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High-temperature crystal structures and chemical modifications in RbH_2PO_4 RONALD J. TACKETT, HEBER MARTINEZ, RUSSEL R. CHIANELLI, University of Texas at El Paso, JIANZHONG ZHANG, YUSHENG ZHAO, Los Alamos National Laboratory, CRISTIAN E. BOTEZ, University of Texas at El Paso — We have used labortatory and synchrotron x-ray diffraction to investigate the structural and chemical changes undergone by polycrystalline RbH_2PO_4 upon heating within the 30-250 °C temperature regime. We report no evidence of the previously reported onset of partial polymerization at $T = 96$°C which was proposed as an explanation for the observed high-temperature several-order-of-magnitude increase in proton conductivity observed in phosphate-based solid acids. Instead, we found that a tetragonal-to-monoclinic polymorphic transition initiates at $T \sim 90$°C. The transition is complete at $T \sim 130$°C, and the new monoclinic RbH_2PO_4 polymorph is stable upon further heating to $T = 200$°C. Moreover, this reported monoclinic phase is *isomorphic* to that of monoclinic CsH_2PO_4. This remarkable similarity suggests that the microscopic structures and dynamics responsible for the high-temperature superprotonic behavior of RbH_2PO_4 could be the same as those of its Cs-based counterpart.

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