Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Hydrogen adsorption on inorganic benzenes decorated with alkali metal cations: theoretical study

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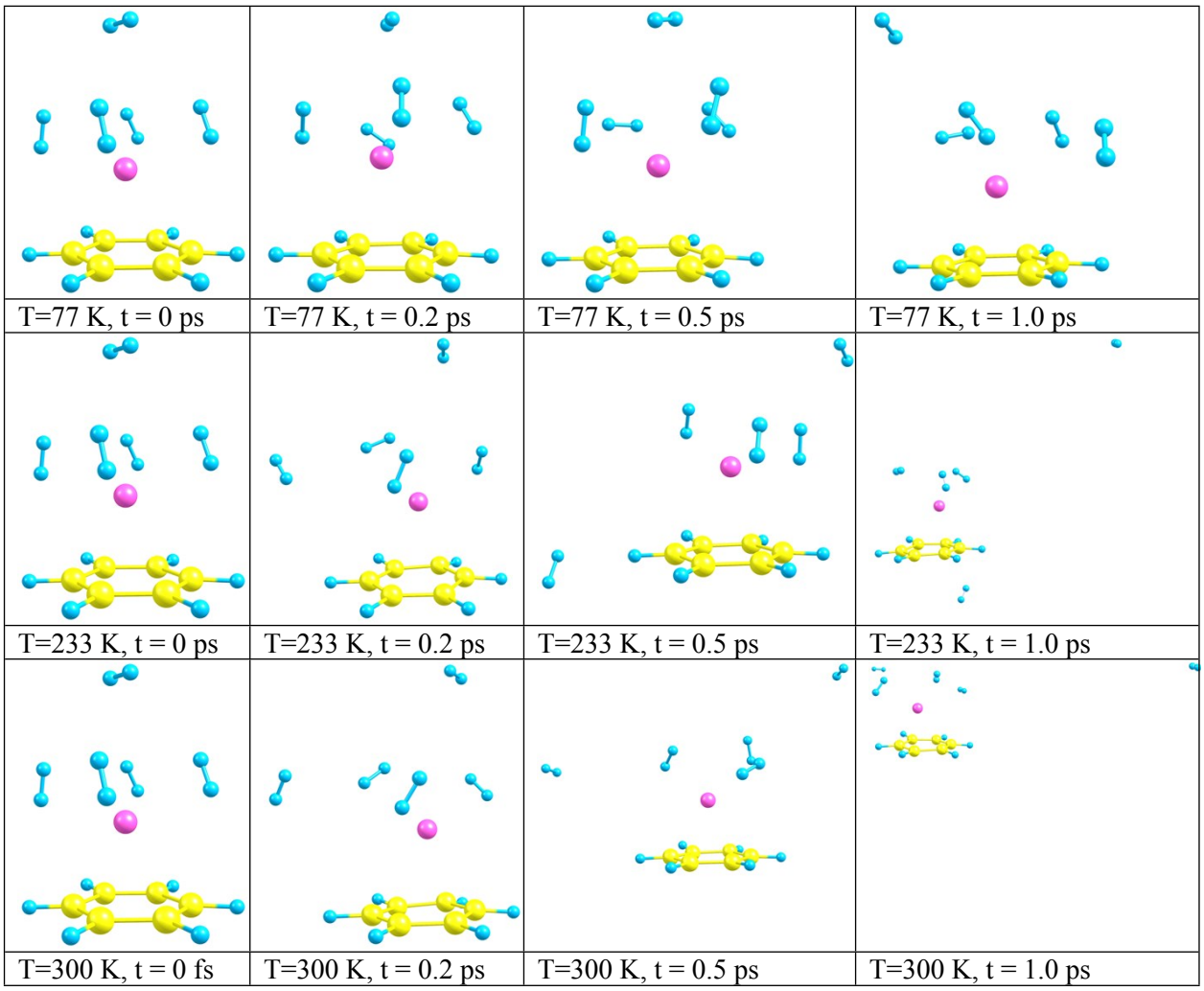


Fig. 1SI. Snap shots of 5 H_2 molecules adsorbed on $Li^+@C_6H_6$ complexes under different simulation conditions. Atomic color code: yellow – carbon, light-blue – hydrogen, magenta – lithium cation.

