2f-Cr-exo: E= -2094.111748

| | | | |
|----|--------------|--------------|--------------|
| C | 4.278675000 | -1.207018000 | 0.027844000 |
| C | 3.135691000 | -1.909718000 | 0.005360000 |
| C | 2.045180000 | -0.994659000 | -0.524512000 |
| C | 3.947037000 | 0.201636000 | -0.451929000 |
| C | 2.863211000 | -0.127010000 | -1.501953000 |
| H | 5.247186000 | -1.522569000 | 0.421164000 |
| H | 2.966405000 | -2.923200000 | 0.372156000 |
| H | 1.179465000 | -1.508047000 | -0.940654000 |
| H | 4.798269000 | 0.816867000 | -0.775835000 |
| H | 2.305514000 | 0.742573000 | -1.884190000 |
| H | 3.249242000 | -0.700039000 | -2.357204000 |
| C | 1.695420000 | 0.082601000 | 0.597993000 |
| C | 3.089343000 | 0.836937000 | 0.692724000 |
| H | 3.552579000 | 0.642836000 | 1.669531000 |
| C | 0.365194000 | 0.839809000 | 0.314502000 |
| Cr | -1.519158000 | -0.306302000 | -0.039744000 |
| C | -0.779377000 | -2.016641000 | 0.328913000 |
| C | -0.851379000 | -0.320680000 | -1.813544000 |
| C | -1.953799000 | -0.049022000 | 1.796649000 |
| C | -3.035322000 | -1.326779000 | -0.445196000 |
| C | -2.646782000 | 1.117546000 | -0.569092000 |
| O | -0.452210000 | -3.107027000 | 0.505989000 |
| O | -3.968176000 | -1.958237000 | -0.689844000 |
| O | -3.436834000 | 1.871481000 | -0.941748000 |
| O | -2.177458000 | 0.146573000 | 2.907807000 |
| O | -0.423560000 | -0.280502000 | -2.882346000 |
| N | 0.372672000 | 2.168024000 | 0.202582000 |
| C | 1.410528000 | 3.041086000 | -0.382012000 |
| H | 3.036429000 | 1.920379000 | 0.610459000 |
| H | 0.889951000 | 3.747283000 | -1.047285000 |
| H | 1.947072000 | 3.627619000 | 0.379933000 |
| H | 2.115343000 | 2.478303000 | -0.993682000 |
| C | 1.438199000 | -0.528298000 | 2.003497000 |
| H | 0.581085000 | -1.205731000 | 2.037694000 |
| H | 2.330616000 | -1.085539000 | 2.322699000 |
| H | 1.260012000 | 0.274181000 | 2.737491000 |
| C | -0.790015000 | 2.996079000 | 0.555276000 |
| H | -1.339892000 | 3.337253000 | -0.333943000 |
| H | -1.461515000 | 2.455729000 | 1.223871000 |
| H | -0.411587000 | 3.883673000 | 1.087591000 |

Reaction of 2,3-dimethyl-1,3-cyclopentadiene with **1d-W**

2,3-dimethyl-1,3-cyclopentadiene: E= -272.408883

| | | | |
|---|--------------|--------------|--------------|
| C | 0.251556000 | 0.742293000 | -0.000068000 |
| C | 0.251557000 | -0.742292000 | -0.000069000 |
| C | -1.030338000 | -1.177639000 | -0.000104000 |
| C | -1.964500000 | 0.000000000 | 0.000042000 |
| C | -1.030339000 | 1.177639000 | -0.000098000 |
| H | -1.355083000 | -2.219699000 | -0.000045000 |
| H | -2.634927000 | 0.000001000 | -0.881657000 |
| H | -2.633676000 | -0.000003000 | 0.882758000 |
| H | -1.355084000 | 2.219699000 | -0.000025000 |
| C | 1.503556000 | 1.564992000 | 0.000039000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 2.127190000 | 1.344973000 | 0.884086000 |
| H | 2.127070000 | 1.345234000 | -0.884167000 |
| H | 1.279982000 | 2.642078000 | 0.000194000 |
| C | 1.503555000 | -1.564993000 | 0.000045000 |
| H | 2.127196000 | -1.344956000 | 0.884084000 |
| H | 1.279979000 | -2.642077000 | 0.000221000 |
| H | 2.127067000 | -1.345252000 | -0.884167000 |

