Supplementary Material

Solid-State and Theoretical Investigations of some Banister-Type Macrocycles with 2,2’-Aldoxime-1,1’-Biphenyl Units

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Single-crystal X-ray diffraction measurement

Single-crystal diffraction data for 4 were collected on Oxford Diffraction SuperNova dual wavelength diffractometer exhibiting an operating mirror monochromated MoKα radiation mode (λ = 0.71073Å). X-ray data collection was monitored and all the data were corrected for Lorentzian, polarization and absorption effects using CrysAlisPro program [Agilent Technologies, CrysAlis PRO, Yarnton Oxfordshire, England: Agilent Technologies, 2010]. Olex2 program was used for the crystal structure solution and refinement [Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. &Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341], SHELXS [Sheldrick, G.M. (2008). A64, 112-122] were used for structure solutions. SHELXL was used for full matrix least-squares refinement on F2 [Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8].

CCDC 2100390 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

| Identification code | 4 |
|---------------------|---|
| CCDC number         | 2100390 |
| Empirical formula   | C_{22}H_{18}N_{2}O_{2} |
| Formula weight      | 342.38 |
| μ (Mo Kα)/mm^{-1}    | 0.71073 |
| Temperature/K        | 293(2) |
| Crystal system      | monoclinic |
| Space group          | P 2_1/n |
| a/Å                  | 13.0101(6) |
| b/Å                  | 9.8134(4) |
| c/Å                  | 14.5485(7) |
| α/°                  | 90.00 |
| β/°                  | 104.166(5) |
| γ/°                  | 90.00 |
| Volume/Å³            | 1800.97(15) |
| Z                    | 4 |
| Density (calculated)/g cm^{-3} | 1.263 |
| Absortion coefficient /mm^{-1} | 0.082 |
| F(000)               | 720 |
Reflections collected | 8753
---|---
Data/restraints/parameters | 4103/0/235
Goodness-of-fit on $F^2$ | 1.059
Final R indexes [$I>=2\sigma (I)$] | $R_1 = 0.0548$, $wR_2 = 0.1568$
Final R indexes [all data] | $R_1 = 0.0843$, $wR_2 = 0.1871$
Largest diff. peak/hole / e Å$^{-3}$ | 0.19/-0.20

**Supplementary Table S1:** Crystallographic data for 4

**Supplementary Figure S1:** Supramolecular associations occurring within species 4 and their DFT estimated interaction energies. A–B dimer case (left side), displaying reciprocal C–H•••O and C–H•••π interactions. Computed interaction energy is of ca. 10.0 kcal/mol ($\Delta E^\circ$/dioxime molecule = 5 kcal mol$^{-1}$). A–C dimer case (right side), revealing π ••π interactions. Computed interaction energy is of ca. 6.4 kcal/mol ($\Delta E^\circ$/dioxime molecule = 3.2 kcal mol$^{-1}$). Interaction energies were estimated using the formula: $\Delta E = E$ (Dimer) $- 2 \times E$ (Monomer). The coordinates of the atoms (for both dimers and monomers) were imported from crystallographic data without performing optimization of the molecular geometries (i.e. single-point calculations only). All these analyses were carried out within the framework of the DFT method, employing the D3 dispersion-corrected version of the PBE0 hybrid functional and the valence triple-zeta Def2-TZVP basis set.
Supplementary Scheme S1: General homodesmotic reactions used to compute the strain energies in macrocycles 1-4. All structures were optimized at the same level of theory (PBE0-D3/Def2-TZVP) and at default temperature (298 K).

| Macrocycle | Strain energy (-ΔH, kcal mol\(^{-1}\)) |
|------------|----------------------------------------|
| 1          | 0.5                                    |
| 2          | -1.4                                   |
| 3          | 0.5                                    |
| 4          | -0.6                                   |

Supplementary Table S2: Strain energies for macrocycles 1-4 based on homodesmotic reactions. Strain energies were calculated using the formula: ΔH = H (product) – H (macrocycle) – H (biphenyl).

| Name | Racemization barrier (kcal mol\(^{-1}\)) |
|------|-----------------------------------------|
|      | Theoretical                             | Experimental |
|      | PBE0-D3       | B3LYP-D3       |         |
| 1    | 26.4          | 26.8           | 25.0     |
| 2    | 26.8          | 26.4           | 24.8     |
| 3    | 27.5          | 27.6           | 24.7     |
| 4    | 33.0          | 33.7           | 31.7     |

Supplementary Table S3: DFT (PBE0-D3/Def2-TZVP and B3LYP-D3/Def2-TZVP) and experimental racemization barriers determined for banisters 1-4.
Supplementary Figure S2: Top view of the optimized molecular structures of macrocycles 1-3 and their alkali metal ion (Li⁺, Na⁺, K⁺) complexes.
Supplementary Figure S3: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 1.

Supplementary Figure S4: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 2.
Supplementary Figure S5: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 3.

Supplementary Figure S6: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 1-Li⁺.
Supplementary Figure S7: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 1-Na⁺.

Supplementary Figure S8: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 1-K⁺.
**Supplementary Figure S9:** Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of $2-\text{Li}^+$. 

**Supplementary Figure S10:** Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of $2-\text{Na}^+$. 
Supplementary Figure S11: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 2-K⁺.

Supplementary Figure S12: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 3-Li⁺.
Supplementary Figure S13: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 3-Na⁺.

Supplementary Figure S14: Theoretical relative enthalpies profile (353 K, 1 atm) for the racemization mechanism of 3-K⁺.
Supplementary Figure S15: Top view of optimized ground state geometries of complexed 9-crown-3, 12-crown-4 and 15-crown-5.
Supplementary Figure S16: Side view of optimized ground state geometries of complexed 9-crown-3, 12-crown-4 and 15-crown-5.

DFT coordinates

1-a

H (353 K, 1 atm) = -1030.651589 a.u.

|   |   |   |
|---|---|---|
| H | 0.39592100 | -0.07942300 | 0.01108000 |
| C | 0.29710800 | -0.08156600 | 1.09053600 |
| C | 0.04101100 | -0.09831900 | 3.87318500 |
| C | -0.31586500 | -1.14557000 | 1.72334700 |
| C | 0.77044800 | 0.98951100 | 1.83807800 |
| C | 0.63835300 | 0.97611300 | 3.21559100 |
| C | -0.45634600 | -1.17109100 | 3.11249700 |
H  -0.71127900  -1.97630900  1.15168300
H   1.24541700   1.83185100  1.34831600
H   1.02367900   1.79927100  3.80731900
C  -0.04860000  -0.07532600  5.35192100
C  -0.31763100  -0.00187300  8.13362300
C   0.52935300  -1.08101700  6.14504000
C  -0.73278900   0.96506200  5.97730800
C  -0.87037700   1.00595300  7.35454700
H  -1.18290200   1.73655300  5.36221000
H  -1.41287500   1.82127600  7.81928600
H   0.84244200  -1.81023500  8.12709300
H  -0.42054000   0.02346400  9.21236300
C   1.30088200  -2.15329800  5.51785400
H   1.81737400  -1.95801600  4.57848900
C  -1.14061200  -2.28384700  3.76922000
H  -1.54609900  -2.13907100  4.76969100
N  -1.24856100  -3.41173000  3.19161500
N   1.34364500  -3.30945000  6.04633500
O   2.15405500  -4.15635300  5.33470900
O  -1.96843100  -4.29633200  3.95602300
C   1.91494000  -5.50848900  5.68035600
H   2.79479700  -5.91281400  6.19669900
H   1.06398700  -5.55244900  6.36268000
C   1.67052600  -6.30164800  4.41378900
H   2.52283100  -6.16982200  3.74243100
H   1.60650000  -7.37102700  4.67030100
C  -1.80778100  -5.62298100  3.49073000
H  -1.63836100  -5.61493300  2.41087200
H  -2.75100600  -6.13122000  3.70873000
C  -0.68284000  -6.34125200  4.19460700
H  -0.78411700  -7.42594600  4.02365200
H  -0.77702900  -6.16153400  5.27448000
|   | X     | Y     | Z     |
|---|-------|-------|-------|
| O | 0.54249500 | -5.87908500 | 3.69489700 |

1-TS-a

H (353 K, 1 atm) = -1030.641146 a.u.
O  3.70698700  0.14241500 -0.09659900
O  -1.41409200 -0.56219300 -0.17751600
C  3.38000200 -0.87392500 -1.03433600
H  4.35120600 -1.30139100 -1.28965000
C  2.43389400 -1.94801100 -0.54036400
H  2.74746900 -2.92662000 -0.93695100
H  2.47240400 -2.00004900  0.55603300
C -1.20433100 -1.80855200 -0.80972500
H -1.26464100 -1.68415800 -1.89499800
H -2.01443400 -2.45915200 -0.47032200
C  0.12520600 -2.41036200 -0.42100000
H  0.17106300 -3.45567400 -0.77167800
H  0.21023000 -2.41836200  0.67615300
O  1.14239100 -1.63872800 -0.98861400
H  2.94515000 -0.42481200 -1.93452300

1-b

H (353 K, 1 atm) = -1030.644045 a.u.

H  1.13886200  3.02899500 -4.45649800
C  0.80071900  2.78112900 -3.45721100
C -0.07915700  2.10311800 -0.87858600
C  0.24222100  1.54314400 -3.20292300
C  0.91599900  3.69691400 -2.42450300
C  0.47480400  3.35118400 -1.15755400
C -0.20542900  1.17273500 -1.92861200
H  0.13968800  0.82868200 -4.01289800
H  1.34775900  4.67553600 -2.59942300
H  0.56614000  4.06143400 -0.34323300
C -0.52937500  1.88272600  0.51813900
C -1.37808800  1.67371400  3.17076900
C  0.10873000  0.99175600  1.39030900
| Element | x    | y    | z    |
|---------|------|------|------|
| C       | -1.5849 | 2.6568 | 0.9951 |
| C       | -2.0174 | 2.5513 | 2.3057 |
| C       | -0.3225 | 0.9076 | 2.7152 |
| H       | -2.0764 | 3.3427 | 0.3140 |
| H       | -2.8456 | 3.1585 | 2.6527 |
| H       | 0.1924  | 0.2268 | 3.3819 |
| H       | -1.6983 | 1.5934 | 4.2033 |
| C       | 1.1769  | 0.1223 | 0.9028 |
| H       | 1.6819  | 0.3501 | -0.0347 |
| C       | -0.7845 | -0.1653 | -1.8560 |
| H       | -0.8539 | -0.6979 | -2.8068 |
| N       | -1.1897 | -0.7623 | -0.8066 |
| N       | 1.4351  | -0.9403 | 1.5475 |
| O       | 2.4145  | -1.7114 | 0.9713 |
| O       | -1.6800 | -1.9956 | -1.1488 |
| C       | 2.2675  | -3.0451 | 1.4294 |
| H       | 3.2708  | -3.4439 | 1.6115 |
| H       | 1.7263  | -3.0234 | 2.3783 |
| C       | 1.5824  | -3.9408 | 0.4059 |
| H       | 2.2454  | -0.4083 | 2.4050 |
| H       | 1.4344  | -4.9250 | 0.8836 |
| C       | -1.8934 | -2.8265 | -0.0230 |
| H       | -2.3053 | -3.7377 | -0.4611 |
| H       | -2.6377 | -2.3829 | 0.6492 |
| C       | -0.6365 | -3.1353 | 0.7641 |
| H       | -0.8565 | -3.9767 | 1.4422 |
| H       | -0.3573 | -2.2720 | 1.3749 |
| O       | 0.3867  | -3.4599 | -0.1417 |
1-TS-rac

H (353 K, 1 atm) = -1030.609564 a.u.

\[
\begin{array}{cccc}
\text{H} & -1.95052700 & 0.07128800 & 0.35907400 \\
\text{C} & -1.42833100 & 0.04067000 & 1.30798400 \\
\text{C} & -0.13209200 & -0.10273300 & 3.84563400 \\
\text{C} & -0.92065500 & -1.14653900 & 1.78929800 \\
\text{C} & -1.16579700 & 1.19434500 & 2.02457600 \\
\text{C} & -0.53506900 & 1.10673400 & 3.24897600 \\
\text{C} & -0.23038600 & -1.24211000 & 3.00510900 \\
\text{H} & -0.99470200 & -2.04863000 & 1.19540700 \\
\text{H} & -1.44624400 & 2.16726100 & 1.63769000 \\
\text{H} & -0.33599900 & 2.03833000 & 3.75572700 \\
\text{C} & 0.26895400 & -0.02091300 & 5.29666100 \\
\text{C} & 0.92321500 & 0.52985800 & 8.02905900 \\
\text{C} & 0.91459000 & -0.97835700 & 6.11186500 \\
\text{C} & -0.12147800 & 1.15290600 & 5.97267200 \\
\text{C} & 0.19776000 & 1.43986600 & 7.28397400 \\
\text{C} & 1.24313900 & -0.67341200 & 7.43614000 \\
\text{H} & -0.74776200 & 1.87107400 & 5.46797000 \\
\text{H} & -0.14262700 & 2.37163000 & 7.72101400 \\
\text{H} & 1.74934700 & -1.43737700 & 8.01456600 \\
\text{H} & 1.19308800 & 0.72753600 & 9.05955400 \\
\text{C} & 1.24819600 & -2.38477300 & 5.78751400 \\
\text{H} & 2.18995900 & -2.65607000 & 5.31060700 \\
\text{C} & 0.51065200 & -2.50221700 & 3.14570200 \\
\text{H} & 1.56758100 & -2.45137000 & 3.39399100 \\
\text{N} & 0.01293100 & -3.60495000 & 2.75284300 \\
\text{N} & 0.47479000 & -3.27728500 & 6.24947900 \\
\text{O} & 0.95103400 & -4.54262200 & 6.02251800 \\
\text{O} & 0.96630600 & -4.59073700 & 2.67574100 \\
\end{array}
\]
1-c

H (353 K, 1 atm) = -1030.648032 a.u.
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 1.68911000| 3.92913900| 1.73275400|
| C       | 1.43251400| 1.83636000| 2.84985000|
| H       | 0.57526700| 4.13310100| -0.08324700|
| H       | 2.11991700| 4.92137500| 1.66520800|
| H       | 1.66726300| 1.18315900| 3.68374500|
| H       | 2.67473600| 3.42179200| 3.57584100|
| C       | 0.06122700| 0.01106900| 2.08559500|
| H       | 0.35983900| -0.46676700| 3.02063800|
| C       | 0.69246100| 0.06630600| -1.20686600|
| H       | 1.49087700| 0.31434600| -0.50886100|
| N       | 0.72136100| -1.02620200| -1.85461200|
| N       | -0.64113400| -0.64460700| 1.25216900|
| O       | -0.91502600| -1.90186300| 1.71145000|
| O       | 1.83722600| -1.76746500| -1.55618600|
| C       | -1.53970800| -2.69736700| 0.71464700|
| H       | -2.56241200| -2.92320100| 1.04031900|
| H       | -1.58425400| -2.12625200| -0.21468900|
| C       | -0.76661500| -3.98849900| 0.54616100|
| H       | -0.57262600| -4.41612000| 1.53351300|
| H       | -1.38815200| -4.70567300| -0.01132300|
| C       | 1.66293300| -3.09501200| -2.01624600|
| H       | 2.55851100| -3.61893300| -1.67734400|
| H       | 1.62514900| -3.11861900| -3.11270900|
| C       | 0.42091600| -3.75735800| -1.47187400|
| H       | 0.34623600| -4.77009400| -1.89925500|
| H       | -0.45257000| -3.18671200| -1.80681100|
| O       | 0.48486800| -3.81620700| -0.06947700|

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1-d

H (353 K, 1 atm) = -1030.651589 a.u.

H  0.39592100  -0.07942300  -0.01108000
C  0.29710800  -0.08156600  -1.09053600
C  0.04101100  -0.09831900  -3.87318500
C -0.31586500  -1.14557000  -1.72334700
C  0.77044800   0.98951100  -1.83807800
C  0.63835300   0.97611300  -3.21559100
C -0.45634600  -1.17109100  -3.11249700
H -0.71127900  -1.97630900  -1.15168300
H  1.24541700   1.83185100  -1.34831600
H  1.02367900   1.79927100  -3.80731900
C -0.04860000  -0.07532600  -5.35192100
C -0.31763100  -0.00187300  -8.13362300
C  0.52935300  -1.08101700  -6.14504000
C -0.73278900   0.96506200  -5.97730800
C -0.87037700   1.00595300  -7.35454700
C  0.38184900  -1.03126900  -7.53159500
H -1.18290200   1.73655300  -5.36221000
H -1.41287500   1.82127600  -7.81928600
H  0.84244200  -1.81023500  -8.12709300
H -0.42054000   0.02346400  -9.21236300
C  1.30088200  -2.15329800  -5.51785400
H  1.81737400  -1.95801600  -4.57848900
C -1.14061200  -2.28384700  -3.76922000
H -1.54609900  -2.13907100  -4.76969100
N -1.24856100  -3.41173000  -3.19161500
N  1.34364500  -3.30945000  -6.04633500
O  2.15405500  -4.15635300  -5.33470900
O  -1.96843100  -4.29633200  -3.95602300
C   1.91494000  -5.50848900  -5.68035600
H   2.79479700  -5.91281400  -6.19669900
H   1.06398700  -5.55244900  -6.36280000
C   1.67052600  -6.30164800  -4.41378900
H   2.52283100  -6.16982200  -3.74243100
H   1.60650000  -7.37102700  -4.67030100
C  -1.80778100  -5.62298100  -3.49073000
H  -1.63836100  -5.61493300  -2.41087200
H  -2.75100600  -6.13122000  -3.70873000
C  -0.68284000  -6.34125200  -4.19460700
H  -0.78411700  -7.42594600  -4.02365200
H  -0.77702900  -6.16153400  -5.27448000
O   0.54249500  -5.87908500  -3.69489700

2-a

H (353 K, 1 atm) = -1184.308997 a.u.

H  0.91949800  2.94469100  -3.51301900
C  0.92343100  3.03488700  -2.43280500
C  0.93224800  3.25333100  0.35495200
C  0.47035900  1.98982700  -1.65364200
C  1.37516600  4.20244000  -1.82942500
C  1.37306300  4.30417600  -0.45019700
C  0.46471800  2.07792300  -0.25838100
H  0.09997600  1.08099100  -2.11183000
H  1.73080000  5.02969600  -2.43285800
H  1.73543800  5.20717700  0.02861600
C  0.95260100  3.44175400  1.82627300
C  0.90419200  3.88633300  4.58675400
C  1.70233500  2.62234000  2.68639500
C  0.20403700  4.48383900  2.37260400
2-b

H (353 K, 1 atm) = -1184.307929 a.u.
### 2-TS-rac

| Element | X-Coordinates | Y-Coordinates | Z-Coordinates |
|---------|---------------|---------------|---------------|
| H       | -4.08450600   | 0.06586200    | 3.42783800    |
| C       | -3.01896400   | 0.09549300    | 3.62253200    |
| C       | -0.23081400   | 0.20219800    | 4.22556700    |
| C       | -2.47109500   | -0.66832200   | 4.62816900    |
| C       | -2.15846600   | 0.82196500    | 2.81867900    |
| C       | -0.81343100   | 0.85565400    | 3.12124700    |

H (353 K, 1 atm) = -1184.266244 a.u.
C   -1.09976900  -0.67816900   4.92246500
H   -3.09924600  -1.33750600   5.20157700
H   -2.52348000   1.35621500   1.94903000
H   -0.17972000   1.40534800   2.44268400
C    1.20933300   0.56234000   4.48796000
C    1.66193200   1.74997000   3.87561200
C    2.19195100  -0.11151200   5.24621500
H    0.94267300   2.41696300   3.42590900
H    3.24278100   3.07754300   3.34364200
H    4.25822600  -0.30611300   5.72664900
H    5.00038900   1.64208900   4.40710300
C   -0.70865100  -1.76815300   5.82536600
H    0.20017800  -2.32612600   5.62551600
C    2.00224100  -1.13909500   6.29310900
H    2.35259900  -2.16267900   6.13918600
N   -1.51313600  -2.17905500   6.72012400
N    1.60424400  -0.75478000   7.43355200
O    1.64484900  -1.76329200   8.35770900
O   -1.06932000  -3.33312000   7.32434300
C    1.04903400  -1.33244400   9.56921600
H    1.40639400  -0.33108900   9.82436800
H   -0.03828600  -1.30530300   9.45955600
C   -2.11380600  -3.88451000   8.10633400
H   -1.77577900  -4.89392300   8.34970900
H   -3.02819400  -3.94861100   7.50735300
C    1.44934800  -2.32688500  10.63748700
H    2.53590400  -2.30269400  10.77028000
H    1.16026100  -3.33554400  10.32876200
C   -2.39498800  -3.12589000   9.37731700
H   -3.33970000  -3.49452900   9.80864400
H (353 K, 1 atm) = -1184.308306 a.u.
|     | x         | y         | z         |
|-----|-----------|-----------|-----------|
| H   | 4.42734500| 1.12809500| -1.41434200|
| H   | 4.74744000| 0.72754000| -3.82106100|
| C   | -0.40305900| -0.81073400| -0.93338800|
| H   | 0.67330700| -0.93341200| -1.04463700|
| C   | 2.25669300| 1.46879000| -0.07285500|
| H   | 3.20615900| 1.70278800| 0.41365400|
| N   | -1.10519200| -1.75720800| -0.45596500|
| N   | 1.20282500| 1.37081500| 0.63255200|
| O   | 1.45587700| 1.63797800| 1.95124100|
| O   | -0.32592000| -2.83044300| -0.10449500|
| C   | 0.30596300| 1.37336100| 2.73627200|
| H   | 0.44703300| 1.93661600| 3.66086600|
| H   | -0.58759400| 1.74082100| 2.22503600|
| C   | -1.12209900| -3.86905300| 0.43296000|
| H   | -0.39727100| -4.62412400| 0.74302700|
| H   | -1.77070100| -4.29506000| -0.34287400|
| C   | 0.18087900| -0.10227500| 3.05161500|
| H   | 1.13166800| -0.46597300| 3.46913800|
| H   | -0.03072900| -0.67601700| 2.14356800|
| C   | -1.97647600| -3.44714500| 1.60176900|
| H   | -2.51268900| -4.33664400| 1.97178000|
| H   | -2.72534100| -2.71704100| 1.26912000|
| H   | -1.77070100| -4.29506000| -0.34287400|
| H   | -2.77462400| -1.83139200| 3.34895200|
| H   | -2.77462400| -1.83139200| 3.34895200|
| C   | -1.03775600| -1.50345000| 4.54208000|
| H   | -1.53531100| -1.35917600| 5.50586600|
| H   | -0.07090100| -1.99255900| 4.72803100|
2-TS-b

H (353 K, 1 atm) = -1184.302503 a.u.

