

SUPPLEMENTARY INFORMATION

Versatility of the Cyano Group in Intermolecular Interactions

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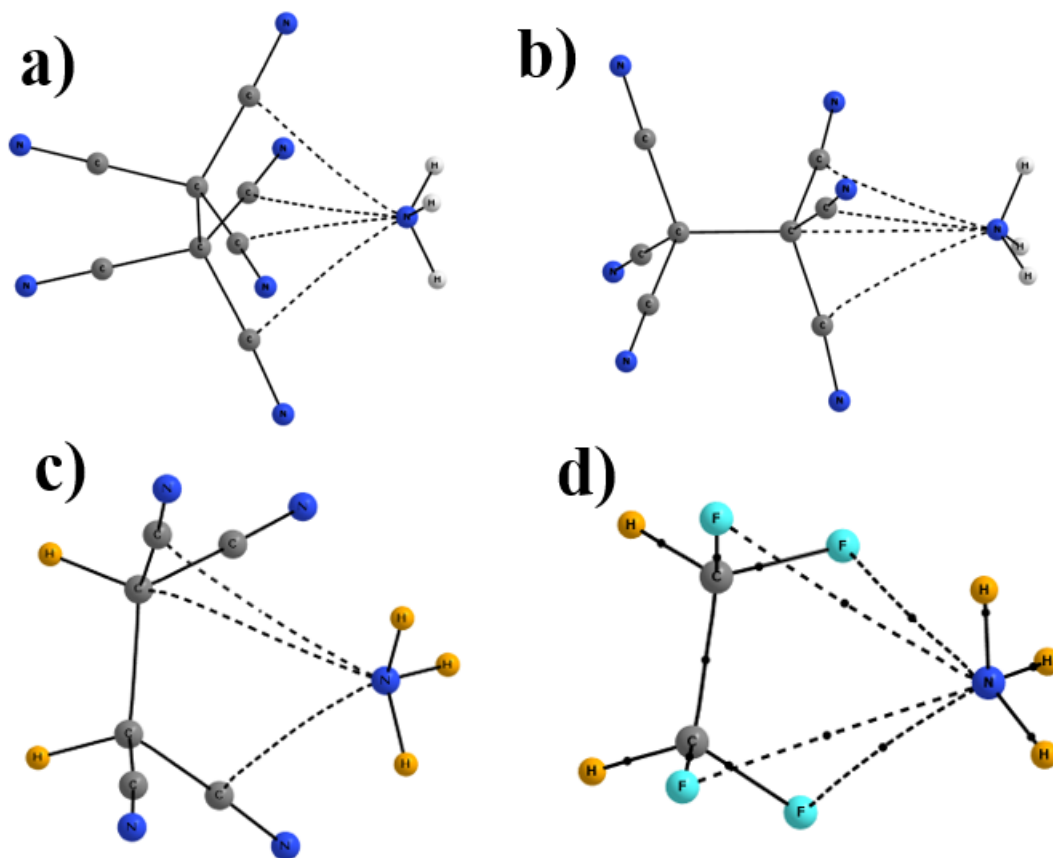


Fig S1. AIM bond paths in complexes of NH_3 with $(\text{CN})_3\text{C}-\text{C}(\text{CN})_3$ in a) side-on and b) end-on complexes, c) $(\text{CN})_2\text{HC}-\text{CH}(\text{CN})_2$ and d) $\text{F}_2\text{HC}-\text{CHF}_2$