TS-endo-cy: E= -2831.682396

| | | | |
|----|--------------|--------------|--------------|
| C | -0.132700000 | 1.534066000 | -1.644041000 |
| C | 1.074464000 | 2.253049000 | -1.870726000 |
| H | 1.185037000 | 2.715216000 | -2.856731000 |
| C | -0.217809000 | 0.522360000 | -0.634220000 |
| W | -2.104839000 | -0.538893000 | 0.075532000 |
| C | -3.269733000 | 1.190171000 | -0.050353000 |
| C | -3.855542000 | -1.461188000 | 0.721947000 |
| C | -2.583037000 | -1.105844000 | -1.885650000 |
| C | -1.212349000 | -2.380852000 | 0.441102000 |
| C | -1.733441000 | -0.065698000 | 2.071092000 |
| O | 0.940729000 | 0.183653000 | -0.078975000 |
| O | -1.556709000 | 0.159591000 | 3.195250000 |
| O | -3.948558000 | 2.130422000 | -0.069977000 |
| O | -2.854403000 | -1.440406000 | -2.959228000 |
| O | -4.831917000 | -1.973377000 | 1.079836000 |
| O | -0.780396000 | -3.434655000 | 0.682146000 |
| H | 2.005063000 | 1.847401000 | -1.474087000 |
| C | -0.832175000 | 3.555223000 | 0.433372000 |
| C | 0.290684000 | 3.280923000 | 1.180691000 |
| C | 1.444255000 | 3.646757000 | 0.413167000 |
| C | 1.031619000 | 3.994332000 | -0.896401000 |
| C | -0.453153000 | 4.296988000 | -0.804718000 |
| H | -1.859746000 | 3.369065000 | 0.743403000 |
| H | 1.689490000 | 4.589513000 | -1.536133000 |
| H | -1.061794000 | 4.078838000 | -1.688658000 |
| H | -0.562629000 | 5.383238000 | -0.610876000 |
| C | -1.297560000 | 1.766507000 | -2.581705000 |
| H | -2.241676000 | 1.990038000 | -2.069445000 |
| H | -1.085694000 | 2.591664000 | -3.278032000 |
| H | -1.480068000 | 0.871769000 | -3.197578000 |
| Ti | 2.445232000 | -0.956024000 | -0.067722000 |
| C | 3.387707000 | -1.693795000 | -2.189112000 |
| C | 2.096263000 | -1.168858000 | -2.443306000 |
| C | 1.152786000 | -2.005005000 | -1.798452000 |
| C | 1.854887000 | -3.017732000 | -1.108931000 |
| C | 3.246758000 | -2.821748000 | -1.351969000 |
| H | 4.326927000 | -1.267605000 | -2.528998000 |
| H | 1.867086000 | -0.266132000 | -3.004562000 |
| H | 0.079996000 | -1.839282000 | -1.767253000 |
| H | 1.399511000 | -3.811355000 | -0.524095000 |
| H | 4.058846000 | -3.447990000 | -0.991740000 |
| C | 2.057493000 | -2.366358000 | 1.824409000 |
| C | 1.705113000 | -1.058926000 | 2.233123000 |
| C | 2.866846000 | -0.259140000 | 2.199015000 |
| C | 3.962707000 | -1.091195000 | 1.826677000 |
| C | 3.467829000 | -2.389217000 | 1.604664000 |
| H | 1.373195000 | -3.205552000 | 1.745329000 |
| H | 0.695343000 | -0.718962000 | 2.435278000 |
| H | 2.921769000 | 0.808070000 | 2.396143000 |
| H | 4.990440000 | -0.763823000 | 1.694314000 |
| H | 4.055443000 | -3.258460000 | 1.321990000 |
| Cl | 4.098406000 | 0.695106000 | -0.598526000 |

| | | | |
|---|--------------|-------------|-------------|
| C | 0.337215000 | 2.662156000 | 2.541189000 |
| H | -0.658694000 | 2.594557000 | 2.995845000 |
| H | 0.741603000 | 1.641929000 | 2.475526000 |
| H | 0.991946000 | 3.233461000 | 3.218853000 |
| C | 2.849507000 | 3.572808000 | 0.892230000 |
| H | 2.926878000 | 3.867972000 | 1.950463000 |
| H | 3.232309000 | 2.541190000 | 0.801989000 |
| H | 3.517759000 | 4.208528000 | 0.293513000 |

