

=====

1

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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	-4.398417000	-3.108011000	2.893129000
C	-3.718069000	-4.263581000	3.218805000
O	-2.479999000	-3.879224000	3.599770000
N	-2.369784000	-2.479036000	3.514480000
C	-3.522376000	-2.099890000	3.096597000
C	-3.967675000	-0.709110000	2.847951000
O	-4.152319000	-5.366427000	3.168093000
H	-4.278244000	-0.627186000	1.796861000
H	-4.883058000	-0.559741000	3.443262000
C	-2.922163000	0.304261000	3.184233000
H	-2.485965000	0.227744000	4.180569000
C	-2.538931000	1.267341000	2.341335000
H	-3.015612000	1.311473000	1.357774000
C	-1.542696000	2.308801000	2.594989000
C	-0.688608000	2.283217000	3.705683000
C	-1.429468000	3.373790000	1.694084000
C	0.233892000	3.297612000	3.912413000
C	-0.506334000	4.391571000	1.900874000
C	0.327518000	4.357997000	3.013050000
H	-0.734592000	1.451340000	4.405663000
H	-2.082397000	3.400400000	0.822215000
H	0.891549000	3.258940000	4.777736000
H	-0.437231000	5.211732000	1.190049000
H	1.053706000	5.150610000	3.176621000

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2

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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	2.243046000	-0.808075000	-0.853271000
N	4.411098000	0.078410000	-0.528531000
C	3.035328000	0.042482000	-0.541696000
C	2.968483000	1.476666000	0.000717000

H	2.533110000	2.202941000	-0.693431000
H	2.479473000	1.567601000	0.973719000
H	5.102891000	-0.631696000	-0.728597000
C	4.512382000	1.434827000	0.014765000
H	4.938660000	1.463057000	1.029055000
C	5.224334000	2.435341000	-0.884015000
H	4.772059000	2.381332000	-1.884831000
C	5.136654000	3.830231000	-0.332096000
C	5.942321000	4.213702000	0.742959000
C	4.221183000	4.751802000	-0.842026000
C	5.835548000	5.484435000	1.295692000
C	4.111663000	6.025504000	-0.292934000
C	4.917674000	6.394455000	0.778699000
H	6.667580000	3.504818000	1.144006000
H	3.594037000	4.468255000	-1.687309000
H	6.473500000	5.767790000	2.129903000
H	3.396040000	6.732745000	-0.706195000
H	4.834701000	7.390244000	1.207736000
H	6.276531000	2.133946000	-0.992467000

PA

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	4.296801000	2.786186000	2.941922000
N	2.422384000	1.525949000	2.799023000
C	3.487136000	2.185376000	2.261545000
C	3.617233000	2.063714000	0.750600000
H	4.255804000	1.180735000	0.580843000
H	2.651711000	1.842318000	0.275255000
H	2.302404000	1.565068000	3.799788000
C	4.248540000	3.272988000	0.147925000
H	5.097387000	3.668472000	0.706247000
C	3.822309000	3.853177000	-0.977792000
H	2.954967000	3.420061000	-1.485449000
C	4.393668000	5.029863000	-1.635113000
C	5.497814000	5.727686000	-1.126156000
C	3.817045000	5.486887000	-2.825939000

C	6.001168000	6.838523000	-1.786375000
C	4.320532000	6.599359000	-3.489357000
C	5.416248000	7.280773000	-2.971705000
H	5.965723000	5.397627000	-0.200883000
H	2.957859000	4.954394000	-3.233178000
H	6.858027000	7.366349000	-1.373345000
H	3.854768000	6.934623000	-4.413470000
H	5.813880000	8.152223000	-3.486553000
H	1.717534000	1.078819000	2.237023000

CO₂

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
C	2.847419000	0.605324000	4.332178000
O	2.984323000	1.253333000	3.310379000
O	2.710730000	-0.042709000	5.353985000

HCl

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
Cl	0.449891000	0.000000000	-3.293878000
H	0.449891000	0.000000000	-4.577553000

L1

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
C	4.357291000	-0.055388000	-2.229952000
C	0.630696000	-1.975304000	-2.662058000
C	0.545311000	-3.300716000	-3.100461000
C	-0.709218000	-3.882547000	-3.209955000
C	-1.829528000	-3.131794000	-2.882672000
C	-1.652800000	-1.816020000	-2.447511000

N	-0.446218000	-1.254024000	-2.339200000
H	1.445669000	-3.868574000	-3.321402000
H	-0.811694000	-4.914497000	-3.538653000
H	-2.829818000	-3.553058000	-2.955372000
C	1.954455000	-1.310096000	-2.530876000
C	2.988779000	-1.611016000	-3.423012000
C	4.208109000	-0.968711000	-3.264214000
C	3.269668000	0.189662000	-1.388032000
N	2.094195000	-0.425442000	-1.539997000
H	2.828222000	-2.310825000	-4.239351000
H	5.031176000	-1.171475000	-3.946070000
H	5.297672000	0.468542000	-2.073360000
C	3.362899000	1.162619000	-0.253039000
H	3.194919000	0.649774000	0.700578000
H	4.337147000	1.660040000	-0.215855000
H	2.579688000	1.922848000	-0.343412000
C	-2.818628000	-0.951519000	-2.077426000
H	-2.855887000	-0.068086000	-2.724455000
H	-3.770195000	-1.486129000	-2.159337000
H	-2.705325000	-0.585224000	-1.051449000

(L1)₂Ni(0)

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
C	4.359347000	-0.155464000	-2.023290000
C	0.692229000	-2.030672000	-2.777216000
C	0.453905000	-3.167052000	-3.557968000
C	-0.836131000	-3.640143000	-3.688932000
C	-1.871224000	-2.963775000	-3.033211000
C	-1.586480000	-1.843445000	-2.271987000
N	-0.319362000	-1.374817000	-2.139363000
H	1.278898000	-3.670575000	-4.055318000
H	-1.044714000	-4.521368000	-4.290107000
H	-2.900384000	-3.306388000	-3.113391000
C	2.000866000	-1.440639000	-2.565122000
C	3.188745000	-1.931347000	-3.118075000
C	4.378695000	-1.286413000	-2.847545000

C	3.159310000	0.292702000	-1.499063000
N	1.986348000	-0.337895000	-1.762507000
H	3.171620000	-2.812140000	-3.754762000
H	5.313517000	-1.649695000	-3.266585000
H	5.276858000	0.378891000	-1.787452000
Ni	0.225518000	0.186764000	-1.100597000
C	3.077304000	1.491845000	-0.614755000
H	2.633641000	1.222232000	0.353245000
H	4.062640000	1.939023000	-0.447743000
H	2.408619000	2.244808000	-1.053416000
C	-2.648484000	-1.081288000	-1.552348000
H	-2.657246000	-0.034236000	-1.884313000
H	-3.639184000	-1.518839000	-1.712958000
H	-2.435968000	-1.054200000	-0.475033000
C	-1.222238000	3.944059000	-2.459874000
C	-0.811355000	1.691293000	1.045497000
C	-1.193601000	2.047788000	2.343352000
C	-0.976456000	1.163192000	3.380273000
C	-0.376792000	-0.069772000	3.098923000
C	-0.015361000	-0.377834000	1.798823000
N	-0.227079000	0.488622000	0.775422000
H	-1.657487000	3.012803000	2.530441000
H	-1.265597000	1.418718000	4.396419000
H	-0.189375000	-0.792557000	3.889774000
C	-0.988767000	2.534489000	-0.121910000
C	-1.562040000	3.810551000	-0.095772000
C	-1.680980000	4.523720000	-1.271467000
C	-0.662343000	2.678497000	-2.436092000
N	-0.542105000	1.973492000	-1.282129000
H	-1.909556000	4.234067000	0.843010000
H	-2.122950000	5.516753000	-1.274843000
H	-1.299710000	4.475005000	-3.405969000
C	-0.158033000	2.009932000	-3.671133000
H	-0.675817000	1.053547000	-3.825458000
H	-0.293919000	2.640194000	-4.556020000
H	0.906744000	1.762510000	-3.563984000
C	0.627607000	-1.675657000	1.439690000
H	1.601716000	-1.499788000	0.963506000
H	0.765899000	-2.314778000	2.317828000
H	0.020600000	-2.209731000	0.696186000

(L1)Ni(I)H

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
C	-2.766685000	-0.642401000	-1.555321000
C	0.380600000	0.216202000	1.094167000
C	1.198097000	1.343504000	1.077207000
C	2.161398000	1.484178000	2.065406000
C	2.281772000	0.501891000	3.039975000
C	1.439882000	-0.606990000	3.001220000
N	0.511902000	-0.739987000	2.036906000
H	1.084068000	2.102794000	0.309446000
H	2.811859000	2.355070000	2.077224000
H	3.023125000	0.583137000	3.830641000
C	-0.695300000	-0.029034000	0.114516000
C	-0.975560000	0.825540000	-0.948337000
C	-2.027189000	0.506371000	-1.795852000
C	-2.435735000	-1.461108000	-0.474667000
N	-1.405545000	-1.154154000	0.331324000
H	-0.385924000	1.721755000	-1.116602000
H	-2.268877000	1.152343000	-2.636284000
H	-3.600441000	-0.916891000	-2.196374000
H	-0.935446000	-3.914225000	1.841426000
Ni	-0.590471000	-2.391272000	1.754331000
C	-3.208065000	-2.696511000	-0.160575000
H	-3.738104000	-2.578650000	0.791966000
H	-3.936875000	-2.921754000	-0.945059000
H	-2.526165000	-3.542554000	-0.013949000
C	1.518385000	-1.700393000	4.013811000
H	0.568418000	-1.790801000	4.553773000
H	1.685003000	-2.666564000	3.520695000
H	2.320458000	-1.522959000	4.736470000

(L1)Ni(I)Cl

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
C	-2.388392000	-0.298623000	0.046111000
C	-0.479454000	1.042145000	0.030901000
C	-1.241779000	2.205823000	0.011649000
C	-2.624953000	2.093891000	0.009885000
C	-3.203684000	0.832558000	0.027225000
H	-0.768419000	3.182874000	-0.001751000
H	-3.246843000	2.985368000	-0.004951000
H	-4.283653000	0.710999000	0.026356000
C	0.995414000	1.030481000	0.034905000
C	1.776146000	2.181892000	0.019662000
C	3.157386000	2.048121000	0.025473000
H	1.318419000	3.166303000	0.003499000
C	2.882830000	-0.340370000	0.060662000
C	3.716056000	0.777797000	0.046135000
H	3.793381000	2.929641000	0.013898000
H	4.793950000	0.639130000	0.051188000
N	-1.048891000	-0.180104000	0.047699000
N	1.545446000	-0.200627000	0.054895000
C	-2.947189000	-1.680536000	0.065280000
H	-2.591172000	-2.252120000	-0.800211000
H	-2.594314000	-2.226622000	0.948333000
H	-4.040986000	-1.669407000	0.063107000
C	3.419521000	-1.730999000	0.083045000
H	3.054255000	-2.270863000	0.964889000
H	3.058210000	-2.297439000	-0.783635000
H	4.513354000	-1.737279000	0.085653000
Ni	0.236111000	-1.710756000	0.074051000
Cl	0.218799000	-3.852035000	0.106318000

(L1)Ni(I)Cl₂

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
C	4.295253000	-0.194482000	-1.833086000
C	0.587544000	-1.776679000	-2.921027000
C	0.360589000	-2.868494000	-3.744704000
C	-0.883424000	-3.486201000	-3.690666000

C	-1.822475000	-3.030592000	-2.783365000
C	-1.554017000	-1.905611000	-1.995735000
N	-0.379668000	-1.266574000	-2.120958000
H	1.140800000	-3.243825000	-4.399347000
H	-1.098609000	-4.342193000	-4.324932000
H	-2.779675000	-3.532085000	-2.666760000
C	1.911066000	-1.162592000	-2.715546000
C	3.073527000	-1.606067000	-3.326979000
C	4.286244000	-1.084824000	-2.891316000
C	3.091347000	0.244359000	-1.270955000
N	1.923139000	-0.201641000	-1.760466000
H	3.039313000	-2.355533000	-4.111351000
H	5.217650000	-1.405837000	-3.350369000
H	5.229291000	0.180036000	-1.422437000
Ni	0.131423000	0.590233000	-1.765960000
C	3.112355000	1.159087000	-0.094620000
H	2.173487000	1.112102000	0.460666000
H	3.946271000	0.885837000	0.562153000
H	3.239355000	2.198221000	-0.412765000
C	-2.549449000	-1.457620000	-0.981077000
H	-3.327465000	-0.843774000	-1.444858000
H	-3.018865000	-2.335598000	-0.522398000
H	-2.080924000	-0.843164000	-0.209867000
Cl	0.898821000	2.609059000	-1.755491000
Cl	-1.851592000	1.334841000	-2.189388000

Int0-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -23.20 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
C	0.112509000	-2.146191000	-0.058947000
C	1.492090000	-2.030857000	0.068186000
C	2.084038000	-0.830674000	0.481940000
C	1.243057000	0.251798000	0.781888000
C	-0.133596000	0.136873000	0.658234000
C	-0.707163000	-1.061274000	0.233403000
H	-0.321515000	-3.088394000	-0.387790000

H	2.133255000	-2.880419000	-0.169720000
H	1.675429000	1.187656000	1.133066000
H	-0.767446000	0.986998000	0.901682000
H	-1.787549000	-1.148829000	0.143517000
C	3.539677000	-0.748000000	0.562643000
H	4.063800000	-1.709065000	0.550189000
C	4.281003000	0.372749000	0.592631000
H	3.811106000	1.357168000	0.600268000
C	5.775436000	0.366361000	0.752216000
H	6.200716000	-0.622610000	0.543486000
H	6.216737000	1.079064000	0.039293000
C	6.175227000	0.730676000	2.129165000
O	5.737089000	1.895707000	2.657852000
O	6.987005000	0.822025000	4.091631000
N	6.915438000	0.041074000	2.919235000
C	1.633297000	2.532379000	-1.882885000
C	1.271583000	0.388660000	-2.715378000
C	-0.078768000	0.649949000	-2.926517000
C	-0.572289000	1.907030000	-2.607969000
C	0.290246000	2.856765000	-2.082919000
H	-0.738103000	-0.111287000	-3.332099000
H	-1.621723000	2.141535000	-2.768065000
H	-0.061131000	3.851938000	-1.822036000
C	1.894882000	-0.913282000	-3.019114000
C	1.189534000	-2.002591000	-3.527840000
C	1.866625000	-3.189324000	-3.758403000
H	0.124910000	-1.930556000	-3.728389000
C	3.877965000	-2.135469000	-2.977654000
C	3.226231000	-3.259378000	-3.477092000
H	1.339753000	-4.054536000	-4.152701000
H	3.788249000	-4.174636000	-3.644280000
N	2.108011000	1.318223000	-2.207831000
N	3.216271000	-0.983828000	-2.763165000
C	2.584760000	3.511911000	-1.282046000
H	2.711811000	3.309837000	-0.209309000
H	3.576852000	3.407978000	-1.737128000
H	2.218017000	4.537964000	-1.384293000
C	5.332604000	-2.143199000	-2.644572000
H	5.840235000	-1.296424000	-3.123774000
H	5.473116000	-2.020037000	-1.562511000

H	5.814464000	-3.075935000	-2.952082000
Ni	4.071668000	0.717086000	-2.102221000
H	5.255816000	1.748749000	-1.990453000
C	6.262649000	1.949289000	3.930581000
O	6.097788000	2.824327000	4.716387000

Int-A'

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
C	0.128851000	-1.807656000	0.252506000
C	1.505211000	-1.651871000	0.147978000
C	2.127087000	-0.428030000	0.445653000
C	1.310117000	0.628802000	0.879643000
C	-0.065434000	0.474611000	0.976240000
C	-0.668355000	-0.741822000	0.659071000
H	-0.322726000	-2.768338000	0.011382000
H	2.123445000	-2.487180000	-0.185917000
H	1.763934000	1.581125000	1.151631000
H	-0.674870000	1.311331000	1.312618000
H	-1.746209000	-0.859160000	0.742182000
C	3.567600000	-0.297680000	0.243102000
H	4.114366000	-1.248061000	0.242889000
C	4.339152000	0.876450000	0.274648000
H	3.877117000	1.821498000	0.566692000
C	5.826269000	0.795603000	0.549868000
H	6.286439000	-0.048725000	0.020702000
H	6.327834000	1.706264000	0.201446000
C	6.089852000	0.595179000	1.992568000
O	5.690096000	1.537029000	2.876599000
O	6.602030000	-0.154628000	3.915488000
N	6.635214000	-0.433891000	2.532948000
C	1.553661000	2.401402000	-1.975278000
C	1.270399000	0.211835000	-2.715785000
C	-0.074087000	0.435664000	-2.998293000
C	-0.607671000	1.691635000	-2.751750000
C	0.216964000	2.688169000	-2.253224000
H	-0.695781000	-0.354335000	-3.408041000

H	-1.654996000	1.893716000	-2.961370000
H	-0.160814000	3.690617000	-2.068257000
C	1.946983000	-1.068123000	-2.988878000
C	1.301988000	-2.189098000	-3.511833000
C	2.044241000	-3.332865000	-3.756004000
H	0.235782000	-2.172152000	-3.716160000
C	3.993990000	-2.186226000	-2.953452000
C	3.408135000	-3.331613000	-3.482066000
H	1.565337000	-4.220933000	-4.160446000
H	4.020154000	-4.210213000	-3.669298000
N	2.057755000	1.176620000	-2.194420000
N	3.265699000	-1.081901000	-2.715379000
C	2.466211000	3.443254000	-1.420716000
H	2.515620000	3.370685000	-0.325994000
H	3.483146000	3.291811000	-1.802488000
H	2.111363000	4.448717000	-1.667557000
C	5.442649000	-2.113185000	-2.603265000
H	5.868071000	-1.164503000	-2.956208000
H	5.573834000	-2.139001000	-1.512440000
H	6.007230000	-2.948327000	-3.027849000
Ni	3.933619000	0.528074000	-1.661449000
H	4.944153000	1.526807000	-2.343176000
C	6.021790000	1.046676000	4.120756000
O	5.829226000	1.590922000	5.158690000

Int-A'-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -636.64 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
C	-4.012435000	-1.687012000	-2.379433000
C	-2.632826000	-1.609276000	-2.508160000
C	-1.925543000	-0.433413000	-2.185585000
C	-2.683489000	0.657451000	-1.713729000
C	-4.062277000	0.575070000	-1.584452000
C	-4.744132000	-0.593837000	-1.920417000
H	-4.521962000	-2.613331000	-2.640766000
H	-2.072127000	-2.469272000	-2.879749000

H	-2.180708000	1.585601000	-1.442497000
H	-4.614079000	1.438213000	-1.215002000
H	-5.824819000	-0.653685000	-1.816042000
C	-0.490638000	-0.379078000	-2.414503000
H	0.019090000	-1.341873000	-2.510942000
C	0.330987000	0.798941000	-2.293282000
H	-0.068193000	1.611034000	-1.675985000
C	1.810321000	0.560449000	-2.021155000
H	2.240126000	-0.117401000	-2.767907000
H	2.373402000	1.501806000	-2.069195000
C	2.002654000	-0.069667000	-0.698895000
O	1.573879000	0.571114000	0.410756000
O	2.454214000	-1.360783000	0.927286000
N	2.534064000	-1.216318000	-0.472465000
C	-2.596044000	2.766929000	-4.574542000
C	-2.949044000	0.604752000	-5.353607000
C	-4.320347000	0.823433000	-5.467676000
C	-4.827927000	2.064991000	-5.120145000
C	-3.956746000	3.051472000	-4.679160000
H	-4.985046000	0.031360000	-5.798319000
H	-5.894516000	2.261958000	-5.192596000
H	-4.319361000	4.039270000	-4.405810000
C	-2.312941000	-0.677065000	-5.702357000
C	-2.991654000	-1.733044000	-6.311002000
C	-2.291996000	-2.882352000	-6.634836000
H	-4.050686000	-1.653267000	-6.535777000
C	-0.305515000	-1.870232000	-5.741803000
C	-0.929179000	-2.948693000	-6.355738000
H	-2.798499000	-3.718397000	-7.110051000
H	-0.346163000	-3.830212000	-6.609597000
N	-2.106910000	1.562109000	-4.907159000
N	-0.995347000	-0.759474000	-5.415446000
C	-1.631163000	3.788911000	-4.069022000
H	-1.377288000	3.590625000	-3.019715000
H	-0.694256000	3.743660000	-4.633435000
H	-2.051043000	4.797872000	-4.129482000
C	1.145361000	-1.886751000	-5.395410000
H	1.613358000	-0.931698000	-5.664087000
H	1.275712000	-2.017188000	-4.312607000
H	1.671880000	-2.701119000	-5.901982000

Ni	-0.372807000	0.640298000	-4.168615000
H	0.517189000	1.737429000	-3.521072000
C	1.864427000	-0.270482000	1.463028000
O	1.639083000	-0.057776000	2.609107000

Int-B'

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
C	4.264730000	2.045225000	1.876825000
H	3.481009000	2.026998000	2.647643000
H	5.021887000	1.301666000	2.152286000
C	4.905629000	3.370360000	1.877548000
C	5.004679000	5.539776000	1.685591000
O	4.705996000	6.682051000	1.544536000
O	4.137559000	4.473263000	1.691814000
O	6.240121000	5.030571000	1.867124000
N	6.160517000	3.625972000	1.987786000
C	3.641332000	1.696544000	0.509570000
H	2.944747000	2.500460000	0.229032000
H	4.450940000	1.716441000	-0.237292000
C	2.909863000	0.352613000	0.524053000
H	2.092723000	0.440753000	1.260807000
C	3.787558000	-0.780979000	0.925705000
C	4.972784000	-1.084016000	0.229201000
C	3.480162000	-1.599282000	2.025899000
C	5.787712000	-2.144691000	0.599647000
C	4.284937000	-2.675253000	2.389633000
C	5.447126000	-2.957239000	1.680276000
H	5.248089000	-0.472559000	-0.631795000
H	2.587401000	-1.372795000	2.611397000
H	6.697081000	-2.344817000	0.035281000
H	4.008441000	-3.286714000	3.247243000
H	6.082951000	-3.791665000	1.966679000
Ni	2.099032000	-0.059591000	-1.264520000
C	0.079742000	-2.322419000	-0.968273000
C	0.260780000	-1.371593000	-3.082890000
C	-0.730454000	-2.204311000	-3.593578000

C	-1.326113000	-3.126505000	-2.745114000
C	-0.917744000	-3.187182000	-1.422221000
H	-1.032520000	-2.141637000	-4.634298000
H	-2.101938000	-3.791840000	-3.115370000
H	-1.361764000	-3.897314000	-0.729728000
C	0.967135000	-0.366610000	-3.900378000
C	0.687945000	-0.140683000	-5.245569000
C	1.420772000	0.819336000	-5.927294000
H	-0.088719000	-0.701279000	-5.756198000
C	2.638501000	1.253145000	-3.903484000
C	2.408529000	1.521233000	-5.251495000
H	1.223396000	1.017027000	-6.977717000
H	3.004681000	2.277507000	-5.755040000
N	0.653459000	-1.432124000	-1.795037000
N	1.919961000	0.326337000	-3.245900000
C	0.544153000	-2.347708000	0.446017000
H	1.620006000	-2.556326000	0.503632000
H	0.399464000	-1.364186000	0.909023000
H	0.004728000	-3.100529000	1.028307000
C	3.691188000	1.974863000	-3.130627000
H	3.256583000	2.463827000	-2.250369000
H	4.445380000	1.268257000	-2.762402000
H	4.191108000	2.730598000	-3.743224000

Int-A'_β

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
C	0.068596000	-1.454306000	-0.211959000
C	1.445905000	-1.386279000	-0.358903000
C	2.200749000	-0.456318000	0.367854000
C	1.530208000	0.388328000	1.260906000
C	0.146015000	0.328398000	1.399429000
C	-0.590900000	-0.589920000	0.661621000
H	-0.499093000	-2.178939000	-0.791902000
H	1.959992000	-2.025287000	-1.074852000
H	2.105121000	1.081713000	1.874463000
H	-0.353836000	0.994148000	2.100020000

H	-1.672002000	-0.639794000	0.769870000
C	3.672501000	-0.380764000	0.207237000
H	4.206952000	-1.334214000	0.248881000
C	4.386004000	0.808649000	0.431524000
H	3.824365000	1.711135000	0.684750000
C	5.816437000	0.821451000	0.910712000
H	6.394582000	-0.017237000	0.504745000
H	6.326404000	1.748591000	0.610374000
C	5.868517000	0.697906000	2.385589000
O	5.228401000	1.612147000	3.150186000
O	6.149131000	0.074286000	4.399534000
N	6.434883000	-0.240431000	3.054038000
C	6.968477000	-0.352475000	-2.330898000
C	6.413553000	1.880142000	-2.710078000
C	7.684635000	2.153702000	-3.210751000
C	8.618966000	1.130379000	-3.257086000
C	8.253547000	-0.137295000	-2.826204000
H	7.937483000	3.146138000	-3.571393000
H	9.618372000	1.315977000	-3.642128000
H	8.952102000	-0.968798000	-2.872010000
C	5.325774000	2.873093000	-2.685178000
C	5.471224000	4.196975000	-3.096522000
C	4.356608000	5.022129000	-3.087012000
H	6.434707000	4.578722000	-3.420731000
C	3.049275000	3.178581000	-2.271212000
C	3.131300000	4.506944000	-2.682275000
H	4.440459000	6.058933000	-3.402526000
H	2.236154000	5.123549000	-2.681096000
N	6.077231000	0.652473000	-2.259629000
N	4.139371000	2.393233000	-2.267567000
C	6.517002000	-1.702541000	-1.885248000
H	6.470477000	-1.770739000	-0.790536000
H	5.499593000	-1.884464000	-2.257800000
H	7.196951000	-2.483817000	-2.237708000
C	1.769904000	2.551134000	-1.830996000
H	1.617795000	1.600475000	-2.360612000
H	1.791799000	2.306079000	-0.760016000
H	0.915041000	3.208845000	-2.012275000
Ni	4.145149000	0.472602000	-1.578595000
H	3.532047000	-0.537404000	-2.628172000

C	5.411992000	1.203271000	4.453549000
O	4.997261000	1.753590000	5.420822000

Int-A'_g-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -635.22 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
C	0.291294000	-0.288834000	1.822021000
C	1.650436000	-0.119113000	1.581246000
C	2.196106000	-0.372961000	0.318025000
C	1.337157000	-0.799347000	-0.698410000
C	-0.022436000	-0.970010000	-0.459977000
C	-0.551924000	-0.714618000	0.800981000
H	-0.108448000	-0.088025000	2.813720000
H	2.307827000	0.208787000	2.385629000
H	1.746994000	-0.979786000	-1.691329000
H	-0.672756000	-1.298343000	-1.268266000
H	-1.615909000	-0.844470000	0.986149000
C	3.676826000	-0.210243000	0.130116000
H	4.236993000	-1.140109000	0.302750000
C	4.305240000	0.985480000	0.628951000
H	3.654982000	1.738203000	1.076451000
C	5.694474000	0.908861000	1.236778000
H	6.444917000	0.517431000	0.536948000
H	6.035521000	1.904950000	1.544242000
C	5.702898000	0.007566000	2.410241000
O	4.989221000	0.332904000	3.513883000
O	5.891951000	-1.643375000	3.745153000
N	6.263170000	-1.148220000	2.474207000
C	6.914413000	-0.153021000	-2.628278000
C	6.380504000	2.074758000	-3.058406000
C	7.590355000	2.279094000	-3.720282000
C	8.476444000	1.220516000	-3.835757000
C	8.133741000	-0.008456000	-3.285857000
H	7.840804000	3.251054000	-4.134376000
H	9.426281000	1.351341000	-4.347816000
H	8.804552000	-0.860746000	-3.357648000

C	5.371135000	3.129649000	-2.886289000
C	5.490240000	4.405587000	-3.436271000
C	4.459787000	5.312702000	-3.255610000
H	6.369735000	4.682571000	-4.009402000
C	3.264717000	3.636530000	-2.014399000
C	3.329313000	4.919133000	-2.546491000
H	4.528187000	6.313125000	-3.674911000
H	2.492025000	5.597556000	-2.405142000
N	6.050347000	0.876276000	-2.527142000
N	4.285841000	2.767972000	-2.165774000
C	6.521340000	-1.451739000	-2.008040000
H	6.539253000	-1.388391000	-0.911689000
H	5.491384000	-1.706046000	-2.286832000
H	7.197685000	-2.257246000	-2.308818000
C	2.067877000	3.151409000	-1.270198000
H	1.682461000	2.229065000	-1.723288000
H	2.331726000	2.899387000	-0.235979000
H	1.271005000	3.900682000	-1.259474000
Ni	4.329735000	0.936590000	-1.385551000
H	3.785827000	-0.502944000	-1.491581000
C	5.114693000	-0.736971000	4.371793000
O	4.627239000	-0.823478000	5.452238000

