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Table S1. B3LYP infrared frequencies for $[(H_3N)BH_3]_2$, $[(H_3N)AlH_3]_2$, and $[(H_3N)GaH_3]_2$.[a]

Molecule	Symmetry	Frequency, cm^{-1} (Intensity, Km/mol)
$[(H_3N)BH_3]_2$	A_g[b]	168, 205, 716, 725, 1090, 1169, 1206, 1394, 1645, 2403, 2504, 3302, 3493
	A_u	86 (70), 213 (0), 271 (0), 683 (3), 1078 (50), 1185 (4), 1632 (20), 2446 (400), 3551 (60)
	B_g[b]	67, 337, 686, 1064, 1182, 1628, 2436, 3551
	B_u	238 (20), 714 (9), 746 (20), 1073 (100), 1177 (100), 1207 (40), 1378 (200), 1637 (20), 2411 (200), 2502 (500), 3318 (600), 3493 (100)
$[(H_3N)AlH_3]_2$	A	43 (30), 49 (1), 110 (0), 181 (0), 237 (0), 419 (9), 434 (2), 458 (1), 710 (5), 744 (8), 761 (20), 793 (300), 851 (100), 1305 (5), 1637 (1), 1652 (6), 1755 (100), 1845 (400), 1851 (100), 3222 (0), 3483 (1), 3546 (70)
	B	48 (10), 201 (30), 237 (40), 424 (0), 438 (20), 508 (60), 703 (20), 729 (80), 762 (600), 790 (500), 817 (300), 1299 (200), 1633 (20), 1650 (40), 1772 (1000), 1842 (200), 1849 (100), 3241 (1000), 3483 (100), 3546 (4)
$[(H_3N)GaH_3]_2$	A	44 (20), 49 (3), 95 (1), 177 (0), 219 (0), 356 (1), 428 (6), 443 (0), 698 (60), 729 (2), 745 (2), 761 (200), 814 (100), 1268 (2), 1639 (0), 1652 (6), 1813 (200), 1917 (400), 1926 (10), 3297 (1), 3498 (0), 3560 (60)
	B	74 (20), 184 (7), 225 (30), 356 (40), 432 (0), 481 (30), 682 (35), 704 (100), 746 (300), 765 (400), 798 (200), 1263 (200), 1636 (20), 1650 (20), 1823 (700), 1913 (200), 1923 (200), 3312 (800), 3498 (200), 3560 (2)

[a] cc-pVDZ basis set for $[(H_3N)BH_3]_2$ and $[(H_3N)AlH_3]_2$, pVDZ basis set for $[(H_3N)GaH_3]_2$. [b] All IR intensities are zero for this irrep.

Table S2. Absolute energies (au) for $(H_3N)BH_3$, $(H_3N)AlH_3$, and $(H_3N)GaH_3$.[a]

		Geometry		
Molecule	Energy	RHF	B3LYP	MP2
$(H_3N)BH_3$	RHF	–82.624 35	–82.623 60	–82.623 63
	B3LYP	–83.218 17	–83.218 86	–83.218 86
	MP2	–82.921 62	–82.922 31	–82.922 32
$(H_3N)AlH_3$	RHF	–299.872 61	–299.872 01	–299.871 99
	B3LYP	–300.821 04	–300.821 59	–300.821 57
	MP2	–300.142 63	–300.143 19	–300.143 21
$(H_3N)GaH_3$	RHF[b]	–1980.945 75	–1980.945 11	–1980.944 75
	B3LYP[b]	–1983.021 15	–1983.021 74	–1983.021 58
	MP2[b]	–1981.366 89	–1981.367 68	–1981.367 85
	RHF[c]	–59.914 66	–59.914 01	–59.914 00
	B3LYP[c]	–60.427 88	–60.428 47	–60.428 36
	MP2[c]	–60.173 73	–60.174 23	–60.174 36

[a] Calculations used the cc-pVDZ basis set unless otherwise indicated. [b] pVDZ basis set used for energies and geometries. [c] pVDZ basis set for H and N, ECP for Ga, used for energies and geometries.

Table S3. Absolute energies (au) for $[(H_3N)BH_3]_2$, $[(H_3N)AlH_3]_2$, and $[(H_3N)GaH_3]_2$.[a]

		Geometry		
Molecule	Energy	RHF	B3LYP	MP2
$[(H_3N)BH_3]_2$	RHF	–165.265 11	–165.261 81	–165.262 17
	B3LYP	–166.457 72	–166.460 67	–166.460 61
	MP2	–165.866 03	–165.868 68	–165.868 74
$[(H_3N)AlH_3]_2$	RHF	–599.758 49	–599.754 97	–599.755 49
	B3LYP	–601.659 02	–601.662 02	–601.661 61
	MP2	–600.302 67	–600.304 86	–600.305 20
$[(H_3N)GaH_3]_2$	RHF[b]	–3961.902 43	–3961.899 00	–3961.898 43
	B3LYP[b]	–3966.056 25	–3966.059 20	–3966.058 27
	MP2[b]	–3962.749 15	–3962.752 01	–3962.752 75
	RHF[c]	–119.840 55	–119.837 12	–119.837 83
	B3LYP[c]	–120.870 11	–120.872 98	–120.872 68
	MP2[c]	–120.362 59	–120.364 66	–120.364 96

[a] Calculations used the cc-pVDZ basis set unless otherwise indicated. [b] pVDZ basis set used for energies and geometries. [c] pVDZ basis set for H and N, ECP for Ga, used for energies and geometries.