

Supporting Information

Synergic effect of pore size engineering and applied electric field on the controlled permeation of alkali metal atoms and ions across pristine and defected *h*-BN sheet

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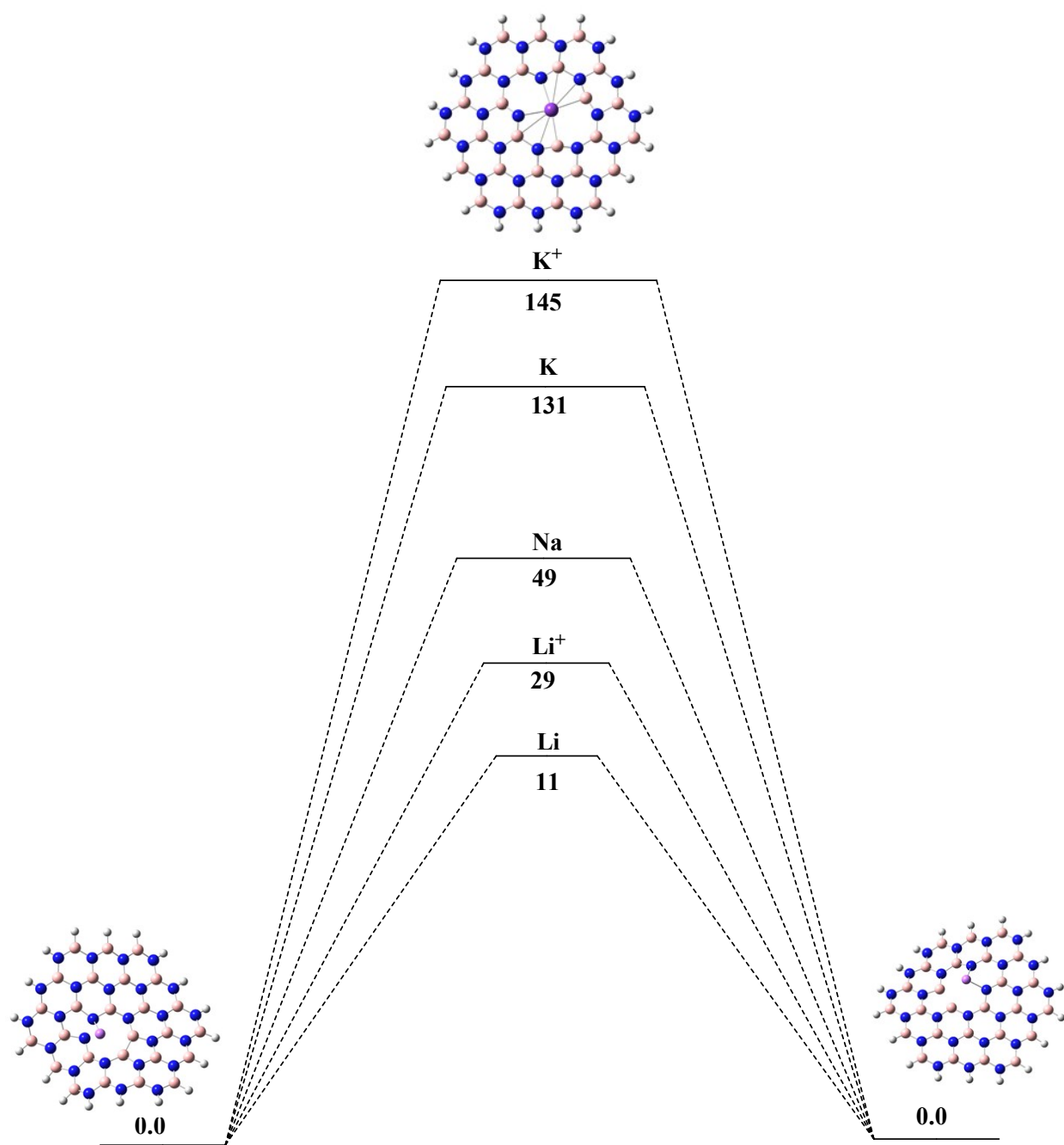


Figure S1 Energy profile diagram showing energy barriers (kcal mol⁻¹) for the permeation of alkali metal atoms/ions across V_{BN} *h*-BN.

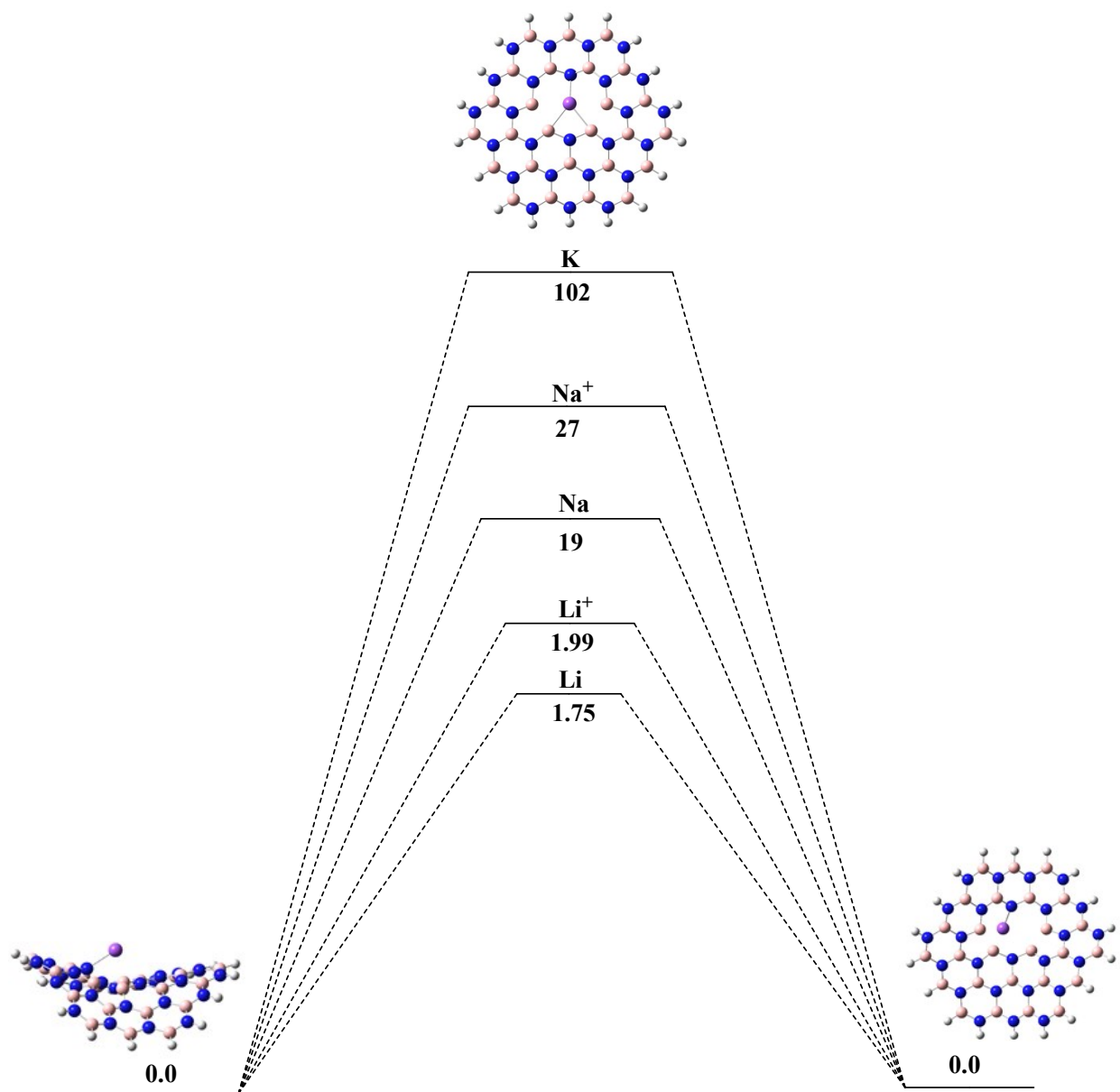


Figure S2 Energy profile diagram showing energy barriers (kcal mol⁻¹) for the permeation of alkali metal atoms/ions across V_{N2B} *h*-BN.

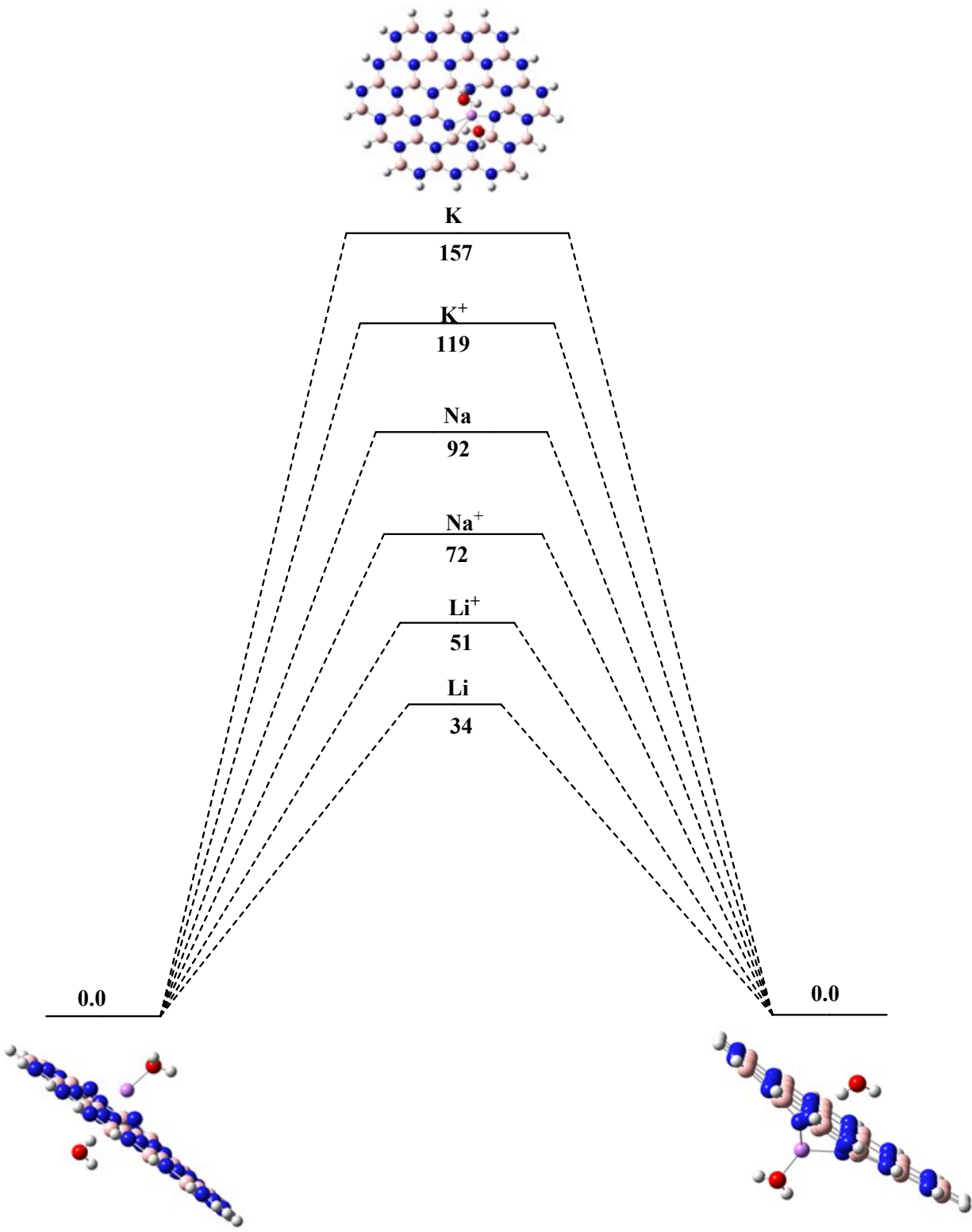


Figure S3 Energy profile diagram showing energy barriers (kcal mol⁻¹) for the permeation of alkali metal atoms/ions across H₂O-V_B h-BN-H₂O.

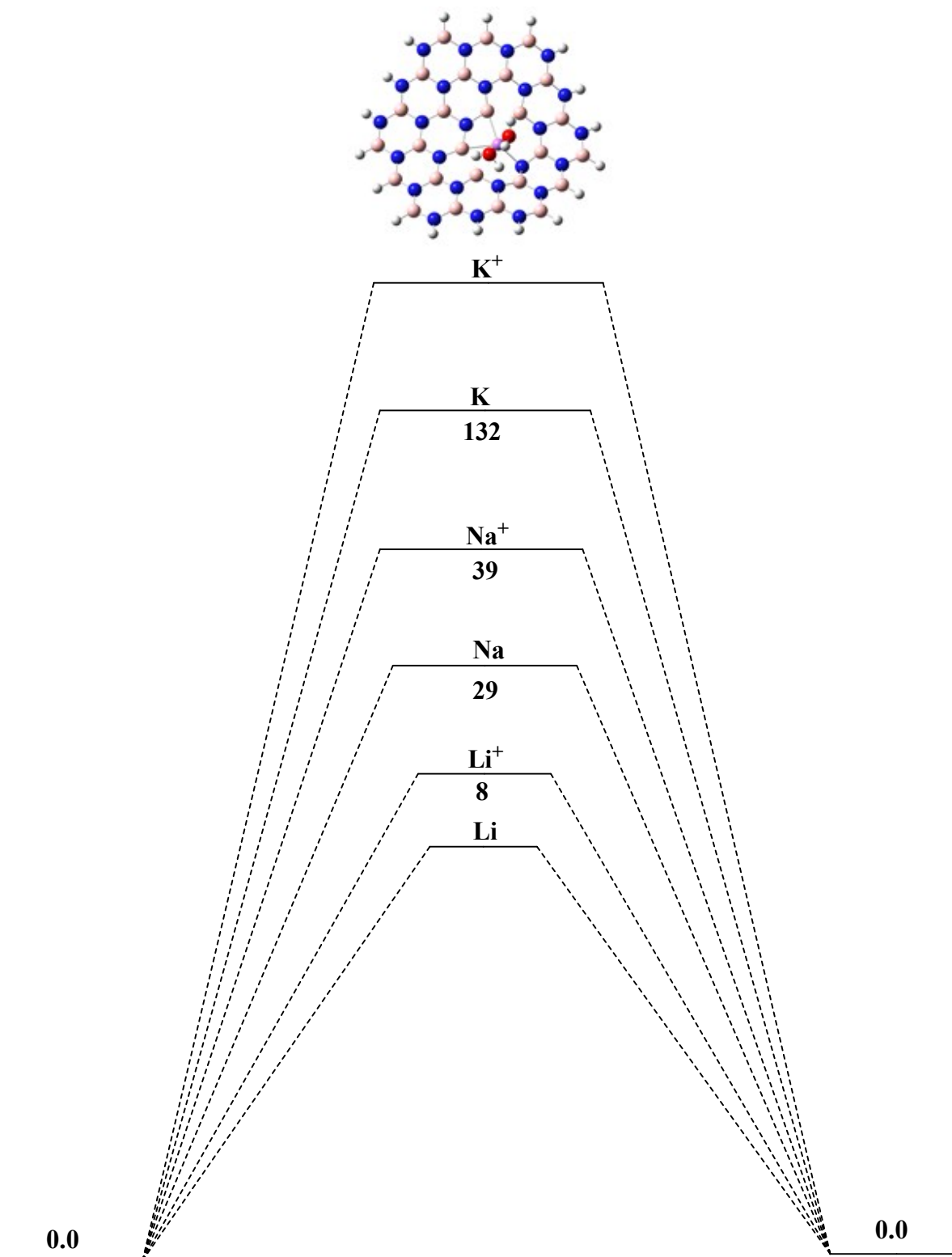


Figure S4 Energy profile diagram showing energy barriers (kcal mol⁻¹) for the permeation of alkali metal atoms/ions across $\text{H}_2\text{O}-\text{V}_{\text{N}_2\text{B}} h\text{-BN}-\text{H}_2\text{O}$.

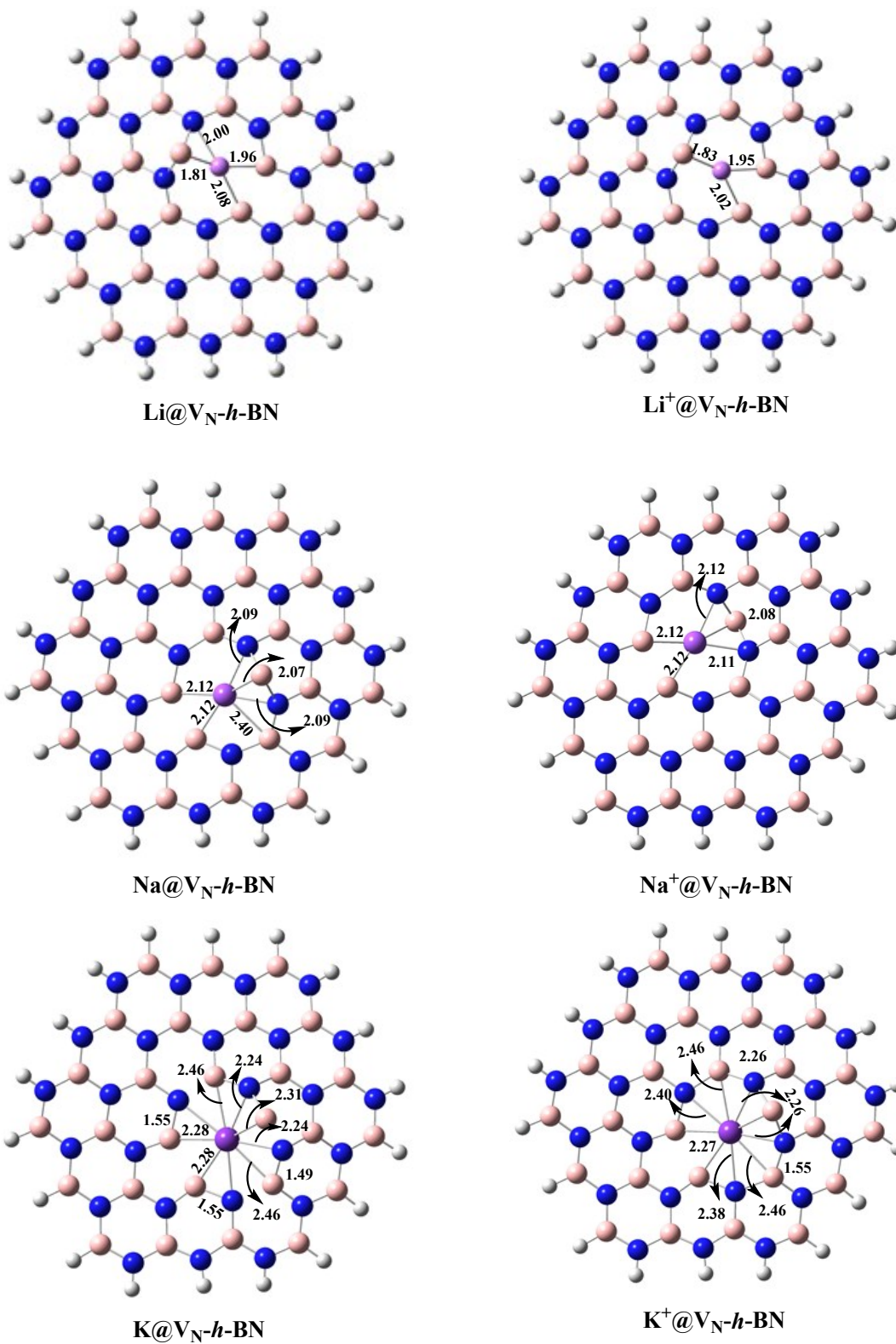
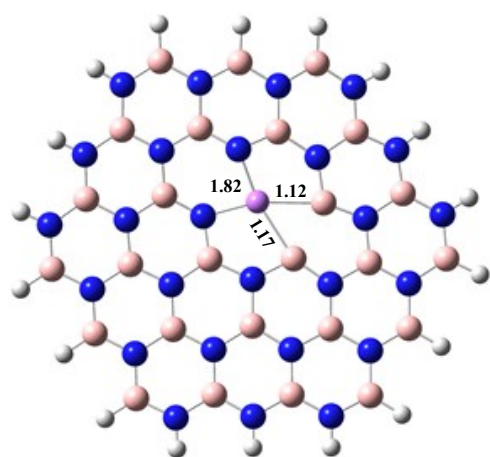
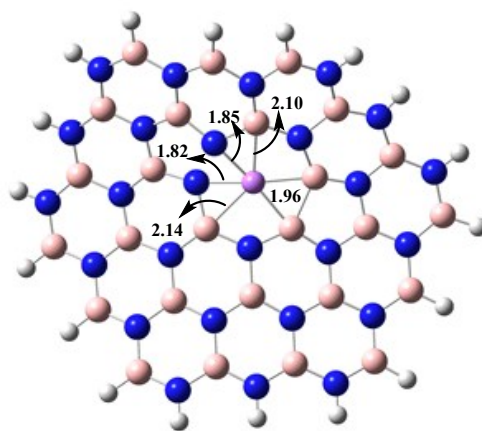