Int-B'_β

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
C	-0.671317000	-3.938859000	3.795702000
C	-0.256664000	-3.392232000	2.583221000
C	-0.966316000	-2.351474000	1.983332000
C	-2.124781000	-1.891688000	2.618151000
C	-2.547742000	-2.435915000	3.823668000
C	-1.817065000	-3.460725000	4.421405000
H	-0.089320000	-4.734620000	4.255819000
H	0.652064000	-3.759306000	2.106239000
H	-2.693180000	-1.082213000	2.156222000
H	-3.447053000	-2.057009000	4.304894000
H	-2.136290000	-3.877613000	5.373565000

C	-0.499237000	-1.695361000	0.705823000
H	0.302559000	-2.309371000	0.262414000
C	-0.011494000	-0.239408000	0.844693000
H	-0.725090000	0.282618000	1.511006000
C	1.368842000	-0.130867000	1.507254000
H	2.150526000	-0.612398000	0.900935000
H	1.649627000	0.928638000	1.595523000
C	1.494897000	-0.733864000	2.857367000
O	0.675682000	-0.329067000	3.855744000
O	2.028336000	-1.888290000	4.567783000
N	2.332066000	-1.644093000	3.209542000
C	1.635668000	-0.023475000	-3.097462000
C	0.541991000	2.016916000	-3.338727000
C	1.253861000	2.313212000	-4.497792000
C	2.185889000	1.394697000	-4.957868000
C	2.373092000	0.211370000	-4.257547000
H	1.083740000	3.240792000	-5.035825000
H	2.757318000	1.597848000	-5.859952000
H	3.086858000	-0.534588000	-4.596894000
C	-0.505350000	2.894104000	-2.783192000
C	-0.890001000	4.099545000	-3.363902000
C	-1.922039000	4.819095000	-2.779944000
H	-0.399492000	4.469844000	-4.258974000
C	-2.099745000	3.112601000	-1.098154000
C	-2.539375000	4.318098000	-1.641737000
H	-2.246524000	5.761784000	-3.212980000
H	-3.356876000	4.852809000	-1.165443000
N	0.747742000	0.878396000	-2.646625000
N	-1.093005000	2.424944000	-1.664487000
C	1.790041000	-1.280120000	-2.309458000
H	2.057861000	-1.047832000	-1.271793000
H	0.838798000	-1.824130000	-2.268705000
H	2.553287000	-1.933758000	-2.741314000
C	-2.709553000	2.534206000	0.135548000
H	-3.013879000	1.494501000	-0.034645000
H	-1.976117000	2.516191000	0.951369000
H	-3.580187000	3.111626000	0.459860000
Ni	-0.203499000	0.809219000	-0.829421000
H	-1.331989000	-1.724415000	-0.015655000
C	1.011962000	-1.087470000	4.950575000

O	0.511020000	-1.021909000	6.027620000
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Int-A-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -785.14 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	7.227755000	0.636940000	-1.233031000
C	6.884646000	-0.645577000	-1.735357000
O	5.618828000	-0.854992000	-1.491926000
N	5.056932000	0.466667000	-0.671813000
C	6.130809000	1.174205000	-0.698090000
O	7.695874000	-1.328481000	-2.280117000
C	3.050525000	1.911317000	4.380497000
C	1.214452000	1.867345000	0.601585000
C	0.001243000	2.462156000	0.254389000
C	-0.434809000	2.376361000	-1.056639000
C	0.337618000	1.683143000	-1.984053000
C	1.528619000	1.090389000	-1.579072000
N	1.957896000	1.195745000	-0.305862000
H	-0.584280000	2.996436000	0.996755000
H	-1.372767000	2.837705000	-1.355518000
H	0.020112000	1.587616000	-3.019268000
C	1.783804000	1.915321000	1.952801000
C	1.180488000	2.563024000	3.030751000
C	1.826297000	2.563006000	4.255617000
C	3.594567000	1.268381000	3.275120000
N	2.962857000	1.273123000	2.088099000
H	0.234643000	3.082700000	2.910095000
H	1.383861000	3.073235000	5.107580000
H	3.584239000	1.893739000	5.327563000
H	3.183415000	-1.293784000	0.834565000
Ni	3.547851000	0.207984000	0.474551000
C	4.890582000	0.534049000	3.319312000
H	5.319431000	0.513017000	4.325353000
H	4.741541000	-0.495521000	2.962206000
H	5.616850000	1.001418000	2.639666000
C	2.381337000	0.304178000	-2.515138000

H	3.352578000	0.792787000	-2.660391000
H	2.599058000	-0.683559000	-2.087186000
H	1.899422000	0.181701000	-3.489262000
C	6.257823000	2.580292000	-0.217533000
H	6.864044000	2.576370000	0.700495000
H	6.869293000	3.101652000	-0.971630000
C	4.956179000	3.277993000	0.002605000
H	4.233660000	3.211374000	-0.813118000
C	4.687551000	3.989786000	1.102094000
H	5.435792000	4.002135000	1.900784000
C	3.478473000	4.763308000	1.381550000
C	2.446008000	4.937031000	0.448456000
C	3.339714000	5.361817000	2.639948000
C	1.316625000	5.675485000	0.771060000
C	2.208222000	6.099282000	2.965173000
C	1.189760000	6.258885000	2.030863000
H	2.522369000	4.486047000	-0.540803000
H	4.133994000	5.231718000	3.374720000
H	0.526916000	5.795260000	0.031701000
H	2.122634000	6.552953000	3.950151000
H	0.305192000	6.841473000	2.277707000

Int-B

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
O	5.075001000	-1.082693000	1.662766000
N	6.236951000	0.253682000	0.205218000
C	5.412272000	0.019539000	1.252038000
C	4.922707000	1.280621000	2.005490000
H	3.832428000	1.166394000	2.067751000
H	5.305678000	1.203272000	3.031088000
Ni	5.665559000	0.831860000	-1.378727000
C	5.281014000	2.581408000	1.377626000
H	6.293588000	2.956452000	1.551090000
C	4.456133000	3.262101000	0.569569000
H	3.469691000	2.831003000	0.371699000
C	4.741314000	4.517394000	-0.123128000

C	5.790234000	5.372616000	0.247234000
C	3.927054000	4.905676000	-1.196706000
C	6.017920000	6.558703000	-0.435565000
C	4.153787000	6.094160000	-1.881470000
C	5.203227000	6.927336000	-1.505712000
H	6.420549000	5.110657000	1.095419000
H	3.104035000	4.253423000	-1.492727000
H	6.833041000	7.209521000	-0.124486000
H	3.502550000	6.372198000	-2.708602000
H	5.376038000	7.865002000	-2.029451000
C	3.848284000	0.951245000	-3.696167000
C	5.334921000	2.724107000	-3.368616000
C	4.718122000	3.476819000	-4.363379000
C	3.629091000	2.943119000	-5.032054000
C	3.205488000	1.664363000	-4.707392000
H	5.083449000	4.467448000	-4.612137000
H	3.127864000	3.511582000	-5.811199000
H	2.374322000	1.200370000	-5.231208000
C	6.548404000	3.181643000	-2.664658000
C	7.158995000	4.400495000	-2.941904000
C	8.338663000	4.714544000	-2.285538000
H	6.720437000	5.103381000	-3.641739000
C	8.230633000	2.580612000	-1.174025000
C	8.885729000	3.793024000	-1.410154000
H	8.830491000	5.666881000	-2.468383000
H	9.826452000	3.991022000	-0.903130000
N	4.884219000	1.494365000	-3.019508000
N	7.061263000	2.303553000	-1.777572000
C	3.399239000	-0.432587000	-3.365349000
H	4.253634000	-1.108604000	-3.267064000
H	2.876117000	-0.455040000	-2.402860000
H	2.724713000	-0.809833000	-4.140426000
C	8.844734000	1.565201000	-0.272422000
H	8.237380000	1.413890000	0.625263000
H	8.869258000	0.584376000	-0.757495000
H	9.859656000	1.863721000	0.006054000
H	4.605156000	-0.108328000	-1.138560000

Int-B-1

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
O	4.312568000	-0.397926000	-0.260326000
N	6.119155000	0.375065000	-1.493636000
C	4.868946000	0.418380000	-0.985085000
C	4.162286000	1.675222000	-1.537705000
H	4.056959000	2.436779000	-0.756801000
H	3.151863000	1.379295000	-1.847544000
C	4.983910000	2.162455000	-2.697508000
H	5.777812000	2.871083000	-2.450056000
C	4.668671000	1.989036000	-4.041145000
H	3.733811000	1.470401000	-4.274888000
C	5.161123000	2.866066000	-5.130926000
C	6.318104000	3.643842000	-5.016178000
C	4.426870000	2.939190000	-6.316568000
C	6.722955000	4.469004000	-6.056845000
C	4.830687000	3.765169000	-7.359474000
C	5.981436000	4.534932000	-7.234350000
H	6.914640000	3.597623000	-4.105536000
H	3.526219000	2.334377000	-6.419141000
H	7.626097000	5.065889000	-5.948589000
H	4.241891000	3.806775000	-8.273207000
H	6.300937000	5.182058000	-8.047670000
H	5.827346000	0.527267000	-4.854092000
Ni	5.928618000	0.482773000	-3.386220000
C	8.522796000	-0.600909000	-3.498164000
C	6.880836000	-2.206608000	-3.919067000
C	7.843466000	-3.213418000	-3.978969000
C	9.178489000	-2.890530000	-3.798526000
C	9.522242000	-1.568544000	-3.566304000
H	7.537192000	-4.243178000	-4.133698000
H	9.941770000	-3.663697000	-3.833201000
H	10.557577000	-1.270953000	-3.424920000
C	5.447088000	-2.524685000	-4.118665000
C	5.069092000	-3.616685000	-4.903165000
C	3.717513000	-3.908747000	-5.017395000

H	5.810784000	-4.209057000	-5.431403000
C	3.256692000	-2.028435000	-3.597404000
C	2.799317000	-3.117607000	-4.344990000
H	3.385830000	-4.747910000	-5.624274000
H	1.733657000	-3.328273000	-4.394895000
N	7.227583000	-0.930925000	-3.666015000
N	4.558490000	-1.736861000	-3.506631000
C	8.845634000	0.832559000	-3.244896000
H	8.421138000	1.460158000	-4.040136000
H	8.396159000	1.151799000	-2.296325000
H	9.927293000	0.993102000	-3.205562000
C	2.308549000	-1.145011000	-2.853127000
H	2.673846000	-0.985576000	-1.830332000
H	2.241371000	-0.162489000	-3.339841000
H	1.301039000	-1.570955000	-2.822167000

Int-B-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -442.87 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	4.345821000	-0.287858000	-0.242442000
N	5.849792000	0.641735000	-1.763297000
C	4.681187000	0.544122000	-1.067260000
C	3.912249000	1.748885000	-1.593264000
H	3.762350000	2.523960000	-0.834733000
H	2.935522000	1.477835000	-2.012897000
C	4.929706000	2.140343000	-2.644057000
H	5.658130000	2.896929000	-2.353898000
C	4.667398000	2.013919000	-4.048828000
H	3.666058000	1.662310000	-4.315409000
C	5.255211000	2.948063000	-5.038611000
C	6.429175000	3.671367000	-4.798775000
C	4.609918000	3.129208000	-6.266325000
C	6.938168000	4.542003000	-5.755581000
C	5.116824000	3.998881000	-7.222859000
C	6.286193000	4.711398000	-6.972943000
H	6.959527000	3.551892000	-3.854607000

H	3.698510000	2.567224000	-6.469817000
H	7.852098000	5.093924000	-5.545781000
H	4.594414000	4.122180000	-8.169188000
H	6.684991000	5.393666000	-7.719795000
H	5.556589000	0.381787000	-5.077261000
Ni	5.734892000	0.417079000	-3.600424000
C	8.424767000	-0.563611000	-3.767318000
C	6.870842000	-2.290504000	-3.963996000
C	7.889770000	-3.241930000	-3.999159000
C	9.209205000	-2.825327000	-3.926347000
C	9.480898000	-1.470816000	-3.817803000
H	7.646411000	-4.298344000	-4.051533000
H	10.017265000	-3.552245000	-3.946511000
H	10.501643000	-1.102924000	-3.759535000
C	5.446887000	-2.694584000	-4.043640000
C	5.076821000	-3.916313000	-4.610767000
C	3.732996000	-4.260216000	-4.615952000
H	5.815835000	-4.573197000	-5.060154000
C	3.258574000	-2.174038000	-3.530592000
C	2.811067000	-3.388005000	-4.057577000
H	3.408940000	-5.201559000	-5.053326000
H	1.751685000	-3.631393000	-4.030751000
N	7.147653000	-0.980625000	-3.837366000
N	4.552231000	-1.839741000	-3.541299000
C	8.664781000	0.901704000	-3.631546000
H	8.174092000	1.445953000	-4.450027000
H	8.229683000	1.262125000	-2.690158000
H	9.734452000	1.131870000	-3.643310000
C	2.315296000	-1.193029000	-2.915175000
H	2.626518000	-0.978863000	-1.884319000
H	2.340615000	-0.248363000	-3.474076000
H	1.286122000	-1.564223000	-2.912540000

Int-C

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
O	4.335878000	-1.412502000	-1.414318000

N	5.618859000	0.365341000	-2.314307000
C	4.524386000	-0.259834000	-1.760714000
C	3.626066000	0.990608000	-1.807259000
H	3.398951000	1.438334000	-0.834148000
H	2.692714000	0.865434000	-2.370524000
C	4.814484000	1.601463000	-2.565400000
H	5.250978000	2.503107000	-2.114326000
C	4.734878000	1.644385000	-4.077771000
H	3.870661000	1.063244000	-4.440890000
C	4.901954000	2.887483000	-4.858165000
C	4.723297000	2.862657000	-6.250864000
C	5.227553000	4.116683000	-4.271361000
C	4.879871000	4.002701000	-7.021293000
C	5.393106000	5.263537000	-5.044911000
C	5.226225000	5.214843000	-6.422390000
H	4.488358000	1.910036000	-6.725674000
H	5.354029000	4.188131000	-3.193011000
H	4.738854000	3.948215000	-8.098951000
H	5.650329000	6.203035000	-4.559503000
H	5.359748000	6.109271000	-7.026440000
C	10.270210000	1.196654000	-4.030169000
C	7.757126000	-2.166141000	-3.779211000
C	8.150211000	-3.457390000	-3.441754000
C	7.196116000	-4.465789000	-3.456632000
C	5.891494000	-4.164533000	-3.811975000
C	5.555415000	-2.847549000	-4.127324000
N	6.485436000	-1.885201000	-4.104222000
H	9.176089000	-3.677081000	-3.163834000
H	5.122191000	-4.931478000	-3.835800000
C	8.684757000	-1.018750000	-3.832680000
C	10.058178000	-1.153400000	-3.645428000
C	10.858018000	-0.025141000	-3.744405000
C	8.887539000	1.269254000	-4.205412000
N	8.122948000	0.173068000	-4.105050000
H	10.498950000	-2.122580000	-3.435230000
H	11.933433000	-0.101476000	-3.604806000
H	10.866257000	2.100947000	-4.119355000
H	5.964760000	0.231865000	-5.703757000
Ni	6.029232000	0.114843000	-4.209377000
C	8.206825000	2.561235000	-4.495254000

H	8.928384000	3.368730000	-4.648516000
H	7.564213000	2.479167000	-5.380226000
H	7.550953000	2.837491000	-3.660918000
C	4.161463000	-2.450474000	-4.475638000
H	3.687897000	-2.020402000	-3.582713000
H	4.163086000	-1.698284000	-5.273733000
H	3.568682000	-3.312595000	-4.795201000
H	7.473468000	-5.483396000	-3.193500000

Int-B-2

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
O	3.957960000	-1.741825000	-1.566476000
N	5.709582000	-0.365291000	-2.234917000
C	4.435352000	-0.669636000	-1.914296000
C	3.559904000	0.603144000	-2.037781000
H	3.126991000	0.839449000	-1.058635000
H	2.731572000	0.363101000	-2.720135000
C	4.395176000	1.719486000	-2.568553000
H	5.072056000	2.189736000	-1.853405000
C	4.311017000	2.219246000	-3.830148000
H	3.549474000	1.795601000	-4.492375000
C	4.988409000	3.421763000	-4.333790000
C	5.946755000	4.124945000	-3.590782000
C	4.678002000	3.889401000	-5.616206000
C	6.583224000	5.238195000	-4.121839000
C	5.316773000	5.002056000	-6.150941000
C	6.276234000	5.680348000	-5.407169000
H	6.203969000	3.794255000	-2.585438000
H	3.920986000	3.363014000	-6.198122000
H	7.324411000	5.767140000	-3.526678000
H	5.061018000	5.341189000	-7.152599000
H	6.777459000	6.551975000	-5.821127000
C	8.081363000	2.268019000	-6.872321000
C	4.358783000	0.306493000	-6.601128000
C	3.268716000	0.745493000	-7.354479000
C	2.048785000	0.103188000	-7.172747000

C	1.967047000	-0.952247000	-6.278210000
C	3.113366000	-1.343874000	-5.574061000
N	4.276486000	-0.703787000	-5.732107000
H	3.363256000	1.583395000	-8.041328000
H	1.030317000	-1.481788000	-6.120090000
C	5.676257000	0.978923000	-6.716370000
C	6.099798000	1.485529000	-7.942349000
C	7.314835000	2.147870000	-8.019582000
C	7.626089000	1.718331000	-5.675282000
N	6.431376000	1.095234000	-5.603337000
H	5.482736000	1.338874000	-8.824112000
H	7.663813000	2.555266000	-8.965083000
H	9.041730000	2.775915000	-6.887743000
H	6.762241000	-0.691407000	-4.106191000
Ni	5.863621000	0.415221000	-3.864248000
C	8.455213000	1.787366000	-4.437440000
H	8.698948000	0.776019000	-4.089609000
H	9.381305000	2.342564000	-4.615545000
H	7.906682000	2.273094000	-3.622384000
C	3.092010000	-2.484831000	-4.612101000
H	2.259485000	-3.166196000	-4.814489000
H	4.037093000	-3.033731000	-4.663690000
H	3.006665000	-2.137062000	-3.572973000
H	1.170633000	0.426023000	-7.727215000

Int-B-TS-i

Charge = 0 Multiplicity = 2

Imaginary frequency = -531.48 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	4.149302000	-1.645197000	-1.521888000
N	5.488511000	0.157904000	-2.197852000
C	4.327132000	-0.499372000	-1.883708000
C	3.329264000	0.639698000	-2.055268000
H	2.826873000	0.916741000	-1.122864000
H	2.569750000	0.417730000	-2.816557000
C	4.352162000	1.659019000	-2.516433000
H	4.783566000	2.305499000	-1.752416000

C	4.350330000	2.141705000	-3.844930000
H	3.585219000	1.736254000	-4.512866000
C	4.990469000	3.377072000	-4.279583000
C	5.946971000	4.056827000	-3.505568000
C	4.675601000	3.908393000	-5.541087000
C	6.560223000	5.208980000	-3.978235000
C	5.290817000	5.060067000	-6.012696000
C	6.240440000	5.717933000	-5.235382000
H	6.226125000	3.665979000	-2.527056000
H	3.927487000	3.400336000	-6.150666000
H	7.297850000	5.714972000	-3.358586000
H	5.025986000	5.448094000	-6.994285000
H	6.723617000	6.620159000	-5.602322000
C	8.132584000	2.164315000	-6.991791000
C	4.380783000	0.280699000	-6.620145000
C	3.273912000	0.738346000	-7.337372000
C	2.054137000	0.106821000	-7.125913000
C	1.989407000	-0.958627000	-6.240273000
C	3.153047000	-1.371320000	-5.579808000
N	4.318235000	-0.740620000	-5.763257000
H	3.359025000	1.585238000	-8.014410000
H	1.051983000	-1.478991000	-6.058364000
C	5.698531000	0.944971000	-6.765989000
C	6.115133000	1.406964000	-8.011012000
C	7.347647000	2.031262000	-8.124863000
C	7.674061000	1.676973000	-5.768679000
N	6.466455000	1.083380000	-5.664473000
H	5.481454000	1.248139000	-8.878866000
H	7.695961000	2.397463000	-9.087263000
H	9.107762000	2.641267000	-7.035735000
H	6.764561000	-0.580173000	-4.018319000
Ni	5.843734000	0.550571000	-3.904022000
C	8.513228000	1.785009000	-4.541016000
H	8.641925000	0.797242000	-4.082458000
H	9.493561000	2.211700000	-4.773473000
H	8.026580000	2.420358000	-3.791833000
C	3.158539000	-2.535958000	-4.645111000
H	2.185624000	-3.035853000	-4.615151000
H	3.919039000	-3.259018000	-4.958822000
H	3.429069000	-2.230962000	-3.625323000

H	1.162068000	0.445686000	-7.647605000
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Int-C-i

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
O	-0.540008000	-2.811219000	3.603672000
N	0.587867000	-1.012575000	2.521322000
C	-0.309453000	-1.646097000	3.381558000
C	-0.932624000	-0.321731000	3.865313000
H	-0.671341000	-0.037569000	4.889514000
H	-2.020622000	-0.259274000	3.739897000
C	-0.071861000	0.303829000	2.758165000
H	0.617433000	1.097695000	3.083206000
C	-0.748657000	0.580223000	1.432228000
H	-1.795763000	0.247229000	1.418700000
C	-0.529615000	1.768027000	0.626175000
C	0.607082000	2.592714000	0.747360000
C	-1.448667000	2.092863000	-0.392366000
C	0.802686000	3.676451000	-0.096645000
C	-1.248207000	3.174994000	-1.238598000
C	-0.118344000	3.976703000	-1.099881000
H	1.349859000	2.370940000	1.513110000
H	-2.342222000	1.475968000	-0.505410000
H	1.690090000	4.294971000	0.027326000
H	-1.983915000	3.395713000	-2.010462000
H	0.040324000	4.828502000	-1.757000000
C	3.411365000	0.957109000	-1.283161000
C	-0.482252000	-0.446624000	-1.969955000
C	-1.254353000	-0.290939000	-3.120298000
C	-2.497004000	-0.899866000	-3.173439000
C	-2.936238000	-1.659178000	-2.092635000
C	-2.125482000	-1.785491000	-0.969845000
N	-0.926751000	-1.176465000	-0.929428000
H	-0.890079000	0.300605000	-3.954776000
H	-3.902263000	-2.156526000	-2.111226000
C	0.867274000	0.109415000	-1.792564000
C	1.517309000	0.885715000	-2.747220000

C	2.805878000	1.321313000	-2.477760000
C	2.711429000	0.177301000	-0.362725000
N	1.457076000	-0.219544000	-0.626742000
H	1.023521000	1.154893000	-3.675941000
H	3.337846000	1.936349000	-3.199044000
H	4.425406000	1.270911000	-1.049885000
H	0.769531000	-2.525017000	0.461299000
Ni	0.190862000	-1.121883000	0.678822000
C	3.317267000	-0.260709000	0.925641000
H	4.350487000	0.086051000	1.015252000
H	2.733262000	0.098571000	1.781424000
H	3.288736000	-1.354277000	1.000793000
C	-2.514409000	-2.580120000	0.229602000
H	-2.688045000	-1.926569000	1.095337000
H	-3.425424000	-3.158052000	0.051908000
H	-1.700206000	-3.259551000	0.516057000
H	-3.122046000	-0.790411000	-4.055954000

Int-D

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	3.747827000	1.093302000	2.485452000
N	5.152772000	1.407365000	0.705737000
C	4.096913000	1.717999000	1.485370000
C	3.303340000	2.965481000	1.071107000
H	2.462273000	2.624380000	0.449706000
H	2.872855000	3.362973000	1.999431000
H	5.507938000	0.498653000	0.998079000
Ni	5.533187000	1.961320000	-1.026635000
C	4.067188000	4.017406000	0.348592000
H	4.933853000	4.426530000	0.877434000
C	3.750640000	4.484662000	-0.868715000
H	2.895301000	4.028927000	-1.377275000
C	4.444902000	5.518331000	-1.632609000
C	5.502443000	6.281054000	-1.114390000
C	4.049338000	5.765264000	-2.955494000
C	6.136688000	7.241736000	-1.889956000

C	4.685411000	6.723569000	-3.734142000
C	5.736374000	7.468205000	-3.205725000
H	5.831221000	6.120824000	-0.087983000
H	3.227080000	5.183051000	-3.372399000
H	6.953329000	7.820811000	-1.461463000
H	4.358045000	6.890806000	-4.758538000
H	6.231144000	8.226852000	-3.808125000
H	4.300666000	1.279564000	-1.303032000
C	5.062127000	2.162329000	-3.929674000
C	6.757036000	3.471783000	-3.010542000
C	7.007890000	4.080766000	-4.236044000
C	6.252055000	3.715788000	-5.336845000
C	5.275881000	2.747860000	-5.178784000
H	7.788376000	4.827130000	-4.333346000
H	6.427696000	4.176624000	-6.305436000
H	4.668067000	2.425405000	-6.019673000
C	7.554183000	3.783933000	-1.809232000
C	8.494885000	4.811204000	-1.793067000
C	9.225017000	5.026986000	-0.636382000
H	8.630916000	5.457621000	-2.653464000
C	8.069033000	3.170350000	0.372158000
C	9.019176000	4.191806000	0.448730000
H	9.955359000	5.830895000	-0.587592000
H	9.593101000	4.309760000	1.364081000
N	5.797041000	2.526815000	-2.855973000
N	7.324958000	2.996837000	-0.738348000
C	4.005581000	1.117020000	-3.792741000
H	4.396585000	0.222853000	-3.299097000
H	3.181178000	1.478579000	-3.167603000
H	3.610332000	0.845575000	-4.776831000
C	7.897197000	2.235373000	1.518862000
H	6.886681000	2.305784000	1.934009000
H	8.005421000	1.198368000	1.181690000
H	8.641560000	2.435489000	2.294782000

Int-D-1

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	3.566162000	0.845881000	2.309577000
N	5.390659000	1.940139000	1.392624000
C	4.084495000	1.775068000	1.698407000
C	3.254108000	2.918334000	1.106461000
H	2.510771000	2.477165000	0.428358000
H	2.695107000	3.420555000	1.905475000
H	5.910279000	1.100740000	1.650928000
Ni	5.635958000	2.675703000	-0.368991000
C	4.163208000	3.858090000	0.379437000
H	4.684352000	4.581347000	1.011287000
C	4.211184000	4.042417000	-0.996107000
H	3.513814000	3.458927000	-1.605605000
C	4.718653000	5.268243000	-1.659151000
C	5.554732000	6.186695000	-1.015307000
C	4.333283000	5.532983000	-2.975352000
C	5.990560000	7.330562000	-1.670997000
C	4.767506000	6.678242000	-3.633062000
C	5.599730000	7.583295000	-2.983748000
H	5.873180000	6.003648000	0.010314000
H	3.685421000	4.822905000	-3.488941000
H	6.640292000	8.032311000	-1.152164000
H	4.452779000	6.863373000	-4.657834000
H	5.941751000	8.480018000	-3.494972000
C	3.884152000	-0.289915000	-1.758022000
C	6.171033000	-0.026114000	-1.887528000
C	6.255670000	-0.826854000	-3.028069000
C	5.083886000	-1.376074000	-3.531601000
C	3.885227000	-1.119340000	-2.884274000
H	7.207428000	-0.996983000	-3.523949000
H	5.108565000	-2.000789000	-4.421398000
H	2.951495000	-1.547503000	-3.241534000
C	7.394369000	0.541940000	-1.272220000
C	8.608642000	-0.137028000	-1.363180000
C	9.741759000	0.411809000	-0.784565000
H	8.648087000	-1.102045000	-1.859113000
C	8.398647000	2.264424000	-0.056327000
C	9.636052000	1.629021000	-0.130660000
H	10.695219000	-0.107441000	-0.838460000

H	10.500194000	2.098021000	0.331784000
N	5.011129000	0.249960000	-1.286317000
N	7.300578000	1.714546000	-0.613806000
C	2.621244000	0.037376000	-1.028351000
H	2.280363000	1.045300000	-1.302721000
H	1.817391000	-0.662779000	-1.276320000
H	2.791446000	0.032442000	0.055491000
C	8.240461000	3.582281000	0.623585000
H	7.875688000	4.330428000	-0.093756000
H	7.492043000	3.508599000	1.422999000
H	9.190500000	3.928280000	1.042086000
H	5.822711000	3.084704000	-1.766296000

Int-D-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -490.69 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	3.871573000	0.841981000	2.070528000
N	5.141908000	2.515495000	1.033523000
C	4.001890000	1.854279000	1.418276000
C	2.971833000	2.840931000	0.889923000
H	2.348400000	2.457888000	0.076472000
H	2.322796000	3.201805000	1.694085000
H	5.999085000	2.304849000	1.546934000
Ni	5.557611000	2.712308000	-0.935967000
C	3.998097000	3.855826000	0.446130000
H	4.237930000	4.637996000	1.168953000
C	4.176983000	4.127865000	-0.946149000
H	3.385217000	3.737663000	-1.592767000
C	4.767202000	5.405683000	-1.398105000
C	5.557954000	6.215071000	-0.571498000
C	4.540393000	5.846723000	-2.709437000
C	6.093405000	7.413275000	-1.034208000
C	5.073826000	7.040030000	-3.172639000
C	5.855819000	7.835773000	-2.337076000
H	5.770362000	5.903694000	0.451650000
H	3.942912000	5.221838000	-3.373220000