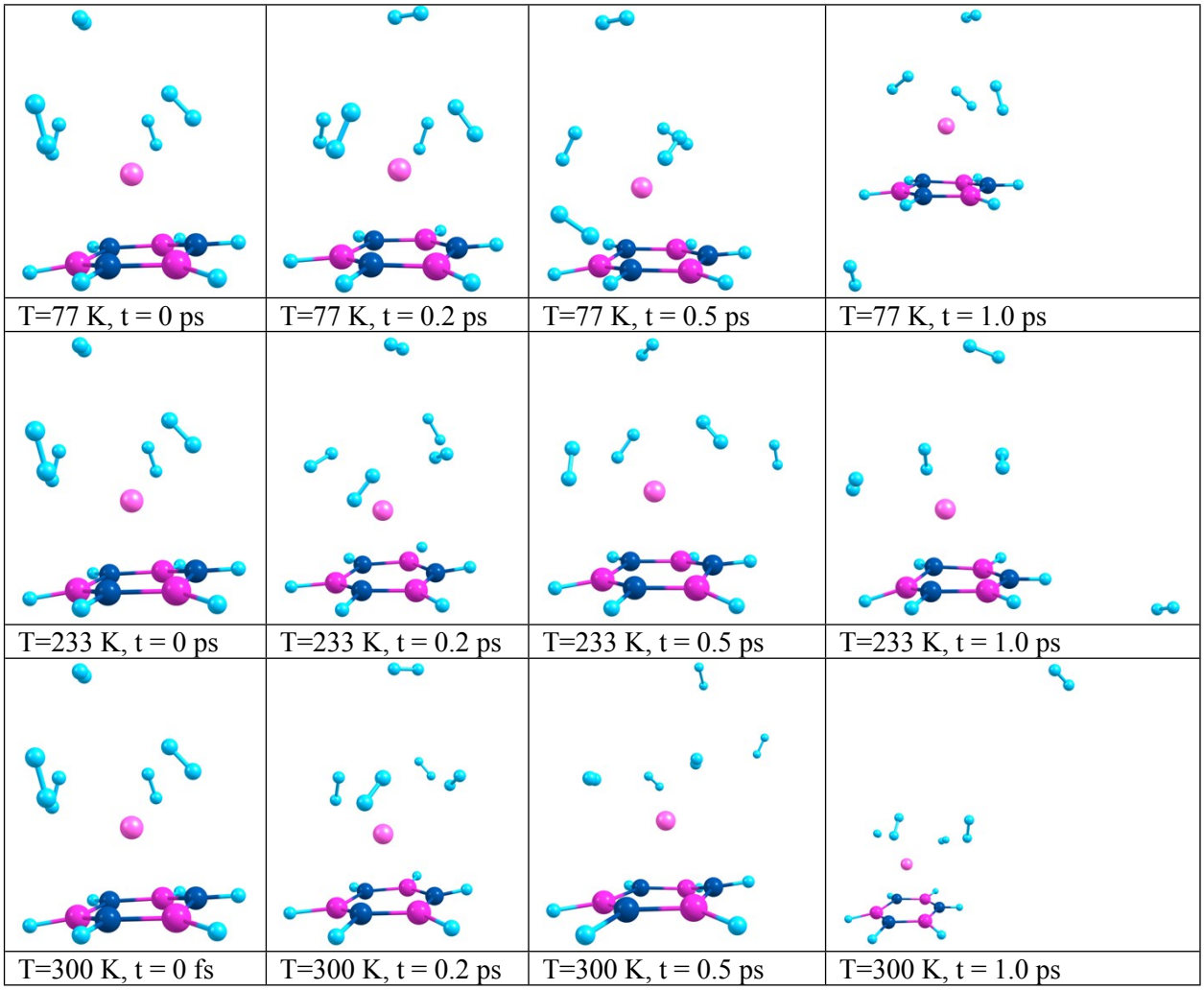


Fig. 2SI. Snap shots of 5 H_2 molecules adsorbed on Li+@ $B_3N_3H_6$ complexes under different simulation conditions. Atomic color code: blue – nitrogen, light-blue – hydrogen, pale-red – boron, magenta – lithium cation.

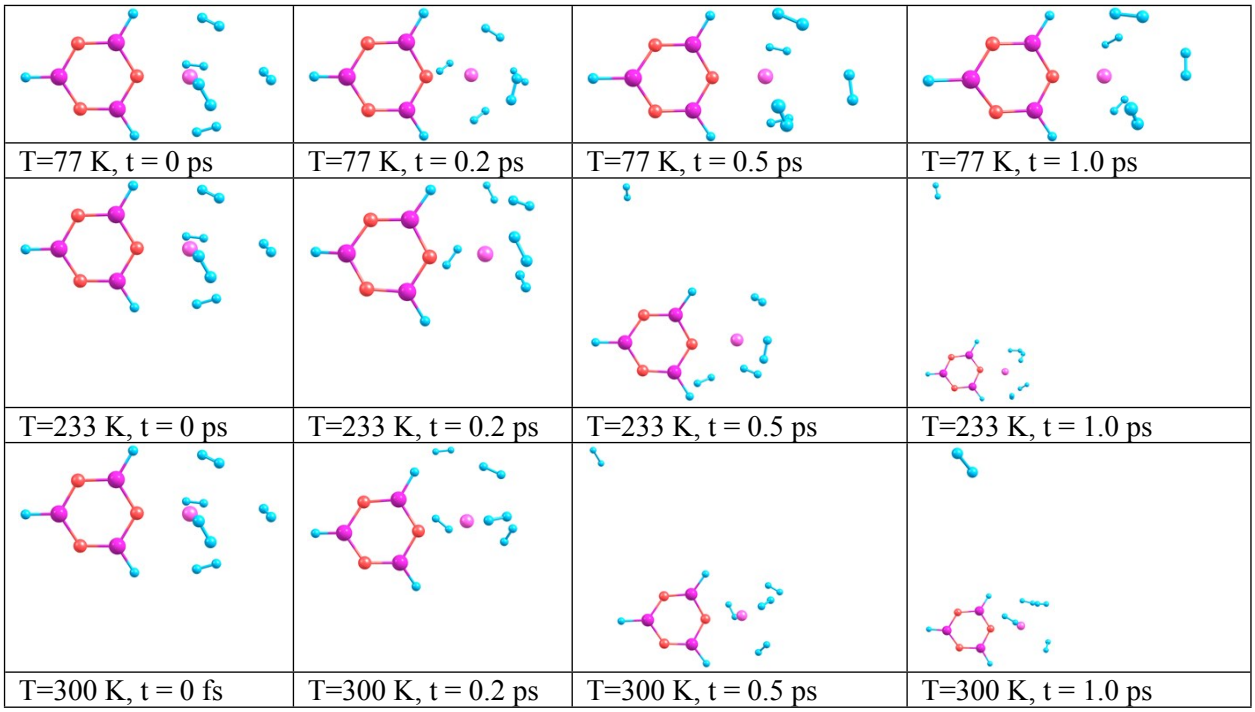
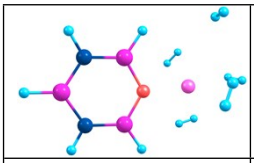
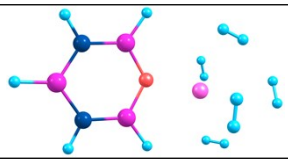
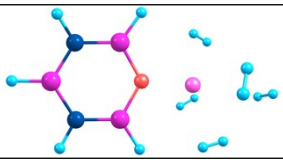
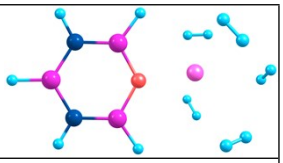


