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Crystal Structure of the 2:1 Adduct of 1,2-Benzenediol and Hexamethylenetetramine. Kadsada Sala¹, Kenneth J. Haller¹, Seik Weng Ng², ¹School of Chemistry, Suranaree Univ. of Technology, Nakhon Ratchasima 30000 Thailand, ² Institute of Postgraduate Studies, Univ. of Malaya, Kuala Lumpur 50603 Malaysia.

The cocrystal product of an aqueous solution of 1,2-benzenediol (catechol) and hexamethylenetetramine (HMT) has been characterized by single crystal X-ray diffraction. The crystal structure consists of a zigzag arrangement of HMT along the *c* direction, with adjacent molecules connected by strong O–H···N hydrogen bonds from two catechol molecules. Each catechol molecule is hydrogen bonded to two HMT molecules, and each HMT molecule is hydrogen bonded to four catechol molecules. Thus, pairs of catechol molecules connect adjacent HMT molecules along the chain. Only weak interactions are observed between the chains in the *a* and *b* directions.

Crystal Data: 2C₆H₆O₂:C₆H₁₂N₄, *M_r* = 360.41, monoclinic, C2/*c*, *a* = 23.5925(7), *b* = 6.8339(2), *c* = 13.1856(3) Å, *beta* = 123.136(2)°, *V* = 1780.2(1) Å³, *Z* = 4, *D_{calc}* = 1.345 Mg m⁻³, *T* = 200 K, *m* = 0.097 mm⁻¹, 2264 refl, 1956 refl > 2σ(*I*), *R* = 0.053, ρ_{max} = 0.39 e Å⁻³.