

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

3a: E= -2032.116330

O	-1.276566000	1.698370000	-0.080822000
O	0.356557000	-2.263363000	-2.211494000
O	3.895240000	-1.497900000	0.032782000
O	2.117675000	1.626276000	-2.144860000
C	-0.855022000	0.450502000	-0.034303000
C	-2.045129000	-0.390060000	-0.009961000
C	-2.251237000	-1.762510000	0.006313000
H	-1.486463000	-2.531719000	0.011743000
C	-3.652350000	-1.978669000	0.010322000
H	-4.175192000	-2.932195000	0.021481000
C	-4.218416000	-0.727123000	-0.002943000

H	-5.252085000	-0.386496000	-0.003748000
C	-0.443454000	2.865861000	-0.161224000
H	-0.023369000	2.917545000	-1.176616000
H	0.385068000	2.777360000	0.552671000
C	-1.312920000	4.070517000	0.137803000
H	-0.712190000	4.989504000	0.056794000
H	-1.726124000	4.015023000	1.156346000
H	-2.150149000	4.138578000	-0.573133000
C	0.621837000	-1.517283000	-1.378941000
C	2.839727000	-1.040327000	0.021758000
C	1.698465000	0.927491000	-1.332781000
C	0.593010000	-1.539185000	1.350029000
O	0.324646000	-2.297634000	2.170654000
C	1.630771000	0.897261000	1.390551000
O	1.996629000	1.578082000	2.242803000
Cr	1.101408000	-0.294811000	0.001423000
O	-3.279806000	0.224795000	-0.016492000

3b: 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

4a: E= -3834.447434

Cr	-4.005236000	0.267741000	0.078220000
C	-5.834175000	0.761242000	0.186559000
O	-6.941900000	1.060698000	0.251452000
C	-3.595794000	1.664018000	1.310011000
O	-3.385148000	2.513744000	2.053555000
C	-4.258760000	-0.907857000	1.562615000
O	-4.440922000	-1.592110000	2.466940000
C	-4.485319000	-1.099950000	-1.160751000
O	-4.812508000	-1.898765000	-1.920004000
C	-3.790080000	1.459303000	-1.392382000
O	-3.687259000	2.184985000	-2.277223000
C	-1.988379000	-0.219974000	-0.029453000
O	-1.391089000	-1.390346000	-0.008751000
C	-2.008799000	-2.686824000	0.062669000
H	-3.085019000	-2.584933000	0.236684000

H	-1.554495000	-3.166962000	0.943041000
C	-1.703992000	-3.462070000	-1.205701000
H	-2.209354000	-3.016261000	-2.075167000
H	-2.062021000	-4.497620000	-1.095768000
H	-0.621991000	-3.482999000	-1.401884000
Cr	3.514367000	-0.701766000	0.109367000
C	4.239152000	-2.444211000	0.328336000
O	4.678244000	-3.498260000	0.458928000
C	2.212696000	-1.128804000	1.449472000
O	1.464573000	-1.432232000	2.263876000
C	4.684208000	-0.086303000	1.482854000
O	5.394383000	0.230396000	2.330120000
C	4.838321000	-0.383209000	-1.222571000
O	5.649969000	-0.259326000	-2.028082000
C	2.341709000	-1.402124000	-1.230513000
O	1.660595000	-1.866288000	-2.028924000
C	2.655549000	1.155177000	-0.134889000
O	3.196994000	2.354540000	-0.276536000
C	4.609722000	2.621227000	-0.316672000
H	5.094389000	2.130240000	0.537317000
H	5.017530000	2.190692000	-1.242656000
O	0.372533000	0.330760000	-0.082009000
C	4.797352000	4.124067000	-0.276420000
H	4.301375000	4.608522000	-1.131284000
H	5.871029000	4.362762000	-0.321196000
H	4.388584000	4.549545000	0.652754000
C	-0.913918000	0.777487000	-0.121205000
C	-0.892769000	2.163450000	-0.249726000
H	-1.752033000	2.822503000	-0.311947000
C	0.460325000	2.550912000	-0.288892000
H	0.861637000	3.555975000	-0.382728000
C	1.210202000	1.384905000	-0.176007000