Fig. 3SI. Snap shots of 5 H_2 molecules adsorbed on $Li^+@B_3O_3H_3$ complexes in the in-plane configuration under different simulation conditions. Atomic color code: blue – nitrogen, light-blue – hydrogen, pale-red – boron, red – oxygen, magenta – lithium cation.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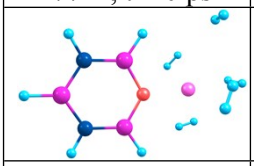	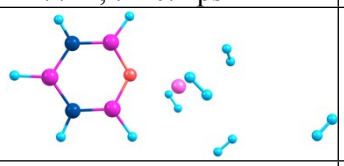	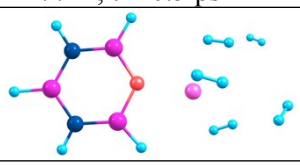	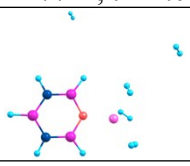
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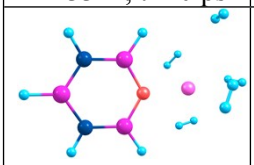	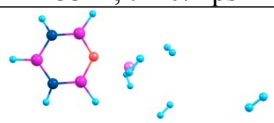	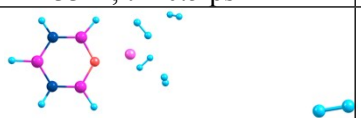	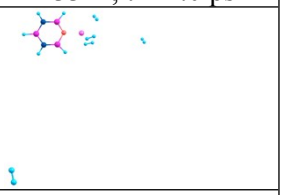
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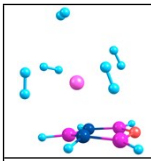
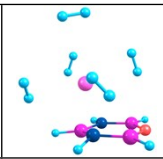
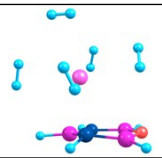
Fig. 4SI. Snap shots of 5 H_2 molecules adsorbed on $Li^+@B_3N_2OH_5$ complexes in the in-plane configuration under different simulation conditions. Atomic color code: blue – nitrogen, light-blue – hydrogen, pale-red – boron, red – oxygen, magenta – lithium cation.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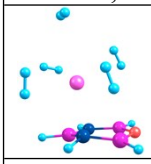	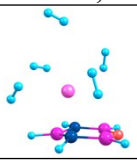	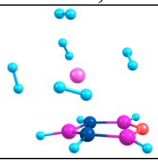	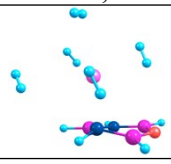
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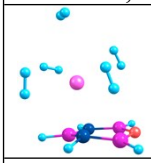	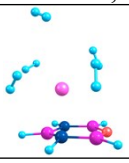	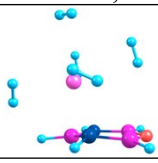	
T=300 K, t = 0 fs	T=300 K, t = 0.2 ps	T=300 K, t = 0.5 ps	T=300 K, t = 1.0 ps

Fig. 5SI. Snap shots of 5 H_2 molecules adsorbed on $Li^+@B_3N_2OH_5$ complexes in the out-of-plane configuration under different simulation conditions. Atomic color code: blue – nitrogen, light-blue – hydrogen, pale-red – boron, red – oxygen, magenta – lithium cation.

Independent gradient model (IGM)

We involved the so-called Independent Gradient Model (IGM) method proposed elsewhere [1, 2]. This straightforward approach "provides chemists with a visual understanding of interactions present in chemical systems" [2]. The new descriptors, which are defined in the framework of this method, allow obtaining a measure of electron sharing (δg), and separately describe interactions inside each fragment (δg^{intra}) or between fragments (δg^{inter}).

$$\delta g = |\nabla \rho^{IGM}| - |\nabla \rho|.$$

$$\delta g^{inter} = |\nabla \rho^{IGM,\ inter}| - |\nabla \rho|.$$

$$\delta g^{intra} = |\nabla \rho^{IGM}| - |\nabla \rho^{IGM,\ inter}|.$$

$$\delta g = \delta g^{inter} + \delta g^{intra}.$$

Where δg^{intra} and δg^{inter} are the intramolecular and intermolecular contributions; $\nabla \rho$ is the electron density gradient, $\nabla \rho^{IGM}$ is the gradient vector of density in independent gradient model; $\nabla \rho^{IGM,\ inter}$ is the gradient vector, where the interaction between molecules canceled while intramolecular part has been divided into two additions, which corresponds to intramolecular interaction in separate molecules.

[1] C. Lefebvre, G. Rubez, H. Khartabil, J.-C. Boisson, J. Contreras-García, E. Hénon, Accurately extracting the signature of intermolecular interactions present in the NCI plot of the reduced density gradient versus electron density, Physical Chemistry Chemical Physics, 19 (2017) 17928-17936.
[2] C. Lefebvre, H. Khartabil, J.-C. Boisson, J. Contreras-García, J.-P. Piquemal, E. Hénon, The Independent Gradient Model: A New Approach for Probing Strong and Weak Interactions in Molecules from Wave Function Calculations, Chemphyschem : a European journal of chemical physics and physical chemistry, 19 (2018) 724-735.

