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Supporting Information for:

A Practical Computational Approach to Study Molecular Instability Using the Pseudo Jahn-Teller Effect

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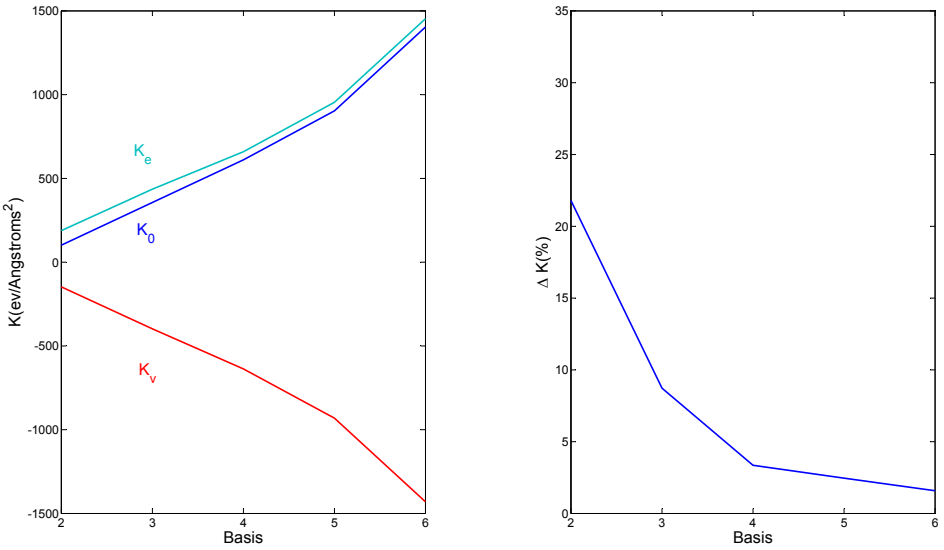

Figure S1: Calculation of the total contributions to the force constant at LDA level, (left) K_0 (blue), K_v (red) and K_e (green) varying the basis quality along the series cc-pvXz (X=d, t, q, 5, 6) in NH_3; (right) Comparison of the absolute value of K_v and K_e, $\Delta K = |Kv/Ke| - 1$ in % varying the basis quality

