Hydrothermal Crystal Growth and Crystal Structures of the Mercury(II) Chromates(VI) α -HgCrO₄, β -HgCrO₄, and HgCrO₄·H₂O

Berthold Stöger and Matthias Weil

Institute for Chemical Technologies and Analytics – Division of Structural Chemistry, Vienna University of Technology, Getreidemarkt 9/164-SC, A-1060 Vienna, Austria

Reprint requests to PD Dr. M. Weil. E-mail: mweil@mail.zserv.tuwien.ac.at

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Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70th birthday

Single crystals of α -HgCrO₄, β -HgCrO₄ and HgCrO₄ · H₂O were obtained by reacting yellow HgO in chromic acid of various concentrations under hydrothermal conditions at 200 °C (4 d). All crystal structures were solved and refined from single crystal diffractometer data sets [α -HgCrO₄: $P2_1/n$, Z = 4, a = 5.5079(8), b = 8.5266(12), c = 7.3503(10) Å, $\beta = 94.022(3)^\circ$, 955 structure factors, $R[F^2 > 2\sigma(F^2)] = 0.0296$; β -HgCrO₄: *Cmcm*, Z = 4, a = 5.7187(9), b = 9.0169(14), c = 7.0114(11) Å, 361 structure factors, $R[F^2 > 2\sigma(F^2)] = 0.0275$; HgCrO₄ · H₂O: $P\overline{1}$, Z = 2, a = 5.6157(15), b = 6.1115(16), c = 7.590(2) Å, $\alpha = 108.850(5)$, $\beta = 91.666(5)$, $\gamma = 116.569(5)^\circ$, 1235 structure factors, $R[F^2 > 2\sigma(F^2)] = 0.0316]$. The previously reported structure of α -HgCrO₄ has been re-determined. It contains distorted [HgO₇] pentagonal bipyramids in which the short bonds are directed towards the apices. The new polymorph β -HgCrO₄ adopts the CrVO₄ (β -CrPO₄) structure type and is composed of slightly distorted [HgO₆] octahedra. The previously unknown monohydrate HgCrO₄ · H₂O crystallizes in an unique structure and is composed of one nearly regular [HgO₄(H₂O)₂] octahedron and one considerably distorted [HgO₆] octahedron. All three structures contain tetrahedral chromate anions CrO₄²⁻ as the second building units with average Cr-O distances of *ca*. 1.65 Å.

Key words: Mercury(II), Chromates(VI), Crystal Structure, Hydrothermal Synthesis