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Theoretical study on the ability of bicyclic cryptands to separate alkali-metal isotopes by ion exchange

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Supporting Information

Table S1. Optimized geometries and total energies of the cryptands from [1.1.1] to [3.3.3] obtained by the B3LYP method with the aug−cc−pVDZ basis set.

Table S2. Total energies of the alkali-metal cations obtained by the B3LYP method with the SDD basis set for Li, Na, K, Rb, and Cs atoms and the MWB pseudo potentials for K to Cs atoms.

Table S3. Optimized geometries and total energies of the alkali-metal cryptates from [M^+⊂1.1.1] to [M^+⊂3.3.3] obtained by the B3LYP method with the aug−cc−pVDZ basis set for C, H, N, and O atoms and the SDD basis set for Li, Na, K, Rb, and Cs atoms with the MWB pseudo potentials for K to Cs atoms.

Table S1. Optimized geometries and energies of the cryptands from [1.1.1] to [3.3.3] by the B3LYP method with the aug−cc−pVDZ basis set.

[1.1.1] cryptand C_{3h} symmetry

N	0.000000	0.000000	2.000350
N	0.000000	0.000000	−2.000350
O	−1.182243	1.840101	0.000000
O	2.184695	0.103802	0.000000
O	−1.002453	−1.943902	0.000000
C	−0.742074	1.215962	2.283570
C	−0.572428	2.283563	1.203205
C	−0.742074	1.215962	−2.283570
C	−0.572428	2.283563	−1.203205
H	−1.809904	0.970354	2.352596
H	−0.459906	1.666449	3.259845
H	−1.035402	3.228227	1.546446
H	0.498310	2.475367	1.031764
H	−0.459906	1.666449	−3.259845
H	−1.809904	0.970354	−2.352596
H	0.498310	2.475367	−1.031764
H	−1.035402	3.228227	−1.546446
C	1.424091	0.034674	2.283570
C	2.263838	−0.646044	1.203205
C	1.424091	0.034674	−2.283570
C	2.263838	−0.646044	−1.203205
H	1.745304	1.082246	2.352596
H	1.673141	−0.434934	3.259845
H	3.313428	−0.717430	1.546446
H	1.894576	−1.669233	1.031764
H	1.673141	−0.434934	−3.259845
H	1.745304	1.082246	−2.352596
H	1.894576	−1.669233	−1.031764
H	3.313428	−0.717430	−1.546446
C	−0.682017	−1.250636	2.283570
C	−1.691410	−1.637519	1.203205
C	−0.682017	−1.250636	−2.283570

C	−1.691410	−1.637519	−1.203205
H	0.064601	−2.052600	2.352596
H	−1.213234	−1.231515	3.259845
H	−2.278026	−2.510798	1.546446
H	−2.392886	−0.806134	1.031764
H	−1.213234	−1.231515	−3.259845
H	0.064601	−2.052600	−2.352596
H	−2.392886	−0.806134	−1.031764
H	−2.278026	−2.510798	−1.546446

Total Energy= −806.91953701 au

[2.1.1] cryptand C_2 symmetry

C	2.76656400	−0.10890300	0.88716800
C	2.32997400	1.09962700	1.72605500
O	0.98936900	1.05551000	2.18475800
C	−0.98936900	1.99162000	−1.88767600
C	−2.07465800	1.63347000	−0.87089900
O	0.29831100	1.83874700	−1.31412300
C	2.45682500	0.75380900	−1.37098500
C	1.30638800	1.36263600	−2.18288700
C	−1.30638800	−1.36263600	−2.18288700
C	−2.45682500	−0.75380900	−1.37098500
C	2.07465800	−1.63347000	−0.87089900
C	0.98936900	−1.99162000	−1.88767600
N	2.07664300	−0.25711000	−0.39104400
O	−0.29831100	−1.83874700	−1.31412300
N	−2.07664300	0.25711000	−0.39104400
C	0.73863600	0.16927400	3.26270500
C	−0.73863600	−0.16927400	3.26270500
O	−0.98936900	−1.05551000	2.18475800
C	−2.32997400	−1.09962700	1.72605500
C	−2.76656400	0.10890300	0.88716800
H	3.87146100	−0.03184700	0.76233600
H	2.59088800	−1.02145500	1.46915100
H	3.02956100	1.19085700	2.57916900
H	2.40171900	2.02556600	1.14206200

H	−1.08175300	1.38103700	−2.79862700
H	−1.14920700	3.04236200	−2.19422600
H	−1.92746500	2.28650200	−0.00170700
H	−3.05014700	1.91718300	−1.33247700
H	3.20043200	0.35957800	−2.09752000
H	2.95496500	1.57726900	−0.84457500
H	0.88291600	0.62490800	−2.87952600
H	1.72160800	2.18349700	−2.80109900
H	−1.72160800	−2.18349700	−2.80109900
H	−0.88291600	−0.62490800	−2.87952600
H	−3.20043200	−0.35957800	−2.09752000
H	−2.95496500	−1.57726900	−0.84457500
H	1.92746500	−2.28650200	−0.00170700
H	3.05014700	−1.91718300	−1.33247700
H	1.08175300	−1.38103700	−2.79862700
H	1.14920700	−3.04236200	−2.19422600
H	1.31377200	−0.76508800	3.16520100
H	1.01514900	0.64490400	4.22317500
H	−1.01514900	−0.64490400	4.22317500
H	−1.31377200	0.76508800	3.16520100
H	−2.40171900	−2.02556600	1.14206200
H	−3.02956100	−1.19085700	2.57916900
H	−2.59088800	1.02145500	1.46915100
H	−3.87146100	0.03184700	0.76233600

Total Energy= −960.75350499 au

[2.2.1] cryptand C_2 symmetry

N	2.73653800	−0.64143800	0.46005100
N	−2.73653800	0.64143800	0.46005100
C	2.45259700	−0.18214900	1.80927400
C	1.10329000	−0.48482000	2.49035500
O	0.00000000	0.00000000	1.72569200
C	−2.45259700	0.18214900	1.80927400
C	−1.10329000	0.48482000	2.49035500
H	3.22688000	−0.60583300	2.47076900
H	2.59272300	0.90740000	1.83962500

H	0.97319300	−1.56575100	2.67021900
H	1.12901400	0.00984300	3.47739500
H	−3.22688000	0.60583300	2.47076900
H	−2.59272300	−0.90740000	1.83962500
H	−0.97319300	1.56575100	2.67021900
H	−1.12901400	−0.00984300	3.47739500
C	2.01218600	−0.04064000	−0.66395100
C	2.02464100	1.48606200	−0.63760900
O	1.31138800	1.91733900	−1.79236500
C	0.97387600	3.29244600	−1.82830700
C	−3.12295400	2.03100100	0.28669700
C	−2.03758500	3.11834600	0.31415400
O	−1.17355500	2.95890600	−0.79986000
C	0.00000000	3.74740700	−0.74352200
H	2.50933800	−0.37381300	−1.58509300
H	0.97001100	−0.37301500	−0.73518700
H	1.52879000	1.85087600	0.27156500
H	3.05826800	1.87886100	−0.65393800
H	1.87940000	3.92638100	−1.76051400
H	0.51843400	3.44896900	−2.81454900
H	−3.64884700	2.11526500	−0.67708500
H	−3.85146500	2.28545800	1.07428200
H	−2.52983800	4.11107900	0.28092500
H	−1.45403500	3.07204800	1.24944900
H	−0.23019900	4.81723400	−0.91475500
H	0.45604200	3.67170100	0.25901900
C	3.12295400	−2.03100100	0.28669700
C	2.03758500	−3.11834600	0.31415400
O	1.17355500	−2.95890600	−0.79986000
C	0.00000000	−3.74740700	−0.74352200
C	−2.01218600	0.04064000	−0.66395100
C	−2.02464100	−1.48606200	−0.63760900
O	−1.31138800	−1.91733900	−1.79236500
C	−0.97387600	−3.29244600	−1.82830700
H	3.64884700	−2.11526500	−0.67708500
H	3.85146500	−2.28545800	1.07428200

H	2.52983800	−4.11107900	0.28092500
H	1.45403500	−3.07204800	1.24944900
H	0.23019900	−4.81723400	−0.91475500
H	−0.45604200	−3.67170100	0.25901900
H	−2.50933800	0.37381300	−1.58509300
H	−0.97001100	0.37301500	−0.73518700
H	−1.52879000	−1.85087600	0.27156500
H	−3.05826800	−1.87886100	−0.65393800
H	−1.87940000	−3.92638100	−1.76051400
H	−0.51843400	−3.44896900	−2.81454900

Total Energy= −1114.60980397 au

[2.2.2] cryptand C_3 symmetry

N	0.00000000	0.00000000	−2.46926700
N	0.00000000	0.00000000	2.74034100
C	1.37919800	0.33920800	−2.82206100
C	2.08045200	1.20114900	−1.78008000
O	1.59202100	2.54754000	−1.85007600
C	2.10969900	3.42422200	−0.86212400
C	0.75609700	1.17450600	3.18656000
C	0.53899300	2.42468400	2.34237000
O	1.35741300	2.36659100	1.18193100
C	1.23645000	3.53127800	0.37848500
H	1.94787800	−0.59391600	−2.89020300
H	1.44489900	0.83874400	−3.81007800
H	1.90442300	0.78403600	−0.77944000
H	3.16760800	1.20869800	−1.98416100
H	3.13414300	3.13089700	−0.57577100
H	2.15854400	4.42197300	−1.32454400
H	0.52196600	1.41496100	4.24615700
H	1.82750300	0.94408600	3.14984600
H	−0.51953600	2.53057600	2.04964400
H	0.81281600	3.31476300	2.94015400
H	0.18498000	3.67745900	0.07351400
H	1.55061000	4.42176500	0.95863800
C	−0.98336100	1.02481700	−2.82206100

C	−2.08045200	1.20114900	−1.78008000
O	−3.00224500	0.10496000	−1.85007600
C	−4.02031300	0.11494300	−0.86212400
C	−1.39520100	0.06754600	3.18656000
C	−2.36933400	−0.74556000	2.34237000
O	−2.72823400	−0.00774200	1.18193100
C	−3.67640100	−0.69484200	0.37848500
H	−0.45959200	1.98387000	−2.89020300
H	−1.44882300	0.83194700	−3.81007800
H	−1.63120600	1.25726100	−0.77944000
H	−2.63056700	2.13888000	−1.98416100
H	−4.27850800	1.14879900	−0.57577100
H	−4.90881300	−0.34163200	−1.32454400
H	−1.48637500	−0.25544400	4.24615700
H	−1.73135400	1.11062100	3.14984600
H	−1.93177500	−1.71521900	2.04964400
H	−3.27707700	−0.95346200	2.94015400
H	−3.27726300	−1.67853200	0.07351400
H	−4.60466600	−0.86801400	0.95863800
C	−0.39583700	−1.36402400	−2.82206100
C	0.00000000	−2.40229900	−1.78008000
O	1.41022400	−2.65250000	−1.85007600
C	1.91061300	−3.53916400	−0.86212400
C	0.63910400	−1.24205300	3.18656000
C	1.83034100	−1.67912400	2.34237000
O	1.37082200	−2.35884900	1.18193100
C	2.43995200	−2.83643600	0.37848500
H	−1.48828600	−1.38995400	−2.89020300
H	0.00392400	−1.67069100	−3.81007800
H	−0.27321700	−2.04129700	−0.77944000
H	−0.53704100	−3.34757800	−1.98416100
H	1.14436500	−4.27969600	−0.57577100
H	2.75026900	−4.08034000	−1.32454400
H	0.96440900	−1.15951700	4.24615700
H	−0.09614900	−2.05470700	3.14984600
H	2.45131100	−0.81535600	2.04964400

H	2.46426100	−2.36130100	2.94015400
H	3.09228300	−1.99892700	0.07351400
H	3.05405600	−3.55375000	0.95863800

Total Energy= −1268.48112275 au

[3.2.2] cryptand C_2 symmetry

N	2.43756200	−2.81835900	−0.60094500
N	−2.43756200	2.81835900	−0.60094500
O	0.00000000	0.00000000	2.89838000
C	1.17092500	−0.14493000	3.68791200
H	1.11621600	−1.07427100	4.28339100
H	1.26423100	0.70577500	4.38862100
C	−1.17092500	0.14493000	3.68791200
H	−1.26423100	−0.70577500	4.38862100
H	−1.11621600	1.07427100	4.28339100
C	1.27356900	−3.62229200	−0.26569000
C	0.00000000	−2.84723800	0.07031400
O	−0.59399100	−2.35235000	−1.13212800
C	−1.58229500	−1.36109300	−0.89255300
C	−2.74936100	2.60886300	−2.00404500
C	−2.22777100	1.30528900	−2.60530100
O	−2.98844500	0.19560800	−2.11921900
C	−2.29852600	−1.04872900	−2.20744200
H	1.04298400	−4.31317600	−1.09589900
H	1.51152000	−4.24138100	0.61366300
H	−0.71800400	−3.52166500	0.57466700
H	0.23987900	−2.01867400	0.75272900
H	−2.30957700	−1.71898600	−0.14269700
H	−1.12010100	−0.44316800	−0.49368000
H	−3.84140000	2.64081100	−2.14539300
H	−2.32085000	3.43072300	−2.60526300
H	−2.31816400	1.34930800	−3.70699400
H	−1.16653000	1.19588900	−2.34543000
H	−3.04421200	−1.82143000	−2.43706600
H	−1.56461000	−1.03621400	−3.02857200
C	3.51211100	−2.72791900	0.37016500