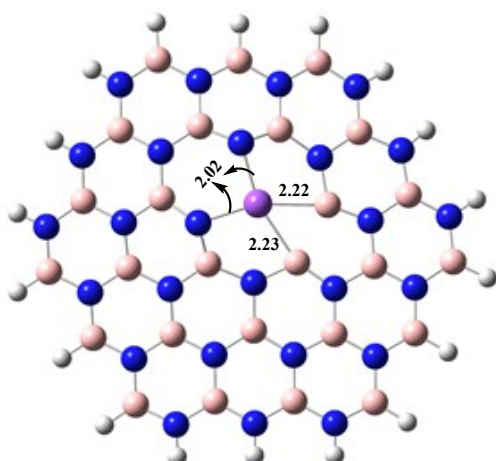
Figure S5 Optimized geometries (bond lengths, Å) of Transition states of V_N h -BN with alkali metal atoms/ions



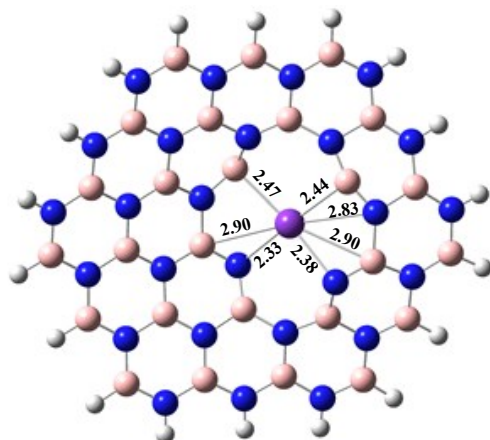
Li@V_{BN} *h*-BN



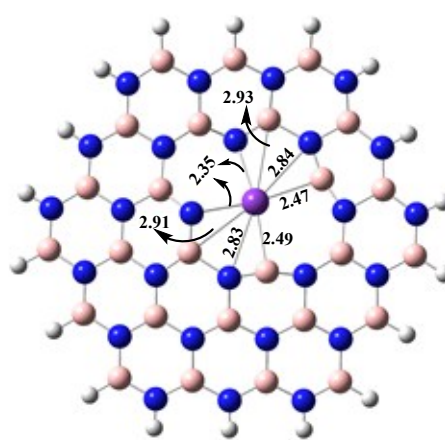
Li⁺@V_{BN} *h*-BN



Na@V_{BN} *h*-BN

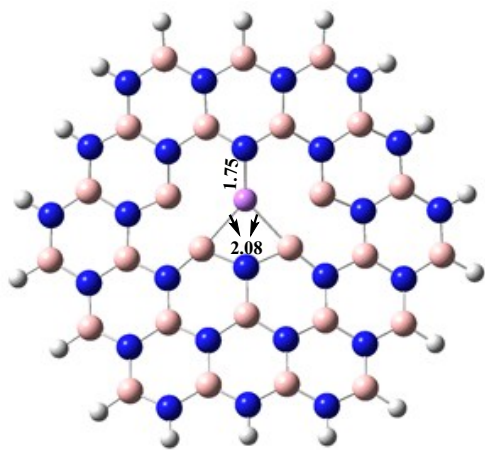


K@V_{BN} *h*-BN

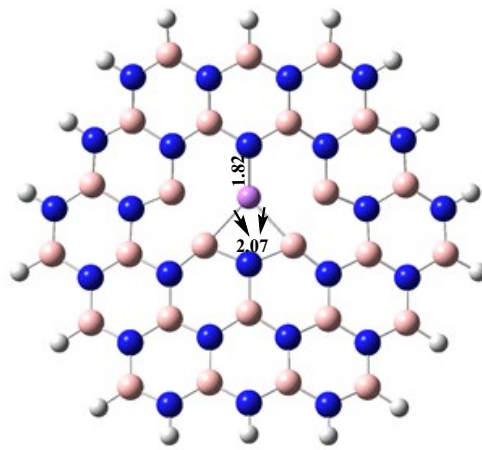


K⁺@V_{BN} *h*-BN

Figure S6 Optimized geometries (bond lengths, Å) of Transition states of V_{BN} *h*-BN with alkali metal atoms/ions

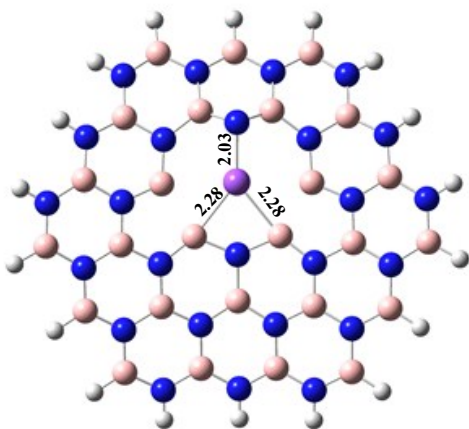


$\text{Li@V}_{\text{N2B}} h\text{-BN}$

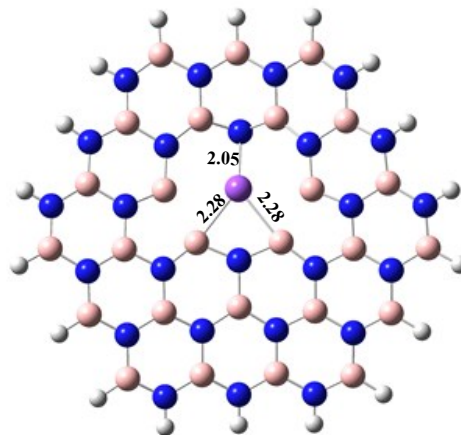


$\text{Li}^+\text{@V}_{\text{N2B}} h\text{-BN}$

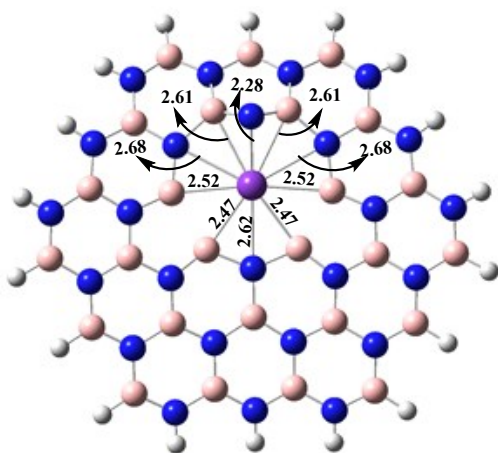
2.05



$\text{Na@V}_{\text{N2B}} h\text{-BN}$



$\text{Na}^+\text{@V}_{\text{N2B}} h\text{-BN}$



$\text{K@V}_{\text{N2B}} h\text{-BN}$

Figure S7 Optimized geometries (bond lengths, Å) of Transition states of $\text{V}_{\text{N2B}} h\text{-BN}$ with alkali metal atoms/ions

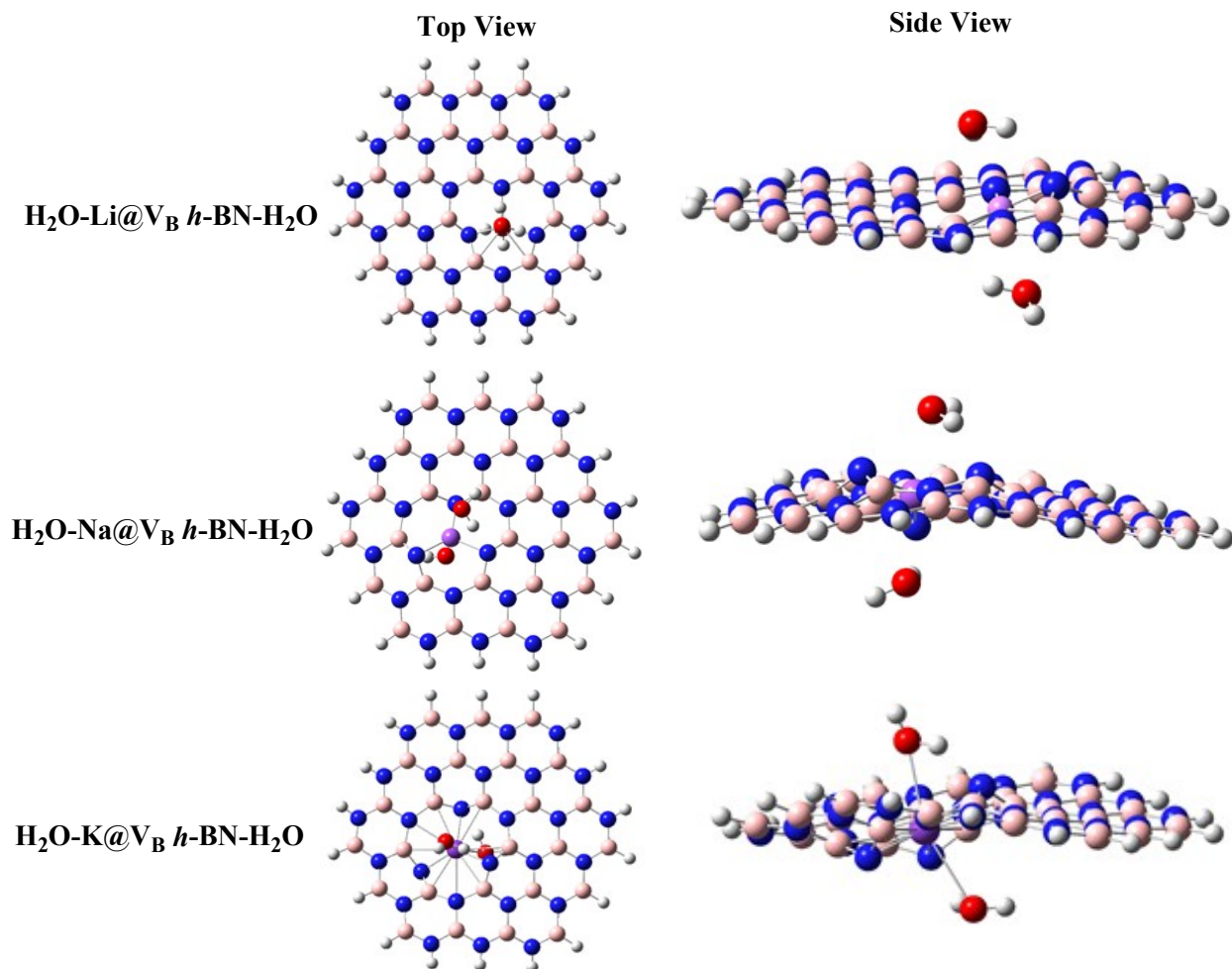


Figure S8 Optimized geometries of Transition states of $\text{H}_2\text{O-V}_\text{B} \text{ } h\text{-BN-H}_2\text{O}$ with alkali metal atoms

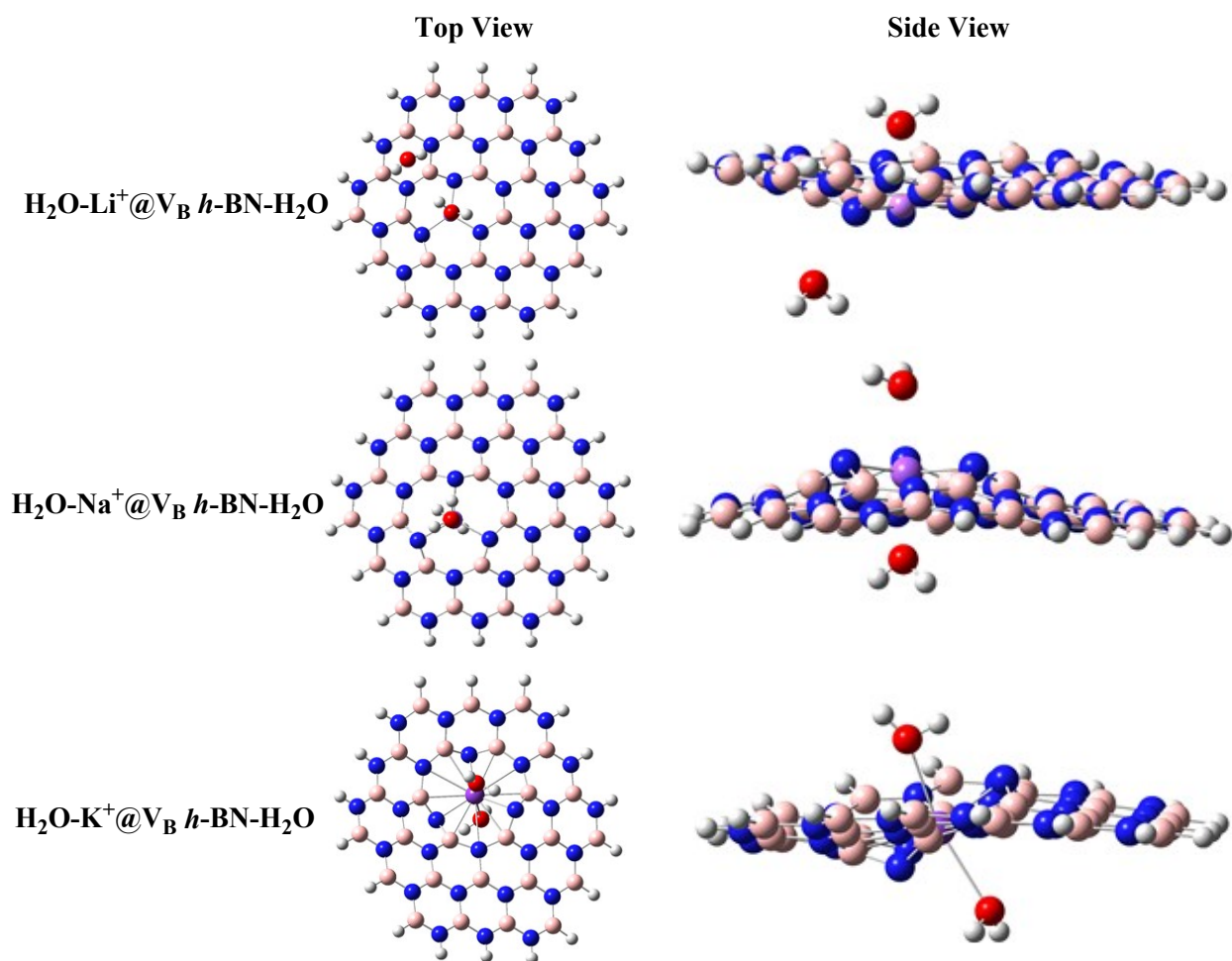


Figure S9 Optimized geometries of Transition states of $\text{H}_2\text{O-V}_{\text{B}} h\text{-BN-H}_2\text{O}$ with alkali metal ions

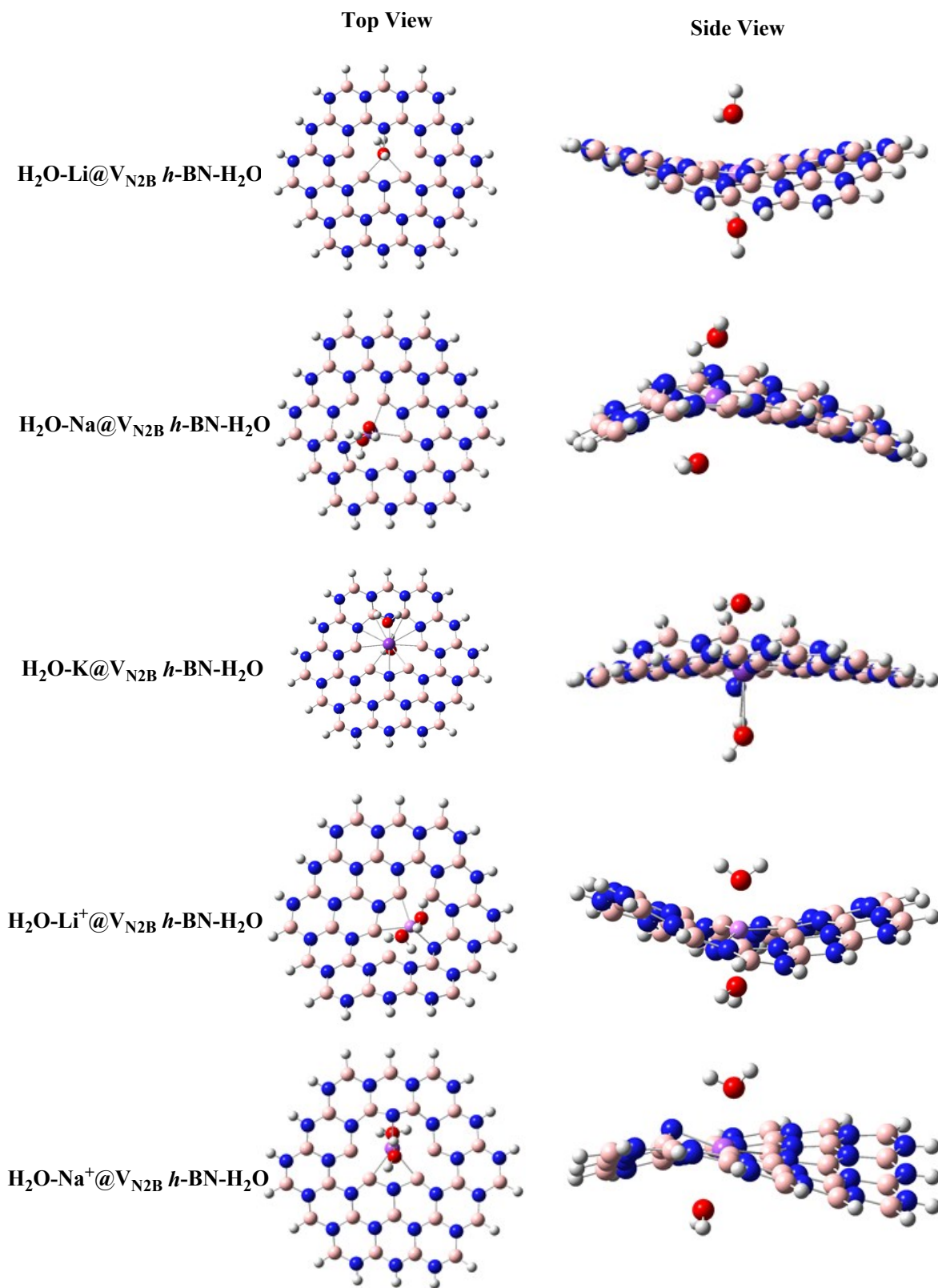


Figure S10 Optimized geometries of Transition states of $\text{H}_2\text{O-V}_{\text{N}_2\text{B}} h\text{-BN-H}_2\text{O}$ with alkali metal atoms/ions

