Molecular RMC simulation on amorphous [$(PhSn)_4S_6$] without using potentials

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The structure of the white-light generating amorphous material [$(PhSn)_4S_6$] is investigated using X-ray scattering coupled with a rigid molecular RMC modelling approach. For this RMC_POT is modified to treat molecules in a constrained fashion and to prepare the necessary molecular starting configurations in cases where no crystal structure is available. This way experimental proof for an adamantane-like molecule structure is found. The intermediate-range structure is analysed, indicating a strong preference for distinct cluster orientations. It is shown that rigid molecular RMC simulations are feasible for structure analysis without using force fields.