H	6.701562000	8.020873000	-0.366355000
H	4.878358000	7.353974000	-4.196244000
H	6.274268000	8.771952000	-2.699012000
C	3.868179000	-0.544919000	-1.670585000
C	6.153613000	-0.289798000	-1.768737000
C	6.280173000	-1.308290000	-2.716613000
C	5.131693000	-1.963087000	-3.137168000
C	3.909978000	-1.587090000	-2.600635000
H	7.249683000	-1.561574000	-3.136568000
H	5.190520000	-2.756285000	-3.878750000
H	2.989456000	-2.083880000	-2.898104000
C	7.358716000	0.415029000	-1.273570000
C	8.577120000	-0.258602000	-1.188467000
C	9.705519000	0.423572000	-0.764339000
H	8.624111000	-1.316001000	-1.430895000
C	8.346457000	2.389612000	-0.533250000
C	9.589765000	1.767907000	-0.447163000
H	10.662352000	-0.086002000	-0.683790000
H	10.451640000	2.348056000	-0.128270000
N	4.973913000	0.092664000	-1.273478000
N	7.245494000	1.711987000	-0.921886000
C	2.573565000	-0.085931000	-1.080133000
H	2.327688000	0.912050000	-1.467807000
H	1.750104000	-0.760066000	-1.335238000
H	2.655327000	-0.011353000	0.011777000
C	8.193759000	3.840686000	-0.215970000
H	7.656936000	4.355028000	-1.024047000
H	7.601761000	3.991046000	0.696014000
H	9.168620000	4.315894000	-0.067635000
H	5.716012000	2.950859000	-2.376703000

Int-D-2

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	3.493954000	1.381972000	2.491863000
N	4.499181000	1.399034000	0.421024000
C	3.812409000	1.937114000	1.447490000

C	3.410916000	3.384982000	1.158446000
H	2.352670000	3.374425000	0.863650000
H	3.478019000	3.950128000	2.094769000
H	4.701866000	0.421146000	0.596989000
Ni	4.980736000	2.251690000	-1.153745000
C	4.243733000	4.012337000	0.094999000
H	5.192577000	4.450498000	0.413176000
C	3.804713000	4.237904000	-1.177102000
H	2.809836000	3.855716000	-1.428353000
C	4.361332000	5.190987000	-2.146436000
C	5.421608000	6.052722000	-1.839587000
C	3.793453000	5.276785000	-3.424952000
C	5.909981000	6.945969000	-2.784887000
C	4.284285000	6.164611000	-4.372963000
C	5.351702000	7.001499000	-4.058579000
H	5.870222000	6.029006000	-0.847298000
H	2.951463000	4.629926000	-3.672983000
H	6.734848000	7.605117000	-2.520104000
H	3.828856000	6.206581000	-5.360071000
H	5.733660000	7.704113000	-4.795564000
H	5.467140000	0.916336000	-1.470015000
C	4.849589000	2.209684000	-3.997254000
C	6.755224000	3.298007000	-3.207799000
C	7.194551000	3.525746000	-4.510626000
C	6.426459000	3.093381000	-5.578543000
C	5.239882000	2.429449000	-5.316619000
H	8.146776000	4.017517000	-4.681356000
H	6.755540000	3.263183000	-6.600492000
H	4.607707000	2.066027000	-6.122279000
C	7.564418000	3.757751000	-2.051460000
C	8.509627000	4.779838000	-2.176067000
C	9.206368000	5.172220000	-1.041819000
H	8.658921000	5.298031000	-3.119258000
C	8.003714000	3.513191000	0.207275000
C	8.954442000	4.537301000	0.166679000
H	9.935121000	5.977553000	-1.099459000
H	9.483261000	4.822992000	1.073332000
N	5.595704000	2.645738000	-2.960668000
N	7.325878000	3.152747000	-0.886485000
C	3.589981000	1.469001000	-3.697154000

H	3.814483000	0.557761000	-3.130229000
H	2.920622000	2.060805000	-3.061858000
H	3.061104000	1.203460000	-4.618027000
C	7.713416000	2.751980000	1.460898000
H	6.679079000	2.388932000	1.455283000
H	8.358356000	1.866122000	1.518606000
H	7.899512000	3.355069000	2.355617000

Int-D-TS-i

Charge = 0 Multiplicity = 1

Imaginary frequency = -517.16 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	3.109927000	0.547068000	1.692357000
N	4.628546000	2.067604000	0.756045000
C	3.385411000	1.560606000	1.098612000
C	2.542600000	2.755461000	0.682530000
H	1.945707000	2.592517000	-0.221489000
H	1.881567000	3.091089000	1.487039000
H	5.423985000	1.678107000	1.263232000
Ni	5.140897000	2.375085000	-1.089782000
C	3.749697000	3.644496000	0.455123000
H	4.068326000	4.234509000	1.319055000
C	4.017149000	4.141444000	-0.854145000
H	3.235407000	3.921273000	-1.588307000
C	4.771094000	5.359553000	-1.130160000
C	5.595451000	5.999398000	-0.187694000
C	4.705955000	5.930125000	-2.414355000
C	6.303416000	7.148133000	-0.511609000
C	5.417237000	7.078117000	-2.738906000
C	6.224552000	7.698770000	-1.789754000
H	5.694404000	5.581793000	0.814825000
H	4.075850000	5.451543000	-3.166741000
H	6.933595000	7.616069000	0.243276000
H	5.337177000	7.492012000	-3.742886000
H	6.780443000	8.599822000	-2.038344000
H	5.719434000	0.998053000	-1.211062000
C	4.706896000	2.213655000	-3.872215000

C	6.579848000	3.483453000	-3.279032000
C	6.816584000	3.794909000	-4.618546000
C	5.960643000	3.319489000	-5.595695000
C	4.893029000	2.518810000	-5.216673000
H	7.676840000	4.395454000	-4.893918000
H	6.130583000	3.559791000	-6.642045000
H	4.201632000	2.115628000	-5.951692000
C	7.486370000	3.967794000	-2.209288000
C	8.448779000	4.952822000	-2.448705000
C	9.289458000	5.324006000	-1.411014000
H	8.525820000	5.447983000	-3.411646000
C	8.148947000	3.759063000	-0.004827000
C	9.153189000	4.712579000	-0.172646000
H	10.043492000	6.091621000	-1.567881000
H	9.800207000	4.976310000	0.660730000
N	5.536560000	2.698976000	-2.922767000
N	7.341189000	3.405383000	-1.006088000
C	3.586845000	1.333122000	-3.432767000
H	3.972228000	0.541716000	-2.777931000
H	2.853832000	1.895902000	-2.840964000
H	3.071217000	0.891021000	-4.291219000
C	7.909061000	3.089381000	1.311334000
H	6.941083000	3.405217000	1.724447000
H	7.869334000	2.001885000	1.177923000
H	8.686828000	3.329713000	2.042400000

Int-E

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	2.489576000	-1.122730000	-0.495501000
N	4.570513000	-0.010237000	-0.339613000
C	3.218889000	-0.204129000	-0.208161000
C	3.053648000	1.183740000	0.426040000
H	2.393550000	1.863489000	-0.124038000
H	2.758619000	1.161010000	1.479217000
C	5.067075000	4.795494000	-4.856015000
C	8.404986000	4.364892000	-2.350727000

C	9.375830000	5.326746000	-2.094345000
C	10.520833000	4.950321000	-1.407234000
C	10.666971000	3.628537000	-1.014237000
C	9.646791000	2.711893000	-1.270194000
N	8.524805000	3.088347000	-1.910681000
H	9.240344000	6.352846000	-2.421857000
H	11.297953000	5.679517000	-1.193148000
H	11.564152000	3.293246000	-0.500377000
C	7.202979000	4.627730000	-3.165752000
C	6.991898000	5.811972000	-3.862280000
C	5.889788000	5.899209000	-4.702946000
C	5.321995000	3.637436000	-4.117221000
N	6.345648000	3.586374000	-3.254404000
H	7.680221000	6.645928000	-3.767687000
H	5.695726000	6.813329000	-5.258312000
H	4.224651000	4.811778000	-5.543490000
H	5.282697000	-0.507092000	-0.860886000
Ni	6.701741000	2.371769000	-1.695943000
C	4.473043000	2.420498000	-4.298593000
H	4.917530000	1.558531000	-3.793838000
H	3.463622000	2.571434000	-3.896553000
H	4.364166000	2.195532000	-5.365796000
C	9.764560000	1.288625000	-0.842632000
H	9.115584000	1.098749000	0.020406000
H	9.420042000	0.620193000	-1.637771000
H	10.796986000	1.040961000	-0.577121000
C	4.568065000	1.375902000	0.137776000
H	5.176706000	1.512497000	1.042446000
C	4.921696000	2.384815000	-0.928458000
H	4.186897000	2.262941000	-1.740824000
C	4.924129000	3.804330000	-0.471781000
C	5.759228000	4.246596000	0.570348000
C	4.141105000	4.772480000	-1.119041000
C	5.826984000	5.588960000	0.920503000
C	4.213494000	6.118366000	-0.776385000
C	5.062723000	6.537407000	0.242882000
H	6.385469000	3.520024000	1.087314000
H	3.462830000	4.454870000	-1.912692000
H	6.488020000	5.899981000	1.727604000
H	3.595731000	6.842816000	-1.304768000

H	5.121036000	7.588878000	0.515388000
H	6.998783000	1.491906000	-0.568692000

Int-E-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -620.61 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	2.788158000	-0.794966000	-1.451875000
N	4.707735000	0.035934000	-0.342570000
C	3.386175000	-0.039030000	-0.728927000
C	3.041678000	1.207869000	0.097973000
H	2.571960000	2.023939000	-0.462221000
H	2.454646000	0.993830000	0.995403000
C	4.881546000	4.737316000	-4.687414000
C	8.649141000	4.253517000	-2.884850000
C	9.776970000	5.002789000	-3.210161000
C	11.000563000	4.638201000	-2.669684000
C	11.062994000	3.530570000	-1.832608000
C	9.901476000	2.823907000	-1.533824000
N	8.708751000	3.197207000	-2.039393000
H	9.701136000	5.837686000	-3.900902000
H	11.899410000	5.199755000	-2.911101000
H	12.007417000	3.208742000	-1.401155000
C	7.322636000	4.512267000	-3.479622000
C	6.979622000	5.722084000	-4.079873000
C	5.732732000	5.834185000	-4.680362000
C	5.276331000	3.563644000	-4.042953000
N	6.461411000	3.472323000	-3.421452000
H	7.664484000	6.565342000	-4.062284000
H	5.432986000	6.767409000	-5.150929000
H	3.913581000	4.779183000	-5.182211000
H	5.532070000	-0.364392000	-0.777886000
Ni	6.938104000	2.635107000	-1.528195000
C	4.384261000	2.361040000	-4.019772000
H	4.951816000	1.465388000	-3.748275000
H	3.566941000	2.474318000	-3.292184000
H	3.915732000	2.203386000	-4.997237000

C	9.912378000	1.636796000	-0.632271000
H	9.246334000	1.811480000	0.221900000
H	9.517321000	0.758352000	-1.155699000
H	10.921468000	1.414103000	-0.271479000
C	4.566624000	1.345471000	0.305136000
H	4.899813000	1.349202000	1.352810000
C	5.208384000	2.463379000	-0.512617000
H	4.766124000	2.350785000	-1.514104000
C	4.946161000	3.842356000	0.008113000
C	5.389629000	4.230201000	1.278091000
C	4.244599000	4.777600000	-0.760268000
C	5.133521000	5.506269000	1.764675000
C	3.994803000	6.057952000	-0.279275000
C	4.435535000	6.427210000	0.987904000
H	5.955613000	3.521902000	1.883236000
H	3.897789000	4.494054000	-1.755342000
H	5.486604000	5.786490000	2.755023000
H	3.448129000	6.768525000	-0.896032000
H	4.238400000	7.427067000	1.367721000
H	6.458612000	2.140951000	-0.201049000

Int-F

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	3.788222000	0.428011000	2.134062000
N	5.344545000	1.128247000	0.613300000
C	4.140878000	1.191483000	1.244119000
C	3.202543000	2.325098000	0.810392000
H	2.474976000	1.894827000	0.105526000
H	2.639902000	2.607889000	1.709671000
H	5.762616000	0.221460000	0.815922000
Ni	5.621088000	1.744482000	-1.110566000
C	3.880265000	3.501715000	0.203724000
H	4.664469000	3.957489000	0.810597000
C	3.597283000	4.031868000	-0.997015000
H	2.796928000	3.571037000	-1.583563000
C	4.282845000	5.147613000	-1.649467000

C	5.304379000	5.888613000	-1.035059000
C	3.952804000	5.462441000	-2.974176000
C	5.984247000	6.879204000	-1.729167000
C	4.630530000	6.455873000	-3.670697000
C	5.656014000	7.165140000	-3.053669000
H	5.570981000	5.684719000	0.000488000
H	3.154659000	4.903813000	-3.464566000
H	6.777728000	7.433791000	-1.231810000
H	4.357230000	6.674375000	-4.701210000
H	6.188690000	7.943838000	-3.594741000
C	4.808264000	2.305635000	-3.893907000
C	6.790038000	3.270531000	-3.134469000
C	7.039231000	3.846057000	-4.375065000
C	6.151186000	3.608065000	-5.412617000
C	5.024457000	2.846754000	-5.163869000
H	7.891768000	4.500735000	-4.520149000
H	6.322416000	4.041725000	-6.394518000
H	4.283200000	2.669932000	-5.938994000
C	7.643026000	3.532329000	-1.962237000
C	8.897061000	4.116066000	-2.100070000
C	9.624982000	4.414803000	-0.958814000
H	9.307661000	4.317460000	-3.083739000
C	7.804774000	3.531377000	0.354143000
C	9.065318000	4.134002000	0.272662000
H	10.611972000	4.863957000	-1.033483000
H	9.590391000	4.370506000	1.194275000
N	5.709713000	2.493058000	-2.911604000
N	7.114088000	3.208990000	-0.758490000
C	3.547476000	1.547652000	-3.639700000
H	3.672127000	0.491847000	-3.900740000
H	3.264101000	1.569475000	-2.585241000
H	2.738432000	1.968095000	-4.248555000
C	7.209780000	3.300407000	1.701081000
H	6.492188000	4.098828000	1.937014000
H	6.656010000	2.357096000	1.730113000
H	7.984486000	3.322572000	2.472651000
Cl	5.341439000	-0.295383000	-1.833375000

Int-F-1

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	3.404904000	1.114770000	2.326961000
N	4.401589000	1.317940000	0.270416000
C	3.794764000	1.779305000	1.376885000
C	3.579769000	3.290446000	1.309757000
H	2.548509000	3.461706000	0.973881000
H	3.665936000	3.696541000	2.323760000
H	4.508345000	0.306961000	0.266219000
Ni	5.174900000	2.241042000	-1.121546000
C	4.549388000	3.950085000	0.397089000
H	5.529305000	4.185801000	0.815992000
C	4.227282000	4.444551000	-0.830805000
H	3.212020000	4.250157000	-1.190174000
C	4.969568000	5.466691000	-1.579842000
C	6.132055000	6.075130000	-1.087459000
C	4.474320000	5.891873000	-2.819028000
C	6.788018000	7.051996000	-1.824842000
C	5.129886000	6.867857000	-3.557516000
C	6.294615000	7.449124000	-3.064815000
H	6.532054000	5.784439000	-0.116858000
H	3.560969000	5.439979000	-3.206635000
H	7.690552000	7.508764000	-1.423690000
H	4.728585000	7.177997000	-4.519637000
H	6.807641000	8.218008000	-3.637622000
Cl	5.767063000	0.258904000	-1.956978000
C	5.198968000	2.910318000	-3.893600000
C	7.181201000	3.488553000	-2.800582000
C	7.748908000	3.911279000	-4.000071000
C	7.009300000	3.836357000	-5.168833000
C	5.720625000	3.334550000	-5.114019000
H	8.771558000	4.272471000	-4.022665000
H	7.439513000	4.159538000	-6.113283000
H	5.108295000	3.251600000	-6.007759000
C	7.943533000	3.545903000	-1.529289000
C	9.131464000	4.270911000	-1.406347000

C	9.794613000	4.245506000	-0.187601000
H	9.519367000	4.867175000	-2.226950000
C	8.069792000	2.812981000	0.666907000
C	9.272154000	3.499016000	0.859091000
H	10.719613000	4.802435000	-0.058005000
H	9.780603000	3.442626000	1.818724000
N	5.923157000	3.000096000	-2.761514000
N	7.427465000	2.863556000	-0.503615000
C	3.831188000	2.319353000	-3.823067000
H	3.912103000	1.236869000	-3.662071000
H	3.261665000	2.712889000	-2.973589000
H	3.275293000	2.508578000	-4.746508000
C	7.443501000	1.995994000	1.751208000
H	6.652829000	2.557988000	2.266483000
H	6.964285000	1.109590000	1.323785000
H	8.180574000	1.697388000	2.502770000

Int-F-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -507.39 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	2.910524000	0.333790000	1.605744000
N	4.511202000	1.793365000	0.732551000
C	3.243137000	1.342124000	1.034388000
C	2.436641000	2.565161000	0.620170000
H	1.857367000	2.421077000	-0.298574000
H	1.764679000	2.897504000	1.416439000
H	5.288525000	1.283012000	1.157980000
Ni	5.101419000	2.223188000	-1.051116000
C	3.642492000	3.449248000	0.431567000
H	3.977058000	4.004251000	1.309370000
C	3.988111000	3.923114000	-0.863225000
H	3.224512000	3.729332000	-1.623764000
C	4.737367000	5.170256000	-1.086066000
C	5.545556000	5.769332000	-0.109723000
C	4.661444000	5.793432000	-2.339794000
C	6.244068000	6.939039000	-0.377167000

C	5.362760000	6.961932000	-2.610602000
C	6.159274000	7.543986000	-1.629149000
H	5.650018000	5.301769000	0.869406000
H	4.041315000	5.340824000	-3.115513000
H	6.868578000	7.377992000	0.398636000
H	5.282046000	7.421867000	-3.593542000
H	6.707000000	8.460524000	-1.835143000
Cl	6.046118000	0.196282000	-1.271515000
C	4.786216000	2.226830000	-3.864242000
C	6.668135000	3.409131000	-3.128086000
C	7.001943000	3.738430000	-4.441086000
C	6.186853000	3.319661000	-5.478697000
C	5.068833000	2.554380000	-5.188220000
H	7.904756000	4.301772000	-4.650224000
H	6.431704000	3.574227000	-6.506754000
H	4.414259000	2.189790000	-5.974966000
C	7.527880000	3.825462000	-1.991015000
C	8.551355000	4.763889000	-2.144287000
C	9.353046000	5.051275000	-1.049350000
H	8.712877000	5.280137000	-3.085427000
C	8.054774000	3.504701000	0.237701000
C	9.119325000	4.403937000	0.155189000
H	10.157553000	5.777441000	-1.138130000
H	9.740976000	4.593728000	1.026995000
N	5.568305000	2.673496000	-2.861033000
N	7.279977000	3.243362000	-0.815700000
C	3.627001000	1.352614000	-3.522054000
H	3.986441000	0.466607000	-2.982503000
H	2.919734000	1.864056000	-2.857610000
H	3.092036000	1.042239000	-4.424499000
C	7.722142000	2.781101000	1.503029000
H	6.713691000	3.051154000	1.844409000
H	7.723089000	1.699862000	1.318669000
H	8.431793000	3.007214000	2.304274000

Int-F-2

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	3.650689000	1.461780000	1.850739000
N	5.329371000	2.337204000	0.532256000
C	4.050969000	2.203712000	0.964048000
C	3.122403000	3.110422000	0.166458000
H	2.416145000	2.481712000	-0.392236000
H	2.532480000	3.723713000	0.858443000
H	5.904842000	1.612244000	0.959460000
Ni	5.535505000	2.492168000	-1.338215000
C	3.944001000	3.952641000	-0.746758000
H	4.520771000	4.738671000	-0.256485000
C	3.901909000	3.931802000	-2.108734000
H	3.243141000	3.208667000	-2.595517000
C	4.452448000	4.977193000	-2.983884000
C	5.322278000	5.972511000	-2.523758000
C	4.055700000	5.003870000	-4.323679000
C	5.779756000	6.963185000	-3.381435000
C	4.504192000	6.000432000	-5.180091000
C	5.369976000	6.983290000	-4.712370000
H	5.653923000	5.972684000	-1.486381000
H	3.399128000	4.218353000	-4.693749000
H	6.458080000	7.727378000	-3.008532000
H	4.183841000	6.003688000	-6.219214000
H	5.727454000	7.761921000	-5.382096000
C	3.945003000	-0.828492000	-1.586392000
C	6.229631000	-0.553908000	-1.681238000
C	6.395881000	-1.714904000	-2.436500000
C	5.264509000	-2.449575000	-2.764074000
C	4.024070000	-2.010705000	-2.327963000
H	7.376633000	-2.017403000	-2.792185000
H	5.351913000	-3.354377000	-3.360787000
H	3.118212000	-2.564923000	-2.562003000
C	7.404395000	0.264782000	-1.296669000
C	8.652855000	-0.327395000	-1.114668000
C	9.743345000	0.464449000	-0.791901000
H	8.753737000	-1.404393000	-1.205355000
C	8.295464000	2.377925000	-0.831350000
C	9.565926000	1.832138000	-0.660882000
H	10.722807000	0.017149000	-0.642905000

H	10.397174000	2.489946000	-0.423152000
N	5.034019000	-0.121345000	-1.279089000
N	7.243906000	1.590908000	-1.125856000
C	2.635690000	-0.284509000	-1.112617000
H	2.714504000	0.045978000	-0.069330000
H	2.359675000	0.588125000	-1.721062000
H	1.831463000	-1.021366000	-1.201020000
C	8.056723000	3.845912000	-0.716696000
H	7.655455000	4.232990000	-1.663803000
H	7.315675000	4.050082000	0.066479000
H	8.983684000	4.377730000	-0.482449000
Cl	5.862975000	2.272821000	-3.529720000

Int-F-TS-i

Charge = 0 Multiplicity = 1

Imaginary frequency = -514.82 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	4.102385000	0.915660000	1.905092000
N	5.234533000	2.591101000	0.732487000
C	4.136870000	1.886684000	1.188231000
C	3.020986000	2.786977000	0.679751000
H	2.431174000	2.353916000	-0.133135000
H	2.350794000	3.080848000	1.493056000
H	6.108134000	2.426607000	1.235908000
Ni	5.549747000	2.730749000	-1.182872000
C	3.944547000	3.885815000	0.229957000
H	4.166028000	4.661917000	0.963755000
C	4.134558000	4.158215000	-1.151077000
H	3.391262000	3.722385000	-1.823972000
C	4.719806000	5.442083000	-1.584503000
C	5.527625000	6.218893000	-0.743258000
C	4.469188000	5.919849000	-2.877481000
C	6.059155000	7.429113000	-1.174653000
C	4.997384000	7.128128000	-3.307979000
C	5.795702000	7.891712000	-2.459423000
H	5.758121000	5.870903000	0.264207000
H	3.864240000	5.315475000	-3.550498000

H	6.682548000	8.013362000	-0.500594000
H	4.787446000	7.475919000	-4.317126000
H	6.210181000	8.838273000	-2.798386000
C	3.930162000	-0.545472000	-1.907184000
C	6.215395000	-0.332096000	-1.812403000
C	6.404606000	-1.388167000	-2.705922000
C	5.285684000	-2.038534000	-3.204294000
C	4.029945000	-1.616812000	-2.797666000
H	7.401340000	-1.666009000	-3.036296000
H	5.393696000	-2.857357000	-3.911469000
H	3.128069000	-2.098044000	-3.168254000
C	7.393708000	0.402772000	-1.295846000
C	8.606424000	-0.259770000	-1.104404000
C	9.721848000	0.462823000	-0.714398000
H	8.659686000	-1.334900000	-1.246222000
C	8.364773000	2.441569000	-0.725283000
C	9.605336000	1.833402000	-0.545073000
H	10.674158000	-0.036425000	-0.554105000
H	10.462382000	2.443682000	-0.273391000
N	5.006952000	0.080779000	-1.424976000
N	7.275930000	1.722255000	-1.059355000
C	2.598647000	-0.035760000	-1.459366000
H	2.559694000	0.008545000	-0.364642000
H	2.447764000	0.980036000	-1.849331000
H	1.778307000	-0.664291000	-1.818646000
C	8.207274000	3.920559000	-0.585770000
H	7.748415000	4.339372000	-1.490821000
H	7.549309000	4.181257000	0.252752000
H	9.174654000	4.404072000	-0.419109000
Cl	5.723479000	2.815619000	-3.361609000

Int-G

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	3.655767000	-2.909334000	-4.163927000
N	5.445355000	-1.612699000	-3.318145000
C	4.183778000	-2.152780000	-3.387117000

C	3.767915000	-1.425555000	-2.100592000
H	3.013336000	-0.642617000	-2.236097000
H	3.458397000	-2.093184000	-1.291814000
C	5.022500000	3.913847000	-4.981145000
C	7.429148000	3.867988000	-1.540825000
C	7.336165000	4.734164000	-0.459860000
C	8.271551000	4.612761000	0.560288000
C	9.266477000	3.656902000	0.447194000
C	9.292665000	2.804373000	-0.662980000
N	8.367847000	2.900034000	-1.631843000
H	6.528977000	5.458922000	-0.400198000
H	8.224670000	5.262464000	1.430632000
H	10.031196000	3.551452000	1.212779000
C	6.509806000	3.940488000	-2.690107000
C	5.849527000	5.102628000	-3.072251000
C	5.074319000	5.075425000	-4.223224000
C	5.709341000	2.777259000	-4.555355000
N	6.394904000	2.797984000	-3.396501000
H	5.967250000	6.014608000	-2.494587000
H	4.540884000	5.965725000	-4.546569000
H	4.460826000	3.875716000	-5.910497000
H	6.320052000	-1.846784000	-3.773599000
Ni	7.182404000	1.272190000	-2.536785000
C	5.745927000	1.529219000	-5.372539000
H	5.260968000	0.686607000	-4.865795000
H	5.260802000	1.683265000	-6.340540000
H	6.786160000	1.226018000	-5.540808000
C	10.352030000	1.767450000	-0.806437000
H	9.944402000	0.775625000	-0.573014000
H	10.695607000	1.710018000	-1.843662000
H	11.200539000	1.976098000	-0.147976000
C	5.236877000	-0.922877000	-2.043022000
H	5.810837000	-1.368687000	-1.222552000
C	5.416882000	0.571107000	-2.117432000
H	4.719433000	0.951422000	-2.878822000
C	5.217797000	1.315337000	-0.847355000
C	5.936641000	1.000918000	0.319693000
C	4.327170000	2.399231000	-0.794991000
C	5.770354000	1.744856000	1.480537000
C	4.163098000	3.145030000	0.366603000

C	4.886788000	2.822598000	1.511152000
H	6.656161000	0.182822000	0.292403000
H	3.754497000	2.652159000	-1.689489000
H	6.340686000	1.484651000	2.370100000
H	3.460013000	3.976093000	0.380680000
H	4.759930000	3.402066000	2.423037000
Cl	8.301082000	-0.524606000	-2.094111000

Int-H-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -670.47 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	4.023896000	0.550919000	0.464232000
C	4.813845000	-0.637822000	0.405599000
O	5.869124000	-0.395547000	-0.312732000
N	5.736420000	1.211595000	-0.839097000
C	4.635842000	1.496338000	-0.239598000
C	3.982059000	2.839630000	-0.238823000
O	4.460261000	-1.622569000	0.977374000
H	3.141498000	2.815646000	-0.947721000
H	3.529519000	2.951273000	0.758610000
C	5.512776000	4.489298000	-5.459219000
C	8.476298000	4.033935000	-2.506763000
C	9.580517000	4.860843000	-2.313088000
C	10.461212000	4.566076000	-1.283439000
C	10.232719000	3.448945000	-0.491806000
C	9.120707000	2.646620000	-0.743656000
N	8.256551000	2.960070000	-1.723765000
H	9.748422000	5.722255000	-2.951923000
H	11.328813000	5.197128000	-1.107252000
H	10.913541000	3.180417000	0.311555000
C	7.475213000	4.256467000	-3.569750000
C	7.516393000	5.333513000	-4.451775000
C	6.517145000	5.445788000	-5.406902000
C	5.529880000	3.430422000	-4.552418000
N	6.500230000	3.333480000	-3.632411000
H	8.294209000	6.087480000	-4.381113000