Li@V_B *h*-BN

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.00009100 | -1.10982100 | 0.47365700 |
| B | 1.35466300 | 0.69196500 | 0.47186200 |
| B | -1.35495500 | 0.69154500 | 0.47205200 |
| B | 2.66930700 | -1.44217400 | 0.36274600 |
| B | 3.84170900 | 0.71763900 | 0.02385500 |
| B | 2.53684100 | 2.86729800 | 0.05564900 |
| B | -0.00048600 | 2.80113600 | 0.19648700 |
| B | -2.53784100 | 2.86649300 | 0.05587900 |
| B | -3.84196600 | 0.71639000 | 0.02386100 |
| B | -2.66884700 | -1.44300100 | 0.36291700 |
| B | -1.27557900 | -3.58301400 | 0.11933600 |
| B | 1.27679200 | -3.58259500 | 0.11886500 |
| N | 0.00049600 | -2.95114800 | 0.04391700 |
| N | 1.59133800 | -0.67270600 | 0.83066300 |
| N | 2.56573700 | -2.88738400 | 0.15926400 |
| N | -2.56474500 | -2.88817700 | 0.15941000 |
| N | -1.59117900 | -0.67317400 | 0.83096200 |
| N | -3.89704000 | -0.72684700 | 0.06518100 |
| N | -2.57607700 | 1.43274100 | 0.16651700 |
| N | -0.00024400 | 1.34085400 | 0.41526800 |
| N | -1.25590000 | 3.54210500 | 0.10377600 |
| N | 1.25468700 | 3.54250000 | 0.10369000 |
| N | 2.57555900 | 1.43356100 | 0.16635500 |
| N | 3.89728300 | -0.72558300 | 0.06517600 |
| B | 3.80162400 | -3.61566000 | -0.08481100 |
| B | 5.11565500 | -1.45489900 | -0.19076200 |
| B | 1.24940400 | 4.99664200 | 0.02038800 |

| | | | |
|---|-------------|-------------|-------------|
| B | -1.25108300 | 4.99622800 | 0.02033200 |
| B | -5.11509200 | -1.45657400 | -0.19117800 |
| B | -3.80035600 | -3.61688300 | -0.08478000 |
| N | -1.26067400 | -5.05786700 | 0.01682700 |
| N | 1.26235100 | -5.05744000 | 0.01583300 |
| N | 5.06977900 | 1.46089100 | -0.21192200 |
| N | 3.78286700 | 3.60440000 | -0.11453900 |
| N | -3.78415200 | 3.60319700 | -0.11403600 |
| N | -5.07025400 | 1.45923300 | -0.21207100 |
| B | 0.00095400 | -5.75745400 | -0.00958100 |
| B | 5.03433000 | 2.90042500 | -0.24985500 |
| B | -5.03534700 | 2.89879300 | -0.24960000 |
| B | -2.50576100 | -5.77814500 | -0.12870500 |
| B | 3.75866000 | 5.04818300 | -0.16509200 |
| N | -3.72746600 | -5.05193500 | -0.18754500 |
| N | 2.50135700 | 5.70019300 | -0.07610000 |
| N | -0.00095400 | 5.68644500 | 0.02586700 |
| N | -5.03918300 | -2.89147400 | -0.21199400 |
| N | -6.31296800 | -0.68537400 | -0.40781000 |
| N | -2.50325400 | 5.69936900 | -0.07632300 |
| B | 2.50765700 | -5.77726300 | -0.12998600 |
| B | 6.31446500 | 0.74146900 | -0.41153200 |
| B | -6.31464500 | 0.73939000 | -0.41199000 |
| B | -3.76040000 | 5.04698200 | -0.16475400 |
| N | 6.31330800 | -0.68329300 | -0.40718100 |
| N | 5.04028700 | -2.88983000 | -0.21132600 |
| N | 3.72918300 | -5.05066900 | -0.18811800 |
| H | -7.33333600 | 1.33584000 | -0.58849300 |

| | | | |
|---|-------------|-------------|-------------|
| H | -6.04552900 | 3.51380800 | -0.40122900 |
| H | -4.76709300 | 5.67649200 | -0.28082300 |
| H | 0.00113800 | -6.95001700 | -0.05523600 |
| H | -2.51135500 | -6.96903600 | -0.21383800 |
| H | 2.51359300 | -6.96808800 | -0.21602000 |
| H | 7.33297200 | 1.33826900 | -0.58791500 |
| H | 6.04428700 | 3.51577600 | -0.40162400 |
| H | 4.76511800 | 5.67800100 | -0.28154200 |
| H | -4.57878300 | -5.58367900 | -0.30619500 |
| H | -5.88277200 | -3.42048800 | -0.38876200 |
| H | -7.19481900 | -1.15284500 | -0.56632700 |
| H | -2.49390600 | 6.70884700 | -0.12124200 |
| H | -0.00111800 | 6.69533600 | -0.03660800 |
| H | 2.49169500 | 6.70967400 | -0.12090600 |
| H | 7.19539200 | -1.15046200 | -0.56529100 |
| H | 5.88410100 | -3.41854600 | -0.38791700 |
| H | 4.58063800 | -5.58208900 | -0.30722200 |

Li@V_B *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Li | -0.00002100 | 1.47686800 | -1.62150900 |
| B | -1.29370000 | -0.64996500 | -0.32479400 |
| B | 1.29372400 | -0.64993200 | -0.32480300 |
| B | -2.62050400 | 1.43459200 | -0.28319500 |
| B | -3.81788300 | -0.71325700 | -0.03916000 |
| B | -2.52000900 | -2.84427000 | -0.01339100 |
| B | 0.00004000 | -2.80638800 | -0.11044000 |
| B | 2.52008900 | -2.84420400 | -0.01338800 |
| B | 3.81790500 | -0.71315600 | -0.03916100 |
| B | 2.62046500 | 1.43465800 | -0.28321000 |

| | | | |
|---|-------------|-------------|-------------|
| B | 1.28182600 | 3.52043000 | -0.05378600 |
| B | -1.28192600 | 3.52040000 | -0.05378000 |
| N | -0.00004300 | 2.86992600 | -0.16459200 |
| N | -1.45215600 | 0.73645300 | -0.66307400 |
| N | -2.56821200 | 2.87249900 | -0.07947300 |
| N | 2.56812900 | 2.87256400 | -0.07948500 |
| N | 1.45214000 | 0.73648500 | -0.66309500 |
| N | 3.86873700 | 0.72695100 | -0.09112200 |
| N | 2.54101800 | -1.40483900 | -0.09999700 |
| N | 0.00002000 | -1.35213000 | -0.28834700 |
| N | 1.25279500 | -3.54291100 | -0.03423600 |
| N | -1.25269600 | -3.54294400 | -0.03423800 |
| N | -2.54097600 | -1.40490500 | -0.09999600 |
| N | -3.86875600 | 0.72684800 | -0.09111700 |
| B | -3.80516900 | 3.60634500 | 0.09496600 |
| B | -5.10522400 | 1.45179000 | 0.09515400 |
| B | -1.25048100 | -4.99502100 | 0.04361600 |
| B | 1.25061800 | -4.99498800 | 0.04361900 |
| B | 5.10518300 | 1.45192800 | 0.09515200 |
| B | 3.80506600 | 3.60644400 | 0.09495700 |
| N | 1.24787100 | 4.99263700 | 0.06883400 |
| N | -1.24801100 | 4.99260700 | 0.06884000 |
| N | -5.06231500 | -1.45426600 | 0.11542800 |
| N | -3.77362900 | -3.58694600 | 0.09524900 |
| N | 3.77372900 | -3.58684500 | 0.09525600 |
| N | 5.06235700 | -1.45413000 | 0.11543300 |
| B | -0.00007800 | 5.69913800 | 0.13108700 |
| B | -5.03139300 | -2.89097600 | 0.16316100 |

| | | | |
|---|-------------|-------------|------------|
| B | 5.03147400 | -2.89084100 | 0.16317000 |
| B | 2.48869100 | 5.73321100 | 0.19660400 |
| B | -3.75856700 | -5.03063000 | 0.15080600 |
| N | 3.72512600 | 5.03951400 | 0.21254800 |
| N | -2.50578900 | -5.69490500 | 0.11331700 |
| N | 0.00007800 | -5.68608100 | 0.05240200 |
| N | 5.04777700 | 2.88604400 | 0.13716100 |
| N | 6.31518700 | 0.68307200 | 0.23202500 |
| N | 2.50594500 | -5.69483800 | 0.11332500 |
| B | -2.48885000 | 5.73314700 | 0.19661300 |
| B | -6.31734000 | -0.74067200 | 0.23613500 |
| B | 6.31736100 | -0.74050000 | 0.23614400 |
| B | 3.75870500 | -5.03052900 | 0.15081600 |
| N | -6.31520700 | 0.68290000 | 0.23201900 |
| N | -5.04785900 | 2.88590900 | 0.13716700 |
| N | -3.72526700 | 5.03941700 | 0.21255700 |
| H | 7.34468100 | -1.33830400 | 0.34810200 |
| H | 6.04792100 | -3.50662400 | 0.26325100 |
| H | 4.77422200 | -5.65260400 | 0.22852500 |
| H | -0.00009300 | 6.88554700 | 0.24826800 |
| H | 2.46372600 | 6.92228100 | 0.29871600 |
| H | -2.46391700 | 6.92221800 | 0.29872500 |
| H | -7.34464300 | -1.33850600 | 0.34808800 |
| H | -6.04782300 | -3.50678800 | 0.26323700 |
| H | -4.77406700 | -5.65273100 | 0.22851100 |
| H | 4.56955700 | 5.58347300 | 0.32129200 |
| H | 5.90457000 | 3.40725900 | 0.26443700 |
| H | 7.20252700 | 1.15358300 | 0.34283900 |

| | | | |
|---|-------------|-------------|------------|
| H | 2.50489400 | -6.70414900 | 0.15966000 |
| H | 0.00009100 | -6.69524400 | 0.10867900 |
| H | -2.50471100 | -6.70421600 | 0.15965200 |
| H | -7.20256000 | 1.15338600 | 0.34283100 |
| H | -5.90466800 | 3.40709700 | 0.26444100 |
| H | -4.56971300 | 5.58335400 | 0.32130100 |

Li@V_B *h*-BN (product)

| | | | |
|----|-------------|-------------|------------|
| Li | -0.00006200 | 1.47664600 | 1.62192900 |
| B | -1.29373200 | -0.64995400 | 0.32488700 |
| B | 1.29380200 | -0.64986000 | 0.32491600 |
| B | -2.62064000 | 1.43448400 | 0.28334300 |
| B | -3.81797600 | -0.71338100 | 0.03960500 |
| B | -2.51995400 | -2.84428000 | 0.01341700 |
| B | 0.00011500 | -2.80629300 | 0.11027600 |
| B | 2.52018800 | -2.84408700 | 0.01340700 |
| B | 3.81804000 | -0.71308700 | 0.03961000 |
| B | 2.62052600 | 1.43467500 | 0.28338800 |
| B | 1.28171500 | 3.52037700 | 0.05355500 |
| B | -1.28200600 | 3.52028900 | 0.05354000 |
| N | -0.00012600 | 2.86989000 | 0.16456600 |
| N | -1.45221600 | 0.73646900 | 0.66320700 |
| N | -2.56829300 | 2.87239200 | 0.07937500 |
| N | 2.56805300 | 2.87258100 | 0.07940900 |
| N | 1.45216900 | 0.73656300 | 0.66327100 |
| N | 3.86882200 | 0.72705300 | 0.09156400 |
| N | 2.54110400 | -1.40473200 | 0.10023100 |
| N | 0.00005900 | -1.35204600 | 0.28831600 |
| N | 1.25289200 | -3.54279800 | 0.03392100 |

| | | | |
|---|-------------|-------------|-------------|
| N | -1.25260600 | -3.54289400 | 0.03392600 |
| N | -2.54098200 | -1.40492300 | 0.10022600 |
| N | -3.86887600 | 0.72675500 | 0.09154400 |
| B | -3.80525100 | 3.60619800 | -0.09501200 |
| B | -5.10537500 | 1.45168700 | -0.09468200 |
| B | -1.25034800 | -4.99494700 | -0.04435900 |
| B | 1.25074600 | -4.99485100 | -0.04436900 |
| B | 5.10525800 | 1.45208600 | -0.09467100 |
| B | 3.80495200 | 3.60648700 | -0.09498800 |
| N | 1.24774300 | 4.99256500 | -0.06946000 |
| N | -1.24815000 | 4.99247700 | -0.06946900 |
| N | -5.06237700 | -1.45440700 | -0.11473200 |
| N | -3.77356700 | -3.58700200 | -0.09507500 |
| N | 3.77385800 | -3.58671100 | -0.09510200 |
| N | 5.06250000 | -1.45401200 | -0.11474600 |
| B | -0.00022800 | 5.69901100 | -0.13192700 |
| B | -5.03139600 | -2.89112200 | -0.16257200 |
| B | 5.03163100 | -2.89072900 | -0.16260300 |
| B | 2.48852500 | 5.73316400 | -0.19732500 |
| B | -3.75845000 | -5.03067400 | -0.15102600 |
| N | 3.72501600 | 5.03953400 | -0.21288000 |
| N | -2.50562700 | -5.69488500 | -0.11408100 |
| N | 0.00022500 | -5.68596300 | -0.05354800 |
| N | 5.04775600 | 2.88616500 | -0.13687900 |
| N | 6.31529900 | 0.68321700 | -0.23130200 |
| N | 2.50607900 | -5.69469100 | -0.11410400 |
| B | -2.48898900 | 5.73297900 | -0.19733500 |
| B | -6.31745000 | -0.74083900 | -0.23528300 |

| | | | |
|---|-------------|-------------|-------------|
| B | 6.31751300 | -0.74034000 | -0.23530300 |
| B | 3.75885100 | -5.03038300 | -0.15106100 |
| N | -6.31535300 | 0.68271800 | -0.23129500 |
| N | -5.04799300 | 2.88577100 | -0.13690000 |
| N | -3.72542700 | 5.03925300 | -0.21289600 |
| H | 7.34485200 | -1.33815600 | -0.34700800 |
| H | 6.04810400 | -3.50649200 | -0.26251100 |
| H | 4.77439100 | -5.65243500 | -0.22863900 |
| H | -0.00027000 | 6.88537000 | -0.24963900 |
| H | 2.46351800 | 6.92220200 | -0.29979700 |
| H | -2.46407600 | 6.92202000 | -0.29980100 |
| H | -7.34474100 | -1.33874100 | -0.34697200 |
| H | -6.04782100 | -3.50696600 | -0.26246200 |
| H | -4.77394300 | -5.65280400 | -0.22858800 |
| H | 4.56944100 | 5.58349200 | -0.32165100 |
| H | 5.90451400 | 3.40743700 | -0.26415000 |
| H | 7.20265100 | 1.15373200 | -0.34201600 |
| H | 2.50502800 | -6.70398900 | -0.16070200 |
| H | 0.00026400 | -6.69511100 | -0.11008100 |
| H | -2.50449800 | -6.70418300 | -0.16067300 |
| H | -7.20274600 | 1.15315800 | -0.34200200 |
| H | -5.90479700 | 3.40696900 | -0.26416600 |
| H | -4.56989400 | 5.58314600 | -0.32166300 |

Li⁺@V_B *h*-BN

| | | | |
|----|-------------|-------------|------------|
| Li | 1.32617300 | 0.91351800 | 0.38692100 |
| B | -1.31264100 | 0.79572800 | 0.38608700 |
| B | -0.08343600 | -1.48141100 | 0.16938800 |
| B | 0.09298000 | 2.96210500 | 0.39697400 |

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|---|-------------|-------------|-------------|
| B | -2.40679800 | 3.03782000 | 0.06060900 |
| B | -3.77553300 | 0.90464500 | 0.01395400 |
| B | -2.59415900 | -1.32420100 | 0.09963800 |
| B | -1.44460800 | -3.57566000 | 0.04315100 |
| B | 1.08203300 | -3.69358900 | 0.01436100 |
| B | 2.47418900 | -1.60947800 | 0.09472700 |
| B | 3.94462000 | 0.53521400 | 0.21611900 |
| B | 2.74957700 | 2.83740000 | 0.31145800 |
| N | 2.99628300 | 1.48097900 | 0.71505000 |
| N | -0.24125200 | 1.63280200 | 0.85904600 |
| N | 1.44966400 | 3.51438900 | 0.24727500 |
| N | 3.75843700 | -0.90453600 | 0.07673000 |
| N | 1.23098700 | -0.86288800 | 0.16264300 |
| N | 2.39183400 | -3.04028100 | 0.00775500 |
| N | -0.15160300 | -2.91220200 | 0.08181000 |
| N | -1.28853200 | -0.65624000 | 0.22959000 |
| N | -2.64704400 | -2.76994500 | 0.04221500 |
| N | -3.80832800 | -0.53943900 | 0.03378600 |
| N | -2.49615700 | 1.58378800 | 0.14606500 |
| N | -1.11045800 | 3.71171300 | 0.12735300 |
| B | 1.50556100 | 4.96865900 | -0.03140100 |
| B | -1.02134500 | 5.15242300 | -0.07497500 |
| B | -5.10249500 | -1.20921700 | -0.06549400 |
| B | -3.94685600 | -3.44338300 | -0.02398500 |
| B | 3.60660800 | -3.83640100 | -0.11100100 |
| B | 4.97559100 | -1.70226200 | -0.12407800 |
| N | 5.19823000 | 1.21670500 | -0.09358400 |
| N | 4.02319000 | 3.46778800 | -0.02954700 |

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|---|-------------|-------------|-------------|
| N | -3.60789000 | 3.80686900 | -0.14527000 |
| N | -4.97379700 | 1.69868000 | -0.13871700 |
| N | -1.50252100 | -5.02001800 | -0.01183000 |
| N | 1.00407300 | -5.13081100 | -0.05281400 |
| B | 5.22432000 | 2.66549100 | -0.19840100 |
| B | -4.89295700 | 3.13713200 | -0.21663600 |
| B | -0.28906100 | -5.79318600 | -0.05256500 |
| B | 6.38309100 | 0.39351500 | -0.29804000 |
| B | -6.25962700 | 1.02456100 | -0.22027600 |
| N | 6.23400700 | -1.01832000 | -0.26023000 |
| N | -6.28170000 | -0.39569800 | -0.16651200 |
| N | -5.12907500 | -2.64030200 | -0.06392600 |
| N | 4.85448500 | -3.12886900 | -0.18246500 |
| N | 3.47951600 | -5.26113900 | -0.16612000 |
| N | -3.96593500 | -4.87825300 | -0.05067700 |
| B | 4.03213600 | 4.90768700 | -0.23757600 |
| B | -3.52501100 | 5.25243800 | -0.27969800 |
| B | 2.22117000 | -5.92680700 | -0.13427400 |
| B | -2.79543700 | -5.68346700 | -0.04804800 |
| N | -2.24307700 | 5.87703700 | -0.24772800 |
| N | 0.29234000 | 5.72289700 | -0.11314800 |
| N | 2.79016900 | 5.59079300 | -0.20101000 |
| H | 2.16368400 | -7.11357900 | -0.18031000 |
| H | -0.33830900 | -6.98000300 | -0.09478000 |
| H | -2.86888500 | -6.87049800 | -0.07981800 |
| H | 6.24356800 | 3.20697100 | -0.48000100 |
| H | 7.44017400 | 0.90128900 | -0.49562500 |
| H | 5.05245800 | 5.48068200 | -0.44770400 |

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|---|-------------|-------------|-------------|
| H | -4.50937800 | 5.90404500 | -0.42373400 |
| H | -5.88341800 | 3.78153400 | -0.34639700 |
| H | -7.26657700 | 1.64859400 | -0.33082400 |
| H | 7.07236200 | -1.56708800 | -0.39982600 |
| H | 5.70188500 | -3.67027700 | -0.30093900 |
| H | 4.30587700 | -5.83994100 | -0.23446500 |
| H | -4.85554200 | -5.35799600 | -0.08359300 |
| H | -6.02520700 | -3.10614000 | -0.12203600 |
| H | -7.18582600 | -0.84443200 | -0.22862400 |
| H | -2.21792800 | 6.88125000 | -0.36510600 |
| H | 0.37427200 | 6.71852400 | -0.27507500 |
| H | 2.81776300 | 6.58922100 | -0.36219000 |

Li⁺@V_B *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Li | 1.35645500 | 0.62963400 | -1.76903600 |
| B | -1.23068700 | 0.83795100 | -0.27614500 |
| B | -0.14031500 | -1.45083700 | -0.23837500 |
| B | 0.24004200 | 2.91136900 | -0.19707900 |
| B | -2.26587400 | 3.11244300 | -0.05347100 |
| B | -3.71338900 | 1.04599500 | -0.04135100 |
| B | -2.63195000 | -1.22374600 | -0.05578300 |
| B | -1.56810400 | -3.49951200 | -0.02876800 |
| B | 0.94654000 | -3.71378800 | -0.03444600 |
| B | 2.41147300 | -1.66890700 | -0.16179000 |
| B | 3.88534900 | 0.39892000 | -0.17365800 |
| B | 2.78697300 | 2.69459300 | -0.16941100 |
| N | 2.81420300 | 1.29520400 | -0.56537000 |
| N | -0.00145000 | 1.53627700 | -0.62102500 |
| N | 1.57224100 | 3.47108600 | -0.05980900 |