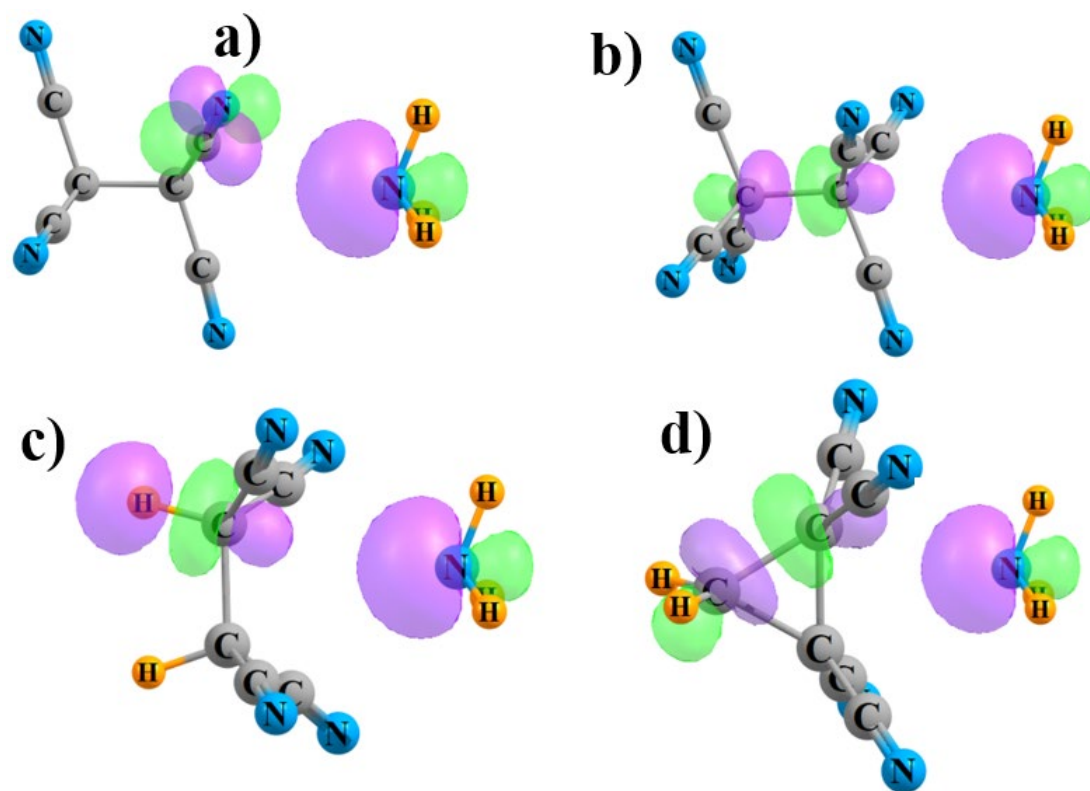


Fig S2. Overlap of NH₃ N lone pair orbital with a) $\pi^*(\text{C}\equiv\text{N})$, b) $\sigma^*(\text{C}-\text{C})$, c) $\sigma^*(\text{H}-\text{C})$, and d) $\sigma^*(\text{C}-\text{C})$ orbital of cyclopropane derivative.

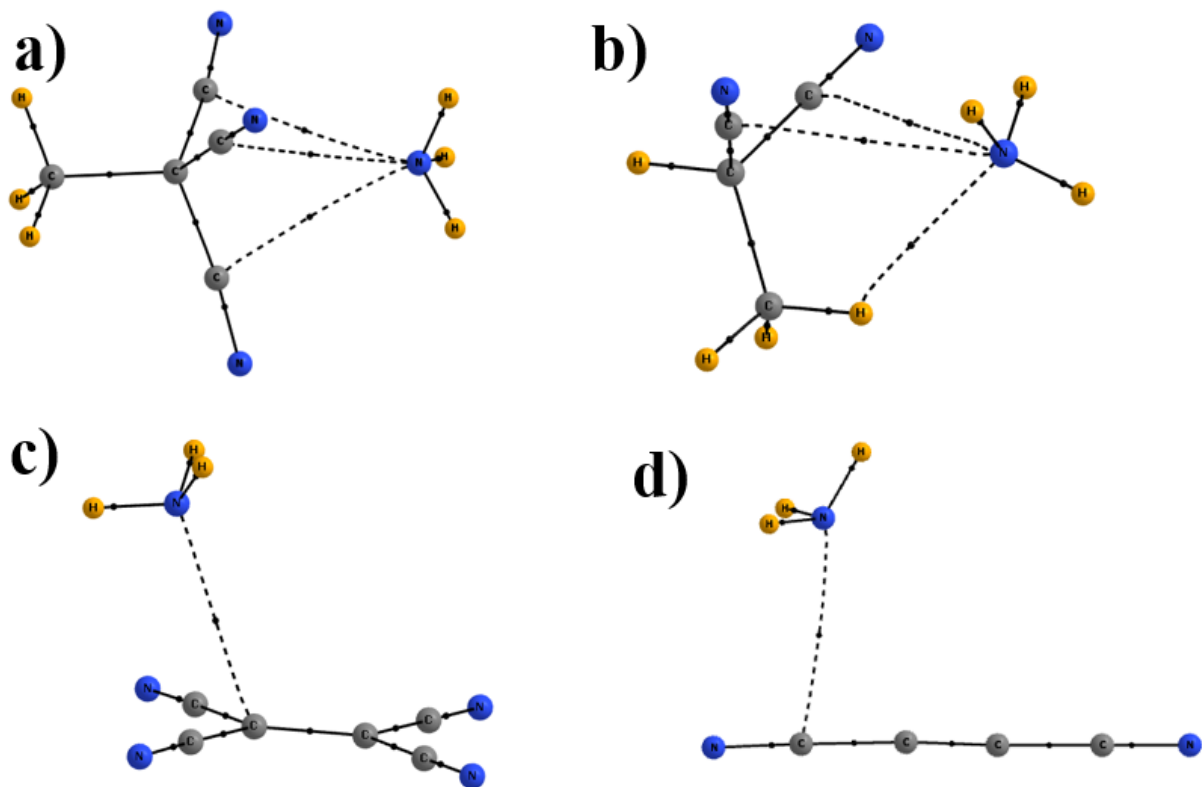


Fig S3. AIM bond paths in complexes of NH₃ with a) H₃C-C(CN)₃, b) H₃C-CH(CN)₂, c) (CN)₂C=C(CN)₂ and d) (CN)C≡C(CN).