TS-exo-cy: E= -2831.687417

| | | | |
|----|--------------|--------------|--------------|
| C | -1.167160000 | 4.414098000 | 0.081860000 |
| C | -2.064190000 | 3.544011000 | 0.781828000 |
| C | -1.315781000 | 2.589010000 | 1.441306000 |
| C | 0.148963000 | 3.915203000 | 0.211900000 |
| C | 0.132271000 | 2.934849000 | 1.365279000 |
| H | -1.720210000 | 1.759630000 | 2.022298000 |
| H | 1.025718000 | 4.534220000 | 0.005073000 |
| H | 0.822556000 | 2.090723000 | 1.273523000 |
| H | 0.421655000 | 3.483944000 | 2.284059000 |
| C | -0.618772000 | 1.584216000 | -1.178641000 |
| C | 0.320765000 | 2.635616000 | -1.333040000 |
| H | 0.140944000 | 3.345072000 | -2.146574000 |
| C | -0.294356000 | 0.384260000 | -0.468847000 |
| W | -1.635767000 | -1.379397000 | -0.015195000 |
| C | -3.310988000 | -0.219860000 | 0.446049000 |
| C | -1.086770000 | -1.155249000 | 1.984004000 |
| C | -2.122631000 | -1.462569000 | -2.054209000 |
| C | -2.860422000 | -3.004029000 | 0.430231000 |
| C | -0.167908000 | -2.832023000 | -0.258000000 |
| O | -4.258666000 | 0.381132000 | 0.739892000 |
| O | -3.542479000 | -3.908487000 | 0.676586000 |
| O | 0.614176000 | -3.689230000 | -0.344079000 |
| O | -2.375090000 | -1.488080000 | -3.181960000 |
| O | -0.781566000 | -0.997464000 | 3.091737000 |
| O | 0.946781000 | 0.312147000 | -0.012196000 |
| H | 1.373249000 | 2.437018000 | -1.132120000 |
| C | -1.950398000 | 1.756285000 | -1.862827000 |
| H | -2.767285000 | 1.233889000 | -1.355403000 |
| H | -2.217555000 | 2.822181000 | -1.928536000 |
| H | -1.910500000 | 1.370949000 | -2.896506000 |
| Ti | 2.771817000 | -0.077273000 | -0.000686000 |
| Cl | 3.526780000 | 2.194470000 | -0.021634000 |
| C | 4.059258000 | 0.016312000 | -2.046341000 |
| C | 2.689049000 | 0.128936000 | -2.403910000 |
| C | 2.046628000 | -1.085537000 | -2.068088000 |
| C | 3.000845000 | -1.935158000 | -1.464445000 |
| C | 4.254713000 | -1.251625000 | -1.461645000 |
| H | 4.808677000 | 0.796353000 | -2.149825000 |
| H | 2.209950000 | 1.007426000 | -2.828651000 |
| H | 0.981900000 | -1.291698000 | -2.160498000 |
| H | 2.797648000 | -2.933766000 | -1.087783000 |
| H | 5.196736000 | -1.639197000 | -1.079662000 |
| C | 4.423506000 | -0.620634000 | 1.660708000 |
| C | 3.669563000 | -1.796813000 | 1.417989000 |
| C | 2.335138000 | -1.556551000 | 1.826220000 |
| C | 2.279523000 | -0.249884000 | 2.382993000 |
| C | 3.560712000 | 0.321647000 | 2.286120000 |
| H | 5.476009000 | -0.466082000 | 1.429833000 |
| H | 4.043443000 | -2.720312000 | 0.983575000 |
| H | 1.501926000 | -2.246379000 | 1.728934000 |
| H | 1.383836000 | 0.230885000 | 2.764951000 |

| | | | |
|---|--------------|-------------|--------------|
| H | 3.833721000 | 1.330799000 | 2.579460000 |
| C | -3.558255000 | 3.652743000 | 0.737499000 |
| H | -3.896690000 | 4.598074000 | 1.194498000 |
| H | -3.925973000 | 3.649252000 | -0.301807000 |
| H | -4.039208000 | 2.817971000 | 1.262964000 |
| C | -1.588275000 | 5.577298000 | -0.754141000 |
| H | -0.731126000 | 6.061166000 | -1.243843000 |
| H | -2.310203000 | 5.275994000 | -1.533048000 |
| H | -2.103112000 | 6.333821000 | -0.136530000 |

Adduct-endo-cy: E= -2831.719379

| | | | |
|----|--------------|--------------|--------------|
| C | 0.152527000 | 1.998952000 | 1.189234000 |
| C | -1.277871000 | 2.466301000 | 1.634558000 |
| H | -1.301859000 | 2.625339000 | 2.723909000 |
| C | 0.221242000 | 0.618160000 | 0.496066000 |
| W | 2.135342000 | -0.455761000 | -0.059530000 |
| C | 3.317537000 | 1.268397000 | 0.089160000 |
| C | 3.938582000 | -1.445469000 | -0.411707000 |
| C | 2.370240000 | -0.921492000 | 1.972541000 |
| C | 1.260632000 | -2.300669000 | -0.427978000 |
| C | 2.062611000 | -0.126669000 | -2.124318000 |
| O | -0.923332000 | 0.094589000 | 0.293561000 |
| O | 2.035384000 | 0.012116000 | -3.271680000 |
| O | 4.026563000 | 2.179836000 | 0.139581000 |
| O | 2.499148000 | -1.197881000 | 3.086409000 |
| O | 4.938310000 | -1.998247000 | -0.592910000 |
| O | 0.850565000 | -3.361186000 | -0.679058000 |
| H | -2.066582000 | 1.752905000 | 1.388035000 |
| C | 0.535311000 | 3.158154000 | 0.160496000 |
| C | -0.416662000 | 3.077652000 | -1.035890000 |
| C | -1.630635000 | 3.478382000 | -0.602728000 |
| C | -1.482649000 | 3.815425000 | 0.877356000 |
| C | -0.052520000 | 4.388968000 | 0.885393000 |
| H | 1.602147000 | 3.180689000 | -0.089084000 |
| H | -2.283532000 | 4.441517000 | 1.296336000 |
| H | 0.357166000 | 4.573377000 | 1.890077000 |
| H | 0.047638000 | 5.304793000 | 0.284255000 |
| C | 1.094145000 | 1.981008000 | 2.411729000 |
| H | 2.143464000 | 1.826668000 | 2.137679000 |
| H | 1.028677000 | 2.929681000 | 2.961370000 |
| H | 0.806241000 | 1.178463000 | 3.108694000 |
| Ti | -2.449457000 | -1.053856000 | 0.059183000 |
| C | -3.479944000 | -1.959476000 | 2.054037000 |
| C | -2.240526000 | -1.379182000 | 2.422713000 |
| C | -1.206585000 | -2.125989000 | 1.801162000 |
| C | -1.803383000 | -3.134686000 | 1.014324000 |
| C | -3.218201000 | -3.026650000 | 1.165736000 |
| H | -4.461546000 | -1.601513000 | 2.350728000 |
| H | -2.110197000 | -0.495285000 | 3.043829000 |
| H | -0.144092000 | -1.898913000 | 1.839609000 |
| H | -1.266444000 | -3.871876000 | 0.426446000 |
| H | -3.963660000 | -3.676038000 | 0.712858000 |
| C | -1.950568000 | -2.365179000 | -1.859558000 |
| C | -1.439086000 | -1.072624000 | -2.105580000 |
| C | -2.526878000 | -0.164998000 | -2.152189000 |
| C | -3.722747000 | -0.911499000 | -1.988132000 |
| C | -3.372943000 | -2.264308000 | -1.786344000 |
| H | -1.356143000 | -3.269355000 | -1.775363000 |
| H | -0.386094000 | -0.811598000 | -2.143590000 |
| H | -2.455737000 | 0.914338000 | -2.253166000 |
| H | -4.727607000 | -0.500405000 | -1.954701000 |