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|---|-------------|-------------|-------------|
| N | 3.70232200 | -1.02552500 | -0.04000500 |
| N | 1.19810300 | -0.95695300 | -0.55425600 |
| N | 2.26624900 | -3.09600700 | -0.02956100 |
| N | -0.24705600 | -2.88268200 | -0.11548800 |
| N | -1.30667200 | -0.60161400 | -0.17462300 |
| N | -2.74254800 | -2.66194200 | -0.00990600 |
| N | -3.81270300 | -0.39307200 | -0.01786600 |
| N | -2.39869800 | 1.66594300 | -0.14249700 |
| N | -0.94201000 | 3.72105300 | -0.04246500 |
| B | 1.69319100 | 4.91940300 | 0.17451300 |
| B | -0.81545900 | 5.16266500 | 0.15259300 |
| B | -5.13428600 | -1.01201500 | 0.06444400 |
| B | -4.06311600 | -3.28495900 | 0.06842100 |
| B | 3.45504900 | -3.93048300 | 0.14518000 |
| B | 4.89131600 | -1.86278300 | 0.16375200 |
| N | 5.18449900 | 1.02524100 | -0.01869700 |
| N | 4.10014000 | 3.29368500 | 0.00155500 |
| N | -3.44621200 | 3.93163800 | 0.07158000 |
| N | -4.88890000 | 1.88477300 | 0.04414200 |
| N | -1.67551400 | -4.94017700 | 0.05125500 |
| N | 0.81743500 | -5.14556600 | 0.08048300 |
| B | 5.28621400 | 2.46628400 | 0.05380000 |
| B | -4.75863800 | 3.31811900 | 0.09070000 |
| B | -0.49350300 | -5.75967200 | 0.09706400 |
| B | 6.35869100 | 0.18651700 | 0.17280100 |
| B | -6.20275600 | 1.26633200 | 0.10970800 |
| N | 6.17155200 | -1.21721900 | 0.24973300 |
| N | -6.28318700 | -0.15186800 | 0.10888800 |

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|---|-------------|-------------|------------|
| N | -5.21614500 | -2.43932700 | 0.09761300 |
| N | 4.72682500 | -3.27908700 | 0.23516700 |
| N | 3.27760100 | -5.34799600 | 0.23035100 |
| N | -4.13398600 | -4.71796800 | 0.11260100 |
| B | 4.20568500 | 4.73083200 | 0.20403000 |
| B | -3.31824600 | 5.37242400 | 0.20307400 |
| B | 2.00220600 | -5.97784000 | 0.19575000 |
| B | -2.98980600 | -5.55865300 | 0.11300400 |
| N | -2.01344200 | 5.94069900 | 0.24512800 |
| N | 0.50519200 | 5.70763700 | 0.25136400 |
| N | 3.00790000 | 5.48514700 | 0.28191000 |
| H | 1.90813600 | -7.16131700 | 0.26758300 |
| H | -0.58830800 | -6.94315900 | 0.15776900 |
| H | -3.10005300 | -6.74234900 | 0.16562500 |
| H | 6.34973300 | 2.97287700 | 0.20812500 |
| H | 7.43907100 | 0.67326900 | 0.27248400 |
| H | 5.27046700 | 5.24910700 | 0.31133900 |
| H | -4.28308800 | 6.06342600 | 0.28270800 |
| H | -5.72752800 | 4.00406500 | 0.15608900 |
| H | -7.18566400 | 1.93488200 | 0.16545700 |
| H | 6.99724900 | -1.78553700 | 0.38526000 |
| H | 5.55083700 | -3.85126600 | 0.36636600 |
| H | 4.08686000 | -5.94601600 | 0.33024500 |
| H | -5.03885400 | -5.16676200 | 0.15914800 |
| H | -6.12948900 | -2.86995200 | 0.15569200 |
| H | -7.20578100 | -0.56275100 | 0.15833000 |
| H | -1.94938000 | 6.94381100 | 0.35562500 |
| H | 0.60352300 | 6.70427900 | 0.39562900 |

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|--|-------------|-------------|-------------|
| H | 3.09972600 | 6.48159800 | 0.42943700 |
| Li ⁺ @V _B <i>h</i> -BN (product) | | | |
| Li | 1.35739600 | 0.62826400 | 1.76899800 |
| B | -1.23007200 | 0.83884800 | 0.27573900 |
| B | -0.14148300 | -1.45078100 | 0.23794900 |
| B | 0.24233700 | 2.91112300 | 0.19684700 |
| B | -2.26354900 | 3.11412400 | 0.05348000 |
| B | -3.71262900 | 1.04873900 | 0.04123500 |
| B | -2.63292600 | -1.22179800 | 0.05543200 |
| B | -1.57077700 | -3.49835400 | 0.02857900 |
| B | 0.94371200 | -3.71452400 | 0.03438200 |
| B | 2.41017400 | -1.67061300 | 0.16176100 |
| B | 3.88572800 | 0.39611500 | 0.17376200 |
| B | 2.78902400 | 2.69257000 | 0.16900800 |
| N | 2.81527600 | 1.29330100 | 0.56523400 |
| N | -0.00022600 | 1.53615300 | 0.62057500 |
| N | 1.57487700 | 3.46996700 | 0.05943900 |
| N | 3.70154700 | -1.02824100 | 0.04018500 |
| N | 1.19719400 | -0.95784700 | 0.55389500 |
| N | 2.26386900 | -3.09766300 | 0.02964400 |
| N | -0.24927300 | -2.88255900 | 0.11524500 |
| N | -1.30714900 | -0.60065700 | 0.17392500 |
| N | -2.74459300 | -2.65992800 | 0.00969800 |
| N | -3.81303900 | -0.39024100 | 0.01771400 |
| N | -2.39747000 | 1.66770100 | 0.14233400 |
| N | -0.93921600 | 3.72168100 | 0.04250600 |
| B | 1.69687700 | 4.91823900 | -0.17458900 |
| B | -0.81158300 | 5.16324800 | -0.15213500 |

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|---|-------------|-------------|-------------|
| B | -5.13511800 | -1.00817400 | -0.06436500 |
| B | -4.06565400 | -3.28194000 | -0.06845000 |
| B | 3.45204000 | -3.93301600 | -0.14484200 |
| B | 4.88994800 | -1.86645800 | -0.16323700 |
| N | 5.18538400 | 1.02137000 | 0.01884200 |
| N | 4.10265800 | 3.29061900 | -0.00222500 |
| N | -3.44326500 | 3.93422600 | -0.07144300 |
| N | -4.88749600 | 1.88843600 | -0.04409900 |
| N | -1.67922800 | -4.93896100 | -0.05136900 |
| N | 0.81359600 | -5.14620500 | -0.08053000 |
| B | 5.28810400 | 2.46233700 | -0.05426000 |
| B | -4.75614900 | 3.32169100 | -0.09050000 |
| B | -0.49782100 | -5.75932100 | -0.09716300 |
| B | 6.35892200 | 0.18169700 | -0.17245300 |
| B | -6.20182500 | 1.27100600 | -0.10951400 |
| N | 6.17072200 | -1.22190900 | -0.24903600 |
| N | -6.28335200 | -0.14714700 | -0.10861900 |
| N | -5.21803400 | -2.43543000 | -0.09750300 |
| N | 4.72437000 | -3.28262000 | -0.23458700 |
| N | 3.27362800 | -5.35042600 | -0.23003700 |
| N | -4.13755900 | -4.71489600 | -0.11259600 |
| B | 4.20924200 | 4.72770400 | -0.20467200 |
| B | -3.31421400 | 5.37495700 | -0.20251400 |
| B | 1.99777200 | -5.97934100 | -0.19570200 |
| B | -2.99398800 | -5.55643400 | -0.11304700 |
| N | -2.00897900 | 5.94225100 | -0.24429000 |
| N | 0.50944400 | 5.70733800 | -0.25094000 |
| N | 3.01201700 | 5.48295400 | -0.28218500 |

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|---|-------------|-------------|-------------|
| H | 1.90282300 | -7.16274700 | -0.26757200 |
| H | -0.59351700 | -6.94273600 | -0.15792300 |
| H | -3.10517800 | -6.74004500 | -0.16566100 |
| H | 6.35196700 | 2.96806500 | -0.20900400 |
| H | 7.43968600 | 0.66761000 | -0.27214300 |
| H | 5.27440000 | 5.24513500 | -0.31225700 |
| H | -4.27853400 | 6.06669700 | -0.28195600 |
| H | -5.72453500 | 4.00833500 | -0.15585700 |
| H | -7.18425300 | 1.94027500 | -0.16507800 |
| H | 6.99600800 | -1.79086700 | -0.38434200 |
| H | 5.54791400 | -3.85548800 | -0.36569300 |
| H | 4.08249100 | -5.94898700 | -0.32986000 |
| H | -5.04272400 | -5.16309100 | -0.15916000 |
| H | -6.13170200 | -2.86538500 | -0.15550400 |
| H | -7.20627900 | -0.55729700 | -0.15791000 |
| H | -1.94413300 | 6.94534600 | -0.35448000 |
| H | 0.60836200 | 6.70395100 | -0.39498000 |
| H | 3.10462400 | 6.47933300 | -0.42970200 |

Li@V_{BN} *h*-BN

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|----|-------------|-------------|-------------|
| Li | -0.31388300 | 1.28674200 | 0.04373300 |
| B | 1.60331000 | 0.28192900 | -0.00198400 |
| B | -0.71688700 | -1.08885600 | -0.05626900 |
| B | 1.53930300 | 2.31817800 | -0.03774000 |
| B | -0.87169200 | 3.56758200 | 0.12580700 |
| B | -3.09574200 | 2.41521000 | 0.22316600 |
| B | -3.00171600 | -0.02892300 | -0.03672600 |
| B | -2.83793600 | -2.49675500 | -0.11964200 |
| B | -0.60193700 | -3.61884100 | -0.05307500 |

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|---|-------------|-------------|-------------|
| B | 1.54027500 | -2.25507500 | 0.04762400 |
| B | 3.75523000 | -1.08128300 | 0.07056900 |
| B | 3.76680800 | 1.38501000 | -0.05049200 |
| N | 3.03173900 | 0.15521000 | 0.01173600 |
| N | 2.95019800 | 2.55998300 | -0.09938400 |
| N | 2.99922700 | -2.29568900 | 0.10425500 |
| N | 0.79325500 | -0.95691800 | 0.00401500 |
| N | 0.84654200 | -3.53691500 | 0.02676400 |
| N | -1.37424500 | -2.40606700 | -0.07894200 |
| N | -1.59387500 | 0.01110800 | -0.13023700 |
| N | -3.66278100 | -1.31906500 | -0.08926200 |
| N | -3.79967000 | 1.16832900 | 0.09682600 |
| N | -1.68994200 | 2.44666000 | 0.33422500 |
| N | 0.63343100 | 3.48827300 | -0.02128900 |
| B | 3.59033200 | 3.85002100 | -0.18409400 |
| B | 1.29164300 | 4.82000700 | -0.12875500 |
| B | -5.23767300 | 1.12406400 | 0.07484900 |
| B | -5.11118500 | -1.38429900 | -0.09313600 |
| B | 1.59293000 | -4.79015300 | 0.08277300 |
| B | 3.74342800 | -3.54510000 | 0.16952800 |
| N | 5.21468200 | -1.05434300 | 0.08993200 |
| N | 5.20548400 | 1.43633600 | -0.06229600 |
| N | -1.60186300 | 4.85206000 | 0.09521300 |
| N | -3.82956600 | 3.68089700 | 0.22195600 |
| N | -3.49492400 | -3.79836300 | -0.17597400 |
| N | -1.27359700 | -4.91415500 | -0.09956100 |
| B | 5.93350700 | 0.19247600 | 0.01830400 |
| B | -3.05426000 | 4.88675200 | 0.17198000 |

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| B | -2.70957400 | -4.99561300 | -0.17344900 |
| B | 5.93694500 | -2.30521800 | 0.17321100 |
| B | -5.27702800 | 3.64666200 | 0.20228700 |
| N | 5.18326000 | -3.50483500 | 0.21948100 |
| N | -5.94198400 | 2.38529600 | 0.15097800 |
| N | -5.87071900 | -0.16453200 | -0.02579400 |
| N | 3.01884400 | -4.76589100 | 0.17431300 |
| N | 0.89358300 | -6.04408300 | 0.04316300 |
| N | -5.71366800 | -2.69199200 | -0.16717300 |
| B | 5.84990400 | 2.73246700 | -0.14990000 |
| B | -0.89380200 | 6.09384500 | -0.01957500 |
| B | -0.51613800 | -6.13957300 | -0.05503100 |
| B | -4.94180800 | -3.88368700 | -0.20954200 |
| N | 0.51738300 | 6.02843500 | -0.12865900 |
| N | 2.71729600 | 4.96350400 | -0.22525800 |
| N | 5.03065900 | 3.89613700 | -0.21662600 |
| H | -1.05449600 | -7.20332500 | -0.09583500 |
| H | -3.23909100 | -6.06280600 | -0.22492200 |
| H | -5.48081600 | -4.94770000 | -0.26707200 |
| H | 7.12536200 | 0.19932900 | 0.02449200 |
| H | 7.12923700 | -2.32766300 | 0.20045700 |
| H | 7.03900900 | 2.82342600 | -0.16636800 |
| H | -1.45723700 | 7.14514900 | -0.02833600 |
| H | -3.60166600 | 5.94738900 | 0.16860600 |
| H | -5.91050200 | 4.65993400 | 0.22514900 |
| H | 5.69094500 | -4.37705500 | 0.27227800 |
| H | 3.51981400 | -5.64253400 | 0.21403300 |
| H | 1.42682300 | -6.90146500 | 0.07825000 |

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|---|-------------|-------------|-------------|
| H | -6.71989500 | -2.78295100 | -0.18272500 |
| H | -6.88002800 | -0.21988300 | -0.03840900 |
| H | -6.95246000 | 2.39488600 | 0.13867200 |
| H | 1.01734300 | 6.90332600 | -0.20602500 |
| H | 3.09062900 | 5.90077900 | -0.28659400 |
| H | 5.49624500 | 4.79113400 | -0.27711900 |

Li@V_{BN} *h*-BN (reactant)

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|----|-------------|-------------|-------------|
| Li | -0.49049600 | 1.28025100 | 1.43858700 |
| B | 1.54392900 | 0.35638400 | 0.12230000 |
| B | -0.66608000 | -1.07271000 | 0.11787600 |
| B | 1.41822700 | 2.28710500 | -0.05520900 |
| B | -0.94986600 | 3.45202500 | -0.14991600 |
| B | -3.09261100 | 2.33362900 | 0.42469700 |
| B | -2.94099300 | -0.10626100 | 0.46024600 |
| B | -2.74564300 | -2.52753600 | -0.03122800 |
| B | -0.49536000 | -3.56230900 | -0.33203800 |
| B | 1.59940100 | -2.18346800 | -0.01715300 |
| B | 3.74369900 | -0.96338100 | 0.32717300 |
| B | 3.67968900 | 1.49266900 | 0.25506100 |
| N | 2.97930300 | 0.24523100 | 0.28547400 |
| N | 2.82858800 | 2.61742700 | 0.02751500 |
| N | 3.04544600 | -2.19926000 | 0.15027400 |
| N | 0.81624600 | -0.91823500 | 0.05639800 |
| N | 0.94868100 | -3.46324500 | -0.25369300 |
| N | -1.29457900 | -2.38471800 | -0.11244500 |
| N | -1.52161900 | -0.02153200 | 0.52382000 |
| N | -3.58066800 | -1.39555000 | 0.27070000 |
| N | -3.77298200 | 1.07267600 | 0.54624700 |

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|---|-------------|-------------|-------------|
| N | -1.67037700 | 2.40281700 | 0.46667200 |
| N | 0.52601800 | 3.42401500 | -0.30790200 |
| B | 3.43799300 | 3.90579100 | -0.18030300 |
| B | 1.14310200 | 4.72430500 | -0.66459300 |
| B | -5.21021300 | 0.99184200 | 0.52310900 |
| B | -5.02745400 | -1.49964600 | 0.29430000 |
| B | 1.73324300 | -4.68528900 | -0.38119500 |
| B | 3.82534300 | -3.42424200 | 0.10209900 |
| N | 5.19265300 | -0.89632500 | 0.50188600 |
| N | 5.11038300 | 1.59622000 | 0.39694700 |
| N | -1.73487500 | 4.65464700 | -0.50156700 |
| N | -3.87278400 | 3.55002700 | 0.20160500 |
| N | -3.37706400 | -3.82117500 | -0.27062200 |
| N | -1.13506200 | -4.84816200 | -0.59262400 |
| B | 5.86801300 | 0.37740800 | 0.55442300 |
| B | -3.16566200 | 4.70202800 | -0.27754700 |
| B | -2.56951200 | -4.96607200 | -0.57431300 |
| B | 5.94707300 | -2.13042700 | 0.52878700 |
| B | -5.31689100 | 3.49337500 | 0.28505700 |
| N | 5.24664300 | -3.35029200 | 0.33224000 |
| N | -5.94947300 | 2.23348300 | 0.49503400 |
| N | -5.81429800 | -0.31287800 | 0.48824200 |
| N | 3.15000400 | -4.64360300 | -0.18373900 |
| N | 1.06917200 | -5.92129100 | -0.69359600 |
| N | -5.60558700 | -2.80456500 | 0.09087900 |
| B | 5.71156400 | 2.91098900 | 0.28575800 |
| B | -1.09127500 | 5.83349200 | -1.01229000 |
| B | -0.33981600 | -6.03295100 | -0.80427700 |

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|---|-------------|-------------|-------------|
| B | -4.81809600 | -3.95076600 | -0.19835900 |
| N | 0.32234400 | 5.82256700 | -1.09365100 |
| N | 2.55845900 | 4.94543600 | -0.57405800 |
| N | 4.86669500 | 4.02203700 | -0.00260200 |
| H | -0.84968700 | -7.08323600 | -1.05072300 |
| H | -3.08095500 | -6.02030100 | -0.79656100 |
| H | -5.33978000 | -5.00885600 | -0.38354700 |
| H | 7.05054000 | 0.42373800 | 0.70097600 |
| H | 7.12845900 | -2.12602800 | 0.69703600 |
| H | 6.88866200 | 3.05888700 | 0.41450400 |
| H | -1.71276800 | 6.79814600 | -1.33969700 |
| H | -3.76078900 | 5.70703600 | -0.52383900 |
| H | -5.97375800 | 4.48384100 | 0.15941400 |
| H | 5.78616200 | -4.20481700 | 0.32968500 |
| H | 3.67755400 | -5.50305400 | -0.24895200 |
| H | 1.62217100 | -6.75780300 | -0.81686900 |
| H | -6.60931900 | -2.91801800 | 0.11649200 |
| H | -6.82201900 | -0.38959400 | 0.46549300 |
| H | -6.95971400 | 2.21630900 | 0.51078800 |
| H | 0.78189900 | 6.66680100 | -1.40541200 |
| H | 2.91044100 | 5.87040300 | -0.77871600 |
| H | 5.30649900 | 4.92562700 | -0.11018900 |

Li@V_{BN} *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.48873500 | 1.27994200 | 1.43802300 |
| B | -1.54391200 | 0.35625900 | 0.12258500 |
| B | 0.66621800 | -1.07275200 | 0.11821500 |
| B | -1.41823100 | 2.28703700 | -0.05521900 |
| B | 0.94972300 | 3.45185000 | -0.15010300 |

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|---|-------------|-------------|-------------|
| B | 3.09213200 | 2.33378500 | 0.42554400 |
| B | 2.94098200 | -0.10609700 | 0.46096100 |
| B | 2.74584900 | -2.52728800 | -0.03117300 |
| B | 0.49553900 | -3.56220300 | -0.33226300 |
| B | -1.59923500 | -2.18342200 | -0.01723000 |
| B | -3.74354000 | -0.96348600 | 0.32772300 |
| B | -3.67962400 | 1.49260300 | 0.25590400 |
| N | -2.97918500 | 0.24518700 | 0.28622000 |
| N | -2.82856200 | 2.61731500 | 0.02821400 |
| N | -3.04527100 | -2.19929900 | 0.15036800 |
| N | -0.81610800 | -0.91820500 | 0.05652000 |
| N | -0.94849300 | -3.46313900 | -0.25405400 |
| N | 1.29474600 | -2.38461500 | -0.11250100 |
| N | 1.52163200 | -0.02171800 | 0.52497000 |
| N | 3.58073400 | -1.39535200 | 0.27103300 |
| N | 3.77275700 | 1.07292000 | 0.54684200 |
| N | 1.66991100 | 2.40301000 | 0.46750200 |
| N | -0.52613800 | 3.42370300 | -0.30855500 |
| B | -3.43803200 | 3.90553600 | -0.18035600 |
| B | -1.14330500 | 4.72372400 | -0.66595100 |
| B | 5.21004700 | 0.99221500 | 0.52355600 |
| B | 5.02753000 | -1.49932000 | 0.29434500 |
| B | -1.73304500 | -4.68516800 | -0.38189800 |
| B | -3.82516600 | -3.42428300 | 0.10179700 |
| N | -5.19248600 | -0.89647800 | 0.50260200 |
| N | -5.11029900 | 1.59607400 | 0.39777900 |
| N | 1.73467500 | 4.65438500 | -0.50219300 |
| N | 3.87232500 | 3.55025300 | 0.20243100 |