Symmetry-adapted perturbation theory (SAPT)

Symmetry-adapted perturbation theory (SAPT) is a method for direct calculations of the non-covalent interaction between two molecules. In other words, the interaction energy is determined without computing the total energy of the monomers or dimer. Thus, the result obtained is free from the basis set superposition error (BSSE). In addition, SAPT provides a decomposition of the

interaction energy into meaningful components: *i.e.*, electrostatic, exchange, induction (polarization) and dispersion terms. In SAPT, the Hamiltonian of the dimer is partitioned into contributions from each monomer and the interaction.

$$H = F_A + W_A + F_B + W_B + V$$

the Hamiltonian (H) is written as a sum of the usual monomer Fock operators (F), the fluctuation potential of each monomer (W), and the interaction potential (V). Fock operators are treated as the zeroth-order Hamiltonian and the interaction energy is evaluated through a perturbative expansion of V, W_A and W_B. Through first-order in V, electrostatic and exchange interactions are included; induction and dispersion first appear at second-order in V.

Several truncations of the closed-shell SAPT expansion are available in PSI4. The simplest truncation of SAPT is denoted SAPT0 and defined in the following equation:

$$E_{SAPT0} = E_{elst}^{(10)} + E_{exch}^{(10)} + E_{ind,resp}^{(20)} + E_{exch-ind,resp}^{(20)} + E_{disp}^{(20)} + E_{exch-disp}^{(20)} + \delta_{HF}^{(2)}$$

In this notation, $E^{(vw)}$ defines the order in V and in WA+WB; the subscript (resp) indicates that orbital relaxation effects are included.

The $\delta_{HF}^{(2)}$ term takes into account the higher-order induction effects, and it is included in the definition of SAPT terms.

Normally, the adsorption energy terms are calculated as following:

$E_{ad} = E_{el} + E_{ex} + E_{ind} + E_{disp}$,

Where $E_{el} = E_{elst}^{(10)}$, $E_{ex} = E_{exch}^{(10)}$,

$E_{ind} = E_{ind,resp}^{(20)} + E_{exch-ind,resp}^{(20)} + \delta_{HF}^{(2)}$,

$E_{disp} = E_{disp}^{(20)} + E_{exch-disp}^{(20)}$

For the SAPT2 method, we can write down the following equation:

$$E_{SAPT2} = E_{SAPT0} + E_{elst,resp}^{(12)} + E_{exch}^{(11)} + E_{exch}^{(12)} + E_{ind}^{t(22)} + E_{exch-ind}^{t(22)},$$

where some second order corrections in energy have been added with amendments to the energy terms mentioned above.

1) Full description of the SAPT method can be found elsewhere [B. Jeziorski, R. Moszynski, K. Szalewicz, Chem. Rev. 1994, 94, 1887 – 1930; K. Szalewicz, WIREs Comput. Mol. Sci. 2012, 2, 254 – 272].
2) Additional information can be founded in the PSI4 manual [http://www.psicode.org/psi4manual/master/sapt.html].
3) Besides this, we refer the reader to the comprehensive review of K. Patkowski, WIREs Comput Mol Sci. 2019; e1452.

Cartesian coordinates of studied structures

$1H_2/Li^+@C_6H_6$

C	-0.895828630	-0.710086944	0.885667819
C	-0.482001651	-0.905787250	2.208430715
C	0.039200382	-0.376942382	-0.102980507
H	-1.208353024	-1.171088224	2.964375481
H	-0.289782304	-0.230918665	-1.122292579
C	0.870657032	-0.759796565	2.539127489
C	1.391659375	-0.225056184	0.228326171
H	1.197508090	-0.925888953	3.555945666
H	2.112847414	0.027294485	-0.536921564
C	1.805020487	-0.412877880	1.554243634
H	2.844132770	-0.276317870	1.820403534
H	-1.934958989	-0.839027478	0.617474522
Li	0.193360704	1.218231113	1.547224920
H	0.600817466	3.234140310	1.451780466
H	1.194265473	2.901839371	1.147857413

$2H_2/Li^+@C_6H_6$

C	-0.830870961	-0.559636582	0.865012603
C	-0.384681464	-0.651533344	2.188709900
C	0.098142768	-0.539074434	-0.183746844
H	-1.096294800	-0.624940902	3.002269344
H	-0.232334651	-0.463715410	-1.210050086
C	0.983319460	-0.786308580	2.463950127
C	1.467219926	-0.637203538	0.090744462
H	1.313490597	-0.926946136	3.482685270

H	2.183980776	-0.614440080	-0.719306148
C	1.909226492	-0.795320253	1.410188803
H	2.958868194	-0.951671956	1.605581015
H	-1.890717186	-0.513212665	0.660308733
Li	0.637854282	1.204036457	1.292701506
H	-1.151686696	2.156469083	0.838189386
H	-0.888710331	2.834714521	0.993470424
H	1.530367147	3.020064864	1.796886114
H	1.784680900	2.577797447	2.339466530

$3H_2/Li^+@C_6H_6$

C	-0.807102313	-0.624006916	0.877868702
C	-0.363458857	-0.784491689	2.195433769
C	0.121556561	-0.489774852	-0.160171783
H	-1.085662352	-0.895820586	2.992305682
H	-0.215465108	-0.355454838	-1.179457220
C	1.004907489	-0.822815807	2.476990131
C	1.493981404	-0.539499981	0.118101334
H	1.327047092	-0.978890063	3.497387279
H	2.208589538	-0.453227270	-0.689019112
C	1.938428720	-0.718709542	1.433764181
H	2.995922862	-0.790653784	1.640482712
H	-1.866526996	-0.637664070	0.666795707
Li	0.571512693	1.224946244	1.381864767
H	1.012596922	2.372087450	-0.427877743
H	0.685175474	2.943234337	-0.083871870
H	-0.691445786	2.747910133	2.302702865
H	-1.151765267	2.427894555	1.814522270

