Hydrothermal Crystal Growth and Crystal Structures of the Mercury(II) Chromates(VI) $\alpha$-HgCrO$_4$, $\beta$-HgCrO$_4$, and HgCrO$_4 \cdot$H$_2$O

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Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70$^{th}$ birthday

Single crystals of $\alpha$-HgCrO$_4$, $\beta$-HgCrO$_4$ and HgCrO$_4 \cdot$H$_2$O were obtained by reacting yellow HgO in chromic acid of various concentrations under hydrothermal conditions at 200 $^\circ$C (4 d). All crystal structures were solved and refined from single crystal diffractometer data sets [$\alpha$-HgCrO$_4$: $P2_1/n$, $Z = 4$, $a = 5.5079(8)$, $b = 8.5266(12)$, $c = 7.3503(10)$ Å, $\beta = 94.022(3)^\circ$, 955 structure factors, $R[F^2 > 2\sigma(F^2)] = 0.0296$; $\beta$-HgCrO$_4$: $Cmcm$, $Z = 4$, $a = 5.7187(9)$, $b = 9.0169(14)$, $c = 7.0114(11)$ Å, 361 structure factors, $R[F^2 > 2\sigma(F^2)] = 0.0275$; HgCrO$_4 \cdot$H$_2$O: $P\overline{1}$, $Z = 2$, $a = 5.6157(15)$, $b = 6.1115(16)$, $c = 7.590(2)$ 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 $\alpha$-HgCrO$_4$ has been re-determined. It contains distorted [HgO$_7$] pentagonal bipyramids in which the short bonds are directed towards the apices. The new polymorph $\beta$-HgCrO$_4$ adopts the CrVO$_4$ ($\beta$-CrPO$_4$) structure type and is composed of slightly distorted [HgO$_6$] octahedra. The previously unknown monohydrate HgCrO$_4 \cdot$H$_2$O crystallizes in an unique structure and is composed of one nearly regular [HgO$_4$(H$_2$O)$_2$] octahedron and one considerably distorted [HgO$_6$] octahedron. All three structures contain tetrahedral chromate anions CrO$_4^{2-}$ 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