C	3.56461600	−1.43463700	1.18006800
O	2.43849600	−1.36935700	2.05076000
C	2.39882700	−0.16969600	2.80263800
C	−3.51211100	2.72791900	0.37016500
C	−3.56461600	1.43463700	1.18006800
O	−2.43849600	1.36935700	2.05076000
C	−2.39882700	0.16969600	2.80263800
H	3.44399900	−3.57038700	1.07859100
H	4.48286400	−2.81865400	−0.14516300
H	4.49701500	−1.41965400	1.77807300
H	3.57274800	−0.56912600	0.49886600
H	3.29518400	−0.09357900	3.44753700
H	2.38961600	0.70618300	2.13140600
H	−3.44399900	3.57038700	1.07859100
H	−4.48286400	2.81865400	−0.14516300
H	−4.49701500	1.41965400	1.77807300
H	−3.57274800	0.56912600	0.49886600
H	−3.29518400	0.09357900	3.44753700
H	−2.38961600	−0.70618300	2.13140600
C	2.74936100	−2.60886300	−2.00404500
C	2.22777100	−1.30528900	−2.60530100
O	2.98844500	−0.19560800	−2.11921900
C	2.29852600	1.04872900	−2.20744200
C	−1.27356900	3.62229200	−0.26569000
C	0.00000000	2.84723800	0.07031400
O	0.59399100	2.35235000	−1.13212800
C	1.58229500	1.36109300	−0.89255300
H	3.84140000	−2.64081100	−2.14539300
H	2.32085000	−3.43072300	−2.60526300
H	2.31816400	−1.34930800	−3.70699400
H	1.16653000	−1.19588900	−2.34543000
H	3.04421200	1.82143000	−2.43706600
H	1.56461000	1.03621400	−3.02857200
H	−1.04298400	4.31317600	−1.09589900
H	−1.51152000	4.24138100	0.61366300
H	0.71800400	3.52166500	0.57466700

H	−0.23987900	2.01867400	0.75272900
H	2.30957700	1.71898600	−0.14269700
H	1.12010100	0.44316800	−0.49368000

Total Energy= −1422.32954596 au

[3.3.2] cryptand C_2 symmetry

N	−2.89915700	3.13941300	0.63630400
N	2.89915700	−3.13941300	0.63630400
O	−1.82477000	−1.85697300	−1.19158300
O	1.82477000	1.85697300	−1.19158300
C	−2.44648000	−1.33767300	−2.35582300
H	−3.53789800	−1.50806200	−2.31761300
H	−2.05237300	−1.85120300	−3.25310800
C	2.07270000	3.24408300	−1.01940800
H	1.70758200	3.81159900	−1.89481100
H	3.16038000	3.42242500	−0.92601600
C	−2.07270000	−3.24408300	−1.01940800
H	−3.16038000	−3.42242500	−0.92601600
H	−1.70758200	−3.81159900	−1.89481100
C	2.44648000	1.33767300	−2.35582300
H	2.05237300	1.85120300	−3.25310800
H	3.53789800	1.50806200	−2.31761300
C	−3.40441600	2.38056900	1.76639200
C	−2.81581400	0.97949700	1.91426400
O	−1.44029200	1.08550500	2.25668300
C	−0.74523700	−0.15182200	2.19041900
C	3.40441600	−2.38056900	1.76639200
C	2.81581400	−0.97949700	1.91426400
O	1.44029200	−1.08550500	2.25668300
C	0.74523700	0.15182200	2.19041900
H	−3.19685700	2.94005700	2.69081600
H	−4.50404200	2.26885200	1.70003900
H	−3.36492700	0.43857900	2.71011400
H	−2.92702400	0.42383400	0.97060500
H	−1.00418000	−0.78991600	3.05527800
H	−1.00824700	−0.68878300	1.26642000

H	3.19685700	−2.94005700	2.69081600
H	4.50404200	−2.26885200	1.70003900
H	3.36492700	−0.43857900	2.71011400
H	2.92702400	−0.42383400	0.97060500
H	1.00418000	0.78991600	3.05527800
H	1.00824700	0.68878300	1.26642000
C	−3.58708800	3.02066400	−0.63549600
C	−2.81581400	2.28656900	−1.73305500
O	−2.92860500	0.87801300	−1.54146400
C	−2.16897300	0.14524500	−2.48712800
C	2.19307200	−4.37598300	0.91549300
C	0.70267900	−4.22844700	1.20972900
O	0.00675800	−3.86357100	0.02237500
C	−1.38887900	−3.74399200	0.23554200
H	−4.54556700	2.49751900	−0.48933300
H	−3.83069700	4.02480600	−1.02541800
H	−3.24185500	2.55037900	−2.72110100
H	−1.75739800	2.59229200	−1.71118200
H	−2.44432000	0.45696800	−3.51290700
H	−1.09235500	0.34150600	−2.34713500
H	2.30168100	−5.04884500	0.05302400
H	2.64064500	−4.89678000	1.78542000
H	0.31802400	−5.19880200	1.58158300
H	0.54165400	−3.46557800	1.98756200
H	−1.81629800	−4.73005300	0.50147100
H	−1.59547300	−3.05063000	1.06850200
C	−2.19307200	4.37598300	0.91549300
C	−0.70267900	4.22844700	1.20972900
O	−0.00675800	3.86357100	0.02237500
C	1.38887900	3.74399200	0.23554200
C	3.58708800	−3.02066400	−0.63549600
C	2.81581400	−2.28656900	−1.73305500
O	2.92860500	−0.87801300	−1.54146400
C	2.16897300	−0.14524500	−2.48712800
H	−2.30168100	5.04884500	0.05302400
H	−2.64064500	4.89678000	1.78542000

H	−0.31802400	5.19880200	1.58158300
H	−0.54165400	3.46557800	1.98756200
H	1.81629800	4.73005300	0.50147100
H	1.59547300	3.05063000	1.06850200
H	4.54556700	−2.49751900	−0.48933300
H	3.83069700	−4.02480600	−1.02541800
H	3.24185500	−2.55037900	−2.72110100
H	1.75739800	−2.59229200	−1.71118200
H	2.44432000	−0.45696800	−3.51290700
H	1.09235500	−0.34150600	−2.34713500

Total Energy= −1576.18657548 au

[3.3.3] cryptand D_3 symmetry

N	0.00000000	0.00000000	4.01939400
N	0.00000000	0.00000000	−4.01939400
O	0.00000000	3.13711500	0.00000000
O	2.71682100	−1.56855700	0.00000000
O	−2.71682100	−1.56855700	0.00000000
C	0.90625100	3.91310500	0.76588800
H	0.36096400	4.53494900	1.49926800
H	1.48361700	4.58813800	0.10642900
C	2.93572300	−2.74138800	0.76588800
H	3.74689900	−2.58007900	1.49926800
H	3.23163600	−3.57891900	0.10642900
C	−3.84197300	−1.17171600	0.76588800
H	−4.10786300	−1.95487000	1.49926800
H	−4.71525200	−1.00921900	0.10642900
C	−0.90625100	3.91310500	−0.76588800
H	−1.48361700	4.58813800	−0.10642900
H	−0.36096400	4.53494900	−1.49926800
C	3.84197300	−1.17171600	−0.76588800
H	4.71525200	−1.00921900	−0.10642900
H	4.10786300	−1.95487000	−1.49926800
C	−2.93572300	−2.74138800	−0.76588800
H	−3.23163600	−3.57891900	−0.10642900
H	−3.74689900	−2.58007900	−1.49926800

C	1.29566900	0.61379900	4.25941300
C	1.97117300	1.21145800	3.03041700
O	1.22786200	2.33604300	2.56094500
C	1.87026800	2.98769800	1.47916000
C	−1.29566900	0.61379900	−4.25941300
C	−1.97117300	1.21145800	−3.03041700
O	−1.22786200	2.33604300	−2.56094500
C	−1.87026800	2.98769800	−1.47916000
H	1.21315600	1.40377500	5.02875100
H	1.98295200	−0.14979800	4.65241300
H	2.99273500	1.53547300	3.31150700
H	2.04546700	0.45202900	2.23661700
H	2.73286300	3.57480700	1.84810600
H	2.24808600	2.24539500	0.75632800
H	−1.21315600	1.40377500	−5.02875100
H	−1.98295200	−0.14979800	−4.65241300
H	−2.99273500	1.53547300	−3.31150700
H	−2.04546700	0.45202900	−2.23661700
H	−2.73286300	3.57480700	−1.84810600
H	−2.24808600	2.24539500	−0.75632800
C	−0.11626900	−1.42898200	4.25941300
C	0.06356700	−2.31281500	3.03041700
O	1.40914200	−2.23138100	2.56094500
C	1.65228800	−3.11354800	1.47916000
C	1.17940000	0.81518300	−4.25941300
C	2.03474000	1.10135600	−3.03041700
O	2.63700400	−0.10466200	−2.56094500
C	3.52255600	0.12585000	−1.47916000
H	0.60912700	−1.75251100	5.02875100
H	−1.12120400	−1.64238800	4.65241300
H	−0.16660900	−3.35952100	3.31150700
H	−0.63126500	−1.99744100	2.23661700
H	1.72944200	−4.15413200	1.84810600
H	0.82052600	−3.06959800	0.75632800
H	1.82228300	0.34873600	−5.02875100
H	0.86174700	1.79218500	−4.65241300

H	2.82612700	1.82404800	−3.31150700
H	1.41420200	1.54541200	−2.23661700
H	4.46230500	0.57932600	−1.84810600
H	3.06861300	0.82420200	−0.75632800
C	−1.17940000	0.81518300	4.25941300
C	−2.03474000	1.10135600	3.03041700
O	−2.63700400	−0.10466200	2.56094500
C	−3.52255600	0.12585000	1.47916000
C	0.11626900	−1.42898200	−4.25941300
C	−0.06356700	−2.31281500	−3.03041700
O	−1.40914200	−2.23138100	−2.56094500
C	−1.65228800	−3.11354800	−1.47916000
H	−1.82228300	0.34873600	5.02875100
H	−0.86174700	1.79218500	4.65241300
H	−2.82612700	1.82404800	3.31150700
H	−1.41420200	1.54541200	2.23661700
H	−4.46230500	0.57932600	1.84810600
H	−3.06861300	0.82420200	0.75632800
H	−0.60912700	−1.75251100	−5.02875100
H	1.12120400	−1.64238800	−4.65241300
H	0.16660900	−3.35952100	−3.31150700
H	0.63126500	−1.99744100	−2.23661700
H	−1.72944200	−4.15413200	−1.84810600
H	−0.82052600	−3.06959800	−0.75632800

Total Energy= −1730.03970314 au

Table S2. Energies of the alkali metal cations by the B3LYP method with the SDD basis set for Li, Na, K, Rb, and Cs atom and the MWB pseudo potentials for K to Cs atoms.

Li^+ B3LYP SDD
Total Energy= −7.28499742 au

Na^+ B3LYP SDD
Total Energy= −162.08122918 au

K^+ B3LYP SDD+MWB10
Total Energy= −28.14995475 au

Rb^+ B3LYP SDD+MWB28
Total Energy= −23.93949095 au

Cs^+ B3LYP SDD+MWB46
Total Energy= −20.00175184 au

Table S3. Optimized geometries and energies of the alkali metal cryptates from [M^+⊂1.1.1] to [M^+⊂3.3.3] by the B3LYP method with the aug−cc−pVDZ basis set for C, H, N, and O atoms , and the SDD basis set for Li, Na, K, Rb, and Cs atom with the MWB pseudo potentials for K to Cs atoms.

