High-pressure Crystal Phase of 1,2-ethylenediamine

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1,2-Ethylenediamine ($\rm H_2N~CH_2~CH_2~NH_2$) is the simplest of α,ω -alkanediamines. Its m.p. is 284.29 K [1], and it was crystallized at low temperature and its structure determined at 213 K [2] and 130 K [3]. The crystals are monoclinic, space group $P2_1/c$, a=5.047(2), b=7.14(2), c=5.475(2) and $\beta=115.36(3)$ [3] (hereafter phase II).

In our study we have crystallized $C_2H_8N_2$ by pressure-freezing in Merrill-Bassett diamond-anvil cell. In this way three distinct phases of $C_2H_8N_2$ have been obtained and their structures determinated: phase II with the unit cell parameters similar to those listed above for the low-temperature phase; phase I (which is stable at lower pressure and higher temperature, than for phase II) – monoclinic, space group $P2_1/c$ a = 5.031(10), b = 5.132(3), c = 7.167(5), $\beta = 110.60(12)^\circ$ at 0.3 GPa and 293(2) K; at 1.5 GPa the crystal is transformed to phase III with the unit-cell doubled.

The structures have been solved by direct methods and refined by full matrix least squares.

[1] Messerly J.F., Finke H.L., Osborn A.G., Douslin D.R., *J. Chem. Thermodyn*, 1975, 7, 1029. [2] Jamet-Delcroix P.S., *Acta Cryst.*, 1973, **B29**, 977. [3] Thalladi V.R., Boese R., Weiss H.-C., *Angew. Chem. Int. Ed.*, 2000, **39**, 918.

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