Supplemental Material for

CuN_{10}: A High-Energy-Density Pentazolates with Antiferromagnetic State

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Tab. S1. Calculated lattice constants and atomic positions of the $P2_12_12_1$-CuN_{10} structures.

Allotrope	Lattice(Å)	Space group	Atomic positions	
$P2_12_12_1$-CuN_{10}	a=8.307 b=8.166 c=9.031	$P2_12_12_1$	Cu1(0.750 0.215 0.239)	
			N1(0.075 0.142 0.094)	N2(0.954 0.099 0.185)
			N3(0.989 0.961 0.253)	N4(0.132 0.919 0.205)
			N5(0.186 0.030 0.106)	N6(0.953 0.671 0.801)
			N7(0.039 0.700 0.924)	N8(0.149 0.586 0.931)
			N9(0.128 0.488 0.812)	N10(0.006 0.540 0.732)

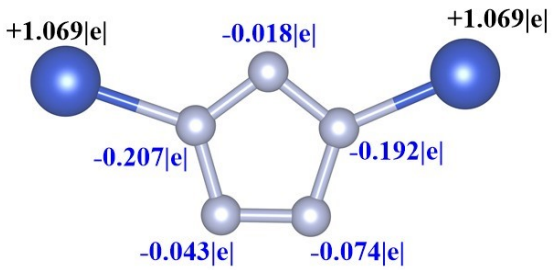

Fig. S1. The atomic Bader charge transfer in $P2_12_12_1$-CuN_{10} crystal.

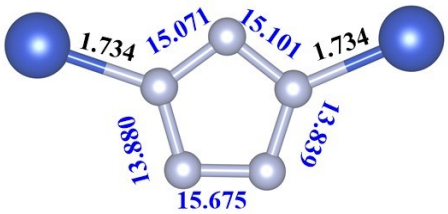

Fig. S2. The integral crystal orbital Hamilton populations (-ICOHP) of Cu-N and N-N bonds in $P2_12_12_1$-CuN_{10} crystal.

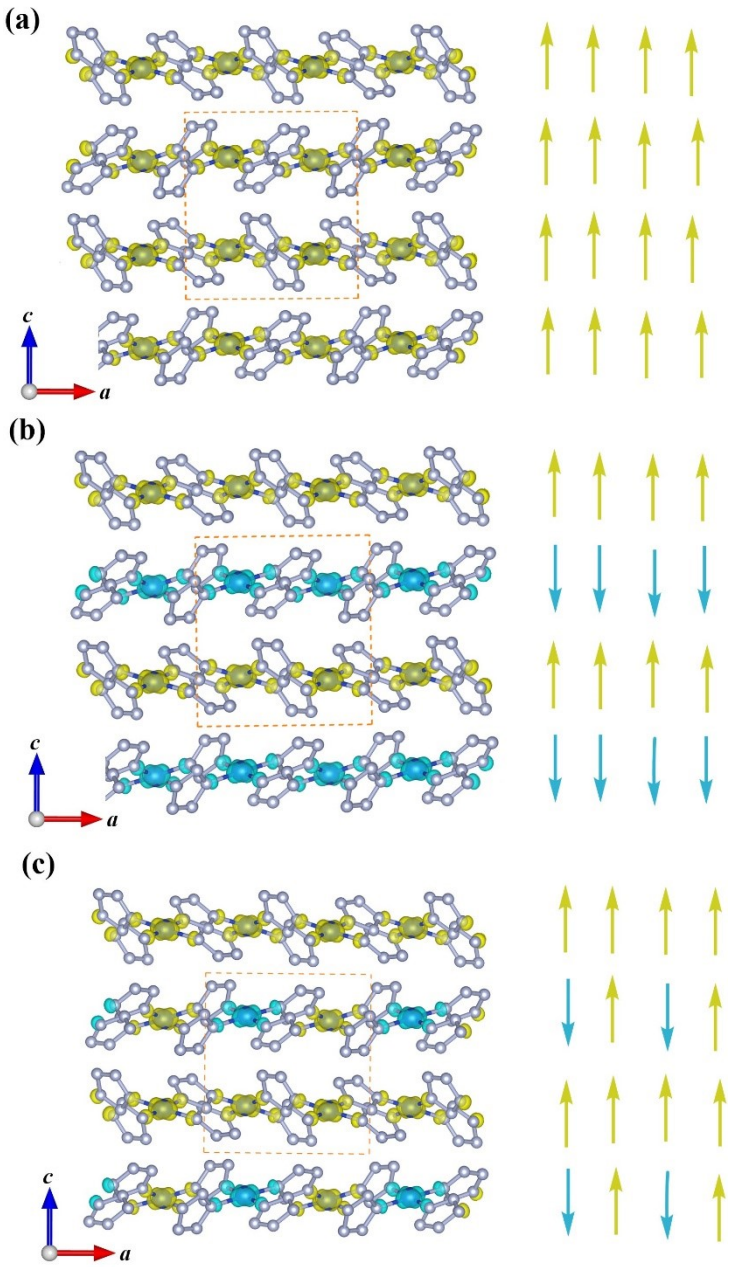

Fig. S3. Spin charge distribution of $P2_12_12_1$-CuN_{10} crystal in (a) FM, (b) AFM2 and (c) FIM state. When referring to the energy of AFM1 ordering state, the energy of FM, AFM2 and FIM ordering states are 0.121, 0.118 and 0.061 eV/unit, respectively.