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Supplementary Information

Fock-Space Coupled Cluster Theory: Systematic Study of Partial Fourth order Triples Schemes for Ionization Potential and Comparison with Bondonic Formalism

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Nitrogen Molecule BASIS A (Gamess Format)

Nitrogen 7.0 0.000 0.000 1.035
S 8
1 11420.0000000 0.0005230
2 1712.0000000 0.0040450
3 389.3000000 0.0207750
4 110.0000000 0.0807270
5 35.5700000 0.2330740
6 12.5400000 0.4335010
7 4.6440000 0.3474720
8 0.5118000 -0.0085080
S 8
1 11420.0000000 -0.0001150
2 1712.0000000 -0.0008950
3 389.3000000 -0.0046240
4 110.0000000 -0.0185280
5 35.5700000 -0.0573390
6 12.5400000 -0.1320760
7 4.6440000 -0.1725100
8 0.5118000 0.5999440
S 1
1 1.2930000 1.0000000
S 1

```
  1      0.1787000           1.0000000
S   1
  1      0.0576000           1.0000000
P   3
  1     26.6300000           0.0146700
  2      5.9480000           0.0917640
  3      1.7420000           0.2986830
P   1
  1      0.5550000           1.0000000
P   1
  1      0.1725000           1.0000000
P   1
  1      0.0491000           1.0000000
D   1
  1      1.6540000           1.0000000
D   1
  1      0.4690000           1.0000000
F   1
  1      1.0930000           1.0000000
```