H  -4.06016500  2.47768500  -2.16992900
C  -3.00697500  2.22486200  -2.21485800
C  -0.29646200  1.56575000  -2.32079100
C  -2.56772600  1.01541200  -1.71473800
C  -2.09904500  3.11170600  -2.78016100
C  -0.75698900  2.77681500  -2.83273100
C  -1.21516700  0.66718300  -1.75843400
H  -3.26719900  0.31027400  -1.28240000
H  -2.43610400  4.06161200  -3.17901400
H  -0.04106100  3.46448500  -3.26950300
C  1.15728100  1.26770100  -2.41218200
C  3.89638200  0.78060900  -2.68267900
C  2.00467400  1.37715500  -1.30331500
C  1.70317300  0.91399600  -3.64421400
C  3.05944600  0.66775400  -3.78238000
C  3.36820500  1.14039500  -1.45387800
H  1.04359400  0.82722300  -4.50062000
H  3.46181500  0.38776500  -4.74921300
H  4.01674500  1.23338500  -0.58960000
H  4.95862500  0.58873000  -2.78031200
C  -0.75233600  -0.61615900  -1.24130100
H  0.29889100  -0.87590000  -1.34523500
C  1.48761600  1.79576400  0.01822000
H  1.60503800  2.83425200  0.33762700
N  -1.55078100  -1.42159300  -0.66595800
N  0.91806500  0.95175900  0.77127900
O  0.48661100  1.51806900  1.94346600
O  -0.89951200  -2.56554600  -0.27372300
C   -0.12389800   0.54109500   2.76995200
H   -0.64459700   1.11484900   3.53898500
H   -0.85006600  -0.03722800   2.19222200
C   -1.77876600  -3.40343700   0.44582400
H   -1.23221400  -4.34220900   0.55655200
H   -2.69041600  -3.58277000  -0.13568000
C    0.89759600  -0.35944000   3.44873800
H    1.77375700   0.24978300   3.69663900
H    1.21023500  -1.16552100   2.77844200
C   -2.15211500  -2.86693600   1.80425200
H   -2.85169300  -3.57963400   2.26974200
H   -2.67321400  -1.90460500   1.70071600
O    0.37358900  -0.86477100   4.65958500
O   -0.99591300  -2.72196600   2.58642100
C   -1.27277300  -2.54749300   3.95294500
H   -1.70794800  -3.47148900   4.36741100
H   -1.99957800  -1.73632200   4.11034300
C    0.00439200  -2.21825000   4.69230200
H   -0.13567900  -2.45453200   5.75057800
H    0.80919500  -2.85905400   4.30521400

2-d

H (353 K, 1 atm) = -1184.304957 a.u.
H  -3.38412300  0.44214500  -1.60635700
H  -2.43321700  4.02934200  -3.74881100
H  -0.03398600  3.45520700  -3.61460800
C   1.10210000  1.34511900  -2.44967100
C   3.80292700  0.64754800  -2.31438500
C   1.74827500  1.25509200  -1.20697600
C   1.83467700  1.11339800  -3.60972800
C   3.17601500  0.76924500  -3.54658500
C   3.09280300  0.89527700  -1.15219500
H   1.33211400  1.17712400  -4.56867400
H   3.72941500  0.58636400  -4.46055600
H   3.57305400  0.83123400  -0.18312300
H   4.84978400  0.37209600  -2.25995900
C  -0.88195400  -0.48075800  -1.35407200
H   0.14408400  -0.81404100  -1.50045900
C   1.00530200  1.57427900   0.01325800
H   0.30304900  2.40911700   0.00129000
N  -1.68284400  -1.19936400  -0.67439600
N   1.15397100   0.88095800   1.06708200
O   0.43553200  1.42015400   2.11414500
O  -1.06616900  -2.35349800  -0.25918900
C   0.03194400  0.40576000   3.01643200
H  -0.41426100  0.94672400   3.85292200
H  -0.73244400  -0.22028700  2.54669500
C  -1.94619900  -3.14289100   0.51405300
H  -1.48413800  -4.13231200   0.52992500
H  -2.92172500  -3.20784900  0.02057500
C   1.17121200  -0.45183400   3.54395600
H   2.01680900  0.19799000   3.78967400
H   1.49729200  -1.17584900   2.79267600
C  -2.12912600  -2.65036700  1.92706400
H  -2.86063200  -3.30938900   2.42106300
H  -2.54672200  -1.63267800   1.92372400
| Atom | x   | y   | z    |
|------|-----|-----|------|
| O    | 0.77107700 | -1.09396400 | 4.73774600 |
| O    | -0.89762500 | -2.68118800 | 2.60027800 |
| C    | -1.02651400 | -2.61416300 | 3.99983000 |
| H    | -1.47847500 | -3.54641000 | 4.37475700 |
| H    | -1.68152700 | -1.78275700 | 4.29983800 |
| C    | 0.33595100  | -2.42480200 | 4.63352500 |
| H    | 0.29405700  | -2.79392900 | 5.66166500 |
| H    | 1.06389800  | -3.03665400 | 4.08183200 |

2-e

H (353 K, 1 atm) = -1184.308997 a.u.
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 2.52700300| 1.54416000| -2.14493400|
| H       | 2.83449600| 1.58069200| -1.10004000|
| C       | -0.04290500| 0.97168100| -0.55023100|
| H       | -0.18216900| 1.11534300| -1.62038000|
| N       | -0.31511000| -0.15297700| -0.02085100|
| N       | 2.86341600| 0.56104600| -2.87931400|
| O       | 3.65355100| -0.32680800| -2.20418600|
| O       | -0.77027300| -1.04772000| -0.95084400|
| C       | 3.85725100| -1.48754400| -2.98860400|
| H       | 4.39756100| -1.22847500| -3.90755900|
| H       | 2.88932600| -1.92153700| -3.26075500|
| C       | 4.67037500| -2.45107200| -2.15967300|
| H       | 5.53454500| -1.92445000| -1.74531100|
| H       | 5.04791100| -3.25331200| -2.80951100|
| C       | -1.07712600| -2.28410900| -0.33443700|
| H       | -1.81320400| -2.13124000| 0.46336900|
| H       | -1.53129400| -2.87613200| -1.13136900|
| C       | 0.11680500| -3.00991900| 0.22995700|
| H       | -0.25444400| -3.91918400| 0.73101200|
| H       | 0.61226300| -2.38610900| 0.98635600|
| O       | 1.00970700| -3.33376700| -0.80086000|
| O       | 3.95217900| -2.97133300| -1.07062100|
| C       | 3.17935800| -4.10867600| -1.36509000|
| H       | 3.80081400| -5.01433300| -1.29627400|
| H       | 2.75981700| -4.06292300| -2.37874000|
| C       | 2.04073100| -4.19211600| -0.38474200|
| H       | 2.41474500| -3.90590500| 0.60822400|
| H       | 1.67170800| -5.22777100| -0.32263400|
3-a

H (353 K, 1 atm) = -1337.96462 a.u.

H    -4.60260300  3.38110700  2.79114700
C    -3.56718600  3.06078900  2.80799900
C    -0.89931700  2.22578200  2.84416600
C    -3.20946000  1.85815200  2.23217900
C    -2.60017500  3.85056700  3.41800200
C    -1.28243200  3.42968600  3.43486500
C    -1.88164300  1.42246700  2.24097200
H    -3.95581400  1.22325000  1.77055300
H    -2.87271700  4.79405100  3.87685700
H    -0.51984300  4.04752400  3.89605200
C     0.53077400  1.83564800  2.89551700
C     3.21721200  1.09724900  3.11941500
C     1.30950800  1.65265000  1.74020700
C     1.12541800  1.66121200  4.14517500
C     2.45337900  1.29271400  4.26375100
C     2.65055100  1.28174000  1.87432300
H     0.51855800  1.80176600  5.03287700
H     2.89145700  1.15519100  5.24566600
H     3.23980700  1.15196500  0.97484100
H     4.25912000  0.80956100  3.20106100
C    -1.51923900  0.13426000  1.65490100
H    -0.54547400 -0.29729300  1.88334800
C     0.73217300  1.87725800  0.41650700
H    -0.23761200  2.36635900  0.33496400
N    -2.32237100 -0.47769300  0.88049400
N     1.35288300  1.51063900 -0.63187700
O    -1.79958900 -1.66660000  0.45141900
O     0.66633300  1.83691900 -1.77027000
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 1.38874400| 1.41029700| -2.9100700|
| H       | 2.44681900| 1.66456900| -2.8009180|
| H       | 0.97519900| 1.97847700| -3.7453820|
| C       | 1.24322200| -0.07538600| -3.1632580|
| H       | 0.19478900| -0.33044400| -3.3727530|
| H       | 1.54935500| -0.64451300| -2.2788100|
| O       | 2.06348700| -0.34979300| -4.2773920|
| C       | 0.47560200| -4.01129000| -3.4723470|
| H       | 0.87925200| -4.93614500| -3.9154600|
| H       | -0.14554000| -3.51945300| -4.2339360|
| C       | -0.39550100| -4.37649400| -2.3040370|
| H       | 0.23169500| -4.73765100| -1.4755390|
| H       | -1.05922600| -5.20143600| -2.6103850|
| O       | -1.14915600| -3.26382500| -1.9048570|
| C       | -2.07731900| -3.57849500| -0.9021390|
| H       | -1.58810000| -4.09684700| -0.0639170|
| H       | -2.85787200| -4.24779600| -1.2978300|
| C       | -2.72511000| -2.32212000| -0.3956210|
| H       | -2.99630400| -1.67072000| -1.2322960|
| H       | -3.63146900| -2.57096700| 0.1684650|
| C       | 1.86337500| -1.59271900| -4.8940590|
| H       | 2.41775100| -1.54660900| -5.8363030|
| H       | 0.79990900| -1.73297700| -5.1406450|
| C       | 2.37545100| -2.77769400| -4.0942190|
| H       | 2.56240900| -3.62044800| -4.7784690|
| H       | 3.32822100| -2.50018100| -3.6349970|
| O       | 1.52521100| -3.18387100| -3.0468150|

Supplementary Material
3-b

H (353 K, 1 atm) = -1337.962062 a.u.

H  -2.78743700  -1.51489500  -4.27844500
C  -2.14918800  -0.71197400  -3.92780700
C  -0.50129900   1.35419000  -3.00325700
C  -2.17770500  -0.34041400  -2.59985400
C  -1.30002400  -0.05470100  -4.80973600
C  -0.49201200   0.96578000  -4.34496400
C  -1.36607900   0.69048600  -2.11455500
H  -2.83786700  -0.84204000  -1.90329900
H  -1.26439500  -0.34059000  -5.85471100
H   0.18169100   1.47516300  -5.02498600
C   0.38157000   2.48237300  -2.61398000
C   1.99415800   4.68839700  -2.00655500
C   1.38102000   2.37878600  -1.63276100
C   0.22068900   3.69836600  -3.27956000
C   1.01204100   4.79367900  -2.98268100
C   2.17581700   3.49026200  -1.34374700
H  -0.55767500   3.77987500  -4.03020500
H   0.86187300   5.72805600  -3.51128000
H   2.94705200   3.38663600  -0.59033900
H   2.62374300   5.53843000  -1.76986700
C  -1.43104700   1.06274800  -0.70111800
H  -0.83005800   1.89250500  -0.33549200
C   1.58035700   1.12702300  -0.90381600
H   1.29700500   0.18018700  -1.36336200
N  -2.16411000   0.40546900   0.10525800
N   2.01668600   1.16531600   0.29076200
O  -2.02158600   0.84498000   1.39458200
O   2.10002300  -0.07414600   0.85176700
|  |  |  |  |
|---|---|---|---|
| C | 2.39264300 | 0.04472900 | 2.23669200 |
| H | 3.47014200 | 0.18467800 | 2.38087900 |
| H | 1.86090200 | 0.91111600 | 2.63854200 |
| C | 1.91996100 | -1.19607600 | 2.93366000 |
| H | 1.91918500 | -1.00530000 | 4.01894400 |
| H | 0.89439200 | -1.41623500 | 2.61896100 |
| O | 2.79528000 | -2.26136700 | 2.63620200 |
| C | -0.66073900 | -3.75351200 | 3.24963000 |
| H | -0.79824700 | -4.80016300 | 3.56470900 |
| H | -0.26338500 | -3.19424600 | 4.10832900 |
| C | -1.99627500 | -3.17829900 | 2.86791000 |
| H | -2.29725500 | -3.59988100 | 1.89792800 |
| H | -2.74800500 | -3.47857300 | 3.61550400 |
| O | -1.91796200 | -1.77789600 | 2.79429300 |
| C | -3.08113800 | -1.22574600 | 2.23708300 |
| H | -3.22994500 | -1.59586000 | 1.21481200 |
| H | -3.96634800 | -1.51069200 | 2.83034900 |
| C | -3.01745200 | 0.27947400 | 2.22887100 |
| H | -2.77421500 | 0.65228100 | 3.22567400 |
| H | -4.00370400 | 0.66336500 | 1.93919000 |
| C | 2.41627100 | -3.48850900 | 3.19939100 |
| H | 3.32877500 | -4.08502800 | 3.30621300 |
| H | 2.00773000 | -3.34139700 | 4.21054800 |
| C | 1.45546200 | -4.27896400 | 2.33053200 |
| H | 1.34652200 | -5.29130700 | 2.75520400 |
| H | 1.89089600 | -4.37206600 | 1.33286500 |
| O | 0.19410800 | -3.68673000 | 2.14025400 |
3-TS-rac

H (353 K, 1 atm) = -1337.920734 a.u.

H -3.84842000 -1.15461600  2.91565500
C -2.85294000 -0.85939400  3.22519000
C -0.21296500 -0.12147100  4.08258600
C -2.27824000 -1.40158500  4.35312200
C -2.12070200  0.07451600  2.52023600
C -0.85932800  0.42388100  2.95567300
C -0.99287100 -1.06523600  4.80380100
H -2.82734800 -2.13217000  4.93214900
H -2.52625300  0.55230800  1.63571900
H -0.38197000  1.20295800  2.38732200
H -2.27824000 -1.40158500  4.35312200
H -2.12070200  0.07451600  2.52023600
C  1.14106600  0.46900000  4.41675800
C  1.68070300  1.39916500  3.50741500
C  2.77524900  2.19884500  3.76734000
C  2.99107800  1.13911500  5.86652700
H  1.42238000  1.51960500  2.3067200
H  3.11786300  2.89056300  3.00630600
H  3.52451900  0.97257200  6.79381700
H  4.25237800  2.75459900  5.23789700
C -0.65536600 -1.82490900  6.02651200
H  0.15555500 -2.54586000  6.04090400
C  1.84201700 -0.84442900  6.52326400
H  1.93621100 -1.85126600  6.12144400
N -1.47503700 -1.77919100  6.99713600
N  1.88859000 -0.65245100  7.77788900
O -1.17410300 -2.69929500  7.97102500
O  2.01590500 -1.82615000  8.46641400
|     | X        | Y        | Z        |
|-----|----------|----------|----------|
| C   | 1.974514 | -1.565748| 9.859522 |
| H   | 2.879167 | -1.029059| 10.166834|
| H   | 1.100637 | -0.945420| 10.083392|
| C   | 1.852617 | -2.870598| 10.586803|
| H   | 1.565092 | -2.653497| 11.628135|
| C   | 0.288820 | -6.024695| 11.187241|
| H   | 0.305937 | -7.049288| 11.591072|
| C   | -1.074558| -5.730920| 10.621614|
| H   | -1.226963| -6.332439| 9.713949 |
| H   | -1.844697| -6.016848| 11.355303|
| O   | -1.149578| -4.362954| 10.321252|
| C   | -2.302073| -3.992588| 9.613979 |
| H   | -2.500683| -4.703342| 8.798970 |
| H   | -3.180757| -3.984177| 10.278513|
| C   | -2.113958| -2.619853| 9.028587 |
| H   | -1.755860| -1.924227| 9.796865 |
| H   | -3.065190| -2.250367| 8.636944 |
| O   | 3.094450 | -4.735725| 11.318375|
| C   | 4.137569 | -4.939768| 11.583493|
| H   | 2.546401 | -4.592844| 12.262387|
| C   | 2.757939 | -5.950845| 10.566494|
| H   | 2.752511 | -6.846344| 11.186504|
| H   | 3.154582 | -6.058557| 9.644832 |
| O   | 1.232624 | -5.880452| 10.160674|
3-c

H (353 K, 1 atm) = -1337.96462 a.u.

H  -4.60260300  3.38110700  -2.79114700
C  -3.56718600  3.06078900  -2.80799900
C  -0.89931700  2.22578200  -2.84416600
C  -3.20946000  1.85815200  -2.23217900
C  -2.60017500  3.85056700  -3.41800200
C  -1.28243200  3.42968600  -3.43486500
C  -1.88164300  1.42246700  -2.24097200
H  -3.95581400  1.22325000  -1.77055300
H  -2.87271700  4.79405100  -3.87685700
H  -0.51984300  4.04752400  -3.89605200
C  0.53077400  1.83564800  -2.89551700
C  3.21721200  1.09724900  -3.11941500
C  1.30950800  1.65265000  -1.74020700
C  1.12541800  1.66121200  -4.14517500
C  2.45337900  1.29271400  -4.26375100
C  2.65055100  1.28174000  -1.87432300
H  0.51855800  1.80176600  -5.03287700
H  2.89145700  1.15519100  -5.24566600
H  3.23980700  1.15196500  -0.97484100
H  4.25912000  0.80956100  -3.20106100
C  -1.51923900  0.13426000  -1.65490100
H  -0.54547400  -0.29729300  -1.88334800
C  0.73217300  1.87725800  -0.41650700
H  -0.23761200  2.36635900  -0.33496400
N  -2.32237100  -0.47769300  -0.88049400
N  1.35288300  1.51063900  0.63187700
O  -1.79958900  -1.66660000  -0.45141900
O  0.66633300  1.83691900  1.77027000
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | 1.388744     | 1.410297     | 2.910070     |
| H       | 2.446819     | 1.664569     | 2.800918     |
| H       | 0.975199     | 1.978477     | 3.745382     |
| C       | 1.243222     | -0.075386    | 3.163258     |
| H       | 0.194789     | -0.330444    | 3.372753     |
| H       | 1.549355     | -0.644513    | 2.278810     |
| O       | 2.063487     | -0.349793    | 4.277392     |
| C       | 0.475602     | -4.01129     | 3.472347     |
| H       | 0.879252     | -4.936145    | 3.915460     |
| H       | -0.145540    | -3.519453    | 4.233936     |
| C       | -0.395501    | -4.376494    | 2.304037     |
| H       | 0.231695     | -4.737651    | 1.475539     |
| H       | -1.059227    | -5.201436    | 2.610385     |
| O       | -1.149157    | -3.263825    | 1.904857     |
| C       | -2.077319    | -3.578495    | 0.902139     |
| H       | -1.588100    | -4.096847    | 0.063917     |
| H       | -2.857872    | -4.247796    | 1.297830     |
| C       | -2.725110    | -2.322120    | 0.395621     |
| H       | -2.996304    | -1.670720    | 1.232296     |
| H       | -3.631469    | -2.570967    | -0.168465    |
| C       | 1.863375     | -1.592719    | 4.894059     |
| H       | 2.417751     | -1.546609    | 5.836303     |
| H       | 0.799909     | -1.732977    | 5.140645     |
| C       | 2.375451     | -2.777694    | 4.094219     |
| H       | 2.562409     | -3.620448    | 4.778469     |
| H       | 3.328221     | -2.500181    | 3.634997     |
| O       | 1.525211     | -3.183871    | 3.046815     |
4-a

\[ H \text{ (393 K, 1 atm)} = -1107.763925 \text{ a.u.} \]

\begin{align*}
\text{C} & \quad 2.83222700 \quad -0.41984700 \quad 0.09757300 \\
\text{C} & \quad 3.34774100 \quad -2.94309600 \quad 1.18041700 \\
\text{C} & \quad 1.95339200 \quad -1.48681000 \quad -0.15207600 \\
\text{C} & \quad 3.96986700 \quad -0.64711000 \quad 0.86827200 \\
\text{C} & \quad 4.22960500 \quad -1.89515000 \quad 1.40941500 \\
\text{C} & \quad 2.22567400 \quad -2.74032000 \quad 0.39935800 \\
\text{H} & \quad 4.64363000 \quad 0.18087500 \quad 1.05946500 \\
\text{H} & \quad 5.11772300 \quad -2.04894700 \quad 2.01153200 \\
\text{H} & \quad 1.54446900 \quad -3.55540400 \quad 0.18730500 \\
\text{H} & \quad 3.54457800 \quad -3.92332900 \quad 1.59902300 \\
\text{C} & \quad 2.57369900 \quad 0.94443900 \quad -0.42387400 \\
\text{C} & \quad 2.13352300 \quad 3.49317700 \quad -1.36705400 \\
\text{C} & \quad 3.44412000 \quad 1.48673300 \quad -1.36705400 \\
\text{C} & \quad 1.47670400 \quad 1.70755400 \quad 0.01013900 \\
\text{C} & \quad 1.27170700 \quad 2.97904100 \quad -0.53023100 \\
\text{C} & \quad 3.22947100 \quad 2.74786500 \quad -1.89595400 \\
\text{H} & \quad 4.28897800 \quad 0.89300600 \quad -1.69832400 \\
\text{H} & \quad 0.42614000 \quad 3.55779100 \quad -0.17898200 \\
\text{H} & \quad 3.91486700 \quad 3.14841000 \quad -2.63403700 \\
\text{H} & \quad 1.95931500 \quad 4.48189600 \quad -1.88776900 \\
\text{C} & \quad 0.57903300 \quad 1.18055400 \quad 1.03607800 \\
\text{H} & \quad 0.91085400 \quad 0.34066100 \quad 1.64610600 \\
\text{C} & \quad 0.78436600 \quad -1.29287200 \quad -1.00930700 \\
\text{H} & \quad 0.79840900 \quad -0.50270200 \quad -1.75961300 \\
\text{N} & \quad -0.57873000 \quad 1.67744500 \quad 1.20808700 \\
\text{N} & \quad -0.24116500 \quad -2.03465900 \quad -0.87304600 \\
\text{O} & \quad -1.19425000 \quad -1.77036000 \quad -1.82477100 \\
\text{O} & \quad -1.23914100 \quad 1.06267400 \quad 2.25034600 \\
\end{align*}
Supplementary Material

C       -2.47618700  -2.21126400  -1.38871500
H       -3.00432400  -2.52800000  -2.29058700
H       -2.33845900  -3.07701900  -0.73437500
C       -2.62438100   1.32630100   2.15028000
H       -2.79110100   2.40593300   2.06905200
H       -3.03514200   0.98506600   3.10484700
C       -3.22875800  -1.10796700  -0.69965700
C       -4.51232800   1.04172400   0.51380600
C       -2.66299600  -0.47498200   0.40219300
C       -4.45734000  -0.66915200  -1.17389500
C       -5.10493700   0.39303000  -0.55666800
C       -3.28090000   0.61202700   0.99892100
H       -4.90372800  -1.14728200  -2.03999000
H       -5.00277800   1.89818200   0.96647300
H       -6.06256700   0.73481800  -0.93301500
H       -1.70605800  -0.81373200   0.77722700

4-TS-a

H (393 K, 1 atm) = -1107.749651 a.u.

