Electronic Supplementary Material for PCCP

Theoretical Study of the interaction between HNZ (Z = O, S) and H_2XNH_2 (X = B, Al). Conventional and dihydrogen bonds.

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Supporting Information
Cartesian coordinates and energies including ZPE correction of monomers and complexes at the MP2/6-311++G(2d,2p) level of theory

HNO	x	y	z
N	-0.582100	0	0.130603
H	-0.563620	0	1.177304
O	0.579790	0	-0.261441
E(ZPE)= -130.215899 a.u.			

HNS	x	y	z
N	-1.007702	0	0.288014
H	-1.001878	0	1.313269
S	0.503487	0	-0.208085
E(ZPE)= -452.832032 a.u.			

H_2BNH_2	x	y	z
B	0	0	-0.780678
N	0	0	0.612996
H	0.840740	0	1.160627
H	-0.840740	0	1.160627
H	-1.041983	0	-1.354417
H	1.041983	0	-1.354417
E(ZPE)= -81.775090 a.u.			

H_2AlNH_2	x	y	z
Al	-0.547805	0	-0.356823
N	0.942851	0	0.614143
H	0.976448	0	1.618904
H	1.875449	0	0.238730
H	-0.405551		-1.925197
H	-1.924837	0	0.407257
E(ZPE)= -298.989477 a.u.			

H_2NBH_2•••HNO	x	y	z
H	-0.840987	0	0.771610
H	-0.963502	0	2.456148
H	1.539449	0	2.830535
H	1.677211	0	0.757458
N	0.250515	0	-2.025123
O	-0.844795	0	-1.466753
H	0.981340	0	-1.279292
N	-0.360060	0	1.654521
B	1.026332	0	1.758355
E(ZPE)= -211.994762 a.u.			

H_2NBH_2•••HNS	x	y	z
H	-0.507902	0	1.330046
H	-0.387013	0	3.013981
H	2.141505	0	3.033811
H	1.991340	0	0.962741
N	0.523804	0	-1.718048
H	1.094249	0	-0.865495
N	0.096793	0	2.134636
B	1.484435	0	2.043454
S	-1.006158	0	-1.288029
E(ZPE)= -534.610915 a.u.			

H_2NAlH_2•••HNO	x	y	z
H	-1.466541	0	0.602501
H	-1.500602	0	2.258856
H	1.651688	0	2.790171
H	1.580619	0	0.023272
N	0.131326	0	-2.547660
O	-0.865269	0	-1.829233
H	0.963806	0	-1.915237
Al	0.859200	0	1.431280
N	-0.913672	0	1.443040
E(ZPE)= -429.208733 a.u.			

H_2NAlH_2•••HNS	x	y	z
H	-1.167784	0	1.159314
H	-1.112488	0	2.815764
H	2.078838	0	3.161600
H	1.812935	0	0.399658
N	0.439512	0	-2.234540
H	1.020881	0	-1.387665
Al	1.200047	0	1.858010
N	-0.569976	0	1.969502
S	-1.082485	0	-1.777970
E(ZPE)= -751.825188 a.u.			