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Supplementary Information for Crystal Structure of Silver Pentazolates AgN_5 and AgN_6

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Table S1: Crystallographic information for AgN_5-$P2_1/c$ and AgN_6-$P2_12_12$ at 0 GPa.

Crystal	Lattice parameters (Å, °)	Atomic positions
AgN_5-$P2_1/c$	a=3.44644; b=9.15045; c=9.25141 α=γ=90; β=90.6714	Ag (0.943, 0.250, 0.501) N1 (0.826, 0.086, 0.323) N2 (0.696, 0.957, 0.365) N3 (0.834, 0.086, 0.179) N4 (0.620, 0.878, 0.248) N5 (0.709, 0.957, 0.133)
AgN_6-$P2_12_12$	a=9.707103; b=12.097535; c=3.341592 α=β=γ=90	Ag (0.822, 0.091, 0.007) N1 (0.716, 0.245, 0.120) N2 (0.763, 0.343, 0.007) N3 (0.587, 0.254, 0.250) N4 (0.661, 0.413, 0.069) N5 (0.553, 0.358, 0.220) N6 (0.055, 0.488, 0.475)

From the electronic band structure calculations at 0 GPa presented in Fig. S1 it is evident that AgN_5-$P2_1/c$ is an insulator with a band gap of 3.03 eV and from Fig. S2 that AgN_6-$P2_12_12$ is an insulator with a band gap of 3.15 eV.

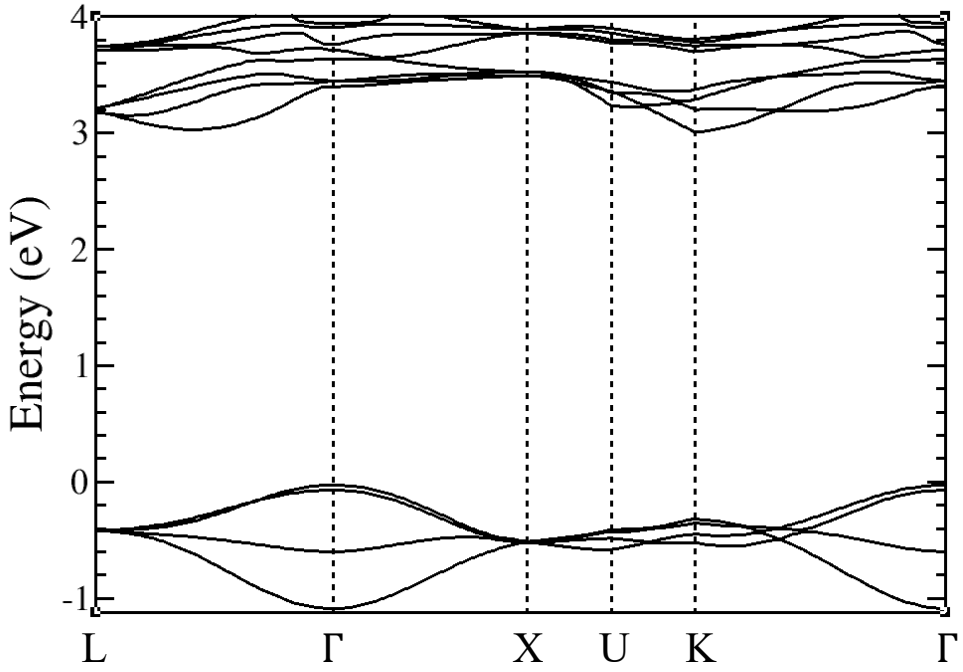

Figure S1: Electronic band structure of AgN_5-$P2_1/c$.

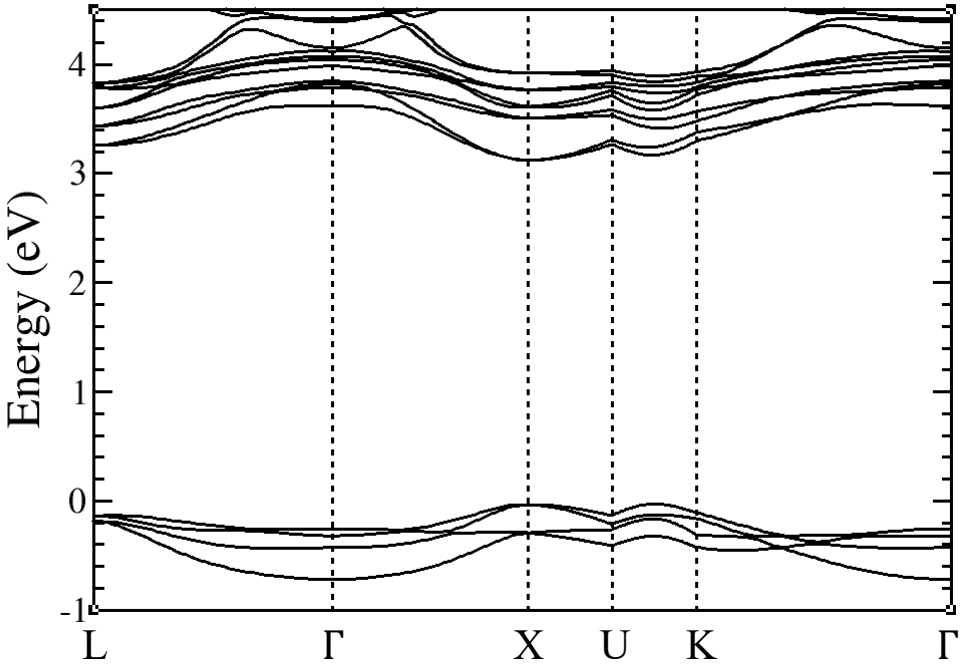

Figure S2: Electronic band structure of AgN_6-$P2_12_12_12$.