H       0.42219600   4.41324400  -3.60338600
C       0.50177500   4.15844000  -2.55278500
C       0.69215300   3.50151100   0.15201400
C      -0.01976000   2.96433500  -2.09261200
C      -1.11485600   5.03447600  -1.66662600
C      -1.20471600   4.70388700  -0.32421700
C      -0.06993000   2.61721300  -0.74289200
H      -0.51312700   2.27823300  -2.77041400
H       1.51868900   5.97639000  -2.01986200
H       1.68369300   5.38225700   0.37335200
C       0.82136200   3.16008300   1.59246500
|     |        |        |        |
|-----|--------|--------|--------|
| C   | 0.97129400 | 2.43636200 | 4.28350700 |
| C   | 1.89499100 | 2.39100300 | 2.05250100 |
| C   | -0.15651600 | 3.56870000 | 2.49466500 |
| C   | -0.08331900 | 3.21520200 | 3.83294900 |
| C   | 1.95480000 | 2.03094000 | 3.39565200 |
| H   | -0.99124700 | 4.15785600 | 2.13086700 |
| H   | -0.85576900 | 3.54030200 | 4.52045300 |
| H   | 2.78409900 | 1.42281200 | 3.73854400 |
| H   | 1.02926800 | 2.14346000 | 5.32541700 |
| C   | 2.99477900 | 1.98246800 | 1.14820800 |
| H   | 3.79209000 | 2.69244300 | 0.91502100 |
| C   | -0.45523200 | 1.34126200 | -0.25876800 |
| H   | -0.61556900 | 1.20113200 | 0.80900300 |
| N   | -0.67774700 | 0.38827200 | -1.07104000 |
| N   | 3.02084500 | 0.80100600 | 0.69296900 |
| O   | 4.18078900 | 0.54214300 | -0.00006400 |
| O   | -1.20141600 | -0.71763500 | -0.43552700 |
| C   | 4.02332000 | -0.51562100 | -0.95774100 |
| H   | 5.01967700 | -0.95605700 | -1.03541100 |
| C   | -0.73681300 | -1.89953000 | -1.08661300 |
| H   | -0.81486800 | -1.75733000 | -2.16900200 |
| H   | -1.42705300 | -2.68479000 | -0.77408900 |
| C   | 0.67036400 | -2.21647100 | -0.66814100 |
| C   | 3.26102600 | -2.56465200 | 0.30368800 |
| C   | 0.95317100 | -3.23661100 | 0.23186300 |
| C   | 1.70832500 | -1.39742400 | -1.09460800 |
| C   | 2.99170000 | -1.53446800 | -0.58999900 |
| C   | 2.24758300 | -3.42373200 | 0.69847800 |
| H   | 0.15402400 | -3.88432900 | 0.57840800 |
| H   | 1.49546500 | -0.59312900 | -1.78987900 |
| H   | 2.46037400 | -4.22983700 | 1.39155600 |
| H   | 4.26295800 | -2.68338800 | 0.70316000 |
| H   | 3.76585400 | -0.06328900 | -1.92206400 |
4-b

H (393 K, 1 atm) = -1107.756577 a.u.

H  0.88973400  4.24983400  -3.56259400
C  0.90094100  3.98970000  -2.51032000
C  0.90687800  3.32416400   0.19965800
C  0.18415100  2.89715800  -2.06300000
C  1.63026100  4.75408300  -1.60864700
C  1.62413100  4.42257800  -0.26461100
C  0.18391700  2.54480300  -0.71143400
H  -0.38641600  2.28964400  -2.75486500
H  2.19545900  5.61356000  -1.95069200
H  2.18388300  5.02012500   0.44625100
C  0.88562900  3.06413800   1.66394000
C  0.78395400  2.83877200   4.45633300
C  1.84565500  2.29145700   2.33970000
C  -0.11118900  3.69168000   2.40589200
C  -0.17549900  3.58033500   3.78606900
C  1.78234400  2.21136900   3.73484700
H  -0.84610200  4.28869900   1.87718600
H  -0.96580200  4.08124200   4.33308300
H  2.53361200  1.62699900   4.25594800
H  0.75678200  2.74951400   5.53599800
C  2.92390100  1.52830700   1.71404200
H  3.74968900  1.22604100   2.36191200
C  -0.47481300  1.32279000  -0.25753800
H  -0.59070300  1.13966100   0.80997400
N  -0.81106000  0.43995300  -1.10773300
N  2.91517700  1.14375600   0.50241100
O  4.05203900  0.42359500   0.21173400
4-TS-b

H (393 K, 1 atm) = -1107.753452 a.u.
# Supplementary Material

|  |  |  |
|---|---|---|
| C | 0.64158700 | 3.50651400 | 4.46370700 |
| C | 1.64169000 | 2.49593100 | 2.48449200 |
| C | -0.00478900 | 4.24193400 | 2.28208400 |
| C | -0.12499900 | 4.33302300 | 3.65961800 |
| C | 1.51069600 | 2.60834600 | 3.87468600 |
| H | -0.81286100 | 5.04713500 | 4.09723700 |
| H | 2.11545200 | 1.96334200 | 4.50337600 |
| H | 0.56669200 | 3.56045800 | 5.54340400 |
| C | 2.60385200 | 1.48545500 | 2.05165400 |
| H | 2.31908200 | 0.99381300 | 2.85313700 |
| C | -0.45240800 | 1.33104600 | 0.00954300 |
| H | -0.52354600 | 1.27288000 | 1.07634300 |
| N | -0.75209900 | 0.32535500 | 0.72849200 |
| N | 2.82830000 | 1.11676000 | 0.85342300 |
| O | 3.80409200 | 0.14399100 | 0.83886400 |
| O | -1.13776100 | -0.75799600 | 0.03551500 |
| C | 3.92015900 | -0.47969100 | -0.43506400 |
| H | 4.94686300 | -0.84945300 | -0.47229300 |
| C | -0.85215700 | -1.94866100 | -0.67634800 |
| H | -1.26127700 | -1.86648900 | -1.69061600 |
| H | -1.40114200 | -2.73116300 | -0.14721300 |
| C | 0.61728500 | -2.29031900 | -0.74296200 |
| C | 3.33959400 | -2.88846800 | -0.98477700 |
| C | 1.02932400 | -3.57470600 | -1.09253700 |
| C | 1.58815700 | -1.33018000 | -0.51187700 |
| C | 2.94256200 | -1.60545300 | -0.63783300 |
| C | 2.37908700 | -3.86891500 | -1.20842200 |
| H | 0.29236100 | -4.35151800 | -1.27372100 |
| H | 1.30761100 | -0.32791200 | -0.24497500 |
| H | 2.68804600 | -4.87400500 | -1.47319700 |
| H | 4.39382200 | -3.12784500 | -1.08176700 |
| H | 3.79304700 | 0.28387700 | -1.20899600 |
4-c

H (393 K, 1 atm) = -1107.754527 a.u.

|   |   |   |   |
|---|---|---|---|
| H | 0.84592100 | 3.83906700 | -3.66663500 |
| C | 0.86625100 | 3.71282100 | -2.59024700 |
| C | 0.90032200 | 3.38860300 | 0.18304000 |
| C | 0.16291600 | 2.67875400 | -2.00481900 |
| C | 1.59792300 | 4.58731000 | -1.79693300 |
| C | 1.60480500 | 4.42563700 | -0.42211900 |
| C | 0.17459000 | 2.49849300 | -0.62018200 |
| H | -0.40276800 | 1.98212900 | -2.61136400 |
| H | 2.15581200 | 5.39990000 | -2.24809300 |
| H | 2.16490500 | 5.11129200 | 0.20382600 |
| C | 0.86073800 | 3.33841200 | 1.66964800 |
| C | 0.64158700 | 3.50651400 | 4.46370700 |
| C | 1.64169000 | 2.49593100 | 2.48449200 |
| C | -0.00478900 | 4.24193400 | 2.28208400 |
| C | -0.12499900 | 4.33302300 | 3.65961800 |
| C | 1.51069600 | 2.60834600 | 3.87468600 |
| H | -0.60000100 | 4.88764200 | 1.64596900 |
| H | -0.81286100 | 5.04713500 | 4.09723700 |
| H | 2.11545200 | 1.96334200 | 4.50337600 |
| H | 0.56669200 | 3.56045800 | 5.54340400 |
| C | 2.60385200 | 1.48545500 | 2.05165400 |
| H | 3.15908200 | 0.99381300 | 2.85313700 |
| C | -0.45240800 | 1.33104600 | -0.00954300 |
| H | -0.52354600 | 1.27288000 | 1.07634300 |
| N | -0.75209900 | 0.32535500 | -0.72849200 |
| N | 2.82830000 | 1.11676000 | 0.85342300 |
| O | 3.80409200 | 0.14399100 | 0.83886400 |
| O | -1.13776100 | -0.75799600 | 0.03551500 |
H (393 K, 1 atm) = -1107.71285 a.u.

4-TS-rac
4-d

H (393 K, 1 atm) = -1107.754527 a.u.

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 1.01017200 | 3.21387900 | 3.71968000 |
| C    | 0.99541300 | 3.22583700 | 2.63587600 |
| C    | 0.94767800 | 3.24663600 | -0.15745100 |
| C    | 0.33540500 | 2.22910000 | 1.94532300 |
| C    | 1.64030000 | 4.23878900 | 1.93786700 |
| C    | 1.60578500 | 4.24730200 | 0.55444400 |
| C    | 0.30529300 | 2.22058600 | 0.54935200 |
| H    | -0.16315000| 1.42662700 | 2.47491200 |
| H    | 2.16496200 | 5.02396300 | 2.47020500 |
| H    | 2.10147900 | 5.03873400 | 0.00334700 |
| C    | 0.87107200 | 3.38474000 | -1.63582400 |
| C    | 0.57838000 | 3.89369800 | -4.38438900 |
| C    | 1.53529000 | 2.57186600 | -2.57587100 |
| C    | 0.08928400 | 4.43773100 | -2.10683700 |
| C    | -0.06368700| 4.69917200 | -3.45901500 |
| C    | 1.36434200 | 2.84866900 | -3.93790200 |
| H    | -0.41911000| 5.05924400 | -1.37818100 |
| H    | -0.68592400| 5.52523100 | -3.78324800 |
| H    | 1.87513500 | 2.22043500 | -4.66007800 |
| H    | 0.47056800 | 4.07668500 | -5.44696700 |
| C    | 2.41342700 | 1.43989400 | -2.29524700 |
| H    | 2.79221000 | 0.90833500 | -3.17102600 |
| C    | -0.30193300| 1.10744900 | -0.17235700 |
| H    | -0.33903400| 1.13913800 | -1.26073800 |
| N    | -0.66932200| 0.06292900 | 0.45026000 |
| N    | 2.76360200 | 1.02861300 | -1.14213700 |
| O    | 3.59904700 | -0.06150000| -1.26857300 |
O  -1.05658200  -0.94165400  -0.41917900
C   3.93017300  -0.60792100  -0.00810700
H   4.88409100  -1.11856100  -0.16451900
C  -0.81192700  -2.18961900   0.21213700
H  -1.48531900  -2.31491300  1.06797800
H  -1.07575700  -2.93038900  -0.54765100
C   0.61767400  -2.33349400   0.66787500
C   3.22226800  -2.35274400  1.64609500
C   0.94260200  -3.11058200  1.76987600
C   1.61828200  -1.60193700   0.03766100
C   2.90488400  -1.56131800   0.54561100
C   2.24960000  -3.14093600  2.23859400
H   0.17031200  -3.67551400   2.28248100
H   1.36753900  -1.00110100  -0.82338900
H   2.50146400  -3.75601600  3.09526400
H   4.22938800  -2.33961900   2.05195700
H   4.09235800   0.20967600   0.70288900

4-e

H (393 K, 1 atm) = -1107.763925 a.u.

C   2.83222700  -0.41984700  -0.09757300
C   3.34774100  -2.94309600  -1.18041700
C   1.95339200  -1.48681000   0.15207600
C   3.96986700  -0.64711000  -0.86827200
C   4.22960500  -1.89515000  -1.40941500
C   2.22567400  -2.74032000  -0.39935800
H   4.64363000   0.18087500  -1.05946500
H   5.11772300  -2.04894700  -2.01153200
H   1.54446900  -3.55540400  -0.18730500
H   3.54457800  -3.92332900  -1.59902300
C   2.57369900   0.94443900   0.42387400

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| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | 2.13352300 | 3.49317700 | 1.47921900 |
| C       | 3.44412000  | 1.48673300  | 1.36705400  |
| C       | 1.47670400  | 1.70755400  | -0.01013900 |
| C       | 1.27170700  | 2.97904100  | 0.53023100  |
| C       | 3.22947100  | 2.74786500  | 1.89595400  |
| H       | 4.28897800  | 0.89300600  | 1.69832400  |
| H       | 0.42614000  | 3.55779100  | 0.17898200  |
| H       | 3.91486700  | 3.14841000  | 2.63403700  |
| H       | 1.95931500  | 4.48189600  | 1.88776900  |
| C       | 0.57903300  | 1.18055400  | -1.03607800 |
| H       | 0.91085400  | 0.34066100  | -1.64610600 |
| C       | 0.78436600  | -1.29287200 | 1.00930700  |
| H       | 0.79840900  | -0.50270200 | 1.75961300  |
| N       | -0.57873000 | 1.67744500  | -1.20808700 |
| N       | -0.24116500 | -2.03475900 | 0.87304600  |
| O       | -1.19425000 | -1.77036000 | 1.82477100  |
| O       | -1.23914100 | 1.06267400  | -2.25034600 |
| C       | -2.47618700 | -2.21126400 | 1.38871500  |
| H       | -3.00432400 | -2.52800000 | 2.29058700  |
| H       | -2.33845900 | -3.07701900 | 0.73437500  |
| C       | -2.62438100 | 1.32630100  | -2.15028000 |
| H       | -2.79110100 | 2.40593300  | -2.06905200 |
| H       | -3.03514200 | 0.98506600  | -3.10484700 |
| C       | -3.22875800 | -1.10796700 | 0.69965700  |
| C       | -4.51232800 | 1.04172400  | -0.51380600 |
| C       | -2.66299600 | -0.47498200 | -0.40219300 |
| C       | -4.45734000 | -0.66915200 | 1.17389500  |
| C       | -5.10493700 | 0.39303000  | 0.55666800  |
| C       | -3.28090000 | 0.61202700  | -0.99892100 |
| H       | -4.90372800 | -1.14728200 | 2.03999000  |
| H       | -5.00277800 | 1.89818200  | -0.96647300 |
| H       | -6.06256700 | 0.73481800  | 0.93301500  |
| H       | -1.70605800 | -0.81373200 | -0.77722700 |
1-Li⁺-a

H (353 K, 1 atm) = -1038.036725 a.u.
1-Li⁺-rac

H (353 K, 1 atm) = -1037.987773 a.u.
|    |    |    |    |
|----|----|----|----|
| C  | -0.16137600 | 1.14741200 | 5.98642100 |
| C  | 0.17419600  | 1.44957300 | 7.29088100 |
| C  | 1.28038600  | -0.63414300 | 7.44355900 |
| H  | -0.81297000 | 1.84506400 | 5.48436900 |
| H  | -0.18223900 | 2.37419200 | 7.72887200 |
| H  | 1.81454500  | -1.37781600 | 8.02415100 |
| H  | 1.22291900  | 0.78231600 | 9.05199800 |
| C  | 1.28334700  | -2.34933200 | 5.80980000 |
| H  | 2.25845400  | -2.59996300 | 5.38126600 |
| C  | 0.45592000  | -2.51839600 | 3.17231700 |
| H  | 1.52515800  | -2.46108300 | 3.37978600 |
| N  | -0.06768100 | -3.62645500 | 2.83464200 |
| N  | 0.48018600  | -3.24095500 | 6.21160000 |
| O  | 0.94621200  | -4.54212300 | 5.97641300 |
| O  | 0.91114100  | -4.64695400 | 2.74572600 |
| C  | -0.08190100 | -5.46329700 | 6.37034100 |
| H  | -0.16214300 | -5.48886400 | 7.45967100 |
| H  | -1.02940700 | -5.10859000 | 5.96051400 |
| C  | 0.31104500  | -6.82062800 | 5.83302300 |
| H  | 1.17431500  | -7.22036700 | 6.36886800 |
| H  | -0.51701700 | -7.52518400 | 5.95362100 |
| C  | 0.28624500  | -5.86464600 | 2.32464500 |
| H  | 1.08949400  | -6.46396600 | 1.88941900 |
| H  | -0.45842600 | -5.65027500 | 1.55764600 |
| C  | -0.32970300 | -6.56427600 | 3.50909300 |
| H  | -0.73323800 | -7.54025100 | 3.22335400 |
| H  | -1.13594100 | -5.94950600 | 3.92000600 |
| O  | 0.71842700  | -6.73145400 | 4.46906300 |
| Li | 1.80462500  | -5.16221900 | 4.36792200 |
**1-Li⁺-c**

H (353 K, 1 atm) = -1038.023442 a.u.

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -3.1226200 | 1.59304200 | -3.35874000 |
| C    | -2.45113200 | 1.69961600 | -2.51542800 |
| C    | -0.68280200 | 1.99916100 | -0.35556600 |
| C    | -1.33441500 | 0.89402800 | -2.41303500 |
| C    | -2.70021000 | 2.64872600 | -1.53422700 |
| C    | -1.82058900 | 2.79679500 | -0.47561600 |
| C    | -0.45168300 | 1.02586300 | -1.34054800 |
| H    | -1.12144200 | 0.15317500 | -3.17397200 |
| H    | -3.57560300 | 3.28141200 | -1.59763500 |
| H    | -2.01652600 | 3.54320400 | 0.28544200 |
| C    | 0.23942900  | 2.31457000 | 0.77003800 |
| C    | 1.90754300  | 3.25462600 | 2.84538600 |
| C    | 0.59992600  | 1.46518400 | 1.84108900 |
| C    | 0.73993400  | 3.61570700 | 0.78252100 |
| C    | 1.56187000  | 4.08698600 | 1.79443100 |
| C    | 1.42874200  | 1.95968300 | 2.85684200 |
| H    | 0.47672400  | 4.27291900 | -0.03806900 |
| H    | 1.92977900  | 5.10545200 | 1.73530600 |
| H    | 1.69411400  | 1.30246200 | 3.67832800 |
| H    | 2.54409800  | 3.60801200 | 3.64702900 |
| C    | 0.23292900  | 0.06641100 | 2.00332000 |
| H    | 0.69279200  | -0.45466500 | 2.84795300 |
| C    | 0.66216700  | 0.09722200 | -1.20259600 |
| H    | 1.52141000  | 0.38660000 | -0.59425200 |
| N    | 0.57977700  | -1.06212000 | -1.71916500 |
| N    | -0.51728200 | -0.58324900 | 1.20431000 |
| O    | -0.47538300 | -1.96161100 | 1.50163700 |
O                  1.67521700   -1.87652500   -1.35009200
C                 -1.48473200   -2.66095200    0.75804400
H                 -2.40628700   -2.71735800    1.34307200
H                 -1.67630600   -2.10330200   -0.16206300
C                -0.92987600   -4.03926000    0.48044000
H                -0.75224200   -4.58168100    1.41120900
H                -1.63260000   -4.62013000   -0.12261700
C                  1.55316300   -3.12895500   -2.03539300
H                  2.45837100   -3.67908400   -1.76936600
H                  1.54041800   -2.96509800   -3.11474300
C                 0.31020500   -3.86721500   -1.59500400
H                 -0.75224200   -4.58168100    1.41120900
H                 -1.63260000   -4.62013000   -0.12261700
O                  0.33971300   -3.93528400   -0.16750700
Li                 1.19317000   -2.37171000    0.51225100

1-Li\textsuperscript{2-}c

H (353 K, 1 atm) = -1038.036725 a.u.

H            0.97331700    2.01393700    4.43377300
C            0.64796700    2.09288900    3.40351900
C            -0.21437500    2.30713900    0.74654700
C            -0.04662400    1.04985700    2.81552100
C            0.89234800    3.25064900    2.67881100
C            0.46389400    3.35311500    1.36407000
C            -0.48809300    1.14690300    1.49383500
H            -0.30492500    0.17001000    3.39418800
H            1.42190900    4.07722900    3.13747800
H            0.68180900    4.24651100    0.78989500
C            -0.57587000    2.40150300   -0.68506900
C            -1.30624000    2.54651900    -3.37804000
C            -0.07930700    1.46748800   -1.61127100
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -1.418079 | 3.413142  | -1.136842 |
| C       | -1.782060 | 3.485606  | -2.471545 |
| C       | -0.456117 | 1.543439  | -2.950746 |
| H       | -1.806388 | 4.133703  | -0.425913 |
| H       | -2.442633 | 4.276638  | -2.806101 |
| H       | -0.054552 | 0.822671  | -3.652722 |
| H       | -1.589070 | 2.606452  | -4.422000 |
| C       | 0.851130  | 0.445495  | -1.139650 |
| H       | 1.518731  | 0.702833  | -0.314430 |
| C       | -1.302991 | 0.070431  | 0.926280  |
| H       | -2.187514 | 0.311295  | 0.336596  |
| N       | -0.989490 | -1.148636 | 1.132399  |
| N       | 0.846857  | -0.728554 | -1.623139 |
| O       | 1.736876  | -1.559397 | -0.915230 |
| O       | -1.910484 | -2.030575 | 0.610428  |
| C       | 1.767270  | -2.859056 | -1.513806 |
| H       | 2.668762  | -2.967691 | -2.122630 |
| H       | 0.893287  | -2.949729 | -2.160011 |
| C       | 1.752465  | -3.870946 | -0.389231 |
| H       | 2.682545  | -3.834015 | 0.183084  |
| H       | 1.645026  | -4.885048 | -0.785735 |
| C       | -1.640107 | -3.368170 | 1.003948  |
| H       | -1.384689 | -3.404544 | 2.067717  |
| H       | -2.586451 | -3.892139 | 0.859901  |
| C       | -0.583657 | -4.047442 | 0.169198  |
| H       | -0.622620 | -5.128649 | 0.341727  |
| H       | -0.778289 | -3.851013 | -0.890405 |
| O       | 0.710436  | -3.567685 | 0.536278  |
| Li      | 0.906255  | -1.724166 | 0.938444  |
1-Na⁺-a

H (353 K, 1 atm) = -1192.722415 a.u.

