

## Supplementary information

### Pressure-induced planar N<sub>6</sub> rings in potassium azide

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Table S1. Structural parameters of metastable phases of KN<sub>3</sub> at 100 GPa.

Space group	Lattice parameters( $\text{\AA}$ , $^\circ$ )	Atomic coordinates(fractional)
Imma	$a=4.740, b=4.034, c=6.245$ $\alpha=\beta=\gamma=90$	K $4e$ (0.0000, 0.2500, 0.3271)
		N $4e$ (0.0000, 0.2500, 0.9421)
		N $8i$ (0.2569, 0.2500, 0.6438)
$P\bar{1}$	$a=5.002, b=2.799, c=5.017$ $\alpha=81.629, \beta=111.488, \gamma=74.331$	K $2i$ (0.0481, 0.2675, 0.3157)
		N $2i$ (0.6327, 0.0237, 0.0558)
		N $2i$ (0.3153, 0.7159, 0.1381)
		N $2i$ (0.5470, 0.5328, 0.3966)

Fig. S1. The electronic band structure of I4/mcm phase at 0 GPa.

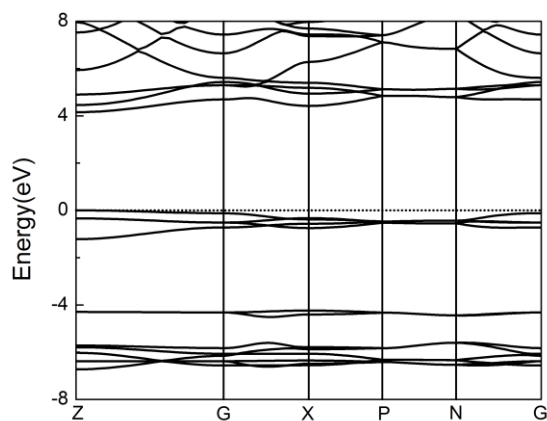


Fig. S2. The electronic band structure of C2/m phase at 30 GPa.

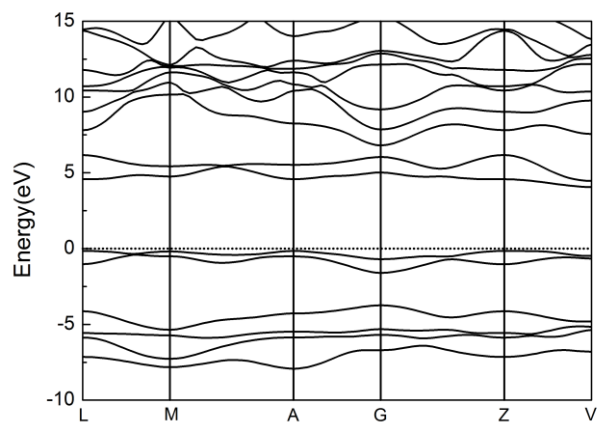


Fig. S3. The electronic band structure of Imma phase at 100 GPa.

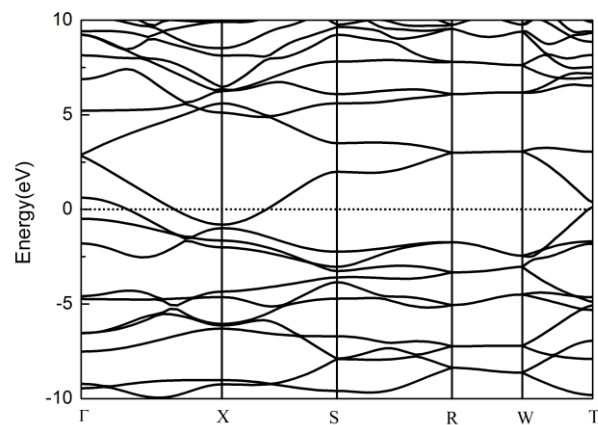


Fig. S4. The electronic band structure of  $P\bar{1}$  phase at 100 GPa.