H	1.852255597	2.758937592	2.228281997
H	2.066632327	2.152793089	2.600362335

$4H_2/Li^+@C_6H_6$

C	-0.879966165	-0.639084495	0.924666446
C	-0.408674869	-0.767577133	2.234937114
C	0.022858549	-0.480868573	-0.132656342
H	-1.111996451	-0.940880814	3.038142767
H	-0.336257471	-0.398873988	-1.148827765
C	0.963608660	-0.712570241	2.489682656
C	1.401685444	-0.453900043	0.115621114
H	1.303801068	-0.840064601	3.508606412
H	2.101403646	-0.367324651	-0.702271520
C	1.872436745	-0.560696241	1.430935066
H	2.932059040	-0.510349399	1.645456641
H	-1.940569999	-0.702066295	0.734992250
Li	0.498108296	1.374273051	1.370749200
H	1.443678945	2.342023153	-0.434101420
H	1.258373567	3.050485373	-0.319376974
H	-0.434072844	2.751727435	2.916728496
H	-0.511753861	2.045390485	3.132825133
H	-1.429045529	2.100701515	0.351129748
H	-1.284069992	2.827751523	0.381964364
H	2.156282486	2.715326026	2.142546951
H	2.242184734	2.068614912	2.493673666

$5H_2/Li^+@C_6H_6$

C	-0.929366214	-0.666526280	1.102984005
C	-0.276134067	-0.760476064	2.337692657
C	-0.193933263	-0.496549982	-0.078036676
H	-0.845569507	-0.948396910	3.236043293
H	-0.696487526	-0.459576848	-1.034704228
C	1.113237627	-0.652320861	2.398948784
C	1.202800357	-0.402205336	-0.016389157
H	1.643844085	-0.743050410	3.336802419
H	1.810470647	-0.296126450	-0.905509669
C	1.846929308	-0.469517748	1.223672211
H	2.919653323	-0.356538256	1.281675686
H	-2.005654498	-0.767059240	1.060146515
Li	0.422625739	1.428664053	1.294175457
H	1.799630800	2.236636211	-0.159259376
H	1.717289965	2.957015302	0.001985610
H	-0.631899084	2.598943020	2.878228568
H	-0.891581884	1.903185001	2.828051451
H	0.456059385	4.760022985	1.464255441
H	-0.278374916	4.683658801	1.517205115
H	-1.171218385	2.115263532	-0.053643112
H	-0.957297342	2.821910080	0.024392168
H	1.995738233	2.779605092	2.586857620
H	1.986992555	2.079157600	2.831310812

$1H_2/Li^+@B_3N_3H_6$

N	-0.880188783	-0.550563770	0.878964905
B	-0.498247162	-0.820214620	2.245019452

B	0.051128520	-0.480784832	-0.223956575
H	-1.279081315	-1.079846047	3.092185967
H	-0.308933754	-0.457726896	-1.348166662
N	0.904824591	-0.616317787	2.518382048
N	1.428491935	-0.297145302	0.169265007
H	1.211140285	-0.748923263	3.472803375
H	2.111103403	-0.214554987	-0.571751700
B	1.928559786	-0.545770116	1.501866536
H	3.080390082	-0.576429403	1.759189354
H	-1.860494058	-0.643090459	0.648635214
Li	0.337319806	1.220517926	1.400010526
H	0.306227316	3.246261995	1.397780810
H	0.906303942	3.112304444	1.818434923

$2H_2/Li^+@B_3N_3H_6$

B	-0.898150202	-0.652159606	0.773914523
N	-0.461216900	-0.607709942	2.149998564
N	0.150561292	-0.445663573	-0.194220685
H	-1.168806836	-0.726826192	2.861860638
H	-0.122477602	-0.436998189	-1.167297274
B	0.914520565	-0.793128724	2.554547950
B	1.556649399	-0.603924560	0.094755571
H	1.231504559	-0.995244010	3.674563048
H	2.382172630	-0.628718928	-0.750570730
N	1.881394709	-0.623765056	1.500645956
H	2.855047326	-0.729076401	1.750769574
H	-2.032938308	-0.746997797	0.460368199
Li	0.485972718	1.228079334	1.309052119

H	-1.294551524	2.270945061	1.326450381
H	-0.858078278	2.870890569	1.267594318
H	1.636622047	2.952070649	1.643607740
H	2.133628860	2.397305854	1.661021247

$3H_2/Li^+@B_3N_3H_6$

N	-0.789521219	-0.486930361	0.796353737
B	-0.477671326	-0.738755830	2.180788846
B	0.179947437	-0.523475687	-0.269026970
H	-1.308619303	-0.886876945	3.008329402
H	-0.141693679	-0.491793062	-1.405414392
N	0.928477915	-0.681098107	2.498164868
N	1.557376114	-0.471734402	0.160721226
H	1.189879037	-0.829777696	3.463097195
H	2.268607385	-0.482850187	-0.557025039
B	1.983019900	-0.730279341	1.514184921
H	3.116100228	-0.883503067	1.812153686
H	-1.763436822	-0.508223381	0.527028025
Li	0.625926754	1.282411358	1.330708374
H	0.593420830	2.338890548	-0.529813270
H	0.616910777	2.935872371	-0.086095053
H	-0.604864697	2.537130816	2.631173937
H	-1.098353978	2.220333261	2.174098063
H	1.994539144	2.780178461	2.052503613
H	2.227135504	2.157275255	2.384534837