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| H    | 0.51964900 | -0.19852800 | 0.05815600 |
| C    | 0.39699100 | -0.17645500 | 1.13449600 |
| C    | 0.03523800 | -0.09395700 | 3.91128100 |
| C    | -0.31654900 | -1.17861800 | 1.77094900 |
| C    | 0.91105600 | 0.87846300  | 1.87575800 |
| C    | 0.72401100 | 0.91810700  | 3.24896400 |
| C    | -0.50285200 | -1.15249200 | 3.15707800 |
| H    | -0.79720300 | -1.95946900 | 1.19058400 |
| H    | 1.45429400 | 1.67592200  | 1.38288000 |
| H    | 1.13840300 | 1.73420200  | 3.83009400 |
| C    | -0.08919400 | -0.06766000 | 5.38665000 |
| C    | -0.41467800 | -0.06626700 | 8.15931300 |
| C    | 0.47962600 | -1.08549400 | 6.16978800 |
| C    | -0.79409900 | 0.95370300  | 6.01513300 |
| C    | -0.95704400 | 0.95564600  | 7.39142100 |
| C    | 0.30487600 | -1.07953800 | 7.55206500 |
| H    | -1.23728500 | 1.73859400  | 5.41256600 |
| H    | -1.51258300 | 1.75582000  | 7.86583700 |
| H    | 0.76061700  | -1.86483000 | 8.14289800 |
| H    | -0.54065000 | -0.06376700 | 9.23526000 |
| C    | 1.28413900 | -2.11574800 | 5.51490800 |
| H    | 1.88830400 | -1.82139400 | 4.65218700 |
| C    | -1.29150800 | -2.20227000 | 3.80973200 |
| H    | -1.94188400 | -1.95571800 | 4.64813700 |
| N    | -1.19186100 | -3.40413100 | 3.39627000 |
| N    | 1.26513800  | -3.32088200 | 5.91379700 |
| O    | 2.06244100  | -4.14065300 | 5.11625200 |
| O    | -2.02176300 | -4.26775900 | 4.05681400 |
C                  1.99480000   -5.48830400    5.58564400
H                  2.95564600   -5.76836400    6.02727700
H                  1.22925300   -5.53525500    6.36026300
C                  1.67659700   -6.39459600    4.41610100
H                  2.50104000   -6.39452800    3.69694300
H                  1.55457800   -7.42536900    4.76796500
C                 -1.85225800   -5.60711900    3.61902000
H                 -1.75097000   -5.63732300    2.52958800
H                 -2.78514500   -6.10335000    3.89189000
C                 -0.71056300   -6.32852400    4.29152300
H                 -0.85151200   -7.41021600    4.17537300
H                 -0.71972500   -6.08837300    5.36035300
O                  0.53011100   -5.95692400    3.70210400
Na                 1.04502500
                    -3.88829700    2.85416800
1-Na+\textsuperscript{b}

H (353 K, 1 atm) = -1192.703607 a.u.

H                  0.99526900    2.98561400   -4.46582200
C                  0.67764500    2.76755800   -3.45338000
C                 -0.19006800    2.21361800   -0.84153700
C                 -0.18352800    1.71262500   -3.20999700
C                  1.11301100    3.54934600   -2.39410400
C                  0.66919700    3.27827200   -1.10965900
C                 -0.60284100    1.40312400   -1.91147000
H                 -0.54294800    1.11046200   -4.03865300
H                  1.77863800    4.38617800   -2.56925600
H                  0.97509000    3.91502500   -0.28711500
C                 -0.70520100    2.07110000    0.54761900
C                 -1.69630900    1.94224000    3.15735700
C                 -0.07728400    1.26665400    1.50564400
| Atom | X  | Y  | Z   |
|------|----|----|-----|
| C    | -1.83196700 | 2.79907200 | 0.91600600 |
| C    | -2.32748400 | 2.73538300 | 2.20859400 |
| C    | -0.57833100 | 1.20984600 | 2.80621300 |
| H    | -2.32002400 | 3.42459200 | 0.17719000 |
| H    | -3.20246700 | 3.31501100 | 2.47792000 |
| H    | -0.07203100 | 0.59118200 | 3.53720400 |
| H    | -2.07234900 | 1.90244000 | 4.17253300 |
| C    | 1.04245800  | 0.42445700 | 1.09791600 |
| H    | 1.69692200  | 0.76692300 | 0.28996000 |
| C    | -1.46208100 | 0.21237800 | -1.79390900 |
| H    | -2.27913500 | 0.08686800 | -2.50717700 |
| N    | -1.18985500 | -0.73200600 | -0.98232000 |
| N    | 1.18211500  | -0.72033400 | 1.62965700 |
| O    | 2.19296000  | -1.48381800 | 1.05266100 |
| O    | -1.97795600 | -1.83537600 | -1.21104400 |
| C    | 2.09593500  | -2.81515400 | 1.57175600 |
| H    | 3.10872800  | -3.15808400 | 1.79442500 |
| H    | 1.53032900  | -2.76614200 | 2.50190400 |
| C    | 1.45377300  | -3.75802400 | 0.56023800 |
| H    | 2.16464900  | -4.00784200 | -0.23238900 |
| H    | 1.18931300  | -4.69510200 | 1.06577300 |
| C    | -2.04466000 | -2.76465100 | -0.13215500 |
| H    | -2.31480500 | -3.69932000 | -0.62597500 |
| H    | -2.85796100 | -2.47848100 | 0.54475900 |
| C    | -0.80399600 | -2.94229200 | 0.70854800 |
| H    | -0.99409600 | -3.79285500 | 1.37541000 |
| H    | -0.61819600 | -2.06031500 | 1.32710600 |
| O    | 0.32923600  | -3.21284500 | -0.11060600 |
| Na   | 1.10356000  | -1.33775300 | -1.17210700 |
1-Na\(^+\)-rac

\[
H \text{(353 K, 1 atm)} = -1192.671347 \text{ a.u.}
\]

\[
\begin{align*}
\text{H} & \quad -1.96061800 \quad 0.04449900 \quad 0.37379500 \\
\text{C} & \quad -1.44283600 \quad 0.01460700 \quad 1.32446200 \\
\text{C} & \quad -0.15515500 \quad -0.11954000 \quad 3.87038700 \\
\text{C} & \quad -0.94995600 \quad -1.17540600 \quad 1.81580600 \\
\text{C} & \quad -1.17279200 \quad 1.16821700 \quad 2.03561700 \\
\text{C} & \quad -0.54661100 \quad 1.08616400 \quad 3.26431900 \\
\text{C} & \quad -0.26991400 \quad -1.26440800 \quad 3.03803900 \\
\text{H} & \quad -1.02840400 \quad -2.07586700 \quad 1.22057200 \\
\text{H} & \quad -1.44512400 \quad 2.14014500 \quad 1.64174800 \\
\text{H} & \quad -0.34422600 \quad 2.01912600 \quad 3.76712500 \\
\text{C} & \quad 0.24641100 \quad -0.02215300 \quad 5.31792100 \\
\text{C} & \quad 0.94975700 \quad 0.57985100 \quad 8.02780100 \\
\text{C} & \quad 0.93512100 \quad -0.94602500 \quad 6.13360500 \\
\text{C} & \quad -0.16759500 \quad 1.14444800 \quad 5.98982100 \\
\text{C} & \quad 0.17485600 \quad 1.45461000 \quad 7.29044000 \\
\text{C} & \quad 1.29091000 \quad -0.62284100 \quad 7.44509700 \\
\text{H} & \quad -0.82658100 \quad 1.83639700 \quad 5.48972500 \\
\text{H} & \quad -0.18397900 \quad 2.37926500 \quad 7.72647400 \\
\text{H} & \quad 1.82959000 \quad -1.36276500 \quad 8.02645000 \\
\text{H} & \quad 1.23919600 \quad 0.80103600 \quad 9.04757500 \\
\text{C} & \quad 1.28179400 \quad -2.35041000 \quad 5.82366000 \\
\text{H} & \quad 2.26148100 \quad -2.59971600 \quad 5.40255600 \\
\text{C} & \quad 0.46601300 \quad -2.52617300 \quad 3.17139900 \\
\text{H} & \quad 1.53263700 \quad -2.46191600 \quad 3.39042100 \\
\text{N} & \quad -0.04432200 \quad -3.63150900 \quad 2.80701900 \\
\text{N} & \quad 0.48065500 \quad -3.24316100 \quad 6.22558200
\end{align*}
\]
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| O    | 0.94439100 | -4.53831400| 6.01471200 |
| O    | 0.92360100 | -4.64176200| 2.68540000 |
| C    | -0.11272300| -5.44978000| 6.34664000 |
| H    | -0.25079700| -5.48307200| 7.42794700 |
| H    | -1.03424000| -5.06932600| 5.89589000 |
| C    | 0.26060100 | -6.81393700| 5.82293600 |
| H    | 1.10611000 | -7.22456800| 6.38096500 |
| H    | -0.58633100| -7.49423700| 5.96480900 |
| C    | 0.28003100 | -5.86101100| 2.31954700 |
| H    | 1.06868100 | -6.48783100| 1.89377000 |
| H    | -0.46641700| -5.66456600| 1.54795900 |
| C    | -0.35232300| -6.52773500| 3.51332800 |
| H    | -0.83120400| -7.46732000| 3.21720800 |
| H    | -1.11333800| -5.86188100| 3.92940700 |
| O    | 0.67646200 | -6.78492200| 4.46520500 |
| Na   | 2.40005500 | -5.26811700| 4.35194800 |

1-Na⁺-c

H (353 K, 1 atm) = -1192,719114 a.u.
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 0.25794500 | 1.38817000 | 1.55377300 |
| C       | 1.01421500 | 3.47367000 | 0.62509900 |
| C       | 2.06388300 | 3.50076600 | 1.53344600 |
| C       | 1.31941900 | 1.41687400 | 2.45870900 |
| H       | 0.90601900 | 4.26802100 | -0.10484500 |
| H       | 2.75869700 | 4.33216500 | 1.52706200 |
| H       | 1.38981500 | 0.64369400 | 3.21716100 |
| H       | 3.03888700 | 2.49156000 | 3.15902900 |
| C       | -0.74103800| 0.31308100 | 1.63045000 |
| H       | -1.79789600| 0.55902900 | 1.73761400 |
| C       | 0.32371100 | 0.46311500 | -1.43518300|
| H       | 1.25769400 | 0.88120600 | -1.05160100|
| N       | 0.29038700 | -0.74018700| -1.84246100|
| N       | -0.37276600| -0.90361100| 1.58536900 |
| O       | -1.42620200| -1.76632000| 1.84569300 |
| O       | 1.54358100 | -1.34165400| -1.68235200|
| C       | -1.52229400| -2.82821500| 0.90762900 |
| H       | -2.40690800| -3.37289300| 1.24228000 |
| H       | -1.73275500| -2.41844500| -0.08694300|
| C       | -0.54702000| -3.78487600| 0.86237600 |
| H       | 0.05375000 | -3.92873100| 1.86835900 |
| H       | 0.69441400 | -4.75995300| 0.50182000 |
| C       | 1.49849500 | -2.69713100| -2.12141200|
| H       | 2.51773000 | -3.06076300| -1.97265300|
| H       | 1.26337900 | -2.74306300| -3.18805000|
| C       | 0.50032500 | -3.51944600| -1.34374800|
| H       | 0.61042000 | -4.57678500| -1.61451000|
| H       | -0.51109300| -3.19798200| -1.60451800|
| O       | 0.73333900 | -3.34073700| 0.04565400 |
| Na      | 1.76852700 | -1.41361200| 0.71869100 |
**1-Na⁺-d**

H (353 K, 1 atm) = -1192.722415 a.u.

|   |     |     |     |
|---|-----|-----|-----|
| H | 0.51964900 | -0.19852800 | -0.05815600 |
| C | 0.39699100 | -0.17645500 | -1.13449600 |
| C | 0.03523800 | -0.09395700 | -3.91128100 |
| C | -0.31654900 | -1.17861800 | -1.77094900 |
| C | 0.91105600 | 0.87846300 | -1.87575800 |
| C | 0.72401100 | 0.91810700 | -3.24896400 |
| C | -0.50285200 | -1.15249200 | -3.15707800 |
| H | -0.79720300 | -1.95946900 | -1.19058400 |
| H | 1.45429400 | 1.67592200 | -1.38288000 |
| H | 1.13840300 | 1.73420200 | -3.83009400 |
| C | -0.08919400 | -0.06766000 | -5.38665000 |
| C | -0.41467800 | -0.06626700 | -8.15931300 |
| C | 0.47962600 | -1.08549400 | -6.16978800 |
| C | -0.79409900 | 0.95370300 | -6.01513300 |
| C | -0.95704400 | 0.95564600 | -7.39142100 |
| C | 0.30487600 | -1.07953800 | -7.55206500 |
| H | -1.23728500 | 1.73859400 | -5.41256600 |
| H | -1.51258300 | 1.75582000 | -7.86583700 |
| H | 0.76061700 | -1.86483000 | -8.14289800 |
| H | -0.54065000 | -0.06376700 | -9.23526000 |
| C | 1.28413900 | -2.11574800 | -5.51490800 |
| H | 1.88830400 | -1.82139400 | -4.65218700 |
| C | -1.29150800 | -2.20227000 | -3.80973200 |
| H | -1.94188400 | -1.95571800 | -4.64813700 |
| N | -1.19186100 | -3.40413100 | -3.39627000 |
| N | 1.26513800 | -3.32088200 | -5.91379700 |
| O | 2.06244100 | -4.14065300 | -5.11625200 |
6-K^-a

H (353 K, 1 atm) = -1630.295581 a.u.
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| C       | 0.49995500 | -1.08919700| 6.17862400 |
| C       | -0.75263200| 0.96129100 | 6.00905100 |
| C       | -0.91438100| 0.97934000 | 7.38503500 |
| C       | 0.32664900 | -1.06622800| 7.56127700 |
| H       | -1.18996700| 1.74413500 | 5.39949900 |
| H       | -1.46123100| 1.78992800 | 7.85179700 |
| H       | 0.77537700 | -1.85103000| 8.15801800 |
| H       | -0.50628700| -0.02837300| 9.23734400 |
| C       | 1.29715700 | -2.13799900| 5.54357200 |
| H       | 1.92104400 | -1.86176100| 4.68965400 |
| C       | -1.24467500| -2.23051600| 3.81301300 |
| H       | -1.80732500| -2.02895400| 4.72354000 |
| N       | -1.19483200| -3.40877500| 3.32832300 |
| N       | 1.25758000 | -3.33475100| 5.96476300 |
| O       | 2.07105200 | -4.17943000| 5.22687600 |
| O       | -1.97135300| -4.29070700| 4.02802600 |
| C       | 1.92398900 | -5.51993100| 5.69024900 |
| H       | 2.84255900 | -5.83321700| 6.19658600 |
| H       | 1.10701900 | -5.54049300| 6.41188900 |
| C       | 1.65685500 | -6.42394700| 4.50747500 |
| H       | 2.52000200 | -6.42832000| 3.83402100 |
| H       | 1.52140400 | -7.45483800| 4.85678100 |
| C       | -1.82044100| -5.62237900| 3.56621900 |
| H       | -1.68573100| -5.63020000| 2.48031900 |
| H       | -2.76906900| -6.11036100| 3.79884200 |
| C       | -0.71229700| -6.37293900| 4.26105000 |
| H       | -0.85904500| -7.45072000| 4.11202800 |
| H       | -0.76638100| -6.16193100| 5.33484800 |
| O       | 0.54999800 | -5.99346800| 3.73576300 |
| K       | 1.38736100 | -3.83654500| 2.38247300 |
1-K$^+$-a

H (353 K, 1 atm) = -1630.276383 a.u.

| Atoms | x | y | z |
|-------|---|---|---|
| H     | 0.39744200 | 2.98583600 | -4.54078400 |
| C     | 0.17958200 | 2.84508200 | -3.48882700 |
| C     | -0.43748300 | 2.48419900 | -0.78037600 |
| C     | -0.32261000 | 1.63834800 | -3.04378900 |
| C     | 0.37320900 | 3.88287500 | -2.58694900 |
| C     | 0.05943400 | 3.69973200 | -1.25248100 |
| C     | -0.62831800 | 1.43446000 | -1.69329300 |
| H     | -0.52327400 | 0.83990200 | -3.74724400 |
| H     | 0.75929600 | 4.83729700 | -2.92478100 |
| H     | 0.21342800 | 4.50606400 | -0.54458300 |
| C     | -0.75218600 | 2.38087000 | 0.66128600 |
| C     | -1.39078200 | 2.31903600 | 3.38369400 |
| C     | -0.14693300 | 1.44022000 | 1.50730300 |
| C     | -1.66814800 | 3.28205500 | 1.20450000 |
| C     | -1.99193900 | 3.25221200 | 2.54897500 |
| C     | -0.47430600 | 1.42540500 | 2.86574300 |
| H     | -2.14024600 | 4.00483000 | 0.54874200 |
| H     | -2.70892100 | 3.96036600 | 2.94709800 |
| H     | 0.02035100 | 0.71144500 | 3.51222000 |
| H     | -1.62680700 | 2.29931700 | 4.44087900 |
| C     | 0.82022200 | 0.46909700 | 0.98638900 |
| H     | 1.42360800 | 0.71362400 | 0.11138500 |
| C     | -1.18336200 | 0.13388000 | -1.28700300 |
| H     | -1.85660700 | 0.08190000 | -0.43207800 |
| N     | -0.84898200 | -0.87158400 | -1.99520700 |
| N     | 0.88965400 | -0.65467000 | 1.57205400 |
| O     | 1.79459000 | -1.55296200 | 1.03487500 |
| O     | -1.37540300 | -2.12569500 | -1.81847500 |
| Atoms | X-Position | Y-Position | Z-Position |
|-------|------------|------------|------------|
| C     | 1.65749700 | -2.77723600 | 1.75918900 |
| H     | 2.65099200 | -3.09434700 | 2.08697100 |
| H     | 1.05564400 | -2.56680300 | 2.64239200 |
| C     | 1.03077000 | -3.87984300 | 0.90515700 |
| H     | 1.79372500 | -4.37510900 | 0.29662100 |
| H     | 0.61507200 | -4.64583100 | 1.57283700 |
| C     | -2.04674900 | -2.52763500 | -0.62596300 |
| H     | -2.54237300 | -3.44553100 | -0.94347400 |
| H     | -2.81898800 | -1.81554200 | -0.31984900 |
| C     | -1.08948400 | -2.80932200 | 0.52077900 |
| H     | -1.59122000 | -3.47832000 | 1.23216000 |
| H     | -0.81666000 | -1.89497400 | 1.05402400 |
| O     | 0.06572100 | -3.42939200 | -0.01968000 |
| K     | 1.47447000 | -2.21827100 | -2.00648400 |

**1-K^+-rac**

H (353 K, 1 atm) = -1630.244987 a.u.

| Atoms | X-Position | Y-Position | Z-Position |
|-------|------------|------------|------------|
| H     | -1.99102800 | 0.02926000 | 0.38543900 |
| C     | -1.46591100 | 0.00552500 | 1.33230600 |
| C     | -0.16022000 | -0.11441200 | 3.86996500 |
| C     | -0.96110500 | -1.17944900 | 1.82338000 |
| C     | -1.19853500 | 1.16280700 | 2.03856300 |
| C     | -0.56369100 | 1.08728200 | 3.26290500 |
| C     | -0.27171600 | -1.26212600 | 3.04083800 |
| H     | -1.03827100 | -2.08247700 | 1.23188500 |
| H     | -1.48012900 | 2.13210400 | 1.64466700 |
| H     | -0.36511000 | 2.02351100 | 3.76070500 |
| C     | 0.24849100 | -0.01350300 | 5.31605700 |
| C     | 0.94610600 | 0.57653700 | 8.03116400 |
| C     | 0.91867600 | -0.94848700 | 6.13502100 |
| C     | -0.14529400 | 1.16189200 | 5.98511900 |
| C     | 0.19535300 | 1.46669100 | 7.28740300 |
| Symbol | X          | Y          | Z          |
|--------|------------|------------|------------|
| C      | 1.26929500 | -0.63152700| 7.44967900 |
| H      | -0.78818800| 1.86711100 | 5.48318400 |
| H      | -0.14772200| 2.39896300 | 7.71998400 |
| H      | 1.79016500 | -1.38179500| 8.03385700 |
| H      | 1.23099000 | 0.79161000 | 9.05357400 |
| C      | 1.25580700 | -2.35395600| 5.82043400 |
| H      | 2.22544100 | -2.60396600| 5.38000700 |
| C      | 0.47133800 | -2.52130100| 3.17254400 |
| H      | 1.53808300 | -2.45373500| 3.38607700 |
| N      | -0.03682900 | -3.62787700| 2.80968300 |
| N      | 0.46284100 | -3.24817500| 6.23547600 |
| O      | 0.92278900 | -4.53857200| 6.02002700 |
| O      | 0.92445900 | -4.63470500| 2.68691200 |
| C      | -0.13936200| -5.43921400| 6.33410800 |
| H      | -0.29268900| -5.48101300| 7.41701400 |
| H      | -1.05631700| -5.06066300| 5.87908000 |
| C      | 0.22805000 | -6.81107500| 5.81883900 |
| H      | 1.06849800 | -7.22234900| 6.38523000 |
| H      | -0.62350800| -7.48501100| 5.97103600 |
| C      | 0.27517400 | -5.84956900| 2.32619800 |
| H      | 1.05920300 | -6.48701100| 1.90658000 |
| H      | -0.46625100| -5.65612300| 1.54801100 |
| C      | -0.37091600| -6.50863100| 3.51587200 |
| H      | -0.87851700| -7.43064900| 3.20926400 |
| H      | -1.11524600| -5.82486100| 3.93269700 |
| O      | 0.64475200 | -6.80330800| 4.46518800 |
| K      | 2.94391500 | -5.41485000| 4.33927000 |
1-K⁺-c

H (353 K, 1 atm) = -1630.290979 a.u.

