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$(CuI)_3(As_4Q_4)_2$ (Q = S, Se)

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The crystal structures of the adduct compounds $(CuI)_3(As_4S_4)_2$ and $(CuI)_3(As_4Se_4)_2$ were determined by single crystal X-ray diffraction analysis. They crystallize isotypically in the space group $C2/c$ (No. 15), $Z = 4$, with $a = 16.529(2)$ Å, $b = 12.404(2)$ Å, $c = 13.324(2)$ Å, $b = 127.28(1)°$ for $(CuI)_3(As_4S_4)_2$ and $a = 16.779(2)$ Å, $b = 12.717(2)$ Å, $c = 13.693(2)$ Å, $b = 127.69(1)°$ for $(CuI)_3(As_4Se_4)_2$, respectively. Both structures consist of cage-like As_4Q_4 (Q = S, Se) molecules which are identical to those in a-As_4S_4 (realgar). The molecules that have almost point group symmetry D_{2d} are embedded in a matrix of copper(I) iodide, see Figure 1. Raman spectra indicate strong interactions between the embedded molecules and the surrounding matrix.

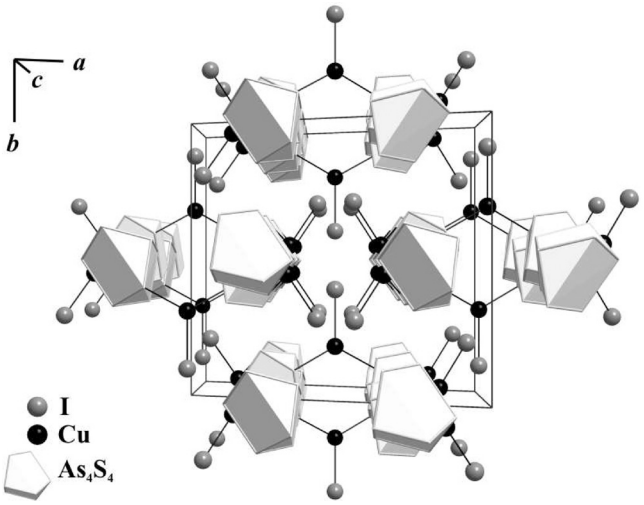

Figure 1. Section of the crystal structure of $(CuI)_3(As_4S_4)_2$ with view along c. Copper(I) is exclusively coordinated to sulfur atoms of the As_4S_4 cages and iodide ions.

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