[Li^+⊂1.1.1] C_{3h} symmetry

Li	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.02226000
N	0.00000000	0.00000000	−2.02226000
O	−1.67678500	−0.95609100	0.00000000
O	0.01039400	1.93018400	0.00000000
O	1.66639200	−0.97409300	0.00000000
C	−1.25306700	−0.71255600	2.33905500
C	−2.29870900	−0.54296700	1.22960500
C	−1.25306700	−0.71255600	−2.33905500
C	−2.29870900	−0.54296700	−1.22960500
H	−1.02390800	−1.78058000	2.43793400
H	−1.69054600	−0.38709400	3.29806900
H	−3.18356400	−1.16145200	1.44226000
H	−2.62218000	0.50629700	1.13962400
H	−1.69054600	−0.38709400	−3.29806900
H	−1.02390800	−1.78058000	−2.43793400
H	−2.62218000	0.50629700	−1.13962400
H	−3.18356400	−1.16145200	−1.44226000
C	0.00944200	1.44146600	2.33905500
C	0.67913200	2.26222400	1.22960500
C	0.00944200	1.44146600	−2.33905500
C	0.67913200	2.26222400	−1.22960500
H	−1.03007400	1.77702000	2.43793400
H	0.51004000	1.65760300	3.29806900
H	0.58593500	3.33777300	1.44226000
H	1.74955600	2.01772600	1.13962400
H	0.51004000	1.65760300	−3.29806900
H	−1.03007400	1.77702000	−2.43793400
H	1.74955600	2.01772600	−1.13962400
H	0.58593500	3.33777300	−1.44226000

C	1.24362500	−0.72891000	2.33905500
C	1.61957800	−1.71925700	1.22960500
C	1.24362500	−0.72891000	−2.33905500
C	1.61957800	−1.71925700	−1.22960500
H	2.05398200	0.00356000	2.43793400
H	1.18050600	−1.27050900	3.29806900
H	2.59762900	−2.17632100	1.44226000
H	0.87262400	−2.52402300	1.13962400
H	1.18050600	−1.27050900	−3.29806900
H	2.05398200	0.00356000	−2.43793400
H	0.87262400	−2.52402300	−1.13962400
H	2.59762900	−2.17632100	−1.44226000

Total Energy= −814.37428493 au

[Li^+⊂2.1.1] C_2 symmetry

Li	0.00000000	0.00000000	0.22001800
C	0.62839000	2.89011700	0.86596800
C	−0.59358600	2.57431200	1.72793900
O	−0.67612800	1.16947400	1.99716700
C	−2.08215300	−0.68038800	−1.84675700
C	−1.98700600	−1.87618500	−0.90370800
O	−1.47498400	0.44912000	−1.21025800
C	−0.35340700	2.58219400	−1.34621200
C	−1.11009800	1.49350700	−2.11408800
C	1.11009800	−1.49350700	−2.11408800
C	0.35340700	−2.58219400	−1.34621200
C	1.98700600	1.87618500	−0.90370800
C	2.08215300	0.68038800	−1.84675700
N	0.63067400	2.07726200	−0.36622800
O	1.47498400	−0.44912000	−1.21025800
N	−0.63067400	−2.07726200	−0.36622800
C	0.00000000	0.75499400	3.18851600
C	0.00000000	−0.75499400	3.18851600
O	0.67612800	−1.16947400	1.99716700
C	0.59358600	−2.57431200	1.72793900
C	−0.62839000	−2.89011700	0.86596800

H	0.65940700	3.97598800	0.65873600
H	1.53749100	2.65028700	1.43072300
H	−0.55244000	3.14739100	2.66605000
H	−1.52887700	2.83801300	1.22014000
H	−1.57868700	−0.87962300	−2.80451300
H	−3.14059800	−0.47153100	−2.06856800
H	−2.65391600	−1.69610700	−0.05169400
H	−2.36832100	−2.76852900	−1.43596800
H	0.11987500	3.25890500	−2.08029400
H	−1.09195000	3.18164200	−0.80434100
H	−0.50622900	1.07019100	−2.93026000
H	−2.00929600	1.93837700	−2.57065600
H	2.00929600	−1.93837700	−2.57065600
H	0.50622900	−1.07019100	−2.93026000
H	−0.11987500	−3.25890500	−2.08029400
H	1.09195000	−3.18164200	−0.80434100
H	2.65391600	1.69610700	−0.05169400
H	2.36832100	2.76852900	−1.43596800
H	1.57868700	0.87962300	−2.80451300
H	3.14059800	0.47153100	−2.06856800
H	1.03523400	1.13090400	3.20044000
H	−0.52523100	1.13590100	4.07854700
H	0.52523100	−1.13590100	4.07854700
H	−1.03523400	−1.13090400	3.20044000
H	1.52887700	−2.83801300	1.22014000
H	0.55244000	−3.14739100	2.66605000
H	−1.53749100	−2.65028700	1.43072300
H	−0.65940700	−3.97598800	0.65873600

Total Energy= −968.23418833 au

[Li^+⊂2.2.1] C_2 symmetry

Li	0.00000000	0.00000000	−0.36033000
N	0.76112300	2.37773100	0.59475100
N	−0.76112300	−2.37773100	0.59475100
C	0.00000000	2.41896400	1.83983600
C	0.19981600	1.17144600	2.69014200

O	0.00000000	0.00000000	1.88861800
C	0.00000000	−2.41896400	1.83983600
C	−0.19981600	−1.17144600	2.69014200
H	0.25367000	3.29966600	2.46494600
H	−1.06534600	2.50044400	1.59261200
H	1.20828500	1.13596800	3.13345400
H	−0.52441000	1.18889700	3.51995100
H	−0.25367000	−3.29966600	2.46494600
H	1.06534600	−2.50044400	1.59261200
H	−1.20828500	−1.13596800	3.13345400
H	0.52441000	−1.18889700	3.51995100
C	0.29018900	3.32699200	−0.42062400
C	−1.02193400	2.91403400	−1.06374700
O	−0.86484900	1.61561500	−1.64972100
C	−2.05087600	1.14248300	−2.30217600
C	−2.22056200	−2.41203900	0.77907700
C	−2.86835600	−1.04978500	0.52406900
O	−2.25476800	−0.50198400	−0.64221000
C	−3.00113700	0.51958700	−1.29470800
H	0.17043300	4.35429500	−0.02203200
H	1.04721300	3.36889700	−1.21098800
H	−1.84795800	2.90842100	−0.33594500
H	−1.27829500	3.64281200	−1.84941200
H	−2.54272300	1.95639900	−2.85572200
H	−1.71894800	0.38092900	−3.01804600
H	−2.65267000	−3.13418500	0.07604600
H	−2.49506000	−2.76035500	1.78847000
H	−3.95046700	−1.18116500	0.36573100
H	−2.72825400	−0.35683600	1.36906300
H	−3.87998800	0.09561500	−1.80842400
H	−3.36091000	1.26161400	−0.56270300
C	2.22056200	2.41203900	0.77907700
C	2.86835600	1.04978500	0.52406900
O	2.25476800	0.50198400	−0.64221000
C	3.00113700	−0.51958700	−1.29470800
C	−0.29018900	−3.32699200	−0.42062400

C	1.02193400	−2.91403400	−1.06374700
O	0.86484900	−1.61561500	−1.64972100
C	2.05087600	−1.14248300	−2.30217600
H	2.65267000	3.13418500	0.07604600
H	2.49506000	2.76035500	1.78847000
H	3.95046700	1.18116500	0.36573100
H	2.72825400	0.35683600	1.36906300
H	3.87998800	−0.09561500	−1.80842400
H	3.36091000	−1.26161400	−0.56270300
H	−0.17043300	−4.35429500	−0.02203200
H	−1.04721300	−3.36889700	−1.21098800
H	1.84795800	−2.90842100	−0.33594500
H	1.27829500	−3.64281200	−1.84941200
H	2.54272300	−1.95639900	−2.85572200
H	1.71894800	−0.38092900	−3.01804600

Total Energy= −1122.08193169 au

[Li^+⊂2.2.2] C_3 symmetry

Li	0.00000000	0.00000000	0.31064900
N	0.00000000	0.00000000	−1.97803200
N	0.00000000	0.00000000	2.58469700
C	1.28544400	0.56150400	−2.49950300
C	1.85070900	1.71859600	−1.69705600
O	1.03474100	2.87977800	−1.85492500
C	1.10937500	3.83371300	−0.80687500
C	0.26655800	1.37152600	3.07859700
C	−0.40222800	2.44760700	2.24610000
O	0.16889300	2.41548400	0.93520100
C	0.00000000	3.65178000	0.21409200
H	2.02782800	−0.23962200	−2.48382700
H	1.15922000	0.87097000	−3.55123300
H	1.92822000	1.44609300	−0.63322700
H	2.86979000	1.93521700	−2.06133600
H	2.09346300	3.80376700	−0.31291000
H	0.99007800	4.82660600	−1.26392300
H	−0.04758100	1.47386000	4.13299400

H	1.34667000	1.55222000	3.04480500
H	−1.49583300	2.31971700	2.18913500
H	−0.20620500	3.42337700	2.71641600
H	−0.98379900	3.66185200	−0.28097600
H	0.03796100	4.49348700	0.92354800
C	−1.12899900	0.83247500	−2.49950300
C	−2.41370200	0.74346300	−1.69705600
O	−3.01133100	−0.54377700	−1.85492500
C	−3.87478000	−0.95611000	−0.80687500
C	−1.32105600	−0.45491700	3.07859700
C	−1.91857600	−1.57214300	2.24610000
O	−2.17631700	−1.06147600	0.93520100
C	−3.16253400	−1.82589000	0.21409200
H	−0.80639500	1.87596200	−2.48382700
H	−1.33389200	0.56842900	−3.55123300
H	−2.21646400	0.94684100	−0.63322700
H	−3.11084300	1.51770300	−2.06133600
H	−4.34089100	−0.08889200	−0.31291000
H	−4.67500200	−1.55587000	−1.26392300
H	−1.25261000	−0.77813600	4.13299400
H	−2.01759700	0.39014100	3.04480500
H	−1.26101700	−2.45528800	2.18913500
H	−2.86162900	−1.89026700	2.71641600
H	−2.67935700	−2.68292100	−0.28097600
H	−3.91045400	−2.21386800	0.92354800
C	−0.15644500	−1.39397900	−2.49950300
C	0.56299300	−2.46205900	−1.69705600
O	1.97659000	−2.33600100	−1.85492500
C	2.76540600	−2.87760300	−0.80687500
C	1.05449700	−0.91661000	3.07859700
C	2.32080400	−0.87546400	2.24610000
O	2.00742400	−1.35400700	0.93520100
C	3.16253400	−1.82589000	0.21409200
H	−1.22143300	−1.63633900	−2.48382700
H	0.17467200	−1.43939900	−3.55123300
H	0.28824300	−2.39293400	−0.63322700

H	0.24105200	−3.45292000	−2.06133600
H	2.24742800	−3.71487600	−0.31291000
H	3.68492400	−3.27073500	−1.26392300
H	1.30019100	−0.69572400	4.13299400
H	0.67092700	−1.94236100	3.04480500
H	2.75685000	0.13557100	2.18913500
H	3.06783400	−1.53310900	2.71641600
H	3.66315600	−0.97893100	−0.28097600
H	3.87249300	−2.27961900	0.92354800

Total Energy= −1275.91504177 au

[Li^+⊂2.2.2] C_1 symmetry

Li	−0.35331300	0.41192900	0.19202700
N	−0.73528100	−1.84636600	−0.11262800
N	0.99336100	2.26506000	−0.05515200
C	−0.39538600	−2.32534800	−1.48856300
C	−0.65194300	−1.33172900	−2.60950100
O	−2.05434500	−1.08538300	−2.76654100
C	−2.42998800	0.22066500	−3.17378900
C	0.65740500	2.73141600	−1.41545900
C	−0.82777800	2.69109900	−1.74006600
O	−1.39273800	1.44577000	−1.30274700
C	−2.63794500	1.13946900	−1.97681800
H	0.67336900	−2.55698900	−1.50402300
H	−0.93458200	−3.26497100	−1.69955300
H	−0.11754100	−0.39239600	−2.41266200
H	−0.25496100	−1.75726000	−3.54632200
H	−1.69733000	0.64464700	−3.88060200
H	−3.38670000	0.12339400	−3.70668300
H	1.01313400	3.76559400	−1.59025600
H	1.18653800	2.08602300	−2.12449600
H	−1.38487100	3.51783300	−1.27340300
H	−0.93790500	2.79626100	−2.82904500
H	−3.28502200	0.64658900	−1.24287600
H	−3.12534000	2.07608800	−2.28472300
C	−2.19643200	−2.05625700	0.13355900