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | -3.34910500 | 2.03371900 | -3.58457200 |
| C    | -2.68932100 | 2.13215000 | -2.73093500 |
| C    | -0.96473500 | 2.39636100 | -0.54015600 |
| C    | -1.63520100 | 1.25550300 | -2.56919200 |
| C    | -2.88684000 | 3.14990400 | -1.80632800 |
| C    | -2.02970700 | 3.27800200 | -0.72832200 |
| C    | -0.76519400 | 1.37217500 | -1.48173400 |
| H    | -1.45287100 | 0.47643600 | -3.29902600 |
| H    | -3.70861600 | 3.84574200 | -1.92710300 |
| H    | -2.19107700 | 4.06361600 | 0.00101600  |
| C    | -0.09144700 | 2.59583800 | 0.63878600  |
| C    | 1.57163600  | 3.09544000 | 2.83849800  |
| C    | 0.14144700  | 1.59583800 | 2.83849800  |
| C    | 0.51802300  | 3.83838700 | 0.81339000  |
| C    | 1.34273500  | 4.08914100 | 1.89578800  |
| C    | 0.97232200  | 1.85983300 | 2.68838800  |
| H    | 0.35007800  | 4.60992000 | 0.07067900  |
| H    | 1.80495500  | 5.06294100 | 2.00621800  |
| H    | 1.11286900  | 1.08762500 | 3.43492300  |
| H    | 2.20258000  | 3.29115400 | 3.69718700  |
| C    | -0.49407400 | 0.28066100 | 1.47603400  |
| H    | -1.48736600 | 0.21828200 | 1.03464900  |
| C    | 0.34973800  | 0.43392300 | -1.34392000 |
| H    | 1.23688300  | 0.73669000 | -0.78640200 |
| N    | 0.24874400  | -0.72748100| -1.84975000 |
| N    | 0.15567400  | -0.73899400| 1.87359700  |
| O    | -0.39587000 | -1.99867600| 1.77180700  |
| O    | 1.35915500  | -1.52546900| 1.61681300  |
C       -1.43637600    -2.27077600    0.82853300
H       -2.41901200    -2.18690600    1.30375800
H       -1.37864800    -1.57578200    -0.01475900
C       -1.16320300    -3.68008400    0.35230600
H       -1.06831900    -4.34964400    1.21019900
H       -1.99462500    -4.03982000   -0.26240400
C        1.15327000    -2.77828400   -2.26858500
H        2.06838000    -3.34729200   -2.08260400
H        1.06083600    -2.62769700   -3.34809200
C       -0.06206700    -3.50893600   -1.75501500
H       -0.15849100    -4.46398600   -2.28544000
H       -0.94840600    -2.90526100   -1.96723000
O        0.06325500    -3.73709900   -0.35955900
K       2.16841100    -2.38602300    0.99669400

1-K^+-d

H (353 K, 1 atm) = -1630.295581 a.u.

H      0.34424000    -0.08813800   -0.03552900
C      0.28051200    -0.10206700   -1.11734000
C      0.04511300    -0.09936700   -3.90990700
C     -0.39798700   -1.12438500   -1.75897000
C      0.83254800    0.93057200   -1.86392400
C      0.70347700    0.93194500   -3.24358700
C     -0.51324100   -1.14588300   -3.15332100
H     -0.90759600   -1.88921700   -1.18171200
H      1.35097700    1.74366800   -1.36981500
H      1.13343300    1.73784300   -3.82768100
C     -0.05940600   -0.07330400   -5.38745900
C     -0.38191400   -0.04106300   -8.16124400
C      0.49995500   -1.08919700   -6.17862400
2-Li$^+$-a

H (353 K, 1 atm) = -1191.711135 a.u.

H  -4.69179500  2.23069700  2.18453200
C  -3.60972800  2.18012100  2.19113200
C  -0.80921400  2.03916300  2.22477300
C  -2.96928400  1.03547800  1.76240200
C  -2.85971000  3.25987300  2.64065200
C  -1.47887200  3.18486000  2.65679600
C  -1.57475500  0.94871200  1.77545800
H  -3.54135600  0.17929900  1.42699500
H  -3.35307800  4.16359000  2.97844400
H  -0.89592000  4.03552800  2.99043700
C  0.67039200  2.03296400  2.27480300
C  3.46505200  2.06893700  2.50419400
C  1.48260000  1.71845600  1.17101600
C  1.39094000  2.43655700  3.79271000
C  2.66865900  2.38522500  3.59789300
C  2.87358800  1.73834800  1.30208900
H  0.67210000  2.59654900  4.33916700
H  3.12336800  2.64516100  4.54652100
H  3.48175400  1.50782100  0.43618500
H  4.54475300  2.08958500  2.58957800
C -0.92276200 -0.28276000  1.33455100
H  0.07764500 -0.52015600  1.69594300
C  0.88270800  1.38416100 -0.11911200
H  -0.12135200  1.73792700 -0.35256800
N -1.51291800 -1.05324500  0.51128400
N  1.52258300  0.66008200 -0.94733800
O -0.68421900 -2.13722500  0.14294800
2-Li$^2$-b

H (353 K, 1 atm) = -1191.705465 a.u.
| Atom | x     | y     | z      |
|------|-------|-------|--------|
| C    | -1.46085500 | 0.66281300 | -2.13161200 |
| H    | -2.98329300  | -0.73513400 | -2.68834800 |
| H    | -1.32173200  | 1.57913200  | -5.88271500 |
| H    | 0.16333000   | 2.71278300  | -4.28374800 |
| C    | 0.34073800   | 2.40826000  | -1.66772400 |
| C    | 1.97673600   | 3.98331500  | -0.01500800 |
| C    | 1.24560100   | 1.80907700  | -0.77099300 |
| C    | 0.28702200   | 3.80189600  | -1.71309400 |
| C    | 1.09040000   | 4.58234600  | -0.90094000 |
| C    | 2.05015600   | 2.60669400  | 0.04687100  |
| H    | -0.41740900  | 4.27457000  | -2.38763200 |
| H    | 1.02377600   | 5.66238900  | -0.95853200 |
| H    | 2.75242400   | 2.12392000  | 0.71534100  |
| H    | 2.61410900   | 4.59037000  | 0.61635400  |
| C    | -1.50591200  | 0.30723900  | -0.72007800 |
| H    | -1.04987900  | 0.98417300  | 0.00046500  |
| C    | 1.36523900   | 0.35668400  | -0.69943400 |
| H    | 1.09801600   | -0.24433600 | -1.56941800 |
| N    | -2.00751000  | -0.79143400 | -0.31406400 |
| N    | 1.74871800   | -0.21633100 | 0.37357800  |
| O    | -1.71002800  | -0.95085500 | 1.05743200  |
| O    | 1.70931400   | -1.62132600 | 0.21565800  |
| C    | 2.81591500   | -2.22413200 | 0.88540600  |
| H    | 2.75428600   | -3.27494800 | 0.59811000  |
| H    | 3.75586800   | -1.80639900 | 0.51633700  |
| C    | 2.71943900   | -2.08424500 | 2.38675900  |
| H    | 3.46836000   | -2.72511700 | 2.86573800  |
| H    | 2.88401600   | -1.04867500 | 2.70490800  |
| O    | 1.40692500   | -2.49566500 | 2.72495100  |
| C    | 1.06287000   | -2.47303000 | 4.09937500  |
| H    | 1.67684300   | -3.17815800 | 4.66976200  |
| H    | 1.20865700   | -1.46565000 | 4.50961700  |
| C    | -0.38948400  | -2.87180700 | 4.15360800  |
H    -0.50332000   -3.90320100    3.79772200
H    -0.77741900   -2.80598400    5.17532200
O    -1.07934700   -1.98367300    3.29019200
C    -2.31254300   -2.46423500    2.78077600
H    -2.14676000   -3.41902700    2.26358500
H    -3.04004300   -2.62726500    3.58373300
C    -2.82284400   -1.41654800    1.81834900
H    -3.25335100   -0.56218800    2.34781300
H    -3.57250900   -1.84003700    1.14757900
Li    0.07529600  -1.55360100    1.63159500

2-Li⁺-rac

H (353 K, 1 atm) = -1191.668668 a.u.

H    -3.90562900   -0.63999600    2.51147300
C    -2.97024500   -0.37002700    2.98571200
C    -0.46795800    0.27694400    4.21469100
C    -2.30647000  -1.27218300    3.79066900
C    -2.43519100    0.89654200    2.86082800
C    -1.23489400    1.19573600    3.47280700
C    -1.09312400   -0.97589000    4.42095500
H    -2.74209600   -2.24912700    3.96176600
H    -2.95291000    1.66680700    2.30182600
H    -0.89979800    2.21825000    3.39824200
C    0.84420400    0.81367000    4.71820900
C    2.99778800    2.38050000    5.74533500
C    1.62172100    0.37574600    5.81947600
C    1.33594600    1.96040000    4.07317900
C    2.37616000    2.72897600    4.55974500
C    2.63937700    1.18778100    6.33549800
H    0.89885800    2.26822400    3.13544300
H    2.69680600    3.60143800    4.00293100
|  | X             | Y             | Z             |
|---|---------------|---------------|---------------|
| H | 3.19387600    | 0.81744900    | 7.18843300    |
| H | 3.79391300    | 2.98433900    | 6.16278200    |
| C | -0.70651300   | -2.09176600   | 5.32142000    |
| H | 0.03308900    | -2.84262700   | 5.04204800    |
| C | 1.65502800    | -0.99130800   | 6.32654200    |
| H | 1.60217300    | -1.79777700   | 5.60100000    |
| N | -1.43514900   | -2.23428900   | 6.34855100    |
| N | 1.95438500    | -1.27182100   | 7.53151900    |
| O | -1.13353300   | -3.39679000   | 7.08787500    |
| O | 2.13460200    | -2.68008500   | 7.65166200    |
| C | 3.18705800    | -2.95020000   | 8.58083300    |
| H | 3.53902700    | -3.94997300   | 8.31839600    |
| H | 4.00049500    | -2.23660200   | 8.44299100    |
| C | 2.66835700    | -2.93492200   | 9.99617100    |
| H | 3.44173000    | -3.28028600   | 10.69146100   |
| H | 2.35058200    | -1.92673800   | 10.28881400   |
| O | 1.55776600    | -3.81560400   | 9.98463200    |
| C | 0.79203300    | -3.89793900   | 11.17288600   |
| H | 1.34258300    | -4.41719400   | 11.96435300   |
| H | 0.53129700    | -2.89169100   | 11.52427100   |
| C | -0.44883300   | -4.66358600   | 10.79237200   |
| H | -0.18848700   | -5.69095300   | 10.50899900   |
| H | -1.16290000   | -4.69442900   | 11.62161100   |
| O | -0.99468000   | -3.97720200   | 9.67769900    |
| C | -1.95546600   | -4.68207500   | 8.91375200    |
| H | -1.52868300   | -5.62693800   | 8.55116500    |
| H | -2.84755000   | -4.91234000   | 9.50681000    |
| C | -2.33360000   | -3.77203500   | 7.77949500    |
| H | -2.80867800   | -2.86265000   | 8.15308300    |
| H | -3.01516600   | -4.27682800   | 7.08981900    |
| Li| 0.40317800    | -3.34871900   | 8.41328800    |
2-Li\(^+\)-c

H (353 K, 1 atm) = -1191.711135 a.u.

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| H    | -4.69179500 | 2.23069700 | -2.18453200 |
| C    | -3.60972800 | 2.18012100 | -2.19113200 |
| C    | -0.80921400 | 2.03916300 | -2.22477300 |
| C    | -2.96928400 | 1.03547800 | -1.76240200 |
| C    | -2.85971000 | 3.25987300 | -2.64065200 |
| C    | -1.47887200 | 3.18486000 | -2.65679600 |
| C    | -1.57475500 | 0.94871200 | -1.77545800 |
| H    | -3.54135600 | 0.17929900 | -1.42699500 |
| H    | -3.35307800 | 4.16359000 | -2.97844400 |
| H    | -0.89592000 | 4.03552800 | -2.99043700 |
| C    | 0.67039200  | 2.03296400 | -2.27480300 |
| C    | 3.46505200  | 2.06893700 | -2.50419400 |
| C    | 1.48260000  | 1.71845600 | -1.17101600 |
| C    | 1.29090400  | 2.36755700 | -3.47927100 |
| C    | 2.66865900  | 2.38522500 | -3.59789300 |
| C    | 2.87358800  | 1.73834800 | -1.30208900 |
| H    | 0.67210000  | 2.59654900 | -4.33916700 |
| H    | 3.12336800  | 2.64516100 | -4.54652100 |
| H    | 3.48175400  | 1.50782100 | -0.43618500 |
| H    | 4.54475300  | 2.08958500 | -2.58957800 |
| C    | -0.92276200 | -0.28276000 | -1.33455100 |
| H    | 0.07764500  | -0.52015600 | -1.69594300 |
| C    | 0.88270800  | 1.38416100 | 0.11911200 |
| H    | -0.12135200 | 1.73792700 | 0.35256800 |
| N    | -1.51291800 | -1.05324500 | -0.51128400 |
| N    | 1.52258300  | 0.66008200 | 0.94733800 |
| O    | -0.68421900 | -2.13722500 | -0.14294800 |
| O    | 0.73979400  | 0.37777300 | 2.08979700 |
C      1.59069700  0.35649200  3.23869600
H      2.57962800  0.01011600  2.92844300
H      1.67695200  1.36309500  3.65719400
C      0.98482200 -0.59275300  4.23328000
H      1.63773800 -0.68073400  5.10873100
H     -0.00195700 -0.24706900  4.56798400
O      0.86177900 -1.83232000  3.55916800
C      0.23148800 -2.87329200  4.28440600
H      0.86414600 -3.21816900  5.10917300
H     -0.72302800 -2.51974600  4.69428900
C     -0.00072800 -3.97970500  3.28980900
H      0.95575000 -4.39366600  2.94646700
H     -0.59463700 -4.78481100  3.73535300
O     -0.68643400 -3.38111700  2.20428300
C     -0.82629800 -4.17924300  1.04259400
H      0.15961900 -4.51687100  0.69732100
H     -1.44636700 -5.06079200  1.23965000
C     -1.49513500 -3.82270500 -0.93518100
C     -1.59931700 -3.30328100  0.02146900
C     -2.48236800 -2.98993300  0.36989900
H     -2.74942600  1.19670600  1.54570500
C     -2.94922100  3.49898000  2.18393700
C     -1.38478900  3.33590500  2.35499200

2-Na\textsuperscript{+}-a

H (353 K, 1 atm) = -1346.398884 a.u.
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -1.57408200 | 1.02068100 | 1.71707200 |
| H       | -3.55492700 | 0.34531600 | 1.26011000 |
| H       | -3.20384300 | 4.46438000 | 2.37290700 |
| H       | -0.76999100 | 4.17483000 | 2.66066000 |
| C       | 0.69150200  | 1.97721500 | 2.26530900 |
| C       | 3.44808200  | 1.66914800 | 2.62084900 |
| C       | 1.51969300  | 1.67228100 | 1.17138600 |
| C       | 1.27033600  | 2.14502800 | 3.52029700 |
| C       | 2.63485700  | 1.99102100 | 3.70043500 |
| C       | 2.89444700  | 1.51724100 | 1.36465100 |
| H       | 0.63240000  | 2.37958400 | 4.36482200 |
| H       | 3.06569800  | 2.12224200 | 4.68600900 |
| H       | 3.52312700  | 1.30346700 | 0.50886400 |
| H       | 4.51657500  | 1.55519700 | 2.75832100 |
| C       | -0.97132800 | -0.29915800| 1.54847600 |
| H       | -0.04617400 | -0.52937600| 2.07920800 |
| C       | 0.94724700  | 1.58289100 | -0.16950300|
| H       | 0.01509900  | 2.10858600 | -0.38240800|
| N       | -1.51763900 | -1.17647800| 0.79967900 |
| N       | 1.52768400  | 0.90835400 | -1.08435200|
| O       | -0.76969800 | -2.35750700| 0.76390000 |
| O       | 0.80439000  | 0.93845100 | -2.28078000|
| C       | 1.64148000  | 0.57981800 | -3.38374200|
| H       | 2.59354900  | 0.21512300 | -2.99342400|
| H       | 1.82245700  | 1.46962200 | -3.99286100|
| C       | 0.96254200  | -0.48383800| -4.20314000|
| H       | 1.57328100  | -0.70269400| -5.08797200|
| H       | -0.02382500 | -0.14171300| -4.54448100|
| O       | 0.82573700  | -1.63407200| -3.38993400|
| C       | 0.14499600  | -2.71369300| -4.00197100|
| H       | 0.70558100  | -3.08593500| -4.86790000|
| H       | -0.84427000 | -2.38857600| -4.34446300|
| C       | 0.00714900  | -3.81034800| -2.98013900|
Supplementary Material

2-Na⁺-b

H (353 K, 1 atm) = -1346.394968 a.u.

H  -2.44870600  -1.01653100  -4.77223400
C  -1.89752800  -0.32147400  -4.15045700
C  -0.47791900  1.48048800  -2.55385600
C  -2.10192000  -0.30641800  -2.78420100
C  -1.00111800  0.57038300  -4.72651700
C  -0.29922100  1.46394700  -3.93298700
C  -1.40321300  0.59231200  -1.97644700
H  -2.82437900  -0.97181800  -2.32704400
H  -0.84742900  0.56881200  -5.79917600
H  0.41275600  2.14801800  -4.38059300
C  0.31734200  2.40225600  -1.70681100
C  1.70294100  4.14333100  -0.01354200
C  1.28718900  1.90755500  -0.81666300
C  0.07935400  3.77174000  -1.74909400
C  0.76416300  4.63725000  -0.91015800
C  1.96845100  2.78731900  0.02693300
H  -0.66827000  4.15476900  -2.43436700
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 0.56378800 | 5.70117800 | -0.95582600 |
| H    | 2.73352900 | 2.39560500 | 0.68677600 |
| H    | 2.24330200 | 4.82023600 | 0.63716300 |
| C    | -1.65897200 | 0.67741700 | -0.54411400 |
| H    | -1.41804300 | 1.61397500 | -0.03651100 |
| C    | 1.62611600 | 0.48777500 | -0.84467600 |
| H    | 1.48966100 | -0.06419100 | -1.77581300 |
| N    | -2.15024900 | -0.28918400 | 0.12965300 |
| N    | 2.08751200 | -0.12095600 | 0.17989600 |
| O    | -2.25093000 | 0.07922900 | 1.47777500 |
| O    | 2.33550200 | -1.45296600 | -0.11994000 |
| C    | 3.22818400 | -2.05535700 | 0.80440100 |
| H    | 3.33080200 | -3.07119500 | 0.42085800 |
| H    | 4.20606200 | -1.56389900 | 0.77196200 |
| C    | 2.72747200 | -2.08972900 | 2.23250200 |
| H    | 3.35704500 | -2.78792400 | 2.79754500 |
| H    | 2.80931700 | -1.10525500 | 2.71167500 |
| O    | 1.37912500 | -2.51703300 | 2.21964600 |
| C    | 0.87467100 | -2.98029100 | 3.45839100 |
| H    | 1.39227300 | -3.89576100 | 3.76840700 |
| H    | 1.01447300 | -2.22307300 | 4.24239000 |
| C    | -0.59027800 | -3.26246500 | 3.26011100 |
| H    | -0.71688500 | -3.98920400 | 2.44750200 |
| H    | -1.02278300 | -3.68261100 | 4.17559200 |
| O    | -1.22472200 | -2.04088700 | 2.92497100 |
| C    | -2.52341100 | -2.18478300 | 2.37808900 |
| H    | -2.47070400 | -2.72013500 | 1.42169200 |
| H    | -3.17337100 | -2.75349200 | 3.05478400 |
| C    | -3.10759200 | -0.80519500 | 2.19408100 |
| H    | -3.23323400 | -0.31489400 | 3.16068900 |
| H    | -4.07946900 | -0.87235600 | 1.69861900 |
| Na   | 0.06673400 | -0.71574200 | 1.49988200 |
2-Na\textsuperscript{+}-rac

H (353 K, 1 atm) = -1346.346631 a.u.

\begin{align*}
\text{H} & : -3.95382200 \quad -0.56749800 \quad 2.56726700 \\
\text{C} & : -3.00891700 \quad -0.31995600 \quad 3.03477000 \\
\text{C} & : -0.47003900 \quad 0.26011500 \quad 4.23413000 \\
\text{C} & : -2.36049300 \quad -1.23704100 \quad 3.83377700 \\
\text{C} & : -2.44069600 \quad 0.93048700 \quad 2.90287000 \\
\text{C} & : -1.22562200 \quad 1.19598800 \quad 3.50127400 \\
\text{C} & : -1.13035900 \quad -0.97688600 \quad 4.45314100 \\
\text{H} & : -2.81459700 \quad -2.20456400 \quad 4.00336400 \\
\text{H} & : -2.94079900 \quad 1.71513500 \quad 2.34780800 \\
\text{H} & : -0.87314000 \quad 2.21121200 \quad 3.42119200 \\
\text{C} & : 0.85516900 \quad 0.77664400 \quad 4.73446200 \\
\text{C} & : 2.99190600 \quad 2.34626000 \quad 5.80849500 \\
\text{C} & : 1.66686000 \quad 0.29996700 \quad 5.79819500 \\
\text{C} & : 1.32770900 \quad 1.95633700 \quad 4.13375300 \\
\text{C} & : 2.35629500 \quad 2.72664100 \quad 4.64129000 \\
\text{C} & : 2.66958900 \quad 1.11702400 \quad 6.34096200 \\
\text{H} & : 0.88281200 \quad 2.29573400 \quad 3.21161400 \\
\text{H} & : 2.65482300 \quad 3.62545200 \quad 4.11499800 \\
\text{H} & : 3.25134300 \quad 0.71678500 \quad 7.16134900 \\
\text{H} & : 3.77669400 \quad 2.94908300 \quad 6.24814900 \\
\text{C} & : -0.76192300 \quad -2.09728200 \quad 5.34704800 \\
\text{H} & : 0.09296100 \quad -2.74766800 \quad 5.17009600 \\
\text{C} & : 1.79498900 \quad -1.09068600 \quad 6.22707400 \\
\text{H} & : 1.82664600 \quad -1.86053500 \quad 5.45790700 \\
\text{N} & : -1.61881400 \quad -2.38494300 \quad 6.24469100 \\
\text{N} & : 2.10518800 \quad -1.40591600 \quad 7.42596300 \\
\text{O} & : -1.29020300 \quad -3.53691700 \quad 6.96371500 \\
\end{align*}
2-Na⁺-c

