Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Ammonia Borane in External Electric Field: Structure, Charge transfer, and Chemical Bonding

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General Comments

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Table S1. The optimized structural parameters and Dipole moment (μ) of BH_3NH_3 in different external electric fields[a].

$E_{ext} \times 10^{-4}$ au	r (B-N)	r(B-H)	r(N-H)	H-B-H	H-N-H	H_1-B-H_2-H_3	H_1'-N-H_2'-H_3'	μ_1	μ_2
-767	1.653	1.263	1.045	106.7	101.0	113.9	103.7	13.33	6.30
-750	1.634	1.263	1.044	106.2	100.8	112.7	103.4	13.01	6.36
-700	1.617	1.258	1.040	106.1	101.1	112.7	103.7	12.26	6.35
-650	1.611	1.253	1.037	106.5	101.5	113.5	104.4	11.63	6.31
-600	1.608	1.247	1.034	107.1	102.0	114.6	105.2	11.04	6.25
-550	1.606	1.242	1.032	107.7	102.5	115.9	106.0	10.49	6.18
-519	1.606	1.239	1.031	108.1	102.8	116.8	106.5	10.15	6.14
-500	1.606	1.237	1.030	108.3	102.9	117.3	106.8	9.96	6.12
-450	1.607	1.233	1.028	108.9	103.4	118.7	107.6	9.46	6.05
-400	1.609	1.229	1.026	109.5	103.9	120.1	108.5	8.98	5.99
-350	1.611	1.226	1.024	110.1	104.4	121.5	109.3	8.52	5.92
-300	1.614	1.222	1.023	110.6	104.9	122.9	110.2	8.06	5.86
-250	1.617	1.219	1.022	111.1	105.4	124.3	111.1	7.61	5.79
-200	1.621	1.217	1.021	111.6	105.8	125.7	112.1	7.18	5.73
-150	1.626	1.214	1.020	112.1	106.3	127.2	113.0	6.74	5.66
-100	1.633	1.212	1.019	112.6	106.8	128.7	114.1	6.31	5.59
-50	1.641	1.210	1.018	113.1	107.4	130.3	115.3	5.87	5.51
0	1.649	1.208	1.017	113.6	107.9	131.9	116.3	5.44	5.44
50	1.660	1.207	1.016	114.1	108.5	133.6	117.8	5.44	5.35
100	1.674	1.205	1.015	114.6	109.1	135.6	119.2	4.99	5.25
150	1.692	1.204	1.015	115.2	109.8	137.7	120.9	4.52	5.14
200	1.716	1.202	1.014	115.8	110.6	140.4	122.9	4.04	4.99
250	1.751	1.201	1.013	116.5	111.6	143.8	125.5	3.51	4.80
300	1.820	1.199	1.011	117.5	113.2	149.2	130.7	2.90	4.42
320	1.902	1.197	1.009	118.3	114.9	154.7	136.8	1.80	3.97
321	3.207	1.192	1.021	119.7	102.3	168.3	105.7	4.20	2.01

[a]The bond distance are in angstroms; angles, in degrees; dipole moment, in Debye.

Table S2. NBO charge q_1 of BH_3NH_3 in external electric fields and NBO charge q_2 of BH_3NH_3 after external electric fields.The Laplacian of the electron density ($\nabla^2\rho_{(r)}$) and electron density (ρ) of the bond critical points (BCPs).

