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Supporting information

Dual role of Lewis acid and base for pnicogen and unexpected interplay between pnicogen bond and coordination interaction in $H_3N\cdots FH_2X\cdots MCN$(X = P and As; M = Cu, Ag, and Au)

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Table S1 Changes of bond lengths (Δr, Å) and frequency shifts of stretch vibrations (Δv, cm^{-1}) for F-X, M-C and C-N bonds in the dyads.

	$\Delta r_{F\text{-}X}$	$\Delta r_{M\text{-}C}$	$\Delta r_{C\text{-}N}$	$\Delta v_{F\text{-}X}$	$\Delta v_{M\text{-}C}$	$\Delta v_{C\text{-}N}$
$H_3N\cdots FH_2P$	0.026	---	---	-69	---	---
$H_3N\cdots FH_2As$	0.033	---	---	-60	---	---
$FH_2P\cdots CuCN$	-0.032	0.042	0.001	62	-1	-3
$FH_2P\cdots AgCN$	-0.032	0.010	0.001	64	17	-2
$FH_2P\cdots AuCN$	-0.037	0.095	0.001	73	-48	-7
$FH_2As\cdots CuCN$	-0.030	0.035	0.001	43	-1	-3
$FH_2As\cdots AgCN$	-0.030	0.007	0.001	46	17	-2
$FH_2As\cdots AuCN$	-0.033	0.083	0.001	49	-44	-6

Table S2 Angles (α, deg) in the triads and their differences ($\Delta\alpha$, deg) relative to the dyads.

	α_1	α_2	α_3	α_4	α_5	$\Delta\alpha_1$	$\Delta\alpha_2$
$H_3N\cdots FH_2P\cdots CuCN$	168.1	112.9	78.9	44.0	57.0	0.3	-3.7
$H_3N\cdots FH_2P\cdots AgCN$	168.2	110.8	80.9	46.6	52.5	0.1	-4.9
$H_3N\cdots FH_2P\cdots AuCN$	167.6	110.0	82.3	45.2	52.5	-0.2	-6.5
$H_3N\cdots FH_2As\cdots CuCN$	167.7	110.7	81.6	44.9	53.5	2.5	-4.2
$H_3N\cdots FH_2As\cdots AgCN$	167.8	109.5	82.7	47.1	50.2	2.6	-4.9
$H_3N\cdots FH_2As\cdots AuCN$	167.9	108.6	83.5	46.4	50.0	2.7	-6.3

Table S3 Changes of bond lengths (Δr, Å) and frequency shifts of stretch vibrations (Δv, cm^{-1}) for F-X, M-C, and C-N bonds in the triads.

	$\Delta r_{F\text{-}X}$	$\Delta r_{M\text{-}C}$	$\Delta r_{C\text{-}N}$	$\Delta v_{F\text{-}X}$	$\Delta v_{M\text{-}C}$	$\Delta v_{C\text{-}N}$
$H_3N\cdots FH_2P\cdots CuCN$	-0.009	0.037	0.001	-6	-4	-8
$H_3N\cdots FH_2P\cdots AgCN$	-0.006	0.007	0.001	-14	14	-4
$H_3N\cdots FH_2P\cdots AuCN$	-0.012	0.090	0.001	-4	-58	-8
$H_3N\cdots FH_2As\cdots CuCN$	0.003	0.031	0.001	-19	-4	-8
$H_3N\cdots FH_2As\cdots AgCN$	0.005	0.005	0.001	-22	15	-4
$H_3N\cdots FH_2As\cdots AuCN$	0.001	0.080	0.001	-17	-47	-8

Table S4 Total interaction energy (ΔE_{total}, kcal/mol) and interaction energy (ΔE, kcal/mol) between two molecular pairs in the trimers.

	ΔE_{total}	$\Delta E_{X\cdots N}$	$\Delta E_{X\cdots M}$	$\Delta E_{N\cdots M}$
$H_3N\cdots FH_2P\cdots CuCN$	-57.9	-2.3	-41.8	-9.6
$H_3N\cdots FH_2P\cdots AgCN$	-50.1	-3.9	-35.1	-8.6
$H_3N\cdots FH_2P\cdots AuCN$	-70.6	-2.9	-55.4	-8.7
$H_3N\cdots FH_2As\cdots CuCN$	-51.4	-1.4	-35.2	-8.5
$H_3N\cdots FH_2As\cdots AgCN$	-45.7	-6.3	-30.4	-7.7
$H_3N\cdots FH_2As\cdots AuCN$	-63.5	-2.2	-47.8	-8.1