H (353 K, 1 atm) = -1346.398884 a.u.

|   | 2.40746500 | -2.77649900 | 7.50780900 |
|---|-------------|-------------|------------|
| C | 3.31011300  | -3.03366300 | 8.58138500 |
| H | 3.61583000  | -4.06754200 | 8.41491600 |
| H | 4.18626000  | -2.38474800 | 8.50339000 |
| C | 2.67800900  | -2.90067400 | 9.94985200 |
| H | 3.38747900  | -3.25908000 | 10.70605900|
| H | 2.44077600  | -1.85243800 | 10.18006000|
| O | 1.50429100  | -3.68585900 | 9.92965100 |
| C | 0.74798400  | -3.74803700 | 11.12150500|
| H | 1.30925600  | -4.24094100 | 11.92413800|
| H | 0.48001900  | -2.73829400 | 11.46635100|
| C | -0.48733700 | -4.54940700 | 10.79391000|
| H | -0.18564800 | -5.55205100 | 10.46977000|
| H | -1.12844600 | -4.64460200 | 11.67706000|
| O | -1.17781500 | -3.89253900 | 9.74165300 |
| C | -1.94689800 | -4.74663800 | 8.91204800 |
| H | -1.33483900 | -5.59631700 | 8.58323600 |
| H | -2.81743800 | -5.13894300 | 9.45138700 |
| C | -2.42867800 | -3.95803600 | 7.72552300 |
| H | -2.98779500 | -3.07361100 | 8.04091900 |
| H | -3.07683200 | -4.58077600 | 7.10247600 |
| Na| 0.16516500  | -2.52206900 | 8.43112100 |

H     -4.60125300  2.55179500  -1.64363100
C     -3.53261100  2.42814200  -1.77120000
C     -0.77590500  2.10728500  -2.11425000
C     -2.94922100  1.19670600  -1.54570500
C     -2.74942600  3.49898000  -2.18393700
C     -1.38478900  3.33590500  -2.35499200
C     -1.57408200   1.02068100   -1.71707200
H     -3.55492700   0.34531600   -1.26011000
H     -3.20384300   4.46438000   -2.37290700
H     -0.76999100   4.17483000   -2.66066000
C      0.69150200   1.97721500   -2.26530900
C      3.44808200   1.66914800   -2.62084900
C      1.51969300   1.67228100   -1.17138600
C      1.27033600   2.14502800   -3.52029700
C      2.63485700   1.99102100   -3.70043500
C      2.89444700   1.51724100   -1.36465100
H      0.63240000   2.37958400   -4.36482200
H      3.06569800   2.12224200   -4.68600900
H      3.52312700   1.30346700   -0.50886400
H      4.51657500   1.55519700   -2.75832100
C     -0.97132800   -0.29915800   -1.54847600
H     -0.04617400   -0.52937600   -2.07920800
C      0.94724700   1.58289100    0.16950300
H      0.01509900   2.10858600    0.38240800
N     -1.51763900   -1.17647800   -0.79967900
N      1.52768400    0.90835400    1.08435200
O     -0.76969800   -2.35750700   -0.76390000
O      0.80439000   0.93845100    2.28078000
C      1.64148000   0.57981800    3.38374200
H      2.59354900   0.21512300    2.99342400
H      1.82245700   1.46962200    3.99286100
C      0.96254200   -0.48383800    4.20314000
H      1.57328100   -0.70269400    5.08797200
H     -0.02382500   -0.14171300    4.54448100
O      0.82573700   -1.63407200    3.38993400
C      0.14499600   -2.71369300    4.00197100
H      0.70558100   -3.08593500    4.86790000
H     -0.84642700   -2.38857600    4.34446300
C     0.00714900   -3.81034800    2.98013900

Supplementary Material
H                  0.99894000   -4.15228200    2.65553900
H                 -0.52460300   -4.66113200    3.42292900
O                 -0.71135700   -3.28799800    1.87813500
C                 -0.85541400   -4.18045900    0.78917000
H                 0.13049000   -4.52412700    0.44804100
H                -1.44167000   -5.06054000    1.08170700
C                -1.57512900   -3.44946600   -0.31144400
H                -2.52687500   -3.05377800    0.04829800
H                -1.76296000   -4.12155400   -1.15320000
Na               0.02824300   -1.16707700   1.24826400

2-K'-a

H (353 K, 1 atm) = -1783.971162 a.u.

H                  1.16067000    3.16447000   -3.56244200
C                  1.09968100    3.19223300   -2.48113300
C                  0.93556900    3.26963600    0.30577500
C                  0.57336500    2.11647100   -1.79274600
C                 1.53042700    4.31604700   -1.78669700
C                 1.44539100    4.35237800   -0.40467100
C                 0.48232400    2.14252100   -0.40000600
H                  0.20392700    1.24846700   -2.32515800
H                 1.93387400    5.16627300   -2.32381700
H                 1.79440900    5.22222800    0.14024500
C                 0.88967200    3.31619000   1.78674800
C                  0.70038400    3.38050600    4.57675800
C                 1.68063900    2.45779800    2.56983000
C                  0.03171500    4.20909400    2.42292200
C                -0.06922500    4.24114400    3.80422900
C                 1.57550000    2.50372100    3.96319900
H                -0.57622000    4.87165000    1.81733700
H                -0.74529800    4.94213500    4.27926200
H   2.22606800  1.87322600  4.55849500
H   0.63776000  3.41546600  5.65792700
C   2.65264100  1.57405400  1.92759600
H   3.03576200  1.83203400  0.94066000
C  -0.12883900  1.04027700  0.33510000
H  -0.50966800  1.24557100  1.33762200
N  -0.24000300 -0.12517100 -0.16195200
N   3.06066600  0.51846300  2.51628800
O   3.99415600 -0.16082200  1.76578700
O  -0.86203100 -0.99145500  0.73143100
C   4.71487500 -1.10577800  2.54776500
H   5.77858100 -0.89849700  2.40116300
H   4.47771100 -0.96308200  3.60446000
C   4.42600600 -2.51622100  2.11550100
H   4.49915500 -2.58073500  1.02275200
H   5.18127000 -3.18504500  2.54928000
C  -1.13846100 -2.22929900  0.08489600
H  -1.71582500 -2.05168800 -0.82622400
H  -1.76103500 -2.77718500  0.79535400
C   0.10561900 -3.00959200 -0.24428600
H  -0.18554800 -3.94598900 -0.73892500
H   0.73724500 -2.43624700 -0.93351400
O   0.81137400 -3.27913600  0.95218400
O   3.13643800 -2.90256600  2.55691400
C   2.71751100 -4.15921000  2.04915900
H   3.57182200 -4.83584500  1.93504400
H   2.04741000 -4.59669000  2.79458200
C   1.99078200 -4.02576800  0.73540600
H   2.62246400 -3.52223900 -0.00933600
H   1.74807500 -5.02510300  0.34924300
K   0.93649700 -1.30554500  2.91674300
2-K$^{+}$-b

H (353 K, 1 atm) = -1783.963867 a.u.

H  -2.38043000  -1.04782100  -4.95358700
C  -1.84259600  -0.36788900  -4.30392700
C  -0.46060300   1.39280200  -2.63413200
C  -2.12661900  -0.33659700  -2.95219400
C  -0.88179300   0.48634400  -4.83027800
C  -0.19805900   1.35985300  -3.99941900
C  -1.44552000   0.54070600  -2.10703100
H  -2.89417700  -0.97683000  -2.53448700
H  -0.66461500   0.47263300  -5.89178600
H   0.56096100   2.01798200  -4.40697700
C   0.31414400   2.30167200  -1.75017600
C   1.68223700   4.02873600  -0.02653900
C   1.32873000   1.80733500  -0.91153800
C   0.01837800   3.66109300  -1.72161500
C   0.69041400   4.51995600  -0.86596100
C   2.00542400   2.68445100  -0.05763700
H  -0.76119400   4.04126800  -2.37207500
H   0.44495600   5.57534200  -0.85945500
H   2.81924500   2.30145500   0.54789600
H   2.22303900   4.70076700   0.62923800
C  -1.76613200   0.62480100  -0.68707200
H  -1.50573500   1.54881000  -0.16454200
C   1.69479000   0.39319200  -0.97411400
H   1.47635400  -0.17000500  -1.88137600
N  -2.34042300  -0.31982900  -0.05453300
N   2.25455700  -0.18892800   0.01470900
O  -2.51610200   0.02229600   1.28175700
O   2.50927500  -1.50679300  -0.26802300
2-K\textsuperscript{+}-rac

H (353 K, 1 atm) = -1783.915733 a.u.
C  -1.12703100  -0.94578800  4.48647400
H  -2.83022200  -2.16405000  4.08402000
H  -3.04323900   1.81464300  2.57767900
H  -0.92528200   2.28035300  3.56038200
C   0.85535100   0.79187300  4.77937100
C   3.06277500   2.25262700  5.86062600
C   1.70678300   0.22784900  5.76514400
C   1.30243000   2.01841400  4.25753200
C   2.36496000   2.73702100  4.76987000
C   2.75034900   0.98827800  6.31219300
H   0.81188500   2.43983300  3.39447700
H   2.64243700   3.67639800  4.30670000
H   3.36760800   0.51868000  7.06763300
H   3.88149900   2.80867300  6.30038100
C  -0.68515100  -2.11165700  5.28422100
H   0.10330300  -2.78746100  4.96041100
C   1.80398600  -1.19083100  6.12355100
H   1.85082300  -1.92411400  5.32136200
N  -1.40537100  -2.40802900  6.29127600
N   2.06150100  -1.55938400  7.31690900
O  -0.98668500  -3.56702100  6.93129200
O   2.31626400  -2.91662600  7.37884800
C   3.13948100  -3.23643700  8.48952400
H   3.29150200  -4.31229600  8.39272400
H   4.10907200  -2.73388100  8.40416100
C   2.53127300  -2.92649600  9.83583200
H   3.20614000  -3.30739300 10.61472400
H   2.43972000  -1.84017200  9.98536900
O   1.27181700  -3.54885400  9.89971000
C   0.60034100  -3.42764900 11.12615500
H   1.19039900  -3.83574500 11.95798300
H   0.41046500  -2.36609300 11.36743100
C  -0.69781900  -4.19137100 10.99891500
H (353 K, 1 atm) = -1783.965614 a.u.
2-K⁺-d

H (353 K, 1 atm) = -1783.971162 a.u.

\[
\begin{array}{ccc}
\text{H} & 1.16067000 & 3.16447000 & 3.56244200 \\
\text{C} & 1.09968100 & 3.19223300 & 2.48113300 \\
\text{C} & 0.93556900 & 3.26963600 & -0.30577500 \\
\text{C} & 0.57336500 & 2.11647100 & 1.79274600 \\
\text{C} & 1.53042700 & 4.31604700 & 1.78669700 \\
\text{C} & 1.44539100 & 4.35237800 & 0.40467100 \\
\text{C} & 0.48232400 & 2.14252100 & 0.40000600 \\
\text{H} & 0.20392700 & 1.24846700 & 2.32515800 \\
\text{H} & 1.93387400 & 5.16627300 & 2.32381700 \\
\text{H} & 1.79440900 & 5.2222800 & -0.14024500 \\
\text{C} & 0.88967200 & 3.31619000 & -1.78674800 \\
\text{C} & 0.70038400 & 3.38050600 & -4.57675800 \\
\text{C} & 1.68063900 & 2.45779800 & -2.56983000 \\
\text{C} & 0.03171500 & 4.20909400 & -2.42292200 \\
\text{C} & -0.06922500 & 4.24114400 & -3.80422900 \\
\text{C} & 1.57550000 & 2.50372100 & -3.96319900 \\
\text{H} & -0.57622000 & 4.87165000 & -1.81733700 \\
\text{H} & -0.74529800 & 4.94213500 & -4.27926200 \\
\text{H} & 2.22606800 & 1.87322600 & -4.55849500 \\
\text{H} & 0.63776000 & 3.41546600 & -5.65792700 \\
\text{C} & 2.65264100 & 1.57405400 & -1.92759600 \\
\text{H} & 3.03576200 & 1.83203400 & -0.94066000 \\
\text{C} & -0.12883900 & 1.04027700 & -0.33510000 \\
\text{H} & -0.50966800 & 1.24557100 & -1.33762200 \\
\text{N} & -0.24000300 & -0.12517100 & 0.16195200 \\
\text{N} & 3.06066600 & 0.51846300 & -2.51628800 \\
\text{O} & 3.99415600 & -0.16082200 & -1.76578700 \\
\end{array}
\]
3-Li²⁻-a

H (353 K, 1 atm) = -1345.380076 a.u.
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -0.60823500| 3.33562500 | -0.35949300|
| H       | -1.22203600| 3.23228200 | -2.40506100|
| H       | 0.02458300  | 7.09309900 | -1.02504800|
| H       | 0.46020100  | 6.14609800 | 1.21390100  |
| C       | 0.19343900  | 3.59023400 | 1.99709500  |
| C       | 0.70669100  | 2.45023900 | 4.50257500  |
| C       | 1.14025300  | 2.55864100 | 2.13146600  |
| C       | -0.46476900 | 4.04585800 | 3.13551100  |
| C       | -0.21602400 | 3.48141400 | 4.37582400  |
| C       | 1.38581900  | 1.99910300 | 3.38745400  |
| H       | -1.19841600 | 4.83741100 | 3.03445900  |
| H       | -0.74360500 | 3.84747900 | 5.24874500  |
| H       | 2.15337300  | 1.23994500 | 3.48692500  |
| H       | 0.91030200  | 2.01759500 | 5.47463500  |
| C       | 1.93375800  | 2.15652700 | 0.97554100  |
| H       | 2.09523300  | 2.87525300 | 0.17285600  |
| C       | -0.92575600 | 1.93889000 | -0.06591400|
| H       | -1.27899000 | 1.68053400 | 0.93309900  |
| N       | -0.79441700 | 1.03184800 | -0.94541000 |
| N       | 2.46722500  | 1.00376600 | 0.88738900  |
| O       | 3.23038500  | 0.88402300 | -0.29250600 |
| O       | -1.21400900 | -0.19085100| -0.45843900 |
| C       | 4.56873400  | 0.51594300 | 0.01779900  |
| H       | 5.15005400  | 0.80489800 | -0.86053600 |
| H       | 4.92335700  | 1.09674700 | 0.87474900  |
| C       | 4.76725200  | -0.95903900| 0.26096600  |
| H       | 4.43117500  | -1.54181800| -0.60705700 |
| H       | 5.83721300  | -1.14935000| 0.41282500  |
| C       | -0.86915500 | -1.20760800| -1.37150300 |
| H       | -1.12230700 | -0.91024100| -2.39410300 |
| H       | -1.49637300 | -2.05946500| -1.10005500 |
| C       | 0.60131500  | -1.55492400| -1.32028100 |
| H       | 0.80336200  | -2.37404500| -2.02232200 |
H                  1.19946000   -0.68902900   -1.60817800
O                  1.06440400   -1.91982000   -0.02224000
O                  4.03248600   -1.34678300    1.41011900
C                  1.32445400   -3.64731400    1.55602200
H                  2.10613200   -4.14968700    0.97651800
C                  0.36174200   -2.97794700    0.61209600
H                  0.01294900   -3.71391800   -0.12069300
H                 -0.50829800   -2.58092500    1.14667600
H                  0.80826900   -4.39468800    2.16797400
C                  4.24026600   -2.68313800    1.82495600
H                  5.24532600   -2.81039500    2.24437600
H                  4.14324000   -3.36103500    0.96685800
C                  3.19362700   -2.96770700    2.87857100
H                  3.35490100   -2.32718800    3.74771400
H                  3.24381500   -4.01063700    3.20671000
O                  1.89719900   -2.64556700    2.38849100
Li                 2.09539900   -0.92977200    1.31787000

3-Li⁺-rac

H (353 K, 1 atm) = -1345.330837 a.u.
|  |  |  |  |
|---|---|---|---|
| C | 2.80749000 | 2.29193000 | 5.58073900 |
| C | 1.40273800 | 0.37022200 | 6.10647500 |
| C | 1.57364300 | 1.16868600 | 3.86903900 |
| C | 2.48822300 | 2.13411900 | 4.24536200 |
| C | 2.28851700 | 1.38739200 | 6.48400200 |
| H | 1.35847500 | 1.07278900 | 2.81460400 |
| H | 2.94422100 | 2.76051000 | 3.48786900 |
| H | 2.60465300 | 1.41740400 | 7.51887000 |
| H | 3.49337100 | 3.06302900 | 5.90923600 |
| C | -0.53491100 | -2.37006000 | 5.89665400 |
| H | 0.16812900 | -3.20229700 | 5.98695400 |
| C | 1.28458000 | -0.67013500 | 7.13549600 |
| H | 1.49912300 | -1.69578000 | 6.84239200 |
| N | -1.26909200 | -2.00171100 | 6.85964200 |
| N | 1.15774200 | -0.38896300 | 8.36825100 |
| O | -1.05081500 | -2.71945500 | 8.02461300 |
| O | 1.35866200 | -1.55647500 | 9.16622700 |
| C | 2.56273300 | -1.36658300 | 9.89387600 |
| H | 3.40215800 | -1.31556700 | 9.19103100 |
| H | 2.51954000 | -0.43336800 | 10.46351000 |
| C | 2.72036000 | -2.54964500 | 10.80764300 |
| H | 3.73269700 | -2.55646300 | 11.22622100 |
| H | 2.00101300 | -2.51712100 | 11.63671300 |
| O | 2.48542400 | -3.70281800 | 10.01803700 |
| C | 0.01404200 | -6.05138500 | 10.71396900 |
| H | -0.10839100 | -7.13733100 | 10.79787900 |
| H | 0.46595200 | -5.68204100 | 11.64169700 |
| C | -1.31783800 | -5.39538500 | 10.50788300 |
| H | -1.80386000 | -5.80151900 | 9.61231900 |
| H | -1.96591100 | -5.57859400 | 11.37249700 |
| O | -1.08687400 | -4.00729400 | 10.33237500 |
| C | -2.25573400 | -3.28643300 | 9.95701500 |
| H | -2.92420200 | -3.94621300 | 9.39368300 |
$3$-Li$^+$-b

H (353 K, 1 atm) = $-1345.380076$ a.u.
| Element | x   | y   | z      |
|---------|-----|-----|--------|
| H       | -1.19841600 | 4.83741100 | -3.03445900 |
| H       | -0.74360500  | 3.84747900  | -5.24874500  |
| H       | 2.15337300   | 1.23994500   | -3.48692500   |
| H       | 0.91030200   | 2.01759500   | -5.47463500   |
| C       | 1.93375800   | 2.15652700   | -0.97554100   |
| H       | 2.09523300   | 2.87525300   | -0.17285600   |
| C       | -0.92575600  | 1.93889000   | 0.06591400    |
| H       | -1.27899000  | 1.68053400   | -0.93309900   |
| N       | -0.79441700  | 1.03184800   | 0.94541000    |
| N       | 2.46722500   | 1.00376600   | -0.88738900   |
| O       | 3.23038500   | 0.88402300   | 0.29250600    |
| O       | -1.21400900  | -0.19085100  | 0.45843900    |
| C       | 4.56873400   | 0.51594300   | -0.01779900   |
| H       | 5.15005400   | 0.80489800   | 0.86053600    |
| H       | 4.24026600   | -2.68313800  | -1.82495600   |
| C       | 1.06404000   | -1.91982000  | 0.02224000    |
| C       | 1.32445400   | -3.64731400  | -1.55602200   |
| H       | 2.10613200   | -4.14968700  | -0.97651800   |
| C       | 0.36174200   | -2.97794700  | -0.61209600   |
| H       | 0.01294900   | -3.71391800  | 0.12069300    |
| H       | -0.50829800  | -2.58092500  | -1.14667600   |
| H       | 0.80826900   | -4.39468800  | -2.16797400   |
| C       | 4.24026600   | -2.68313800  | -1.82495600   |
H 5.24532600 -2.81039500 -2.24437600
H 4.14324000 -3.36103500 -0.96685800
C 3.19362700 -2.96770700 -2.87857100
H 3.35490100 -2.32718800 -3.74771400
H 3.24381500 -4.01063700 -3.20671000
O 1.89719900 -2.64556700 -2.38849100
Li 2.09539900 -0.92977200 -1.31787000

3-Na⁺-a

H (353 K, 1 atm) = -1500.066985 a.u.
H  -0.73351500  -0.28698200   1.93312000
C   0.50677300   1.84086600   0.31644300
H  -0.20214000   2.66866500   0.29836900
N  -2.31253000  -0.16918700   0.63915400
N   0.74100400   1.19163800  -0.75385000
O  -1.79364800  -1.37854800   0.17862200
O  -0.00683800   1.71222200  -1.82263300
C   0.81551700   1.89432000  -2.96814600
H   1.82016800   2.19203800  -2.65636800
H   0.36285700   2.72460500  -3.51591100
C   0.88283700   0.69806200  -3.88069500
H   1.46342900   0.98170200  -4.76864400
H  -0.12272800   0.40640500  -4.21391200
O   1.50611700  -0.38158800  -3.21122900
C   0.85049600  -4.02445700  -2.90751400
H   1.44329700  -4.92773600  -3.09777000
H   0.43135900  -3.67952100  -3.86046300
C  -0.27064300  -4.34364900  -1.96309900
H   0.12357500  -4.71731500  -1.00845800
H  -0.90113800  -5.12604300  -2.40413400
O  -1.01579100  -3.16133400  -1.74931600
C  -2.18463800  -3.37587400  -0.98054400
H  -1.93674500  -3.93515000  -0.06900200
H  -2.91936700  -3.95549500  -1.55304300
C  -2.76676400  -2.04286100  -0.61584500
H  -2.99429200  -1.44669500  -1.50609100
H  -3.68734000  -2.18361100  -0.04292600
C   1.99594600  -1.38398100  -4.07655900
H   2.76298700  -0.97345300  -4.74634000
H   1.18409600  -1.77919300  -4.70256700
C   2.60685700  -2.46421400  -3.21827800
H   3.05191800  -3.24208600  -3.84925500
H   3.39772400  -2.03350800  -2.60033600
O                  1.65925200   -3.02074500   -2.32249600
Na                 0.36895000   -1.20466400   -1.23415100

3-\text{Na}^+\text{-b}

H (353 K, 1 atm) = -1500.065749 a.u.

