

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

1: E= -3452.560915

Cr	-2.082751000	-0.438276000	-0.073553000
C	-3.557017000	-1.530743000	-0.520982000
O	-4.454410000	-2.197445000	-0.794939000
C	-2.256447000	0.436102000	-1.752284000
O	-2.387759000	0.908366000	-2.794662000
C	-3.317710000	0.757445000	0.747247000
O	-4.119171000	1.419359000	1.241578000
C	-1.938051000	-1.355023000	1.595039000
O	-1.886758000	-1.920299000	2.593174000
C	-0.960579000	-1.714052000	-0.925687000
O	-0.337516000	-2.513364000	-1.471425000
C	-0.421213000	0.720659000	0.488644000
O	-0.278439000	2.033157000	0.413744000
C	-1.218005000	2.958810000	-0.155531000
H	-2.172318000	2.880274000	0.381674000
H	-1.387282000	2.695704000	-1.208538000
C	-0.627714000	4.348892000	-0.023234000
H	-0.456685000	4.607072000	1.033046000
H	-1.322946000	5.088048000	-0.450191000
H	0.329968000	4.426266000	-0.560413000
Fe	2.566462000	-0.182000000	0.126494000
C	0.799500000	0.213419000	1.133835000
C	1.881257000	1.043425000	1.633525000
H	1.892008000	2.129618000	1.619386000
C	2.893140000	0.197375000	2.153226000
H	3.834568000	0.523708000	2.593262000
C	2.479945000	-1.158746000	1.969956000
H	3.051661000	-2.044734000	2.242060000
C	1.207039000	-1.158534000	1.343457000
H	0.649270000	-2.049133000	1.073246000
C	2.272962000	-0.052233000	-1.929203000
H	1.308159000	0.089427000	-2.413473000
C	3.150737000	0.985036000	-1.486417000
H	2.979168000	2.055994000	-1.583028000
C	4.289127000	0.367075000	-0.883610000
H	5.135292000	0.884329000	-0.433205000
C	4.111147000	-1.048949000	-0.951697000
H	4.798590000	-1.799087000	-0.563066000
C	2.863482000	-1.308252000	-1.598016000
H	2.421366000	-2.285283000	-1.783720000

3: E= -2355.048309

O	-1.068277000	1.700050000	-0.074981000
O	0.571639000	-2.266826000	-2.224120000
O	4.092218000	-1.497090000	0.036995000
O	2.312865000	1.619272000	-2.142402000
C	-0.664495000	0.438926000	-0.034180000
C	-1.875890000	-0.375215000	-0.012444000
C	-2.043329000	-1.757254000	-0.002739000
H	-1.214936000	-2.460947000	-0.006697000
C	-3.395953000	-2.168819000	0.007494000
H	-3.714807000	-3.211736000	0.015590000
C	-4.268583000	-1.100602000	0.006474000

H	-5.358210000	-1.138266000	0.015634000
C	-0.231783000	2.866367000	-0.154927000
H	0.197456000	2.912403000	-1.166424000
H	0.588751000	2.779791000	0.567972000
C	-1.101736000	4.073968000	0.130861000
H	-0.497042000	4.990640000	0.054035000
H	-1.526206000	4.023563000	1.145056000
H	-1.930170000	4.144335000	-0.590241000
C	0.825585000	-1.524661000	-1.385074000
C	3.035255000	-1.043173000	0.024393000
C	1.892013000	0.920203000	-1.331268000
C	0.792289000	-1.547131000	1.354916000
O	0.531746000	-2.301646000	2.181053000
C	1.821867000	0.890223000	1.390024000
O	2.187841000	1.571955000	2.241626000
Cr	1.294904000	-0.302337000	0.001529000
S	-3.459889000	0.410851000	-0.011135000

4: E= -2413.715244

16	0.107432000	3.364809000	0.389230000
6	-0.711289000	1.922906000	-0.235478000
6	-2.005201000	2.254611000	-0.597268000
6	-2.323554000	3.626461000	-0.405079000
6	-1.283294000	4.346357000	0.130252000
6	0.001757000	0.636931000	-0.318460000
24	-0.982493000	-1.218881000	0.066007000
6	0.238983000	-1.551135000	1.487833000
8	0.969305000	-1.762816000	2.351831000
7	1.292084000	0.819753000	-0.579845000
6	2.388520000	-0.143811000	-0.648938000
6	3.689176000	0.468595000	-0.127233000
6	-2.202572000	-0.910117000	-1.359384000
8	-2.952270000	-0.762203000	-2.220275000
6	-1.870110000	-2.830582000	0.461149000
8	-2.410560000	-3.818183000	0.705474000
6	0.102812000	-2.167958000	-1.172140000
8	0.713716000	-2.788986000	-1.925212000
6	-2.145488000	-0.330843000	1.294252000
8	-2.869518000	0.155661000	2.041208000
1	-2.707236000	1.538155000	-1.017924000
1	-3.296540000	4.060436000	-0.639576000
1	-1.272704000	5.395772000	0.423169000
1	2.515947000	-0.477128000	-1.693975000
1	2.121332000	-1.026575000	-0.059591000
6	4.872219000	-0.501260000	-0.203844000
1	3.538622000	0.794124000	0.917376000
1	3.927618000	1.381069000	-0.706527000
6	6.179031000	0.099970000	0.314287000
1	4.630259000	-1.412210000	0.371955000
1	5.004415000	-0.831667000	-1.249835000
1	7.006875000	-0.622752000	0.244874000
1	6.467983000	0.993611000	-0.263873000
1	6.089798000	0.403521000	1.370511000
1	1.598640000	1.773038000	-0.793417000