| | | | |
|----|--------------|--------------|--------------|
| H | -4.066991000 | -3.088354000 | -1.638628000 |
| Cl | -4.138191000 | 0.524423000 | 0.576431000 |
| C | -0.019884000 | 2.559588000 | -2.379325000 |
| H | 0.970541000 | 2.936714000 | -2.682432000 |
| H | 0.055296000 | 1.462596000 | -2.381035000 |
| H | -0.745385000 | 2.840357000 | -3.157650000 |
| C | -2.940742000 | 3.521564000 | -1.317320000 |
| H | -2.833050000 | 3.340165000 | -2.397862000 |
| H | -3.629714000 | 2.763294000 | -0.907637000 |
| H | -3.429706000 | 4.502622000 | -1.186681000 |

Adduct-exo-cy: E= -2831.718534

| | | | |
|----|--------------|--------------|--------------|
| C | -2.459941000 | 4.123892000 | 0.192103000 |
| C | -3.173377000 | 3.006492000 | -0.060758000 |
| C | -2.341469000 | 1.830871000 | 0.434374000 |
| C | -1.155811000 | 3.678039000 | 0.853334000 |
| C | -1.644585000 | 2.456785000 | 1.656952000 |
| H | -2.907754000 | 0.912776000 | 0.607259000 |
| H | -0.615197000 | 4.462177000 | 1.403807000 |
| H | -0.829816000 | 1.834133000 | 2.065859000 |
| H | -2.346602000 | 2.709734000 | 2.464684000 |
| C | -1.102483000 | 1.656745000 | -0.541817000 |
| C | -0.302017000 | 2.973315000 | -0.239180000 |
| H | -0.181863000 | 3.594523000 | -1.138696000 |
| C | -0.322869000 | 0.361679000 | -0.222748000 |
| W | -1.259379000 | -1.659710000 | 0.066320000 |
| C | -3.115984000 | -1.077393000 | -0.712761000 |
| C | -1.788058000 | -1.088682000 | 2.013967000 |
| C | -0.629209000 | -2.125785000 | -1.874993000 |
| C | -2.170860000 | -3.527179000 | 0.272891000 |
| C | 0.407113000 | -2.646487000 | 0.808197000 |
| O | -4.156632000 | -0.809980000 | -1.140894000 |
| O | -2.675314000 | -4.562013000 | 0.384456000 |
| O | 1.298417000 | -3.282471000 | 1.204159000 |
| O | -0.250235000 | -2.357297000 | -2.942867000 |
| O | -2.046868000 | -0.742772000 | 3.085015000 |
| O | 0.939914000 | 0.521727000 | -0.233341000 |
| H | 0.706179000 | 2.760602000 | 0.125558000 |
| C | -1.463880000 | 1.546250000 | -2.035748000 |
| H | -2.065651000 | 0.653049000 | -2.251403000 |
| H | -2.021946000 | 2.439760000 | -2.351434000 |
| H | -0.545059000 | 1.492311000 | -2.641666000 |
| Ti | 2.842338000 | 0.490695000 | -0.048934000 |
| Cl | 3.263407000 | 2.744956000 | -0.574654000 |
| C | 4.621481000 | -0.069433000 | -1.523470000 |
| C | 3.571349000 | 0.392961000 | -2.367252000 |
| C | 2.488468000 | -0.494816000 | -2.244720000 |
| C | 2.855937000 | -1.520891000 | -1.329489000 |
| C | 4.189234000 | -1.277679000 | -0.920132000 |
| H | 5.583960000 | 0.418883000 | -1.380762000 |
| H | 3.583673000 | 1.310781000 | -2.947648000 |
| H | 1.518262000 | -0.395848000 | -2.723686000 |
| H | 2.227735000 | -2.348066000 | -1.013265000 |
| H | 4.770549000 | -1.903171000 | -0.247451000 |
| C | 4.309940000 | 0.025954000 | 1.764716000 |
| C | 3.196242000 | -0.863589000 | 1.864098000 |
| C | 2.049906000 | -0.088623000 | 2.144089000 |
| C | 2.437025000 | 1.274426000 | 2.185834000 |
| C | 3.839352000 | 1.338606000 | 1.982938000 |
| H | 5.343659000 | -0.255597000 | 1.574514000 |
| H | 3.209859000 | -1.944034000 | 1.751923000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.031379000 | -0.465167000 | 2.209545000 |
| H | 1.773348000 | 2.126236000 | 2.318484000 |
| H | 4.432634000 | 2.247238000 | 1.933185000 |
| C | -4.481598000 | 2.821753000 | -0.759312000 |
| H | -4.384622000 | 2.126568000 | -1.610428000 |
| H | -5.225982000 | 2.366866000 | -0.081900000 |
| H | -4.896479000 | 3.769857000 | -1.132613000 |
| C | -2.728929000 | 5.544609000 | -0.178474000 |
| H | -2.729591000 | 6.195826000 | 0.713610000 |
| H | -1.936639000 | 5.931613000 | -0.845000000 |
| H | -3.693482000 | 5.669490000 | -0.692512000 |