5a: E= -2090.791495

O	-0.546491000	3.298166000	-0.275500000
C	-1.048630000	2.024739000	-0.058912000
C	-2.368655000	2.154734000	0.324069000
C	-2.676233000	3.545231000	0.340392000
C	-1.527648000	4.187869000	-0.033598000
C	-0.143218000	0.891624000	-0.260619000
Cr	-0.785370000	-1.134299000	0.017349000
C	0.796528000	-1.557149000	0.981233000
O	1.738714000	-1.842679000	1.579672000
N	1.060182000	1.317157000	-0.628897000
C	2.280624000	0.572404000	-0.908950000
C	3.404910000	0.913453000	0.074180000
C	-2.387495000	-0.758438000	-0.939876000
O	-3.364912000	-0.574372000	-1.517536000
C	-1.380671000	-2.899829000	0.267382000
O	-1.744649000	-3.982320000	0.421438000
C	0.007225000	-1.649402000	-1.634397000
O	0.463050000	-1.988016000	-2.635364000
C	-1.599900000	-0.643454000	1.666049000
O	-2.100645000	-0.383033000	2.668323000
H	-3.050311000	1.347650000	0.569044000
H	-3.626850000	4.007437000	0.596306000
H	-1.272571000	5.237019000	-0.166275000
H	2.598316000	0.811436000	-1.939857000
H	2.056365000	-0.497097000	-0.884196000
C	4.701724000	0.156454000	-0.227980000
H	3.066617000	0.678924000	1.097698000
H	3.597306000	2.002599000	0.049456000
C	5.838846000	0.502593000	0.733839000
H	4.500844000	-0.928652000	-0.186069000
H	5.016533000	0.368021000	-1.266122000

H	6.752978000	-0.062447000	0.493236000
H	6.089708000	1.575803000	0.690956000
H	5.566572000	0.267203000	1.775902000
H	1.187119000	2.328241000	-0.709297000

5b: E= -2413.715244

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

3a⁺: E= -2032.166350

O	1.278414000	1.702785000	-0.249412000
O	-0.556795000	-2.343540000	2.163017000
O	-4.012928000	-1.340671000	-0.202925000
O	-2.014112000	1.580580000	2.229821000
C	0.896768000	0.392908000	0.004324000
C	2.045181000	-0.433141000	0.021278000
C	2.245556000	-1.825930000	0.125024000
H	1.469046000	-2.579566000	0.201353000
C	3.645747000	-2.054267000	0.112401000
H	4.155475000	-3.015313000	0.177444000
C	4.242715000	-0.823281000	-0.001437000
H	5.281251000	-0.502766000	-0.054631000
C	0.638182000	2.775521000	0.390404000
H	0.674244000	2.650447000	1.490716000
H	-0.429712000	2.832627000	0.111739000
C	1.350458000	4.055635000	-0.019478000
H	0.888894000	4.931756000	0.465584000
H	1.295066000	4.191223000	-1.111558000
H	2.414644000	4.013262000	0.262128000
C	-0.761119000	-1.571504000	1.327993000
C	-2.922622000	-0.939759000	-0.126169000

C	-1.672431000	0.887188000	1.367555000
C	-0.616885000	-1.481801000	-1.391130000
O	-0.303332000	-2.195444000	-2.242448000
C	-1.536549000	1.006788000	-1.332172000
O	-1.772968000	1.795733000	-2.143847000
Cr	-1.186665000	-0.304765000	-0.015409000
O	3.306849000	0.158374000	-0.059767000