C	−2.80409800	−1.08686900	1.13226600
O	−2.18956000	−1.23747100	2.40957700
C	−2.31490600	−0.12529800	3.28538600
C	0.34967100	3.10266800	0.98299100
C	0.21459100	2.37661400	2.30792900
O	−0.66871400	1.25663400	2.12962800
C	−1.01165300	0.64251900	3.39154900
H	−2.72793900	−1.92231100	−0.81177700
H	−2.37653500	−3.09238200	0.46533600
H	−2.68528500	−0.04847600	0.78122500
H	−3.88743100	−1.28482100	1.20812900
H	−3.12936900	0.54175400	2.96442400
H	−2.56636800	−0.50822000	4.28543600
H	0.90476200	4.04502400	1.14064500
H	−0.65872100	3.37526400	0.65627500
H	1.18283700	2.02531100	2.69728900
H	−0.21712800	3.06633400	3.04907800
H	−0.19410900	−0.02526700	3.70389400
H	−1.12822600	1.43025700	4.15183900
C	0.01399900	−2.68124000	0.87938500
C	1.46743200	−2.30876900	1.10280800
O	2.27132800	−2.71155100	−0.00643300
C	3.63147600	−2.29806200	0.07142800
C	2.46635200	2.33033300	0.13362900
C	3.29180300	1.31013000	−0.63249400
O	3.07920900	0.03146200	−0.06461400
C	3.86863600	−0.99324000	−0.66737200
H	−0.49313600	−2.57196600	1.84096200
H	−0.04978200	−3.74500400	0.59079000
H	1.57079100	−1.22739600	1.27667400
H	1.81644500	−2.83203900	2.01030300
H	3.94748600	−2.20704900	1.12287500
H	4.23743800	−3.08412600	−0.40037000
H	2.82486900	3.34174800	−0.13525300
H	2.68193100	2.18459800	1.19762500
H	3.05847200	1.29732400	−1.71111100

H	4.35362000	1.59905400	−0.53817000
H	3.59043800	−1.10231200	−1.72985600
H	4.94067400	−0.73107000	−0.61539900

Total Energy= −1275.91824488 au

[Na^+⊂1.1.1] C_{3h} symmetry

Na	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.15861100
N	0.00000000	0.00000000	−2.15861100
O	−1.82340100	−1.15197300	0.00000000
O	−0.08593700	2.15509900	0.00000000
O	1.90933900	−1.00312500	0.00000000
C	−1.26681300	−0.72415600	2.36977200
C	−2.31648000	−0.58486000	1.23858300
C	−1.26681300	−0.72415600	−2.36977200
C	−2.31648000	−0.58486000	−1.23858300
H	−1.03157600	−1.78886700	2.49277200
H	−1.76645300	−0.40349900	3.30099200
H	−3.23245600	−1.11002500	1.54748500
H	−2.57297800	0.47459000	1.07652400
H	−1.76645300	−0.40349900	−3.30099200
H	−1.03157600	−1.78886700	−2.49277200
H	−2.57297800	0.47459000	−1.07652400
H	−3.23245600	−1.11002500	−1.54748500
C	0.00626900	1.45917100	2.36977200
C	0.65173600	2.29856100	1.23858300
C	0.00626900	1.45917100	−2.36977200
C	0.65173600	2.29856100	−1.23858300
H	−1.03341700	1.78780500	2.49277200
H	0.53378600	1.73154300	3.30099200
H	0.65491800	3.35440100	1.54748500
H	1.69749600	1.99096900	1.07652400
H	0.53378600	1.73154300	−3.30099200
H	−1.03341700	1.78780500	−2.49277200
H	1.69749600	1.99096900	−1.07652400
H	0.65491800	3.35440100	−1.54748500

C	1.26054400	−0.73501400	2.36977200
C	1.66474400	−1.71370000	1.23858300
C	1.26054400	−0.73501400	−2.36977200
C	1.66474400	−1.71370000	−1.23858300
H	2.06499200	0.00106300	2.49277200
H	1.23266700	−1.32804300	3.30099200
H	2.57753800	−2.24437600	1.54748500
H	0.87548200	−2.46555900	1.07652400
H	1.23266700	−1.32804300	−3.30099200
H	2.06499200	0.00106300	−2.49277200
H	0.87548200	−2.46555900	−1.07652400
H	2.57753800	−2.24437600	−1.54748500

Total Energy= −969.07632460 au

[Na^+⊂2.1.1] C_2 symmetry

Na	0.00000000	0.00000000	0.34259700
C	−0.38467800	−3.00988000	0.80116000
C	0.63290800	−2.63591500	1.89082900
O	0.66968500	−1.22659200	2.16228000
C	1.76210200	0.99332400	−2.10312500
C	1.51229600	2.23161300	−1.23106200
O	1.60082000	−0.19350200	−1.32280200
C	0.96187400	−2.53599500	−1.20239800
C	1.51229600	−1.40249100	−2.08037700
C	−1.51229600	1.40249100	−2.08037700
C	−0.96187400	2.53599500	−1.20239800
C	−1.51229600	−2.23161300	−1.23106200
C	−1.76210200	−0.99332400	−2.10312500
N	−0.26343600	−2.22169000	−0.44522100
O	−1.60082000	0.19350200	−1.32280200
N	0.26343600	2.22169000	−0.44522100
C	−0.03333400	−0.75937700	3.32080500
C	0.03333400	0.75937700	3.32080500
O	−0.66968500	1.22659200	2.16228000
C	−0.63290800	2.63591500	1.89082900
C	0.38467800	3.00988000	0.80116000

H	−0.29500500	−4.09975000	0.62327100
H	−1.39414100	−2.83870400	1.19555400
H	0.38841200	−3.19915100	2.80340700
H	1.65480600	−2.91333600	1.60276000
H	1.08523900	0.95710500	−2.96852400
H	2.78994100	1.05673600	−2.49756200
H	2.34323400	2.30491300	−0.51929600
H	1.57900900	3.11827100	−1.89091000
H	0.82158700	−3.42021700	−1.85389700
H	1.74121400	−2.79946200	−0.47939800
H	0.88436600	−1.23375300	−2.96677000
H	2.50985800	−1.70165500	−2.44250100
H	−2.50985800	1.70165500	−2.44250100
H	−0.88436600	1.23375300	−2.96677000
H	−0.82158700	3.42021700	−1.85389700
H	−1.74121400	2.79946200	−0.47939800
H	−2.34323400	−2.30491300	−0.51929600
H	−1.57900900	−3.11827100	−1.89091000
H	−1.08523900	−0.95710500	−2.96852400
H	−2.78994100	−1.05673600	−2.49756200
H	−1.08435600	−1.08929500	3.29896600
H	0.44120400	−1.14595300	4.23656700
H	−0.44120400	1.14595300	4.23656700
H	1.08435600	1.08929500	3.29896600
H	−1.65480600	2.91333600	1.60276000
H	−0.38841200	3.19915100	2.80340700
H	1.39414100	2.83870400	1.19555400
H	0.29500500	4.09975000	0.62327100

Total Energy= −1122.98153486 au

[Na^+⊂2.2.1] C_2 symmetry

Na	0.00000000	0.00000000	−0.52621300
N	0.14382400	2.49034400	0.50930800
N	−0.14382400	−2.49034400	0.50930800
C	−0.51347700	2.35816300	1.81515800
C	0.00000000	1.20108000	2.66733400

O	0.00000000	0.00000000	1.89154900
C	0.51347700	−2.35816300	1.81515800
C	0.00000000	−1.20108000	2.66733400
H	−0.42210400	3.28559800	2.41640400
H	−1.58349700	2.19485500	1.64342400
H	1.01564500	1.38868700	3.05178400
H	−0.66646000	1.09460000	3.53800800
H	0.42210400	−3.28559800	2.41640400
H	1.58349700	−2.19485500	1.64342400
H	−1.01564500	−1.38868700	3.05178400
H	0.66646000	−1.09460000	3.53800800
C	−0.62610000	3.34725200	−0.41243300
C	−1.91078600	2.71608400	−0.92759400
O	−1.59210500	1.51652000	−1.63820400
C	−2.73659800	0.79924400	−2.11566900
C	−1.55175200	−2.92190600	0.60572700
C	−2.56041800	−1.78151600	0.50198100
O	−2.27896700	−1.03666000	−0.68248500
C	−3.30635400	−0.11752700	−1.04615700
H	−0.88659700	4.32321000	0.04356500
H	0.01020400	3.55276200	−1.28063300
H	−2.61925900	2.50379600	−0.11186400
H	−2.40040800	3.43050500	−1.60975600
H	−3.51152300	1.49489900	−2.47308700
H	−2.38757000	0.20293500	−2.96792400
H	−1.75938300	−3.61880600	−0.21455900
H	−1.74333900	−3.47506200	1.54268400
H	−3.57394800	−2.21304500	0.45033600
H	−2.52396400	−1.10811400	1.37308800
H	−4.18466900	−0.65514400	−1.44179000
H	−3.63220000	0.45529700	−0.16143400
C	1.55175200	2.92190600	0.60572700
C	2.56041800	1.78151600	0.50198100
O	2.27896700	1.03666000	−0.68248500
C	3.30635400	0.11752700	−1.04615700
C	0.62610000	−3.34725200	−0.41243300

C	1.91078600	−2.71608400	−0.92759400
O	1.59210500	−1.51652000	−1.63820400
C	2.73659800	−0.79924400	−2.11566900
H	1.75938300	3.61880600	−0.21455900
H	1.74333900	3.47506200	1.54268400
H	3.57394800	2.21304500	0.45033600
H	2.52396400	1.10811400	1.37308800
H	4.18466900	0.65514400	−1.44179000
H	3.63220000	−0.45529700	−0.16143400
H	0.88659700	−4.32321000	0.04356500
H	−0.01020400	−3.55276200	−1.28063300
H	2.61925900	−2.50379600	−0.11186400
H	2.40040800	−3.43050500	−1.60975600
H	3.51152300	−1.49489900	−2.47308700
H	2.38757000	−0.20293500	−2.96792400

Total Energy= −1276.85196842 au

[Na^+⊂2.2.2] C_3 symmetry

Na	0.00000000	0.00000000	0.01290100
N	0.00000000	0.00000000	3.17844500
N	0.00000000	0.00000000	−3.18274800
C	−1.17703200	0.75894000	3.61416100
C	−2.39478000	0.52621500	2.73869800
O	−2.11876700	0.99642200	1.41716700
C	−3.30627300	1.14959600	0.64332500
C	−1.32736100	0.44728400	−3.61688700
C	−1.90514300	1.54132000	−2.73778000
O	−2.10451400	1.02716300	−1.41881500
C	−2.96789100	1.85625600	−0.64502100
H	−1.44668800	0.53013400	4.66463000
H	−0.94112200	1.82870700	3.57468900
H	−2.68526500	−0.53684600	2.70196100
H	−3.24367700	1.08920100	3.16071600
H	−3.75755700	0.16474200	0.43391500
H	−4.04211000	1.75659500	1.19725500
H	−1.31716300	0.80423200	−4.66623200

H	−2.01616500	−0.40469700	−3.58015800
H	−1.25342700	2.42971400	−2.69540400
H	−2.87312100	1.85753400	−3.16058700
H	−2.48333800	2.82513000	−0.43520100
H	−3.90225200	2.04952100	−1.19863800
C	1.24577700	0.63987000	3.61416100
C	1.65310600	1.81083300	2.73869800
O	1.92231000	1.33669500	1.41716700
C	2.64871600	2.28851800	0.64332500
C	1.05104000	0.92588600	−3.61688700
C	2.28739400	0.87924200	−2.73778000
O	1.94180700	1.30898100	−1.41881500
C	3.09151000	1.64214100	−0.64502100
H	1.18245400	0.98780200	4.66463000
H	2.05426700	−0.09931800	3.57468900
H	0.87771000	2.59393100	2.70196100
H	2.56511400	2.26450600	3.16071600
H	2.02144900	3.17176900	0.43391500
H	3.54231100	2.62227300	1.19725500
H	1.35506700	0.73858100	−4.66623200
H	0.65760500	1.94839800	−3.58015800
H	2.73090800	−0.12935800	−2.69540400
H	3.04523200	1.55942900	−3.16058700
H	3.68830400	0.73806900	−0.43520100
H	3.72606400	2.35468900	−1.19863800
C	−0.06874500	−1.39880900	3.61416100
C	0.74167400	−2.33704800	2.73869800
O	0.19645600	−2.33311700	1.41716700
C	0.65755700	−3.43811500	0.64332500
C	0.27632100	−1.37317000	−3.61688700
C	−0.38225100	−2.42056300	−2.73778000
O	0.16270700	−2.33614400	−1.41881500
C	−0.12361900	−3.49839600	−0.64502100
H	0.26423400	−1.51793600	4.66463000
H	−1.11314600	−1.72938900	3.57468900
H	1.80755500	−2.05708500	2.70196100