Reaction of 2,3-dimethyl-1,3-butadiene with **1d-W**

2,3-dimethyl-1,3-cyclobutadiene: E= -234.322763

| | | | |
|---|--------------|--------------|--------------|
| C | 0.746142000 | 0.127250000 | 0.024790000 |
| C | -0.746156000 | 0.127255000 | -0.024797000 |
| C | -1.432310000 | 1.194146000 | -0.469093000 |
| C | 1.432340000 | 1.194110000 | 0.469096000 |
| H | -2.526335000 | 1.200313000 | -0.483769000 |
| H | 2.526368000 | 1.200202000 | 0.483763000 |
| C | 1.447740000 | -1.133348000 | -0.426512000 |
| H | 1.217232000 | -1.981118000 | 0.240898000 |
| H | 1.120660000 | -1.429574000 | -1.438148000 |
| H | 2.539684000 | -1.003331000 | -0.439526000 |
| C | -1.447767000 | -1.133329000 | 0.426510000 |
| H | -1.120836000 | -1.429447000 | 1.438220000 |
| H | -2.539720000 | -1.003359000 | 0.439352000 |
| H | -1.217119000 | -1.981164000 | -0.240779000 |
| H | 0.921274000 | 2.085498000 | 0.841413000 |
| H | -0.921140000 | 2.085478000 | -0.841386000 |