H	6.518840000	6.281827000	-6.102024000
H	4.717167000	4.548913000	-6.197393000
Ni	6.724202000	1.758145000	-2.348404000
C	4.493540000	2.358986000	-4.552156000
H	4.001076000	2.307632000	-3.571379000
H	3.732577000	2.530041000	-5.318901000
H	4.972666000	1.383835000	-4.715631000
C	8.847616000	1.405668000	0.037055000
H	7.897281000	1.485307000	0.577621000
H	8.744229000	0.546161000	-0.637972000
H	9.647212000	1.203283000	0.754915000
C	4.908572000	3.970724000	-0.540631000
H	5.851186000	3.971671000	0.010809000
C	4.611370000	4.961299000	-1.387490000
H	3.662715000	4.907428000	-1.930484000
C	5.428373000	6.136910000	-1.687535000
C	6.659867000	6.390854000	-1.066787000
C	4.967697000	7.053451000	-2.640711000
C	7.400794000	7.517195000	-1.395024000
C	5.709547000	8.180494000	-2.972304000
C	6.931683000	8.417010000	-2.350724000
H	7.047303000	5.699239000	-0.318950000
H	4.012754000	6.867126000	-3.131626000
H	8.353515000	7.694420000	-0.899523000
H	5.330502000	8.878184000	-3.715780000
H	7.512488000	9.301571000	-2.601538000
Cl	7.227585000	0.116404000	-3.793066000

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1'

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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	2.893699000	0.561321000	3.016058000
C	3.270853000	0.911857000	4.297208000
O	3.338901000	2.261400000	4.315293000
N	3.000910000	2.771184000	3.048509000
C	2.759163000	1.726308000	2.343915000
C	2.344615000	1.700105000	0.927729000

O	3.487218000	0.161519000	5.189899000
H	2.302092000	2.734720000	0.572582000
H	3.109310000	1.178476000	0.338178000
C	0.987914000	1.000726000	0.739117000
H	1.053180000	-0.027933000	1.119073000
H	0.230339000	1.508301000	1.352971000
C	0.581255000	0.997049000	-0.656134000
C	0.272016000	1.014212000	-1.827148000
C	-0.104529000	1.033354000	-3.203696000
C	0.035730000	-0.114887000	-3.995750000
C	-0.618899000	2.203184000	-3.780303000
C	-0.331621000	-0.089851000	-5.333987000
C	-0.983659000	2.220865000	-5.119239000
C	-0.841311000	1.076147000	-5.898873000
H	0.434343000	-1.021216000	-3.546037000
H	-0.727333000	3.092153000	-3.163408000
H	-0.219781000	-0.985468000	-5.940511000
H	-1.381817000	3.132871000	-5.557653000
H	-1.128114000	1.092589000	-6.947645000

1'-int-A'

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
O	-1.516022000	5.744052000	1.925158000
C	-1.271327000	7.006007000	2.423557000
O	-0.225395000	6.883785000	3.269779000
N	0.198209000	5.541440000	3.309469000
C	-0.599476000	4.936357000	2.505629000
O	-1.873101000	7.992423000	2.152475000
C	-0.318696000	3.263210000	0.669938000
H	0.645019000	3.703912000	0.377167000
H	-1.072550000	3.777883000	0.059740000
C	-0.318610000	1.827933000	0.338079000
C	-0.452428000	0.618055000	0.676252000
C	-0.581299000	-0.707518000	1.186519000
C	0.556821000	-1.430579000	1.590891000
C	-1.825581000	-1.365237000	1.188920000

C	0.449363000	-2.760010000	1.975394000
C	-1.920231000	-2.695556000	1.570038000
C	-0.786087000	-3.403074000	1.964284000
H	1.527370000	-0.935295000	1.582758000
H	-2.713137000	-0.817670000	0.875951000
H	1.342678000	-3.300190000	2.282834000
H	-2.891337000	-3.186449000	1.559234000
H	-0.865576000	-4.445459000	2.263055000
C	3.893550000	-0.976631000	-1.034570000
C	-0.082952000	-2.006639000	-1.921265000
C	-0.588163000	-3.292426000	-2.101588000
C	-1.938109000	-3.443910000	-2.378433000
C	-2.742743000	-2.315422000	-2.471096000
C	-2.180735000	-1.056693000	-2.270152000
N	-0.873040000	-0.918521000	-1.999924000
H	0.057429000	-4.161189000	-2.015224000
H	-2.360730000	-4.435345000	-2.520403000
H	-3.803884000	-2.398665000	-2.692222000
C	1.329859000	-1.718962000	-1.622009000
C	2.322543000	-2.696780000	-1.586178000
C	3.620253000	-2.315777000	-1.284858000
C	2.859992000	-0.043935000	-1.088476000
N	1.604470000	-0.421363000	-1.383588000
H	2.086482000	-3.736447000	-1.791979000
H	4.415314000	-3.056342000	-1.248481000
H	4.900769000	-0.643961000	-0.796797000
H	0.133972000	1.974222000	-2.361200000
Ni	-0.028155000	0.818673000	-1.307276000
C	3.084474000	1.401364000	-0.797961000
H	2.672099000	1.654572000	0.187994000
H	4.149886000	1.650499000	-0.801265000
H	2.545162000	2.018273000	-1.527997000
C	-2.988279000	0.196576000	-2.327332000
H	-2.474638000	0.947114000	-2.940685000
H	-3.990442000	0.013972000	-2.726514000
H	-3.089707000	0.633951000	-1.325065000
C	-0.581880000	3.502340000	2.162847000
H	-1.547243000	3.056500000	2.437273000
H	0.188572000	3.020897000	2.774752000

1'-int-A'-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -578.24 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	1.268777000	2.017288000	2.629765000
C	1.739678000	1.259372000	3.677029000
O	0.714743000	1.118365000	4.539256000
N	-0.432872000	1.748203000	4.016709000
C	-0.036937000	2.247842000	2.902657000
O	2.843060000	0.825980000	3.775773000
C	-0.467520000	2.781714000	0.490352000
H	0.546054000	3.165902000	0.303215000
H	-1.129402000	3.364468000	-0.163846000
C	-0.519418000	1.341789000	0.130337000
C	-0.823190000	0.181800000	0.618570000
C	-1.366494000	-0.510084000	1.758572000
C	-0.549753000	-1.362737000	2.518583000
C	-2.704756000	-0.338833000	2.149986000
C	-1.043925000	-1.983844000	3.657068000
C	-3.198941000	-0.986338000	3.274670000
C	-2.370890000	-1.802951000	4.040135000
H	0.483162000	-1.514408000	2.203602000
H	-3.347316000	0.314813000	1.559834000
H	-0.388635000	-2.620343000	4.247885000
H	-4.237742000	-0.840805000	3.564657000
H	-2.757512000	-2.297521000	4.927851000
C	4.310099000	-0.585608000	-1.690303000
C	0.603732000	-2.068973000	-2.982728000
C	0.389467000	-3.082038000	-3.916206000
C	-0.910620000	-3.458701000	-4.207371000
C	-1.960369000	-2.812627000	-3.563462000
C	-1.688413000	-1.807057000	-2.641906000
N	-0.420586000	-1.448215000	-2.356978000
H	1.226762000	-3.566151000	-4.409819000
H	-1.106914000	-4.246540000	-4.930021000
H	-2.993460000	-3.081530000	-3.768039000
C	1.934573000	-1.589261000	-2.595755000

C	3.124331000	-2.126907000	-3.084406000
C	4.326455000	-1.612985000	-2.627122000
C	3.092772000	-0.086425000	-1.238087000
N	1.926735000	-0.577158000	-1.701869000
H	3.111415000	-2.939472000	-3.804611000
H	5.269361000	-2.013812000	-2.990156000
H	5.234342000	-0.167755000	-1.299829000
H	0.033095000	1.530378000	-1.526599000
Ni	0.095418000	0.033950000	-1.102002000
C	3.014372000	0.995467000	-0.218054000
H	2.498257000	0.637685000	0.682640000
H	4.007169000	1.351917000	0.070045000
H	2.422412000	1.835322000	-0.605413000
C	-2.775616000	-1.080759000	-1.927363000
H	-2.692990000	-0.000947000	-2.106200000
H	-3.763427000	-1.421939000	-2.250570000
H	-2.679179000	-1.225719000	-0.843574000
C	-0.856156000	3.031343000	1.948557000
H	-0.747776000	4.098972000	2.183611000
H	-1.902145000	2.762663000	2.138813000

1'-int-A-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -786.50 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	6.629040000	1.242004000	-1.787690000
C	6.484929000	-0.061896000	-2.313684000
O	5.702996000	-0.740812000	-1.518588000
N	5.172411000	0.303463000	-0.361729000
C	5.839975000	1.341509000	-0.717644000
C	5.789229000	2.677655000	-0.053569000
O	7.022523000	-0.377056000	-3.332986000
H	5.846762000	2.546612000	1.032499000
H	6.675965000	3.228071000	-0.386441000
C	3.199527000	1.662193000	4.598501000
C	1.521543000	1.801161000	0.743440000
C	0.444375000	2.584734000	0.330550000

C	0.004651000	2.478506000	-0.979329000
C	0.636010000	1.584427000	-1.835973000
C	1.713258000	0.832271000	-1.374453000
N	2.150084000	0.956415000	-0.106041000
H	-0.041787000	3.267367000	1.021349000
H	-0.830827000	3.080593000	-1.327670000
H	0.311424000	1.466443000	-2.867045000
C	2.058866000	1.816624000	2.110241000
C	1.493318000	2.539431000	3.161453000
C	2.074586000	2.463198000	4.416516000
C	3.716253000	0.958518000	3.518245000
N	3.153224000	1.045207000	2.297540000
H	0.604551000	3.143368000	3.003730000
H	1.651722000	3.016406000	5.251136000
H	3.675167000	1.574896000	5.572094000
H	3.109270000	-1.607783000	1.029302000
Ni	3.638926000	-0.143278000	0.734644000
C	4.896976000	0.055908000	3.626036000
H	5.292261000	0.015140000	4.645015000
H	4.613029000	-0.956515000	3.303177000
H	5.699077000	0.383144000	2.950583000
C	2.426188000	-0.140197000	-2.248440000
H	3.434550000	0.223764000	-2.481331000
H	2.550455000	-1.098371000	-1.726595000
H	1.896856000	-0.291975000	-3.194518000
C	4.509391000	3.458414000	-0.414732000
H	3.683704000	3.102580000	0.216566000
H	4.661129000	4.516972000	-0.168019000
C	4.146786000	3.277597000	-1.811373000
C	3.886813000	2.964044000	-2.952862000
C	3.554423000	2.541469000	-4.273563000
C	4.405950000	1.667038000	-4.965239000
C	2.348091000	2.941670000	-4.865087000
C	4.046856000	1.200149000	-6.222340000
C	1.999565000	2.471459000	-6.124144000
C	2.846001000	1.599015000	-6.803658000
H	5.342163000	1.350084000	-4.506548000
H	1.693060000	3.618808000	-4.320397000
H	4.708842000	0.516873000	-6.748299000
H	1.062749000	2.786237000	-6.578244000

H	2.568860000	1.228695000	-7.787806000
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int-B_{chiral}

Charge = 0 Multiplicity = 2

Cartesian coordinates:

ATOM	X	Y	Z
O	7.484058000	-1.050302000	-10.826847000
C	7.484414000	-1.281755000	-9.625664000
C	6.351922000	-2.132050000	-8.996576000
H	6.763118000	-2.887198000	-8.312428000
H	5.843160000	-2.632866000	-9.829354000
C	5.449781000	-1.200376000	-8.266348000
H	5.015613000	-0.404109000	-8.877179000
C	5.231035000	-1.216918000	-6.945070000
H	5.648203000	-2.047312000	-6.365018000
C	4.516629000	-0.201571000	-6.172335000
C	4.224705000	1.070738000	-6.691466000
C	4.146715000	-0.468413000	-4.847204000
C	3.563390000	2.019400000	-5.925477000
C	3.490250000	0.483495000	-4.075604000
C	3.191860000	1.732066000	-4.612248000
H	4.545612000	1.319298000	-7.703042000
H	4.374963000	-1.447146000	-4.423816000
H	3.354849000	3.000791000	-6.349445000
H	3.208247000	0.247637000	-3.051617000
H	2.677560000	2.479309000	-4.011937000
Ni	8.041501000	0.538347000	-7.681346000
C	7.234747000	1.632152000	-5.234855000
C	6.674151000	2.423622000	-4.249498000
C	6.369806000	3.739083000	-4.576101000
C	6.641751000	4.186627000	-5.857615000
H	6.478672000	2.000635000	-3.268898000
H	5.926495000	4.405038000	-3.840422000
H	6.417751000	5.208877000	-6.151792000
N	7.490783000	2.048766000	-6.500390000
C	7.550035000	3.815584000	-8.197504000
H	7.334406000	2.964042000	-8.860146000
C	7.646098000	0.254643000	-4.997853000

C	8.598383000	-1.713896000	-5.364050000
H	8.220259000	-2.485771000	-6.052801000
C	10.124556000	-1.911846000	-5.231979000
C	10.740976000	-0.854654000	-4.318130000
H	11.819792000	-1.029906000	-4.225390000
H	10.606801000	0.152871000	-4.730594000
H	10.321886000	-0.871660000	-3.302881000
C	10.378981000	-3.308531000	-4.664476000
H	9.984878000	-3.436174000	-3.647532000
H	9.932188000	-4.081991000	-5.303226000
H	11.457656000	-3.501393000	-4.618018000
C	10.765289000	-1.819741000	-6.614496000
H	10.338825000	-2.557994000	-7.304418000
H	10.608749000	-0.838230000	-7.073725000
H	11.844674000	-2.002900000	-6.535318000
C	9.040632000	4.071977000	-8.306963000
C	9.744990000	3.571580000	-9.402563000
C	9.728995000	4.810410000	-7.341658000
C	11.108664000	3.810625000	-9.534745000
H	9.220820000	2.974327000	-10.146825000
C	11.092270000	5.053140000	-7.474101000
H	9.192180000	5.201758000	-6.476736000
C	11.785335000	4.552987000	-8.572295000
H	11.644275000	3.406625000	-10.390453000
H	11.614586000	5.631798000	-6.715339000
H	12.852355000	4.736992000	-8.674262000
C	6.662216000	4.963572000	-8.640153000
C	5.309209000	4.691907000	-8.873544000
C	7.121130000	6.267412000	-8.814799000
C	4.435144000	5.696807000	-9.263546000
H	4.946700000	3.669831000	-8.749005000
C	6.245471000	7.278295000	-9.207553000
H	8.173254000	6.493623000	-8.653633000
C	4.903050000	6.998706000	-9.430288000
H	3.388485000	5.464034000	-9.446691000
H	6.621029000	8.290092000	-9.343655000
H	4.222896000	7.788706000	-9.739987000
O	7.411287000	-0.345430000	-3.829833000
N	8.252720000	-0.401008000	-5.912891000
C	7.202212000	3.325931000	-6.809927000

C	7.818100000	-1.720924000	-4.031845000
H	8.408392000	-2.024147000	-3.162625000
H	6.905557000	-2.328549000	-4.072811000
N	8.409051000	-0.857185000	-8.727801000
H	7.757425000	1.201062000	-8.935934000

int-B_{R-a}-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -427.30 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	5.586264000	1.137179000	1.338927000
N	4.308583000	0.373427000	-0.449943000
C	5.004607000	1.289895000	0.278998000
C	4.833085000	2.539337000	-0.569251000
H	5.786068000	3.000286000	-0.856957000
H	4.216650000	3.300112000	-0.079369000
C	4.114175000	1.866101000	-1.723022000
H	3.026422000	1.946586000	-1.730678000
C	4.734738000	1.689220000	-3.012765000
H	5.779020000	2.015649000	-3.072184000
C	3.966521000	1.920607000	-4.261023000
C	2.642079000	1.499534000	-4.418897000
C	4.575344000	2.604844000	-5.315811000
C	1.950495000	1.755751000	-5.594477000
C	3.883629000	2.862971000	-6.494602000
C	2.566948000	2.440751000	-6.639210000
H	2.152284000	0.934257000	-3.625095000
H	5.607035000	2.938295000	-5.206514000
H	0.927240000	1.398456000	-5.697530000
H	4.377886000	3.398225000	-7.302712000
H	2.024873000	2.638627000	-7.561028000
H	5.072990000	-0.231738000	-3.623162000
Ni	4.783300000	-0.088938000	-2.173169000
C	5.830243000	-2.839442000	-1.976902000
C	5.807044000	-4.226324000	-1.922649000
C	4.576336000	-4.870701000	-1.939916000
C	3.425352000	-4.106976000	-1.994640000

H	6.742645000	-4.771378000	-1.861031000
H	4.520299000	-5.955353000	-1.900656000
H	2.440454000	-4.567134000	-1.987115000
N	4.707363000	-2.096491000	-2.057700000
C	2.262088000	-1.870235000	-2.118048000
H	2.589717000	-0.837518000	-1.912935000
C	7.111979000	-2.122124000	-1.929244000
C	8.702279000	-0.607287000	-1.801700000
H	9.011471000	-0.010268000	-2.674995000
C	9.049000000	0.216832000	-0.544851000
C	10.565790000	0.391501000	-0.474948000
H	10.825803000	1.064898000	0.351040000
H	11.093873000	-0.554263000	-0.296563000
H	10.960803000	0.832881000	-1.400795000
C	8.400520000	1.590377000	-0.684973000
H	8.806504000	2.134434000	-1.549918000
H	7.320159000	1.483690000	-0.812165000
H	8.571623000	2.193745000	0.215266000
C	8.530125000	-0.461846000	0.720221000
H	7.434192000	-0.483907000	0.744345000
H	8.910865000	-1.487374000	0.827898000
H	8.855339000	0.101234000	1.603727000
C	1.334137000	-2.259549000	-0.978041000
C	1.600070000	-1.737114000	0.290502000
C	0.279310000	-3.160200000	-1.136489000
C	0.819533000	-2.108059000	1.379572000
H	2.428783000	-1.035425000	0.408717000
C	-0.499199000	-3.531501000	-0.044300000
H	0.055285000	-3.560806000	-2.124886000
C	-0.231105000	-3.006464000	1.215723000
H	1.033576000	-1.690918000	2.360994000
H	-1.321193000	-4.230966000	-0.180971000
H	-0.842422000	-3.294515000	2.068028000
C	1.623350000	-1.861669000	-3.496049000
C	2.254912000	-2.392789000	-4.620297000
C	0.390720000	-1.219850000	-3.666179000
C	1.666610000	-2.299230000	-5.879724000
H	3.225878000	-2.875664000	-4.523248000
C	-0.199554000	-1.130194000	-4.919937000
H	-0.110076000	-0.792344000	-2.798152000

C	0.436695000	-1.673710000	-6.034262000
H	2.179193000	-2.717302000	-6.742955000
H	-1.161836000	-0.633725000	-5.027830000
H	-0.023920000	-1.603855000	-7.016883000
O	8.208276000	-2.911628000	-1.890795000
N	7.260748000	-0.859545000	-1.909015000
C	3.516802000	-2.713649000	-2.052094000
C	9.331385000	-2.015745000	-1.859516000
H	9.937783000	-2.266967000	-0.982053000
H	9.930532000	-2.187143000	-2.760397000

int-B_{R-b}-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -443.86 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	5.969356000	-0.202958000	1.121263000
N	4.183823000	-0.294283000	-0.367738000
C	5.157212000	0.315069000	0.373157000
C	4.936109000	1.776612000	0.012878000
H	5.834000000	2.245895000	-0.406533000
H	4.586035000	2.380320000	0.856909000
C	3.864518000	1.520450000	-1.027801000
H	2.828678000	1.562967000	-0.692935000
C	4.094714000	1.763690000	-2.423567000
H	5.063682000	2.211226000	-2.667502000
C	2.997743000	2.151883000	-3.339655000
C	1.657749000	1.827829000	-3.097942000
C	3.302787000	2.877385000	-4.495861000
C	0.660615000	2.214779000	-3.985330000
C	2.307298000	3.266073000	-5.382683000
C	0.978358000	2.936317000	-5.132079000
H	1.389230000	1.249974000	-2.213922000
H	4.343314000	3.130591000	-4.698975000
H	-0.373890000	1.948668000	-3.778004000
H	2.570542000	3.831288000	-6.274291000
H	0.196660000	3.239119000	-5.824743000
H	4.569816000	0.067781000	-3.664416000

Ni	4.414011000	-0.167252000	-2.198581000
C	7.150880000	-2.054546000	-2.143770000
C	8.284589000	-2.830024000	-1.922454000
C	9.513182000	-2.180798000	-1.885507000
C	9.557460000	-0.811629000	-2.089102000
H	8.197117000	-3.902915000	-1.785178000
H	10.426860000	-2.742296000	-1.707651000
H	10.501521000	-0.271385000	-2.085651000
N	7.181609000	-0.728848000	-2.318709000
C	8.342294000	1.382924000	-2.520277000
H	7.386991000	1.573622000	-3.037614000
C	5.825493000	-2.683278000	-2.206858000
C	3.635517000	-3.076947000	-2.260237000
H	3.161857000	-2.849016000	-1.289588000
C	2.540876000	-3.022337000	-3.339962000
C	1.588617000	-4.195592000	-3.099700000
H	0.748549000	-4.148658000	-3.803291000
H	2.075275000	-5.169557000	-3.241841000
H	1.173009000	-4.166871000	-2.083130000
C	1.754565000	-1.720095000	-3.199294000
H	1.357859000	-1.602425000	-2.180771000
H	2.381040000	-0.847088000	-3.423990000
H	0.908025000	-1.708740000	-3.898553000
C	3.135775000	-3.097596000	-4.743518000
H	3.813306000	-2.254766000	-4.925747000
H	3.690384000	-4.028932000	-4.918917000
H	2.333024000	-3.054282000	-5.490181000
C	9.456867000	1.810989000	-3.457975000
C	9.285402000	1.630826000	-4.832198000
C	10.669781000	2.322405000	-2.994104000
C	10.298626000	1.957954000	-5.725243000
H	8.341143000	1.226712000	-5.198890000
C	11.687577000	2.647186000	-3.886265000
H	10.810969000	2.477181000	-1.925016000
C	11.504995000	2.467738000	-5.253335000
H	10.145324000	1.817702000	-6.792981000
H	12.626331000	3.047542000	-3.509598000
H	12.298684000	2.727813000	-5.949912000
C	8.301856000	2.162764000	-1.217210000
C	8.338767000	1.553331000	0.034986000

C	8.161065000	3.555332000	-1.283150000
C	8.239260000	2.316856000	1.197543000
H	8.381387000	0.470503000	0.126291000
C	8.072173000	4.317107000	-0.126758000
H	8.125640000	4.038864000	-2.259664000
C	8.113796000	3.697097000	1.122104000
H	8.230897000	1.811615000	2.160000000
H	7.962996000	5.397130000	-0.198027000
H	8.034327000	4.291213000	2.029678000
O	5.780751000	-4.005460000	-1.990832000
N	4.712392000	-2.089721000	-2.430694000
C	8.361819000	-0.115874000	-2.307717000
C	4.410814000	-4.399905000	-2.182411000
H	4.359606000	-4.983694000	-3.110972000
H	4.116834000	-5.037519000	-1.344696000

int-B_{S-a}-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -442.58 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	4.066363000	-0.472203000	-0.502334000
N	5.771204000	0.488772000	-1.768857000
C	4.535017000	0.407562000	-1.210723000
C	3.900786000	1.700068000	-1.696542000
H	3.745296000	2.420803000	-0.887178000
H	2.946588000	1.557233000	-2.221032000
C	5.035520000	2.097433000	-2.621376000
H	5.753270000	2.819495000	-2.231811000
C	4.879118000	2.055387000	-4.051134000
H	3.910347000	1.682016000	-4.400868000
C	5.470257000	3.087117000	-4.936880000
C	6.621161000	3.811672000	-4.609785000
C	4.836074000	3.362011000	-6.153106000
C	7.120627000	4.779232000	-5.473532000
C	5.335541000	4.328502000	-7.016570000
C	6.481292000	5.043805000	-6.681401000
H	7.143881000	3.609893000	-3.675221000

H	3.939842000	2.798366000	-6.416738000
H	8.017588000	5.331061000	-5.199657000
H	4.824676000	4.526874000	-7.956620000
H	6.873080000	5.802477000	-7.354914000
H	5.925769000	0.609897000	-5.093669000
Ni	5.929969000	0.447932000	-3.615398000
C	5.403915000	-2.808241000	-3.926822000
C	5.145754000	-4.173208000	-4.033987000
C	3.827561000	-4.586823000	-3.896580000
C	2.840593000	-3.641604000	-3.653995000
H	5.954537000	-4.873963000	-4.215297000
H	3.571657000	-5.640740000	-3.972555000
H	1.801793000	-3.935386000	-3.527970000
N	4.461407000	-1.892579000	-3.702674000
C	2.200209000	-1.186337000	-3.294538000
H	2.707598000	-0.559250000	-2.548883000
C	6.771010000	-2.291847000	-4.068643000
C	8.567950000	-0.983501000	-4.243422000
H	8.652383000	-0.442821000	-5.201985000
C	9.406729000	-0.212519000	-3.205551000
C	10.878126000	-0.346296000	-3.606060000
H	11.503962000	0.254640000	-2.935356000
H	11.242736000	-1.379920000	-3.544443000
H	11.047012000	0.015013000	-4.630122000
C	9.035009000	1.269025000	-3.242609000
H	9.124477000	1.681826000	-4.257282000
H	8.006779000	1.429479000	-2.894612000
H	9.702015000	1.838436000	-2.582393000
C	9.180580000	-0.751173000	-1.795032000
H	8.137783000	-0.612177000	-1.483510000
H	9.433066000	-1.816225000	-1.704463000
H	9.819697000	-0.208799000	-1.086934000
C	0.931151000	-1.676217000	-2.632389000
C	0.886034000	-1.737078000	-1.238011000
C	-0.171868000	-2.103824000	-3.373331000
C	-0.249244000	-2.221832000	-0.596302000
H	1.752992000	-1.394593000	-0.669072000
C	-1.304288000	-2.592388000	-2.729912000
H	-0.140434000	-2.044159000	-4.461661000
C	-1.344702000	-2.651816000	-1.339578000

H	-0.279016000	-2.260742000	0.490399000
H	-2.160132000	-2.921910000	-3.315304000
H	-2.232406000	-3.028640000	-0.836252000
C	1.949457000	-0.308340000	-4.508140000
C	2.423585000	-0.607168000	-5.784719000
C	1.220769000	0.873615000	-4.327833000
C	2.191254000	0.260093000	-6.850616000
H	2.996536000	-1.516689000	-5.953234000
C	0.989904000	1.741669000	-5.386730000
H	0.825288000	1.103083000	-3.337547000
C	1.477480000	1.437004000	-6.656541000
H	2.574058000	0.010847000	-7.837795000
H	0.426719000	2.657534000	-5.222439000
H	1.298482000	2.113967000	-7.489042000
O	7.716720000	-3.178470000	-4.408721000
N	7.134320000	-1.071342000	-3.927508000
C	3.198007000	-2.293149000	-3.558290000
C	8.962871000	-2.460804000	-4.413854000
H	9.567424000	-2.841666000	-3.581633000
H	9.479159000	-2.676088000	-5.353484000

int-B_{S-b}-TS

Charge = 0 Multiplicity = 2

Imaginary frequency = -539.59 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	3.622029000	-2.296293000	-1.853528000
N	4.870437000	-0.330155000	-2.126561000
C	3.755787000	-1.085621000	-1.877163000
C	2.752477000	0.022495000	-1.596944000
H	2.429978000	0.045553000	-0.550901000
H	1.865617000	-0.030436000	-2.240795000
C	3.686341000	1.163156000	-1.955393000
H	4.196317000	1.670950000	-1.137220000
C	3.492018000	1.892128000	-3.150723000
H	2.708960000	1.530344000	-3.824174000
C	3.957144000	3.251722000	-3.383907000
C	4.903596000	3.895303000	-2.566635000

C	3.471556000	3.956437000	-4.499037000
C	5.348239000	5.177503000	-2.861246000
C	3.915412000	5.239830000	-4.790634000
C	4.863110000	5.858498000	-3.977405000
H	5.317145000	3.372311000	-1.705063000
H	2.734096000	3.473895000	-5.141636000
H	6.086615000	5.648813000	-2.215425000
H	3.517654000	5.762413000	-5.658670000
H	5.212711000	6.862728000	-4.204047000
H	5.951252000	-0.582002000	-4.184300000
Ni	5.055726000	0.477462000	-3.708150000
C	3.944945000	0.143333000	-6.799339000
C	3.610909000	-0.122364000	-8.125496000
C	2.761220000	-1.194143000	-8.369545000
C	2.297072000	-1.948548000	-7.302372000
H	4.019593000	0.483369000	-8.928076000
H	2.474573000	-1.446868000	-9.387443000
H	1.654361000	-2.810559000	-7.462978000
N	3.472256000	-0.555582000	-5.763539000
C	2.190977000	-2.338569000	-4.774642000
H	2.989913000	-2.206545000	-4.029395000
C	4.903166000	1.209189000	-6.477546000
C	6.396325000	2.546997000	-5.482163000
H	6.063131000	3.346010000	-4.806615000
C	7.854286000	2.213050000	-5.103600000
C	8.363485000	0.997441000	-5.871837000
H	9.420301000	0.818963000	-5.637207000
H	7.801291000	0.096421000	-5.598166000
H	8.290085000	1.131038000	-6.960265000
C	8.704613000	3.446347000	-5.423394000
H	8.780678000	3.649384000	-6.499095000
H	8.295321000	4.342204000	-4.934261000
H	9.726154000	3.301129000	-5.051642000
C	7.956830000	1.961070000	-3.599059000
H	7.620400000	2.841963000	-3.034683000
H	7.356659000	1.099107000	-3.279846000
H	9.001092000	1.763552000	-3.324356000
C	2.052066000	-3.829687000	-5.002029000
C	3.116484000	-4.669066000	-4.671838000
C	0.891189000	-4.389420000	-5.541630000