H	0.67856200	−3.35370700	3.16071600
H	1.73610800	−3.33651100	0.43391500
H	0.49979900	−4.37886800	1.19725500
H	−0.03790400	−1.54281300	−4.66623200
H	1.35856000	−1.54370200	−3.58015800
H	−1.47748100	−2.30035600	−2.69540400
H	−0.17211100	−3.41696300	−3.16058700
H	−1.20496600	−3.56319900	−0.43520100
H	0.17618900	−4.40421000	−1.19863800

Total Energy= −1430.71130260 au

[K^+⊂2.2.1] C_1 symmetry

K	0.00004000	0.00001200	−1.07251200
N	1.91853300	−1.68182200	0.39040200
N	−1.91858100	1.68186400	0.39033500
C	2.10619300	−1.21631400	1.77380500
C	0.84818100	−0.84421800	2.56033900
O	−0.00013800	−0.00004700	1.78134700
C	−2.10624700	1.21659200	1.77382000
C	−0.84825900	0.84433800	2.56031900
H	2.66215800	−1.96472200	2.37533200
H	2.73085800	−0.31866300	1.73830400
H	0.28235500	−1.72843700	2.89284900
H	1.18222100	−0.31813300	3.46950300
H	−2.66199900	1.96521300	2.37527500
H	−2.73112200	0.31908100	1.73849800
H	−0.28225300	1.72848800	2.89271100
H	−1.18233100	0.31839300	3.46955300
C	3.17241300	−1.52982000	−0.38174500
C	3.60890900	−0.09313100	−0.65415100
O	2.63880600	0.56553800	−1.47134800
C	2.85022500	1.97184200	−1.64186400
C	−1.42670000	3.06982400	0.29739100
C	0.08011100	3.27016600	0.44792700
O	0.77584600	2.62230000	−0.61801800
C	2.18958100	2.80468300	−0.55275000

H	4.02276400	−2.04220200	0.11240800
H	3.02677500	−2.02048300	−1.35227600
H	3.77009000	0.47139400	0.27661500
H	4.57512200	−0.12782900	−1.18506800
H	3.92687400	2.20093300	−1.67575800
H	2.41772200	2.23044000	−2.61721100
H	−1.70313600	3.45913700	−0.69038600
H	−1.92242100	3.72135600	1.04445000
H	0.27720000	4.35574500	0.41443200
H	0.45937400	2.89614100	1.40980500
H	2.44564700	3.86735500	−0.70832900
H	2.55796000	2.51324400	0.44618200
C	1.42664800	−3.06979600	0.29768800
C	−0.08018000	−3.27009000	0.44811200
O	−0.77580300	−2.62235300	−0.61798300
C	−2.18953900	−2.80477200	−0.55284400
C	−3.17246100	1.52971100	−0.38178100
C	−3.60881200	0.09296000	−0.65409300
O	−2.63873500	−0.56560500	−1.47139900
C	−2.85010800	−1.97190600	−1.64198100
H	1.70317700	−3.45930700	−0.68998500
H	1.92229300	−3.72118500	1.04492100
H	−0.27728100	−4.35567100	0.41474600
H	−0.45953100	−2.89592300	1.40989900
H	−2.44556700	−3.86744500	−0.70847800
H	−2.55800800	−2.51337700	0.44606700
H	−4.02285100	2.04203400	0.11236100
H	−3.02689800	2.02032800	−1.35234500
H	−3.76979100	−0.47155600	0.27671400
H	−4.57510200	0.12751700	−1.18488000
H	−3.92675100	−2.20101800	−1.67597600
H	−2.41751600	−2.23045500	−2.61730200

Total Energy= −1142.87274783 au

[K^+⊂2.2.2] C_3 symmetry

K	0.00000000	0.00000000	0.00040000

N	0.00000000	0.00000000	3.09142000
N	0.00000000	0.00000000	−3.09199400
C	−1.07341500	0.89867900	3.55008700
C	−2.37490400	0.78651800	2.76973200
O	−2.17268400	1.23121600	1.42830500
C	−3.38956300	1.30143300	0.68735300
C	−1.36839200	0.29537300	−3.55094000
C	−2.07969100	1.38964400	−2.76867300
O	−2.30930700	0.95306100	−1.42902100
C	−3.11401800	1.86784700	−0.68727800
H	−1.30118800	0.73468800	4.62265500
H	−0.72505800	1.93369200	3.45779400
H	−2.76939900	−0.24359900	2.76357300
H	−3.12863000	1.42430400	3.26236700
H	−3.84174200	0.29836700	0.60212000
H	−4.10850100	1.96087000	1.20328000
H	−1.37825600	0.57786400	−4.62295100
H	−1.97103400	−0.61561000	−3.46092100
H	−1.50763200	2.33274200	−2.75819600
H	−3.04478700	1.59545300	−3.26241700
H	−2.60252300	2.84197600	−0.60174800
H	−4.07662000	2.02806200	−1.20270600
C	1.31498600	0.48026500	3.55008700
C	1.86859600	1.66346800	2.76973200
O	2.15260600	1.26599200	1.42830500
C	2.82185500	2.28473100	0.68735300
C	0.93999600	1.03737600	−3.55094000
C	2.24331200	1.10624300	−2.76867300
O	1.98002900	1.52338800	−1.42902100
C	3.17461200	1.76289500	−0.68727800
H	1.28685200	0.75951800	4.62265500
H	2.03715600	−0.33892700	3.45779400
H	1.17373700	2.52016900	2.76357300
H	2.79779800	1.99732100	3.26236700
H	2.17926500	3.17786300	0.60212000
H	3.75241400	2.57763100	1.20328000

H	1.18957300	0.90467300	−4.62295100
H	0.45238300	2.01477100	−3.46092100
H	2.77403000	0.13927700	−2.75819600
H	2.90409600	1.83913600	−3.26241700
H	3.76248500	0.83286300	−0.60174800
H	3.79466300	2.51642500	−1.20270600
C	−0.24157200	−1.37894400	3.55008700
C	0.50630800	−2.44998600	2.76973200
O	0.02007800	−2.49720700	1.42830500
C	0.56770800	−3.58616400	0.68735300
C	0.42839600	−1.33274800	−3.55094000
C	−0.16362100	−2.49588700	−2.76867300
O	0.32927800	−2.47644900	−1.42902100
C	−0.06059400	−3.63074300	−0.68727800
H	0.01433600	−1.49420600	4.62265500
H	−1.31209800	−1.59476500	3.45779400
H	1.59566200	−2.27657000	2.76357300
H	0.33083200	−3.42162500	3.26236700
H	1.66247800	−3.47623000	0.60212000
H	0.35608700	−4.53850100	1.20328000
H	0.18868300	−1.48253700	−4.62295100
H	1.51865100	−1.39916000	−3.46092100
H	−1.26639800	−2.47201900	−2.75819600
H	0.14069100	−3.43458900	−3.26241700
H	−1.15996200	−3.67483900	−0.60174800
H	0.28195700	−4.54448700	−1.20270600

Total Energy= −1296.75300922 au

[K^+⊂3.2.2] C_2 symmetry

K	0.00000000	0.00000000	0.13231700
N	−2.23978800	2.59363100	−0.66571800
N	2.23978800	−2.59363100	−0.66571800
O	0.00000000	0.00000000	3.25947200
C	−1.07353800	0.48043700	4.06402100
H	−0.76821600	1.41269600	4.56869100
H	−1.33308000	−0.26328400	4.83765300

C	1.07353800	−0.48043700	4.06402100
H	1.33308000	0.26328400	4.83765300
H	0.76821600	−1.41269600	4.56869100
C	−1.44617100	3.52372300	−1.48105400
C	0.00000000	3.66681100	−1.03165700
O	0.70230800	2.45720300	−1.33139500
C	2.11736800	2.61284600	−1.42386800
C	3.35610000	−2.03223300	−1.43894600
C	2.97259000	−0.86647200	−2.33488100
O	2.55781000	0.24911000	−1.54022800
C	2.68521000	1.47995000	−2.24796800
H	−1.42836900	3.16173300	−2.51590700
H	−1.90938100	4.53072900	−1.50368600
H	0.45629700	4.50263000	−1.58693200
H	0.07913900	3.89612300	0.04401800
H	2.36101800	3.56187400	−1.92920400
H	2.57549300	2.63363000	−0.41979400
H	4.12129500	−1.66989900	−0.74370200
H	3.84218500	−2.80661000	−2.06621400
H	3.85925200	−0.58796900	−2.92847000
H	2.16909700	−1.13179700	−3.04220000
H	3.75007600	1.68395600	−2.45592400
H	2.14921300	1.42549300	−3.21062200
C	−2.72510900	3.25598200	0.55377100
C	−3.14041200	2.29368600	1.65224500
O	−1.97927200	1.66864900	2.19167200
C	−2.29357400	0.72647500	3.20891300
C	2.72510900	−3.25598200	0.55377100
C	3.14041200	−2.29368600	1.65224500
O	1.97927200	−1.66864900	2.19167200
C	2.29357400	−0.72647500	3.20891300
H	−1.92296900	3.88749300	0.95445900
H	−3.57921500	3.92788800	0.33203400
H	−3.65796100	2.85938900	2.44633900
H	−3.84152200	1.52735200	1.28158600
H	−3.09434400	1.11403600	3.86206500

H	−2.65277200	−0.21541300	2.75709300
H	1.92296900	−3.88749300	0.95445900
H	3.57921500	−3.92788800	0.33203400
H	3.65796100	−2.85938900	2.44633900
H	3.84152200	−1.52735200	1.28158600
H	3.09434400	−1.11403600	3.86206500
H	2.65277200	0.21541300	2.75709300
C	−3.35610000	2.03223300	−1.43894600
C	−2.97259000	0.86647200	−2.33488100
O	−2.55781000	−0.24911000	−1.54022800
C	−2.68521000	−1.47995000	−2.24796800
C	1.44617100	−3.52372300	−1.48105400
C	0.00000000	−3.66681100	−1.03165700
O	−0.70230800	−2.45720300	−1.33139500
C	−2.11736800	−2.61284600	−1.42386800
H	−4.12129500	1.66989900	−0.74370200
H	−3.84218500	2.80661000	−2.06621400
H	−3.85925200	0.58796900	−2.92847000
H	−2.16909700	1.13179700	−3.04220000
H	−3.75007600	−1.68395600	−2.45592400
H	−2.14921300	−1.42549300	−3.21062200
H	1.42836900	−3.16173300	−2.51590700
H	1.90938100	−4.53072900	−1.50368600
H	−0.45629700	−4.50263000	−1.58693200
H	−0.07913900	−3.89612300	0.04401800
H	−2.36101800	−3.56187400	−1.92920400
H	−2.57549300	−2.63363000	−0.41979400

Total Energy= −1450.59483455 au

[K^+⊂3.3.2] C_1 symmetry

K	0.51671700	0.10406900	0.03521000
N	3.76159500	−0.67402500	−0.52525900
N	−3.87005400	−0.06187200	−0.97442300
O	−0.30226700	−1.19519800	2.68799800
O	0.15960600	2.97636200	0.32220800
C	0.61883800	−0.95095200	3.74778100

H	1.01746500	−1.91151600	4.11492200
H	0.11858500	−0.44042400	4.58979700
C	1.14747000	3.85483400	−0.21369800
H	1.84495400	4.17067400	0.58065700
H	0.66257500	4.75583500	−0.62584400
C	−1.32861000	−2.10945900	3.08570700
H	−0.87735900	−2.93570400	3.66030600
H	−2.05903800	−1.59680100	3.73311700
C	−0.76958400	3.66422800	1.16147300
H	−0.26229200	4.03342000	2.07028600
H	−1.17978700	4.53024900	0.61690000
C	3.77184700	−1.70427500	−1.57398000
C	2.53100900	−2.58471300	−1.58260600
O	1.41680200	−1.79087900	−1.99510200
C	0.25490300	−2.54676700	−2.31844100
C	−3.54595800	−0.25901200	−2.38299100
C	−2.14852300	0.25628700	−2.73136900
O	−1.10590000	−0.56947000	−2.18440500
C	−0.73408500	−1.65059100	−3.03446100
H	3.82308900	−1.21038500	−2.55187500
H	4.66671900	−2.35206000	−1.49765700
H	2.68277000	−3.41027400	−2.29822700
H	2.33623900	−3.02868100	−0.59105700
H	0.51565800	−3.38413400	−2.98780100
H	−0.19579300	−2.97157900	−1.40341300
H	−3.59894700	−1.33075700	−2.61620200
H	−4.27859500	0.23459800	−3.05193100
H	−2.02621200	0.32577400	−3.82461000
H	−2.00128900	1.25470400	−2.30208000
H	−1.61217000	−2.25737700	−3.31220900
H	−0.28185300	−1.25796400	−3.96051500
C	4.27273100	−1.18346400	0.75422400
C	3.75270200	−0.41207600	1.95821200
O	2.37252400	−0.73340000	2.13822300
C	1.76289500	−0.09092400	3.25331600
C	−4.54986700	−1.18197200	−0.33149200

