

Estimation of the thermodynamic and physicochemical properties of the alkali astatides: how weak are the bonds in molecular astatine (At₂) and tennesseine (Ts₂)?

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Astatine, element 85, occurs on earth with an estimated total abundance of less than 1 g [1]. One of its longest-lived isotopes, ²¹¹At, with a half-life of 7.2 h, is of considerable interest as an α particle emitting radionuclide for targeted alpha therapy (TAT), but only nanogram quantities are available through synthetic methods. Recently, sodium astatide, NaAt, was produced and successfully used as a therapeutic drug, leading to marked tumor regression effects in mice that had received grafts of thyroid cancer cells [2]. Thus, there is renewed interest in the properties of astatine and astatine containing compounds. The recent [3] accurate and precise determination of the electron affinity (*EA*) of the astatine atom At⁰ warrants a re-investigation of the estimated thermodynamic properties of At⁰ and astatine containing molecules as this *EA* was found to be much lower (by 0.4 eV) than previous estimated values. In this contribution we estimate, from available data sources, the following thermodynamic and physicochemical properties of the alkali astatides (MAt, M = Li, Na, K, Rb, Cs): their solid and gaseous heats of formation, lattice and gas-phase binding enthalpies, sublimation energies and melting temperatures. Use of Born-Haber cycles together with the new *EA*(At⁰) value allows the evaluation of $\Delta H_f^\circ(\text{At}^0)_a$ from which it is concluded that At₂ (and Ts₂) are weakly bonded species (*D_e* < 50 kJ/mol), in agreement with the finding from theory that spin-orbit coupling considerably reduces these bond strengths [4]. Bond order assessments of the dihalogens X₂ (X = F, Cl, Br, I, At, Ts) with and without spin-orbit coupling confirm these findings. Like F₂, At₂ belongs to the charge-shift bonding systems [5], but for a different reason. A comparison of the potential energy curves for the X₂ diatomics will be presented.

References

1. R. Si, C. Froese Fischer; Phys. Rev. A, **98**, 052504 (2018)
2. T. Watabe *et al.*; J. Nucl. Med., **60**, 1301 (2019)
3. D. Leimbach *et al.*; Nat. Commun. **11**, 3824 (2020)
4. J. Graton *et al.*; Phys. Chem. Chem. Phys., **20**, 29616 (2018)
5. S. Shaik *et al.*; Nat. Chem., **1**, 443 (2009)