C	3.030672000	-6.039635000	-4.894844000
H	4.006746000	-4.237735000	-4.215086000
C	0.806347000	-5.758353000	-5.770291000
H	0.041030000	-3.743811000	-5.765252000
C	1.878276000	-6.586804000	-5.449715000
H	3.864790000	-6.683322000	-4.624544000
H	-0.103960000	-6.181530000	-6.189828000
H	1.809641000	-7.658782000	-5.621011000
C	0.940679000	-1.727765000	-4.165940000
C	0.212246000	-0.701560000	-4.765269000
C	0.521466000	-2.214691000	-2.921683000
C	-0.910493000	-0.166099000	-4.133087000
H	0.522598000	-0.303631000	-5.730812000
C	-0.598182000	-1.686133000	-2.296001000
H	1.117095000	-2.986297000	-2.435266000
C	-1.319743000	-0.656767000	-2.900124000
H	-1.465767000	0.637138000	-4.612950000
H	-0.905702000	-2.071223000	-1.326172000
H	-2.195239000	-0.239184000	-2.408038000
O	5.255405000	2.016131000	-7.486609000
N	5.455508000	1.417945000	-5.337540000
C	2.672659000	-1.596314000	-6.000637000
C	6.183284000	2.973225000	-6.946068000
H	7.089646000	2.936414000	-7.559280000
H	5.733604000	3.968441000	-7.033437000

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int-D_{chiral}

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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	8.332614000	-3.889509000	-7.175759000
C	7.767199000	-2.819588000	-7.432096000
C	6.264559000	-2.728306000	-7.118405000
H	6.113389000	-3.190070000	-6.132287000
H	5.790728000	-3.409251000	-7.841126000
C	5.628052000	-1.386465000	-7.179890000
H	5.648838000	-0.887642000	-8.150463000
C	5.048404000	-0.787501000	-6.127653000

H	5.026368000	-1.332652000	-5.177604000
C	4.455035000	0.547393000	-6.086141000
C	4.449753000	1.417226000	-7.189182000
C	3.889335000	1.007394000	-4.888578000
C	3.896788000	2.685971000	-7.094879000
C	3.333747000	2.277824000	-4.792946000
C	3.335555000	3.125577000	-5.896105000
H	4.897893000	1.091380000	-8.128123000
H	3.890456000	0.347504000	-4.020727000
H	3.915359000	3.345537000	-7.962619000
H	2.896119000	2.606203000	-3.852394000
H	2.900604000	4.120166000	-5.826465000
Ni	8.089428000	0.034448000	-7.568342000
C	7.450470000	1.960438000	-5.690733000
C	6.948758000	3.083292000	-5.059866000
C	6.756704000	4.223479000	-5.829968000
C	7.082521000	4.181698000	-7.174801000
H	6.713436000	3.042944000	-4.000779000
H	6.360420000	5.132440000	-5.385145000
H	6.950933000	5.055045000	-7.808633000
N	7.732795000	1.890684000	-7.015414000
C	7.965580000	2.950570000	-9.209893000
H	7.688122000	1.938151000	-9.539422000
C	7.764783000	0.725279000	-4.978135000
C	8.572272000	-1.308778000	-4.611201000
H	8.148434000	-2.234017000	-5.028951000
C	10.065982000	-1.583123000	-4.333220000
C	10.755267000	-0.359043000	-3.735486000
H	11.813368000	-0.582949000	-3.551756000
H	10.714980000	0.494201000	-4.424303000
H	10.320582000	-0.048005000	-2.775840000
C	10.152628000	-2.768853000	-3.372607000
H	9.679036000	-2.567037000	-2.402217000
H	9.677983000	-3.656935000	-3.810484000
H	11.202919000	-3.015524000	-3.174451000
C	10.758015000	-1.968397000	-5.640024000
H	10.261174000	-2.825732000	-6.115203000
H	10.755921000	-1.131508000	-6.348944000
H	11.802662000	-2.238315000	-5.437370000
C	9.471510000	3.043919000	-9.359695000

C	10.115372000	2.213251000	-10.277977000
C	10.234161000	3.953619000	-8.624621000
C	11.490992000	2.293094000	-10.462661000
H	9.527762000	1.490217000	-10.841937000
C	11.610840000	4.036634000	-8.809269000
H	9.746920000	4.604365000	-7.897944000
C	12.242569000	3.206185000	-9.729243000
H	11.978036000	1.634514000	-11.178047000
H	12.191448000	4.750600000	-8.229271000
H	13.319138000	3.266750000	-9.870472000
C	7.179178000	3.935895000	-10.052418000
C	5.836958000	3.645928000	-10.319794000
C	7.716424000	5.125432000	-10.540927000
C	5.046256000	4.526930000	-11.045489000
H	5.415891000	2.707493000	-9.953850000
C	6.925565000	6.010643000	-11.271060000
H	8.763712000	5.358133000	-10.356194000
C	5.590595000	5.717607000	-11.522316000
H	4.005950000	4.280820000	-11.247183000
H	7.360634000	6.933677000	-11.647928000
H	4.976387000	6.409249000	-12.094096000
O	7.424784000	0.564069000	-3.699628000
N	8.371833000	-0.225180000	-5.579945000
C	7.566888000	3.002986000	-7.753434000
C	7.753685000	-0.817107000	-3.397766000
H	8.299029000	-0.828004000	-2.449622000
H	6.807919000	-1.356470000	-3.271687000
N	8.348823000	-1.754862000	-8.002161000
H	9.315046000	-1.983060000	-8.228673000
H	7.762763000	0.214803000	-8.971396000

int-D_{R-a}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -521.87 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	10.512833000	-0.721814000	-10.381741000
C	9.552287000	-0.838207000	-9.657502000

C	8.606948000	-2.007195000	-9.416381000
H	8.972396000	-2.732757000	-8.681316000
H	8.353146000	-2.532067000	-10.341848000
C	7.510207000	-1.111513000	-8.881598000
H	6.838222000	-0.701593000	-9.640200000
C	7.049894000	-1.256897000	-7.544348000
H	7.387335000	-2.159960000	-7.027081000
C	5.798831000	-0.670147000	-7.069902000
C	5.060885000	0.262888000	-7.817948000
C	5.297480000	-1.006140000	-5.799817000
C	3.892931000	0.827301000	-7.321638000
C	4.142804000	-0.423731000	-5.293644000
C	3.428631000	0.502989000	-6.049400000
H	5.418844000	0.569302000	-8.801805000
H	5.832032000	-1.749878000	-5.205245000
H	3.339162000	1.534149000	-7.940471000
H	3.789674000	-0.705641000	-4.303121000
H	2.518758000	0.952669000	-5.659362000
Ni	8.601697000	0.065873000	-7.056730000
C	7.360821000	2.136883000	-4.802825000
C	7.284661000	3.138544000	-3.834784000
C	6.894460000	4.402964000	-4.249757000
C	6.563121000	4.605386000	-5.582846000
H	7.536974000	2.923545000	-2.801067000
H	6.840630000	5.223967000	-3.538968000
H	6.235121000	5.579973000	-5.934965000
N	7.045851000	2.319446000	-6.084914000
C	6.213103000	3.635155000	-7.925602000
H	5.535563000	2.778643000	-8.064304000
C	7.825215000	0.796119000	-4.422589000
C	8.732295000	-1.247346000	-4.381646000
H	8.197228000	-2.121585000	-4.788482000
C	10.240601000	-1.579713000	-4.411916000
C	11.073195000	-0.359679000	-4.028095000
H	12.137069000	-0.626109000	-4.000158000
H	10.943659000	0.445213000	-4.761831000
H	10.809063000	0.028812000	-3.034583000
C	10.494408000	-2.729932000	-3.433955000
H	10.319887000	-2.451678000	-2.387089000
H	9.861200000	-3.597446000	-3.666509000

H	11.539073000	-3.055208000	-3.508062000
C	10.642043000	-2.056933000	-5.807442000
H	10.061335000	-2.943298000	-6.101096000
H	10.491489000	-1.272951000	-6.562780000
H	11.703362000	-2.336190000	-5.816481000
C	7.355591000	3.427331000	-8.897136000
C	7.057313000	2.985546000	-10.189810000
C	8.684993000	3.688073000	-8.568832000
C	8.062645000	2.796080000	-11.130201000
H	6.016581000	2.793266000	-10.454376000
C	9.696987000	3.494607000	-9.507373000
H	8.940159000	4.015323000	-7.562118000
C	9.390951000	3.045447000	-10.788732000
H	7.813491000	2.441731000	-12.127776000
H	10.731492000	3.677644000	-9.227214000
H	10.184269000	2.872246000	-11.511293000
C	5.406897000	4.886069000	-8.210668000
C	4.059733000	4.915510000	-7.840597000
C	5.972980000	6.027847000	-8.776867000
C	3.291692000	6.056431000	-8.037098000
H	3.620871000	4.028430000	-7.380910000
C	5.206113000	7.173401000	-8.972936000
H	7.020967000	6.015367000	-9.073174000
C	3.864793000	7.190914000	-8.606034000
H	2.242990000	6.060636000	-7.748014000
H	5.660292000	8.055769000	-9.418533000
H	3.266056000	8.084925000	-8.764517000
O	7.702138000	0.472102000	-3.126835000
N	8.365469000	-0.074604000	-5.194578000
C	6.631911000	3.528264000	-6.471326000
C	8.176213000	-0.876413000	-2.993618000
H	8.925947000	-0.889254000	-2.196147000
H	7.329668000	-1.502954000	-2.691029000
N	8.867836000	0.137221000	-8.958867000
H	9.040844000	1.099946000	-9.254652000
H	9.726219000	1.028405000	-6.828659000

int-D_{R-b}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -519.49 cm^{-1}

Cartesian coordinates:

ATOM	X	Y	Z
O	6.853242000	-3.035155000	-9.587036000
C	6.319887000	-2.238161000	-8.854692000
C	5.015597000	-2.282811000	-8.080367000
H	5.050519000	-2.882588000	-7.163843000
H	4.187407000	-2.632109000	-8.704414000
C	5.003188000	-0.788690000	-7.823210000
H	4.454116000	-0.188375000	-8.553539000
C	5.124007000	-0.309274000	-6.484945000
H	5.157083000	-1.098466000	-5.726497000
C	4.551586000	0.950651000	-6.014827000
C	4.028344000	1.942348000	-6.861737000
C	4.512141000	1.212038000	-4.633087000
C	3.511498000	3.128966000	-6.357278000
C	4.000707000	2.400307000	-4.128644000
C	3.501919000	3.376381000	-4.986585000
H	4.020113000	1.780465000	-7.937652000
H	4.896906000	0.452498000	-3.949690000
H	3.104723000	3.868314000	-7.047560000
H	3.994614000	2.565569000	-3.052328000
H	3.101893000	4.308105000	-4.594339000
Ni	7.193856000	-0.253950000	-6.880289000
C	7.506517000	1.865065000	-5.055709000
C	7.637896000	2.479463000	-3.814955000
C	7.981109000	1.704687000	-2.718351000
C	8.212608000	0.350136000	-2.906288000
H	7.472917000	3.549040000	-3.739102000
H	8.088417000	2.153732000	-1.734529000
H	8.530184000	-0.289172000	-2.085813000
N	7.670363000	0.534048000	-5.226307000
C	8.283919000	-1.687266000	-4.421073000
H	8.589683000	-1.734311000	-5.480738000
C	7.307815000	2.702444000	-6.251280000
C	7.541525000	3.638895000	-8.209634000
H	8.569976000	4.048736000	-8.231592000
C	7.126915000	3.462287000	-9.674310000

C	5.806193000	2.713775000	-9.813066000
H	5.552574000	2.598815000	-10.874772000
H	5.876979000	1.713203000	-9.365863000
H	4.975338000	3.246455000	-9.331818000
C	7.008324000	4.844850000	-10.314762000
H	6.183062000	5.427408000	-9.883448000
H	7.934837000	5.422179000	-10.190059000
H	6.816707000	4.752821000	-11.391204000
C	8.226607000	2.669372000	-10.379919000
H	9.174850000	3.223158000	-10.378948000
H	8.403598000	1.710983000	-9.876852000
H	7.952935000	2.474122000	-11.424567000
C	7.026621000	-2.523092000	-4.301695000
C	6.860264000	-3.608885000	-5.164034000
C	6.046328000	-2.273814000	-3.339766000
C	5.736358000	-4.423153000	-5.072681000
H	7.616797000	-3.803517000	-5.924971000
C	4.914777000	-3.080713000	-3.253108000
H	6.162330000	-1.432834000	-2.655779000
C	4.755854000	-4.156651000	-4.120227000
H	5.622101000	-5.261963000	-5.756114000
H	4.154970000	-2.865490000	-2.505236000
H	3.871718000	-4.786158000	-4.054067000
C	9.447376000	-2.207159000	-3.595255000
C	10.735086000	-1.789915000	-3.946579000
C	9.288788000	-3.053594000	-2.499380000
C	11.840012000	-2.207756000	-3.217666000
H	10.858957000	-1.132385000	-4.808561000
C	10.397061000	-3.471985000	-1.765769000
H	8.293216000	-3.396741000	-2.222489000
C	11.672860000	-3.051245000	-2.121273000
H	12.835712000	-1.879803000	-3.507717000
H	10.259207000	-4.135090000	-0.914477000
H	12.537030000	-3.382871000	-1.550267000
O	6.880544000	3.966225000	-6.008937000
N	7.622203000	2.385873000	-7.445260000
C	8.045109000	-0.215825000	-4.168918000
C	6.681961000	4.533605000	-7.316829000
H	5.607775000	4.469501000	-7.549876000
H	6.990842000	5.581794000	-7.289948000

N	6.651328000	-0.912066000	-8.612422000
H	7.239233000	-0.458497000	-9.313533000
H	8.643904000	-0.421416000	-7.217911000

int-D_{R-c}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -459.90 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	6.979494000	0.939243000	-8.870931000
C	7.046677000	0.319205000	-7.831077000
C	6.425763000	-0.999785000	-7.396151000
H	6.992234000	-1.881581000	-7.717696000
H	5.386237000	-1.102109000	-7.721858000
C	6.580475000	-0.691219000	-5.924315000
H	5.783107000	-0.074325000	-5.501696000
C	7.333553000	-1.517423000	-5.030368000
H	7.635403000	-2.483697000	-5.449221000
C	6.922942000	-1.566932000	-3.592434000
C	5.564443000	-1.519820000	-3.245074000
C	7.847552000	-1.704054000	-2.548092000
C	5.146188000	-1.578349000	-1.918818000
C	7.432930000	-1.791153000	-1.223114000
C	6.080556000	-1.718818000	-0.898274000
H	4.814838000	-1.447326000	-4.033280000
H	8.905774000	-1.723681000	-2.799596000
H	4.083847000	-1.529570000	-1.685259000
H	8.176444000	-1.902548000	-0.435771000
H	5.758239000	-1.767174000	0.139965000
Ni	8.855601000	-0.356991000	-5.463958000
N	7.609424000	0.693460000	-6.638117000
H	7.723883000	1.694100000	-6.472042000
H	9.695045000	-1.275623000	-4.676059000
C	9.876162000	2.563885000	-4.209775000
C	10.334822000	3.762837000	-3.665300000
C	9.486476000	4.446583000	-2.805700000
C	8.234824000	3.918092000	-2.525985000
H	11.323074000	4.135042000	-3.914738000

H	9.799758000	5.385789000	-2.356327000
H	7.550090000	4.425691000	-1.851613000
N	8.671401000	2.047904000	-3.947336000
C	6.488141000	2.094845000	-2.911350000
H	6.667652000	1.006556000	-2.862028000
C	10.736063000	1.803892000	-5.130493000
C	11.619447000	0.301274000	-6.519338000
H	11.979017000	-0.625929000	-6.043126000
C	11.347687000	-0.016759000	-8.003631000
C	10.628491000	1.136557000	-8.698831000
H	10.490135000	0.902568000	-9.761490000
H	9.634141000	1.310413000	-8.272020000
H	11.195585000	2.076105000	-8.646438000
C	12.694397000	-0.284262000	-8.681541000
H	13.331812000	0.608028000	-8.730757000
H	13.252132000	-1.075084000	-8.160838000
H	12.531389000	-0.618916000	-9.713203000
C	10.506694000	-1.287418000	-8.111688000
H	11.032349000	-2.146969000	-7.674434000
H	9.550803000	-1.183962000	-7.581631000
H	10.297637000	-1.511710000	-9.165547000
C	5.570093000	2.312947000	-4.103063000
C	4.357922000	1.613993000	-4.138201000
C	5.886148000	3.147892000	-5.173873000
C	3.510251000	1.710717000	-5.233965000
H	4.097647000	0.974018000	-3.294750000
C	5.041234000	3.241743000	-6.278772000
H	6.814516000	3.718485000	-5.163758000
C	3.857756000	2.515334000	-6.318108000
H	2.578018000	1.149861000	-5.247014000
H	5.320307000	3.874764000	-7.117895000
H	3.205220000	2.579876000	-7.185302000
C	5.861725000	2.511839000	-1.596012000
C	6.191778000	1.811827000	-0.434313000
C	5.005041000	3.610042000	-1.500517000
C	5.673111000	2.196042000	0.796987000
H	6.852159000	0.947343000	-0.509229000
C	4.488963000	3.999497000	-0.268191000
H	4.736305000	4.158277000	-2.403266000
C	4.820292000	3.292628000	0.883629000

H	5.932381000	1.633768000	1.691619000
H	3.820566000	4.855791000	-0.209178000
H	4.411067000	3.592877000	1.845609000
O	11.977239000	2.290933000	-5.303379000
N	10.430629000	0.730353000	-5.760873000
C	7.857335000	2.709760000	-3.121417000
C	12.608321000	1.456566000	-6.287244000
H	12.774457000	2.067891000	-7.182713000
H	13.578123000	1.135925000	-5.895882000

int-D_{R-d}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -483.07 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	8.719929000	-0.642151000	-10.958499000
C	8.050422000	-0.567920000	-9.950916000
C	6.773647000	-1.288869000	-9.546276000
H	6.933773000	-2.314477000	-9.196558000
H	6.038551000	-1.301158000	-10.356712000
C	6.445331000	-0.312481000	-8.440958000
H	5.870084000	0.562398000	-8.751333000
C	6.372678000	-0.726949000	-7.077035000
H	6.342187000	-1.808818000	-6.919107000
C	5.636330000	0.073323000	-6.075831000
C	5.361478000	1.437462000	-6.247093000
C	5.213267000	-0.527062000	-4.881710000
C	4.699405000	2.168044000	-5.264625000
C	4.553015000	0.200452000	-3.901888000
C	4.291074000	1.557596000	-4.084083000
H	5.688340000	1.948313000	-7.154461000
H	5.432395000	-1.582879000	-4.722829000
H	4.506391000	3.228222000	-5.423561000
H	4.239432000	-0.295846000	-2.985302000
H	3.778136000	2.130193000	-3.314965000
Ni	8.292121000	-0.262416000	-6.977864000
N	8.158014000	0.304664000	-8.897351000
H	8.649436000	1.184494000	-9.073432000

H	8.236156000	-0.701281000	-5.574814000
C	11.210238000	-0.162604000	-6.702060000
C	12.443537000	0.402482000	-6.394898000
C	12.486835000	1.721190000	-5.965394000
C	11.300695000	2.429068000	-5.870663000
H	13.338979000	-0.202793000	-6.482735000
H	13.433763000	2.187344000	-5.706167000
H	11.283290000	3.461016000	-5.528926000
N	10.055375000	0.531339000	-6.623068000
C	8.799673000	2.589506000	-6.221263000
H	8.006804000	1.818765000	-6.252660000
C	11.139099000	-1.583955000	-7.073511000
C	10.530814000	-3.651891000	-7.451193000
H	10.261588000	-4.122644000	-6.487291000
C	9.823624000	-4.457757000	-8.547214000
C	9.945776000	-3.786705000	-9.911522000
H	9.415091000	-4.379768000	-10.667203000
H	9.522867000	-2.776027000	-9.919981000
H	10.989553000	-3.708110000	-10.242581000
C	10.440407000	-5.855832000	-8.600542000
H	11.481617000	-5.835869000	-8.949237000
H	10.418999000	-6.341017000	-7.614668000
H	9.877989000	-6.491490000	-9.295949000
C	8.352764000	-4.578764000	-8.151322000
H	8.236893000	-5.205746000	-7.256891000
H	7.933396000	-3.593026000	-7.917051000
H	7.766012000	-5.033084000	-8.960231000
C	8.624561000	3.437111000	-7.470214000
C	7.432085000	4.155423000	-7.622330000
C	9.562467000	3.484458000	-8.503175000
C	7.183050000	4.889809000	-8.773373000
H	6.699116000	4.134735000	-6.815851000
C	9.312111000	4.220404000	-9.661391000
H	10.499675000	2.935883000	-8.417981000
C	8.123599000	4.923606000	-9.801323000
H	6.248839000	5.438450000	-8.870526000
H	10.054377000	4.236853000	-10.456004000
H	7.927643000	5.495376000	-10.705087000
C	8.590464000	3.348255000	-4.925955000
C	7.951335000	2.696000000	-3.869571000

C	9.021721000	4.664537000	-4.750360000
C	7.755054000	3.345584000	-2.656059000
H	7.590321000	1.676716000	-4.014133000
C	8.832741000	5.311623000	-3.533366000
H	9.489567000	5.192404000	-5.581870000
C	8.199668000	4.653005000	-2.483413000
H	7.242211000	2.829097000	-1.847567000
H	9.171724000	6.337803000	-3.408657000
H	8.043855000	5.162706000	-1.535246000
O	12.331709000	-2.234367000	-7.033248000
N	10.093998000	-2.249991000	-7.361364000
C	10.098885000	1.815987000	-6.223760000
C	12.054466000	-3.543906000	-7.553607000
H	12.415629000	-3.585186000	-8.591891000
H	12.600374000	-4.278271000	-6.955225000

int-D_{S-a}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -518.31 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	3.420630000	2.723020000	1.520766000
N	5.115576000	3.358118000	0.032287000
C	3.900729000	3.454045000	0.688549000
C	3.491176000	4.833082000	0.195678000
H	2.690941000	4.820939000	-0.552858000
H	3.200699000	5.497507000	1.014664000
H	5.810213000	2.731227000	0.448203000
Ni	5.270944000	3.236314000	-1.887212000
C	4.856595000	5.124836000	-0.394111000
H	5.563972000	5.605168000	0.288012000
C	4.985498000	5.340997000	-1.795824000
H	4.031104000	5.389221000	-2.326486000
C	6.070962000	6.096768000	-2.415597000
C	7.214556000	6.531620000	-1.722493000
C	6.009492000	6.405537000	-3.787435000
C	8.240544000	7.211007000	-2.363927000
C	7.031978000	7.094079000	-4.428743000

C	8.163571000	7.496875000	-3.725742000
H	7.307285000	6.322236000	-0.655805000
H	5.131035000	6.098366000	-4.355536000
H	9.116829000	7.517098000	-1.792679000
H	6.942445000	7.317019000	-5.490747000
H	8.968246000	8.030327000	-4.225912000
H	5.354254000	1.746467000	-1.821280000
C	7.928845000	3.571144000	-3.624566000
C	9.080012000	3.847619000	-4.361944000
C	10.253703000	4.071204000	-3.657988000
C	10.237692000	4.014580000	-2.269716000
H	9.041467000	3.882271000	-5.446171000
H	11.178323000	4.288862000	-4.186935000
H	11.142812000	4.186996000	-1.693423000
N	7.902827000	3.525782000	-2.292016000
C	8.895295000	3.698209000	-0.107405000
H	8.047001000	4.368699000	0.113623000
C	6.669361000	3.241827000	-4.301995000
C	4.655960000	2.408939000	-4.742152000
H	4.713983000	1.329995000	-4.511037000
C	3.162999000	2.773554000	-4.746492000
C	2.515149000	2.313866000	-3.441649000
H	1.439183000	2.530216000	-3.460309000
H	2.645692000	1.234657000	-3.290645000
H	2.960212000	2.814451000	-2.570166000
C	2.917084000	4.267829000	-4.930756000
H	3.337653000	4.842653000	-4.099711000
H	3.339587000	4.659922000	-5.865015000
H	1.837684000	4.462357000	-4.959861000
C	2.517940000	2.008057000	-5.906425000
H	2.710668000	0.929411000	-5.829741000
H	1.430770000	2.151808000	-5.891967000
H	2.877561000	2.351915000	-6.885593000
C	10.105275000	4.257547000	0.612030000
C	10.192350000	5.630580000	0.848304000
C	11.170256000	3.441185000	0.995632000
C	11.316195000	6.179407000	1.455978000
H	9.363254000	6.274395000	0.551089000
C	12.298067000	3.987613000	1.599705000
H	11.107627000	2.367285000	0.822941000

C	12.374146000	5.357472000	1.832399000
H	11.364303000	7.250505000	1.639251000
H	13.119319000	3.338486000	1.895423000
H	13.253578000	5.782755000	2.310364000
C	8.491544000	2.328259000	0.403551000
C	8.729950000	1.152750000	-0.305723000
C	7.872374000	2.244211000	1.654286000
C	8.336496000	-0.077778000	0.213713000
H	9.208513000	1.197481000	-1.282727000
C	7.470636000	1.018497000	2.171477000
H	7.696508000	3.160485000	2.220016000
C	7.699760000	-0.148625000	1.447172000
H	8.519587000	-0.985003000	-0.357510000
H	6.969859000	0.975626000	3.135615000
H	7.378649000	-1.108856000	1.843154000
O	6.750782000	2.970705000	-5.616461000
N	5.523655000	3.068125000	-3.741716000
C	9.031286000	3.748027000	-1.618168000
C	5.405067000	2.705516000	-6.041564000
H	5.027459000	3.604410000	-6.550335000
H	5.426143000	1.873045000	-6.748997000

int-D_{S-b}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -532.33 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	3.194644000	0.492808000	1.589370000
N	4.707978000	2.038340000	0.686704000
C	3.467638000	1.540170000	1.053727000
C	2.628520000	2.771271000	0.756103000
H	1.959834000	2.669918000	-0.106064000
H	2.042544000	3.076115000	1.628668000
H	5.516945000	1.610620000	1.139377000
Ni	5.137678000	2.399964000	-1.161752000
C	3.829173000	3.652093000	0.486946000
H	4.216082000	4.200175000	1.348837000
C	4.040990000	4.174895000	-0.818824000

H	3.226554000	3.986225000	-1.525695000
C	4.821063000	5.381916000	-1.079995000
C	5.642595000	6.001042000	-0.121368000
C	4.792927000	5.957410000	-2.361834000
C	6.391091000	7.128504000	-0.430391000
C	5.552015000	7.078912000	-2.675569000
C	6.359857000	7.676493000	-1.712799000
H	5.714948000	5.577340000	0.880555000
H	4.159416000	5.499343000	-3.124266000
H	7.011671000	7.584526000	0.340749000
H	5.508866000	7.490004000	-3.682897000
H	6.950460000	8.557317000	-1.953229000
C	6.586877000	3.546360000	-3.306837000
C	6.858407000	3.954519000	-4.607055000
C	6.029490000	3.516560000	-5.628289000
C	4.987559000	2.655971000	-5.316076000
H	7.709693000	4.602740000	-4.786831000
H	6.205587000	3.823221000	-6.655895000
H	4.340322000	2.247521000	-6.088896000
N	5.537690000	2.752723000	-2.993475000
C	3.653564000	1.328912000	-3.614443000
H	4.004768000	0.868540000	-2.673793000
C	7.480832000	3.926108000	-2.208019000
C	8.496279000	4.083475000	-0.267783000
H	8.130314000	4.679736000	0.584504000
C	9.347050000	2.933658000	0.310087000
C	8.458450000	2.082669000	1.216541000
H	9.057709000	1.327046000	1.740341000
H	7.958052000	2.702566000	1.974829000
H	7.690476000	1.566455000	0.627586000
C	9.911828000	2.049842000	-0.799618000
H	9.104531000	1.597269000	-1.389284000
H	10.571731000	2.602389000	-1.481506000
H	10.503324000	1.234472000	-0.364391000
C	10.481833000	3.533109000	1.138054000
H	11.157507000	4.153567000	0.534641000
H	10.090405000	4.155053000	1.954500000
H	11.087428000	2.736047000	1.587093000
C	3.523376000	0.214918000	-4.637968000
C	4.511859000	-0.773255000	-4.660977000

