

Electronic Supplementary Material

Planar tetracoordinate carbon species CLi_3E with 12- valence-electron[†]

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[†]All of these calculations are carried out using the Gaussian 09 program¹.

1 Figures and Tables

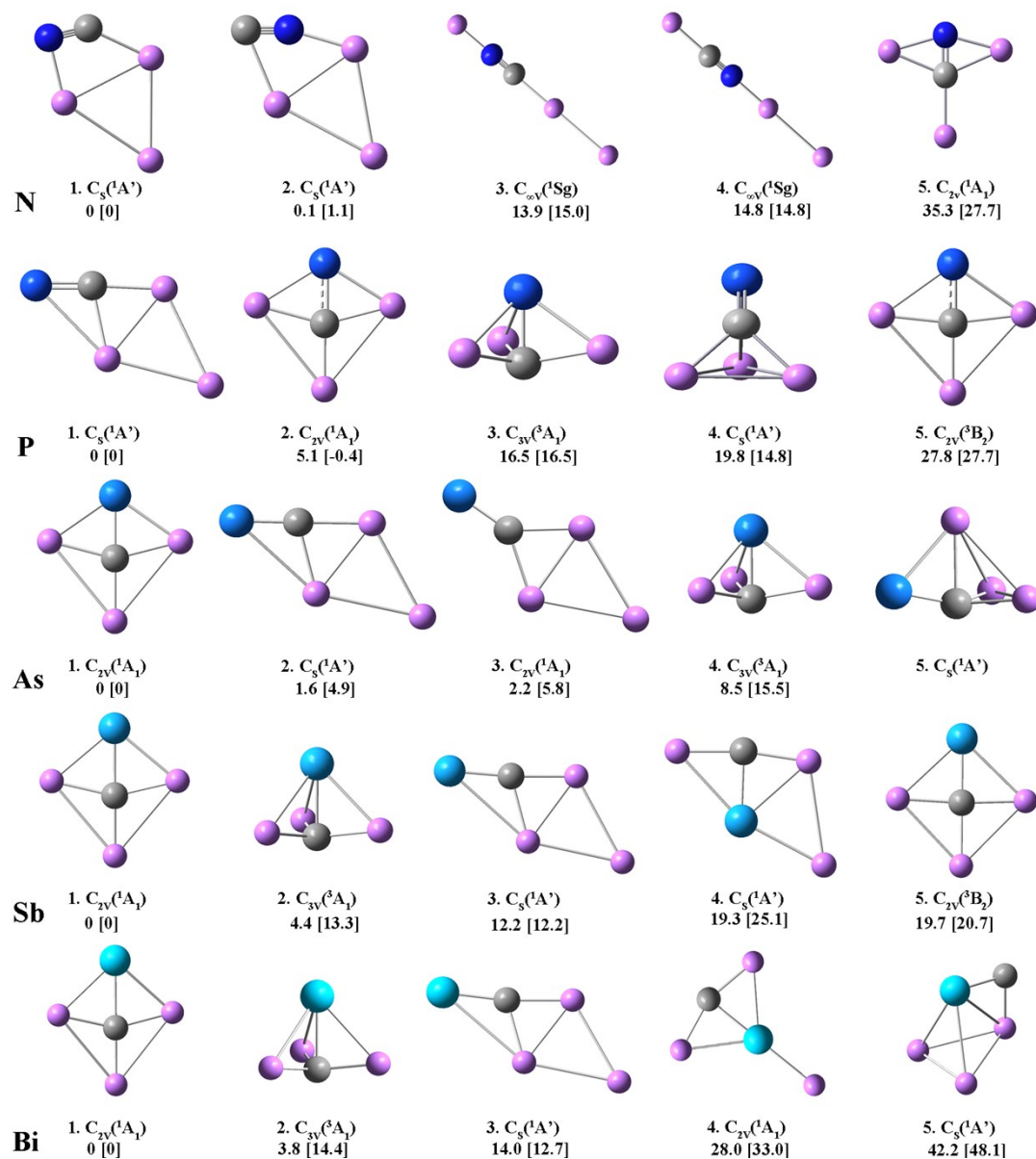


Figure S1. Local minima for the CL_3E ($E = N, P, As, Sb, Bi$) clusters. The energy differences in kcal/mol are computed at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level. The values in square brackets are obtained at the MP2/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level.