TS-endo-acy: E= -2793.596993

| | | | |
|----|--------------|--------------|--------------|
| C | 0.083730000 | 1.573621000 | 1.699463000 |
| C | -1.196853000 | 2.065877000 | 2.045197000 |
| H | -1.322019000 | 2.434387000 | 3.067996000 |
| C | 0.246355000 | 0.581515000 | 0.667346000 |
| W | 2.203080000 | -0.295405000 | -0.094932000 |
| C | 3.189358000 | 1.539791000 | 0.105456000 |
| C | 4.005794000 | -0.980211000 | -0.879558000 |
| C | 2.780054000 | -0.895284000 | 1.828525000 |
| C | 1.528831000 | -2.227937000 | -0.446468000 |
| C | 1.567678000 | 0.234450000 | -2.006621000 |
| O | -0.879976000 | 0.131274000 | 0.140649000 |
| O | 1.203128000 | 0.542374000 | -3.064597000 |
| O | 3.766734000 | 2.540010000 | 0.185579000 |
| O | 3.082299000 | -1.243647000 | 2.889463000 |
| O | 5.010582000 | -1.355043000 | -1.319096000 |
| O | 1.212231000 | -3.326133000 | -0.669385000 |
| H | -2.081514000 | 1.581133000 | 1.633896000 |
| C | 0.490434000 | 3.214805000 | -0.735751000 |
| C | -0.833987000 | 3.330207000 | -1.039202000 |
| C | -1.799649000 | 3.729116000 | -0.038530000 |
| C | -1.425796000 | 3.923256000 | 1.297525000 |
| H | 1.199670000 | 2.841281000 | -1.473833000 |
| H | -2.190247000 | 4.314294000 | 1.974128000 |
| C | 1.260895000 | 2.097383000 | 2.486260000 |
| H | 1.771261000 | 2.940717000 | 1.989114000 |
| H | 0.935401000 | 2.459688000 | 3.473450000 |
| H | 2.024701000 | 1.327328000 | 2.647278000 |
| Ti | -2.312532000 | -1.084730000 | 0.059159000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -3.193696000 | -2.011712000 | 2.130343000 |
| C | -1.950280000 | -1.400026000 | 2.428784000 |
| C | -0.937123000 | -2.113211000 | 1.743697000 |
| C | -1.550223000 | -3.133635000 | 0.984399000 |
| C | -2.955989000 | -3.071003000 | 1.229527000 |
| H | -4.166426000 | -1.683030000 | 2.484646000 |
| H | -1.800215000 | -0.519563000 | 3.048851000 |
| H | 0.118462000 | -1.855826000 | 1.730043000 |
| H | -1.027196000 | -3.837050000 | 0.341607000 |
| H | -3.714950000 | -3.732388000 | 0.817845000 |
| C | -1.598066000 | -2.050410000 | -2.005502000 |
| C | -1.861324000 | -0.687759000 | -2.306259000 |
| C | -3.230686000 | -0.452578000 | -2.104133000 |
| C | -3.840797000 | -1.680692000 | -1.705127000 |
| C | -2.837290000 | -2.670992000 | -1.689575000 |
| H | -0.629927000 | -2.540876000 | -2.046818000 |
| H | -1.113850000 | 0.053706000 | -2.563236000 |
| H | -3.743425000 | 0.500981000 | -2.190464000 |
| H | -4.890352000 | -1.814700000 | -1.451278000 |
| H | -2.975485000 | -3.723011000 | -1.454283000 |
| Cl | -4.062255000 | 0.430599000 | 0.663620000 |
| C | -1.326297000 | 2.953220000 | -2.417248000 |
| H | -0.511827000 | 2.554004000 | -3.035978000 |
| H | -2.118431000 | 2.192909000 | -2.363500000 |
| H | -1.755848000 | 3.825087000 | -2.937960000 |
| C | -3.256056000 | 3.750551000 | -0.402069000 |
| H | -3.431870000 | 4.352044000 | -1.308504000 |
| H | -3.618043000 | 2.728862000 | -0.609248000 |
| H | -3.873366000 | 4.156813000 | 0.410461000 |
| H | 0.921280000 | 3.572540000 | 0.194806000 |
| H | -0.413754000 | 4.253784000 | 1.539092000 |

TS-exo-acy: E= -2793.595596

| | | | |
|----|--------------|--------------|--------------|
| C | 0.372994000 | 4.453943000 | -0.206151000 |
| C | 1.330366000 | 3.693348000 | -0.976772000 |
| C | 1.008777000 | 2.455810000 | -1.459392000 |
| C | -0.878616000 | 3.911638000 | 0.112595000 |
| H | 1.754199000 | 1.847270000 | -1.972219000 |
| H | -1.601234000 | 4.557207000 | 0.619181000 |
| C | 0.458120000 | 1.665592000 | 1.279685000 |
| C | -0.621766000 | 2.533837000 | 1.561058000 |
| H | -0.477427000 | 3.230000000 | 2.392799000 |
| C | 0.273378000 | 0.463203000 | 0.511381000 |
| W | 1.801920000 | -1.139639000 | 0.036483000 |
| C | 3.315729000 | 0.250864000 | -0.354223000 |
| C | 1.289395000 | -0.990828000 | -1.978063000 |
| C | 2.211159000 | -1.216614000 | 2.093671000 |
| C | 3.245528000 | -2.579059000 | -0.388422000 |
| C | 0.516148000 | -2.766940000 | 0.155008000 |
| O | 4.160182000 | 0.999515000 | -0.617230000 |
| O | 4.052202000 | -3.377928000 | -0.621825000 |
| O | -0.157755000 | -3.715851000 | 0.160029000 |
| O | 2.413977000 | -1.241589000 | 3.230947000 |
| O | 0.997306000 | -0.892276000 | -3.095981000 |
| O | -0.951513000 | 0.299538000 | 0.048587000 |
| H | -1.642356000 | 2.174556000 | 1.434907000 |
| C | 1.783411000 | 2.074783000 | 1.857927000 |
| H | 2.021937000 | 3.108587000 | 1.550259000 |
| H | 1.745350000 | 2.072629000 | 2.960503000 |
| H | 2.610904000 | 1.431379000 | 1.550419000 |
| Ti | -2.715735000 | -0.307985000 | -0.052812000 |