H                  -2.71396700   -1.17635900   -4.79426900
C                  -2.11881200   -0.41050900   -4.31167800
C                  -0.59083500    1.57932700   -3.06637600
C                  -2.18617600   -0.24284800   -2.94363300
C                  -1.29712400    0.41743900   -5.06754600
C                  -0.54621200    1.40084200   -4.44846700
C                  -1.43222000    0.74700700   -2.30741600
H                  -2.84303900   -0.86283100   -2.34584000
H                  -1.24180200    0.29509300   -6.14284100
H                   0.10557000    2.03668300   -5.03660100
C                   0.23947900    2.64510100   -2.45959500
C                   1.73879400    4.74074100   -1.36620700
C                   1.20210200    2.38870400   -1.46772000
C                   0.06137500    3.95740600   -2.89582100
C                   0.79792100    4.99685400   -2.35631600
C                   1.94015900    3.44669100   -0.93072800
H                   -0.68414000    4.15866600   -3.65661800
H                   0.63759900    6.00940100   -2.70737600
H                   2.68948000    3.23045200   -0.17927600
H                   2.32220400    5.55070500   -0.94521500
C                  -1.54576700    0.94797600   -0.86681700
H                  -1.20971300    1.89202100   -0.43760700
C                   1.46167500    1.01812800   -1.03509900
H                   1.13407900    0.19405400   -1.67001300
N                   -2.02197100    0.04282600   -0.10688700
N                   2.06677900    0.77861200    0.05855400
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| O    | -1.96703200 | 0.45189600 | 1.23668800 |
| O    | 2.19977200   | -0.60069800 | 0.26647000 |
| C    | 3.30247000   | -0.82767500 | 1.13983900 |
| H    | 3.52379400   | -1.89085200 | 1.03629000 |
| H    | 4.17204800   | -0.26248100 | 0.79268000 |
| C    | 2.98161600   | -0.45483600 | 2.56936400 |
| H    | 3.85341400   | -0.64231700 | 3.20647500 |
| H    | 2.74801400   | 0.61030000  | 2.61947300 |
| O    | 1.84017000   | -1.13433400 | 3.06858300 |
| C    | -0.61355800  | -3.92200700 | 2.98699600 |
| H    | -0.55607700  | -5.01688700 | 3.01681000 |
| H    | -0.52755800  | -3.54158500 | 4.01220900 |
| C    | -1.93304600  | -3.49779300 | 2.40906900 |
| H    | -2.03852300  | -3.87159600 | 1.38167100 |
| H    | -2.74699700  | -3.91685800 | 3.01388600 |
| O    | -1.97790100  | -2.08527600 | 2.42046400 |
| C    | -3.19322400  | -1.55473800 | 1.93022700 |
| H    | -3.37931000  | -1.91671800 | 0.91312700 |
| H    | -4.03338000  | -1.85974900 | 2.56767500 |
| C    | -3.09222000  | -0.05141300 | 1.95082500 |
| H    | -2.94195000  | 0.30940900  | 2.96994000 |
| H    | -4.01391000  | 0.38482400  | 1.55341900 |
| C    | 2.05472600   | -2.40776500 | 3.65569800 |
| H    | 3.09006500   | -2.51036400 | 3.99966000 |
| H    | 1.41161600   | -2.45083600 | 4.53901100 |
| C    | 1.71808400   | -3.54166600 | 2.70542600 |
| H    | 1.82306200   | -4.50186300 | 3.22566200 |
| H    | 2.39753000   | -3.55397600 | 1.85174800 |
| O    | 0.41585800   | -3.39827500 | 2.16696400 |
| Na   | 0.00429900   | -1.07807700 | 1.54151100 |
### 3-Na⁺-rac

H (353 K, 1 atm) = -1500.019697 a.u.

|    | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| H  | -3.1676480 | -2.0231540 | 2.1093930 |
| C  | -2.3849060 | -1.5139210 | 2.6578700 |
| C  | -0.2743390 | -0.2300230 | 4.1018740 |
| C  | -1.8457780 | -2.0735530 | 3.7971350 |
| C  | -1.9401520 | -0.2592980 | 2.2854180 |
| C  | -0.9287980 | 0.3516040  | 2.9978830 |
| C  | -0.8390300 | -1.4477650 | 4.5365180 |
| H  | -2.2333800 | -3.0191170 | 4.1604140 |
| H  | -2.3849700 | 0.2596360  | 1.4447130 |
| H  | -0.6642360 | 1.3519790  | 2.6937460 |
| C  | 0.8875440  | 0.5472090  | 4.6583210 |
| C  | 2.7713800  | 2.5079930  | 5.5303660 |
| C  | 1.5016460  | 0.4653140  | 5.9350760 |
| C  | 1.4131910  | 1.5431610  | 3.8165870 |
| C  | 2.3213040  | 2.5003130  | 4.2231210 |
| C  | 2.3862930  | 1.4703730  | 6.3504100 |
| H  | 1.1142630  | 1.5700980  | 2.7803490 |
| H  | 2.6744690  | 3.2352310  | 3.5094820 |
| H  | 2.8139700  | 1.3800560  | 7.3402450 |
| H  | 3.4607030  | 3.2637340  | 5.8861570 |
| C  | -0.5900930 | -2.1819770 | 5.7981780 |
| H  | 0.0833610  | -3.0433700 | 5.8167460 |
| C  | 1.5107020  | -0.6975190 | 6.8297490 |
| H  | 1.5947950  | -1.6879720 | 6.3890300 |
| N  | -1.3305760 | -1.9035680 | 6.7860760 |
| N  | 1.6358650  | -0.5523170 | 8.0863010 |
| O  | -1.1445190 | -2.7679800 | 7.8554640 |
| O  | 1.8651560  | -1.7874120 | 8.7372220 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 3.03799900 | -1.64876000| 9.53302500 |
| H       | 3.91843400 | -1.83571500| 8.90801100 |
| H       | 3.09037400 | -0.62690600| 9.91820500 |
| C       | 2.98225200 | -2.61625600| 10.68099700|
| H       | 3.93322600 | -2.57048300| 11.22628500|
| H       | 2.17572300 | -2.34496500| 11.37674200|
| O       | 2.75549200 | -3.91686800| 10.17076700|
| C       | -0.06980200| -6.05448300| 11.15726300|
| H       | -0.16240800| -7.08647300| 11.51703900|
| H       | 0.21542000 | -5.41846300| 12.00404600|
| C       | -1.38877200| -5.58903500| 10.60981000|
| H       | -1.70192100| -6.22833700| 9.77372700 |
| H       | -2.15158900| -5.65008800| 11.39590700|
| O       | -1.23173100| -4.25564400| 10.16476000|
| C       | -2.41401000| -3.69101500| 9.62650800 |
| H       | -2.87755100| -4.39433500| 8.92297100 |
| H       | -3.13361500| -3.47120700| 10.42485300|
| C       | -2.04754500| -2.42470500| 8.90913300 |
| H       | -1.56567500| -1.70776400| 9.58249600 |
| H       | -2.93681300| -1.96141800| 8.48017200 |
| C       | 2.82092700 | -4.93260800| 11.15226600|
| H       | 3.86087800 | -5.11688700| 11.44982500|
| H       | 2.26758400 | -4.62256500| 12.04882900|
| C       | 2.22810900 | -6.18596700| 10.55456200|
| H       | 2.28397000 | -7.00967800| 11.27536900|
| H       | 2.79477900 | -6.47434000| 9.66655000 |
| O       | 0.89368700 | -5.97823100| 10.12183400|
| Na      | 0.72871000 | -3.84266900| 8.90619200 |
3-Na\textsuperscript{+}-c

H (353 K, 1 atm) = -1500.066985 a.u.

\begin{tabular}{llll}
H & -4.47161000 & 3.62289300 & -2.98050100 \\
C & -3.45812700 & 3.24153300 & -2.94665300 \\
C & -0.84344700 & 2.25874800 & -2.86313100 \\
C & -3.18754600 & 2.06176500 & -2.28055400 \\
C & -2.43256900 & 3.92747200 & -3.58624400 \\
C & -1.13863500 & 3.43745500 & -3.54456500 \\
C & -1.88800500 & 1.55648800 & -2.23680100 \\
H & -3.98216000 & 1.50259200 & -1.80174500 \\
H & -2.64217400 & 4.84957700 & -4.11532500 \\
H & -0.33413300 & 3.98433500 & -4.02327000 \\
C & 0.55280000 & 1.77664800 & -2.79828700 \\
C & 3.16209300 & 0.76134200 & -2.72831300 \\
C & 1.18220600 & 1.50946300 & -1.56949500 \\
C & 1.26247000 & 1.54753100 & -3.97476800 \\
C & 2.55227600 & 1.04439500 & -3.94407700 \\
C & 2.48156000 & 0.99882000 & -1.54914200 \\
H & 0.77889300 & 1.74507500 & -4.92466400 \\
H & 3.08381300 & 0.87039100 & -4.87233000 \\
H & 2.96220300 & 0.83013200 & -0.59249200 \\
H & 4.17462800 & 0.37680400 & -2.70257500 \\
C & -1.59966800 & 0.27990800 & -1.58985700 \\
H & -0.73351500 & -0.28698200 & -1.93312000 \\
C & 0.50677300 & 1.84086600 & -0.31644300 \\
H & -0.20214000 & 2.66866500 & -0.29836900 \\
N & -2.31253000 & -0.16918700 & -0.63915400 \\
N & 0.74100400 & 1.19163800 & 0.75385000 \\
O & -1.79364800 & -1.37854800 & -0.17862200 \\
O & -0.00683800 & 1.71222200 & 1.82263300 \\
\end{tabular}
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 0.81551700 | 1.89432000 | 2.96814600 |
| H    | 1.82016800  | 2.19203800  | 2.65636800  |
| H    | 0.36285700  | 2.72460500  | 3.51591100  |
| C    | 0.88283700  | 0.69806200  | 3.88069500  |
| H    | 1.46342900  | 0.98170200  | 4.76864400  |
| H    | -0.12272800 | 0.40640500  | 4.21391200  |
| O    | 1.50611700  | -0.38158800 | 3.21122900  |
| C    | 0.85049600  | -4.02445700 | 2.90751400  |
| H    | 1.44329700  | -4.92773600 | 3.09777000  |
| H    | 0.43135900  | -3.67952100 | 3.86046300  |
| C    | -0.27064300 | -4.34364900 | 1.96309900  |
| H    | 0.12357500  | -4.71731500 | 1.00845800  |
| H    | -0.90113800 | -5.12604300 | 2.40413400  |
| O    | -1.01579100 | -3.16133400 | 1.74931600  |
| C    | -2.18463800 | -3.37587400 | 0.98054400  |
| H    | -1.93674500 | -3.93515000 | 0.06900200  |
| H    | -2.91936700 | -3.95549500 | 1.55304300  |
| C    | -2.76676400 | -2.04286100 | 0.61584500  |
| H    | -2.99429200 | -1.44669500 | 1.50609100  |
| H    | -3.68734000 | -2.18361100 | 0.04292600  |
| C    | 1.99594600  | -1.38398100 | 4.07655900  |
| H    | 2.76298700  | -0.97345300 | 4.74634000  |
| H    | 1.18409600  | -1.77919300 | 4.70256700  |
| C    | 2.60685700  | -2.46421400 | 3.21827800  |
| H    | 3.05191800  | -3.24208600 | 3.84925500  |
| H    | 3.39772400  | -2.03350800 | 2.60033600  |
| O    | 1.65925200  | -3.02074500 | 2.32249600  |
| Na   | 0.36895000  | -1.20466400 | 1.23415100  |
3-K⁺-a

H (353 K, 1 atm) = -1937.638731 a.u.

H  -4.65975100  3.51717300  2.35326900
C  -3.62237200  3.22550900  2.46526000
C  -0.94768700  2.46724300  2.75947000
C  -3.20923500  1.97613000  2.04810700
C  -2.70920700  4.09842300  3.04420900
C  -1.38684400  3.71763100  3.19051200
C  -1.87677300  1.58058400  2.19047700
H  -3.91730400  1.27675700  1.62093500
H  -3.02858100  5.07750100  3.38127100
H  -0.66912200  4.40195000  3.62857800
C  0.48356400  2.11991700  2.92208900
C  3.17516400  1.46861100  3.32847300
C  1.32258100  1.85324500  1.82634500
C  1.02171400  2.06858100  4.20681200
C  2.35071600  1.74289900  4.41331800
C  2.66480100  1.52937000  2.04743500
H  0.37458900  2.27380400  5.05193500
H  2.74597200  1.70515000  5.42160000
H  3.30700300  1.35372600  1.19282000
H  4.21921100  1.22489100  3.48475300
C  -1.45928600  0.23641200  1.79883800
H  -0.52686400 -0.15981500  2.20430000
C  0.80443000  1.96787600  0.46526100
H  -0.13694800  2.49045800  0.29723700
N  -2.17258500 -0.46733900  1.01481000
N  1.44006500  1.46798700 -0.52083600
O  -1.59578800 -1.70708200  0.76519900
O  0.75007900  1.64555000 -1.71824500
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 1.66211100 | 1.78193300 | -2.80580300 |
| H    | 2.67239200  | 1.56876500 | -2.44967100 |
| H    | 1.62503800  | 2.81667800 | -3.16058600 |
| C    | 1.29880100  | 0.84558400 | -3.92341000 |
| H    | 1.90207500  | 1.10389700 | -4.80407600 |
| H    | 0.23985000  | 0.95573900 | -4.19478000 |
| O    | 1.57223400  | -0.47923800 | -3.51331500 |
| C    | 0.12502900  | -4.04928900 | -3.34157700 |
| H    | 0.46933100  | -4.91449100 | -3.92300300 |
| H    | -0.57399700 | -3.47428300 | -3.96305200 |
| C    | -0.58587100 | -4.53836800 | -2.11267600 |
| H    | 0.11500500  | -5.07965000 | -1.46226300 |
| H    | -1.37886700 | -5.23529100 | -2.41491700 |
| O    | -1.13778300 | -3.43129900 | -1.43136000 |
| C    | -1.91932200 | -3.79908100 | -0.31293300 |
| H    | -1.29286400 | -4.27677400 | 0.45318600 |
| H    | -2.69599300 | -4.51694500 | -0.60785100 |
| C    | -2.59211200 | -2.57658500 | 0.23747400 |
| H    | -3.14686900 | -2.05539900 | -0.54763000 |
| H    | -3.28932100 | -2.86403800 | 1.03097300 |
| C    | 1.46622800  | -1.43187100 | -4.55004400 |
| H    | 2.07251800  | -1.12727900 | -5.41407800 |
| H    | 0.42385100  | -1.51639700 | -4.88884900 |
| C    | 1.98729300  | -2.75046600 | -4.03296300 |
| H    | 2.02548800  | -3.47859900 | -4.85193900 |
| H    | 3.00411100  | -2.60939000 | -3.65876300 |
| O    | 1.22708000  | -3.25535500 | -2.95011900 |
| K    | 0.61713100  | -1.28618500 | -1.02121900 |
3-K⁺-b

H (353 K, 1 atm) = -1937.636103 a.u.

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 2.49780900 | -1.09566100 | -4.96432900 |
| C    | 1.95893800 | -0.31229400 | -4.44495100 |
| C    | 0.57986200 | 1.72393700  | -3.10898400 |
| C    | 1.10131500 | -0.16365000 | -3.07988900 |
| C    | 1.13916000 | 0.55944300  | -5.15227900 |
| C    | 0.46177600 | 1.67781000  | -4.48809800 |
| C    | 1.42019300 | 0.84878300  | -2.39824800 |
| H    | 2.76552500 | -0.81362200 | -2.52276900 |
| H    | 1.02949900 | 0.45337700  | -6.22513900 |
| H    | 0.18526100 | 2.24202500  | -5.03750700 |
| C    | 0.17188100 | 2.81063500  | -2.43562200 |
| C    | 1.49986100 | 4.92091200  | -1.17144700 |
| C    | 1.17921900 | 2.54999500  | -1.49069900 |
| C    | -0.13483500 | 4.13351300 | -2.74564500 |
| C    | 0.51847800 | 5.18151600  | -2.12015600 |
| C    | 1.83077100 | 3.61597600  | -0.86550700 |
| H    | -0.91147400 | 4.33432900 | -3.47489500 |
| H    | 0.26117200 | 6.20362400  | -2.37172000 |
| H    | 2.61553400 | 3.40044800  | -0.15074900 |
| H    | 2.01600900 | 5.73856800  | -0.68279700 |
| C    | -1.61050000 | 1.04605500 | -0.96619700 |
| H    | -1.28642000 | 1.98716900 | -0.52181800 |
| C    | 1.57896200 | 1.17237200  | -1.22203400 |
| H    | 1.27144400 | 0.39872600  | -1.92767400 |
| N    | 2.13973800 | 0.15548200  | -0.22156200 |
| N    | 2.29888800 | 0.86309200  | -0.21795300 |
| O    | 2.14624500 | 0.58496200  | -1.10661400 |
| O    | 2.57063900 | -0.50286500 | -0.20836000 |
C  3.68561800  -0.77142800  0.63511100
H  4.08411500  -1.72198900  0.27486200
H  4.44160300   0.00561800  0.50366800
C  3.31074800  -0.89766400  2.08855500
H  4.22302600  -1.08423000  2.67048500
H  2.85609000   0.03163600  2.45756600
O  2.41298000  -1.98307400  2.21213500
C  -0.89341800  -3.39882500  3.87692200
H  -0.98680100  -4.34125400  4.43175000
H  -0.66909500  -2.59691000  4.59284200
C  -2.19472800  -3.10234800  3.18900200
H  -2.39300900  -3.86050800  2.41807400
H  -3.00760900  -3.14671300  3.92576100
O  -2.11966700  -1.81395100  2.61733800
C  -3.30923200  -1.40753600  1.97192000
H  -3.41722100  -1.91738900  1.00597500
H  -4.18683900  -1.65836000  2.58263700
C  -3.28230400   0.08973200  1.79898600
H  -3.22145100   0.57388400  2.77511300
H  -4.20033200   0.41622100  1.29933500
C  2.22247200  -2.45581400  3.52873400
H  3.18959300  -2.67136800  4.00267800
H  1.70691300  -1.70258100  4.14224700
C  1.41837500  -3.72929400  3.44111700
H  1.35291700  -4.19676800  4.42968000
H  1.92795200  -4.42576200  2.77030800
O  0.12615900  -3.50438400  2.90307800
K  0.04741100  -1.54834000  0.85051900
3-K-rac

H (353 K, 1 atm) = -1937.58631 a.u.

H  -4.22893900  -0.05113900   3.50164300
C  -3.15531400  -0.04670600   3.64370600
C  -0.33462500   0.03746100   3.50164300
C  -2.58583100  -0.70458100   4.71273600
C  -2.30579500   0.53672500   2.72385000
C  -0.94710100   0.56864100   2.96862500
C  -1.20313400  -0.72766600   4.93941800
H  -3.21024400  -1.27937000   5.38431800
H  -2.69081000   0.97801000   1.81224300
H  -0.34217800   1.03164900   2.20625000
C   1.10020700   0.43718700   4.36425900
C   3.75156600   1.51333000   4.58489600
C   2.00023000   0.00592400   5.37119200
C   1.59557800   1.47742600   3.55522200
C   2.87202500   1.99601200   3.63659000
C   3.29255800   0.54261400   5.44764200
H   0.94686900   1.95549600   2.84108400
H   3.16264000   2.79244000   2.96175800
H   3.94563300   0.16801000   6.22489400
H   4.76013900   1.89810800   4.67215800
C  -0.83519500  -1.79119200   5.88722000
H  -0.18253200  -2.58375700   5.51782900
C   1.76126400  -0.96864700   6.44979200
H   1.51286100  -2.00218300   6.22757100
N  -1.45664000  -1.93412600   6.98403700
N   2.01054300  -0.60041000   7.63834600
O  -1.19072500  -3.16419200   7.58592600
O   1.88956000  -1.62425000   8.56701400
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 2.49396200 | -1.18788400| 9.78215800 |
| H       | 3.58276400 | -1.19498500| 9.66736300 |
| H       | 2.16886900 | -0.16697600| 9.99653800 |
| C       | 2.08011000 | -2.09364500| 10.90435500|
| H       | 2.53983700 | -1.71560000| 11.82662800|
| H       | 0.98906900 | -2.07458200| 11.03779100|
| O       | 2.51031000 | -3.41565000| 10.64063200|
| C       | 0.36309000 | -6.49840200| 11.09233100|
| H       | 0.46222000 | -7.52423300| 11.46906000|
| H       | 0.15393700 | -5.83932800| 11.94270700|
| C       | -0.78958800| -6.41967500| 10.13070900|
| H       | -0.63336000| -7.09225800| 9.27523000 |
| H       | -1.70234200| -6.74249700| 10.64773000|
| O       | -0.90923400| -5.08146800| 9.69219100 |
| C       | -2.13299000| -4.79610300| 9.04531700 |
| H       | -2.26953000| -5.44662900| 8.17029500 |
| H       | -2.97291100| -4.96855400| 9.73100100 |
| C       | -2.14608700| -3.35524400| 8.62616300 |
| H       | -1.91161600| -2.70130800| 9.47282100 |
| H       | -3.13992800| -3.09762800| 8.25247000 |
| C       | 2.41222200 | -4.26345100| 11.76716300|
| H       | 3.19028300 | -4.01474700| 12.50121300|
| H       | 1.43796900 | -4.12656100| 12.25555500|
| C       | 2.58369400 | -5.69307500| 11.31433300|
| H       | 2.63737600 | -6.35447100| 12.18705700|
| H       | 3.52144300 | -5.79377100| 10.76257800|
| O       | 1.55084900 | -6.10171700| 10.43320500|
| K       | 1.32620600 | -4.29894700| 8.31147800 |
3-K⁺-c

H (353 K, 1 atm) = -1937.638731 a.u.