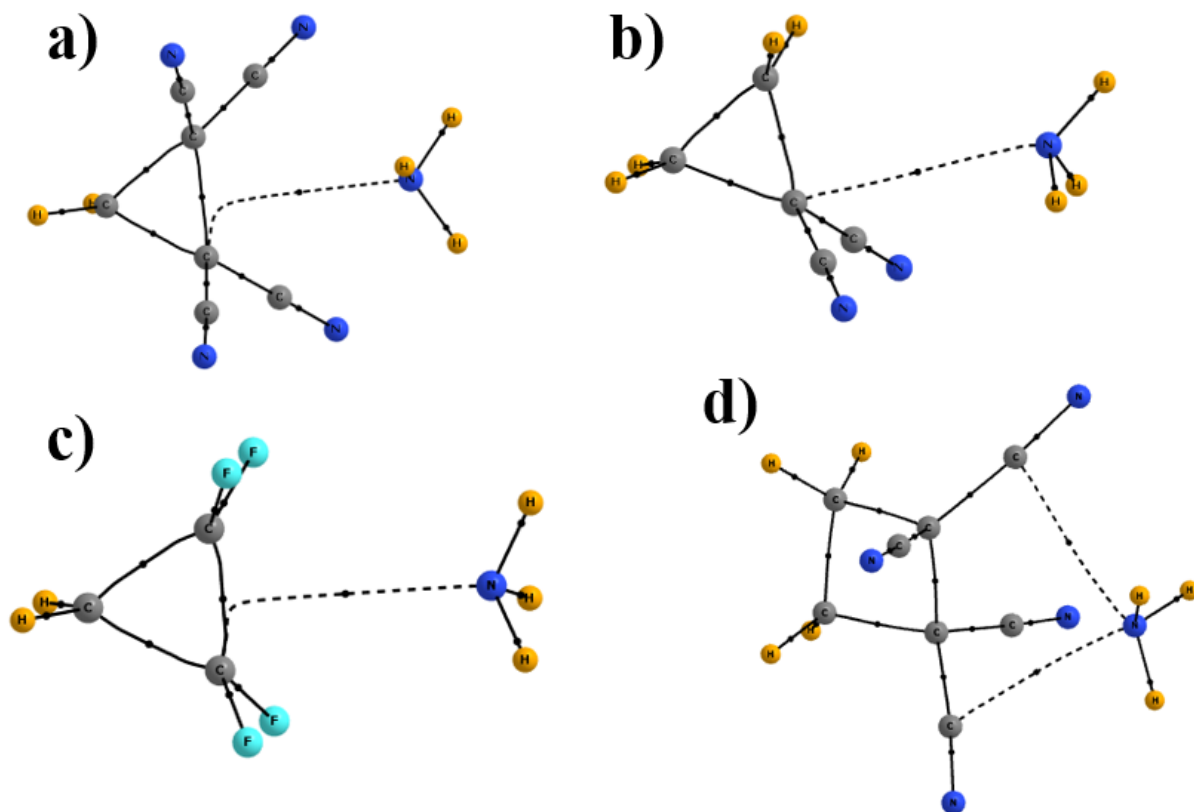


Fig S4. AIM bond paths in complexes of NH_3 with cyclic a) $\text{CH}_2\{\text{C}(\text{CN})_2\}_2$, b) $\text{CH}_2\text{CH}_2\text{C}(\text{CN})_2$, c) $\text{CH}_2\{\text{CF}_2\}_2$ and d) $\text{CH}_2\text{CH}_2\{\text{C}(\text{CN})_2\}_2$.

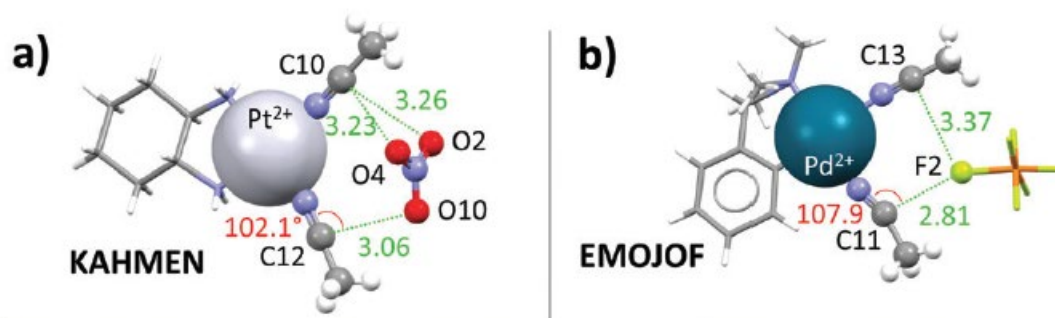


Fig S5. Examples of crystal structures containing short contacts between $\text{C}\equiv\text{N}$ groups and potential electron donors. Reproduced from Ref. 61 with permission from The Royal Society of Chemistry.