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|---|-------------|-------------|-------------|
| N | 3.37731400 | -3.82088500 | -0.27081100 |
| N | 1.13535500 | -4.84800500 | -0.59287300 |
| B | -5.86789000 | 0.37722500 | 0.55518900 |
| B | 3.16531800 | 4.70201700 | -0.27740100 |
| B | 2.56981400 | -4.96579500 | -0.57455100 |
| B | -5.94684600 | -2.13061700 | 0.52924000 |
| B | 5.31641500 | 3.49377100 | 0.28578400 |
| N | -5.24641400 | -3.35041200 | 0.33219500 |
| N | 5.94915100 | 2.23391100 | 0.49563800 |
| N | 5.81421500 | -0.31244200 | 0.48833700 |
| N | -3.14984100 | -4.64350200 | -0.18469200 |
| N | -1.06889100 | -5.92108200 | -0.69441100 |
| N | 5.60578800 | -2.80410600 | 0.09059400 |
| B | -5.71151700 | 2.91084100 | 0.28644900 |
| B | 1.09105600 | 5.83277300 | -1.01391600 |
| B | 0.34013700 | -6.03277400 | -0.80469400 |
| B | 4.81835200 | -3.95037300 | -0.19864900 |
| N | -0.32253600 | 5.82161300 | -1.09591400 |
| N | -2.55864900 | 4.94494500 | -0.57514300 |
| N | -4.86671900 | 4.02179300 | -0.00244500 |
| H | 0.85001100 | -7.08306000 | -1.05113600 |
| H | 3.08130800 | -6.02002500 | -0.79670800 |
| H | 5.34015800 | -5.00835100 | -0.38412700 |
| H | -7.05040700 | 0.42353200 | 0.70182800 |
| H | -7.12822400 | -2.12634000 | 0.69755000 |
| H | -6.88860700 | 3.05871800 | 0.41526400 |
| H | 1.71254900 | 6.79734400 | -1.34159400 |
| H | 3.76046100 | 5.70695600 | -0.52398700 |

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|---|-------------|-------------|-------------|
| H | 5.97321300 | 4.48430800 | 0.16038800 |
| H | -5.78599300 | -4.20490000 | 0.32938600 |
| H | -3.67736300 | -5.50295800 | -0.25006200 |
| H | -1.62183000 | -6.75760400 | -0.81789800 |
| H | 6.60953500 | -2.91746300 | 0.11599300 |
| H | 6.82195300 | -0.38896600 | 0.46552500 |
| H | 6.95939700 | 2.21683400 | 0.51139600 |
| H | -0.78203700 | 6.66572800 | -1.40808800 |
| H | -2.91070500 | 5.86972800 | -0.78048200 |
| H | -5.30655400 | 4.92533700 | -0.11031400 |

Li⁺@V_{BN} *h*-BN

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|----|-------------|-------------|-------------|
| Li | 0.01279200 | 1.19925700 | -0.02260900 |
| B | 1.71369200 | 0.25806500 | -0.26920700 |
| B | -0.75867500 | -0.79962600 | -0.01626500 |
| B | 1.73138300 | 2.08544700 | -0.32278700 |
| B | -0.65717600 | 3.13163600 | 0.46664800 |
| B | -3.03790900 | 2.35749200 | 0.35017900 |
| B | -3.05673100 | 0.21379600 | -0.38759700 |
| B | -2.89081200 | -2.19829600 | -0.51338600 |
| B | -0.78854200 | -3.32632400 | 0.19383100 |
| B | 1.41913300 | -2.15209500 | 0.27204400 |
| B | 3.72660200 | -1.24671200 | -0.16532800 |
| B | 3.86537400 | 1.16109500 | -0.69926300 |
| N | 3.07802600 | -0.01985000 | -0.48802600 |
| N | 3.07231200 | 2.35783300 | -0.67418100 |
| N | 2.86452900 | -2.30579900 | 0.26413100 |
| N | 0.74183200 | -0.80460200 | 0.04158900 |
| N | 0.62248700 | -3.32643300 | 0.49669900 |

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|---|-------------|-------------|-------------|
| N | -1.47022500 | -2.06295200 | -0.13473300 |
| N | -1.64315600 | 0.44776300 | -0.08973100 |
| N | -3.66687100 | -1.01459300 | -0.70501000 |
| N | -3.84507800 | 1.35770200 | -0.19832100 |
| N | -1.61857200 | 1.95983400 | 0.39629000 |
| N | 0.79112600 | 3.15166000 | 0.06593300 |
| B | 3.71846900 | 3.64040400 | -0.68368200 |
| B | 1.49179800 | 4.49759000 | 0.11792300 |
| B | -5.28038900 | 1.39856600 | -0.28374200 |
| B | -5.12298900 | -1.03340500 | -0.89944200 |
| B | 1.26918300 | -4.58815600 | 0.89122700 |
| B | 3.51855100 | -3.55555400 | 0.64415800 |
| N | 5.17232800 | -1.30619700 | -0.23438200 |
| N | 5.28555500 | 1.14937400 | -0.79386300 |
| N | -1.27493500 | 4.33833300 | 1.00108100 |
| N | -3.61770300 | 3.57865800 | 0.79253200 |
| N | -3.55325200 | -3.46997900 | -0.65802600 |
| N | -1.52417400 | -4.57632200 | 0.21303900 |
| B | 5.95186300 | -0.13009900 | -0.57931700 |
| B | -2.69814100 | 4.56892700 | 1.23225700 |
| B | -2.87720300 | -4.67112200 | -0.26402200 |
| B | 5.80056800 | -2.56016200 | 0.14739600 |
| B | -5.07490200 | 3.71099000 | 0.69983700 |
| N | 4.95478500 | -3.62157800 | 0.57862700 |
| N | -5.85973300 | 2.64305400 | 0.15773400 |
| N | -5.89023800 | 0.18380600 | -0.74022000 |
| N | 2.68833400 | -4.63881200 | 1.04297100 |
| N | 0.45575800 | -5.74923500 | 1.08247400 |

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|---|-------------|-------------|-------------|
| N | -5.69527200 | -2.31573700 | -1.17867600 |
| B | 5.93650900 | 2.44640600 | -0.95316400 |
| B | -0.49831000 | 5.55182300 | 1.20647700 |
| B | -0.90521600 | -5.79552400 | 0.69997300 |
| B | -4.95429300 | -3.52557800 | -1.04795600 |
| N | 0.81878000 | 5.60063600 | 0.71616800 |
| N | 2.83087200 | 4.70927600 | -0.36023900 |
| N | 5.13659700 | 3.64178500 | -0.91859900 |
| H | -1.52817200 | -6.80613300 | 0.76980600 |
| H | -3.42882900 | -5.72221300 | -0.31434000 |
| H | -5.48255100 | -4.57675500 | -1.22484300 |
| H | 7.13664800 | -0.20013200 | -0.65027700 |
| H | 6.98236400 | -2.69327900 | 0.11106100 |
| H | 7.11653400 | 2.52203200 | -1.08238500 |
| H | -0.97741800 | 6.49286400 | 1.74697800 |
| H | -3.06471500 | 5.58194300 | 1.72700400 |
| H | -5.59473500 | 4.71350700 | 1.07414100 |
| H | 5.40877900 | -4.48699200 | 0.83951700 |
| H | 3.11211200 | -5.51845900 | 1.30596700 |
| H | 0.88645500 | -6.60931800 | 1.39333000 |
| H | -6.68095400 | -2.39861000 | -1.38829400 |
| H | -6.89586000 | 0.12450700 | -0.83325000 |
| H | -6.86078800 | 2.78541600 | 0.13234200 |
| H | 1.32391700 | 6.46895000 | 0.83180700 |
| H | 3.18158400 | 5.65645500 | -0.29747300 |
| H | 5.63930000 | 4.51715400 | -0.98406400 |

Li⁺@V_{BN} *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.45350300 | -1.72965900 | -1.53823600 |
| B | -1.61338000 | -0.24201000 | -0.08025700 |
| B | 0.73306500 | 0.75047300 | -0.08466200 |
| B | -1.66991200 | -1.97840800 | -0.42112800 |
| B | 0.47922300 | -3.06918500 | 0.43882900 |
| B | 2.79523200 | -2.32458500 | 0.68260600 |
| B | 2.95080100 | -0.36866500 | -0.44074300 |
| B | 2.89444000 | 2.02770200 | -0.76252300 |
| B | 0.88036500 | 3.28839900 | -0.02877800 |
| B | -1.31292000 | 2.18878100 | 0.41104500 |
| B | -3.62890700 | 1.28397200 | 0.26699200 |
| B | -3.82161500 | -1.04452300 | -0.51103700 |
| N | -3.01280600 | 0.05591000 | -0.09831300 |
| N | -3.02933000 | -2.20946900 | -0.78427000 |
| N | -2.74098800 | 2.35801100 | 0.58929000 |
| N | -0.69388800 | 0.84762500 | 0.15400700 |
| N | -0.48236400 | 3.36268000 | 0.43488300 |
| N | 1.49499300 | 1.97837300 | -0.31946400 |
| N | 1.48475600 | -0.56829200 | -0.28472400 |
| N | 3.62396400 | 0.79560900 | -0.85637000 |
| N | 3.68944500 | -1.46009100 | 0.04073900 |
| N | 1.39787000 | -1.91676500 | 0.44450100 |
| N | -0.78969400 | -3.13132800 | -0.30827700 |
| B | -3.66909800 | -3.45806600 | -1.08253900 |
| B | -1.46614400 | -4.46578700 | -0.49457900 |
| B | 5.12227600 | -1.50915800 | 0.16603900 |
| B | 5.09413800 | 0.76909700 | -0.89233000 |

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|---|-------------|-------------|-------------|
| B | -1.07123600 | 4.66199400 | 0.78323300 |
| B | -3.33971300 | 3.63742100 | 0.93857000 |
| N | -5.07816000 | 1.36992900 | 0.26075600 |
| N | -5.24493900 | -1.00389700 | -0.58130100 |
| N | 0.96662300 | -4.27107700 | 1.11388700 |
| N | 3.27209100 | -3.45077200 | 1.41134900 |
| N | 3.60185100 | 3.25459700 | -1.02891700 |
| N | 1.63886800 | 4.51478500 | -0.20599400 |
| B | -5.88635400 | 0.24132400 | -0.16804300 |
| B | 2.28237100 | -4.43151600 | 1.72539900 |
| B | 2.96578800 | 4.51441000 | -0.75669200 |
| B | -5.65855300 | 2.63366000 | 0.68591700 |
| B | 4.72450100 | -3.58523100 | 1.55388000 |
| N | -4.77614100 | 3.70091200 | 1.03091300 |
| N | 5.60097000 | -2.63336800 | 0.93240500 |
| N | 5.81073900 | -0.40878100 | -0.44440400 |
| N | -2.45907600 | 4.74401000 | 1.12493600 |
| N | -0.23291800 | 5.82261300 | 0.72898700 |
| N | 5.72408100 | 1.98675400 | -1.30540100 |
| B | -5.89751000 | -2.23964600 | -0.99674100 |
| B | 0.28319400 | -5.54051000 | 0.92870000 |
| B | 1.07871600 | 5.79337300 | 0.19761000 |
| B | 5.01380500 | 3.22198000 | -1.37702900 |
| N | -0.80241600 | -5.61819200 | 0.02209200 |
| N | -2.77399000 | -4.58010900 | -1.07739100 |
| N | -5.09708400 | -3.41128000 | -1.25581100 |
| H | 1.71392200 | 6.79298900 | 0.08333500 |
| H | 3.54089700 | 5.53520700 | -0.95591700 |

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|---|-------------|-------------|-------------|
| H | 5.58241500 | 4.22497000 | -1.67065400 |
| H | -7.07286000 | 0.32791000 | -0.18093700 |
| H | -6.83895400 | 2.77979500 | 0.73914300 |
| H | -7.08099900 | -2.29638000 | -1.10924300 |
| H | 0.65771500 | -6.51393200 | 1.49730200 |
| H | 2.53301000 | -5.38994400 | 2.37796300 |
| H | 5.17159800 | -4.49733800 | 2.17330700 |
| H | -5.20770100 | 4.57498900 | 1.30063400 |
| H | -2.84367300 | 5.65136900 | 1.35195400 |
| H | -0.61347600 | 6.72264800 | 0.98788900 |
| H | 6.72431900 | 2.02143400 | -1.44927000 |
| H | 6.82110600 | -0.36237500 | -0.41766200 |
| H | 6.59188600 | -2.77235100 | 1.08079900 |
| H | -1.25194400 | -6.51940700 | -0.07295000 |
| H | -3.14155900 | -5.51610700 | -1.19348200 |
| H | -5.60628400 | -4.24969000 | -1.50295300 |

Li⁺@V_{BN} *h*-BN (product)

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|----|-------------|-------------|-------------|
| Li | 0.26711800 | -0.74895400 | 1.66442000 |
| B | -1.59355900 | -0.44213000 | 0.12858700 |
| B | 0.65004800 | 0.79799000 | -0.11206300 |
| B | -1.44213200 | -2.13674900 | -0.35672800 |
| B | 0.88291000 | -3.06680300 | 0.03253600 |
| B | 2.97257500 | -2.05112700 | 0.93511000 |
| B | 2.98944300 | 0.01643400 | 0.02322100 |
| B | 2.67768600 | 2.27946600 | -0.75209600 |
| B | 0.46409100 | 3.32289500 | -0.39627100 |
| B | -1.53230100 | 2.05197900 | 0.42743300 |
| B | -3.72236900 | 0.87640300 | 0.62282700 |

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|---|-------------|-------------|-------------|
| B | -3.70776700 | -1.47273800 | -0.12893700 |
| N | -2.99871000 | -0.30831200 | 0.31537700 |
| N | -2.81478100 | -2.49854200 | -0.56350800 |
| N | -2.94125200 | 2.07188900 | 0.75839000 |
| N | -0.76845800 | 0.75095100 | 0.28242900 |
| N | -0.87237700 | 3.29880700 | 0.15669700 |
| N | 1.24622900 | 2.08199700 | -0.47875500 |
| N | 1.57465500 | -0.36295300 | -0.00984300 |
| N | 3.56755400 | 1.20592900 | -0.44743900 |
| N | 3.78442600 | -0.94947000 | 0.65524900 |
| N | 1.54624200 | -1.79820800 | 0.54824500 |
| N | -0.44703200 | -3.16420200 | -0.52806800 |
| B | -3.33387100 | -3.73546700 | -1.07026500 |
| B | -0.94852400 | -4.47842800 | -1.03353000 |
| B | 5.22039500 | -0.90065700 | 0.74295700 |
| B | 5.02398000 | 1.34242000 | -0.39960400 |
| B | -1.61065800 | 4.55918200 | 0.32794000 |
| B | -3.67381000 | 3.31545100 | 0.96771300 |
| N | -5.16875900 | 0.81275300 | 0.69184100 |
| N | -5.13033700 | -1.56404100 | -0.15714200 |
| N | 1.61719100 | -4.30694400 | 0.29371600 |
| N | 3.56834400 | -3.26019000 | 1.39428400 |
| N | 3.24448200 | 3.52231700 | -1.20552300 |
| N | 1.04036200 | 4.58240800 | -0.83348100 |
| B | -5.87537400 | -0.40048500 | 0.30510400 |
| B | 2.85510100 | -4.44750700 | 1.04245100 |
| B | 2.39847800 | 4.67901000 | -1.30718800 |
| B | -5.86303600 | 2.03807500 | 1.05043300 |

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|---|-------------|-------------|-------------|
| B | 5.01567100 | -3.24230500 | 1.65100200 |
| N | -5.08905100 | 3.22641700 | 1.21542100 |
| N | 5.79514800 | -2.07740400 | 1.34736500 |
| N | 5.82075800 | 0.27952500 | 0.18573200 |
| N | -2.94261000 | 4.53383000 | 0.85163900 |
| N | -0.97670000 | 5.77889100 | -0.07078000 |
| N | 5.53576000 | 2.56837800 | -0.93661900 |
| B | -5.67345200 | -2.81102000 | -0.68996700 |
| B | 1.17222800 | -5.55310600 | -0.32368200 |
| B | 0.29837100 | 5.82187200 | -0.68685800 |
| B | 4.68818100 | 3.64224900 | -1.35168900 |
| N | -0.02068600 | -5.56628200 | -1.07490300 |
| N | -2.32199400 | -4.69093600 | -1.40083600 |
| N | -4.77128000 | -3.83891800 | -1.13569600 |
| H | 0.76061300 | 6.85243600 | -1.06001300 |
| H | 2.82464500 | 5.70914200 | -1.71861200 |
| H | 5.16256500 | 4.64758500 | -1.77631000 |
| H | -7.06394600 | -0.43082400 | 0.34473000 |
| H | -7.04550500 | 2.05939000 | 1.18466800 |
| H | -6.84982500 | -2.97934200 | -0.75933500 |
| H | 1.81876800 | -6.54226100 | -0.19959300 |
| H | 3.29250300 | -5.52274600 | 1.28862300 |
| H | 5.54395500 | -4.22251900 | 2.07001900 |
| H | -5.60134900 | 4.07515400 | 1.41616100 |
| H | -3.43042600 | 5.41344900 | 0.95806600 |
| H | -1.47774400 | 6.65146400 | 0.02734500 |
| H | 6.53315600 | 2.72339200 | -0.99762500 |
| H | 6.82626900 | 0.39073900 | 0.20044500 |

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|---|-------------|-------------|-------------|
| H | 6.79206400 | -2.15026200 | 1.50259000 |
| H | -0.31339400 | -6.45285300 | -1.46316200 |
| H | -2.57440900 | -5.61118300 | -1.73693100 |
| H | -5.20068800 | -4.68225400 | -1.49304000 |

Li@V_{N2B} *h*-BN

| | | | |
|----|-------------|-------------|-------------|
| Li | -0.00003000 | 1.11721400 | 0.11584500 |
| B | -1.39281400 | -0.41558400 | -0.08646600 |
| B | 1.39284600 | -0.41550400 | -0.08646200 |
| B | 0.00006900 | -2.53456800 | 0.29841300 |
| B | 2.47645700 | -2.73062700 | 0.02004900 |
| B | 3.75319900 | -0.69905100 | -0.54254900 |
| B | 2.42878700 | 1.27002000 | -0.14174300 |
| B | 1.19411800 | 3.43762600 | 0.58102500 |
| B | -1.19429200 | 3.43754000 | 0.58120400 |
| B | -2.42886900 | 1.26988800 | -0.14157400 |
| B | -3.75314000 | -0.69923200 | -0.54265100 |
| B | -2.47627900 | -2.73078200 | 0.01975700 |
| N | -2.48556600 | -1.32589900 | -0.24342200 |
| N | 0.00003200 | -1.01596600 | 0.07269200 |
| N | -1.22486800 | -3.31525500 | 0.39843100 |
| N | -3.70751800 | 0.71844600 | -0.54601800 |
| N | -2.41730200 | 2.68509700 | 0.15398600 |
| N | -0.00005300 | 2.74983200 | 0.73720200 |
| N | 2.41713400 | 2.68525500 | 0.15369200 |
| N | 3.70746800 | 0.71862300 | -0.54614600 |
| N | 2.48566500 | -1.32576700 | -0.24325800 |
| N | 1.22504800 | -3.31516500 | 0.39862500 |
| B | -1.23394300 | -4.72914800 | 0.76026700 |