C	−3.59688700	−2.25478000	0.17499100
O	−2.82324500	−1.72345300	1.24573000
C	−2.02581900	−2.70336800	1.88279700
H	3.95630600	−2.22752700	0.86997400
H	5.38048100	−1.18049800	0.78116700
H	4.31996100	−0.71125600	2.85567900
H	3.87494800	0.67540200	1.82537600
H	2.48343900	0.02717400	4.07911900
H	1.41392100	0.91823300	2.96897300
H	−5.11031600	−0.80569000	0.53332400
H	−5.29038000	−1.66158800	−1.00200200
H	−4.18264300	−3.12138700	0.53107300
H	−2.93074100	−2.60709100	−0.63261600
H	−2.65544400	−3.54171600	2.23333300
H	−1.27854800	−3.11811300	1.18056400
C	4.46566000	0.54392700	−0.95307200
C	3.57579000	1.51434700	−1.71322100
O	2.61389200	2.05419500	−0.80441400
C	1.90328100	3.16986300	−1.33005700
C	−4.44434900	1.24444200	−0.65546600
C	−3.89687400	1.82307300	0.64219400
O	−2.58502300	2.32472600	0.38831300
C	−1.90137900	2.74088200	1.55622800
H	4.84165900	1.07035700	−0.06809000
H	5.34861700	0.30552500	−1.57607800
H	4.19702700	2.32994100	−2.12048600
H	3.06465600	1.02125800	−2.55765300
H	2.60683800	3.89798900	−1.76890400
H	1.20749900	2.84616000	−2.12424000
H	−4.20462900	1.95141100	−1.46002400
H	−5.54869800	1.20258300	−0.59160400
H	−4.54310600	2.64754500	0.99248500
H	−3.86329600	1.04915300	1.42617700
H	−2.57390500	3.30394600	2.22762000
H	−1.52904300	1.86432300	2.11822200

Total Energy= −1604.44465819 au

[Rb^{+}⊂2.2.2] D_3 symmetry

Rb	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	3.09508200
N	0.00000000	0.00000000	−3.09508200
C	0.32169000	1.36551800	3.55113200
C	−0.34832100	2.48887200	2.76726400
O	0.18875400	2.55043800	1.44518000
C	−0.30924900	3.65596800	0.69161800
C	−0.32169000	1.36551800	−3.55113200
C	0.34832100	2.48887200	−2.76726400
O	−0.18875400	2.55043800	−1.44518000
C	0.30924900	3.65596800	−0.69161800
H	0.06332700	1.49756100	4.62100700
H	1.40488900	1.51318100	3.47071700
H	−1.44312800	2.36197400	2.71674400
H	−0.15091200	3.43920200	3.29232800
H	−1.40865600	3.59969700	0.61364700
H	−0.04805400	4.60277800	1.19492900
H	−0.06332700	1.49756100	−4.62100700
H	−1.40488900	1.51318100	−3.47071700
H	1.44312800	2.36197400	−2.71674400
H	0.15091200	3.43920200	−3.29232800
H	1.40865600	3.59969700	−0.61364700
H	0.04805400	4.60277800	−1.19492900
C	1.02172800	−0.96135000	3.55113200
C	2.32958700	−0.94278200	2.76726400
O	2.11436700	−1.43868500	1.44518000
C	3.32078500	−1.56016600	0.69161800
C	1.34341800	−0.40416700	−3.55113200
C	1.98126600	−1.54609000	−2.76726400
O	2.30312100	−1.11175300	−1.44518000
C	3.01153600	−2.09580200	−0.69161800
H	1.26526300	−0.80362300	4.62100700
H	0.60800900	−1.97326000	3.47071700
H	2.76709300	0.06879800	2.71674400

H	3.05389200	−1.58890800	3.29232800
H	3.82175700	−0.57991600	0.61364700
H	4.01015000	−2.25977200	1.19492900
H	1.32859000	−0.69393800	−4.62100700
H	2.01289700	0.46007900	−3.47071700
H	1.32396500	−2.43077200	−2.71674400
H	2.90298000	−1.85029400	−3.29232800
H	2.41310100	−3.01978100	−0.61364700
H	3.96209500	−2.34300500	−1.19492900
C	−1.34341800	−0.40416700	3.55113200
C	−1.98126600	−1.54609000	2.76726400
O	−2.30312100	−1.11175300	1.44518000
C	−3.01153600	−2.09580200	0.69161800
C	−1.02172800	−0.96135000	−3.55113200
C	−2.32958700	−0.94278200	−2.76726400
O	−2.11436700	−1.43868500	−1.44518000
C	−3.32078500	−1.56016600	−0.69161800
H	−1.32859000	−0.69393800	4.62100700
H	−2.01289700	0.46007900	3.47071700
H	−1.32396500	−2.43077200	2.71674400
H	−2.90298000	−1.85029400	3.29232800
H	−2.41310100	−3.01978100	0.61364700
H	−3.96209500	−2.34300500	1.19492900
H	−1.26526300	−0.80362300	−4.62100700
H	−0.60800900	−1.97326000	−3.47071700
H	−2.76709300	0.06879800	−2.71674400
H	−3.05389200	−1.58890800	−3.29232800
H	−3.82175700	−0.57991600	−0.61364700
H	−4.01015000	−2.25977200	−1.19492900

Total Energy= −1292.52486051 au

[Rb^{+}⊂3.2.2] C_2 symmetry

Rb	0.00000000	0.00000000	0.19132300
N	−2.21230700	2.58212400	−0.67193600
N	2.21230700	−2.58212400	−0.67193600
O	0.00000000	0.00000000	3.36314400

C	−1.01259600	0.60551800	4.16321900
H	−0.62204600	1.53379600	4.61333400
H	−1.31291700	−0.07491300	4.97881500
C	1.01259600	−0.60551800	4.16321900
H	1.31291700	0.07491300	4.97881500
H	0.62204600	−1.53379600	4.61333400
C	−1.46763100	3.48360100	−1.56650700
C	0.00000000	3.66273900	−1.20711200
O	0.70818300	2.46347400	−1.52496200
C	2.12195900	2.63270900	−1.59684800
C	3.38344300	−2.01813200	−1.36161700
C	3.07786800	−0.86718200	−2.30635800
O	2.62928200	0.27473800	−1.57274000
C	2.72521300	1.46736000	−2.34819100
H	−1.50133200	3.08020200	−2.58513800
H	−1.94422700	4.48377900	−1.60469000
H	0.40501300	4.49693400	−1.80422700
H	0.13909800	3.91689700	−0.14252500
H	2.36309600	3.55854600	−2.14588400
H	2.55872700	2.71292800	−0.58584800
H	4.08836000	−1.64324000	−0.61168400
H	3.92147200	−2.79917400	−1.93671000
H	4.00826000	−0.61754900	−2.84431300
H	2.32171900	−1.13747400	−3.06244900
H	3.78539500	1.68873700	−2.56273300
H	2.19775700	1.34162500	−3.30897600
C	−2.62553400	3.30409700	0.54273500
C	−3.04203200	2.41241500	1.69982800
O	−1.89412700	1.77494400	2.25554100
C	−2.23489000	0.90155900	3.32604500
C	2.62553400	−3.30409700	0.54273500
C	3.04203200	−2.41241500	1.69982800
O	1.89412700	−1.77494400	2.25554100
C	2.23489000	−0.90155900	3.32604500
H	−1.78622000	3.92016400	0.88743100
H	−3.46143100	3.99986000	0.32361500

H	−3.52342200	3.03843700	2.47104700
H	−3.77751600	1.65197900	1.38865300
H	−2.98808000	1.37252900	3.98126500
H	−2.67001200	−0.03276700	2.92865600
H	1.78622000	−3.92016400	0.88743100
H	3.46143100	−3.99986000	0.32361500
H	3.52342200	−3.03843700	2.47104700
H	3.77751600	−1.65197900	1.38865300
H	2.98808000	−1.37252900	3.98126500
H	2.67001200	0.03276700	2.92865600
C	−3.38344300	2.01813200	−1.36161700
C	−3.07786800	0.86718200	−2.30635800
O	−2.62928200	−0.27473800	−1.57274000
C	−2.72521300	−1.46736000	−2.34819100
C	1.46763100	−3.48360100	−1.56650700
C	0.00000000	−3.66273900	−1.20711200
O	−0.70818300	−2.46347400	−1.52496200
C	−2.12195900	−2.63270900	−1.59684800
H	−4.08836000	1.64324000	−0.61168400
H	−3.92147200	2.79917400	−1.93671000
H	−4.00826000	0.61754900	−2.84431300
H	−2.32171900	1.13747400	−3.06244900
H	−3.78539500	−1.68873700	−2.56273300
H	−2.19775700	−1.34162500	−3.30897600
H	1.50133200	−3.08020200	−2.58513800
H	1.94422700	−4.48377900	−1.60469000
H	−0.40501300	−4.49693400	−1.80422700
H	−0.13909800	−3.91689700	−0.14252500
H	−2.36309600	−3.55854600	−2.14588400
H	−2.55872700	−2.71292800	−0.58584800

Total Energy= −1446.37603557 au

[Rb^{+}⊂3.3.2] C_1 symmetry

Rb	0.21345000	0.11828900	0.08605700
N	−3.77128500	0.04281800	−0.92592700
N	3.68872000	−0.66339500	−0.64461900

O	0.24816600	3.12140400	0.64283100
O	−0.28779700	−1.59075100	2.68699700
C	−0.73178000	3.79606900	1.42772000
H	−1.13657800	4.64747500	0.85567600
H	−0.28224100	4.18517300	2.35860400
C	−1.35765700	−2.47517900	3.02235600
H	−2.05295900	−1.97852500	3.71942600
H	−0.95408700	−3.37376400	3.51875200
C	1.29753800	3.98825700	0.21643400
H	0.87675600	4.95450600	−0.10939300
H	1.99333800	4.17812700	1.05097000
C	0.69229000	−1.52130200	3.71846600
H	0.25383000	−1.11376300	4.64679400
H	1.07277800	−2.53434300	3.93174800
C	−3.63628800	−0.16897200	−2.36915200
C	−2.31364300	0.36847300	−2.91117800
O	−1.19900900	−0.41570300	−2.46269100
C	−0.80621000	−1.43707200	−3.37453600
C	3.68626500	−1.52319700	−1.83777600
C	2.46067000	−2.41610800	−1.96250400
O	1.33871900	−1.60754700	−2.32004300
C	0.19466400	−2.35765700	−2.70681800
H	−3.68251600	−1.24626300	−2.57506600
H	−4.47255400	0.29015700	−2.93435600
H	−2.33498900	0.39557000	−4.01195600
H	−2.13871200	1.39098000	−2.55290200
H	−1.67430300	−2.04123200	−3.68873800
H	−0.35839700	−0.98266100	−4.27395300
H	3.71116300	−0.88722100	−2.73085900
H	4.59308200	−2.15876500	−1.87550100
H	2.64266600	−3.16304000	−2.75395800
H	2.25441100	−2.96178700	−1.02543500
H	0.47630900	−3.14528400	−3.42695000
H	−0.25920500	−2.85068900	−1.82766100
C	−4.28584300	1.37392000	−0.59103100
C	−3.77865900	1.89127100	0.74772500

O	−2.43304600	2.34080600	0.58419500
C	−1.85477400	2.84340500	1.77941800
C	4.43390400	0.58100600	−0.88979100
C	3.59463900	1.67894000	−1.52278800
O	2.67509300	2.17599100	−0.54898500
C	2.03423800	3.37845200	−0.95546600
H	−3.96561300	2.08715500	−1.36061500
H	−5.39379500	1.39245900	−0.58511100
H	−4.40717900	2.73638600	1.07849500
H	−3.82556900	1.10563700	1.51974000
H	−2.59984200	3.40411600	2.36968200
H	−1.49029500	2.01170900	2.40989300
H	4.80921600	0.96915900	0.06410000
H	5.32181800	0.39927100	−1.52578800
H	4.26120500	2.49572800	−1.84896200
H	3.04778800	1.31323600	−2.40885400
H	2.78338400	4.10867800	−1.30854900
H	1.33332900	3.18187600	−1.78629400
C	−4.51265700	−1.02812000	−0.25511300
C	−3.64374100	−2.21340200	0.13546200
O	−2.76954900	−1.82231600	1.19121100
C	−2.09228400	−2.92121700	1.77816300
C	4.20614700	−1.37580700	0.53212100
C	3.74594500	−0.78071400	1.85456100
O	2.37918000	−1.13577400	2.06608600
C	1.83844900	−0.63353800	3.28189600
H	−4.95535300	−0.63208800	0.66666200
H	−5.35430400	−1.39505500	−0.87505700
H	−4.29362800	−3.03772600	0.47854100
H	−3.05753800	−2.58317100	−0.72455500
H	−2.81538200	−3.70377300	2.07094400
H	−1.38195500	−3.37078500	1.06008500
H	3.85575400	−2.41485400	0.50016300
H	5.31400900	−1.41329800	0.52541800
H	4.36172600	−1.19230000	2.67247600
H	3.85828900	0.31598000	1.86461500