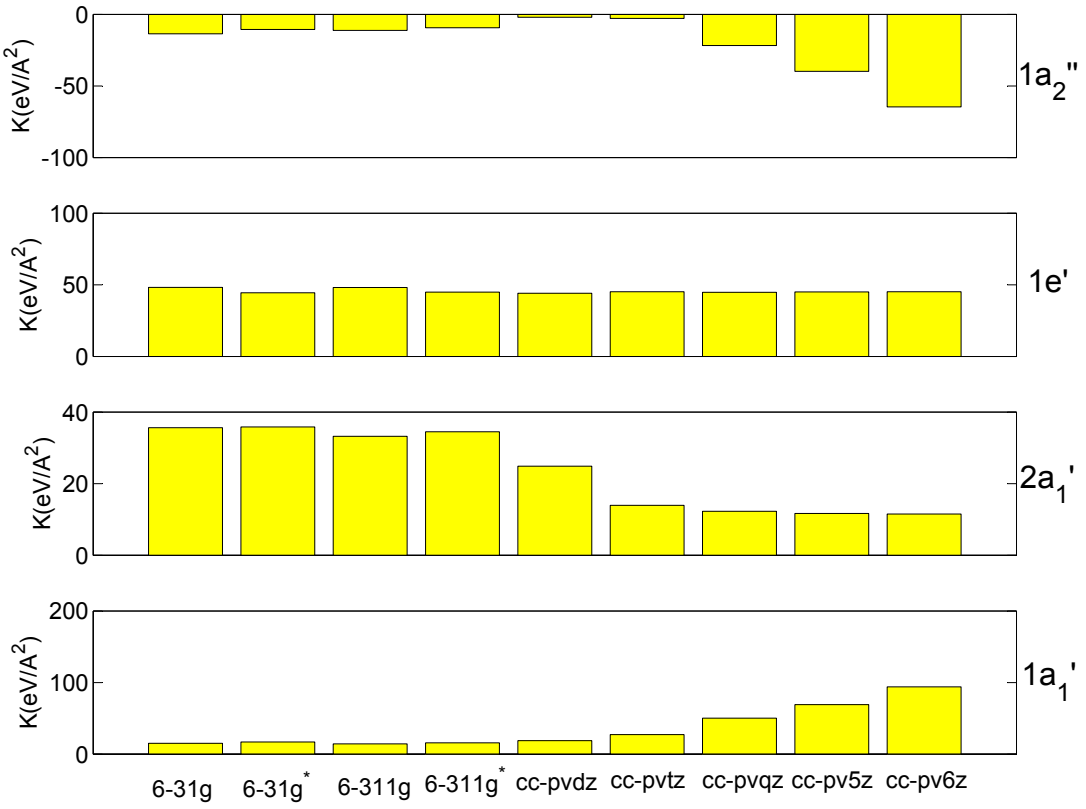

Figure S2: Calculation of the orbital contributions for each of the occupied orbitals of NH_3 to the total force constant for several basis-sets at LDA level of theory

Table S1: Orbital contributions for NH_3 and BH_3 at GGA (BLYP and PBE)/cc-pvtz level of theory. The orbital contributions are given per individual orbital, i.e. the e' orbital total contribution is twice the one in the table due to the degeneracy. Units are eV/Å^2.

		BLYP				PBE			
System	Contribution	K_0	$2K_v$	K_e	K	K_0	$2K_v$	K_e	K
NH_3	$1a'_1$	58.84	-64.14	39.91	34.61	48.24	-64.02	39.97	24.18
	$2a'_1$	84.35	-110.52	40.69	14.53	80.13	-110.09	43.58	13.62
	$1e'$	107.29	-153.53	90.17	43.93	103.76	-152.93	94.85	45.68
	$1a''_2$	171.84	-322.55	147.23	-3.49	168.69	-324.09	153.58	-1.83
	Nuclear	-150.88	0.0	0.0	-150.88	150.88	0.0	0.0	-150.88
	DFT XC	0.0	0.0	14.07	14.07	0.0	0.0	20.18	20.18
	Total	378.74	-804.28	422.24	-3.30	353.70	-804.07	447.01	-3.37
BH_3	$1a'_1$	26.87	-24.16	12.18	14.89	24.77	-24.17	12.14	12.74
	$2a'_1$	30.11	-28.70	8.22	9.62	29.12	-28.35	8.80	9.56
	$1e'$	55.49	-73.29	20.77	20.77	54.24	-72.29	39.27	21.22
	Nuclear	-69.15	0.0	0.0	-69.15	-69.15	0.0	0.0	-69.15
	DFT XC	0.0	0.0	9.26	9.26	0.0	0.0	10.03	10.03
	Total	98.83	-199.44	106.79	6.18	93.22	-197.11	109.51	5.62

Table S2: Contributions of K_0, K_v and K_e to the force constant of the orbital $1a''_2$ NH_3 and their decomposition in kinetic energy (T), electron-electron repulsion (V_{ee}), electron-nuclear interactions (V_{en}) at GGA (BLYP and PBE)/cc-pvtz level of theory. Units are eV/Å^2.

		k_0	$2k_v$	k_e	k
BLYP	T	125.05	-308.90	178.27	-5.58
	V_{en}	94.13	-51.65	-22.47	20.01
	V_{ee}	-47.35	38.00	-8.58	-17.93
	Total	171.84	-322.55	147.23	-3.50
PBE	T	126.18	-310.92	167.03	-17.71
	V_{en}	94.11	-51.31	2.99	45.79
	V_{ee}	-51.61	38.15	-16.44	-29.90
	Total	168.69	-324.09	153.58	-1.82