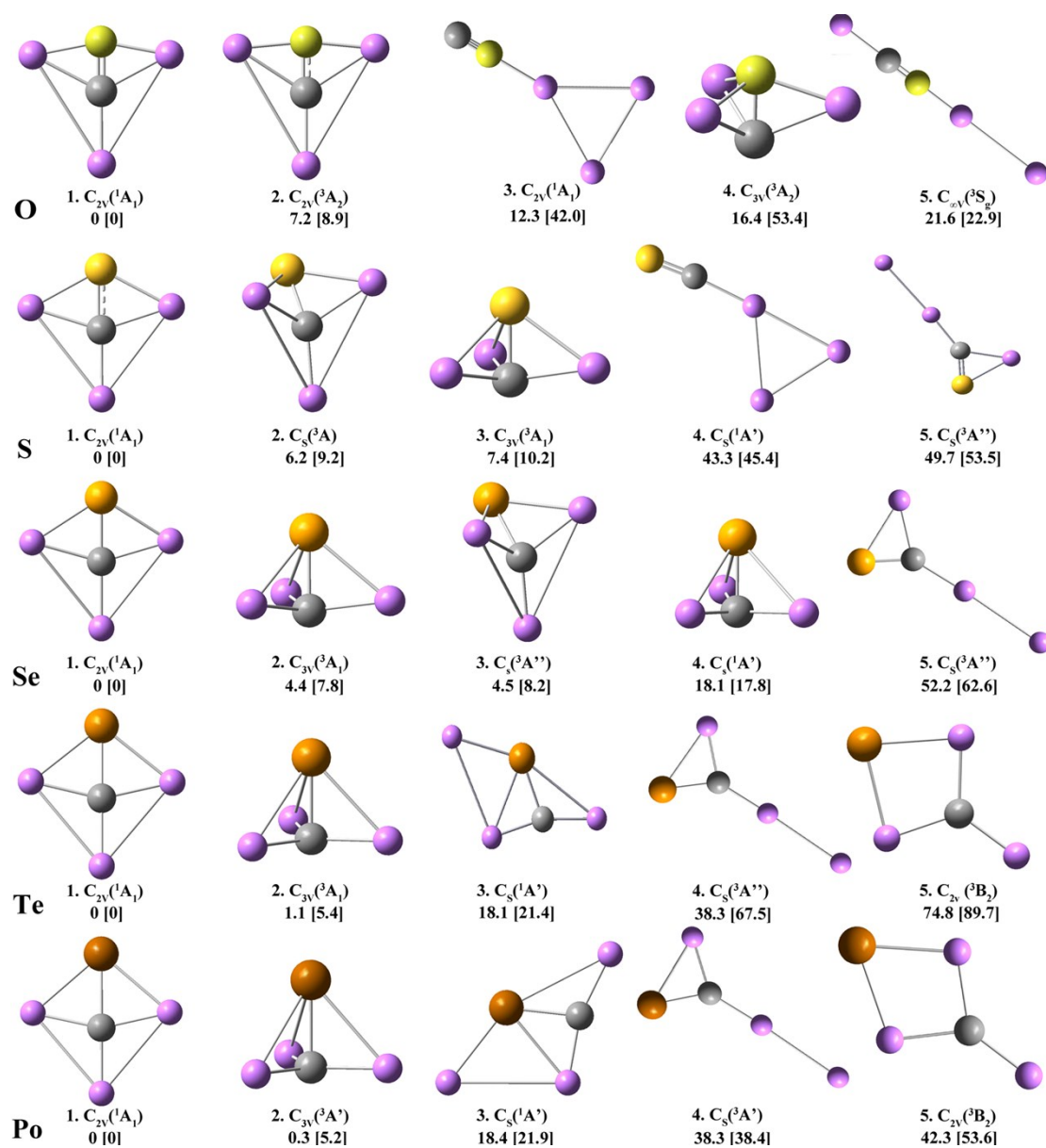


Figure S2. Local minima for the CLi_3E^+ ($E = O, S, Se, Te, Po$) clusters. The energy differences in kcal/mol are computed at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level. The values in square brackets are obtained at the MP2/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level.

