[MS21-04] X-ray scattering of the Pt hexa halides of Cl, Br and I and Ta_6Br_{12} for XFEL

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In X-ray laser experiments the impact of the extreme X-ray pulse flux on atoms is expected to lead to expulsion of atomic electrons starting with the core electrons [1]. These are the source of the anomalous and dispersive differences in MAD. I have suggested that metal atoms as markers can assist in XFEL based protein electron density interpretation [2]. Thus examples of currently challenged structure determination cases such as alpha-crustacyanin , a 320kDa 16mer multi protein complex, which are suited for the XFEL [3], would benefit from such marker atoms. Heavy metal clusters would be needed the larger the complex, as is this case. We have been investigating $PtBr_6$ without and with Ta_6Br_{12} in lysozyme currently with lab X-ray sources in 'zero dose' and progressively increasing X-ray dose conditions, firstly as a support for MAD protein powder diffraction [4]. In addition the related isomorphous PtI_6 lysozyme complex has been studied at progressively increasing X-ray doses and Pt Cl_6 thus far at 'zero dose'. These various experiments were at cryo temperature. The $PtBr_6$ lysozyme case at progressively increasing X-ray doses we have also studied at room temperature. The stability of $PtBr_6$ under UV irradiation has been studied and reported in the literature [5]. The X-ray scattering behaviour of these complexes under femtosecond intense X-ray pulse conditions we plan to investigate at an XFEL and for the sub nano second to longer timescales we have plans to utilise ESRF. These time-resolved X-ray scattering signatures and their stabilities as inorganic metal complexes are of fundamental interest. Their use in structure determination of alpha crustacyanin can follow either under nanocrystal or ultimately single molecule simple forms.

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