$4H_2/Li^+@B_3N_3H_6$

B	-0.964485958	-0.702423243	1.062214310

N	-0.248004865	-0.666000083	2.314151623
N	-0.160501435	-0.442928569	-0.104429269
H	-0.781411530	-0.834163286	3.156128840
H	-0.622893217	-0.450104912	-1.002887578
B	1.188090024	-0.720251926	2.421978799
B	1.278740834	-0.472451719	-0.110428108
H	1.744782049	-0.875580887	3.454756551
H	1.905380379	-0.428757566	-1.114935313
N	1.893436823	-0.440944549	1.195387388
H	2.903194861	-0.449500972	1.230808481
H	-2.134203526	-0.858741914	1.002842352
Li	0.469362289	1.363133118	1.351819321
H	1.767389492	2.158724140	-0.157798261
H	1.628386405	2.859919154	0.041330423
H	-0.714675147	2.700075785	2.869246849
H	-0.970737566	2.007524640	2.940164990
H	-1.202078385	2.105812562	0.043394906
H	-1.003187583	2.814688007	0.136274871
H	1.885730036	2.799497859	2.619022490
H	1.933117818	2.110745817	2.889885098

$5H_2/Li^+@B_3N_3H_6$

B	-0.900602116	-0.778237134	1.302629294
N	-0.019854175	-0.820008091	2.447627578
N	-0.259394774	-0.406724779	0.068177687
H	-0.428510532	-1.056811592	3.341233763
H	-0.846436880	-0.332324225	-0.750864483
B	1.419333898	-0.884230198	2.347717738

B	1.166327077	-0.437941417	-0.141061107
H	2.088386443	-1.085651575	3.304422785
H	1.659830474	-0.292814579	-1.206209018
N	1.956128129	-0.529088146	1.062406017
H	2.961596277	-0.533757624	0.959928199
H	-2.066736843	-0.950394989	1.398040079
Li	0.492166301	1.242295550	1.617504891
H	1.684091484	2.315063706	0.244606806
H	1.429943739	2.936887057	0.563227464
H	-0.855542038	2.696916660	2.377333806
H	-1.150636924	2.040931676	2.562778241
H	0.597937076	4.995643339	1.644498548
H	-0.029046997	4.877819086	1.269253939
H	-1.187651907	2.316839963	-0.680366884
H	-1.249095919	3.053878607	-0.670644087
H	1.638658068	2.449522031	3.155782678
H	1.849805402	1.753576479	3.307734525

$1H_2/Li^+@B_3O_3H_3$

B	-2.336207566	-1.659607622	0.941503211
O	-1.625468949	-1.551797709	2.131831999
O	-2.118787591	-0.694876996	-0.034791235
B	-0.728470605	-0.566672119	2.349169621
B	-1.257671691	0.330364032	0.140973611
H	-0.087021260	-0.478860963	3.340318652
H	-1.076285047	1.169416352	-0.673016723
O	-0.525624896	0.428723863	1.356186356
H	-3.093146323	-2.541263603	0.763581892

Li	0.677712794	1.804800203	1.661494235
H	1.948339254	3.384101093	1.906953471
H	1.644407081	3.543612197	1.245420574

$2H_2/Li^+@B_3O_3H_3$

B	-2.271286202	-1.731594004	0.945398553
O	-1.564288547	-1.539182222	2.128158554
O	-2.159857576	-0.764839242	-0.045374392
B	-0.755312727	-0.473353703	2.311849254
B	-1.407969718	0.348073054	0.108621912
H	-0.090986841	-0.320599830	3.281727919
H	-1.326575282	1.199524746	-0.707723101
O	-0.663373497	0.521338484	1.305889950
H	-2.940133663	-2.684962850	0.786234888
Li	0.588141873	1.882691500	1.589951431
H	2.591482658	2.005637432	1.088043287
H	2.265185304	1.896042734	0.427982450
H	0.488979190	3.920023595	1.740983783
H	-0.195611977	3.688970345	1.920341236

$3H_2/Li^+@B_3O_3H_3$

B	-2.290277266	-1.482447699	1.061309193
O	-1.048812467	-1.680205467	1.653567426
O	-2.560379113	-0.236496027	0.505704181
B	-0.107481499	-0.708111376	1.694096005
B	-1.665471128	0.773656650	0.554538002
H	0.957011569	-0.867831859	2.182517223
H	-1.897110704	1.851707095	0.120997233

O	-0.395157687	0.569828521	1.145793395
H	-3.091588931	-2.342546420	1.032664289
Li	0.742317529	2.052185664	1.210443121
H	2.711414327	1.937547469	1.778537755
H	2.524469957	1.238583014	1.605454319
H	0.357794780	3.226216094	-0.410203124
H	1.069708876	3.416533437	-0.305392916
H	0.160853452	3.583331094	2.490064634
H	0.109431505	2.967049288	2.903464494

$4H_2/Li^+@B_3O_3H_3$

B	-2.199464983	-1.544929677	0.964229691
O	-1.325038362	-1.462266182	2.040194579
O	-2.213248456	-0.492803548	0.057230671
B	-0.487855333	-0.413518726	2.211035460
B	-1.406995677	0.583020766	0.190651515
H	0.277203446	-0.344301958	3.111142798
H	-1.409650501	1.487845761	-0.572170194
O	-0.509224360	0.658892610	1.284806690
H	-2.907511926	-2.473395100	0.824239933
Li	0.691354073	2.111874596	1.424626309
H	2.300311227	1.154435492	0.350858982
H	2.254392874	1.770942279	-0.059884728
H	-0.252800080	3.600798341	2.734951749
H	-0.768309202	3.067089564	2.720755314
H	0.121056621	3.379080707	-0.129213459
H	0.650809205	3.819134992	0.150390088
H	2.315067995	2.226711884	2.758037363

