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Towards a stronger halogen bond involving At — Investigation of halogen-bonded adducts of AtI and Bu3PO

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Astatine (At, Z=85) is a radioelement belonging to the halogen group. One of the astatine isotopes, At-211, is considered as a promising candidate for targeted alpha-immunotherapy. A prerequisite is to efficiently label carrier-targeting agents with At-211, which requires knowledge on astatine chemistry and to investigate its reactivity.
A halogen bond corresponds to the interaction between an electrophilic region of a halogenated compound R-X (called halogen-bond donor) and a Lewis base B (called halogen-bond acceptor). Recently, some of us have evidenced the very first halogen bonds involving astatine, that is between the astatine monoiodide (AtI) and nine Lewis bases. The associated equilibrium constants (log KBAtI) were measured through competition experiments. The present work aims at extending the previous halogen-bond scale and looking for stronger halogen-bond acceptors for AtI. To this end, the Lewis base tri-n-butylphosphine oxide (Bu3PO) was selected. In contrast with the previous study, Bu3PO can not only lead to 1:1 adduct (B···AtI), but also to 1:2 one (B2···AtI). The equilibrium constant for the formation of the 1:1 adduct is 4.16 ± 0.34, which is in good agreement with the theoretical calculations. For now, it is the strongest halogen-bond involving At that has been reported. The nature of the 1:2 adduct, which is quite original from a chemist's point of view, will be revealed by means of relativistic quantum mechanical calculations.

Choix de session parallèle

5.2 La radio-chimie théorique aux interfaces physique/chimie et théorie/expérience

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