| | | | |
|----|--------------|--------------|--------------|
| Cl | -3.767142000 | 1.829841000 | 0.141289000 |
| C | -4.061362000 | -0.550951000 | 1.951911000 |
| C | -2.724844000 | -0.314614000 | 2.369426000 |
| C | -1.933354000 | -1.408367000 | 1.949604000 |
| C | -2.762191000 | -2.301629000 | 1.234300000 |
| C | -4.088078000 | -1.770699000 | 1.245784000 |
| H | -4.901474000 | 0.122137000 | 2.099028000 |
| H | -2.367619000 | 0.565368000 | 2.898416000 |
| H | -0.855831000 | -1.499245000 | 2.069927000 |
| H | -2.432280000 | -3.230808000 | 0.778227000 |
| H | -4.968238000 | -2.226906000 | 0.797911000 |
| C | -3.427386000 | -1.964947000 | -1.640356000 |
| C | -2.090986000 | -1.613608000 | -1.953770000 |
| C | -2.092813000 | -0.267679000 | -2.413706000 |
| C | -3.408732000 | 0.218349000 | -2.338856000 |
| C | -4.240515000 | -0.821409000 | -1.832399000 |
| H | -3.761954000 | -2.940430000 | -1.297027000 |
| H | -1.222141000 | -2.260051000 | -1.867220000 |
| H | -1.213362000 | 0.294626000 | -2.712323000 |
| H | -3.730605000 | 1.229836000 | -2.567793000 |
| H | -5.309503000 | -0.745946000 | -1.641230000 |
| C | 2.734602000 | 4.228354000 | -1.148819000 |
| H | 3.369692000 | 3.512288000 | -1.686930000 |
| H | 2.734337000 | 5.179824000 | -1.706029000 |
| H | 3.215945000 | 4.429121000 | -0.177743000 |
| C | 0.789209000 | 5.773974000 | 0.386415000 |
| H | 1.676741000 | 5.676237000 | 1.034049000 |
| H | 1.070093000 | 6.486526000 | -0.408268000 |
| H | -0.018796000 | 6.227236000 | 0.977145000 |
| H | -1.349350000 | 3.185012000 | -0.550965000 |
| H | -0.005725000 | 2.065843000 | -1.458089000 |

Adduct-endo-acy: E= -2793.661840

| | | | |
|----|--------------|--------------|--------------|
| C | 0.101146000 | 1.984698000 | 1.350867000 |
| C | -1.312824000 | 2.194123000 | 1.968780000 |
| H | -1.210675000 | 2.390652000 | 3.047011000 |
| C | 0.250385000 | 0.626795000 | 0.604878000 |
| W | 2.208144000 | -0.291893000 | -0.063614000 |
| C | 3.413504000 | 1.392099000 | 0.251076000 |
| C | 4.000516000 | -1.216397000 | -0.595930000 |
| C | 2.447138000 | -0.919453000 | 1.925119000 |
| C | 1.376267000 | -2.104698000 | -0.630246000 |
| C | 1.996529000 | 0.373903000 | -2.033666000 |
| O | -0.857771000 | 0.050909000 | 0.369408000 |
| O | 1.867821000 | 0.731286000 | -3.126459000 |
| O | 4.132118000 | 2.288514000 | 0.381583000 |
| O | 2.559423000 | -1.262296000 | 3.022242000 |
| O | 4.990950000 | -1.738531000 | -0.886921000 |
| O | 0.998891000 | -3.141796000 | -1.002175000 |
| H | -1.904204000 | 1.280249000 | 1.875020000 |
| C | 0.368559000 | 3.072634000 | 0.261098000 |
| C | -0.783236000 | 3.245586000 | -0.708741000 |
| C | -2.016649000 | 3.374839000 | -0.178031000 |
| C | -2.119281000 | 3.340493000 | 1.331754000 |
| H | 1.296668000 | 2.828147000 | -0.273796000 |
| H | -3.170496000 | 3.255334000 | 1.645777000 |
| C | 1.146661000 | 2.092060000 | 2.475708000 |
| H | 2.177012000 | 2.021868000 | 2.113472000 |
| H | 1.035097000 | 3.063981000 | 2.981296000 |
| H | 0.998033000 | 1.301242000 | 3.227533000 |
| Ti | -2.371878000 | -1.079849000 | -0.001669000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -3.384439000 | -2.285317000 | 1.833436000 |
| C | -2.169166000 | -1.721232000 | 2.298054000 |
| C | -1.103513000 | -2.341199000 | 1.597329000 |
| C | -1.656214000 | -3.250306000 | 0.669179000 |
| C | -3.075614000 | -3.212265000 | 0.813235000 |
| H | -4.381063000 | -2.003984000 | 2.161321000 |
| H | -2.076634000 | -0.930003000 | 3.039035000 |
| H | -0.048982000 | -2.092455000 | 1.689288000 |
| H | -1.087294000 | -3.879606000 | -0.007388000 |
| H | -3.791957000 | -3.819641000 | 0.265326000 |
| C | -1.865589000 | -2.107035000 | -2.081199000 |
| C | -1.379643000 | -0.783612000 | -2.152893000 |
| C | -2.482423000 | 0.102421000 | -2.071600000 |
| C | -3.663670000 | -0.680691000 | -2.002052000 |
| C | -3.289062000 | -2.042421000 | -1.986493000 |
| H | -1.254285000 | -3.003416000 | -2.122881000 |
| H | -0.333313000 | -0.497096000 | -2.161922000 |
| H | -2.424621000 | 1.186360000 | -2.022187000 |
| H | -4.675164000 | -0.295771000 | -1.908895000 |
| H | -3.968872000 | -2.890119000 | -1.946915000 |
| Cl | -4.075349000 | 0.388980000 | 0.739152000 |
| C | -0.429344000 | 3.295113000 | -2.169932000 |
| H | 0.310278000 | 4.092164000 | -2.364681000 |
| H | 0.045435000 | 2.356581000 | -2.499496000 |
| H | -1.294134000 | 3.480367000 | -2.821217000 |
| C | -3.297417000 | 3.597526000 | -0.933495000 |
| H | -3.161971000 | 3.662645000 | -2.022077000 |
| H | -4.007694000 | 2.781892000 | -0.716106000 |
| H | -3.781743000 | 4.533211000 | -0.601376000 |
| H | 0.556106000 | 4.023540000 | 0.794576000 |
| H | -1.753125000 | 4.307298000 | 1.729028000 |