H	1.799448439	1.864748199	3.152260241

$5H_2/Li^+@B_3O_3H_3$

B	-2.132298742	-1.534227372	0.906327754
O	-1.304023305	-1.441921674	2.017700435
O	-2.151561728	-0.461294580	0.024993826
B	-0.518416397	-0.364139587	2.243366958
B	-1.380536959	0.634095794	0.204971427
H	0.199086978	-0.288810939	3.180394238
H	-1.376688650	1.541736528	-0.553288770
O	-0.529795558	0.723357891	1.333897313
H	-2.791405277	-2.488556117	0.713545423
Li	0.716920731	2.154594383	1.493118993
H	2.276417572	1.105200184	0.407710535
H	2.218618022	1.695486271	-0.039404243
H	-0.112107254	3.622998313	2.777879059
H	-0.682035729	3.155765792	2.859044674
H	0.063367785	3.303890217	-0.149957634
H	0.588668530	3.762641494	0.106786919
H	2.253230604	1.883712657	2.820782547
H	1.726978131	1.589763314	3.254238877
H	2.629169477	4.163095837	1.583183725
H	2.188506462	4.401716308	2.129116571

$1H_2/Li^+@B_3N_2OH_3$ (in-plane)

N	-0.886688629	-0.638634182	0.988885249
B	-0.524180189	-0.696411686	2.344323018
B	0.071624848	-0.519411454	-0.080122540

H	-1.280692524	-0.806582100	3.250195355
H	-0.251919710	-0.478905970	-1.215380229
O	0.855672977	-0.624502183	2.670493202
N	1.454539989	-0.445845057	0.325968943
H	2.159759507	-0.354395608	-0.389269039
B	1.850581318	-0.494955374	1.668476303
H	2.970106188	-0.424468174	2.063884107
H	-1.866321227	-0.692644832	0.752366873
Li	1.547124965	-0.656413293	4.361686553
H	0.434199040	-0.829086676	6.008059882
H	1.098521217	-0.801364003	6.343789177

$2H_2/Li^+@B_3N_2OH_3$ (in-plane)

N	-0.832774431	-0.466962312	1.125781240
B	-0.448233479	-0.586474578	2.470752215
B	0.108669569	-0.459197306	0.035370713
H	-1.194071488	-0.593113997	3.393373841
H	-0.238217354	-0.359195925	-1.089628106
O	0.933370533	-0.705929333	2.767864337
N	1.496418463	-0.572401667	0.410595293
H	2.193178731	-0.568449295	-0.318799329
B	1.915671966	-0.698232425	1.743044812
H	3.041452116	-0.810163335	2.102552838
H	-1.816320677	-0.395811556	0.911519774
Li	1.566795515	-0.778331224	4.490094360
H	0.121537546	-1.467509741	5.689292673
H	0.559250891	-1.208926165	6.233205341
H	3.307627073	0.098745051	5.024353934

H	3.407679956	-0.575531539	5.323664560

$3H_2/Li^+@B_3N_2OH_3$ (in-plane)

N	-0.511884794	-0.179212761	1.327484997
B	-0.091515169	-0.251957608	2.663191060
B	0.296541477	-0.644894427	0.228927063
H	-0.715069315	0.147346917	3.594322447
H	-0.069869382	-0.575365339	-0.892787735
O	1.170112000	-0.823715778	2.956202553
N	1.577888304	-1.192198154	0.592501099
H	2.183568353	-1.530441133	-0.140279089
B	2.019953183	-1.296321193	1.921907494
H	3.059996665	-1.754288511	2.260173692
H	-1.415224394	0.224049619	1.127089423
Li	1.634337238	-0.746470301	4.737522093
H	0.125615880	-1.441211756	5.925529879
H	0.272850082	-0.822804423	6.310493010
H	1.901816920	1.265987433	4.899222699
H	2.229938072	1.088192961	5.542372765
H	3.001938293	-2.042286397	5.518758999
H	3.377473586	-1.407348146	5.613206552

$4H_2/Li^+@B_3N_2OH_3$ (in-plane)

N	-0.585934091	0.065829653	1.896388127
B	0.107971191	-0.236097495	3.075190687
B	-0.058883823	-0.253203117	0.591320458
H	-0.276696020	0.013923163	4.175698489
H	-0.645222987	-0.001342215	-0.403600424

O	1.358320502	-0.885743247	3.002639884
N	1.226736598	-0.899852516	0.587410223
H	1.636350731	-1.144678887	-0.301664212
B	1.937965626	-1.224769261	1.755235689
H	2.990455020	-1.768468942	1.774400537
H	-1.485023393	0.520298757	1.958147864
Li	1.868501789	-1.060896727	4.786515837
H	0.427123564	-2.634261026	4.923496422
H	0.495107804	-2.568812834	5.659965662
H	3.385265091	0.447213026	4.249351218
H	3.429298246	0.537437173	4.984439488
H	1.115699029	-0.325461894	6.673561393
H	1.763583109	0.032323272	6.608803761
H	3.508379628	-2.288380918	5.320454702
H	3.209431386	-2.600428967	4.716185194

$5H_2/Li^+@B_3N_2OH_3$ (in-plane)

N	-0.235236919	0.426726802	1.891546838
B	0.361114418	0.027568803	3.098064267
B	0.058809008	-0.199087313	0.627802079
H	0.151394076	0.534830718	4.150042616
H	-0.449386675	0.142473764	-0.382883094
O	1.277417490	-1.053331628	3.088559064
N	1.022135271	-1.268007670	0.681634455
H	1.264532646	-1.742305573	-0.175429924
B	1.621584521	-1.700989497	1.877050936
H	2.405329273	-2.589436209	1.947671774
H	-0.895273609	1.189634671	1.913260589

