Modelling thorium phosphate diphosphate

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A continuing problem in the nuclear industry is that of storing radioactive waste for long periods of time. Phosphate matrixes are possible candidates because of their resistance to radiation effects and low solubility. A compound has been synthesised as a possible candidate, $Th_4(PO_4)_4P_2O_7$ (Benard *et al.*, 1996). The formulation was derived from the crystal structure and an atomistic simulation has been attempted. The bond distances for the phosphate and diphosphate groups in the original crystal structure were different from those found in other phosphate compounds. There appeared to be some disorder at the diphosphate site related to half occupancy at the bridging oxygen. An infra red spectrum confirms the presence of the diphosphate group. To model both phosphate and diphosphate in the same molecule different parameters were used for each and tested in the compound $Na_6[Th(PO_4)(P_2O_7)]_2$, (Kojic−Prodic *et al.*, 1982).

References:

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