2 Cartesian coordinates of all the ptC species optimized at MP2/aug-cc-pVTZ level.

C_{2v} CLi₃N

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.34322000 |
| Li | 0.00000000 | 1.85916000 | 0.41351900 |
| Li | 0.00000000 | -1.85916000 | 0.41351900 |
| Li | 0.00000000 | 0.00000000 | -2.25392600 |
| N | 0.00000000 | 0.00000000 | 0.90571200 |

C_{2v} CLi₃P

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.76885500 |
| Li | 0.00000000 | 1.95632300 | -0.25823000 |
| Li | 0.00000000 | -1.95632300 | -0.25823000 |
| Li | 0.00000000 | 0.00000000 | -2.66715800 |
| P | 0.00000000 | 0.00000000 | 0.94426600 |

C_{2v} CLi₃As

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.20512400 |
| Li | 0.00000000 | 1.95975300 | -0.70836000 |
| Li | 0.00000000 | -1.95975300 | -0.70836000 |
| Li | 0.00000000 | 0.00000000 | -3.09819900 |
| As | 0.00000000 | 0.00000000 | 0.62956100 |

C_{2v} CLi₃Sb

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.54204800 |
| Li | 0.00000000 | 1.97608000 | -1.10288700 |
| Li | 0.00000000 | -1.97608000 | -1.10288700 |
| Li | 0.00000000 | 0.00000000 | -3.43047900 |
| Sb | 0.00000000 | 0.00000000 | 0.51296200 |

C_{2v} CLi₃Bi

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.79061900 |
| Li | 0.00000000 | 1.97165100 | -1.35618300 |
| Li | 0.00000000 | -1.97165100 | -1.35618300 |
| Li | 0.00000000 | 0.00000000 | -3.67375700 |

| | | | |
|----|------------|------------|------------|
| Bi | 0.00000000 | 0.00000000 | 0.36026600 |
|----|------------|------------|------------|

C_{2v} CLi₃O⁺

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.43694000 |
| Li | 0.00000000 | 1.80529900 | 0.48227300 |
| Li | 0.00000000 | -1.80529900 | 0.48227300 |
| Li | 0.00000000 | 0.00000000 | -2.35168600 |
| O | 0.00000000 | 0.00000000 | 0.84788300 |

C_{2v} CLi₃S⁺

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.79127500 |
| Li | 0.00000000 | 1.99544200 | -0.17409800 |
| Li | 0.00000000 | -1.99544200 | -0.17409800 |
| Li | 0.00000000 | 0.00000000 | -2.72913100 |
| S | 0.00000000 | 0.00000000 | 0.87372700 |

C_{2v} CLi₃Se⁺

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.20048200 |
| Li | 0.00000000 | 2.01722600 | -0.64605900 |
| Li | 0.00000000 | -2.01722600 | -0.64605900 |
| Li | 0.00000000 | 0.00000000 | -3.14032100 |
| Se | 0.00000000 | 0.00000000 | 0.60294700 |

C_{2v} CLi₃Te⁺

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.50764800 |
| Li | 0.00000000 | 2.04375000 | -1.07075400 |
| Li | 0.00000000 | -2.04375000 | -1.07075400 |
| Li | 0.00000000 | 0.00000000 | -3.44939600 |
| Te | 0.00000000 | 0.00000000 | 0.49651200 |

C_{2v} CLi₃Po⁺

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.74731700 |
| Li | 0.00000000 | 2.04016700 | -1.33727600 |
| Li | 0.00000000 | -2.04016700 | -1.33727600 |
| Li | 0.00000000 | 0.00000000 | -3.68516200 |
| Po | 0.00000000 | 0.00000000 | 0.35194100 |

3 Cartesian coordinates and energies (hartree) of all the low-lying isomers calculated at MP2/aug-cc-pVTZ and CCSD(T)/aug-cc-pVTZ level.

CLi₃N

1 MP2=-115.11547939 , CCSD(T)= -115.12713556

| | | | |
|----|-------------|-------------|------------|
| C | 0.00000000 | 1.02457000 | 0.00000000 |
| Li | -0.76970900 | -1.10438100 | 0.00000000 |
| Li | 1.65697600 | -2.89788500 | 0.00000000 |
| Li | 1.78443500 | 0.07444400 | 0.00000000 |
| N | -1.14501500 | 0.80515000 | 0.00000000 |