Li	2.154501026	-1.358563673	4.722744123
H	1.007354700	-3.068971470	5.121661068
H	0.823471956	-2.619183697	5.682700446
H	3.016066224	0.684442853	4.664846403
H	2.667037467	0.706407233	5.318966870
H	0.299217050	-0.434650198	6.833317092
H	0.881505763	0.021377766	6.831556944
H	4.090525416	-2.019528297	4.426163524
H	3.886328730	-1.954781455	3.714663970
H	3.422946004	-1.317968031	6.657939138
H	3.027477165	-1.907385899	6.875989820

$1H_2/Li^+@B_3N_2OH_3$ (out-of-plane)

N	-0.877531519	-0.541292424	0.878333358
B	-0.456647784	-0.828056908	2.227731802
B	0.050289757	-0.475916842	-0.231407527
H	-1.196248703	-1.110779755	3.101652725
H	-0.303480196	-0.478585384	-1.356977938
O	0.896301085	-0.614507944	2.484340157
N	1.427168261	-0.282238008	0.170873350
H	2.123564486	-0.217855441	-0.559722970
B	1.889689386	-0.567856924	1.507371274
H	3.025668927	-0.669547817	1.802177253
H	-1.860244943	-0.649451750	0.662812882
Li	0.324047701	1.272170264	1.387595830
H	0.286135144	3.295557482	1.403510632
H	0.898690398	3.165002450	1.807568173

$2H_2/Li^+@B_3N_2OH_3$ (out-of-plane)

B	-0.902918128	-0.695350887	0.800919979
N	-0.424200477	-0.604142590	2.162886035
N	0.115928275	-0.444829755	-0.192520824
H	-1.090526198	-0.747984962	2.910165360
H	-0.163243115	-0.474983213	-1.164255626
B	0.977810357	-0.740818217	2.489257615
B	1.526139073	-0.556911985	0.096481987
H	1.370978605	-0.925568490	3.586439528
H	2.365903248	-0.581633680	-0.732399412
O	1.869436278	-0.538682991	1.444115742
H	-2.039105533	-0.855228179	0.521473360
Li	0.336426853	1.304533714	1.253310779
H	-1.334853685	2.434024430	1.092489077
H	-0.841309624	2.986674331	1.162371440
H	1.665192412	2.749394981	1.888501735
H	2.105147660	2.149663493	1.847054225

$3H_2/Li^+@B_3N_2OH_3$ (out-of-plane)

O	-0.775834501	-0.531471906	0.804542718
B	-0.476168612	-0.732811108	2.144588373
B	0.155567973	-0.538022171	-0.223247352
H	-1.342816053	-0.860461282	2.935863624
H	-0.200359941	-0.554427231	-1.347747368
N	0.919437295	-0.668362325	2.502368601
N	1.541874130	-0.423132578	0.173086144
H	1.163175005	-0.830228971	3.470209008
H	2.239496510	-0.445941092	-0.558818024

B	1.974670632	-0.727213410	1.520330053
H	3.107068755	-0.901959561	1.807520342
Li	0.739573385	1.378361124	1.334693745
H	0.667889517	2.342287937	-0.473218570
H	0.483713595	2.947378366	-0.080326678
H	-0.607971096	2.452835795	2.588414294
H	-1.077354558	2.152037728	2.095036622
H	2.043168666	2.817441238	2.109091778
H	2.308569165	2.169302126	2.360286619

$4H_2/Li^+@B_3N_2OH_3$ (out-of-plane)

B	-0.977677962	-0.731767293	0.967546225
O	-0.439232390	-0.847263158	2.237292779
N	-0.069682995	-0.377527368	-0.098813731
H	-0.445320129	-0.350009141	-1.036930713
B	0.914238911	-0.806476437	2.517142657
B	1.361349808	-0.461450660	0.055350757
H	1.310438690	-1.012831917	3.611286926
H	2.106748569	-0.422412783	-0.863274147
N	1.797704986	-0.434327202	1.431305053
H	2.791452280	-0.459290342	1.617677684
H	-2.137475314	-0.875887627	0.794311480
Li	0.557652071	1.528233786	1.206513303
H	1.682421522	2.218808750	-0.535547526
H	1.372222936	2.870033656	-0.359237095
H	-0.447061969	2.269720471	3.020743677
H	-0.642765830	1.552941878	3.034477615
H	-1.201408479	2.339006133	0.238556849

H	-1.062980263	2.946675522	0.643232541
H	1.874847928	3.058999423	2.298043456
H	2.231367628	2.407260311	2.303122212

$5H_2/Li^+@B_3N_2OH_3$ (out-of-plane)

B	-0.554305426	-0.563325317	1.854260156
O	0.406432918	-1.078347848	2.677631876
N	-0.140887773	-0.021283692	0.565333389
H	-0.885002186	0.146637081	-0.102479473
B	1.708690128	-1.349522303	2.266863116
B	1.152167218	-0.426071623	0.002305633
H	2.471067228	-1.830435980	3.030749792
H	1.411073426	-0.201247846	-1.131839740
N	2.065166015	-1.014038102	0.916144794
H	2.990561392	-1.256878833	0.593533910
H	-1.675646521	-0.487039640	2.230797630
Li	0.240040019	2.022329843	1.071930466
H	2.328090653	2.133077166	0.600995282
H	2.055253806	2.567782752	0.064112863
H	-1.505317506	2.788639259	2.030063634
H	-1.675644169	2.064331442	2.046444185
H	-0.587733758	2.596188530	-0.768744322
H	-0.506357917	3.272912281	-0.472515977
H	1.122955304	2.445198211	2.956248698
H	1.164583905	1.712116507	3.076295379
H	1.025097342	4.438793196	1.401566759
H	0.305810901	4.576132917	1.520956949