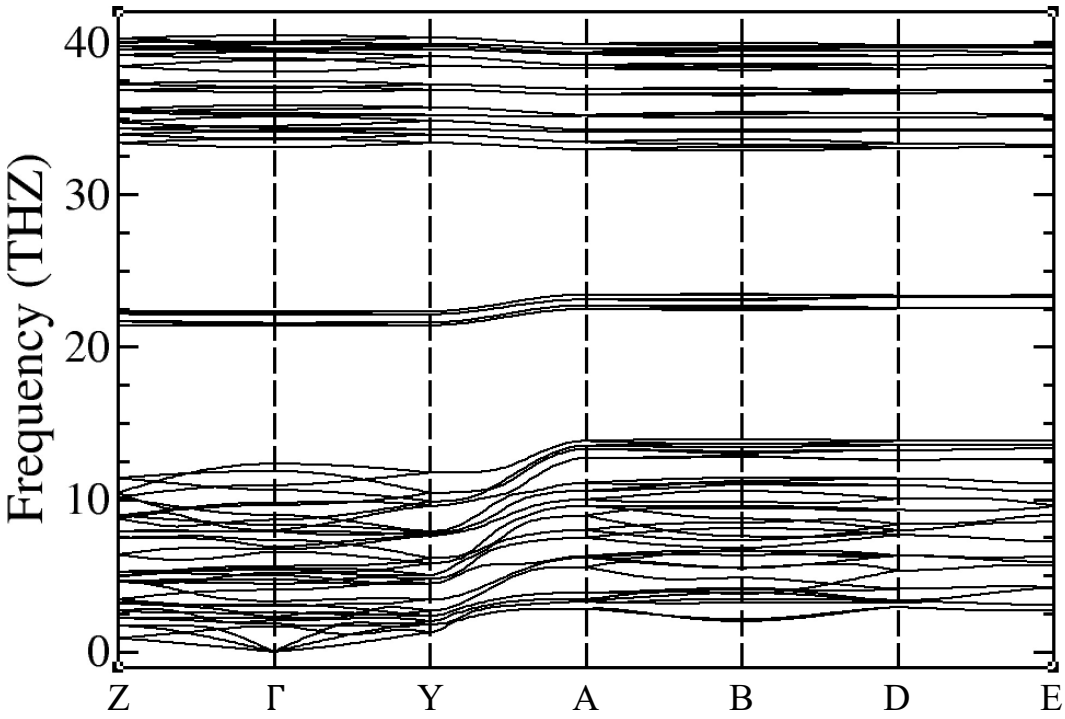

Figure S3: Phonon band structure of AgN_5-$P2_1/c$ at 0 GPa show no negative frequencies, indicating the crystal is dynamically stable.

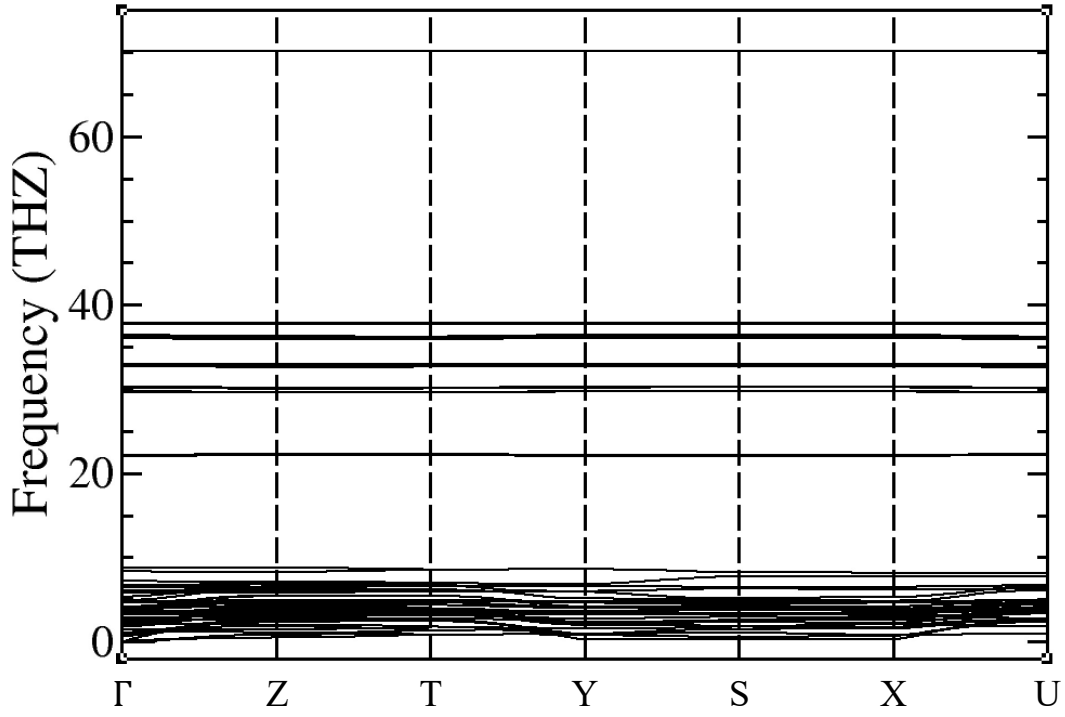

Figure S4: Phonon band structure of AgN_6-$P2_12_12$ at 0 GPa show no negative frequencies, indicating the crystal is dynamically stable.