1⁺: E= -4504.394840

Cr	2.165204000	-0.417793000	0.112603000
C	3.687577000	-1.506740000	0.590577000
O	4.579894000	-2.160037000	0.875208000
C	2.603694000	0.687002000	1.618896000
O	2.916311000	1.285450000	2.544383000
C	3.314019000	0.659713000	-1.003953000

O	4.012225000	1.274036000	-1.669204000
C	1.891464000	-1.608551000	-1.361776000
O	1.758497000	-2.342002000	-2.231822000
C	1.076441000	-1.477840000	1.248521000
O	0.400425000	-2.095221000	1.946425000
C	0.515770000	0.643046000	-0.394118000
O	0.256207000	1.937668000	-0.332885000
C	1.183662000	2.960665000	0.102845000
H	2.167951000	2.758073000	-0.337721000
H	1.267834000	2.894860000	1.197014000
C	0.639822000	4.303817000	-0.334936000
H	0.563359000	4.365741000	-1.431060000
H	1.320933000	5.099335000	0.003209000
H	-0.351656000	4.497864000	0.101830000
Fe	-2.683880000	-0.205027000	-0.153769000
C	-0.703673000	0.039257000	-1.029369000
C	-1.681114000	0.787535000	-1.774959000
H	-1.653499000	1.864672000	-1.924656000
C	-2.671613000	-0.103357000	-2.265773000
H	-3.532058000	0.169834000	-2.876296000
C	-2.339293000	-1.419627000	-1.814960000
H	-2.894993000	-2.333323000	-2.023673000
C	-1.139690000	-1.330575000	-1.048954000
H	-0.653958000	-2.170352000	-0.560296000
C	-2.910842000	0.863754000	1.644382000
H	-2.239014000	1.660132000	1.962033000
C	-4.104272000	1.031059000	0.880033000
H	-4.494898000	1.974069000	0.498006000
C	-4.683654000	-0.252878000	0.678129000
H	-5.587692000	-0.463058000	0.106542000
C	-3.849394000	-1.220156000	1.308455000
H	-4.015137000	-2.297161000	1.319216000
C	-2.750775000	-0.533497000	1.912582000
H	-1.938441000	-0.997866000	2.470794000

3⁺: E= -2354.796693

O	1.050752000	1.717252000	-0.170723000
O	-0.493567000	-2.098964000	2.408106000
O	-4.182416000	-1.514386000	0.117929000
O	-2.057059000	1.614391000	2.302349000
C	0.703010000	0.458708000	-0.077920000
C	1.885274000	-0.357895000	-0.023696000
C	2.036049000	-1.749954000	0.055464000
H	1.205928000	-2.452849000	0.091755000
C	3.376189000	-2.171891000	0.076340000
H	3.691670000	-3.213864000	0.134201000
C	4.258541000	-1.104902000	0.014220000
H	5.348577000	-1.154335000	0.017287000
C	0.204249000	2.881528000	-0.336783000
H	-0.778090000	2.687651000	0.112590000
H	0.076770000	3.022029000	-1.421492000
C	0.893754000	4.067098000	0.301964000
H	0.287573000	4.970643000	0.136639000
H	1.885276000	4.232760000	-0.144062000
H	1.011526000	3.923415000	1.386320000
C	-0.763914000	-1.455840000	1.511510000
C	-3.137095000	-1.079507000	0.077595000
C	-1.767246000	0.933551000	1.438446000
C	-0.814333000	-1.574060000	-1.419315000
O	-0.560899000	-2.291534000	-2.263233000
C	-1.853888000	0.820581000	-1.497163000
O	-2.201145000	1.436771000	-2.387148000
Cr	-1.289271000	-0.311332000	0.003668000
S	3.477773000	0.408987000	-0.073968000

4⁺: E= -2413.471213

S	-0.048605000	3.373812000	0.285535000
C	-0.804763000	1.878276000	-0.280366000
C	-2.144782000	2.118442000	-0.564193000
C	-2.539991000	3.463272000	-0.359533000
C	-1.512720000	4.251634000	0.107101000
C	-0.011415000	0.656039000	-0.402642000
Cr	-0.920275000	-1.225112000	0.078633000
C	0.401084000	-1.382814000	1.492763000
O	1.166287000	-1.459020000	2.333323000
N	1.255490000	0.872290000	-0.702786000
C	2.402330000	-0.037913000	-0.793702000
C	3.638740000	0.555737000	-0.113723000
C	-2.223406000	-1.040550000	-1.352163000
O	-2.977575000	-0.975484000	-2.203193000
C	-1.689363000	-2.991065000	0.598288000
O	-2.121548000	-3.995527000	0.897669000
C	0.112558000	-2.150492000	-1.319109000
O	0.655073000	-2.699297000	-2.153136000
C	-2.053615000	-0.361865000	1.467342000
O	-2.700284000	0.087693000	2.283094000
H	-2.829372000	1.365400000	-0.949390000
H	-3.548777000	3.835984000	-0.540147000
H	-1.549771000	5.304951000	0.386193000
H	2.610225000	-0.229115000	-1.861125000
H	2.137621000	-0.995811000	-0.332847000
C	4.863576000	-0.360502000	-0.217417000
H	3.406373000	0.755637000	0.947035000
H	3.872553000	1.533732000	-0.573532000
C	6.108418000	0.232674000	0.443316000
H	4.627444000	-1.335633000	0.245209000
H	5.071637000	-0.570379000	-1.281754000
H	6.966320000	-0.450257000	0.353051000
H	6.393985000	1.189049000	-0.024122000
H	5.943585000	0.420685000	1.516743000
H	1.518512000	1.839268000	-0.919390000