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Structural variations in mercurian tetrahedrite

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ABSTRACT

The structures of four mercurian tetrahedrite samples, $^{[IV]}[(Cu^{+})_4(Hg,Zn,Fe)_2]\ ^{[III]}(Cu^{+})_6{}^{[III]}(Sb,As)_4{}^{[IV]}S_{12}{}^{[VI]}S$, with Hg-contents ranging from 0.32 to 1.15 apfu were refined by least-squares in space group $I\bar{4}3m$ to agreement factors $R < 0.027$. The *a* cell dimension varied from 10.3310(2) to 10.4033(2) Å; both the *a* cell dimension and the size of the $^{[IV]}$M1 site vary linearly with the Hg content. The magnitude of the observed variation in the *a* cell dimension partially validates the empirical relationship developed by previous investigators. The degree of distortion and amount of rotation of the $^{[IV]}$M1 tetrahedron as a function of the M1-S1 bond length is comparable to that predicted by the empirical relationships of previous investigators when the As content is taken into account. The spinner blade length remains virtually unchanged because the Hg substitution takes place at M1 and the As:Sb ratio varies only slightly. The structural trends as a function of composition in these mercurian tetrahedrites closely follows those previously predicted by modeling using ionic radii and