C	2.486311000	0.155251000	-5.567696000
C	4.465265000	-1.800208000	-5.594312000
H	5.318999000	-0.727979000	-3.928134000
C	2.440367000	-0.873126000	-6.506253000
H	1.704235000	0.913203000	-5.551505000
C	3.427382000	-1.851792000	-6.522185000
H	5.237114000	-2.566559000	-5.595236000
H	1.624360000	-0.910138000	-7.224719000
H	3.386735000	-2.657081000	-7.252033000
C	2.339779000	2.009865000	-3.291855000
C	1.947781000	3.223472000	-3.857066000
C	1.467862000	1.367843000	-2.408143000
C	0.720418000	3.795306000	-3.528124000
H	2.610934000	3.737128000	-4.552818000
C	0.238227000	1.930105000	-2.087683000
H	1.771184000	0.421308000	-1.959087000
C	-0.136311000	3.152259000	-2.642155000
H	0.435967000	4.748784000	-3.967416000
H	-0.423968000	1.418405000	-1.392744000
H	-1.093069000	3.599991000	-2.384245000
O	8.547455000	4.683212000	-2.543410000
N	7.340510000	3.564658000	-0.996317000
C	4.760144000	2.285715000	-3.991348000
C	9.192045000	4.997331000	-1.295446000
H	10.266146000	4.817828000	-1.413765000
H	9.021546000	6.061516000	-1.090243000
H	5.769077000	1.044410000	-1.320651000

int-D_{S-c}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -472.16 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	-1.691851000	2.122777000	-5.964250000
N	-3.229386000	0.961114000	-4.640716000
C	-2.418376000	2.003212000	-4.999933000
C	-2.791745000	2.983892000	-3.894426000
H	-2.002762000	3.133036000	-3.148327000

H	-3.087369000	3.958406000	-4.295479000
H	-3.527416000	0.292377000	-5.352837000
Ni	-3.051664000	0.058586000	-2.867154000
C	-3.953871000	2.158053000	-3.387278000
H	-4.907560000	2.320264000	-3.895661000
C	-3.970678000	1.611118000	-2.067694000
H	-3.181072000	1.991944000	-1.410225000
C	-5.267425000	1.369562000	-1.370143000
C	-6.386957000	2.175850000	-1.619913000
C	-5.396332000	0.379530000	-0.385166000
C	-7.588024000	1.987868000	-0.940929000
C	-6.584246000	0.207173000	0.315684000
C	-7.692548000	1.003880000	0.035987000
H	-6.314065000	2.982246000	-2.349638000
H	-4.540953000	-0.264682000	-0.191484000
H	-8.439402000	2.628119000	-1.165533000
H	-6.648390000	-0.566051000	1.079395000
H	-8.627876000	0.857781000	0.572410000
H	-2.926845000	-0.494834000	-1.507679000
C	-3.907072000	-2.920562000	-3.947630000
C	-4.287703000	-4.251584000	-4.109602000
C	-5.646346000	-4.533267000	-4.098514000
C	-6.557146000	-3.493490000	-3.958655000
H	-3.537643000	-5.025432000	-4.241065000
H	-5.996548000	-5.556433000	-4.211349000
H	-7.627026000	-3.683817000	-3.966329000
N	-4.773573000	-1.916989000	-3.796513000
C	-6.985175000	-0.972964000	-3.743794000
H	-6.646129000	-0.415988000	-2.852622000
C	-2.492522000	-2.528128000	-3.998443000
C	-0.601122000	-1.358174000	-4.019269000
H	-0.555562000	-0.667693000	-4.880865000
C	0.381059000	-0.827351000	-2.959014000
C	0.233718000	-1.571474000	-1.634570000
H	0.954310000	-1.177372000	-0.906884000
H	-0.774532000	-1.438378000	-1.224059000
H	0.429509000	-2.647752000	-1.730742000
C	1.797807000	-1.000191000	-3.513034000
H	2.076826000	-2.054529000	-3.640168000
H	1.908949000	-0.496619000	-4.483125000

H	2.525709000	-0.555462000	-2.823602000
C	0.134696000	0.663760000	-2.732798000
H	0.222396000	1.227947000	-3.671855000
H	-0.867867000	0.837059000	-2.315140000
H	0.873257000	1.062483000	-2.025166000
C	-8.441181000	-1.332996000	-3.533772000
C	-9.297467000	-1.570130000	-4.610868000
C	-8.929620000	-1.492850000	-2.236423000
C	-10.615228000	-1.959296000	-4.394291000
H	-8.925334000	-1.441817000	-5.627084000
C	-10.248156000	-1.877689000	-2.017663000
H	-8.263072000	-1.301982000	-1.394962000
C	-11.094709000	-2.113054000	-3.096713000
H	-11.271895000	-2.138332000	-5.242974000
H	-10.616479000	-1.990504000	-1.000157000
H	-12.126899000	-2.411419000	-2.927517000
C	-6.785832000	-0.041670000	-4.928986000
C	-7.261988000	1.267917000	-4.822634000
C	-6.179284000	-0.433987000	-6.122618000
C	-7.096757000	2.175319000	-5.861848000
H	-7.758983000	1.568719000	-3.900166000
C	-6.014542000	0.472810000	-7.167990000
H	-5.818099000	-1.454953000	-6.239850000
C	-6.460281000	1.782829000	-7.037202000
H	-7.465067000	3.193612000	-5.754066000
H	-5.531156000	0.151250000	-8.087942000
H	-6.320737000	2.492201000	-7.849308000
O	-1.645072000	-3.398788000	-4.572602000
N	-2.015030000	-1.407994000	-3.603967000
C	-6.080860000	-2.186706000	-3.819782000
C	-0.338623000	-2.804347000	-4.468172000
H	0.233528000	-3.382365000	-3.730688000
H	0.153575000	-2.884559000	-5.441030000

int-D_{S-d}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -499.30 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	3.256238000	-0.255439000	0.745035000
N	4.942103000	1.326269000	0.384724000
C	3.660816000	0.840587000	0.422979000
C	2.900561000	2.112731000	0.065425000
H	2.457170000	2.087514000	-0.936071000
H	2.123030000	2.341735000	0.800762000
H	5.663868000	0.835921000	0.917758000
Ni	5.620565000	2.039222000	-1.362217000
C	4.110092000	3.012504000	0.157217000
H	4.331309000	3.415438000	1.147465000
C	4.600470000	3.696867000	-0.991405000
H	3.899204000	3.770504000	-1.826776000
C	5.559715000	4.812139000	-0.871618000
C	6.400113000	4.969390000	0.239984000
C	5.683884000	5.738989000	-1.916010000
C	7.324171000	6.008414000	0.300223000
C	6.606083000	6.774350000	-1.856528000
C	7.436940000	6.917414000	-0.746413000
H	6.351150000	4.253682000	1.062661000
H	5.050586000	5.622036000	-2.795415000
H	7.965119000	6.105635000	1.175740000
H	6.678472000	7.477073000	-2.684578000
H	8.163758000	7.724904000	-0.700074000
H	6.028114000	2.679735000	-2.629497000
C	6.649052000	-0.485632000	-2.384925000
C	7.612186000	-1.422884000	-2.741230000
C	8.935976000	-1.175472000	-2.405259000
C	9.243494000	-0.022847000	-1.699698000
H	7.310498000	-2.315357000	-3.279010000
H	9.716616000	-1.878842000	-2.683002000
H	10.265464000	0.205757000	-1.408008000
N	6.950341000	0.642057000	-1.710635000
C	8.480984000	2.054620000	-0.453685000
H	7.623342000	2.731125000	-0.629548000
C	5.241207000	-0.693871000	-2.753294000
C	3.095456000	-0.464012000	-3.164385000
H	2.292610000	-0.498977000	-2.410915000
C	2.598262000	0.409368000	-4.337834000

C	3.673086000	0.549723000	-5.413600000
H	3.291876000	1.153725000	-6.246626000
H	4.563171000	1.053513000	-5.015999000
H	3.980247000	-0.419407000	-5.828810000
C	1.339690000	-0.226194000	-4.926345000
H	1.532465000	-1.211179000	-5.370783000
H	0.561467000	-0.346700000	-4.160571000
H	0.930218000	0.411378000	-5.719884000
C	2.247510000	1.796926000	-3.804738000
H	1.468607000	1.736184000	-3.030998000
H	3.131471000	2.284958000	-3.375967000
H	1.861354000	2.429335000	-4.614575000
C	9.717866000	2.834594000	-0.845762000
C	10.985951000	2.527606000	-0.348036000
C	9.578056000	3.898713000	-1.738680000
C	12.097748000	3.259286000	-0.752485000
H	11.096940000	1.722778000	0.379340000
C	10.687836000	4.636071000	-2.136025000
H	8.583334000	4.156600000	-2.104913000
C	11.950921000	4.314592000	-1.648178000
H	13.080661000	3.011739000	-0.357396000
H	10.560786000	5.471505000	-2.821103000
H	12.819336000	4.892538000	-1.956311000
C	8.431682000	1.677954000	1.019369000
C	8.196114000	0.378921000	1.473203000
C	8.574181000	2.697999000	1.967779000
C	8.095303000	0.107955000	2.837888000
H	8.078787000	-0.438529000	0.762573000
C	8.475467000	2.429081000	3.325649000
H	8.766066000	3.713607000	1.621959000
C	8.233297000	1.129686000	3.767513000
H	7.906234000	-0.910709000	3.168709000
H	8.586735000	3.237858000	4.044510000
H	8.152821000	0.918164000	4.831010000
O	4.975931000	-1.859766000	-3.387298000
N	4.286651000	0.119739000	-2.543949000
C	8.225905000	0.860929000	-1.343638000
C	3.546657000	-1.887706000	-3.544468000
H	3.326168000	-2.174708000	-4.578127000
H	3.145403000	-2.652890000	-2.870238000

int-F_{chiral}

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	8.613306000	-3.742619000	-7.230045000
C	7.794910000	-2.837247000	-7.424238000
C	6.385084000	-3.014783000	-6.842670000
H	6.508357000	-3.377220000	-5.811545000
H	5.962102000	-3.857748000	-7.408267000
C	5.478721000	-1.838161000	-6.896100000
H	5.224319000	-1.474107000	-7.892550000
C	5.018435000	-1.201691000	-5.809005000
H	5.278105000	-1.607534000	-4.824399000
C	4.242523000	0.037766000	-5.779904000
C	3.887862000	0.742809000	-6.943464000
C	3.877459000	0.583727000	-4.541197000
C	3.196480000	1.942452000	-6.859303000
C	3.183339000	1.785321000	-4.458517000
C	2.841282000	2.473161000	-5.619016000
H	4.181635000	0.361023000	-7.921010000
H	4.148660000	0.049002000	-3.630426000
H	2.937243000	2.473612000	-7.773200000
H	2.905957000	2.183623000	-3.484485000
H	2.295916000	3.412748000	-5.560116000
Ni	7.542758000	0.027054000	-7.894618000
C	6.853693000	2.017353000	-6.106379000
C	6.274899000	3.119993000	-5.506078000
C	6.008435000	4.213421000	-6.323091000
C	6.418825000	4.189185000	-7.648013000
H	6.047563000	3.106843000	-4.444803000
H	5.531208000	5.100414000	-5.914370000
H	6.307615000	5.064061000	-8.282236000
N	7.136616000	1.938941000	-7.424248000
C	7.675155000	2.993334000	-9.541158000
H	7.156467000	2.195488000	-10.092384000
C	7.415006000	0.876761000	-5.391026000
C	8.740099000	-0.889248000	-5.081018000

H	8.527625000	-1.934380000	-5.343627000
C	10.276173000	-0.713929000	-5.082846000
C	10.673745000	0.719114000	-4.734985000
H	11.767217000	0.811020000	-4.746088000
H	10.280148000	1.430923000	-5.474007000
H	10.333301000	1.027512000	-3.737057000
C	10.859551000	-1.695900000	-4.067070000
H	10.526219000	-1.497591000	-3.039637000
H	10.587191000	-2.727897000	-4.324824000
H	11.954294000	-1.629641000	-4.068671000
C	10.824300000	-1.067392000	-6.465195000
H	10.527870000	-2.083266000	-6.760552000
H	10.473323000	-0.359561000	-7.227497000
H	11.921257000	-1.016062000	-6.448288000
C	9.112299000	2.528374000	-9.373772000
C	9.622680000	1.553718000	-10.232086000
C	9.935203000	3.025427000	-8.357687000
C	10.925189000	1.086395000	-10.080794000
H	8.978536000	1.137948000	-11.004904000
C	11.237942000	2.561551000	-8.205897000
H	9.545886000	3.774694000	-7.665363000
C	11.736238000	1.588300000	-9.067955000
H	11.302485000	0.319425000	-10.753226000
H	11.863507000	2.957184000	-7.407999000
H	12.750720000	1.216152000	-8.943741000
C	7.503037000	4.277614000	-10.324035000
C	6.320509000	4.461099000	-11.046572000
C	8.451658000	5.299961000	-10.318915000
C	6.087760000	5.640507000	-11.743794000
H	5.578839000	3.661528000	-11.056616000
C	8.221574000	6.481362000	-11.018723000
H	9.385337000	5.165495000	-9.775544000
C	7.039908000	6.656319000	-11.730482000
H	5.164429000	5.764190000	-12.305250000
H	8.973684000	7.267200000	-11.009982000
H	6.863187000	7.578479000	-12.279203000
O	7.352935000	0.761547000	-4.073245000
N	8.094318000	0.006309000	-6.048243000
C	7.014006000	3.039232000	-8.180174000
C	8.029463000	-0.491031000	-3.772413000

H	8.700920000	-0.305602000	-2.929685000
H	7.258811000	-1.209897000	-3.470585000
N	8.052639000	-1.736143000	-8.147866000
H	8.997672000	-1.786350000	-8.526678000
Cl	6.391803000	0.006118000	-9.765020000

int-F_{R-a}

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	8.884283000	-0.523973000	-11.905045000
C	8.533622000	-0.608257000	-10.734044000
C	7.190166000	-1.187990000	-10.316522000
H	7.300586000	-2.275626000	-10.209898000
H	6.460785000	-0.993951000	-11.111433000
C	6.736030000	-0.569830000	-9.045305000
H	6.360742000	0.453936000	-9.121980000
C	6.578346000	-1.253747000	-7.879674000
H	6.883338000	-2.305500000	-7.869086000
C	5.720824000	-0.834886000	-6.761592000
C	5.297859000	0.488448000	-6.574105000
C	5.250674000	-1.814596000	-5.879263000
C	4.464526000	0.818747000	-5.514627000
C	4.402778000	-1.486234000	-4.825893000
C	4.014565000	-0.164289000	-4.634147000
H	5.642197000	1.267098000	-7.253539000
H	5.548810000	-2.852060000	-6.033402000
H	4.158892000	1.853433000	-5.375754000
H	4.042635000	-2.265692000	-4.158223000
H	3.357275000	0.099780000	-3.809252000
Ni	8.776998000	-0.209560000	-7.877403000
C	8.151354000	2.235023000	-5.945087000
C	8.180979000	3.392385000	-5.174588000
C	8.240122000	4.605110000	-5.852237000
C	8.295061000	4.609726000	-7.239364000
H	8.176190000	3.334643000	-4.090468000
H	8.265634000	5.541197000	-5.299905000
H	8.382210000	5.540051000	-7.795500000

N	8.139470000	2.234431000	-7.278856000
C	8.332807000	3.275358000	-9.435866000
H	9.008987000	2.418769000	-9.599552000
C	8.183565000	0.902075000	-5.331232000
C	8.415126000	-1.292441000	-4.972628000
H	7.680989000	-2.033967000	-5.321643000
C	9.748143000	-2.045555000	-4.784414000
C	10.863739000	-1.114539000	-4.318328000
H	11.784278000	-1.690537000	-4.160886000
H	11.075140000	-0.343421000	-5.067867000
H	10.622773000	-0.625734000	-3.364103000
C	9.509895000	-3.139436000	-3.738782000
H	9.268531000	-2.738605000	-2.745891000
H	8.696401000	-3.813646000	-4.040939000
H	10.416805000	-3.745683000	-3.626992000
C	10.139215000	-2.727835000	-6.095064000
H	9.334439000	-3.389498000	-6.448440000
H	10.371416000	-2.004310000	-6.884657000
H	11.031701000	-3.347559000	-5.941231000
C	8.975782000	4.491070000	-10.070608000
C	8.230614000	5.510107000	-10.662996000
C	10.366076000	4.617253000	-10.008578000
C	8.864455000	6.633957000	-11.186766000
H	7.147048000	5.417333000	-10.724494000
C	10.999617000	5.737228000	-10.532048000
H	10.948119000	3.821306000	-9.542080000
C	10.248701000	6.750195000	-11.123352000
H	8.272188000	7.419151000	-11.651735000
H	12.083221000	5.817680000	-10.483545000
H	10.743119000	7.625601000	-11.538271000
C	7.011662000	2.884860000	-10.063806000
C	5.780041000	3.230362000	-9.504947000
C	7.030706000	2.158917000	-11.257942000
C	4.589575000	2.839499000	-10.115595000
H	5.749841000	3.803666000	-8.577461000
C	5.844406000	1.770295000	-11.869026000
H	7.984427000	1.865329000	-11.696618000
C	4.618702000	2.104955000	-11.296710000
H	3.637241000	3.110306000	-9.664508000
H	5.886200000	1.189501000	-12.788456000

H	3.689775000	1.794475000	-11.769525000
O	7.931991000	0.820122000	-4.025255000
N	8.443899000	-0.190813000	-5.955586000
C	8.246954000	3.392034000	-7.927870000
C	7.876417000	-0.586905000	-3.716024000
H	8.473067000	-0.752967000	-2.814932000
H	6.827316000	-0.837000000	-3.512789000
N	9.252394000	-0.236630000	-9.658989000
H	10.186353000	0.088785000	-9.895066000
Cl	10.840375000	0.556743000	-7.505795000

int-F_{R-b}

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	10.575005000	-0.066770000	-11.167103000
C	10.377855000	0.288258000	-10.013409000
C	11.480887000	0.244528000	-8.962825000
H	12.377173000	0.728664000	-9.373139000
H	11.741738000	-0.810155000	-8.807859000
C	11.074532000	0.871788000	-7.665085000
H	11.364220000	0.341852000	-6.757215000
C	10.666282000	2.182860000	-7.552849000
H	10.496134000	2.745465000	-8.473727000
C	10.714598000	2.989926000	-6.326165000
C	11.193029000	2.493753000	-5.105865000
C	10.278336000	4.319876000	-6.372024000
C	11.178081000	3.281627000	-3.963949000
C	10.270087000	5.113614000	-5.231410000
C	10.707836000	4.592402000	-4.017855000
H	11.582781000	1.479418000	-5.048473000
H	9.929417000	4.723881000	-7.322665000
H	11.543906000	2.870733000	-3.024632000
H	9.919850000	6.141978000	-5.289483000
H	10.698768000	5.208860000	-3.122087000
Ni	8.908052000	0.863965000	-7.700591000
N	9.212933000	0.743728000	-9.508967000
H	8.423097000	0.581211000	-10.128173000

Cl	7.044782000	-0.348406000	-7.961596000
C	7.914730000	2.090406000	-5.303588000
C	7.646413000	2.316290000	-3.962632000
C	7.946880000	1.313053000	-3.050998000
C	8.452492000	0.116796000	-3.525030000
H	7.198407000	3.258222000	-3.664601000
H	7.754052000	1.451655000	-1.990442000
H	8.629145000	-0.724429000	-2.858812000
N	8.496531000	0.956341000	-5.757886000
C	9.222290000	-1.376063000	-5.413898000
H	8.953499000	-1.385255000	-6.481150000
C	7.515352000	3.083159000	-6.308762000
C	7.035239000	4.101884000	-8.199367000
H	7.782945000	4.560237000	-8.868341000
C	5.822572000	3.718483000	-9.074076000
C	4.724449000	3.062129000	-8.240045000
H	3.875736000	2.805146000	-8.886037000
H	5.081946000	2.131752000	-7.781502000
H	4.340102000	3.721166000	-7.449558000
C	5.296632000	4.987733000	-9.743711000
H	4.939835000	5.733772000	-9.020906000
H	6.071435000	5.458890000	-10.363861000
H	4.451444000	4.743606000	-10.398688000
C	6.279280000	2.737012000	-10.151307000
H	7.148086000	3.121993000	-10.702943000
H	6.549143000	1.771354000	-9.709001000
H	5.468893000	2.567804000	-10.871712000
C	8.459032000	-2.522970000	-4.762690000
C	7.124410000	-2.722325000	-5.129864000
C	9.031840000	-3.358215000	-3.803920000
C	6.380080000	-3.738901000	-4.545073000
H	6.685177000	-2.075347000	-5.890802000
C	8.282185000	-4.374813000	-3.216682000
H	10.074738000	-3.223549000	-3.520786000
C	6.955862000	-4.567198000	-3.584621000
H	5.345675000	-3.889166000	-4.845882000
H	8.742217000	-5.021737000	-2.472808000
H	6.372589000	-5.364400000	-3.129339000
C	10.725101000	-1.546517000	-5.329865000
C	11.352848000	-2.319766000	-6.311004000

C	11.506353000	-0.993949000	-4.313714000
C	12.729577000	-2.506778000	-6.298472000
H	10.746150000	-2.760162000	-7.102839000
C	12.887685000	-1.178610000	-4.299663000
H	11.038228000	-0.393352000	-3.533332000
C	13.503692000	-1.928336000	-5.295245000
H	13.200641000	-3.098981000	-7.079706000
H	13.482925000	-0.730444000	-3.507059000
H	14.582279000	-2.064874000	-5.288889000
O	6.945475000	4.213090000	-5.842859000
N	7.642048000	2.930643000	-7.564408000
C	8.719957000	-0.045350000	-4.889052000
C	6.722092000	5.031204000	-7.006602000
H	5.687700000	5.388326000	-6.974609000
H	7.394090000	5.896274000	-6.945526000

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int-F_{R-c}

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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	5.954947000	3.362623000	-4.648795000
C	6.916683000	2.757341000	-5.112038000
C	7.809703000	3.378741000	-6.181349000
H	8.338719000	4.227517000	-5.726320000
H	7.157076000	3.812967000	-6.947617000
C	8.778154000	2.390134000	-6.777510000
H	8.822885000	2.310316000	-7.865352000
C	9.808341000	1.858816000	-6.027137000
H	9.779341000	2.072338000	-4.955325000
C	11.069894000	1.279044000	-6.487617000
C	11.437256000	1.211665000	-7.838175000
C	11.980090000	0.832858000	-5.521541000
C	12.670213000	0.695567000	-8.204643000
C	13.213435000	0.310646000	-5.888240000
C	13.559431000	0.238658000	-7.233492000
H	10.749505000	1.559143000	-8.604206000
H	11.707673000	0.899605000	-4.468351000
H	12.941784000	0.647507000	-9.256339000

H	13.906594000	-0.033477000	-5.124343000
H	14.525491000	-0.165470000	-7.527358000
N	7.314633000	1.513132000	-4.765384000
H	6.632139000	1.076470000	-4.148954000
Ni	8.075555000	0.522143000	-6.144095000
C	4.904189000	-0.201090000	-6.395203000
C	3.534140000	-0.276574000	-6.176518000
C	2.735444000	0.694350000	-6.773754000
C	3.326053000	1.650416000	-7.581513000
H	3.116477000	-1.063617000	-5.556141000
H	1.659890000	0.693820000	-6.616484000
H	2.730479000	2.418064000	-8.069949000
N	5.486282000	0.726265000	-7.162127000
C	5.413315000	2.520057000	-8.773422000
H	6.472722000	2.494845000	-8.474415000
C	5.813657000	-1.196041000	-5.807253000
C	7.618328000	-2.340031000	-5.151020000
H	8.237116000	-2.703833000	-5.987396000
C	8.513020000	-2.280494000	-3.899539000
C	7.800881000	-1.627500000	-2.717629000
H	8.450702000	-1.652787000	-1.833978000
H	7.570697000	-0.576030000	-2.925841000
H	6.867790000	-2.137498000	-2.444536000
C	8.909838000	-3.716911000	-3.549775000
H	8.051158000	-4.332372000	-3.250952000
H	9.403684000	-4.208507000	-4.398650000
H	9.614664000	-3.717737000	-2.709517000
C	9.780815000	-1.492047000	-4.215800000
H	10.305132000	-1.897235000	-5.091040000
H	9.551012000	-0.439694000	-4.427440000
H	10.465916000	-1.520216000	-3.357811000
C	4.964451000	3.970014000	-8.744289000
C	4.949498000	4.759631000	-9.896363000
C	4.669013000	4.575662000	-7.516742000
C	4.622229000	6.110424000	-9.829732000
H	5.199736000	4.314897000	-10.857073000
C	4.345049000	5.926458000	-7.451488000
H	4.721089000	3.998699000	-6.592139000
C	4.312338000	6.698173000	-8.608357000
H	4.613118000	6.705449000	-10.740519000

H	4.125148000	6.374461000	-6.485191000
H	4.055652000	7.753963000	-8.557260000
C	5.337145000	1.805269000	-10.113025000
C	6.385232000	0.963169000	-10.488188000
C	4.206638000	1.881025000	-10.931035000
C	6.315593000	0.230411000	-11.668634000
H	7.252137000	0.856215000	-9.833935000
C	4.139098000	1.152529000	-12.113234000
H	3.375973000	2.526526000	-10.647381000
C	5.195464000	0.326601000	-12.487155000
H	7.141410000	-0.421987000	-11.942976000
H	3.256071000	1.229334000	-12.744113000
H	5.141773000	-0.243632000	-13.411886000
O	5.284856000	-2.390083000	-5.525225000
N	7.067461000	-1.044118000	-5.583161000
C	4.714801000	1.623979000	-7.769016000
C	6.350798000	-3.197095000	-4.989609000
H	6.105731000	-3.417902000	-3.943646000
H	6.379681000	-4.134527000	-5.551443000
Cl	8.800438000	-0.629006000	-7.885626000

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int-F_{R-d}
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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	10.088868000	-1.730227000	-8.257012000
C	9.593383000	-0.751255000	-7.714811000
C	10.317034000	-0.006411000	-6.593856000
H	11.318834000	0.272249000	-6.948867000
H	10.470613000	-0.731051000	-5.784325000
C	9.543650000	1.182530000	-6.085932000
H	9.540192000	1.364022000	-5.010494000
C	9.148290000	2.203200000	-6.938031000
H	9.326798000	2.034747000	-8.002104000
C	8.745931000	3.572092000	-6.617985000
C	8.746276000	4.095318000	-5.317665000
C	8.364405000	4.406853000	-7.677379000
C	8.354083000	5.404902000	-5.089977000

C	7.972272000	5.718920000	-7.449112000
C	7.958722000	6.217634000	-6.151529000
H	9.042081000	3.466613000	-4.482348000
H	8.365610000	4.010555000	-8.694489000
H	8.352049000	5.796235000	-4.075466000
H	7.661016000	6.344816000	-8.282022000
H	7.642607000	7.241726000	-5.965541000
N	8.386012000	-0.208286000	-7.995464000
H	7.826201000	-0.800289000	-8.605728000
Ni	7.606153000	0.717554000	-6.586709000
C	5.166690000	-0.849602000	-6.735143000
C	3.827911000	-1.151780000	-6.925676000
C	3.041349000	-0.237860000	-7.619093000
C	3.629586000	0.906206000	-8.124386000
H	3.423889000	-2.071731000	-6.516386000
H	1.980188000	-0.422815000	-7.763729000
H	3.046043000	1.644784000	-8.667159000
N	5.738309000	0.268242000	-7.226394000
C	5.693144000	2.306892000	-8.587240000
H	6.711819000	2.307897000	-8.167987000
C	6.037327000	-1.736590000	-5.952385000
C	7.678807000	-2.558470000	-4.737340000
H	8.660378000	-2.880854000	-5.118736000
C	7.862168000	-2.153780000	-3.257905000
C	6.546680000	-1.675027000	-2.646852000
H	6.702689000	-1.414639000	-1.592409000
H	6.179727000	-0.776252000	-3.158692000
H	5.763364000	-2.444401000	-2.676768000
C	8.396997000	-3.363554000	-2.491795000
H	7.694096000	-4.206823000	-2.485236000
H	9.345667000	-3.716605000	-2.918543000
H	8.583473000	-3.092133000	-1.445433000
C	8.885113000	-1.023056000	-3.170790000
H	9.833999000	-1.308270000	-3.648248000
H	8.501121000	-0.113433000	-3.647473000
H	9.099313000	-0.791659000	-2.119436000
C	5.079910000	3.647875000	-8.217959000
C	5.022138000	4.709056000	-9.123262000
C	4.676065000	3.870641000	-6.897152000
C	4.548091000	5.956424000	-8.726269000