H	2.59845500	−0.64215100	4.08109500
H	1.50667000	0.41256200	3.15054500

Total Energy= −1600.22462155 au

[Rb^{+}⊂3.3.3] C_1 symmetry

Rb	0.56265000	−0.00059300	0.00101100
N	4.22742200	−0.00176800	0.00017600
N	−4.47485600	−0.00134000	−0.00212200
O	−0.06234000	2.01415400	2.30090100
O	−0.05918100	0.99008200	−2.89188500
O	−0.06205200	−3.00040500	0.59225300
C	0.74584500	3.18326400	2.39990700
H	1.37575600	3.12679100	3.30410900
H	0.10672900	4.08007500	2.47960700
C	0.74761500	0.49183800	−3.95514300
H	1.37908700	1.30265100	−4.35688500
H	0.10747100	0.11539100	−4.77220200
C	0.74463800	−3.67054500	1.55657100
H	1.37532900	−4.42546600	1.05669800
H	0.10438700	−4.18773400	2.29255900
C	−0.85970500	1.83535400	3.47273200
H	−0.20233400	1.70964200	4.35096800
H	−1.48756200	2.72725600	3.63462200
C	−0.85383200	2.09739400	−3.32000100
H	−0.19449000	2.92105900	−3.64571600
H	−1.48067200	1.79613700	−4.17568600
C	−0.85635800	−3.92608800	−0.15147300
H	−0.19669900	−4.62102100	−0.70024200
H	−1.48364900	−4.51525300	0.53793100
C	4.65037300	1.26344800	0.61446600
C	3.69158200	2.41524800	0.35159300
O	2.50623300	2.19600000	1.11897100
C	1.63035800	3.31504500	1.17922400
C	−4.85193000	0.33467400	1.37048400
C	−3.80982700	−0.08148500	2.39915500
O	−2.72744900	0.84896000	2.35113800

C	−1.74586700	0.61689900	3.34102000
H	4.70514800	1.12976400	1.70169100
H	5.66387900	1.55880400	0.27977500
H	4.16549700	3.35937500	0.66931700
H	3.44451400	2.50046900	−0.72025600
H	2.20534400	4.25164900	1.27220800
H	1.02296400	3.38563200	0.25822100
H	−4.97551400	1.42178500	1.45387600
H	−5.82491700	−0.11503100	1.64941800
H	−4.25911500	−0.06425500	3.40836700
H	−3.44417200	−1.10239800	2.19830100
H	−2.21961300	0.43919100	4.32362500
H	−1.14535500	−0.28100000	3.09870000
C	4.65092600	−0.10267100	−1.40244600
C	3.69136100	−0.90481800	−2.26892000
O	2.50604300	−0.13006100	−2.46033500
C	1.62999700	−0.63387200	−3.46119600
C	−4.84979800	1.01982700	−0.97973500
C	−3.80826600	2.11992900	−1.12938400
O	−2.72404800	1.61543200	−1.91005200
C	−1.74128000	2.58914600	−2.19845900
H	4.70713100	0.90575700	−1.83004000
H	5.66390100	−0.54148100	−1.49049000
H	4.16445000	−1.10019100	−3.24612200
H	3.44457500	−1.87641700	−1.80819000
H	2.20477400	−1.02063300	−4.31939600
H	1.02108500	−1.46670700	−3.06399200
H	−4.96949600	0.54913500	−1.96368400
H	−5.82414300	1.48501800	−0.73259600
H	−4.25716600	2.98601300	−1.64808000
H	−3.44467500	2.45476900	−0.14350300
H	−2.21364300	3.53070300	−2.53291500
H	−1.14200800	2.82404900	−1.29776000
C	4.64994000	−1.16624800	0.78914400
C	3.69055000	−1.51378200	1.91773100
O	2.50508300	−2.06773100	1.34355100

C	1.62816900	−2.67902100	2.28185100
C	−4.85096600	−1.35812900	−0.39812600
C	−3.80827700	−2.03958700	−1.27324800
O	−2.72712600	−2.46552700	−0.44313800
C	−1.74316000	−3.20250600	−1.14005300
H	4.70466600	−2.04113000	0.12996500
H	5.66334700	−1.02417200	1.21255400
H	4.16358200	−2.26135900	2.57673500
H	3.44392200	−0.62793400	2.52733400
H	2.20222700	−3.22743800	3.04745800
H	1.02009800	−1.91644300	2.80234800
H	−4.97393500	−1.97443900	0.50135700
H	−5.82400800	−1.37527600	−0.92697600
H	−4.25732100	−2.92088000	−1.76553900
H	−3.44123200	−1.35349900	−2.05483600
H	−2.21436900	−3.96404600	−1.78780100
H	−1.14362800	−2.54036400	−1.79403000

Total Energy= −1754.07477338 au

[Rb^{+}⊂3.3.3] D_3 symmetry

Rb	0.00000000	−0.00000000	0.00004414
N	0.00000000	4.29228011	−0.00229595
N	−0.00000000	−4.29228011	−0.00229595
O	0.00000000	−0.00000000	3.09293005
O	−2.67854475	0.00245334	−1.54428251
O	2.67854475	−0.00245334	−1.54428251
C	−0.86742613	0.79874129	3.89381146
H	−0.27048241	1.45427111	4.55011740
H	−1.49654833	0.15108999	4.52943029
C	−2.93829505	0.79736872	−2.69865478
H	−3.80657199	1.45188034	−2.51295871
H	−3.17176433	0.14670612	−3.55967604
C	3.80675603	0.79315667	−1.18943497
H	4.08110878	1.44846868	−2.03328159
H	4.66930549	0.14311633	−0.95986377
C	0.86742613	−0.79874129	3.89381146

H	1.49654833	−0.15108999	4.52943029
H	0.27048241	−1.45427111	4.55011740
C	−3.80675603	−0.79315667	−1.18943497
H	−4.66930549	−0.14311633	−0.95986377
H	−4.08110878	−1.44846868	−2.03328159
C	2.93829505	−0.79736872	−2.69865478
H	3.17176433	−0.14670612	−3.55967604
H	3.80657199	−1.45188034	−2.51295871
C	−0.64154995	4.68623307	1.25362603
C	−1.66041100	3.67289693	1.75466992
O	−0.95531166	2.53830165	2.26164457
C	−1.75960429	1.64473373	3.01227808
C	0.64154995	−4.68623307	1.25362603
C	1.66041100	−3.67289693	1.75466992
O	0.95531166	−2.53830165	2.26164457
C	1.75960429	−1.64473373	3.01227808
H	0.12578176	4.78552250	2.03133454
H	−1.13525416	5.67412851	1.16878161
H	−2.25430777	4.12707222	2.56674371
H	−2.35068187	3.36747948	0.95042779
H	−2.45507612	2.20039632	3.66502660
H	−2.36999997	1.00731740	2.34499499
H	−0.12578176	−4.78552250	2.03133454
H	1.13525416	−5.67412851	1.16878161
H	2.25430777	−4.12707222	2.56674371
H	2.35068187	−3.36747948	0.95042779
H	2.45507612	−2.20039632	3.66502660
H	2.36999997	−1.00731740	2.34499499
C	−0.76574666	4.68855921	−1.18590630
C	−0.69326927	3.67534017	−2.31907722
O	−1.48723176	2.54272143	−1.96154424
C	−1.73005642	1.64504596	−3.03092359
C	−1.40910948	−4.68394908	−0.07360654
C	−2.35040868	−3.67034129	0.56093619
O	−2.43774667	−2.53494433	−0.30196668
C	−3.48716962	−1.63959474	0.02308910

H	−1.82262679	4.79054059	−0.91003353
H	−0.44272899	5.67569048	−1.57077983
H	−1.09902948	4.13058241	−3.23921569
H	0.34754947	3.36760804	−2.51559313
H	−1.94666412	2.19691971	−3.96211354
H	−0.84470132	1.00933783	−3.22131470
H	−1.70013882	−4.78084087	−1.12689450
H	−1.58352091	−5.67243593	0.39489264
H	−3.35077833	−4.12383006	0.67080231
H	−1.99699396	−3.36595148	1.56043097
H	−4.40028702	−2.19351954	0.30218240
H	−3.21015571	−1.00281064	0.88444143
C	1.40910948	4.68394908	−0.07360654
C	2.35040868	3.67034129	0.56093619
O	2.43774667	2.53494433	−0.30196668
C	3.48716962	1.63959474	0.02308910
C	0.76574666	−4.68855921	−1.18590630
C	0.69326927	−3.67534017	−2.31907722
O	1.48723176	−2.54272143	−1.96154424
C	1.73005642	−1.64504596	−3.03092359
H	1.70013882	4.78084087	−1.12689450
H	1.58352091	5.67243593	0.39489264
H	3.35077833	4.12383006	0.67080231
H	1.99699396	3.36595148	1.56043097
H	4.40028702	2.19351954	0.30218240
H	3.21015571	1.00281064	0.88444143
H	1.82262679	−4.79054059	−0.91003353
H	0.44272899	−5.67569048	−1.57077983
H	1.09902948	−4.13058241	−3.23921569
H	−0.34754947	−3.36760804	−2.51559313
H	1.94666412	−2.19691971	−3.96211354
H	0.84470132	−1.00933783	−3.22131470

Total Energy= −1754.07409302 au

[Cs^+⊂2.2.2] C_3 symmetry

Cs	0.00000000	0.00000000	−0.00093500

N	0.00000000	0.00000000	−3.12189100
N	0.00000000	0.00000000	3.12213400
C	1.12194500	0.85119900	−3.56635200
C	2.41680300	0.72167000	−2.76229000
O	2.26978300	1.33230700	−1.47724000
C	3.46486800	1.30969500	−0.69248000
C	1.36759700	0.33584900	3.56664100
C	2.08223800	1.42444600	2.76407000
O	2.45786400	0.92970200	1.47563500
C	3.19546800	1.87247200	0.69330500
H	1.36720200	0.65562400	−4.62926200
H	0.80699300	1.89983000	−3.50820400
H	2.71712400	−0.33297100	−2.63834500
H	3.22013800	1.22964200	−3.32280100
H	3.84695300	0.27789900	−0.60812700
H	4.24176700	1.92462800	−1.17810500
H	1.37027400	0.64849900	4.62988700
H	1.98416500	−0.56886600	3.50742900
H	1.45490300	2.32480000	2.64676500
H	2.98574100	1.72329800	3.32261700
H	2.63625900	2.82010100	0.60933200
H	4.16186200	2.08675500	1.18086400
C	−1.29813200	0.54603300	−3.56635200
C	−1.83338600	1.73217800	−2.76229000
O	−2.28870400	1.29953600	−1.47724000
C	−2.86666400	2.34581600	−0.69248000
C	−0.97465200	1.01645000	3.56664100
C	−2.27472600	1.09104800	2.76407000
O	−2.03407800	1.66372100	1.47563500
C	−3.21934200	1.83112100	0.69330500
H	−1.25138800	0.85622000	−4.62926200
H	−2.04879800	−0.25103800	−3.50820400
H	−1.07020000	2.51958400	−2.63834500
H	−2.67497100	2.17390100	−3.32280100
H	−2.16414400	3.19260900	−0.60812700
H	−3.78766000	2.71116400	−1.17810500

H	−1.24675400	0.86244200	4.62988700
H	−0.49943000	2.00277100	3.50742900
H	−2.74078700	0.09758300	2.64676500
H	−2.98529000	1.72407900	3.32261700
H	−3.76040800	0.87301700	0.60933200
H	−3.88811300	2.56090100	1.18086400
C	0.17618700	−1.39723200	−3.56635200
C	−0.58341700	−2.45384800	−2.76229000
O	0.01892000	−2.63184400	−1.47724000
C	−0.59820500	−3.65551200	−0.69248000
C	−0.39294500	−1.35229800	3.56664100
C	0.19248800	−2.51549400	2.76407000
O	−0.42378600	−2.59342400	1.47563500
C	0.02387400	−3.70359200	0.69330500
H	−0.11581400	−1.51184400	−4.62926200
H	1.24180400	−1.64879200	−3.50820400
H	−1.64692300	−2.18661300	−2.63834500
H	−0.54516800	−3.40354300	−3.32280100
H	−1.68280900	−3.47050800	−0.60812700
H	−0.45410700	−4.63579200	−1.17810500
H	−0.12352000	−1.51094200	4.62988700
H	−1.48473500	−1.43390400	3.50742900
H	1.28588400	−2.42238300	2.64676500
H	−0.00045100	−3.44737700	3.32261700
H	1.12415000	−3.69311700	0.60933200
H	−0.27374900	−4.64765500	1.18086400

