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CDW - MH phase transition in [Pd(cptn)2Br]Br2 studied by 3D-PDF

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The occurrence of a Mott-Hubbard (MH) to Charge-Density-Wave (CDW) phase transition in the quasi-one-dimensional Bromo-bridged Pd compound [Pd(cptn)2Br]Br2 (cptn = (1R,2R)-trans-1,2-Cyclopentadiamine) was investigated by means of single crystal X-ray diffraction employing the novel 3D-ΔPDF method. Raman and STM measurements indicate that the phase transition occurs slightly above 100K and that should be accompanied by a dimerization of Pd-Br pairs along the 1D chain in order to stabilize the CDW state. The existence of such state is demonstrated by the measured variation of Spin susceptibility with temperature. However, no change of the Orthorombic structure over the relevant temperatures is observed. Clear evidence of the presence of diffuse scattering streaks above 100K allows for modelling of 1D disorder with the program Yell [1], which yields the expected dimerization in a layered fashion along with precise values of the present in- and out-of-plane correlations. The presence of unexpected Bragg peaks that could be assigned to a Monoclinic structure was also investigated and points to a phase separation phenomena.

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