H	5.358730000	4.565247000	-10.147939000
C	4.209406000	5.117989000	-6.500753000
H	4.770758000	3.071480000	-6.161417000
C	4.136471000	6.164889000	-7.415081000
H	4.504619000	6.768556000	-9.449221000
H	3.908905000	5.272143000	-5.466891000
H	3.765878000	7.139517000	-7.105074000
C	5.830438000	2.016704000	-10.074193000
C	7.037897000	1.511999000	-10.560613000
C	4.766350000	2.180212000	-10.967516000
C	7.182815000	1.184449000	-11.906021000
H	7.864033000	1.345164000	-9.868687000
C	4.910591000	1.855907000	-12.311019000
H	3.819912000	2.588768000	-10.615737000
C	6.120598000	1.356429000	-12.785364000
H	8.131499000	0.790391000	-12.263138000
H	4.073787000	1.996448000	-12.991695000
H	6.232536000	1.102722000	-13.836925000
O	5.530989000	-2.943378000	-5.632853000
N	7.207510000	-1.435137000	-5.555511000
C	4.998108000	1.128292000	-7.937276000
C	6.613949000	-3.644824000	-4.990306000
H	6.219948000	-4.113688000	-4.083335000
H	6.959992000	-4.427675000	-5.674713000
Cl	6.680104000	1.687087000	-4.809203000

int-F_{R-a}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -502.82 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	8.651756000	-2.943484000	-9.681209000
C	7.888958000	-2.350558000	-8.959642000
C	6.903086000	-2.854129000	-7.918039000
H	7.367395000	-3.096431000	-6.955552000
H	6.341101000	-3.722068000	-8.273759000
C	6.103447000	-1.576396000	-7.888196000
H	5.273326000	-1.494626000	-8.593148000

C	6.098902000	-0.778531000	-6.708904000
H	6.567988000	-1.265057000	-5.846016000
C	4.986727000	0.126555000	-6.366212000
C	4.142629000	0.689703000	-7.331750000
C	4.772378000	0.479870000	-5.026848000
C	3.149062000	1.591371000	-6.973851000
C	3.782835000	1.387718000	-4.667163000
C	2.966985000	1.954572000	-5.641685000
H	4.287218000	0.453647000	-8.385148000
H	5.396083000	0.027577000	-4.253889000
H	2.519279000	2.019824000	-7.752386000
H	3.645365000	1.647985000	-3.619407000
H	2.192548000	2.666070000	-5.365136000
Ni	7.664877000	0.219954000	-7.518775000
C	6.534507000	3.196775000	-7.052021000
C	6.093475000	4.510309000	-6.931968000
C	5.586311000	5.121223000	-8.073989000
C	5.572124000	4.418264000	-9.269392000
H	6.165759000	5.031803000	-5.982688000
H	5.232443000	6.148449000	-8.035752000
H	5.239888000	4.885580000	-10.194529000
N	6.457657000	2.492644000	-8.182607000
C	6.046987000	2.244637000	-10.543038000
H	6.851668000	1.519396000	-10.347457000
C	7.167804000	2.501679000	-5.925003000
C	8.225147000	1.009424000	-4.638493000
H	7.648142000	0.134588000	-4.291098000
C	9.713972000	0.616061000	-4.571957000
C	10.608186000	1.714906000	-5.139761000
H	11.660286000	1.418676000	-5.044296000
H	10.400493000	1.883116000	-6.203785000
H	10.493026000	2.666390000	-4.602467000
C	10.054893000	0.356135000	-3.102251000
H	9.969606000	1.256718000	-2.480090000
H	9.405759000	-0.418957000	-2.671025000
H	11.090224000	0.004940000	-3.017402000
C	9.937377000	-0.681129000	-5.350321000
H	9.287609000	-1.485362000	-4.974052000
H	9.753548000	-0.551167000	-6.424777000
H	10.976716000	-1.012350000	-5.231977000

C	6.479212000	3.062799000	-11.746528000
C	7.819582000	3.458991000	-11.808305000
C	5.608204000	3.458413000	-12.759779000
C	8.276699000	4.237722000	-12.862584000
H	8.501536000	3.139956000	-11.017718000
C	6.067727000	4.241987000	-13.816599000
H	4.566371000	3.142836000	-12.732650000
C	7.399787000	4.633905000	-13.870484000
H	9.322976000	4.532298000	-12.901616000
H	5.378869000	4.540804000	-14.603879000
H	7.757524000	5.241567000	-14.698624000
C	4.770764000	1.452811000	-10.735174000
C	3.507963000	2.016372000	-10.537431000
C	4.847680000	0.112790000	-11.122228000
C	2.353996000	1.257646000	-10.708843000
H	3.425930000	3.057089000	-10.223508000
C	3.696345000	-0.650594000	-11.289736000
H	5.826454000	-0.338570000	-11.283406000
C	2.444381000	-0.080696000	-11.078724000
H	1.379741000	1.713320000	-10.543930000
H	3.779350000	-1.693977000	-11.586301000
H	1.543190000	-0.676185000	-11.203158000
O	7.165391000	3.124253000	-4.744031000
N	7.737790000	1.352537000	-5.982176000
C	6.015694000	3.089948000	-9.283455000
C	7.840043000	2.255272000	-3.816943000
H	8.703344000	2.800006000	-3.419588000
H	7.148401000	2.037270000	-2.996270000
N	7.532668000	-1.016998000	-8.985020000
H	7.836807000	-0.480926000	-9.802169000
Cl	9.371080000	1.263510000	-8.571401000

int-F_{R-b}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -500.10 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	8.440723000	-2.109968000	-10.306172000

C	7.885321000	-1.749079000	-9.297664000
C	7.039839000	-2.519941000	-8.296980000
H	7.618932000	-3.119148000	-7.585105000
H	6.313564000	-3.164493000	-8.800454000
C	6.425752000	-1.291998000	-7.676286000
H	5.493688000	-0.936149000	-8.117622000
C	6.742432000	-0.940563000	-6.335875000
H	7.345136000	-1.693450000	-5.816395000
C	5.808121000	-0.219111000	-5.453513000
C	4.731726000	0.542549000	-5.923960000
C	5.992714000	-0.297277000	-4.065917000
C	3.889362000	1.212022000	-5.045418000
C	5.158690000	0.380797000	-3.186059000
C	4.102308000	1.145670000	-3.671038000
H	4.559438000	0.631044000	-6.995953000
H	6.807701000	-0.910534000	-3.680584000
H	3.058418000	1.794700000	-5.439933000
H	5.331182000	0.304402000	-2.114177000
H	3.443899000	1.674950000	-2.986349000
Ni	8.212558000	0.226175000	-7.121029000
N	7.689822000	-0.465980000	-8.829664000
H	7.887642000	0.297884000	-9.480835000
Cl	9.949091000	1.332310000	-8.038571000
C	8.146316000	2.116150000	-5.013675000
C	8.347331000	2.648513000	-3.748903000
C	9.145109000	1.948638000	-2.853290000
C	9.772454000	0.790672000	-3.281378000
H	7.902170000	3.606184000	-3.500347000
H	9.316553000	2.331205000	-1.850580000
H	10.486472000	0.268190000	-2.648677000
N	8.679692000	0.934298000	-5.391270000
C	10.277703000	-0.898268000	-5.115176000
H	10.227561000	-0.777786000	-6.209394000
C	7.478153000	2.904610000	-6.063455000
C	6.805871000	3.627530000	-8.015105000
H	7.678499000	3.623463000	-8.694971000
C	5.550471000	3.581604000	-8.894458000
C	4.269952000	3.568691000	-8.062890000
H	3.404754000	3.368505000	-8.707615000
H	4.310460000	2.794472000	-7.288269000

H	4.083767000	4.530270000	-7.567969000
C	5.557731000	4.807897000	-9.807433000
H	5.508613000	5.745063000	-9.236505000
H	6.461865000	4.835930000	-10.429868000
H	4.689904000	4.789422000	-10.478713000
C	5.615142000	2.320684000	-9.754442000
H	6.537545000	2.302628000	-10.351844000
H	5.600624000	1.413650000	-9.137350000
H	4.765348000	2.284129000	-10.447896000
C	9.635863000	-2.229984000	-4.792540000
C	9.703284000	-3.245607000	-5.750001000
C	8.992388000	-2.493225000	-3.582717000
C	9.118990000	-4.485215000	-5.515070000
H	10.208301000	-3.047257000	-6.696394000
C	8.401440000	-3.732327000	-3.346460000
H	8.935609000	-1.717140000	-2.819288000
C	8.457509000	-4.729254000	-4.313877000
H	9.174569000	-5.260486000	-6.276356000
H	7.892346000	-3.915387000	-2.402908000
H	7.990448000	-5.694212000	-4.132580000
C	11.750259000	-0.815797000	-4.744574000
C	12.330221000	-1.611223000	-3.757671000
C	12.536866000	0.126071000	-5.415688000
C	13.678476000	-1.463501000	-3.439599000
H	11.729586000	-2.359859000	-3.242554000
C	13.881201000	0.269229000	-5.098261000
H	12.078840000	0.735510000	-6.197790000
C	14.455312000	-0.523658000	-4.107023000
H	14.122520000	-2.091975000	-2.670595000
H	14.485867000	0.998942000	-5.631967000
H	15.509010000	-0.412863000	-3.860996000
O	7.550859000	4.243296000	-5.883506000
N	6.991070000	2.454986000	-7.148526000
C	9.531678000	0.301587000	-4.567251000
C	6.912534000	4.809926000	-7.042008000
H	5.933611000	5.204067000	-6.734628000
H	7.533250000	5.633721000	-7.403633000

int-F_{R-c}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -514.03 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	8.236776000	2.556472000	-4.566033000
C	8.747874000	1.863321000	-5.413835000
C	9.931489000	0.910646000	-5.338940000
H	9.703424000	-0.059329000	-4.884105000
H	10.773762000	1.367965000	-4.811107000
C	10.127285000	0.824054000	-6.828178000
H	10.784611000	1.569450000	-7.278295000
C	9.834367000	-0.367390000	-7.538475000
H	9.751842000	-1.272332000	-6.929564000
C	10.324935000	-0.550759000	-8.917169000
C	10.579327000	0.533208000	-9.767712000
C	10.544583000	-1.842533000	-9.410819000
C	11.040107000	0.333054000	-11.063771000
C	11.007614000	-2.042871000	-10.703516000
C	11.258071000	-0.956390000	-11.538351000
H	10.391525000	1.550088000	-9.420854000
H	10.337314000	-2.691669000	-8.761639000
H	11.226652000	1.190875000	-11.706991000
H	11.172241000	-3.055847000	-11.064717000
H	11.618421000	-1.114478000	-12.552265000
N	8.511121000	1.847707000	-6.774352000
H	8.015587000	2.654558000	-7.156252000
Ni	7.904135000	0.190651000	-7.569962000
C	5.113396000	-0.448431000	-5.910137000
C	3.981109000	-1.217029000	-5.659097000
C	4.055086000	-2.156557000	-4.639558000
C	5.224979000	-2.257761000	-3.903157000
H	3.083514000	-1.082928000	-6.254702000
H	3.205309000	-2.796843000	-4.416603000
H	5.312232000	-2.967700000	-3.084464000
N	6.247515000	-0.536265000	-5.210803000
C	7.604862000	-1.472749000	-3.440549000
H	7.976059000	-0.434252000	-3.453391000

C	5.085862000	0.542346000	-6.999700000
C	5.583213000	1.924942000	-8.680239000
H	6.146145000	2.857802000	-8.503864000
C	5.784109000	1.556896000	-10.165259000
C	5.087080000	0.243878000	-10.512677000
H	5.229865000	0.022502000	-11.577779000
H	5.507396000	-0.590538000	-9.937556000
H	4.003495000	0.285101000	-10.335998000
C	5.216864000	2.702565000	-11.007139000
H	4.134669000	2.833307000	-10.877472000
H	5.705708000	3.656794000	-10.765670000
H	5.390231000	2.502180000	-12.071235000
C	7.276214000	1.436112000	-10.466868000
H	7.818551000	2.346213000	-10.167987000
H	7.730059000	0.576496000	-9.957825000
H	7.436073000	1.294875000	-11.543566000
C	8.651233000	-2.329133000	-4.135917000
C	9.955388000	-2.335523000	-3.623877000
C	8.378426000	-3.081290000	-5.276253000
C	10.961061000	-3.065658000	-4.242058000
H	10.174423000	-1.753326000	-2.727949000
C	9.386998000	-3.818620000	-5.896321000
H	7.389457000	-3.064666000	-5.729487000
C	10.678251000	-3.813414000	-5.385086000
H	11.968797000	-3.052527000	-3.832599000
H	9.150511000	-4.379404000	-6.798266000
H	11.464936000	-4.383278000	-5.874448000
C	7.391325000	-1.849225000	-1.986851000
C	7.009726000	-0.858864000	-1.079811000
C	7.508506000	-3.165195000	-1.535850000
C	6.752715000	-1.173163000	0.249634000
H	6.915979000	0.170150000	-1.427529000
C	7.247690000	-3.482916000	-0.206388000
H	7.813847000	-3.944019000	-2.233999000
C	6.870329000	-2.488261000	0.690100000
H	6.463165000	-0.388182000	0.944734000
H	7.344603000	-4.512650000	0.130791000
H	6.672570000	-2.736369000	1.730393000
O	3.898698000	1.115233000	-7.233780000
N	6.071028000	0.909610000	-7.730641000

C	6.299647000	-1.416894000	-4.209828000
C	4.113162000	2.104294000	-8.254926000
H	3.395752000	1.915890000	-9.059760000
H	3.904751000	3.086674000	-7.818703000
Cl	7.272703000	-1.787037000	-8.310375000

int-F_{R-d}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -508.19 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	8.448691000	-1.435584000	-9.663708000
C	8.895127000	-0.802220000	-8.734343000
C	9.751435000	0.459645000	-8.720886000
H	9.157710000	1.375504000	-8.816101000
H	10.521733000	0.435372000	-9.497127000
C	10.267708000	0.241742000	-7.325676000
H	11.131254000	-0.417522000	-7.225541000
C	9.913215000	1.101525000	-6.258876000
H	9.571558000	2.100697000	-6.538475000
C	10.542988000	0.956222000	-4.933865000
C	11.086422000	-0.263764000	-4.503876000
C	10.571219000	2.039564000	-4.046093000
C	11.640831000	-0.390811000	-3.234607000
C	11.126276000	1.911163000	-2.780715000
C	11.664368000	0.695026000	-2.365883000
H	11.058590000	-1.135947000	-5.159641000
H	10.129610000	2.984146000	-4.357581000
H	12.058908000	-1.346843000	-2.922984000
H	11.135792000	2.767528000	-2.109818000
H	12.094660000	0.594096000	-1.372394000
N	8.907847000	-1.133104000	-7.399232000
H	8.707928000	-2.109148000	-7.165881000
Ni	8.152474000	0.150290000	-6.161097000
C	5.361776000	-0.671610000	-6.343103000
C	4.190359000	-1.316536000	-5.971646000
C	4.257882000	-2.308236000	-5.000938000
C	5.481764000	-2.601585000	-4.423853000

H	3.252392000	-1.023567000	-6.431850000
H	3.359595000	-2.833435000	-4.686902000
H	5.575311000	-3.345797000	-3.636451000
N	6.551833000	-0.973190000	-5.794805000
C	7.976550000	-2.194338000	-4.230115000
H	8.615696000	-1.338795000	-4.514832000
C	5.326644000	0.428022000	-7.325345000
C	5.759362000	1.937917000	-8.859062000
H	6.466398000	2.765438000	-8.678130000
C	5.696539000	1.709246000	-10.384921000
C	4.840914000	0.488958000	-10.715178000
H	4.755779000	0.371713000	-11.802879000
H	5.299144000	-0.423428000	-10.314690000
H	3.821224000	0.571009000	-10.314312000
C	5.116182000	2.962752000	-11.041783000
H	4.073827000	3.152289000	-10.756315000
H	5.705321000	3.853572000	-10.783431000
H	5.136361000	2.857461000	-12.133589000
C	7.104647000	1.490586000	-10.934183000
H	7.761064000	2.335917000	-10.680999000
H	7.550004000	0.562946000	-10.557906000
H	7.070943000	1.419813000	-12.029243000
C	8.643790000	-3.431402000	-4.804084000
C	9.937997000	-3.745973000	-4.370551000
C	8.059997000	-4.231551000	-5.787169000
C	10.625808000	-4.826045000	-4.904924000
H	10.396116000	-3.129526000	-3.597213000
C	8.751864000	-5.315967000	-6.326817000
H	7.057044000	-4.009915000	-6.149079000
C	10.034037000	-5.616823000	-5.888565000
H	11.630195000	-5.052630000	-4.554227000
H	8.279947000	-5.922873000	-7.095887000
H	10.573384000	-6.461512000	-6.310170000
C	7.908395000	-2.158551000	-2.714330000
C	7.952364000	-0.912324000	-2.084220000
C	7.772646000	-3.312048000	-1.941302000
C	7.865711000	-0.825304000	-0.699840000
H	8.049996000	-0.009233000	-2.691092000
C	7.680677000	-3.221937000	-0.555446000
H	7.756308000	-4.287757000	-2.427121000

C	7.728874000	-1.978972000	0.067489000
H	7.909368000	0.149595000	-0.219741000
H	7.578220000	-4.127285000	0.039018000
H	7.664008000	-1.909761000	1.151086000
O	4.174546000	1.130843000	-7.313195000
N	6.254348000	0.763938000	-8.127447000
C	6.621256000	-1.911919000	-4.839618000
C	4.400868000	2.243682000	-8.191948000
H	3.557448000	2.300419000	-8.888352000
H	4.421712000	3.153065000	-7.581573000
Cl	7.282774000	1.736344000	-4.906905000

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int-F_{S-a}
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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	5.197546000	1.087063000	2.858516000
N	5.208575000	2.279141000	0.902769000
C	5.259347000	1.154056000	1.635491000
C	5.376430000	-0.081638000	0.754513000
H	6.060800000	-0.795785000	1.231314000
H	4.386535000	-0.553421000	0.732214000
H	4.912248000	3.103662000	1.417521000
Ni	5.384030000	2.343183000	-0.917412000
C	5.833049000	0.255212000	-0.635064000
H	5.328784000	-0.241914000	-1.467275000
C	7.046001000	0.864413000	-0.869372000
H	7.585820000	1.274350000	-0.009814000
C	7.826729000	0.765175000	-2.111256000
C	7.547864000	-0.194820000	-3.094078000
C	8.922088000	1.615819000	-2.308943000
C	8.294858000	-0.253864000	-4.264949000
C	9.662782000	1.564849000	-3.482731000
C	9.344440000	0.638402000	-4.471929000
H	6.754698000	-0.921955000	-2.927638000
H	9.174537000	2.334147000	-1.530288000
H	8.067961000	-1.012233000	-5.011536000
H	10.496885000	2.248720000	-3.623290000

H	9.927817000	0.593025000	-5.388492000
Cl	4.045666000	4.134301000	-0.880021000
C	7.176853000	4.284662000	-2.651953000
C	7.887377000	5.282552000	-3.310089000
C	8.624777000	6.161611000	-2.524803000
C	8.607117000	6.022198000	-1.144103000
H	7.852588000	5.363268000	-4.392131000
H	9.200262000	6.959488000	-2.987658000
H	9.152602000	6.710364000	-0.502293000
N	7.189914000	4.119030000	-1.328195000
C	7.794512000	4.733650000	0.924473000
H	6.748111000	4.439892000	1.097080000
C	6.358287000	3.313255000	-3.389203000
C	4.941232000	1.672720000	-3.935006000
H	5.186340000	0.613367000	-3.753006000
C	3.404381000	1.775844000	-4.021739000
C	2.777108000	1.203321000	-2.750723000
H	1.683216000	1.227216000	-2.832935000
H	3.072850000	0.153955000	-2.603826000
H	3.053180000	1.778633000	-1.858697000
C	2.952433000	3.220147000	-4.220659000
H	3.223394000	3.841583000	-3.358950000
H	3.379939000	3.667731000	-5.128691000
H	1.861197000	3.253731000	-4.329559000
C	2.949671000	0.913697000	-5.202802000
H	3.290760000	-0.125599000	-5.096124000
H	1.854143000	0.898478000	-5.248522000
H	3.305012000	1.290971000	-6.170410000
C	8.048142000	5.996880000	1.722871000
C	7.050341000	6.976607000	1.737609000
C	9.240185000	6.239726000	2.403006000
C	7.240262000	8.172821000	2.416549000
H	6.116208000	6.786879000	1.206469000
C	9.432053000	7.439809000	3.084327000
H	10.019841000	5.479978000	2.411719000
C	8.435487000	8.408378000	3.092583000
H	6.451697000	8.921924000	2.423473000
H	10.365345000	7.613386000	3.615652000
H	8.585271000	9.342810000	3.628580000
C	8.636669000	3.541639000	1.332132000

C	9.905152000	3.316820000	0.792402000
C	8.131744000	2.630901000	2.263212000
C	10.642851000	2.191655000	1.152848000
H	10.315043000	4.024171000	0.069193000
C	8.861766000	1.500816000	2.617048000
H	7.142195000	2.778172000	2.692841000
C	10.117753000	1.275030000	2.058725000
H	11.626250000	2.027731000	0.717183000
H	8.429538000	0.793977000	3.322283000
H	10.686737000	0.388609000	2.329768000
O	6.481072000	3.292103000	-4.716304000
N	5.553839000	2.466281000	-2.855148000
C	7.869440000	4.978595000	-0.571776000
C	5.700649000	2.172419000	-5.178429000
H	5.052108000	2.528736000	-5.983946000
H	6.399658000	1.427065000	-5.575928000

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int-F_{S-b}

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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	3.606922000	1.537908000	2.277380000
N	4.849662000	1.610672000	0.350609000
C	3.973204000	2.096350000	1.252925000
C	3.443197000	3.458939000	0.827490000
H	2.449121000	3.322811000	0.378657000
H	3.315440000	4.077702000	1.723568000
H	5.183421000	0.676958000	0.575370000
Ni	5.255953000	2.281737000	-1.313998000
C	4.369952000	4.113644000	-0.135740000
H	5.318939000	4.468258000	0.273302000
C	4.014899000	4.455547000	-1.404934000
H	3.041129000	4.105088000	-1.759231000
C	4.680021000	5.430861000	-2.274669000
C	5.766183000	6.209970000	-1.851143000
C	4.186645000	5.631289000	-3.569406000
C	6.374100000	7.109237000	-2.715546000
C	4.790366000	6.535505000	-4.434448000

C	5.896543000	7.267554000	-4.015492000
H	6.134866000	6.111343000	-0.832240000
H	3.318365000	5.058176000	-3.892748000
H	7.218346000	7.702523000	-2.370230000
H	4.395510000	6.668250000	-5.439346000
H	6.373740000	7.974798000	-4.689762000
Cl	6.342099000	0.378487000	-1.706712000
C	6.652022000	3.386440000	-3.591967000
C	6.940392000	3.654235000	-4.922253000
C	6.078907000	3.167459000	-5.895773000
C	4.993708000	2.401403000	-5.506248000
H	7.829612000	4.225257000	-5.166869000
H	6.269195000	3.360156000	-6.948373000
H	4.333239000	1.945639000	-6.240056000
N	5.559996000	2.692122000	-3.209959000
C	3.611241000	1.273213000	-3.695627000
H	3.959150000	0.826696000	-2.751734000
C	7.563454000	3.835761000	-2.530450000
C	8.530508000	4.236292000	-0.595701000
H	8.163817000	5.051795000	0.054291000
C	9.220339000	3.212928000	0.326075000
C	8.220502000	2.784194000	1.398867000
H	8.690698000	2.076574000	2.093258000
H	7.880131000	3.648489000	1.987767000
H	7.338907000	2.299357000	0.961616000
C	9.676872000	1.987004000	-0.460606000
H	8.823111000	1.458733000	-0.903848000
H	10.383151000	2.242817000	-1.262910000
H	10.192546000	1.288361000	0.210070000
C	10.413971000	3.892160000	0.996541000
H	11.189050000	4.189844000	0.277434000
H	10.103091000	4.787718000	1.552493000
H	10.883908000	3.205613000	1.711365000
C	3.408108000	0.114649000	-4.661221000
C	4.407582000	-0.863603000	-4.713729000
C	2.295674000	-0.010329000	-5.491514000
C	4.297369000	-1.938341000	-5.585348000
H	5.267954000	-0.772802000	-4.048675000
C	2.187644000	-1.089237000	-6.367274000
H	1.498406000	0.729234000	-5.448380000

C	3.186838000	-2.053019000	-6.418866000
H	5.078784000	-2.694506000	-5.609371000
H	1.311875000	-1.175854000	-7.006794000
H	3.098677000	-2.896161000	-7.100224000
C	2.355390000	2.052985000	-3.370913000
C	1.825387000	3.005719000	-4.244328000
C	1.695886000	1.810009000	-2.163988000
C	0.672066000	3.711665000	-3.913718000
H	2.326918000	3.205078000	-5.192300000
C	0.541642000	2.513404000	-1.830930000
H	2.107393000	1.074638000	-1.472102000
C	0.029827000	3.470452000	-2.702561000
H	0.275932000	4.453898000	-4.603317000
H	0.045826000	2.314678000	-0.883179000
H	-0.867851000	4.025051000	-2.440315000
O	8.670656000	4.486684000	-2.940668000
N	7.380444000	3.655000000	-1.286022000
C	4.754502000	2.164722000	-4.150015000
C	9.394128000	4.812783000	-1.739594000
H	10.389716000	4.360084000	-1.812720000
H	9.505192000	5.901849000	-1.695703000

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int-F_{S-c}

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Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	4.649850000	0.773918000	1.982263000
N	4.052973000	0.719538000	-0.233628000
C	4.496304000	1.318328000	0.896383000
C	4.805556000	2.792944000	0.680958000
H	4.210925000	3.376236000	1.397396000
H	5.854333000	2.948667000	0.956133000
H	3.966671000	-0.287764000	-0.121883000
Ni	4.490118000	1.486996000	-1.861140000
C	4.547316000	3.241350000	-0.734155000
H	5.289861000	3.888373000	-1.204831000
C	3.271426000	3.201974000	-1.270597000
H	2.520979000	2.662295000	-0.687244000

C	2.711053000	4.021044000	-2.344982000
C	3.454262000	4.964704000	-3.067648000
C	1.340131000	3.904747000	-2.608747000
C	2.842815000	5.748666000	-4.033579000
C	0.727490000	4.687585000	-3.578094000
C	1.480869000	5.610613000	-4.295835000
H	4.518640000	5.072878000	-2.880210000
H	0.753260000	3.185026000	-2.038579000
H	3.432589000	6.473763000	-4.589102000
H	-0.337767000	4.581255000	-3.769011000
H	1.007448000	6.228842000	-5.055235000
Cl	5.253828000	2.392808000	-3.747955000
C	6.715671000	-0.802675000	-2.252286000
C	7.753083000	-1.717141000	-2.386063000
C	9.033893000	-1.286620000	-2.052611000
C	9.218144000	0.021671000	-1.639063000
H	7.557924000	-2.722550000	-2.745777000
H	9.879831000	-1.964548000	-2.132276000
H	10.208283000	0.403815000	-1.400839000
N	6.879676000	0.449160000	-1.812684000
C	8.245429000	2.318510000	-1.119515000
H	7.303166000	2.779323000	-1.458301000
C	5.340458000	-1.152135000	-2.621742000
C	3.147294000	-1.090715000	-3.027753000
H	2.454872000	-1.053276000	-2.169481000
C	2.395337000	-0.519578000	-4.246085000
C	3.318283000	-0.389057000	-5.454873000
H	2.750030000	-0.010378000	-6.313607000
H	4.131481000	0.318802000	-5.251453000
H	3.755912000	-1.350439000	-5.757460000
C	1.227414000	-1.458664000	-4.556536000
H	1.552942000	-2.459025000	-4.870285000
H	0.565720000	-1.572824000	-3.686609000
H	0.627479000	-1.045653000	-5.376327000
C	1.829917000	0.852106000	-3.890674000
H	1.227645000	0.804084000	-2.971135000
H	2.626462000	1.591001000	-3.750340000
H	1.181611000	1.217833000	-4.697762000
C	9.361675000	2.981783000	-1.903546000
C	10.657095000	3.121836000	-1.403481000