Adduct-exo-acy: E= -2793.653156

| | | | |
|----|--------------|--------------|--------------|
| C | -2.371366000 | 4.299906000 | 0.191519000 |
| C | -3.095741000 | 3.163406000 | 0.185105000 |
| C | -2.352390000 | 1.875145000 | 0.474889000 |
| C | -0.905269000 | 4.166439000 | 0.548468000 |
| H | -3.012398000 | 1.015837000 | 0.325825000 |
| H | -0.361948000 | 5.099994000 | 0.332851000 |
| C | -1.077682000 | 1.747773000 | -0.400598000 |
| C | -0.174933000 | 2.986696000 | -0.133184000 |
| H | 0.275291000 | 3.319604000 | -1.079684000 |
| C | -0.346310000 | 0.407147000 | -0.149565000 |
| W | -1.323534000 | -1.608157000 | 0.060916000 |
| C | -3.171459000 | -1.038753000 | -0.744983000 |
| C | -1.901378000 | -1.059097000 | 2.002002000 |
| C | -0.665940000 | -2.025601000 | -1.881003000 |
| C | -2.234722000 | -3.480430000 | 0.220930000 |
| C | 0.326542000 | -2.626744000 | 0.795128000 |
| O | -4.208792000 | -0.790230000 | -1.192949000 |
| O | -2.736446000 | -4.518884000 | 0.308458000 |
| O | 1.205741000 | -3.287814000 | 1.176505000 |
| O | -0.273876000 | -2.230284000 | -2.949759000 |
| O | -2.193911000 | -0.731634000 | 3.070016000 |
| O | 0.921306000 | 0.523831000 | -0.166793000 |
| H | 0.679642000 | 2.706433000 | 0.490304000 |
| C | -1.457499000 | 1.691847000 | -1.902688000 |
| H | -2.120491000 | 0.844000000 | -2.122763000 |
| H | -1.965514000 | 2.624537000 | -2.188446000 |
| H | -0.552546000 | 1.592285000 | -2.522970000 |
| Ti | 2.826804000 | 0.458999000 | -0.007673000 |

| | | | |
|----|--------------|--------------|--------------|
| C1 | 3.276230000 | 2.720948000 | -0.468203000 |
| C | 4.587294000 | -0.110786000 | -1.499421000 |
| C | 3.560337000 | 0.426586000 | -2.326457000 |
| C | 2.441684000 | -0.420224000 | -2.241315000 |
| C | 2.765758000 | -1.498813000 | -1.370443000 |
| C | 4.105076000 | -1.326093000 | -0.948527000 |
| H | 5.568666000 | 0.331134000 | -1.335553000 |
| H | 3.610761000 | 1.365804000 | -2.869099000 |
| H | 1.477747000 | -0.262490000 | -2.717196000 |
| H | 2.103941000 | -2.312774000 | -1.090396000 |
| H | 4.658726000 | -2.001479000 | -0.301239000 |
| C | 4.310627000 | -0.098757000 | 1.767074000 |
| C | 3.175884000 | -0.961844000 | 1.858435000 |
| C | 2.055028000 | -0.167057000 | 2.183454000 |
| C | 2.479035000 | 1.183014000 | 2.260883000 |
| C | 3.878704000 | 1.218128000 | 2.033550000 |
| H | 5.332855000 | -0.401170000 | 1.548602000 |
| H | 3.160006000 | -2.038316000 | 1.714337000 |
| H | 1.028066000 | -0.518786000 | 2.258356000 |
| H | 1.841870000 | 2.046965000 | 2.436585000 |
| H | 4.494396000 | 2.112593000 | 2.002004000 |
| C | -4.564921000 | 3.028233000 | -0.104411000 |
| H | -4.730718000 | 2.341046000 | -0.953136000 |
| H | -5.090892000 | 2.578557000 | 0.757038000 |
| H | -5.056004000 | 3.982936000 | -0.336148000 |
| C | -2.884531000 | 5.689023000 | -0.065827000 |
| H | -2.691543000 | 6.341931000 | 0.804664000 |
| H | -2.352942000 | 6.148429000 | -0.918540000 |
| H | -3.961197000 | 5.725179000 | -0.279492000 |
| H | -0.837360000 | 4.033993000 | 1.645812000 |
| H | -2.045590000 | 1.838553000 | 1.536822000 |