H  -4.65975100  3.51717300  -2.35326900
C  -3.62237200  3.22550900  -2.46526000
C  -0.94768700  2.46724300  -2.75947000
C  -3.20923500  1.97613000  -2.04810700
C  -2.70920700  4.09842300  -3.04420900
C  -1.38684400  3.71763100  -3.19051200
C  -1.87677300  1.58058400  -2.19047700
H  -3.91730400  1.27675700  -1.62093500
H  -3.02858100  5.07750100  -3.38127100
H  -0.66912200  4.40195000  -3.62857800
C   0.48356400  2.11991700  -2.92208900
C   0.17516400  2.46861100  -3.32847300
C  -3.12258100  1.85324500  -1.82634500
C  -1.45928600  0.23641200  -2.04743500
C  -0.52686400  0.15981500  -2.20430000
C   0.80443000  1.96787600  -0.46526100
H   -0.13694800  2.49045800  -0.29723700
N   -2.17258500  0.46733900  -1.01481000
N   -1.59578800 -1.70708200  -0.76519900
O    0.75007900  1.64555000  1.71824500

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|   |     |     |     |
|---|-----|-----|-----|
| C | 1.66211100 | 1.78193300 | 2.80580300 |
| H | 2.67239200 | 1.56876500 | 2.44967100 |
| H | 1.62503800 | 2.81667800 | 3.16058600 |
| C | 1.29880100 | 0.84558400 | 3.92341000 |
| H | 1.90207500 | 1.10389700 | 4.80407600 |
| H | 0.23985000 | 0.95573900 | 4.19478000 |
| O | 1.57223400 | -0.47923800 | 3.51331500 |
| C | 0.12502900 | -4.04928900 | 3.34157700 |
| H | 0.46933100 | -4.91449100 | 3.92300300 |
| H | -0.57399700 | -3.47428300 | 3.96305200 |
| C | -0.58587100 | -4.53836800 | 2.11267600 |
| H | 0.11500500 | -5.07965000 | 1.46226300 |
| H | -1.37886700 | -3.25329100 | 2.41491700 |
| O | -1.13778300 | -3.43129900 | 1.43136000 |
| C | -1.91932200 | -3.79908100 | 0.31293300 |
| H | -1.29286400 | -4.27677400 | -0.45318600 |
| H | -2.69599300 | -4.51694500 | 0.60785100 |
| C | -2.59211200 | -2.57658500 | -0.23747400 |
| H | -3.14686900 | -2.05539900 | 0.54763000 |
| H | -3.28932100 | -2.86403800 | -1.03097300 |
| C | 1.46622800 | -1.43187100 | 4.55004400 |
| H | 2.07251800 | -1.12727900 | 5.41407800 |
| H | 0.42385100 | -1.51639700 | 4.88884900 |
| C | 1.98729300 | -2.75046600 | 4.03296300 |
| H | 2.02548800 | -3.47859900 | 4.85193900 |
| H | 3.00411100 | -2.60939000 | 3.65876300 |
| O | 1.22708000 | -3.25535500 | 2.95011900 |
| K | 0.61713100 | -1.28618500 | 1.02121900 |
**3-Et₂NH₂⁺-a**

H (353 K, 1 atm) = -1551.856728 a.u.

| Atoms | x-coord  | y-coord  | z-coord  |
|-------|----------|----------|----------|
| C     | -2.314892 | -0.836217 | -5.156492 |
| C     | -1.827719  | -0.136833 | -4.487452 |
| C     | -0.597233  | 1.697568  | -2.769928 |
| C     | -2.366312  | 0.114484  | -3.241262 |
| C     | -0.669276  | 0.519646  | -4.884358 |
| C     | -0.066220  | 1.426858  | -4.030437 |
| C     | -1.764485  | 1.024069  | -2.366294 |
| H     | -3.271356  | -0.387966 | -2.921997 |
| H     | -0.243909  | 0.335324  | -5.863765 |
| H     | 0.829686   | 1.952197  | -4.342702 |
| C     | 0.088322   | 2.704887  | -1.913495 |
| C     | 1.334696   | 4.694561  | -0.387121 |
| C     | 1.307932   | 2.442510  | -1.261861 |
| C     | -0.486315  | 3.966839  | -1.773762 |
| C     | 0.124933   | 4.953986  | -1.020208 |
| C     | 1.916930   | 3.449265  | -0.506325 |
| H     | -1.422599  | 4.172770  | -2.280426 |
| H     | -0.336732  | 5.930712  | -0.935772 |
| H     | 2.859484   | 3.234384  | -0.017399 |
| H     | 1.823564   | 5.467913  | 0.193158 |
| C     | -2.299453  | 1.209179  | -1.017420 |
| H     | -2.015162  | 2.094838  | -0.449957 |
| C     | 1.887923   | 1.103276  | -1.311512 |
| H     | 1.503775   | 0.396813  | -2.047738 |
| N     | -3.024765  | 0.310484  | -0.479029 |
| N     | 2.775136   | 0.725485  | -0.476937 |
| O     | -3.324875  | 0.621087  | 0.825538 |
| O     | 3.057886   | -0.625090 | -0.647319 |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | 4.18834400   | -1.01995900  | 0.12169500   |
| H       | 4.42627100   | -2.01679400  | -0.25350000  |
| H       | 5.02935000   | -0.35215000  | -0.08325100  |
| C       | 3.93711800   | -1.07175800  | 1.60783900   |
| H       | 4.86758300   | -1.38884300  | 2.09930900   |
| H       | 3.68291300   | -0.07355500  | 1.98769900   |
| O       | 2.89354600   | -1.98498200  | 1.88166100   |
| C       | -0.86390700  | -3.20773500  | 3.46843200   |
| H       | -0.66831100  | -4.26868400  | 3.66492100   |
| H       | -1.15198000  | -2.72784500  | 4.41087300   |
| C       | -1.99464400  | -3.13451800  | 2.47634000   |
| H       | -1.68177100  | -3.58619000  | 1.52200600   |
| H       | -2.81649600  | -3.74946700  | 2.87126700   |
| O       | -2.42823700  | -1.81014100  | 2.27850800   |
| C       | -3.58707000  | -1.75821800  | 1.46841000   |
| H       | -3.36638100  | -2.11798500  | 0.45436300   |
| H       | -4.36663400  | -2.41224500  | 1.88532400   |
| C       | -4.16347200  | -0.36509100  | 1.40796100   |
| H       | -4.35168900  | 0.01038100   | 2.41503900   |
| H       | -5.11344800  | -0.41266000  | 0.86497200   |
| C       | 2.65583600   | -2.14034600  | 3.26275600   |
| H       | 3.54896600   | -2.54185100  | 3.76184500   |
| H       | 2.42638800   | -1.16976600  | 3.72326500   |
| C       | 1.52090800   | -3.10090900  | 3.50076300   |
| H       | 1.42120000   | -3.24038000  | 4.58382400   |
| H       | 1.74157300   | -4.07425000  | 3.04516400   |
| O       | 3.01056100   | -2.58864800  | 2.96539600   |
| N       | 0.39968200   | -0.97896200  | 0.75768800   |
| H       | 0.34941900   | -1.64281700  | 1.55465200   |
| H       | 1.39738000   | -0.90882500  | 0.53793800   |
| C       | -0.12839600  | 0.33036400   | 1.21624500   |
| H       | -1.16388300  | 0.16727200   | 1.50450900   |
| H       | -0.10373000  | 1.00450800   | 0.36376700   |
3-Et₂NH₂⁺-TS-rac

H (353 K, 1 atm) = -1551.781752 a.u.
|  |  |  |  |
|---|---|---|---|
| H | 2.74931600 | 0.56830000 | 5.11693700 |
| C | 2.13373700 | -1.47988700 | 5.27945300 |
| H | 1.97444100 | -1.41193300 | 6.36186500 |
| H | 2.51134900 | -2.48286700 | 5.04563100 |
| O | 0.91420100 | -1.25213800 | 4.59051600 |
| N | 1.05481500 | -0.14388000 | 2.16119700 |
| H | 0.97903000 | -0.59035200 | 3.09390700 |
| H | 2.03378300 | 0.12706100 | 2.06341700 |
| C | 0.22773000 | 1.09023000 | 2.19190400 |
| H | -0.77437400 | 0.79896800 | 2.47664100 |
| H | 0.20191200 | 1.51824700 | 1.19566500 |
| C | 0.79866200 | 2.07550100 | 3.18482900 |
| H | 0.82610700 | 1.65392300 | 4.19176300 |
| H | 1.80119100 | 2.40008100 | 2.89847700 |
| C | 0.84662700 | -1.20160400 | 1.14144100 |
| H | -0.17952900 | -1.53474500 | 1.20400600 |
| H | 0.99116800 | -0.75484300 | 0.16037400 |
| C | 1.81676600 | -2.34179800 | 1.35499000 |
| H | 1.70215500 | -2.78475500 | 2.34585300 |
| H | 2.85195200 | -2.02113300 | 1.24753600 |
| H | 1.62163900 | -3.11699100 | 0.61272400 |
| H | 0.16209400 | 2.96070000 | 3.21321800 |

**3-Et₂NH₂⁺⁻**

H (353 K, 1 atm) = -1551.856291 a.u.
C   -1.88718900  1.56517800  -1.93252900
H   -3.89839100  1.38722900  -1.22555200
H   -2.22354700  5.32525200  -1.05241100
H   -0.12762700  4.46186300  -2.02681600
C    0.46533300  1.98907000  -2.77869000
C    2.83963100  1.20572800  -4.03477500
C    1.63375300  1.78894100  -2.02384100
C    0.51157100  1.39317300  -4.15585700
H    -0.12762700  1.94005100  -4.73825700
H     1.69740000  1.24712900  -5.85616000
H     3.70708100  1.25584600  -2.07603100
H     3.76259000  0.91398100  -4.52144700
C   -1.74425900  0.12898900  -2.17867100
H    -0.96273000  0.22691000  -2.84930600
C    1.59847900  1.91927500  -0.56828300
H    0.73794300  2.40178400  -0.10401600
N   -2.48953400  0.69277800  -1.55227400
N    2.52273300  1.41655500  0.14992300
O   -2.17799500  1.99889700  -1.82803800
O    2.23063000  1.51280900  1.50392900
C    3.35730100  1.11530800  2.28382000
H    3.95561000  0.40838500  1.70524500
H    3.96877900  1.99272800  2.51555200
C    2.86766900  0.47816300  3.55437100
H    3.73056100  0.30617100  4.21211300
H    2.17430400  1.15021500  4.07982600
O    2.22810300  0.74064200  3.24085700
C   -1.13331900  3.38590400  3.22826600
H    0.92036500  4.15403600  3.97854000
H   -2.09732800  0.29312580  3.47184800
C   -1.13331900  4.03901700  1.87134700
3-Et$_2$NH$_2^+$-c

H (353 K, 1 atm) = -1551.856728 a.u.

H  -2.31489200  -0.83621700  5.15649200
C  -1.82771900  -0.13683300  4.48745200
C  -0.59723300  1.69756800  2.76992800
C  -2.36631200  0.11448400  3.24126200
C  -0.66927600  0.51964600  4.88435800
C  -0.06622000  1.42685800  4.03043700
C  -1.76448500  1.02409900  2.36629400
H  -3.27135600  -0.38796600  2.92199700
H  -0.24390900  0.33532400  5.86376500
H  0.82968600   1.95219700  4.34270200
C  0.08832200   2.70488700  1.91349500
C  1.33469600   4.69456100  0.38712100
C  1.30793200   2.44251000  1.26186100
C  -0.48631500  3.96683900  1.77376200
C  0.12493300   4.95398600  1.02020800
C  1.91693000   3.44926500  0.50632500
H  -1.42259900  4.17277000  2.28042600
H  -0.33673200  5.93071200  0.93577200
H  2.85948400   3.23438400  0.01739900
H  1.82356400   5.46791300 -0.19315800
C  -2.29945300  1.20917900  1.01742000
H  -2.01516200  2.09483800  0.44995700
C  1.88792300   1.10327600  1.31151200
H  1.50377500   0.39681300  2.04773800
N  -3.02476500  0.31048400  0.47902900
N  2.77513600   0.72548600  0.47693700
O  -3.32487500   0.62108700 -0.82553800
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| O       | 3.0578600  | -0.62500900| 0.64731900 |
| C       | 4.18834400 | -1.01995900| -0.12169500|
| H       | 4.42627100 | -2.01679400| 0.25350000 |
| H       | 5.02935000 | -0.35215000| 0.08325100 |
| C       | 3.93711800 | -1.07175800| -1.60783900|
| H       | 4.86758300 | -1.38884300| -2.09309000|
| H       | 3.68291300 | -0.07355500| -1.98769900|
| O       | 2.89354600 | -1.98498200| -1.88166100|
| C       | -0.86390700| -3.20773500| -3.46832000|
| H       | -0.66831100| -4.26868400| -3.66492100|
| H       | -1.15198000| -2.72784500| -4.41087300|
| C       | -1.99464400| -3.13451800| -2.47634000|
| H       | -1.68177100| -3.58619000| -1.52200600|
| H       | -2.81649600| -3.74946700| -2.87126700|
| O       | -2.42823700| -1.81014100| -2.27850800|
| C       | -3.58707000| -1.75821800| -1.46841000|
| H       | -3.36638100| -2.11798500| -0.45436300|
| H       | -4.36663400| -2.41224500| -1.88532400|
| C       | -4.16347200| -0.36509100| -1.40796100|
| H       | -4.35168900| 0.01038100 | -2.41503900|
| H       | -5.11344800| -0.41266000| -0.86497200|
| C       | 2.65583600 | -2.14034600| -3.26275600|
| H       | 3.54896600 | -2.54185100| -3.76184500|
| H       | 2.42638800 | -1.16976600| -3.72326500|
| C       | 1.52090800 | -3.10090900| -3.50076300|
| H       | 1.42120000 | -3.24038000| -4.58382400|
| H       | 1.74157300 | -4.07425000| -3.04516400|
| O       | 0.31056100 | -2.58864800| -2.96539600|
| N       | 0.39968200 | -0.97896200| -0.75768800|
| H       | 0.34941900 | -1.64281700| -1.55465200|
| H       | 1.39738000 | -0.90882500| -0.53793800|
| C       | -0.12839600| 0.33036400 | -1.21624500|
| H       | -1.16388300| 0.16727200 | -1.50450900|
Supplementary Material

9-crown-3

H (353 K, 1 atm) = -460.947802 a.u.

O 1.04662400 -4.49980100 5.84963100
O 1.05864100 -4.55759300 2.98570800
C -0.06629800 -5.30029000 6.14631900
H -0.28170600 -5.25671200 7.22371000
H -0.96712900 -4.93783100 5.63819500
C 0.21183100 -6.75106200 5.78932800
H 1.03900700 -7.11234100 6.40430500
H -0.68119300 -7.34668600 6.04056900
C 0.42484100 -5.68732800 2.44447600
H 1.22386900 -6.25520400 1.96280500
H -0.30632500 -5.40789900 1.66813500
C -0.27150900 -6.58313500 3.45549000
H -0.63803900 -7.47030700 2.91915700
H -1.15647100 -6.08905200 3.87237100
9-crown-3-Li$^+$

H (353 K, 1 atm) = -468.3237 a.u.
9-crown-3-Na$^+$

H (353 K, 1 atm) = -623.008863 a.u.
9-crown-3-K⁺

H (353 K, 1 atm) = -1060.584967 a.u.

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| O       | 1.03068700 | -4.50870600 | 5.80325300 |
| O       | 1.03808900 | -4.58805200 | 3.01852600 |
| C       | -0.09808000 | -5.28932400 | 6.16243800 |
| H       | -0.27135300 | -5.21459100 | 7.24160300 |
| H       | -0.99719700 | -4.91000400 | 5.66912200 |
| C       | 0.14568500 | -6.74478700 | 5.80276900 |
| H       | 0.92377700 | -7.16326400 | 6.44719600 |
| H       | -0.76751400 | -7.32431100 | 5.98439100 |
| C       | 0.35827700 | -5.68497500 | 2.43244700 |
| H       | 1.12151300 | -6.23978800 | 1.87973800 |
| H       | -0.38649600 | -5.34836100 | 1.70116600 |
| C       | -0.30714800 | -6.59369200 | 3.45155700 |
| H       | -0.64241100 | -7.50677800 | 2.94749900 |
| H       | -1.19660800 | -6.11996900 | 3.87588600 |
| O       | 0.61524700 | -6.92401600 | 4.47751700 |
| C       | 0.21331400 | -3.63061700 | 3.66313600 |
| H       | 0.20363200 | -2.70078100 | 3.08390400 |
| H       | -0.81954000 | -3.98646500 | 3.71029400 |
| C       | 0.75131300 | -3.33893500 | 5.05335100 |
| H       | 1.70259600 | -2.80448100 | 4.98092300 |
| H       | 0.05326200 | -2.68114500 | 5.58514900 |
| K       | 3.08821900 | -5.72695100 | 4.44982100 |

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12-crown-4

H (353 K, 1 atm) = -614.607723 a.u.

O          -0.33848200  -3.39536100   7.01649600
O           2.06361400  -1.74165900   8.21222100
C           2.58841200  -3.04683000   8.31730500
H           2.04041400  -3.75474500   7.68514300
H           3.61109000  -2.96753300   7.93686600
C           2.64979700  -3.59606800   9.73149000
H           3.46366400  -4.32999200   9.79080200
H           2.88454200  -2.78026400  10.42601900
O           1.44761100  -4.24485600  10.09317700
C           0.76431000  -3.74629400  11.21000900
H           1.20305000  -4.11202600  12.15211800
H           0.79949500  -2.64814200  11.23136100
C          -0.67698200  -4.19403700  11.11467700
H          -0.73115300  -5.28913500  11.15739400
H          -1.22911700  -3.79929900  11.97405900
O          -1.28931100  -3.70917700   9.94247700
C         -1.33366300  -4.64056200   8.88068700
H         -0.40994900  -5.22551000   8.83884300
H         -2.17931800  -5.32976300   9.03234900
C        -1.51997200  -3.93807300   7.55701700
H        -2.29542600  -3.16666800   7.65726600
H        -1.88140200  -4.68212800   6.83792700
C       0.66844400  -1.57780600   8.35263200
H       0.52585600  -0.50044600   8.48485400
H       0.27748500  -2.08131800   9.23979500
C      -0.14461400  -2.00409500   7.14619000
H     -1.11633400  -1.49110500   7.18533600
12-crown-4-Li⁺

H (353 K, 1 atm) = -622.007174 a.u.
12-crown-4-Na$^+$

H (353 K, 1 atm) = -776.686464 a.u.
C                 -0.13178200   -2.45537300    6.55572100
H                 -0.85653600   -1.68295300    6.28015400
H                  0.33112500   -2.82162300    5.63640400
Na                 0.92900000    -4.86481100    8.12959200

12-crown-4-K⁺

H (353 K, 1 atm) = -1214.25798 a.u.

O                 -0.82296200   -3.55438400    7.11215400
O                  1.90298800    -2.86909100    7.69256100
C                 2.82762100   -2.58707700    8.73137100
H                  3.70308600    -3.21318600    8.54023200
H                 3.15401100   -1.54119700    8.68434000
C                 2.27843300   -2.86983600   10.10774000
H                  3.02385100   -2.56589900   10.85374600
H                 1.36848800   -2.86221000   10.27921700
O                 1.98988300   -4.25481200   10.24355500
C                 1.11075100   -4.53829000   11.32185300
H                 1.52250000   -5.36533500   11.90668600
H                 1.03443200   -3.67019600   11.98257700
C                 0.26469300   -4.91290700   10.80529600
H                  0.24738100   -5.91619500   10.3455500
H                 1.97441800   -5.36533500   11.64152000
O                 0.63627700   -3.94581900    9.85806900
C                 1.84829500   -4.17508200    9.18068300
H                 0.31427500   -5.22076100    8.3809400
H                 2.71411500   -3.99253000    9.83013700
C                 1.88445000   -3.23852100    8.00155500
H                 1.78799000   -2.21087000    8.36656400
H                 2.84359400   -3.32803700    7.47995600
C                 0.90477500   -1.88229200    7.50007400
H                 1.34793100   -0.97928100    7.06056800
### 15-crown-5

H (353 K, 1 atm) = -768.267015 a.u.
15-crown-5-Li+

H (353 K, 1 atm) = -775.687977 a.u.
15-crown-5-Na$^+$

H (353 K, 1 atm) = -930.372908 a.u.
15-crown-5-K$^+$

H (353 K, 1 atm) = -1367.940279 a.u.

O  -0.82296200  -3.55438400  7.11215400
O   1.90298800  -2.86909100  7.69256100
C   2.82762100  -2.58707700  8.73137100
H   3.70308600  -3.21318600  8.54023200
H   3.15401100  -1.54119700  8.68434000
C   2.27843300  -2.86983600  10.10774000
H   3.02385100  -2.56589900  10.85374600
H   1.36848800  -2.28622100  10.27921700
O   1.98988300  -4.25481200  10.24355500
C   1.11075100  -4.53829000  11.32185300
H   1.52250000  -5.36533500  11.90668600
H   1.03443200  -3.67019600  11.98257700
C  -0.26469300  -4.91290700  10.80529600
H  -0.24738100  -5.91619500  10.34259100
H  -0.97441800  -4.96908500  11.64152000
O  -0.63627700  -3.94581900  9.85806900
C  -1.84829500  -4.17508200  9.18068300
H  -1.91207500  -5.22076100  8.83809400
H  -2.71411500  -3.99253000  9.83013700
C  -1.88445000  -3.23852100  8.00155500
H  -1.78799000  -2.21087000  8.36656400
H  -2.84359400  -3.32803700  7.47995600
C   0.90477500  -1.88229200  7.50007400
H   1.34793100  -0.97928100  7.06056800
H   0.44478300  -1.60738800  8.45631400
C  -0.14480600  -2.43411900  6.56466300
H  -0.85165600  -1.64158400  6.29589900
|   |       |       |       |
|---|-------|-------|-------|
| H | 0.32748000 | -2.77863100 | 5.64096200 |
| K | 1.12238300  | -5.38851600  | 7.81047800  |