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Crystal Structure of a New Monoclinic Phase of KD_2PO_4 at Room Temperature

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The crystal structure of a new monoclinic phase of potassium dideuterium phosphate, KD_2PO_4, at room temperature has been determined by X-ray single crystal diffraction method. Colorless crystals were grown from aqueous solution of KD_2PO_4 reagent with the heavy water(D_2O) by slow evaporation under an argon atmosphere. Crystals are monoclinic, space group $P2_1$ with a=7.1666(4), b=14.7117(10), c=7.4695(7)Å, β=92.324(6)°, V=786.88(10)Å^3, and Z=8. The Structure was refined to $R(F^2)$=0.026 and $wR(F^2)$=0.065 for 1913 reflections with $I > 2\sigma(I)$. The four crystallographically nonequivalent phosphate groups appear to exist as $[H_2PO_4]^{-1}$ ions. This study provides the first example of crystal structure determination of the monoclinic KD_2PO_4 at room temperature.

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