2 MP2=-115.11373476 , CCSD(T)= -115.12697324

| | | | |
|----|-------------|-------------|------------|
| C | -1.14023200 | 1.11277500 | 0.00000000 |
| Li | -0.79453600 | -1.05893700 | 0.00000000 |
| Li | 1.44368900 | -3.05058000 | 0.00000000 |
| Li | 1.63131100 | -0.09192900 | 0.00000000 |
| N | 0.00000000 | 0.84681300 | 0.00000000 |

3 MP2=-115.09155103 , CCSD(T)= -115.10504963

| | | | |
|----|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | 0.17715600 |
| Li | 0.00000000 | 0.00000000 | 3.14606700 |
| Li | 0.00000000 | 0.00000000 | -4.72942600 |
| Li | 0.00000000 | 0.00000000 | -1.89395100 |
| N | 0.00000000 | 0.00000000 | 1.33842800 |

4 MP2=-115.09183506 , CCSD(T)= -115.10354738

| | | | |
|----|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | 1.32476700 |
| Li | 0.00000000 | 0.00000000 | 3.28640400 |
| Li | 0.00000000 | 0.00000000 | -4.58472900 |
| Li | 0.00000000 | 0.00000000 | -1.74289600 |
| N | 0.00000000 | 0.00000000 | 0.16786600 |

5 MP2=-115.07127564 , CCSD(T)= -115.07079836

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.34522300 |
| Li | 0.00000000 | 1.83180700 | 0.42924600 |
| Li | 0.00000000 | -1.83180700 | 0.42924600 |
| Li | 0.00000000 | 0.00000000 | -2.22282100 |
| N | 0.00000000 | 0.00000000 | 0.88061800 |

CLi₃P

1 MP2=-401.2868546 , CCSD(T)= -401.30357879

| | | | |
|----|-------------|-------------|------------|
| C | 0.00000000 | 0.53779500 | 0.00000000 |
| Li | 1.20001100 | -1.18298100 | 0.00000000 |
| Li | 1.88786400 | 1.25932500 | 0.00000000 |
| Li | 4.13991600 | -0.72052200 | 0.00000000 |
| P | -1.44555800 | -0.08628300 | 0.00000000 |

2 MP2=-401.2875448 , CCSD(T)= -401.29551941

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.76733000 |
| Li | 0.00000000 | 0.00000000 | -2.62500600 |
| Li | 0.00000000 | 1.91689600 | -0.25818400 |
| Li | 0.00000000 | -1.91689600 | -0.25818400 |
| P | 0.00000000 | 0.00000000 | 0.93520700 |

3 MP2=-401.26057209 , CCSD(T)=-401.27726253

| | | | |
|----|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.00479500 |
| Li | 0.00000000 | 1.89516000 | -0.62203600 |
| Li | 1.64125700 | -0.94758000 | -0.62203600 |
| Li | -1.64125700 | -0.94758000 | -0.62203600 |
| P | 0.00000000 | 0.00000000 | 0.77514000 |

4 MP2=-401.2632998 , CCSD(T)=-401.27214448

| | | | |
|----|-------------|------------|-------------|
| C | -0.53105100 | 0.40955900 | 0.00000000 |
| Li | -0.53105100 | 1.92588900 | 1.28841800 |
| Li | -0.53105100 | 1.92588900 | -1.28841800 |
| Li | 1.65122800 | 0.77502300 | 0.00000000 |

| | | | |
|---|------------|-------------|------------|
| P | 0.09459500 | -1.08918400 | 0.00000000 |
|---|------------|-------------|------------|

5 MP2=-401.24266289 , CCSD(T)=-401.25945422

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.67222600 |
| Li | 0.00000000 | 0.00000000 | -2.63014800 |
| Li | 0.00000000 | 1.99779800 | -0.44490800 |
| Li | 0.00000000 | -1.99779800 | -0.44490800 |
| P | 0.00000000 | 0.00000000 | 0.97288300 |

CLi₃As

1 MP2=-2294.84663161 , CCSD(T)=-2294.8478539

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.21416100 |
| Li | 0.00000000 | 1.91970600 | -0.71523200 |
| Li | 0.00000000 | -1.91970600 | -0.71523200 |
| Li | 0.00000000 | 0.00000000 | -3.06898900 |
| As | 0.00000000 | 0.00000000 | 0.62979800 |