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|---|-------------|-------------|-------------|
| B | 1.23417500 | -4.72904900 | 0.76049400 |
| B | 4.93386800 | 1.46073600 | -0.71791700 |
| B | 3.65003600 | 3.46936800 | -0.01391400 |
| B | -3.65027600 | 3.46913300 | -0.01345900 |
| B | -4.93397500 | 1.46049100 | -0.71768300 |
| N | -4.96414300 | -1.44970100 | -0.75609900 |
| N | -3.71163300 | -3.49602900 | -0.08195000 |
| N | 3.71187500 | -3.49579200 | -0.08148200 |
| N | 4.96426400 | -1.44946100 | -0.75584800 |
| N | 1.25126800 | 4.90352600 | 0.74172700 |
| N | -1.25152900 | 4.90343100 | 0.74195500 |
| B | -4.93875700 | -2.86777800 | -0.51713000 |
| B | 4.93897700 | -2.86750500 | -0.51667000 |
| B | -0.00014400 | 5.60412700 | 0.89470800 |
| B | -6.17676500 | -0.70877500 | -1.06432100 |
| B | 6.17683400 | -0.70849100 | -1.06417100 |
| N | -6.12430600 | 0.71214400 | -1.06292100 |
| N | 6.12426300 | 0.71242500 | -1.06301800 |
| N | 4.86560300 | 2.85740500 | -0.48922100 |
| N | -4.86582100 | 2.85712900 | -0.48876700 |
| N | -3.65387800 | 4.87191400 | 0.29983800 |
| N | 3.65355200 | 4.87218100 | 0.29924000 |
| B | -3.70825100 | -4.88468000 | 0.31433900 |
| B | 3.70855700 | -4.88441000 | 0.31492500 |
| B | -2.49027800 | 5.61484600 | 0.65339600 |
| B | 2.48994500 | 5.61503600 | 0.65293300 |
| N | 2.48387900 | -5.44181000 | 0.76809000 |
| N | 0.00011500 | -5.37438800 | 1.05974400 |

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|---|-------------|-------------|-------------|
| N | -2.48358700 | -5.44201500 | 0.76762100 |
| H | -2.56381500 | 6.79225200 | 0.84685300 |
| H | -0.00017000 | 6.78295200 | 1.09500600 |
| H | 2.56341600 | 6.79245800 | 0.84631700 |
| H | -5.92750600 | -3.52007600 | -0.64986500 |
| H | -7.19720800 | -1.28369800 | -1.29258700 |
| H | -4.70082500 | -5.54401700 | 0.26916100 |
| H | 4.70118800 | -5.54367200 | 0.26992100 |
| H | 5.92778400 | -3.51974400 | -0.64925700 |
| H | 7.19732700 | -1.28337200 | -1.29231800 |
| H | -6.98696900 | 1.20930600 | -1.23695000 |
| H | -5.69018000 | 3.43419100 | -0.58361000 |
| H | -4.52308700 | 5.37993600 | 0.21274300 |
| H | 4.52271000 | 5.38026700 | 0.21200300 |
| H | 5.68991800 | 3.43451600 | -0.58414900 |
| H | 6.98689000 | 1.20962400 | -1.23711600 |
| H | 2.48287100 | -6.41700100 | 1.03326800 |
| H | 0.00013300 | -6.35761200 | 1.29345100 |
| H | -2.48253900 | -6.41722100 | 1.03274200 |

Li@V_{N2B} *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Li | -0.00001900 | 1.28308000 | 0.79916800 |
| B | 1.38743200 | -0.36693000 | 0.14786700 |
| B | -1.38740300 | -0.36699300 | 0.14785300 |
| B | 0.00006800 | -2.47937400 | -0.28909100 |
| B | -2.47522600 | -2.69092100 | -0.03122700 |
| B | -3.75777900 | -0.69392400 | 0.60480200 |
| B | -2.44270400 | 1.26410100 | 0.25405000 |
| B | -1.19668700 | 3.37687800 | -0.45306700 |

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|---|-------------|-------------|-------------|
| B | 1.19650600 | 3.37690700 | -0.45325200 |
| B | 2.44265700 | 1.26421300 | 0.25387400 |
| B | 3.75780300 | -0.69372400 | 0.60490700 |
| B | 2.47533800 | -2.69084200 | -0.03091000 |
| N | 2.48479400 | -1.29545500 | 0.27453600 |
| N | 0.00002900 | -0.96890300 | -0.00764100 |
| N | 1.22337300 | -3.26058300 | -0.42576400 |
| N | 3.72473800 | 0.72213300 | 0.65300300 |
| N | 2.44318100 | 2.66551000 | -0.06859800 |
| N | -0.00007200 | 2.69153000 | -0.31771200 |
| N | -2.44329400 | 2.66543000 | -0.06828500 |
| N | -3.72475600 | 0.72192600 | 0.65314100 |
| N | -2.48474500 | -1.29556600 | 0.27436400 |
| N | -1.22320100 | -3.26060400 | -0.42597600 |
| B | 1.23265700 | -4.65695500 | -0.84740400 |
| B | -1.23239200 | -4.65696400 | -0.84765900 |
| B | -4.95664300 | 1.46154800 | 0.77951800 |
| B | -3.68084700 | 3.44649900 | 0.00222000 |
| B | 3.68071400 | 3.44662400 | 0.00173700 |
| B | 4.95660400 | 1.46181300 | 0.77925200 |
| N | 4.96881900 | -1.45090000 | 0.79431900 |
| N | 3.70939100 | -3.46507200 | 0.04924300 |
| N | -3.70926800 | -3.46519000 | 0.04872800 |
| N | -4.96877900 | -1.45116500 | 0.79406000 |
| N | -1.25301900 | 4.78497500 | -0.88558100 |
| N | 1.25274000 | 4.78499400 | -0.88581400 |
| B | 4.93880100 | -2.85985300 | 0.50788000 |
| B | -4.93871800 | -2.86006800 | 0.50738300 |

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|---|-------------|-------------|-------------|
| B | -0.00016700 | 5.45802000 | -1.13190400 |
| B | 6.18591800 | -0.71719100 | 1.10363500 |
| B | -6.18589900 | -0.71754400 | 1.10350000 |
| N | 6.14575000 | 0.70582000 | 1.11369600 |
| N | -6.14576800 | 0.70546500 | 1.11383400 |
| N | -4.89720900 | 2.85402400 | 0.50163600 |
| N | 4.89712600 | 2.85424100 | 0.50114200 |
| N | 3.66663300 | 4.81440500 | -0.44211200 |
| N | -3.66684200 | 4.81432300 | -0.44149800 |
| B | 3.70425700 | -4.83701900 | -0.40032000 |
| B | -3.70405800 | -4.83709000 | -0.40097700 |
| B | 2.49873000 | 5.49471400 | -0.90251500 |
| B | -2.49902200 | 5.49467600 | -0.90204500 |
| N | -2.48078300 | -5.37200200 | -0.88259900 |
| N | 0.00016800 | -5.28932600 | -1.17749800 |
| N | 2.48105700 | -5.37199000 | -0.88206700 |
| H | 2.57378400 | 6.63233800 | -1.26264100 |
| H | -0.00021000 | 6.59561900 | -1.50065400 |
| H | -2.57415200 | 6.63231700 | -1.26210000 |
| H | 5.92468700 | -3.52076000 | 0.61927400 |
| H | 7.20557500 | -1.29938800 | 1.31791000 |
| H | 4.69477400 | -5.50092300 | -0.37533900 |
| H | -4.69456900 | -5.50101000 | -0.37619200 |
| H | -5.92459600 | -3.52101400 | 0.61861800 |
| H | -7.20554400 | -1.29980700 | 1.31765600 |
| H | 7.01685800 | 1.19308900 | 1.27290100 |
| H | 5.73347200 | 3.42070100 | 0.53897400 |
| H | 4.53251400 | 5.33538400 | -0.42952500 |

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|---|-------------|-------------|-------------|
| H | -4.53273400 | 5.33528100 | -0.42877000 |
| H | -5.73357300 | 3.42044900 | 0.53956300 |
| H | -7.01689000 | 1.19268200 | 1.27312100 |
| H | -2.47769500 | -6.33561900 | -1.18700300 |
| H | 0.00020000 | -6.26208400 | -1.45131500 |
| H | 2.47802800 | -6.33562800 | -1.18640400 |

Li⁺@V_{N2B} *h*-BN

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|----|-------------|-------------|-------------|
| Li | -0.00007400 | 1.09434400 | -0.22037200 |
| B | -1.39271200 | -0.42890100 | -0.08903800 |
| B | 1.39277400 | -0.42880400 | -0.08913500 |
| B | 0.00010900 | -2.54663400 | 0.30199100 |
| B | 2.48472500 | -2.73227400 | 0.05392100 |
| B | 3.75479500 | -0.69981200 | -0.53694500 |
| B | 2.41704000 | 1.25162800 | -0.20843700 |
| B | 1.24542800 | 3.44345400 | 0.52811900 |
| B | -1.24575200 | 3.44343400 | 0.52755800 |
| B | -2.41708500 | 1.25146000 | -0.20895100 |
| B | -3.75479500 | -0.70012900 | -0.53653300 |
| B | -2.48460400 | -2.73234700 | 0.05492500 |
| N | -2.49285800 | -1.31983800 | -0.20929800 |
| N | 0.00005100 | -1.00865200 | 0.06202200 |
| N | -1.22621400 | -3.31316700 | 0.40977600 |
| N | -3.69012300 | 0.73027600 | -0.58856700 |
| N | -2.40075900 | 2.70071200 | 0.06666100 |
| N | -0.00016500 | 2.72846500 | 0.57115000 |
| N | 2.40064300 | 2.70079400 | 0.06763600 |
| N | 3.69013900 | 0.73062600 | -0.58813600 |
| N | 2.49287600 | -1.31971200 | -0.20997300 |

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|---|-------------|-------------|-------------|
| N | 1.22647900 | -3.31316200 | 0.40919800 |
| B | -1.23589400 | -4.73641400 | 0.76667000 |
| B | 1.23633100 | -4.73642900 | 0.76601200 |
| B | 4.91679700 | 1.47901900 | -0.79703200 |
| B | 3.65247500 | 3.49313200 | -0.08623900 |
| B | -3.65256900 | 3.49299500 | -0.08778800 |
| B | -4.91676000 | 1.47857900 | -0.79790300 |
| N | -4.96471200 | -1.43464600 | -0.73130100 |
| N | -3.72206400 | -3.48252800 | -0.03315700 |
| N | 3.72216500 | -3.48242000 | -0.03472500 |
| N | 4.96468800 | -1.43424000 | -0.73220700 |
| N | 1.26050200 | 4.84179100 | 0.88381900 |
| N | -1.26100900 | 4.84179000 | 0.88316200 |
| B | -4.94942200 | -2.85700800 | -0.46623700 |
| B | 4.94942700 | -2.85673100 | -0.46784300 |
| B | -0.00031400 | 5.52389100 | 1.11677900 |
| B | -6.16849700 | -0.69370700 | -1.07527300 |
| B | 6.16848000 | -0.69312100 | -1.07577100 |
| N | -6.09889400 | 0.73260700 | -1.12406100 |
| N | 6.09892000 | 0.73322000 | -1.12362200 |
| N | 4.83687500 | 2.88913400 | -0.60222200 |
| N | -4.83682400 | 2.88880800 | -0.60387100 |
| N | -3.63907500 | 4.87026800 | 0.32467000 |
| N | 3.63884200 | 4.87030900 | 0.32654300 |
| B | -3.71939700 | -4.87922400 | 0.35876400 |
| B | 3.71965300 | -4.87919100 | 0.35692300 |
| B | -2.51050400 | 5.57186600 | 0.82888900 |
| B | 2.51002900 | 5.57187000 | 0.83025700 |

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|---|-------------|-------------|-------------|
| N | 2.48857100 | -5.43853000 | 0.78568600 |
| N | 0.00029100 | -5.38100000 | 1.04780000 |
| N | -2.48812400 | -5.43850600 | 0.78704100 |
| H | -2.58538800 | 6.71072000 | 1.16124100 |
| H | -0.00039800 | 6.66863200 | 1.43583500 |
| H | 2.58473500 | 6.71070700 | 1.16271000 |
| H | -5.94378200 | -3.49797100 | -0.58329700 |
| H | -7.19183000 | -1.26048000 | -1.29056400 |
| H | -4.71538700 | -5.52891200 | 0.32620600 |
| H | 4.71563000 | -5.52887400 | 0.32384600 |
| H | 5.94375200 | -3.49765600 | -0.58540800 |
| H | 7.19178700 | -1.25979000 | -1.29145900 |
| H | -6.95960000 | 1.22509300 | -1.32305300 |
| H | -5.66685700 | 3.45801400 | -0.70493500 |
| H | -4.50610600 | 5.38886400 | 0.26264000 |
| H | 4.50589500 | 5.38891700 | 0.26493400 |
| H | 5.66691300 | 3.45839400 | -0.70293600 |
| H | 6.95962900 | 1.22581200 | -1.32234000 |
| H | 2.49008800 | -6.41504500 | 1.04824400 |
| H | 0.00034300 | -6.36430400 | 1.28315100 |
| H | -2.48951900 | -6.41497200 | 1.04971700 |

Li⁺@V_{N2B} *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Li | -0.00000200 | 1.22055800 | 1.05502100 |
| B | 1.38372900 | -0.39076000 | 0.13656800 |
| B | -1.38374100 | -0.39061500 | 0.13662900 |
| B | -0.00015100 | -2.51767700 | -0.26152300 |
| B | -2.47761300 | -2.71306000 | -0.02084500 |
| B | -3.77326100 | -0.70387700 | 0.53771700 |

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|---|-------------|-------------|-------------|
| B | -2.45783600 | 1.25831100 | 0.23022200 |
| B | -1.25643200 | 3.45004400 | -0.30050100 |
| B | 1.25688600 | 3.44997000 | -0.30036000 |
| B | 2.45795000 | 1.25805300 | 0.23041100 |
| B | 3.77316400 | -0.70434900 | 0.53759900 |
| B | 2.47731800 | -2.71330700 | -0.02134100 |
| N | 2.48779400 | -1.30015500 | 0.25081700 |
| N | -0.00004600 | -0.98071100 | 0.00255600 |
| N | 1.22210200 | -3.28766800 | -0.38825200 |
| N | 3.74377600 | 0.72448400 | 0.54554200 |
| N | 2.45476400 | 2.69442200 | -0.05307800 |
| N | 0.00020600 | 2.82062200 | 0.03378100 |
| N | -2.45443900 | 2.69464000 | -0.05340100 |
| N | -3.74374900 | 0.72494200 | 0.54531400 |
| N | -2.48793600 | -1.29985100 | 0.25107000 |
| N | -1.22250000 | -3.28757500 | -0.38789200 |
| B | 1.23220300 | -4.70038100 | -0.78442600 |
| B | -1.23280700 | -4.70031500 | -0.78398200 |
| B | -4.99663600 | 1.45215100 | 0.64061300 |
| B | -3.72590700 | 3.46129000 | -0.06214900 |
| B | 3.72630400 | 3.46094200 | -0.06153800 |
| B | 4.99672800 | 1.45155100 | 0.64108700 |
| N | 4.97906100 | -1.45022900 | 0.72541700 |
| N | 3.70771700 | -3.47958800 | 0.06195700 |
| N | -3.70806300 | -3.47923000 | 0.06275400 |
| N | -4.97922700 | -1.44960500 | 0.72570700 |
| N | -1.25479400 | 4.83164900 | -0.72329800 |
| N | 1.25542600 | 4.83157300 | -0.72311900 |

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|---|-------------|-------------|-------------|
| B | 4.94490700 | -2.87358700 | 0.48566000 |
| B | -4.94518400 | -2.87303000 | 0.48635500 |
| B | 0.00035800 | 5.50785300 | -0.96903900 |
| B | 6.21055400 | -0.72464500 | 0.99234600 |
| B | -6.21067200 | -0.72384500 | 0.99236900 |
| N | 6.17773900 | 0.70193400 | 0.96060500 |
| N | -6.17773800 | 0.70271900 | 0.96021400 |
| N | -4.94192200 | 2.84728200 | 0.35525600 |
| N | 4.94218500 | 2.84675600 | 0.35600600 |
| N | 3.69016100 | 4.83499400 | -0.48250600 |
| N | -3.68956900 | 4.83530200 | -0.48321100 |
| B | 3.70410600 | -4.86860400 | -0.35287300 |
| B | -3.70461400 | -4.86833200 | -0.35179000 |
| B | 2.51477100 | 5.54357200 | -0.83632500 |
| B | -2.51404800 | 5.54375100 | -0.83680500 |
| N | -2.47888500 | -5.41135800 | -0.81016100 |
| N | -0.00037400 | -5.33426700 | -1.09650800 |
| N | 2.47824500 | -5.41147600 | -0.81108700 |
| H | 2.55312800 | 6.67735200 | -1.19145000 |
| H | 0.00042300 | 6.62468700 | -1.37470500 |
| H | -2.55222700 | 6.67752200 | -1.19198100 |
| H | 5.93056000 | -3.52739700 | 0.60527600 |
| H | 7.22630400 | -1.30661800 | 1.20368900 |
| H | 4.69671400 | -5.52347500 | -0.31764800 |
| H | -4.69725400 | -5.52313700 | -0.31624000 |
| H | -5.93088100 | -3.52673700 | 0.60618200 |
| H | -7.22648000 | -1.30567100 | 1.20382800 |
| H | 7.05562900 | 1.18548200 | 1.09541100 |

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|---|-------------|-------------|-------------|
| H | 5.78932000 | 3.39905200 | 0.36923300 |
| H | 4.56492300 | 5.34119600 | -0.53168600 |
| H | -4.56427500 | 5.34158300 | -0.53258000 |
| H | -5.78899400 | 3.39967900 | 0.36831000 |
| H | -7.05559600 | 1.18637400 | 1.09484300 |
| H | -2.47569400 | -6.38173500 | -1.09407500 |
| H | -0.00044600 | -6.31078400 | -1.35811000 |
| H | 2.47493100 | -6.38181300 | -1.09513500 |

Li@V_N *h*-BN

| | | | |
|----|-------------|-------------|-------------|
| Li | -0.14707700 | 1.35952800 | 0.81035300 |
| B | 1.54748800 | 0.45657500 | 0.01150500 |
| B | -1.64378000 | 0.90718100 | 1.71950100 |
| B | -0.58535500 | -1.19058300 | 0.36334800 |
| B | 1.25818600 | 2.42280200 | -0.05132700 |
| B | -1.29760600 | 3.37498300 | 0.51404000 |
| B | -3.34397900 | 2.02568700 | 0.37668900 |
| B | -2.94758300 | -0.42003400 | 0.19634500 |
| B | -2.45090800 | -2.80609700 | -0.21132800 |
| B | -0.13816800 | -3.65744300 | 0.11244400 |
| B | 1.79585300 | -2.04860600 | 0.25235100 |
| B | 3.83741100 | -0.65400300 | -0.12221100 |
| B | 3.52733200 | 1.76608800 | -0.46379500 |
| N | 2.95984500 | 0.46924400 | -0.24579900 |
| N | 2.58112300 | 2.83972400 | -0.38849800 |
| N | 3.24642500 | -1.92046700 | 0.18132600 |
| N | 0.88305100 | -0.85346300 | 0.23690400 |
| N | 1.27035900 | -3.40245900 | 0.32104800 |
| N | -1.04373600 | -2.54157000 | 0.04258400 |

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|---|-------------|-------------|-------------|
| N | -1.59602900 | -0.22461100 | 0.71682100 |
| N | -3.39170000 | -1.71703600 | -0.23697000 |
| N | -3.87323100 | 0.69425200 | 0.19233600 |
| N | -1.98184800 | 2.16474300 | 0.87424500 |
| N | 0.21186300 | 3.44642100 | 0.25148700 |
| B | 3.06319600 | 4.19450200 | -0.42932600 |
| B | 0.72670500 | 4.85553700 | 0.19027500 |
| B | -5.24535000 | 0.50880800 | -0.23721700 |
| B | -4.78881600 | -1.93718800 | -0.56626400 |
| B | 2.15847200 | -4.54761600 | 0.48544800 |
| B | 4.13858700 | -3.05757600 | 0.34887100 |
| N | 5.27359100 | -0.46409000 | -0.29318000 |
| N | 4.93429900 | 1.98163600 | -0.67621100 |
| N | -2.12690500 | 4.57293700 | 0.33706800 |
| N | -4.17401700 | 3.18109800 | 0.10687700 |
| N | -2.92368700 | -4.15849900 | -0.46889200 |
| N | -0.63894100 | -5.02143200 | -0.01014000 |
| B | 5.81518500 | 0.83854800 | -0.59535200 |
| B | -3.56070700 | 4.47337100 | 0.19646800 |
| B | -2.01942500 | -5.26457900 | -0.33397100 |
| B | 6.14877100 | -1.60096200 | -0.10266400 |
| B | -5.57328900 | 3.00185900 | -0.21536800 |
| N | 5.56024600 | -2.84812900 | 0.23398200 |
| N | -6.07940700 | 1.67890700 | -0.35368100 |
| N | -5.68681000 | -0.81852300 | -0.55536300 |
| N | 3.56852400 | -4.33763200 | 0.59544100 |
| N | 1.60408200 | -5.87380000 | 0.50010800 |
| N | -5.19966200 | -3.28039700 | -0.87954400 |