Total Energy= −1288.55984055 au

[Cs^{+}⊂3.2.2] C_2 symmetry

Cs	0.00000000	0.00000000	0.23790000
N	−2.19213900	2.58204800	−0.67988700
N	2.19213900	−2.58204800	−0.67988700
O	0.00000000	0.00000000	3.46186800
C	−0.93792100	0.72661000	4.25380200
H	−0.46197300	1.64158900	4.64479200
H	−1.26923200	0.11569000	5.11080600

C	0.93792100	−0.72661000	4.25380200
H	1.26923200	−0.11569000	5.11080600
H	0.46197300	−1.64158900	4.64479200
C	−1.48616400	3.46515400	−1.62644400
C	0.00000000	3.64738100	−1.34929900
O	0.69670800	2.45758800	−1.71987900
C	2.11032500	2.62488900	−1.79088800
C	3.39878100	−2.01384400	−1.30543300
C	3.15306900	−0.88885700	−2.30022200
O	2.67280500	0.27969900	−1.63391900
C	2.72773900	1.42710700	−2.47938200
H	−1.57282400	3.04739100	−2.63568300
H	−1.96163700	4.46586500	−1.65617300
H	0.36677700	4.49172500	−1.95752400
H	0.19782600	3.89065000	−0.29089700
H	2.35209000	3.52537100	−2.38125900
H	2.54007400	2.75499300	−0.78169800
H	4.04799800	−1.61434500	−0.51871000
H	3.98219900	−2.80137900	−1.82541200
H	4.11487600	−0.66277700	−2.79230500
H	2.44048800	−1.17923100	−3.09039000
H	3.77932600	1.65911300	−2.72318100
H	2.19058900	1.23166200	−3.42308400
C	−2.54986500	3.34080200	0.53262400
C	−2.95727400	2.50305100	1.73506800
O	−1.81159900	1.88855200	2.32372900
C	−2.16326400	1.07501900	3.43840700
C	2.54986500	−3.34080200	0.53262400
C	2.95727400	−2.50305100	1.73506800
O	1.81159900	−1.88855200	2.32372900
C	2.16326400	−1.07501900	3.43840700
H	−1.68629300	3.94678300	0.83273100
H	−3.37527900	4.05057700	0.31789400
H	−3.43437100	3.16821400	2.47553900
H	−3.69701500	1.73039500	1.46692000
H	−2.86489700	1.61555700	4.09772800

H	−2.66733600	0.15558700	3.09056200
H	1.68629300	−3.94678300	0.83273100
H	3.37527900	−4.05057700	0.31789400
H	3.43437100	−3.16821400	2.47553900
H	3.69701500	−1.73039500	1.46692000
H	2.86489700	−1.61555700	4.09772800
H	2.66733600	−0.15558700	3.09056200
C	−3.39878100	2.01384400	−1.30543300
C	−3.15306900	0.88885700	−2.30022200
O	−2.67280500	−0.27969900	−1.63391900
C	−2.72773900	−1.42710700	−2.47938200
C	1.48616400	−3.46515400	−1.62644400
C	0.00000000	−3.64738100	−1.34929900
O	−0.69670800	−2.45758800	−1.71987900
C	−2.11032500	−2.62488900	−1.79088800
H	−4.04799800	1.61434500	−0.51871000
H	−3.98219900	2.80137900	−1.82541200
H	−4.11487600	0.66277700	−2.79230500
H	−2.44048800	1.17923100	−3.09039000
H	−3.77932600	−1.65911300	−2.72318100
H	−2.19058900	−1.23166200	−3.42308400
H	1.57282400	−3.04739100	−2.63568300
H	1.96163700	−4.46586500	−1.65617300
H	−0.36677700	−4.49172500	−1.95752400
H	−0.19782600	−3.89065000	−0.29089700
H	−2.35209000	−3.52537100	−2.38125900
H	−2.54007400	−2.75499300	−0.78169800

Total Energy= −1442.42606925 au

[Cs^{+}⊂3.3.2] C_2 symmetry

Cs	0.00000000	0.00000000	−0.10921800
N	0.98069500	3.60861100	0.76839200
N	−0.98069500	−3.60861100	0.76839200
O	−2.73267200	0.71039500	−1.84896700
O	2.73267200	−0.71039500	−1.84896700
C	−2.75540900	1.81260100	−2.74935100

H	−3.55693400	2.51167600	−2.45599700
H	−2.95604200	1.46884800	−3.78000000
C	3.96357400	0.00947600	−1.84702200
H	4.01868000	0.66356000	−2.73357200
H	4.81096100	−0.69621600	−1.88568600
C	−3.96357400	−0.00947600	−1.84702200
H	−4.81096100	0.69621600	−1.88568600
H	−4.01868000	−0.66356000	−2.73357200
C	2.75540900	−1.81260100	−2.74935100
H	2.95604200	−1.46884800	−3.78000000
H	3.55693400	−2.51167600	−2.45599700
C	0.85373300	3.72461800	2.22945500
C	−0.21039400	2.83430200	2.85504600
O	0.22157700	1.46950300	2.82524900
C	−0.31465000	0.68807100	3.89049900
C	−0.85373300	−3.72461800	2.22945500
C	0.21039400	−2.83430200	2.85504600
O	−0.22157700	−1.46950300	2.82524900
C	0.31465000	−0.68807100	3.89049900
H	1.80986300	3.44967700	2.69017100
H	0.65061100	4.77343100	2.52633600
H	−0.34927600	3.15167400	3.90156400
H	−1.18377800	2.93149400	2.34561700
H	−0.09000000	1.17411100	4.85540700
H	−1.41102200	0.59842900	3.79886600
H	−1.80986300	−3.44967700	2.69017100
H	−0.65061100	−4.77343100	2.52633600
H	0.34927600	−3.15167400	3.90156400
H	1.18377800	−2.93149400	2.34561700
H	0.09000000	−1.17411100	4.85540700
H	1.41102200	−0.59842900	3.79886600
C	0.00000000	4.46989700	0.08994700
C	−0.26328200	4.09332700	−1.36062600
O	−1.13756100	2.96578700	−1.40268700
C	−1.42195400	2.52798200	−2.72586600
C	−2.35071300	−3.94035700	0.34528800

C	−3.33725900	−2.79333500	0.48900600
O	−3.09535500	−1.83211700	−0.53701500
C	−4.09718500	−0.82578900	−0.58139200
H	−0.95655700	4.40657100	0.62337200
H	0.31492600	5.53273400	0.12735000
H	−0.74337600	4.94499900	−1.87257800
H	0.67295200	3.86484300	−1.89591200
H	−1.48866200	3.38765900	−3.41388800
H	−0.61308000	1.87044600	−3.09268700
H	−2.34099100	−4.22786300	−0.71201900
H	−2.73861900	−4.81461500	0.90514400
H	−4.36188600	−3.19092000	0.38426200
H	−3.26352700	−2.31438600	1.48071100
H	−5.10047200	−1.28810400	−0.57860700
H	−4.02480800	−0.16921100	0.30435300
C	2.35071300	3.94035700	0.34528800
C	3.33725900	2.79333500	0.48900600
O	3.09535500	1.83211700	−0.53701500
C	4.09718500	0.82578900	−0.58139200
C	0.00000000	−4.46989700	0.08994700
C	0.26328200	−4.09332700	−1.36062600
O	1.13756100	−2.96578700	−1.40268700
C	1.42195400	−2.52798200	−2.72586600
H	2.34099100	4.22786300	−0.71201900
H	2.73861900	4.81461500	0.90514400
H	4.36188600	3.19092000	0.38426200
H	3.26352700	2.31438600	1.48071100
H	5.10047200	1.28810400	−0.57860700
H	4.02480800	0.16921100	0.30435300
H	0.95655700	−4.40657100	0.62337200
H	−0.31492600	−5.53273400	0.12735000
H	0.74337600	−4.94499900	−1.87257800
H	−0.67295200	−3.86484300	−1.89591200
H	1.48866200	−3.38765900	−3.41388800
H	0.61308000	−1.87044600	−3.09268700

Total Energy= −1596.27656106 au

[Cs^+⊂3.3.3] D_3 symmetry

Cs	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	4.23497500
N	0.00000000	0.00000000	−4.23497500
O	0.00000000	3.28188000	0.00000000
O	2.84219200	−1.64094000	0.00000000
O	−2.84219200	−1.64094000	0.00000000
C	0.81673200	4.08072600	0.85035600
H	0.18116200	4.71927600	1.48734200
H	1.46786200	4.73502400	0.24383700
C	3.12564700	−2.74767400	0.85035600
H	3.99643200	−2.51652900	1.48734200
H	3.36672100	−3.63871800	0.24383700
C	−3.94237900	−1.33305200	0.85035600
H	−4.17759400	−2.20274700	1.48734200
H	−4.83458200	−1.09630700	0.24383700
C	−0.81673200	4.08072600	−0.85035600
H	−1.46786200	4.73502400	−0.24383700
H	−0.18116200	4.71927600	−1.48734200
C	3.94237900	−1.33305200	−0.85035600
H	4.83458200	−1.09630700	−0.24383700
H	4.17759400	−2.20274700	−1.48734200
C	−3.12564700	−2.74767400	−0.85035600
H	−3.36672100	−3.63871800	−0.24383700
H	−3.99643200	−2.51652900	−1.48734200
C	0.49422500	1.31337100	4.66468000
C	1.52920100	1.91438000	3.72519900
O	0.85677100	2.41809900	2.57023100
C	1.68361900	3.19860000	1.72195300
C	−0.49422500	1.31337100	−4.66468000
C	−1.52920100	1.91438000	−3.72519900
O	−0.85677100	2.41809900	−2.57023100
C	−1.68361900	3.19860000	−1.72195300
H	−0.34738800	2.01529700	4.70790400
H	0.92129200	1.26897100	5.68625200

H	2.04460000	2.74501600	4.23780100
H	2.28841200	1.16927800	3.43259400
H	2.34256000	3.85328500	2.31841300
H	2.33158600	2.55118800	1.10202200
H	0.34738800	2.01529700	−4.70790400
H	−0.92129200	1.26897100	−5.68625200
H	−2.04460000	2.74501600	−4.23780100
H	−2.28841200	1.16927800	−3.43259400
H	−2.34256000	3.85328500	−2.31841300
H	−2.33158600	2.55118800	−1.10202200
C	0.89030000	−1.08469700	4.66468000
C	0.89330100	−2.28151700	3.72519900
O	1.66575000	−1.95103500	2.57023100
C	1.92825900	−3.05735700	1.72195300
C	1.38452500	−0.22867400	−4.66468000
C	2.42250200	0.36713700	−3.72519900
O	2.52252100	−0.46706400	−2.57023100
C	3.61187800	−0.14124300	−1.72195300
H	1.91899200	−0.70680100	4.70790400
H	0.63831500	−1.43234800	5.68625200
H	1.35495300	−3.14318300	4.23780100
H	−0.13158100	−2.56646200	3.43259400
H	2.16576300	−3.95535900	2.31841300
H	1.04360100	−3.29480700	1.10202200
H	1.57160400	−1.30849500	−4.70790400
H	1.55960700	0.16337700	−5.68625200
H	3.39955300	0.39816800	−4.23780100
H	2.15683100	1.39718300	−3.43259400
H	4.50832200	0.10207400	−2.31841300
H	3.37518700	0.74361900	−1.10202200
C	−1.38452500	−0.22867400	4.66468000
C	−2.42250200	0.36713700	3.72519900
O	−2.52252100	−0.46706400	2.57023100
C	−3.61187800	−0.14124300	1.72195300
C	−0.89030000	−1.08469700	−4.66468000
C	−0.89330100	−2.28151700	−3.72519900

O	−1.66575000	−1.95103500	−2.57023100
C	−1.92825900	−3.05735700	−1.72195300
H	−1.57160400	−1.30849500	4.70790400
H	−1.55960700	0.16337700	5.68625200
H	−3.39955300	0.39816800	4.23780100
H	−2.15683100	1.39718300	3.43259400
H	−4.50832200	0.10207400	2.31841300
H	−3.37518700	0.74361900	1.10202200
H	−1.91899200	−0.70680100	−4.70790400
H	−0.63831500	−1.43234800	−5.68625200
H	−1.35495300	−3.14318300	−4.23780100
H	0.13158100	−2.56646200	−3.43259400
H	−2.16576300	−3.95535900	−2.31841300
H	−1.04360100	−3.29480700	−1.10202200

Total Energy= −1750.12835280 au