2 MP2=-2294.83880286 , CCSD(T)=-2294.845381

| | | | |
|----|-------------|-------------|------------|
| C | 0.00000000 | 0.83658500 | 0.00000000 |
| Li | 2.08811300 | 0.63813600 | 0.00000000 |
| Li | 0.68329500 | 2.73884800 | 0.00000000 |
| Li | 3.64873600 | 3.17316900 | 0.00000000 |
| As | -0.58365000 | -0.74757500 | 0.00000000 |

3 MP2=-2294.83739487 , CCSD(T)=-2294.8443272

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.67723800 |
| Li | 0.00000000 | 1.22418400 | -2.32370500 |
| Li | 0.00000000 | -1.22418400 | -2.32370500 |
| Li | 0.00000000 | 0.00000000 | -5.04424400 |
| As | 0.00000000 | 0.00000000 | 1.00419400 |

4 MP2=-2294.82185274 , CCSD(T)=-2294.8342519

| | | | |
|----|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.40211600 |
| Li | 0.00000000 | 1.89860100 | -1.02651900 |

| | | | |
|----|-------------|-------------|-------------|
| Li | 1.64423700 | -0.94930100 | -1.02651900 |
| Li | -1.64423700 | -0.94930100 | -1.02651900 |
| As | 0.00000000 | 0.00000000 | 0.53489000 |

5 MP2=-2294.82130825 , CCSD(T)= -2294.8191534

| | | | |
|----|-------------|-------------|-------------|
| C | 0.35640700 | -1.02456300 | 0.00000000 |
| Li | -1.83229500 | -0.86759200 | 0.00000000 |
| Li | 0.08611400 | -2.45757800 | 1.30564200 |
| Li | 0.08611400 | -2.45757800 | -1.30564200 |
| As | 0.08611400 | 0.71198900 | 0.00000000 |

CLi₃Sb

1 MP2=-299.87549989 , CCSD(T)= -299.87466922

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.56225900 |
| Li | 0.00000000 | 1.93270000 | -1.11228400 |
| Li | 0.00000000 | -1.93270000 | -1.11228400 |
| Li | 0.00000000 | 0.00000000 | -3.41913100 |
| Sb | 0.00000000 | 0.00000000 | 0.51577800 |

2 MP2=-299.85428355 , CCSD(T)= -299.86769554

| | | | |
|----|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.71082600 |
| Li | 0.00000000 | 1.90938200 | -1.43852700 |
| Li | -1.65357300 | -0.95469100 | -1.43852700 |
| Li | 1.65357300 | -0.95469100 | -1.43852700 |
| Sb | 0.00000000 | 0.00000000 | 0.45513100 |

3 MP2=-299.85606308 , CCSD(T)= -299.85522290

| | | | |
|----|-------------|-------------|------------|
| C | -0.48281500 | -1.09152300 | 0.00000000 |
| Li | 1.25020100 | -2.25625000 | 0.00000000 |
| Li | 0.86962800 | -5.21180400 | 0.00000000 |
| Li | -1.15419800 | -2.99465400 | 0.00000000 |
| Sb | 0.00000000 | 0.74386800 | 0.00000000 |

4 MP2=-299.84250941 , CCSD(T)= -299.84383812

| | | | |
|----|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.45835900 |
| Li | 0.00000000 | 2.00384700 | -1.37316100 |

| | | | |
|----|------------|-------------|-------------|
| Li | 0.00000000 | -2.00384700 | -1.37316100 |
| Li | 0.00000000 | 0.00000000 | -3.43084400 |
| Sb | 0.00000000 | 0.00000000 | 0.53493400 |

5 MP2=-299.8354918, CCSD(T)= -299.84331976

| | | | |
|----|-------------|-------------|------------|
| C | -0.70345100 | -1.59845100 | 0.00000000 |
| Li | 2.72720200 | 0.61510700 | 0.00000000 |
| Li | -2.50505900 | -0.87466000 | 0.00000000 |
| Li | 1.18476000 | -2.03881000 | 0.00000000 |
| Sb | 0.00000000 | 0.32325100 | 0.00000000 |

CLi₃Bi

1 MP2=-274.19977095 , CCSD(T)= -274.19112281

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.82529300 |
| Li | 0.00000000 | 1.92692400 | -1.37388700 |
| Li | 0.00000000 | -1.92692400 | -1.37388700 |
| Li | 0.00000000 | 0.00000000 | -3.68234600 |
| Bi | 0.00000000 | 0.00000000 | 0.36436300 |