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|---|-------------|-------------|-------------|
| B | 5.40016800 | 3.34562600 | -0.84286300 |
| B | -1.55560800 | 5.88754500 | 0.38114300 |
| B | 0.24234300 | -6.14247300 | 0.21110000 |
| B | -4.31108700 | -4.38797600 | -0.81361800 |
| N | -0.14475900 | 5.97115200 | 0.42079400 |
| N | 2.09135600 | 5.17868300 | -0.12531600 |
| N | 4.45647200 | 4.41014700 | -0.72741900 |
| H | -0.15932900 | -7.26418800 | 0.15262100 |
| H | -2.40856000 | -6.38115800 | -0.48609900 |
| H | -4.70489200 | -5.49167400 | -1.03980500 |
| H | 6.98786300 | 0.97784000 | -0.75695000 |
| H | 7.33096100 | -1.49445400 | -0.22108300 |
| H | 6.55153100 | 3.57669700 | -1.05112700 |
| H | -2.23028700 | 6.87006900 | 0.38102700 |
| H | -4.21809800 | 5.46383200 | 0.11146500 |
| H | -6.28726100 | 3.94507900 | -0.37531200 |
| H | 6.17847600 | -3.63785200 | 0.35866400 |
| H | 4.17448900 | -5.13972500 | 0.69930200 |
| H | 2.22222200 | -6.66114800 | 0.63742500 |
| H | -6.16495500 | -3.46639200 | -1.11331700 |
| H | -6.65054800 | -0.96421400 | -0.82333600 |
| H | -7.05063700 | 1.57447700 | -0.61243300 |
| H | 0.26713700 | 6.89392900 | 0.42725900 |
| H | 2.33896200 | 6.15863700 | -0.13954900 |
| H | 4.81046900 | 5.35394300 | -0.80100400 |

Li@V_N *h*-BN (reactant)

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|----|-------------|-------------|------------|
| Li | 0.14725100 | -1.35953800 | 0.81041800 |
| B | -1.54746700 | -0.45671300 | 0.01165100 |

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|---|-------------|-------------|-------------|
| B | 1.64395900 | -0.90700300 | 1.71948900 |
| B | 0.58522500 | 1.19062500 | 0.36336200 |
| B | -1.25794400 | -2.42291300 | -0.05118800 |
| B | 1.29791500 | -3.37487600 | 0.51407200 |
| B | 3.34420600 | -2.02538300 | 0.37671100 |
| B | 2.94752300 | 0.42027800 | 0.19626800 |
| B | 2.45060600 | 2.80630600 | -0.21136300 |
| B | 0.13780600 | 3.65744600 | 0.11253700 |
| B | -1.79606700 | 2.04843800 | 0.25240500 |
| B | -3.83747700 | 0.65362700 | -0.12224200 |
| B | -3.52716900 | -1.76642500 | -0.46376400 |
| N | -2.95980500 | -0.46955800 | -0.24573400 |
| N | -2.58086400 | -2.83993700 | -0.38843900 |
| N | -3.24662100 | 1.92015500 | 0.18131900 |
| N | -0.88315200 | 0.85338800 | 0.23697700 |
| N | -1.27069600 | 3.40233500 | 0.32114600 |
| N | 1.04347300 | 2.54165400 | 0.04261300 |
| N | 1.59598400 | 0.22470800 | 0.71674100 |
| N | 3.39149500 | 1.71733000 | -0.23705500 |
| N | 3.87330300 | -0.69389200 | 0.19231300 |
| N | 1.98209300 | -2.16457400 | 0.87427800 |
| N | -0.21152900 | -3.44641800 | 0.25157600 |
| B | -3.06280300 | -4.19476600 | -0.42925200 |
| B | -0.72622700 | -4.85558300 | 0.19029900 |
| B | 5.24540100 | -0.50830400 | -0.23724700 |
| B | 4.78858200 | 1.93762400 | -0.56638100 |
| B | -2.15891700 | 4.54740700 | 0.48553700 |
| B | -4.13889300 | 3.05718800 | 0.34880700 |

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|---|-------------|-------------|-------------|
| N | -5.27363000 | 0.46359800 | -0.29330300 |
| N | -4.93410600 | -1.98209900 | -0.67625000 |
| N | 2.12739900 | -4.57270300 | 0.33705700 |
| N | 4.17438700 | -3.18069600 | 0.10694800 |
| N | 2.92324600 | 4.15875400 | -0.46894100 |
| N | 0.63845600 | 5.02148200 | -0.01001900 |
| B | -5.81509600 | -0.83909000 | -0.59546900 |
| B | 3.56119300 | -4.47301400 | 0.19651100 |
| B | 2.01889900 | 5.26475500 | -0.33393000 |
| B | -6.14891900 | 1.60040000 | -0.10286800 |
| B | 5.57363900 | -3.00131100 | -0.21529500 |
| N | -5.56052400 | 2.84762000 | 0.23381000 |
| N | 6.07960100 | -1.67830500 | -0.35365100 |
| N | 5.68670100 | 0.81906200 | -0.55545900 |
| N | -3.56895900 | 4.33729100 | 0.59543900 |
| N | -1.60464000 | 5.87363800 | 0.50027600 |
| N | 5.19928100 | 3.28086800 | -0.87970800 |
| B | -5.39984500 | -3.34613500 | -0.84287100 |
| B | 1.55622400 | -5.88737000 | 0.38102600 |
| B | -0.24292300 | 6.14243900 | 0.21127500 |
| B | 4.31060500 | 4.38836300 | -0.81374600 |
| N | 0.14537700 | -5.97112000 | 0.42067000 |
| N | -2.09086300 | -5.17885000 | -0.12523000 |
| N | -4.45605300 | -4.41056000 | -0.72735400 |
| H | 0.15865200 | 7.26419100 | 0.15283500 |
| H | 2.40792700 | 6.38137100 | -0.48606400 |
| H | 4.70429100 | 5.49209600 | -1.03996400 |
| H | -6.98775500 | -0.97848800 | -0.75712300 |

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|---|-------------|-------------|-------------|
| H | -7.33109100 | 1.49379000 | -0.22137100 |
| H | -6.55118000 | -3.57732000 | -1.05116500 |
| H | 2.23099100 | -6.86983300 | 0.38082600 |
| H | 4.21866900 | -5.46341900 | 0.11152300 |
| H | 6.28772200 | -3.94445300 | -0.37519400 |
| H | -6.17883100 | 3.63728900 | 0.35844400 |
| H | -4.17500200 | 5.13932800 | 0.69927800 |
| H | -2.22284900 | 6.66092900 | 0.63761200 |
| H | 6.16454600 | 3.46695300 | -1.11352400 |
| H | 6.65042000 | 0.96485600 | -0.82344600 |
| H | 7.05082200 | -1.57376800 | -0.61239500 |
| H | -0.26641900 | -6.89394200 | 0.42706000 |
| H | -2.33837300 | -6.15882900 | -0.13946900 |
| H | -4.80995500 | -5.35439300 | -0.80092400 |

Li⁺@V_N *h*-BN

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|----|-------------|-------------|-------------|
| Li | -0.14903500 | 1.29233000 | 0.81232400 |
| B | -1.74498900 | 0.85975600 | 1.58697500 |
| B | 1.52497900 | 0.49499600 | -0.00619500 |
| B | -0.53724500 | -1.24516200 | 0.46045700 |
| B | 1.16699600 | 2.47436200 | -0.00163200 |
| B | 3.41822300 | 1.88302000 | -0.56188800 |
| B | 3.82757900 | -0.53757100 | -0.25059600 |
| B | 1.86717100 | -1.99896000 | 0.29528900 |
| B | -0.00881600 | -3.68014100 | 0.26589100 |
| B | -2.35126300 | -2.90736600 | -0.13801400 |
| B | -2.95595500 | -0.53206400 | 0.14739200 |
| B | -3.43036400 | 1.92080600 | 0.31769300 |
| B | -1.39617500 | 3.35502200 | 0.66950400 |

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|---|-------------|-------------|-------------|
| N | -2.09951200 | 2.09781600 | 0.96269700 |
| N | 0.09425500 | 3.44316800 | 0.41396300 |
| N | -3.86628500 | 0.58049900 | 0.04249100 |
| N | -1.62931600 | -0.30822800 | 0.79035200 |
| N | -3.31427200 | -1.83650000 | -0.27266400 |
| N | -0.95952900 | -2.58850100 | 0.17357300 |
| N | 0.89611600 | -0.82109100 | 0.31159600 |
| N | 1.38708600 | -3.35734600 | 0.43318700 |
| N | 3.29364400 | -1.81056500 | 0.12686000 |
| N | 2.89811600 | 0.55806900 | -0.34685900 |
| N | 2.44347800 | 2.93109700 | -0.38921000 |
| B | 0.58108900 | 4.88099900 | 0.40481300 |
| B | 2.89493400 | 4.30544100 | -0.38775600 |
| B | 4.24061900 | -2.91786800 | 0.27149400 |
| B | 2.32770700 | -4.47244800 | 0.59076800 |
| B | -4.68162400 | -2.09760200 | -0.71813200 |
| B | -5.20563200 | 0.35929100 | -0.51013300 |
| N | -4.24079500 | 3.06256500 | 0.03182500 |
| N | -2.26184200 | 4.50452200 | 0.52572400 |
| N | 4.79463900 | 2.14443500 | -0.83725400 |
| N | 5.23415100 | -0.29642800 | -0.50224600 |
| N | -0.47414600 | -5.04931800 | 0.20255200 |
| N | -2.77198500 | -4.26844200 | -0.35723400 |
| B | -3.68244200 | 4.36912600 | 0.26195200 |
| B | 5.71804700 | 1.02434200 | -0.82939400 |
| B | -1.84206300 | -5.34854400 | -0.13286000 |
| B | -5.60106600 | 2.85211700 | -0.45049300 |
| B | 6.16318600 | -1.40299300 | -0.34768000 |

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|---|-------------|-------------|-------------|
| N | -6.03678100 | 1.51889700 | -0.68922500 |
| N | 5.63701300 | -2.65949200 | 0.05231700 |
| N | 3.72883400 | -4.20287000 | 0.60361100 |
| N | -5.57951300 | -0.98111300 | -0.83788200 |
| N | -5.03167700 | -3.45839700 | -0.98822400 |
| N | 1.81069300 | -5.80649000 | 0.69204600 |
| B | -1.72378000 | 5.83915000 | 0.67314000 |
| B | 5.21760500 | 3.52968900 | -0.98007800 |
| B | -4.13117200 | -4.54591200 | -0.78907000 |
| B | 0.45185800 | -6.13613300 | 0.45854100 |
| N | 4.25440900 | 4.56426100 | -0.75862700 |
| N | 1.91535100 | 5.24142400 | 0.03839100 |
| N | -0.31777000 | 5.94571200 | 0.74113600 |
| H | -4.48631400 | -5.66516100 | -0.98000600 |
| H | -2.20197800 | -6.47718800 | -0.23203700 |
| H | 0.08160000 | -7.26667700 | 0.46608200 |
| H | -4.36195900 | 5.33991000 | 0.18673800 |
| H | -6.31960700 | 3.77948900 | -0.64467900 |
| H | -2.43043200 | 6.79180500 | 0.73304100 |
| H | 6.34474100 | 3.79801200 | -1.24753400 |
| H | 6.87019000 | 1.20406000 | -1.06013700 |
| H | 7.32757600 | -1.25628300 | -0.54279400 |
| H | -6.97783800 | 1.40192900 | -1.04125900 |
| H | -6.51554400 | -1.15304200 | -1.18115600 |
| H | -5.96896700 | -3.68604200 | -1.29173600 |
| H | 2.45588200 | -6.57036800 | 0.84198400 |
| H | 4.37104900 | -4.97784100 | 0.70098700 |
| H | 6.29282000 | -3.42255800 | 0.15395600 |

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|---|-------------|-------------|-------------|
| H | 4.58725100 | 5.51776400 | -0.81233400 |
| H | 2.14232100 | 6.22712600 | 0.05820100 |
| H | 0.06874100 | 6.87750100 | 0.81550000 |
| Li ⁺ @V _N <i>h</i> -BN (reactant) | | | |
| Li | 0.23945300 | -3.07253500 | 1.69912700 |
| B | -1.48107300 | -0.36684300 | -0.04133200 |
| B | 0.91512900 | -1.17082900 | 0.56009100 |
| B | 0.52186500 | 1.24294500 | 0.08066600 |
| B | -1.17276600 | -2.33208900 | -0.10760600 |
| B | 1.18952100 | -3.45357900 | -0.38146100 |
| B | 3.21459300 | -2.11722200 | 0.26188600 |
| B | 2.85746600 | 0.33833800 | 0.43805800 |
| B | 2.50913900 | 2.78725200 | 0.13291700 |
| B | 0.21415500 | 3.69043500 | -0.31594500 |
| B | -1.77347000 | 2.14844700 | -0.21898600 |
| B | -3.77105000 | 0.74053800 | 0.20793200 |
| B | -3.46479900 | -1.69907500 | 0.42631200 |
| N | -2.89042700 | -0.40671400 | 0.24131200 |
| N | -2.50788800 | -2.76805500 | 0.26486200 |
| N | -3.20558700 | 2.01739400 | -0.09777900 |
| N | -0.88521000 | 0.95730100 | -0.12529800 |
| N | -1.21006400 | 3.46832500 | -0.39651500 |
| N | 1.08253400 | 2.55964700 | -0.03650000 |
| N | 1.40020200 | 0.13558000 | 0.41739000 |
| N | 3.39098200 | 1.66185700 | 0.37627900 |
| N | 3.73751500 | -0.80965300 | 0.48468800 |
| N | 1.75082300 | -2.31263300 | 0.30644400 |
| N | -0.26488600 | -3.49614600 | -0.39168300 |

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|---|-------------|-------------|-------------|
| B | -3.05101300 | -4.11462000 | 0.15740500 |
| B | -0.83549600 | -4.83803100 | -0.70626900 |
| B | 5.18748200 | -0.61634200 | 0.50965000 |
| B | 4.83218700 | 1.86952900 | 0.48609500 |
| B | -2.08910100 | 4.62239400 | -0.58613200 |
| B | -4.09014000 | 3.17151600 | -0.21395200 |
| N | -5.19123100 | 0.55646000 | 0.44895900 |
| N | -4.85804600 | -1.90722300 | 0.69172600 |
| N | 2.04615400 | -4.52195500 | -0.81755500 |
| N | 4.05706800 | -3.24224200 | -0.05704800 |
| N | 3.05611500 | 4.12125800 | 0.02778200 |
| N | 0.77868500 | 5.01577600 | -0.46545700 |
| B | -5.73378900 | -0.75029100 | 0.71953000 |
| B | 3.48288200 | -4.43667900 | -0.61737100 |
| B | 2.19067000 | 5.23318800 | -0.28712700 |
| B | -6.06846200 | 1.71233600 | 0.34626200 |
| B | 5.50356300 | -3.07608200 | 0.06129900 |
| N | -5.49719900 | 2.96645000 | 0.00171800 |
| N | 6.01066500 | -1.79342500 | 0.39731900 |
| N | 5.68427900 | 0.71658100 | 0.60589300 |
| N | -3.50677900 | 4.43524600 | -0.52273300 |
| N | -1.49138200 | 5.90871000 | -0.80687300 |
| N | 5.32102500 | 3.21395100 | 0.44121800 |
| B | -5.34496300 | -3.26766100 | 0.78551000 |
| B | 1.44243000 | -5.72461500 | -1.36176300 |
| B | -0.09289200 | 6.14203700 | -0.74322400 |
| B | 4.47900900 | 4.33850400 | 0.20376100 |
| N | 0.02876200 | -5.82948100 | -1.28244000 |

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|---|-------------|-------------|-------------|
| N | -2.18384000 | -5.12559800 | -0.36124300 |
| N | -4.42042700 | -4.32750900 | 0.52332700 |
| H | 0.35344700 | 7.23426300 | -0.90060200 |
| H | 2.64534100 | 6.32692000 | -0.39547300 |
| H | 4.93870500 | 5.43452700 | 0.14264100 |
| H | -6.89399100 | -0.89245700 | 0.93923300 |
| H | -7.23838000 | 1.60452400 | 0.53840200 |
| H | -6.48232800 | -3.50317700 | 1.04200700 |
| H | 2.10639200 | -6.60044400 | -1.81301300 |
| H | 4.17334100 | -5.35315200 | -0.92558200 |
| H | 6.23113200 | -3.99734600 | -0.13095100 |
| H | -6.12508200 | 3.75586900 | -0.06903500 |
| H | -4.10688600 | 5.24265900 | -0.62521200 |
| H | -2.08886700 | 6.70692900 | -0.97412300 |
| H | 6.31163100 | 3.39042300 | 0.53967000 |
| H | 6.68472200 | 0.86294000 | 0.63713900 |
| H | 7.01634500 | -1.69709200 | 0.44735700 |
| H | -0.38547700 | -6.69911800 | -1.59231700 |
| H | -2.54435100 | -6.05544000 | -0.53059400 |
| H | -4.79234400 | -5.26805300 | 0.51751000 |

Li@Pristine *h*-BN

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|----|-------------|-------------|------------|
| Li | -0.32297300 | -0.25168300 | 1.02934600 |
| B | -0.97114300 | 1.45040200 | 0.75537200 |
| B | -0.32804400 | -2.00917300 | 1.51495400 |
| B | 1.50635800 | -0.03480400 | 0.66423000 |
| B | -2.98417200 | 0.13293600 | 0.71028000 |
| B | -2.78685500 | -2.52074900 | 0.62467700 |
| B | -0.62542300 | -3.80869600 | 0.09050300 |

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|---|-------------|-------------|-------------|
| B | 1.58275000 | -2.55035200 | 0.19506800 |
| B | 3.66083800 | -1.18959800 | 0.04786700 |
| B | 3.58243600 | 1.30535200 | 0.33077900 |
| B | 1.34583600 | 2.48187100 | 0.35658700 |
| B | -0.80706900 | 3.75121100 | -0.17472700 |
| B | -2.98973200 | 2.48236300 | -0.16089000 |
| N | -1.56091700 | 2.57498800 | 0.09769600 |
| N | -1.76712900 | 0.44253100 | 1.32049700 |
| N | -3.69669700 | 1.24399700 | 0.05773000 |
| N | 0.62922900 | 3.72103800 | 0.05421200 |
| N | 0.63770400 | 1.22023400 | 0.65146200 |
| N | 2.80597500 | 2.51921900 | 0.35732000 |
| N | 2.90628800 | 0.01917300 | 0.36080200 |
| N | 0.92390100 | -1.43767100 | 0.87041800 |
| N | 2.97521400 | -2.44789000 | -0.13588800 |
| N | 0.82301100 | -3.75765700 | -0.07459100 |
| N | -1.30614900 | -2.69231300 | 0.75047300 |
| N | -3.53548100 | -1.26062400 | 0.62258900 |
| B | -5.09398700 | 1.14087600 | -0.25199400 |
| B | -4.97136200 | -1.31749800 | 0.33103500 |
| B | 1.51595600 | -4.90926700 | -0.63576200 |
| B | 3.68685500 | -3.62766200 | -0.59845300 |
| B | 3.51114400 | 3.79329400 | 0.28413200 |
| B | 1.34636200 | 4.97620100 | -0.09921400 |
| N | -1.50880900 | 4.93667400 | -0.64422600 |
| N | -3.67425500 | 3.65228400 | -0.69516400 |
| N | -3.49125900 | -3.77552600 | 0.32374400 |
| N | -1.37560900 | -4.97328600 | -0.30526600 |

