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The first occurrence of the carbide anion, C^{4-}, in an oxide mineral: Mikecoxite, ideally $(CHg_4)OCl_2$, from the McDermitt open-pit mine, Humboldt County, Nevada, U.S.A.

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Abstract

Mikecoxite, ideally $(CHg_4)OCl_2$, is the first mercury-oxide-chloride-carbide containing a C^{4-} anion coordinated by four Hg atoms (a permercurated methane derivative) to be described as a mineral species. It was found at the McDermitt open-pit mine on the eastern margin of the McDermitt Caldera, Humboldt County, Nevada, U.S.A. It is monoclinic, space group $P2_1/n$, Z = 4; a = 10.164(5), b = 10.490(4), c = 6.547(3) Å, V 698.0(5) Å^3. Chemical analysis by electron microprobe gave Hg 86.38, Cl 11.58, Br 0.46, C 1.81, sum = 100.23 wt%, and O was detected but the signal was too weak for quantitative chemical analysis. The empirical formula, calculated on the basis of Hg + Cl + Br = 6 apfu, is $(C_{1.19}Hg_{3.39})(Cl_{2.57}Br_{0.05})_{\Sigma 2.62}$, and the ideal formula based on the chemical analysis and the crystal structure is $(CHg_4)OCl_2$. The seven strongest lines in the X-ray powder diffraction pattern are [d (Å), I, (hkl)]: 2.884, 100, (230); 2.989, 81, ($\bar{3}01$, 301, $\bar{1}12$, 112, $\bar{1}31$, 131); 2.673, 79, ($\bar{1}22$, 122, $\bar{2}12$, 212); 1.7443, 40, (060, $\bar{4}32$, 432); 5.49, 34, ($\bar{1}01$, 101); 4.65, 32, (120); 2.300, 30, ($\bar{3}12$, 312). The Raman spectrum shows three bands at 638, 675, and 704 cm^{-1}, well above the range characteristic of NHg_4 stretching vibrations between 540 and 580 cm^{-1}, that are assigned to CHg_4 stretching vibrations. Mikecoxite forms intergrowths of bladed crystals up to 100 μm long that occur on granular quartz or in vugs associated with kleinite. It is black with a submetallic to metallic luster and strong specular reflections and does not fluoresce under short- or long-wave ultraviolet light. Neither cleavage nor parting were observed, and the calculated density is 8.58 g/cm^3. In the crystal structure of mikecoxite, ($C^{4-}Hg_4^{2+}$) groups link through O^{2-} ions to form three-membered rings that polymerize into corrugated $[CHg_4OCl]^+$ layers with near-linear C^{4-}–Hg^{2+}–O and C^{4-}–Hg^{2+}–Cl linkages. The layers link in the third direction directly via weak Hg^{2+}–O^{2-} and Hg^{2+}–Cl^- bonds to adjacent layers and also indirectly via interlayer Cl^-. A bond-valence parameter has been derived for (Hg^{2+}–C^{4-}) bonds: R_o = 2.073 Å, b = 0.37, which gives bond-valence sums at the C^{4-} ions in accord with the valence-sum rule. The source of carbon for mikecoxite in the volcanic high-desert environment of the type locality seems to be methane, with the reaction catalyzed by microbiota through full mercuration of carbon atoms, beyond the first stage that produces the volatile and highly mobile methylmercury, $[CH_3Hg]^+$, a potent neurotoxin that accumulates in marine food chains. Both the mineral and the mineral name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2021-060). The mineral is named after Michael F. Cox (b. 1958), a founding member of the New Almaden Quicksilver County Park Association (NAQCPA) who was responsible for characterizing and remediating environmental mercury on-site and who recovered the rock containing the new mineral.

Keywords: Mikecoxite, new mineral, mercury-oxide-chloride-carbide, crystal-structure refinement, Raman spectrum, electron-microprobe analysis, McDermitt open-pit mine, Humboldt County, Nevada, U.S.A.