2 MP2=-274.17675762 , CCSD(T)= -274.18511367

| | | | |
|----|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.96437300 |
| Li | 0.00000000 | 1.90678600 | -1.69169200 |
| Li | 1.65132500 | -0.95339300 | -1.69169200 |
| Li | -1.65132500 | -0.95339300 | -1.69169200 |
| Bi | 0.00000000 | 0.00000000 | 0.32543900 |

3 MP2= -274.17952321 , CCSD(T)= -274.16876194

| | | | |
|----|-------------|-------------|------------|
| C | -0.45383100 | -1.41255900 | 0.00000000 |
| Li | 1.25059400 | -2.60709300 | 0.00000000 |
| Li | -1.16179800 | -3.30370000 | 0.00000000 |
| Li | 0.81886600 | -5.55874600 | 0.00000000 |
| Bi | 0.00000000 | 0.51667400 | 0.00000000 |

4 MP2=-274.14726179 , CCSD(T)= -274.14646521

| | | | |
|----|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | -2.03529600 |
| Li | 0.00000000 | 1.92395200 | -1.66656600 |

| | | | |
|----|------------|-------------|-------------|
| Li | 0.00000000 | -1.92395200 | -1.66656600 |
| Li | 0.00000000 | 0.00000000 | 2.66696900 |
| Bi | 0.00000000 | 0.00000000 | 0.17120800 |

5 MP2=-274.12313839 , CCSD(T)= -274.12393112

| | | | |
|----|-------------|-------------|-------------|
| C | -1.82863700 | 0.51953500 | 0.00000000 |
| Li | 0.19734500 | -2.54726400 | 1.40088400 |
| Li | 0.19734500 | -2.54726400 | -1.40088400 |
| Li | -2.19729900 | -1.40348800 | 0.00000000 |
| Bi | 0.19734500 | 0.19731100 | 0.00000000 |

CLi₃O⁺

1 MP2=-135.37767509 , CCSD(T)= -135.3830797

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.44161400 |
| Li | 0.00000000 | 1.77088600 | 0.49415800 |
| Li | 0.00000000 | -1.77088600 | 0.49415800 |
| Li | 0.00000000 | 0.00000000 | -2.32589500 |
| O | 0.00000000 | 0.00000000 | 0.83280200 |

2 MP2=-135.36354341 , CCSD(T)= -135.37156308

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.50962100 |
| Li | 0.00000000 | 1.77917100 | 0.63509600 |
| Li | 0.00000000 | -1.77917100 | 0.63509600 |
| Li | 0.00000000 | 0.00000000 | -2.37867000 |
| O | 0.00000000 | 0.00000000 | 0.79789500 |

3 MP2=-135.31074054 , CCSD(T)= -135.36349093

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | 2.30302500 |
| Li | 0.00000000 | 0.00000000 | -0.84556100 |
| Li | 0.00000000 | 1.44938500 | -3.43887500 |
| Li | 0.00000000 | -1.44938500 | -3.43887500 |
| O | 0.00000000 | 0.00000000 | 1.16897200 |

4 MP2=-135.29254697 , CCSD(T)= -135.35697997

| | | | |
|----|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.80310300 |
| Li | 0.00000000 | 1.82048200 | 0.02687500 |

| | | | |
|----|-------------|-------------|------------|
| Li | -1.57658400 | -0.91024100 | 0.02687500 |
| Li | 1.57658400 | -0.91024100 | 0.02687500 |
| O | 0.00000000 | 0.00000000 | 0.57209200 |

5 MP2=-135.34115471 , CCSD(T)= -135.34861376

| | | | |
|----|------------|------------|-------------|
| C | 0.00000000 | 0.00000000 | 1.34362000 |
| Li | 0.00000000 | 0.00000000 | -1.63819000 |
| Li | 0.00000000 | 0.00000000 | 3.26550200 |
| Li | 0.00000000 | 0.00000000 | -4.70902200 |
| O | 0.00000000 | 0.00000000 | 0.14792700 |

CLi₃S⁺

1 MP2=-457.96778659 , CCSD(T)= -457.98629122

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -0.79847300 |
| Li | 0.00000000 | 1.95983300 | -0.17522000 |
| Li | 0.00000000 | -1.95983300 | -0.17522000 |
| Li | 0.00000000 | 0.00000000 | -2.70457200 |
| S | 0.00000000 | 0.00000000 | 0.87224200 |