3a⁺: E= -2031.864296

O	-1.259769000	1.706666000	-0.199189000
O	0.344641000	-2.312921000	-2.226370000
O	3.986287000	-1.520451000	0.128513000
O	2.008391000	1.417850000	-2.406957000
C	-0.891344000	0.462955000	-0.086739000
C	-2.056029000	-0.376612000	-0.027112000
C	-2.261130000	-1.754354000	0.075649000
H	-1.502421000	-2.528926000	0.142369000
C	-3.653739000	-1.971144000	0.072986000
H	-4.178627000	-2.921494000	0.137780000
C	-4.221649000	-0.717481000	-0.030127000
H	-5.257457000	-0.383092000	-0.068494000
C	-0.421603000	2.876546000	-0.362187000
H	-0.313858000	3.029806000	-1.447427000
H	0.569887000	2.681843000	0.067248000
C	-1.106937000	4.050949000	0.301149000
H	-0.511355000	4.960896000	0.132291000
H	-1.202559000	3.895894000	1.386121000
H	-2.108638000	4.210353000	-0.123569000
C	0.610461000	-1.582651000	-1.397214000
C	2.943253000	-1.080561000	0.084792000
C	1.663876000	0.810638000	-1.510048000
C	0.562018000	-1.426423000	1.521809000
O	0.278446000	-2.060622000	2.420985000
C	1.587048000	0.956789000	1.424839000
O	1.882304000	1.646176000	2.279742000
Cr	1.098976000	-0.304144000	0.005150000
O	-3.289770000	0.231085000	-0.091312000

3a²⁺: E= -2031.425092

O	-0.876356000	1.879561000	-0.290655000
O	-0.353323000	-1.294032000	-2.539330000
O	1.507520000	-3.247299000	0.294458000
O	3.242647000	0.163178000	-2.223210000
C	-0.951757000	0.597475000	-0.122204000
C	-2.230921000	0.036991000	-0.032560000
C	-2.711997000	-1.278964000	0.144526000
H	-2.117768000	-2.185395000	0.253511000
C	-4.105209000	-1.201284000	0.152868000
H	-4.820268000	-2.014726000	0.267087000
C	-4.408713000	0.149971000	-0.017766000
H	-5.360627000	0.681386000	-0.074200000
C	0.434245000	2.497728000	-0.398411000
H	0.682332000	2.553880000	-1.468947000
H	1.179862000	1.834807000	0.127641000
C	0.423101000	3.853395000	0.264244000
H	1.401262000	4.340398000	0.132500000
H	0.196551000	3.783936000	1.337695000
H	-0.337622000	4.484053000	-0.222844000
C	0.104731000	-0.879314000	-1.588794000
C	1.313225000	-2.138999000	0.183791000
C	2.442511000	0.027066000	-1.444226000
C	0.126081000	-0.488849000	1.733068000
O	-0.322579000	-0.653857000	2.758717000

C	2.599956000	0.132183000	1.282909000
O	3.471973000	0.303491000	1.970633000
Cr	1.004452000	-0.233630000	-0.001952000
O	-3.312644000	0.884506000	-0.126898000

