

IUCRData - Supporting information

Ta₆I₁₂(H₂O)₆]I₂·4H₂O

The crystals obtained are washed several times with water and dried for six hours in high vacuum (10⁻⁶ mbar) at 60 °C. The co-crystallized water molecules are thereby removed from the cluster material.

Elemental analysis: M [H₁₂I₁₄O₆Ta₆] = 2970.379 g·mol⁻¹: found H = 0.42 % (calc. 0.41 %).

NMR: MeCN-d₃ is dried by refluxed for several hours with CaH₂ and finally distilled under Schlenk conditions.

¹H NMR (MeCN-d₃), 300 MHz, 300 K, ppm): δ = 2.13 (s, 12H, H₂O).

IR (300 K, ATR, cm⁻¹): $\tilde{\nu}$ = 577 (s), 1581 (m), 1628 (m), 2108 (w), 2353 (w), 3204 (w).