C	9.088007000	3.402708000	-3.207633000
C	11.660556000	3.678073000	-2.191644000
H	10.875647000	2.806583000	-0.383470000
C	10.089948000	3.960015000	-3.993327000
H	8.075853000	3.281333000	-3.599715000
C	11.379405000	4.099380000	-3.487328000
H	12.665304000	3.786138000	-1.788610000
H	9.862013000	4.288402000	-5.004963000
H	12.163160000	4.538326000	-4.100670000
C	8.304942000	2.498561000	0.386594000
C	8.020195000	1.457935000	1.270981000
C	8.517726000	3.779972000	0.909111000
C	7.936838000	1.689979000	2.642058000
H	7.815655000	0.457746000	0.893352000
C	8.450519000	4.009563000	2.276899000
H	8.731125000	4.603709000	0.228929000
C	8.155883000	2.963597000	3.149556000
H	7.670703000	0.871282000	3.305422000
H	8.617302000	5.012673000	2.663623000
H	8.085983000	3.146407000	4.219161000
O	5.099786000	-2.427413000	-2.940410000
N	4.353456000	-0.335523000	-2.652065000
C	8.109108000	0.872582000	-1.539327000
C	3.692138000	-2.519721000	-3.228270000
H	3.588504000	-2.884559000	-4.255591000
H	3.254708000	-3.256042000	-2.546970000

int-F_{S-d}

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	4.264867000	4.210119000	-4.389012000
N	5.487135000	3.162837000	-2.750643000
C	4.393703000	3.786802000	-3.246781000
C	3.264219000	3.899859000	-2.225139000
H	2.925645000	4.944200000	-2.183613000
H	2.427384000	3.319935000	-2.633929000
H	6.138502000	2.889748000	-3.483588000

Ni	5.149935000	2.038693000	-1.317004000
C	3.649143000	3.368961000	-0.869837000
H	2.910068000	2.791639000	-0.313621000
C	4.764324000	3.858420000	-0.207770000
H	5.384152000	4.557094000	-0.774123000
C	5.136845000	3.762145000	1.201451000
C	4.327448000	3.167022000	2.178674000
C	6.359995000	4.326031000	1.590942000
C	4.743042000	3.127021000	3.500156000
C	6.775245000	4.286305000	2.914553000
C	5.967607000	3.681268000	3.871015000
H	3.376557000	2.724725000	1.894838000
H	6.995436000	4.792182000	0.835355000
H	4.108657000	2.659230000	4.249191000
H	7.735749000	4.712080000	3.194621000
H	6.291303000	3.641022000	4.908850000
Cl	4.549640000	0.580775000	0.261358000
C	6.321445000	-0.346171000	-2.415424000
C	7.240727000	-1.355394000	-2.644303000
C	8.555196000	-1.151797000	-2.238234000
C	8.890427000	0.038154000	-1.620712000
H	6.915018000	-2.279302000	-3.110911000
H	9.304483000	-1.924423000	-2.389310000
H	9.899364000	0.213387000	-1.259352000
N	6.653677000	0.818933000	-1.823093000
C	8.253188000	2.329097000	-0.730723000
H	7.298189000	2.875304000	-0.672103000
C	4.900101000	-0.522959000	-2.753151000
C	2.769982000	-0.217658000	-3.192774000
H	2.060185000	0.222851000	-2.472432000
C	2.216086000	0.038135000	-4.611184000
C	3.177834000	-0.482965000	-5.676488000
H	2.750763000	-0.327079000	-6.674932000
H	4.133945000	0.051920000	-5.637374000
H	3.379085000	-1.557742000	-5.571854000
C	0.862928000	-0.662924000	-4.738485000
H	0.939934000	-1.755481000	-4.667492000
H	0.165394000	-0.321129000	-3.961702000
H	0.412279000	-0.434032000	-5.712150000
C	2.004276000	1.535964000	-4.814392000

H	1.297210000	1.932984000	-4.071676000
H	2.937286000	2.107080000	-4.746037000
H	1.572747000	1.723842000	-5.805865000
C	9.178099000	3.169764000	-1.594155000
C	10.543227000	2.892990000	-1.727225000
C	8.644150000	4.241732000	-2.312356000
C	11.347639000	3.663365000	-2.558288000
H	10.993951000	2.084862000	-1.152841000
C	9.448354000	5.013593000	-3.146109000
H	7.577545000	4.454340000	-2.235283000
C	10.801963000	4.726032000	-3.273053000
H	12.407651000	3.434726000	-2.644180000
H	9.009641000	5.840763000	-3.699228000
H	11.432055000	5.327956000	-3.923665000
C	8.698757000	2.096700000	0.707985000
C	7.994661000	1.172472000	1.488810000
C	9.708699000	2.849202000	1.308576000
C	8.309131000	0.994585000	2.829847000
H	7.162006000	0.615011000	1.056544000
C	10.028827000	2.662516000	2.651398000
H	10.248824000	3.593537000	0.727658000
C	9.334514000	1.732050000	3.415500000
H	7.739751000	0.280958000	3.421098000
H	10.825846000	3.252709000	3.099178000
H	9.584976000	1.587273000	4.464186000
O	4.467171000	-1.796795000	-2.764406000
N	4.074944000	0.419296000	-2.976703000
C	7.917279000	1.023816000	-1.425947000
C	3.032662000	-1.699235000	-2.851781000
H	2.691436000	-2.409609000	-3.611348000
H	2.623385000	-1.987154000	-1.877173000

int-F_{s-a}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -510.73 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	5.984357000	2.228996000	2.678328000

N	5.362509000	1.552569000	0.535278000
C	6.200912000	1.690200000	1.615865000
C	7.382271000	0.860710000	1.142319000
H	8.268994000	1.457474000	0.895252000
H	7.663604000	0.100287000	1.876983000
H	4.376448000	1.782878000	0.679889000
Ni	5.755749000	2.211105000	-1.236536000
C	6.674693000	0.307375000	-0.065802000
H	6.126207000	-0.625982000	0.066004000
C	7.084945000	0.682633000	-1.371842000
H	8.012325000	1.265076000	-1.407335000
C	6.863642000	-0.202110000	-2.525670000
C	5.744472000	-1.039506000	-2.633951000
C	7.785885000	-0.196765000	-3.581041000
C	5.553381000	-1.832931000	-3.759147000
C	7.594272000	-0.988328000	-4.707545000
C	6.473514000	-1.809181000	-4.805336000
H	4.993800000	-1.039599000	-1.842949000
H	8.661473000	0.449804000	-3.509891000
H	4.671817000	-2.467442000	-3.824156000
H	8.326432000	-0.966865000	-5.512514000
H	6.320223000	-2.428853000	-5.685408000
Cl	4.317505000	3.900912000	-0.879604000
C	7.588744000	4.550023000	-2.486058000
C	8.167569000	5.724697000	-2.955525000
C	8.717752000	6.589002000	-2.014956000
C	8.648826000	6.257228000	-0.671336000
H	8.162918000	5.955021000	-4.016261000
H	9.176641000	7.522986000	-2.329535000
H	9.031408000	6.926299000	0.096271000
N	7.570710000	4.195243000	-1.198149000
C	7.954698000	4.604392000	1.145829000
H	7.107810000	3.903754000	1.149997000
C	6.887770000	3.645767000	-3.406935000
C	5.510873000	2.132064000	-4.319240000
H	5.685029000	1.049681000	-4.299276000
C	3.993415000	2.341766000	-4.511081000
C	3.224661000	1.581735000	-3.430342000
H	2.145606000	1.677810000	-3.607233000
H	3.476459000	0.512072000	-3.453854000

H	3.431419000	1.976169000	-2.428995000
C	3.619984000	3.820698000	-4.481561000
H	3.821826000	4.258345000	-3.496219000
H	4.159558000	4.399128000	-5.244849000
H	2.548223000	3.937643000	-4.686091000
C	3.618662000	1.723701000	-5.862266000
H	3.939013000	0.673408000	-5.920178000
H	2.529458000	1.747373000	-5.988290000
H	4.050138000	2.260049000	-6.717005000
C	7.553208000	5.755324000	2.045424000
C	6.199145000	6.085256000	2.133873000
C	8.488731000	6.518756000	2.744764000
C	5.789315000	7.163875000	2.908930000
H	5.470477000	5.484471000	1.586336000
C	8.077637000	7.600202000	3.518242000
H	9.544797000	6.253166000	2.692153000
C	6.727261000	7.924506000	3.601784000
H	4.731520000	7.407904000	2.975801000
H	8.814729000	8.186939000	4.062515000
H	6.405366000	8.766092000	4.211239000
C	9.162771000	3.827370000	1.633014000
C	10.306949000	3.634190000	0.859708000
C	9.094752000	3.225187000	2.895999000
C	11.358944000	2.848676000	1.330720000
H	10.381458000	4.089591000	-0.126674000
C	10.141757000	2.444145000	3.364263000
H	8.188457000	3.346337000	3.488009000
C	11.279599000	2.251023000	2.581536000
H	12.242591000	2.706568000	0.712108000
H	10.068031000	1.976997000	4.343956000
H	12.098715000	1.636262000	2.947858000
O	7.094137000	3.842482000	-4.712425000
N	6.070121000	2.711655000	-3.074860000
C	8.064553000	5.041071000	-0.296744000
C	6.395563000	2.782946000	-5.393455000
H	5.843877000	3.230674000	-6.224302000
H	7.146982000	2.089392000	-5.791162000

int-F_{S-b}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -509.92 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	3.300573000	0.339848000	1.676042000
N	4.775864000	1.849232000	0.680406000
C	3.552214000	1.368671000	1.097253000
C	2.674883000	2.576453000	0.800795000
H	1.993281000	2.440837000	-0.046220000
H	2.098545000	2.872609000	1.682159000
H	5.603222000	1.362199000	1.033108000
Ni	5.178920000	2.324001000	-1.132194000
C	3.820791000	3.501698000	0.496246000
H	4.241335000	4.043731000	1.343139000
C	4.029554000	3.989667000	-0.818793000
H	3.211492000	3.775674000	-1.515045000
C	4.745689000	5.249549000	-1.082198000
C	5.573089000	5.871523000	-0.136830000
C	4.626338000	5.855380000	-2.340163000
C	6.261725000	7.037839000	-0.441927000
C	5.325833000	7.015542000	-2.652768000
C	6.152377000	7.613372000	-1.706633000
H	5.707241000	5.419747000	0.845710000
H	3.977497000	5.391918000	-3.085547000
H	6.896062000	7.498707000	0.314189000
H	5.220546000	7.457136000	-3.641725000
H	6.697793000	8.522815000	-1.946994000
Cl	6.263206000	0.370133000	-1.446088000
C	6.621202000	3.536120000	-3.268085000
C	6.939375000	3.914865000	-4.565273000
C	6.131290000	3.471593000	-5.602348000
C	5.061726000	2.643181000	-5.307993000
H	7.812789000	4.535285000	-4.734615000
H	6.348310000	3.750113000	-6.630263000
H	4.431356000	2.230499000	-6.092109000
N	5.542316000	2.779403000	-2.977162000
C	3.626383000	1.397600000	-3.631104000

H	3.912519000	0.926278000	-2.676798000
C	7.494964000	3.925312000	-2.152684000
C	8.499865000	4.088001000	-0.207151000
H	8.122141000	4.664822000	0.653431000
C	9.380346000	2.953273000	0.356358000
C	8.517078000	2.060639000	1.247357000
H	9.147967000	1.350398000	1.796739000
H	7.958866000	2.656036000	1.985260000
H	7.805896000	1.484066000	0.642822000
C	9.975501000	2.102332000	-0.763594000
H	9.185665000	1.628785000	-1.360182000
H	10.626174000	2.681481000	-1.432695000
H	10.587509000	1.300026000	-0.332727000
C	10.491767000	3.580239000	1.196528000
H	11.144138000	4.239127000	0.607883000
H	10.077580000	4.168128000	2.027201000
H	11.127230000	2.796959000	1.627691000
C	3.489067000	0.272284000	-4.643291000
C	4.423869000	-0.766522000	-4.598199000
C	2.496182000	0.255451000	-5.622068000
C	4.363956000	-1.802788000	-5.521189000
H	5.191490000	-0.750630000	-3.821911000
C	2.440031000	-0.783639000	-6.548005000
H	1.755345000	1.053486000	-5.655213000
C	3.372946000	-1.813158000	-6.500205000
H	5.091326000	-2.609972000	-5.472433000
H	1.659133000	-0.789011000	-7.305410000
H	3.325347000	-2.626593000	-7.220731000
C	2.336122000	2.152536000	-3.383709000
C	2.027894000	3.362392000	-4.006303000
C	1.404342000	1.596546000	-2.502471000
C	0.830170000	4.019213000	-3.730970000
H	2.734493000	3.808259000	-4.706110000
C	0.205701000	2.246227000	-2.231127000
H	1.636952000	0.647129000	-2.018020000
C	-0.081271000	3.466467000	-2.838959000
H	0.612420000	4.967916000	-4.216391000
H	-0.503262000	1.801346000	-1.536137000
H	-1.013755000	3.980922000	-2.619914000
O	8.538239000	4.718205000	-2.475264000

N	7.354651000	3.554163000	-0.944891000
C	4.783929000	2.306630000	-3.981659000
C	9.178519000	5.026721000	-1.223757000
H	10.254741000	4.864118000	-1.344119000
H	8.995334000	6.086510000	-1.007810000

int-F_{s-c}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -512.41 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	5.506573000	-1.547198000	2.169621000
N	5.921363000	0.731623000	1.877530000
C	5.152301000	-0.391018000	2.093203000
C	3.804356000	0.260845000	2.357325000
H	3.066791000	0.106130000	1.563126000
H	3.373999000	-0.084862000	3.302522000
H	6.927258000	0.634094000	2.024524000
Ni	5.560591000	1.830380000	0.309600000
C	4.355593000	1.661448000	2.412084000
H	4.683898000	2.008877000	3.392641000
C	4.064132000	2.612487000	1.398954000
H	3.214512000	2.370396000	0.754700000
C	4.315792000	4.049668000	1.625731000
C	5.226029000	4.508177000	2.587270000
C	3.639379000	5.003174000	0.854180000
C	5.452589000	5.867479000	2.770112000
C	3.863182000	6.360147000	1.037744000
C	4.772200000	6.801636000	1.996221000
H	5.788356000	3.795211000	3.191159000
H	2.945267000	4.661311000	0.089123000
H	6.167922000	6.196686000	3.521334000
H	3.325939000	7.080074000	0.424145000
H	4.948974000	7.865369000	2.137590000
Cl	4.969881000	2.949974000	-1.482525000
C	6.395119000	-1.027183000	-1.159495000
C	6.818194000	-2.326672000	-1.408045000
C	5.851380000	-3.327997000	-1.406413000

C	4.525030000	-2.986602000	-1.205131000
H	7.866227000	-2.540006000	-1.594923000
H	6.133454000	-4.363538000	-1.578853000
H	3.742344000	-3.741726000	-1.219466000
N	5.121221000	-0.692039000	-0.934944000
C	2.760655000	-1.162449000	-0.891096000
H	2.843574000	-0.131188000	-0.509557000
C	7.344575000	0.096516000	-1.190444000
C	8.281050000	2.117117000	-1.090587000
H	7.791512000	2.855229000	-1.746773000
C	9.019615000	2.898714000	0.010840000
C	9.661206000	1.970339000	1.039428000
H	10.123029000	2.561811000	1.839574000
H	8.917735000	1.309019000	1.502148000
H	10.448625000	1.336145000	0.612956000
C	10.098870000	3.744745000	-0.668050000
H	10.854784000	3.132881000	-1.178233000
H	9.656733000	4.426575000	-1.406203000
H	10.624460000	4.355390000	0.076303000
C	8.042773000	3.834378000	0.718520000
H	7.502400000	4.478123000	0.011869000
H	7.282767000	3.276722000	1.280898000
H	8.577171000	4.476487000	1.431450000
C	1.874213000	-1.938677000	0.065484000
C	0.482931000	-1.896161000	-0.068552000
C	2.414525000	-2.605006000	1.171124000
C	-0.344031000	-2.518714000	0.859200000
H	0.043375000	-1.367501000	-0.912181000
C	1.585289000	-3.227251000	2.100249000
H	3.493339000	-2.621153000	1.331263000
C	0.204150000	-3.192876000	1.945899000
H	-1.423478000	-2.474524000	0.731432000
H	2.028583000	-3.740333000	2.950986000
H	-0.442213000	-3.682980000	2.670508000
C	2.255234000	-1.032708000	-2.319729000
C	2.485991000	0.163325000	-3.002950000
C	1.659308000	-2.098072000	-2.998137000
C	2.107637000	0.296605000	-4.334740000
H	2.984637000	0.988538000	-2.489798000
C	1.280275000	-1.962804000	-4.329266000

H	1.474149000	-3.035980000	-2.475441000
C	1.501267000	-0.763857000	-5.000596000
H	2.290722000	1.235502000	-4.852209000
H	0.809171000	-2.797884000	-4.843488000
H	1.202429000	-0.657826000	-6.041116000
O	8.425506000	-0.072618000	-1.961507000
N	7.204901000	1.231760000	-0.611165000
C	4.195004000	-1.644153000	-0.978600000
C	9.168526000	1.159000000	-1.903658000
H	10.132360000	0.944762000	-1.425917000
H	9.350356000	1.491572000	-2.929382000

int-F_{S-d}-TS

Charge = 0 Multiplicity = 1

Imaginary frequency = -508.39 cm⁻¹

Cartesian coordinates:

ATOM	X	Y	Z
O	4.606747000	0.191729000	1.694098000
N	5.387575000	2.191572000	0.778424000
C	4.453168000	1.230746000	1.094346000
C	3.176242000	1.920025000	0.626905000
H	2.770203000	1.491874000	-0.295935000
H	2.407947000	1.912657000	1.405563000
H	6.277825000	2.167637000	1.281591000
Ni	5.594226000	2.641487000	-1.096275000
C	3.821176000	3.263347000	0.419028000
H	3.887332000	3.909045000	1.295742000
C	3.984315000	3.820803000	-0.871778000
H	3.338519000	3.416521000	-1.654778000
C	4.431091000	5.215806000	-1.040348000
C	5.183791000	5.875831000	-0.058680000
C	4.138703000	5.908006000	-2.222932000
C	5.616818000	7.183796000	-0.249997000
C	4.572946000	7.212185000	-2.412986000
C	5.314573000	7.859780000	-1.427391000
H	5.457872000	5.356210000	0.860982000
H	3.579892000	5.396740000	-3.004460000
H	6.194973000	7.677351000	0.530060000

H	4.333293000	7.727649000	-3.340578000
H	5.655950000	8.881208000	-1.577753000
Cl	5.716418000	3.094471000	-3.252108000
C	7.517268000	0.472330000	-1.570601000
C	8.755524000	-0.107973000	-1.815581000
C	9.889786000	0.688745000	-1.728153000
C	9.750977000	2.020674000	-1.376776000
H	8.807074000	-1.157870000	-2.082823000
H	10.872503000	0.270829000	-1.930652000
H	10.612076000	2.679374000	-1.297866000
N	7.386433000	1.766572000	-1.224585000
C	8.290200000	3.944470000	-0.602417000
H	7.234105000	4.195693000	-0.805266000
C	6.287890000	-0.325335000	-1.705548000
C	4.213298000	-1.011370000	-1.926464000
H	3.479305000	-1.124558000	-1.112348000
C	3.429520000	-0.742074000	-3.230458000
C	4.373104000	-0.560468000	-4.417926000
H	3.788882000	-0.399852000	-5.332797000
H	5.017782000	0.317080000	-4.279764000
H	5.006512000	-1.441188000	-4.589480000
C	2.482064000	-1.915205000	-3.477803000
H	3.015019000	-2.860755000	-3.642580000
H	1.795300000	-2.056986000	-2.632014000
H	1.874997000	-1.727236000	-4.372073000
C	2.605762000	0.533221000	-3.059688000
H	1.930750000	0.455262000	-2.194337000
H	3.259195000	1.405305000	-2.932458000
H	1.983717000	0.702054000	-3.948086000
C	9.111466000	4.955023000	-1.378252000
C	10.402888000	5.319769000	-0.992880000
C	8.555776000	5.519053000	-2.528839000
C	11.135274000	6.224911000	-1.754422000
H	10.829115000	4.904771000	-0.079025000
C	9.287793000	6.427341000	-3.285500000
H	7.544812000	5.233263000	-2.826758000
C	10.578774000	6.779693000	-2.902912000
H	12.140277000	6.503448000	-1.444685000
H	8.844219000	6.863677000	-4.177551000
H	11.149210000	7.491490000	-3.495542000

C	8.465955000	4.025421000	0.906477000
C	8.759985000	2.919294000	1.705856000
C	8.266693000	5.262833000	1.530913000
C	8.842598000	3.043397000	3.092991000
H	8.924654000	1.941919000	1.253133000
C	8.350131000	5.387527000	2.910445000
H	8.044022000	6.132143000	0.912600000
C	8.637538000	4.275025000	3.699537000
H	9.069660000	2.167368000	3.696184000
H	8.190028000	6.358423000	3.374273000
H	8.701582000	4.371414000	4.780670000
O	6.480160000	-1.633294000	-1.988291000
N	5.098130000	0.110342000	-1.602931000
C	8.480482000	2.533769000	-1.111820000
C	5.166886000	-2.220509000	-1.965115000
H	5.064244000	-2.853749000	-2.852311000
H	5.092075000	-2.846995000	-1.068833000

int-G_R

Charge = 0 Multiplicity = 1

Cartesian coordinates:

ATOM	X	Y	Z
O	10.290501000	-4.670681000	-7.791066000
C	9.354392000	-3.918176000	-7.909989000
C	7.864450000	-3.945637000	-7.536313000
H	7.657870000	-3.959756000	-6.460312000
H	7.295992000	-4.740590000	-8.026968000
C	7.785898000	-2.545124000	-8.205162000
H	7.189785000	-2.535852000	-9.125664000
C	7.408048000	-1.421094000	-7.275664000
H	7.989737000	-1.535478000	-6.348562000
C	5.959136000	-1.282974000	-6.989679000
C	5.486777000	-1.193101000	-5.669466000
C	5.019128000	-1.170764000	-8.029640000
C	4.141139000	-0.986120000	-5.397641000
C	3.673172000	-0.958522000	-7.757751000
C	3.227430000	-0.862541000	-6.442427000
H	6.197023000	-1.301403000	-4.847921000

H	5.356956000	-1.216947000	-9.064790000
H	3.799590000	-0.930280000	-4.365670000
H	2.974487000	-0.853843000	-8.586444000
H	2.173367000	-0.697269000	-6.231077000
Ni	7.573089000	0.410774000	-7.843941000
C	6.641278000	3.001236000	-6.734619000
C	6.081374000	4.226084000	-6.410797000
C	5.464626000	4.940554000	-7.432852000
C	5.418447000	4.384725000	-8.697914000
H	6.144453000	4.600056000	-5.393609000
H	5.027131000	5.916671000	-7.240213000
H	4.962832000	4.917123000	-9.529961000
N	6.613152000	2.450615000	-7.966234000
C	5.853644000	2.461451000	-10.288098000
H	6.647703000	1.704799000	-10.318455000
C	7.353141000	2.196718000	-5.749377000
C	8.693809000	0.650678000	-4.889870000
H	8.484089000	-0.399599000	-4.640384000
C	10.209108000	0.772889000	-5.185081000
C	10.586726000	2.203363000	-5.565572000
H	11.668601000	2.266091000	-5.733634000
H	10.094943000	2.511391000	-6.497579000
H	10.335789000	2.930811000	-4.782278000
C	10.972498000	0.345928000	-3.930092000
H	10.806488000	1.015915000	-3.076765000
H	10.696926000	-0.672293000	-3.624811000
H	12.049854000	0.347284000	-4.133918000
C	10.595850000	-0.167061000	-6.325549000
H	10.360290000	-1.212992000	-6.087834000
H	10.078020000	0.085668000	-7.259741000
H	11.676434000	-0.103095000	-6.505064000
C	6.146098000	3.447283000	-11.405015000
C	7.480126000	3.805426000	-11.621702000
C	5.154811000	4.022145000	-12.199176000
C	7.815425000	4.725052000	-12.606852000
H	8.255538000	3.336542000	-11.013828000
C	5.490533000	4.945653000	-13.186539000
H	4.114244000	3.734679000	-12.053842000
C	6.818808000	5.300665000	-13.391674000
H	8.858369000	4.987622000	-12.769788000

H	4.707966000	5.383806000	-13.802347000
H	7.079518000	6.017848000	-14.166670000
C	4.546647000	1.710277000	-10.456870000
C	3.326571000	2.158284000	-9.948801000
C	4.567111000	0.532321000	-11.209928000
C	2.150345000	1.456571000	-10.201717000
H	3.285857000	3.065265000	-9.346782000
C	3.395556000	-0.172475000	-11.459404000
H	5.521946000	0.170035000	-11.590909000
C	2.180153000	0.291366000	-10.960224000
H	1.207762000	1.823344000	-9.801051000
H	3.431244000	-1.087719000	-12.046109000
H	1.261627000	-0.256294000	-11.158819000
O	7.528191000	2.665658000	-4.512888000
N	7.865479000	1.055562000	-6.038564000
C	5.974807000	3.117433000	-8.935630000
C	8.163140000	1.583732000	-3.791884000
H	8.931088000	2.018638000	-3.147472000
H	7.395054000	1.106546000	-3.170827000
N	9.219442000	-2.671646000	-8.462377000
H	9.826568000	-2.080909000	-9.017672000
Cl	8.172134000	0.012326000	-9.911315000

int-G_S

Charge = 0 Multiplicity = 1

Cartesian coordinates:

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N	5.430234000	0.701951000	2.528151000
C	4.550573000	0.826935000	3.581824000
C	4.580042000	2.357765000	3.484027000
H	3.601929000	2.806411000	3.280968000
H	5.052303000	2.872237000	4.326487000
H	5.519602000	-0.055839000	1.854027000
Ni	5.817501000	1.892090000	-0.661138000
C	5.461786000	2.135376000	2.223831000
H	6.474377000	2.557446000	2.327836000
C	4.846203000	2.503325000	0.905441000

H	3.901216000	1.957511000	0.764525000
C	4.688286000	3.939841000	0.597678000
C	5.351995000	4.960159000	1.296967000
C	3.895003000	4.310001000	-0.502651000
C	5.285808000	6.282191000	0.866254000
C	3.834190000	5.625935000	-0.935119000
C	4.545433000	6.620281000	-0.263288000
H	5.923075000	4.719984000	2.193664000
H	3.342117000	3.535956000	-1.035791000
H	5.807161000	7.057334000	1.425852000
H	3.220805000	5.875703000	-1.799600000
H	4.499408000	7.653560000	-0.599701000
Cl	5.032398000	-0.125250000	-0.677096000
C	6.658663000	3.612072000	-3.042628000
C	6.840444000	4.364154000	-4.194105000
C	6.095053000	4.007421000	-5.313133000
C	5.195012000	2.958742000	-5.217376000
H	7.542685000	5.192047000	-4.201766000
H	6.208979000	4.551538000	-6.247302000
H	4.590133000	2.656513000	-6.069261000
N	5.808957000	2.577153000	-2.945414000
C	3.985681000	1.220461000	-3.793278000
H	4.409572000	0.511213000	-3.065164000
C	7.396920000	3.886443000	-1.811465000
C	8.273398000	3.632646000	0.212549000
H	7.831622000	3.847197000	1.196065000
C	9.337849000	2.521011000	0.388712000
C	8.700115000	1.266168000	0.983818000
H	9.463774000	0.488099000	1.107910000
H	8.265203000	1.461500000	1.972674000
H	7.906712000	0.858488000	0.342560000
C	9.992856000	2.159952000	-0.943647000
H	9.263667000	1.735586000	-1.646111000
H	10.478484000	3.019053000	-1.424448000
H	10.765364000	1.398927000	-0.780119000
C	10.395463000	3.030887000	1.369157000
H	10.957818000	3.891209000	0.984473000
H	9.941257000	3.319956000	2.326434000
H	11.123663000	2.237547000	1.576143000
C	3.675357000	0.455635000	-5.067085000

C	4.619127000	-0.464466000	-5.534464000
C	2.509202000	0.651713000	-5.805611000
C	4.404701000	-1.169168000	-6.711728000
H	5.528234000	-0.629600000	-4.955303000
C	2.292722000	-0.053597000	-6.987384000
H	1.757247000	1.352968000	-5.448558000
C	3.238058000	-0.963682000	-7.444529000
H	5.146617000	-1.886391000	-7.055749000
H	1.375168000	0.107964000	-7.549009000
H	3.065560000	-1.517081000	-8.364720000
C	2.766860000	1.840238000	-3.129038000
C	2.275552000	3.096989000	-3.493186000
C	2.098145000	1.120991000	-2.135979000
C	1.140777000	3.622086000	-2.880400000
H	2.787116000	3.679602000	-4.259932000
C	0.968705000	1.647569000	-1.518094000
H	2.491986000	0.154350000	-1.827562000
C	0.486006000	2.899652000	-1.887951000
H	0.771937000	4.602086000	-3.176668000
H	0.468455000	1.077446000	-0.738718000
H	-0.394427000	3.312944000	-1.401592000
O	8.345966000	4.822619000	-1.816995000
N	7.201999000	3.239170000	-0.717770000
C	5.050527000	2.273877000	-4.001866000
C	8.778324000	4.925696000	-0.439538000
H	9.863909000	5.050794000	-0.440094000
H	8.302732000	5.817571000	-0.013121000