4a²⁺: E= -3833.857884

Cr	-4.020741000	0.266310000	0.052122000
C	-5.976113000	0.811268000	0.086215000
O	-7.063737000	1.114347000	0.104880000
C	-3.628948000	1.696009000	1.345546000
O	-3.418090000	2.509166000	2.108928000
C	-4.340137000	-0.810255000	1.675984000
O	-4.532498000	-1.395096000	2.628929000
C	-4.486830000	-1.139664000	-1.249642000
O	-4.766004000	-1.918237000	-2.026925000
C	-3.762529000	1.357456000	-1.562256000
O	-3.627318000	1.971600000	-2.507417000
C	-1.975495000	-0.248104000	0.021370000
O	-1.426989000	-1.419093000	0.124636000
C	-2.092661000	-2.709091000	0.269193000
H	-3.176980000	-2.555705000	0.316278000
H	-1.747455000	-3.089775000	1.241973000
C	-1.685300000	-3.617219000	-0.870872000
H	-2.049581000	-3.244287000	-1.839674000
H	-2.119437000	-4.614918000	-0.703303000
H	-0.592363000	-3.726343000	-0.921545000
Cr	3.540938000	-0.685706000	0.082435000
C	4.374616000	-2.520810000	0.325600000
O	4.838542000	-3.542205000	0.459219000
C	2.269394000	-1.101294000	1.530035000
O	1.556961000	-1.358939000	2.375559000
C	4.679508000	-0.018733000	1.544780000
O	5.312449000	0.335317000	2.417850000
C	4.834651000	-0.359582000	-1.377597000
O	5.563696000	-0.214017000	-2.233949000
C	2.389894000	-1.404726000	-1.334608000
O	1.730390000	-1.833508000	-2.154399000
C	2.656764000	1.186133000	-0.179240000
O	3.196885000	2.352146000	-0.350418000
C	4.622630000	2.667240000	-0.448598000
H	5.188513000	1.922885000	0.125759000
H	4.875551000	2.570776000	-1.515563000
O	0.385545000	0.309800000	-0.062109000
C	4.839849000	4.073774000	0.058325000
H	4.252057000	4.800914000	-0.520630000
H	5.903899000	4.331266000	-0.056430000
H	4.579467000	4.163595000	1.123292000
C	-0.907445000	0.746822000	-0.110674000
C	-0.903262000	2.127426000	-0.288341000
H	-1.763546000	2.785421000	-0.369188000
C	0.444283000	2.532522000	-0.349916000
H	0.827540000	3.541280000	-0.483448000
C	1.203622000	1.379182000	-0.202825000

4a⁴⁺: E= -3832.739324

Cr	4.179047000	-0.075369000	0.055512000
C	5.268719000	-1.747925000	-0.059355000
O	5.910771000	-2.668984000	-0.121767000
C	3.470515000	-1.110823000	1.549048000
O	3.108883000	-1.714391000	2.434267000
C	5.299499000	0.694504000	1.651681000
O	5.924931000	1.093100000	2.493141000
C	5.652794000	0.878250000	-1.146302000
O	6.454074000	1.352219000	-1.770096000

C	3.621165000	-0.721831000	-1.720999000
O	3.343565000	-1.086998000	-2.753048000
C	2.078764000	0.225477000	0.018666000
O	1.740515000	1.454451000	0.125721000
C	2.786640000	2.492920000	0.266554000
H	3.740941000	2.046064000	-0.114323000
H	2.869743000	2.685249000	1.347081000
C	2.424728000	3.720503000	-0.527101000
H	2.342223000	3.515193000	-1.604115000
H	3.203802000	4.485251000	-0.374323000
H	1.478094000	4.141985000	-0.154004000
Cr	-3.962447000	0.451242000	0.032761000
C	-3.675009000	2.393596000	0.352342000
O	-3.544114000	3.496524000	0.534332000
C	-2.939511000	0.374472000	1.706861000
O	-2.365302000	0.353569000	2.680022000
C	-5.592098000	0.534801000	1.396475000
O	-6.449379000	0.614922000	2.113685000
C	-5.426236000	0.768590000	-1.435790000
O	-6.216624000	0.962089000	-2.207522000
C	-2.831865000	0.933653000	-1.472726000
O	-2.195489000	1.249533000	-2.353406000
C	-2.609498000	-1.124720000	-0.224342000
O	-3.190332000	-2.247047000	-0.413929000
C	-4.670021000	-2.360559000	-0.456729000
H	-5.075111000	-1.467142000	0.083905000
H	-4.933244000	-2.308602000	-1.524519000
O	-0.326354000	-0.215884000	-0.066186000
C	-5.113122000	-3.640753000	0.199812000
H	-4.675990000	-4.502292000	-0.331078000
H	-6.208699000	-3.723824000	0.108827000
H	-4.843687000	-3.684583000	1.264782000
C	0.957179000	-0.693968000	-0.110329000
C	0.934503000	-2.073869000	-0.298324000
H	1.784703000	-2.750442000	-0.376737000
C	-0.419923000	-2.452872000	-0.376341000
H	-0.815519000	-3.457951000	-0.523467000
C	-1.155023000	-1.280225000	-0.226822000