2 MP2=-457.95306653 , CCSD(T)= -457.97633253

| | | | |
|----|-------------|-------------|-------------|
| C | 0.63244100 | 0.54911100 | 0.00000000 |
| Li | -0.50914200 | 0.78527100 | 1.72609500 |
| Li | -0.50914200 | 0.78527100 | -1.72609500 |
| Li | 2.46882900 | 1.13655700 | 0.00000000 |
| S | -0.50914200 | -0.71349800 | 0.00000000 |

3 MP2=-457.95145623 , CCSD(T)= -457.97455564

| | | | |
|----|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.00116800 |
| Li | 0.00000000 | 1.97592800 | -0.65955000 |
| Li | -1.71120400 | -0.98796400 | -0.65955000 |
| Li | 1.71120400 | -0.98796400 | -0.65955000 |
| S | 0.00000000 | 0.00000000 | 0.74643500 |

4 MP2=-457.89547652 , CCSD(T)= -457.91731023

| | | | |
|----|-------------|-------------|------------|
| C | 0.00000000 | 0.42583900 | 0.00000000 |
| Li | 1.12784100 | -3.89315600 | 0.00000000 |
| Li | 1.60520700 | -0.93794400 | 0.00000000 |
| Li | 3.85144500 | -2.97664000 | 0.00000000 |
| S | -1.23459300 | 1.30426100 | 0.00000000 |

5 MP2=-457.88256106 , CCSD(T)= -457.90701558

| | | | |
|----|-------------|-------------|------------|
| C | 0.00000000 | 0.34317200 | 0.00000000 |
| Li | 1.84017100 | 1.22060200 | 0.00000000 |
| Li | -1.97589000 | 1.03421800 | 0.00000000 |
| Li | 4.70089400 | 2.39571800 | 0.00000000 |
| S | -0.85597000 | -1.00066500 | 0.00000000 |

CLi₃Se⁺**1 MP2=-2460.35341802, CCSD(T)= -2460.3656015**

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.22004100 |
| Li | 0.00000000 | 1.98260100 | -0.65418400 |
| Li | 0.00000000 | -1.98260100 | -0.65418400 |
| Li | 0.00000000 | 0.00000000 | -3.13025900 |
| Se | 0.00000000 | 0.00000000 | 0.60694500 |

2 MP2=-2460.3410236 , CCSD(T)= -2460.3586293

| | | | |
|----|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.37108400 |
| Li | 0.00000000 | 1.98710600 | -1.10177400 |
| Li | 1.72088500 | -0.99355300 | -1.10177400 |
| Li | -1.72088500 | -0.99355300 | -1.10177400 |
| Se | 0.00000000 | 0.00000000 | 0.53360200 |

3 MP2=-2460.3404123 , CCSD(T)= -2460.3583495

| | | | |
|----|-------------|-------------|-------------|
| C | -0.91441800 | -0.86661400 | 0.00000000 |
| Li | -1.24096900 | 0.24833100 | 1.71015800 |
| Li | -1.24096900 | 0.24833100 | -1.71015800 |
| Li | -1.24096900 | -2.78067200 | 0.00000000 |

| | | | |
|----|------------|------------|------------|
| Se | 0.48986000 | 0.35446200 | 0.00000000 |
|----|------------|------------|------------|

4 MP2=-2460.32512402 , CCSD(T)= -2460.3367163

| | | | |
|----|-------------|-------------|-------------|
| C | -0.86120800 | -1.01602800 | 0.00000000 |
| Li | 0.28936600 | -1.85343400 | 1.42910900 |
| Li | 0.28936600 | -1.85343400 | -1.42910900 |
| Li | -2.13580300 | 0.51404300 | 0.00000000 |
| Se | 0.28936600 | 0.46101900 | 0.00000000 |

5 MP2=-2460.25359471 , CCSD(T)= -2460.2824629

| | | | |
|----|-------------|-------------|------------|
| C | 0.26829800 | -0.84449100 | 0.00000000 |
| Li | 2.23937000 | -0.17762300 | 0.00000000 |
| Li | -2.14048900 | -5.37605600 | 0.00000000 |
| Li | -0.63547800 | -2.67297800 | 0.00000000 |
| Se | 0.00000000 | 0.87490900 | 0.00000000 |

