

DFT Investigation of Stability of F₂XNY (X = P, As, and Sb; Y = S, Se, and Te)

Joonghan Kim^{1*} AND WONIL SEO¹

¹Department of Chemistry, The Catholic University of Korea, Bucheon 14662,
Republic of Korea
joonghankim@catholic.ac.kr

ABSTRACT

A recent experimental investigation utilizing infrared spectroscopy has detected F₂PNS. [1] Subsequent theoretical analysis revealed that the ground state of F₂PNS is a triplet spin state rather than a singlet state. [2] Despite this finding, no study has explained why F₂PNS exhibits the triplet spin state as its ground state. Consequently, we conducted density functional theory (DFT) calculations to elucidate the stability of the triplet spin state of F₂PNS. We initially assessed the performance of various DFT functionals in calculating the energy difference between the singlet and triplet spin states of F₂PNS, referencing the results obtained using the CCSD(T) method. Notably, the MN15 functional exhibited superior performance in this regard. We calculated the singlet and triplet spin states of F₂XNY (X = P, As, and Sb; Y = S, Se, and Te) using the MN15/QZ4P method. The triplet spin states of F₂XNY are notably more stabilized than the singlet states when X and Y are heavier elements. Energy decomposition analysis was employed to shed light on the observed energetic trends.

References

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- [2] Moon, J.; Baek, H.; Kim, J. Ab Initio Investigation of the Ground States of F₂P(S)N, F₂PNS, and F₂PSN. *J. Phys. Chem. A* **2016**, *120*, 9198-9202.