$E_{ext} \times 10^{-4}$ au	$q_1(NH_3)$	$q_1(BH_3)$	$q_2(NH_3)$	$q_2(BH_3)$	$\nabla^2\rho$(B-N)	$\nabla^2\rho$(B-H)	$\nabla^2\rho$(N-H)	ρ(B-N)	ρ(B-H)	ρ(N-H)
-767	0.706	-0.706	0.318	-0.318	0.124	-0.053	-1.809	0.134	0.140	0.310
-750	0.618	-0.618	0.322	-0.322	0.152	-0.050	-1.811	0.138	0.140	0.312
-700	0.529	-0.529	0.325	-0.325	0.198	-0.050	-1.818	0.141	0.142	0.316
-650	0.490	-0.490	0.327	-0.327	0.235	-0.053	-1.823	0.141	0.145	0.319
-600	0.472	-0.472	0.330	-0.330	0.267	-0.056	-1.826	0.139	0.147	0.323
-550	0.457	-0.457	0.330	-0.330	0.297	-0.060	-1.828	0.137	0.150	0.325
-519	0.449	-0.449	0.329	-0.329	0.314	-0.063	-1.828	0.136	0.151	0.327
-500	0.444	-0.444	0.329	-0.329	0.324	-0.065	-1.828	0.135	0.152	0.328
-450	0.430	-0.430	0.328	-0.328	0.350	-0.070	-1.826	0.133	0.154	0.330
-400	0.419	-0.419	0.327	-0.327	0.374	-0.075	-1.824	0.130	0.156	0.332
-350	0.406	-0.406	0.326	-0.326	0.128	-0.081	-1.820	0.396	0.158	0.334
-300	0.393	-0.393	0.325	-0.325	0.308	-0.087	-1.816	0.125	0.160	0.336
-250	0.380	-0.380	0.324	-0.324	0.435	-0.093	-1.811	0.122	0.161	0.337
-200	0.370	-0.370	0.323	-0.323	0.452	-0.099	-1.805	0.119	0.163	0.339
-150	0.356	-0.356	0.322	-0.322	0.466	-0.106	-1.798	0.115	0.165	0.340
-100	0.344	-0.344	0.321	-0.321	0.479	-0.113	-1.791	0.112	0.166	0.341
-50	0.331	-0.331	0.319	-0.319	0.487	-0.121	-1.785	0.108	0.168	0.342
0	0.316	-0.316	0.316	-0.316	0.494	-0.128	-1.775	0.103	0.169	0.342
50	0.300	-0.300	0.313	-0.313	0.494	-0.137	-1.770	0.099	0.170	0.343
100	0.284	-0.284	0.309	-0.309	0.495	-0.146	-1.763	0.094	0.172	0.343
150	0.267	-0.267	0.303	-0.303	0.487	-0.155	-1.757	0.088	0.173	0.344
200	0.248	-0.248	0.295	-0.295	0.469	-0.167	-1.751	0.081	0.174	0.344
250	0.225	-0.225	0.284	-0.284	0.436	-0.180	-1.748	0.073	0.176	0.344
300	0.191	-0.191	0.262	-0.262		-0.200	-1.757		0.178	0.344
320	0.161	-0.161	0.237	-0.237		-0.217	-1.775		0.180	0.344
321	0.005	-0.005	0.018	-0.018		-0.288	-1.621		0.186	0.335

Table S3. The fragment contribution to HOMO-2 of BH_3NH_3 molecule in a series of $E_{ext} \times 10^{-4}$ au.

$E_{ext} \times 10^{-4}$ au	-767	-750	-700	-650	-600	-550	-519	-500	-450	-400	-350	-300	-250
BH_3% [HOMO-2]	41.27	42.28	44.05	45.69	47.34	49.07	50.18	50.88	52.72	54.58	56.42	58.2	59.91
NH_3% [HOMO-2]	58.73	57.72	55.95	54.31	52.65	50.92	49.82	49.13	47.28	45.42	43.58	41.8	40.09
$E_{ext} \times 10^{-4}$ au	-200	-150	-100	-50	0	50	100	150	200	250	300	320	321
BH_3% [HOMO-2]	61.5	62.97	64.3	65.33	66.37	67.09	67.52	67.61	67.11	65.66	60.97	53.57	3.03
NH_3% [HOMO-2]	38.5	37.03	35.7	34.66	33.63	32.91	32.48	32.39	32.89	34.34	39.03	46.43	96.97

Table S4. The optimized structural parameters of BH_3NH_3 dimers in different external electric fields[a].

$E_{ext} \times 10^{-4}$ au	r(B-N)	H_1-B-H_2-H_3	H_1'-N-H_2'-H_3'
-200	1.606	112.4	123.1
-150	1.610	124.2	124.3
-100	1.614	114.2	114.2
-50	1.620	115.1	115.1
0	1.626	128.1	116.1
50	1.634	129.5	117.2
100	1.643	130.9	118.4
150	1.654	132.5	119.5
200	1.668	134.2	121.0

[a]The bond distance are in angstroms; angles, in degrees.

Optimized Cartesian Coordinates

BH_3NH_3 without external electric field

B	0.00000000	0.00000000	-0.10573900
N	0.00000000	0.00000000	1.54374200
H	1.16752400	0.00000000	-0.41674100
H	-0.58376200	-1.01110600	-0.41674100
H	-0.58376200	1.01110600	-0.41674100
H	-0.94926200	0.00000000	1.90888300
H	0.47463100	0.82208500	1.90888300
H	0.47463100	-0.82208500	1.90888300

Table S5. Potential energy E of eclipsed forms of BH_3NH_3 in different external electric fields.

$E_{ext} \times 10^{-4}$ au	-200	-150	-100	-50	0
E (au)	-82.6896	-82.6754	-82.6619	-82.6490	-82.6368
$E_{ext} \times 10^{-4}$ au	50	100	150	200	
E (au)	-82.6253	-82.6145	-82.6043	-82.5949	