CLi₃Te⁺

1 MP2=-327.47021322 , CCSD(T)= -327.48009553

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.54192300 |
| Li | 0.00000000 | 2.00525900 | -1.08112500 |
| Li | 0.00000000 | -2.00525900 | -1.08112500 |
| Li | 0.00000000 | 0.00000000 | -3.45845600 |
| Te | 0.00000000 | 0.00000000 | 0.50218600 |

2 MP2=-327.46154049 , CCSD(T)= -327.47829378

| | | | |
|----|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.64190724 |
| Li | 0.00000000 | 1.98946714 | -1.56562132 |
| Li | -1.72292908 | -0.99473357 | -1.56562132 |
| Li | 1.72292908 | -0.99473357 | -1.56562132 |
| Te | 0.00000000 | 0.00000000 | 0.46042376 |

3 MP2=-327.4361185 , CCSD(T)= -327.45120596

| | | | |
|----|-------------|-------------|------------|
| C | -0.61186600 | -1.62105700 | 0.00000000 |
| Li | -2.59877200 | -1.75865000 | 0.00000000 |
| Li | 1.30260500 | -2.03570900 | 0.00000000 |
| Li | 2.51990000 | 1.20430600 | 0.00000000 |
| Te | 0.00000000 | 0.33647100 | 0.00000000 |

4 MP2=-327.3626956 , CCSD(T)= -327.41908736

| | | | |
|----|-------------|-------------|------------|
| C | 1.09643185 | 0.66635021 | 0.00000000 |
| Li | 3.06901986 | 0.16464325 | 0.00000000 |
| Li | 0.08827583 | 2.44888620 | 0.00000000 |
| Li | 6.03872688 | -0.71321971 | 0.00000000 |
| Te | -0.65705113 | -0.18651982 | 0.00000000 |

5 MP2=-327.32720532 , CCSD(T)= -327.36087712

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -2.58760200 |
| Li | 0.00000000 | 1.71350300 | -1.36272800 |
| Li | 0.00000000 | -1.71350300 | -1.36272800 |
| Li | 0.00000000 | 0.00000000 | -4.59579900 |
| Te | 0.00000000 | 0.00000000 | 0.72095000 |

CLi₃Po⁺

1 MP2=-297.18711105 , CCSD(T)= -297.19116548

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.79726700 |
| Li | 0.00000000 | 2.00312800 | -1.35910800 |
| Li | 0.00000000 | -2.00312800 | -1.35910800 |
| Li | 0.00000000 | 0.00000000 | -3.71540300 |
| Po | 0.00000000 | 0.00000000 | 0.35814800 |

2 MP2=-297.17875468 , CCSD(T)= -297.19067815

| | | | |
|----|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.87950800 |
| Li | 0.00000000 | 1.98450900 | -1.83753700 |
| Li | -1.71863500 | -0.99225400 | -1.83753700 |
| Li | 1.71863500 | -0.99225400 | -1.83753700 |
| Po | 0.00000000 | 0.00000000 | 0.33113000 |

3 MP2=-297.15226955 , CCSD(T)= -297.16181715

| | | | |
|----|-------------|-------------|------------|
| C | -0.64491400 | -1.81602900 | 0.00000000 |
| Li | 2.65991600 | 0.95943300 | 0.00000000 |
| Li | 1.26412800 | -2.25540200 | 0.00000000 |
| Li | -2.63421700 | -1.93846200 | 0.00000000 |
| Po | 0.00000000 | 0.24523200 | 0.00000000 |

4 MP2=-297.12592932 , CCSD(T)= -297.13008136

| | | | |
|----|-------------|-------------|------------|
| C | -0.41865900 | -1.53893700 | 0.00000000 |
| Li | -2.40016200 | -1.09193500 | 0.00000000 |
| Li | 0.70184400 | -3.23691600 | 0.00000000 |
| Li | 2.53563700 | -5.73177700 | 0.00000000 |
| Po | 0.00000000 | 0.46923200 | 0.00000000 |

5 MP2=-297.10167757 , CCSD(T)= -297.123804

| | | | |
|----|------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -3.25195900 |
| Li | 0.00000000 | 1.50443200 | -1.70609900 |
| Li | 0.00000000 | -1.50443200 | -1.70609900 |
| Li | 0.00000000 | 0.00000000 | -5.26272500 |
| Po | 0.00000000 | 0.00000000 | 0.54210100 |

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