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|---|-------------|-------------|-------------|
| N | 5.09705600 | -1.12447100 | -0.14124500 |
| N | 5.03522900 | 1.33926500 | 0.24409600 |
| B | -2.93295600 | 4.87102200 | -0.90822200 |
| B | -2.80417300 | -4.97223500 | -0.08518200 |
| B | 5.78448900 | 0.13190500 | 0.02181300 |
| B | -0.77208500 | 6.16840900 | -0.79153400 |
| B | -0.68046900 | -6.13068900 | -0.82453900 |
| N | 0.61778600 | 6.15823500 | -0.48354100 |
| N | 0.73551800 | -6.07091800 | -0.96941100 |
| N | 2.93597800 | -4.82664300 | -0.83483200 |
| N | 2.76067500 | 4.99564400 | 0.12257200 |
| N | 4.95060400 | 3.79421600 | 0.34822700 |
| N | 5.10845700 | -3.51717500 | -0.78287700 |
| B | -5.09107900 | 3.55041700 | -0.99106000 |
| B | -4.94167000 | -3.81605300 | 0.30031500 |
| B | 5.72723300 | 2.61015500 | 0.30202100 |
| B | 5.82554800 | -2.31160900 | -0.54187500 |
| N | -5.64515800 | -2.59375900 | 0.35491300 |
| N | -5.71500500 | -0.12951000 | -0.00427500 |
| N | -5.76300600 | 2.31267300 | -0.76909400 |
| H | 6.91891500 | 2.65899400 | 0.29373100 |
| H | 6.97272200 | 0.17352500 | -0.05765000 |
| H | 7.00924900 | -2.27666400 | -0.68369700 |
| H | -3.49481400 | 5.84388100 | -1.31068800 |
| H | -1.30550200 | 7.17254900 | -1.15419700 |
| H | -5.69019500 | 4.49039200 | -1.42030000 |
| H | -5.52231200 | -4.85382400 | 0.20376300 |
| H | -3.42147900 | -5.97108900 | -0.28936100 |

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|---|-------------|-------------|-------------|
| H | -1.27814900 | -7.11749200 | -1.12690200 |
| H | 1.12359200 | 7.02663200 | -0.59021600 |
| H | 3.25742600 | 5.87144200 | 0.03384200 |
| H | 5.44019400 | 4.67826000 | 0.35075600 |
| H | 5.63922600 | -4.32471600 | -1.07854100 |
| H | 3.42154200 | -5.63990900 | -1.18863200 |
| H | 1.19825700 | -6.88610800 | -1.34727600 |
| H | -6.65127100 | -2.62279100 | 0.26554000 |
| H | -6.69961800 | -0.24154000 | -0.20523700 |
| H | -6.74884500 | 2.27428000 | -0.98827400 |

Li@Pristine *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.00004300 | 0.00000000 | 0.00078000 |
| B | 0.00000000 | 0.00000000 | 1.97209545 |
| B | 1.55853497 | 0.00000000 | -1.31790615 |
| B | 0.05672456 | 2.05544910 | -0.07409269 |
| B | 0.43381763 | -2.24356284 | 1.17862833 |
| B | 0.97751028 | -2.63703444 | -1.39828402 |
| B | 0.58599609 | -0.90805496 | -3.24213250 |
| B | 0.17434102 | 1.50630711 | -2.58126207 |
| B | -0.50370556 | 3.78184294 | -1.83556195 |
| B | -0.84224837 | 4.28313663 | 0.60268639 |
| B | -0.90074950 | 2.37840431 | 2.25779749 |
| B | -1.53073356 | 0.49514578 | 3.87111571 |
| B | -0.99442639 | -1.88132977 | 3.20841989 |
| N | -0.89324752 | -0.44273379 | 3.00635045 |
| N | 0.85271385 | -0.90214977 | 1.31167790 |
| N | -0.41189577 | -2.79052645 | 2.25693918 |
| N | -1.43513949 | 1.90921334 | 3.54316732 |

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|---|-------------|-------------|-------------|
| N | -0.22400965 | 1.46289631 | 1.30784290 |
| N | -1.04590758 | 3.79778623 | 1.94433729 |
| N | -0.42518756 | 3.35986869 | -0.43963785 |
| N | 0.64305216 | 1.22727312 | -1.21710069 |
| N | -0.30559351 | 2.82281444 | -2.89771113 |
| N | 0.27706390 | 0.47294307 | -3.59759649 |
| N | 1.00440090 | -1.21860983 | -1.86527886 |
| N | 0.73284842 | -3.09657187 | -0.02429131 |
| B | -0.56205296 | -4.21524486 | 2.43189269 |
| B | 0.59841539 | -4.53815436 | 0.20757142 |
| B | -0.04257512 | 0.81208604 | -4.97748931 |
| B | -0.52488504 | 3.18852437 | -4.28710983 |
| B | -1.49752394 | 4.74113817 | 2.96021951 |
| B | -1.96055011 | 2.84821373 | 4.52065153 |
| N | -2.21261320 | 0.00261360 | 5.05882068 |
| N | -1.74325969 | -2.37116939 | 4.36148982 |
| N | 1.06413021 | -3.63749863 | -2.47656507 |
| N | 0.56411622 | -1.94211838 | -4.25320588 |
| N | -0.83488520 | 5.15455956 | -2.16525293 |
| N | -1.06844113 | 5.68028205 | 0.26196211 |
| B | -2.31937775 | -1.42545439 | 5.28558469 |
| B | 0.90303355 | -3.29121103 | -3.86420798 |
| B | -1.05264865 | 6.11186807 | -1.10989887 |
| B | -2.72812454 | 0.95640642 | 6.01074521 |
| B | 0.27936506 | -1.59694681 | -5.63144315 |
| N | -2.55696427 | 2.34160997 | 5.73035290 |
| N | -0.00421897 | -0.23988256 | -5.95816717 |
| N | -0.38620019 | 2.17144887 | -5.28889357 |

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|---|-------------|-------------|-------------|
| N | -1.88212551 | 4.25064258 | 4.24335886 |
| N | -1.56890084 | 6.14059295 | 2.62468152 |
| N | -0.86144056 | 4.55755215 | -4.56936004 |
| B | -1.87248437 | -3.80464544 | 4.54525316 |
| B | 1.18555522 | -5.05001915 | -2.16684719 |
| B | -1.39161158 | 6.62959644 | 1.30683019 |
| B | -0.99417918 | 5.54410250 | -3.55211390 |
| N | 1.00012331 | -5.45896443 | -0.82884207 |
| N | 0.04918671 | -5.05079150 | 1.43732920 |
| N | -1.28947102 | -4.68614410 | 3.58826802 |
| H | -1.52178797 | 7.78941522 | 1.06099598 |
| H | -1.24935296 | 7.25630081 | -1.37734119 |
| H | -1.24894639 | 6.67352148 | -3.83845137 |
| H | -2.89681955 | -1.81864309 | 6.25309776 |
| H | -3.27756493 | 0.60326410 | 7.00962512 |
| H | -2.46415107 | -4.24481371 | 5.48489266 |
| H | 1.40338812 | -5.84750708 | -3.02707849 |
| H | 1.01081246 | -4.13163855 | -4.70237881 |
| H | 0.28765841 | -2.43033537 | -6.48456661 |
| H | -2.92187317 | 3.00050655 | 6.40416994 |
| H | -2.23072763 | 4.90503353 | 4.93031282 |
| H | -1.83087952 | 6.80331169 | 3.34120760 |
| H | -0.99536605 | 4.85312265 | -5.52641670 |
| H | -0.57059478 | 2.41356319 | -6.25311747 |
| H | -0.20923556 | -0.02377121 | -6.92393535 |
| H | 1.01406580 | -6.44978601 | -0.63092296 |
| H | -0.02588965 | -6.05513397 | 1.52710094 |
| H | -1.40026088 | -5.67856300 | 3.74390463 |

Li@ Pristine *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.00002600 | 0.00000000 | 0.00950000 |
| B | 0.00000000 | 0.00000000 | 2.00084643 |
| B | 1.43697127 | 0.00000000 | -1.25554673 |
| B | -0.21730746 | -1.96456721 | -0.09282748 |
| B | 1.80821545 | 1.55965830 | 1.82494225 |
| B | 3.44737546 | 1.37497606 | -0.26435237 |
| B | 3.54567383 | -0.63736967 | -1.88633718 |
| B | 1.59730060 | -2.28323733 | -1.85836395 |
| B | -0.19801800 | -3.98445893 | -1.58922883 |
| B | -1.91997077 | -3.75668612 | 0.22569809 |
| B | -1.60186447 | -2.01831153 | 2.03694766 |
| B | -1.04211658 | -0.69872457 | 4.14791174 |
| B | 0.82510008 | 0.99815103 | 4.05760721 |
| N | -0.07944038 | 0.05360079 | 3.42276975 |
| N | 0.67016645 | 0.99741333 | 1.28092491 |
| N | 1.83176675 | 1.69470201 | 3.28784749 |
| N | -1.85846055 | -1.66282352 | 3.42654418 |
| N | -0.62377099 | -1.29203085 | 1.21350714 |
| N | -2.33215431 | -3.14602637 | 1.46435406 |
| N | -0.78442881 | -3.21330396 | -0.50041681 |
| N | 0.83275062 | -1.36238981 | -1.04084570 |
| N | 1.04780892 | -3.56518568 | -2.18862032 |
| N | 2.89378451 | -1.85705952 | -2.34956696 |
| N | 2.78321627 | 0.30747979 | -1.08030140 |
| N | 3.00583301 | 1.94031609 | 1.00975886 |
| B | 2.75478762 | 2.57707276 | 3.92395785 |
| B | 3.91487446 | 2.86476999 | 1.69461013 |

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|---|-------------|-------------|-------------|
| B | 3.62610857 | -2.74296472 | -3.24408622 |
| B | 1.73012239 | -4.40278574 | -3.16080124 |
| B | -3.44414667 | -3.74361993 | 2.19390311 |
| B | -2.91630611 | -2.32051161 | 4.17598568 |
| N | -1.17637741 | -0.46060237 | 5.57740910 |
| N | 0.72686890 | 1.18636627 | 5.49643674 |
| N | 4.76665526 | 1.72893196 | -0.79878136 |
| N | 4.88527781 | -0.30333592 | -2.27788456 |
| N | -0.82549952 | -5.21440619 | -2.03220029 |
| N | -2.59676694 | -4.93424709 | -0.29829488 |
| B | -0.28390123 | 0.47232772 | 6.23720184 |
| B | 5.43969307 | 0.94444352 | -1.80028926 |
| B | -2.05862734 | -5.64820869 | -1.42487514 |
| B | -2.23246719 | -1.12942424 | 6.29781503 |
| B | 5.59103323 | -1.15986093 | -3.20173474 |
| N | -3.08617473 | -2.00756148 | 5.57203062 |
| N | 4.94593352 | -2.34609740 | -3.65687745 |
| N | 3.00129456 | -3.96680962 | -3.66209244 |
| N | -3.74932474 | -3.27241491 | 3.50530810 |
| N | -4.18343842 | -4.81498188 | 1.57601525 |
| N | 1.07802499 | -5.61869078 | -3.56517206 |
| B | 1.65792460 | 2.09356493 | 6.14098887 |
| B | 5.51225420 | 2.83477165 | -0.22686859 |
| B | -3.77860458 | -5.43840589 | 0.36988918 |
| B | -0.18366695 | -6.02566306 | -3.04729382 |
| N | 5.04243613 | 3.40682859 | 0.97475563 |
| N | 3.71927395 | 3.22045309 | 3.07735492 |
| N | 2.64174130 | 2.75976088 | 5.35291993 |

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|---|-------------|-------------|-------------|
| H | -4.38466998 | -6.36454564 | -0.07453162 |
| H | -2.61591578 | -6.61683823 | -1.83855458 |
| H | -0.69726088 | -7.03035209 | -3.43369246 |
| H | -0.39065992 | 0.64600482 | 7.41302358 |
| H | -2.39677987 | -0.95260268 | 7.46661389 |
| H | 1.60625343 | 2.27918970 | 7.31980756 |
| H | 6.51429160 | 3.22721101 | -0.74198845 |
| H | 6.49901117 | 1.29667756 | -2.21771159 |
| H | 6.69173765 | -0.88518947 | -3.56974328 |
| H | -3.82243767 | -2.47037872 | 6.08686039 |
| H | -4.49661592 | -3.71687966 | 4.02073382 |
| H | -4.98699136 | -5.19601191 | 2.05597083 |
| H | 1.51130459 | -6.21244107 | -4.25870273 |
| H | 3.49493270 | -4.56252091 | -4.31309003 |
| H | 5.46627357 | -2.93944540 | -4.28824776 |
| H | 5.60388314 | 4.12749881 | 1.40661839 |
| H | 4.38981776 | 3.85407511 | 3.49123093 |
| H | 3.27679599 | 3.38239600 | 5.83294438 |

Li⁺@ Pristine *h*-BN

| | | | |
|----|-------------|-------------|-------------|
| Li | -0.00002300 | -0.00019600 | -0.00085000 |
| B | 1.30472900 | -0.96660400 | -0.00055700 |
| B | -1.48947600 | -0.64619200 | -0.00028300 |
| B | 0.18448700 | 1.61256600 | -0.00152300 |
| B | -0.34002100 | -2.96904800 | 0.00017100 |
| B | -2.87399000 | -2.65786600 | -0.00004700 |
| B | -3.90458400 | -0.28454600 | 0.00016700 |
| B | -2.40169600 | 1.77918900 | -0.00033300 |
| B | -0.86498200 | 3.81757100 | -0.00034200 |

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|---|-------------|-------------|-------------|
| B | 1.70562500 | 3.52315600 | -0.00075400 |
| B | 2.74156700 | 1.19003800 | -0.00072600 |
| B | 3.73915400 | -1.15978200 | 0.00013400 |
| B | 2.19871600 | -3.23875500 | 0.00036200 |
| N | 2.41073700 | -1.78579500 | 0.00004900 |
| N | -0.17514000 | -1.52921100 | -0.00011100 |
| N | 0.85094300 | -3.78746600 | 0.00037800 |
| N | 3.87141500 | 0.28921200 | -0.00006200 |
| N | 1.41202100 | 0.61259500 | -0.00135100 |
| N | 2.85477000 | 2.63046200 | -0.00067400 |
| N | 0.34124200 | 2.97990700 | -0.00134600 |
| N | -1.23704200 | 0.91635300 | -0.00127600 |
| N | -2.18618900 | 3.20787500 | 0.00001500 |
| N | -3.70578400 | 1.15690500 | 0.00030100 |
| N | -2.75193600 | -1.19454400 | 0.00031100 |
| N | -1.68516500 | -3.49709300 | 0.00003800 |
| B | 0.67778800 | -5.24085800 | 0.00035000 |
| B | -1.84518700 | -4.95199400 | -0.00016800 |
| B | -4.87804700 | 2.03361800 | 0.00072900 |
| B | -3.36625900 | 4.07402200 | 0.00063400 |
| B | 4.20010000 | 3.20750800 | -0.00025600 |
| B | 5.21148300 | 0.87832000 | 0.00017800 |
| N | 4.87891600 | -2.03735700 | 0.00045400 |
| N | 3.37034400 | -4.07330600 | 0.00056600 |
| N | -4.20394600 | -3.20615000 | -0.00054500 |
| N | -5.21315200 | -0.88188600 | -0.00005800 |
| N | -0.67463500 | 5.24325200 | 0.00029900 |
| N | 1.84268700 | 4.95494800 | -0.00021500 |

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|---|-------------|-------------|-------------|
| B | 4.69556900 | -3.47832300 | 0.00061200 |
| B | -5.36046900 | -2.32706200 | -0.00054300 |
| B | 0.66490400 | 5.80518800 | 0.00016800 |
| B | 6.21043500 | -1.44478100 | 0.00061500 |
| B | -6.37630100 | -0.00366100 | 0.00029600 |
| N | 6.32886000 | -0.02475900 | 0.00049900 |
| N | -6.17060700 | 1.40645600 | 0.00088000 |
| N | -4.66185600 | 3.45369900 | 0.00093300 |
| N | 5.32197900 | 2.31043300 | 0.00006300 |
| N | 4.30319200 | 4.64040600 | -0.00017700 |
| N | -3.14253600 | 5.49314200 | 0.00087800 |
| B | 3.19129600 | -5.51956600 | 0.00067000 |
| B | -4.35665300 | -4.65550600 | -0.00085900 |
| B | 3.18471600 | 5.52336600 | -0.00013000 |
| B | -1.85336200 | 6.10036100 | 0.00084300 |
| N | -3.18599200 | -5.46806700 | -0.00062100 |
| N | -0.66009400 | -5.76376200 | 0.00007700 |
| N | 1.86729800 | -6.04657000 | 0.00058600 |
| H | 3.34199500 | 6.70228700 | -0.00003600 |
| H | 0.80001200 | 6.98611000 | 0.00045400 |
| H | -1.74017800 | 7.28436300 | 0.00126600 |
| H | 5.65058600 | -4.18597700 | 0.00079000 |
| H | 7.17928400 | -2.13468300 | 0.00084500 |
| H | 4.13339800 | -6.24556900 | 0.00080700 |
| H | -5.43854900 | -5.14961500 | -0.00130700 |
| H | -6.45081500 | -2.80029400 | -0.00098500 |
| H | -7.47610500 | -0.45643800 | 0.00012700 |
| H | 7.26778900 | 0.35156800 | 0.00065400 |

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|---|-------------|-------------|-------------|
| H | 6.25033300 | 2.71333600 | 0.00027600 |
| H | 5.21930900 | 5.06924300 | -0.00006900 |
| H | -3.93780600 | 6.11822600 | 0.00126100 |
| H | -5.47505900 | 4.05610500 | 0.00123600 |
| H | -7.00014600 | 1.98533300 | 0.00115400 |
| H | -3.32955900 | -6.46936900 | -0.00079200 |
| H | -0.77527000 | -6.76921000 | -0.00007100 |
| H | 1.78084600 | -7.05440500 | 0.00064500 |

Li⁺@Pristine *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.00059600 | -0.00076500 | -1.82947900 |
| B | 0.97986700 | 1.10223400 | -0.03337800 |
| B | -1.44456800 | 0.29750000 | -0.03314800 |
| B | 0.46461600 | -1.39965100 | -0.03334100 |
| B | -0.92039000 | 2.77229500 | -0.06725400 |
| B | -3.30283500 | 1.96910700 | 0.01619000 |
| B | -3.81217700 | -0.50404300 | 0.01560000 |
| B | -1.94088400 | -2.18307100 | -0.06792600 |
| B | -0.05405100 | -3.84456700 | 0.01591200 |
| B | 2.34260300 | -3.04910000 | 0.01636600 |
| B | 2.86116400 | -0.58917800 | -0.06767100 |
| B | 3.35683800 | 1.87554900 | 0.01529300 |
| B | 1.46950300 | 3.55315900 | 0.01548200 |
| N | 1.92722100 | 2.16782500 | 0.00689800 |
| N | -0.45450500 | 1.36906100 | -0.14469800 |
| N | 0.04990900 | 3.83252700 | -0.02631500 |
| N | 3.80045800 | 0.49855800 | -0.02671200 |
| N | 1.41278400 | -0.29091700 | -0.14499600 |
| N | 3.29428200 | -1.95944500 | -0.02593100 |

| | | | |
|---|-------------|-------------|-------------|
| N | 0.91386400 | -2.75269800 | 0.00746800 |
| N | -0.95835500 | -1.07799000 | -0.14469400 |
| N | -1.46844700 | -3.54030100 | -0.02670900 |
| N | -3.34421600 | -1.87293200 | -0.02694900 |
| N | -2.84108000 | 0.58506200 | 0.00721100 |
| N | -2.33209000 | 3.04182900 | -0.02572700 |
| B | -0.40832200 | 5.22218500 | 0.01237700 |
| B | -2.79596800 | 4.42962100 | 0.01305000 |
| B | -4.31873100 | -2.96463400 | 0.01106400 |
| B | -2.43850500 | -4.63593700 | 0.01129800 |
| B | 4.72701800 | -2.25757700 | 0.01262100 |
| B | 5.23439900 | 0.20627100 | 0.01169700 |
| N | 4.30723600 | 2.96175400 | 0.05814500 |
| N | 2.43706200 | 4.62414700 | 0.05837000 |
| N | -4.71877800 | 2.24892300 | 0.05965200 |
| N | -5.22348800 | -0.20175700 | 0.05894400 |
| N | 0.41159100 | -5.21056800 | 0.05943300 |
| N | 2.78641300 | -4.42234700 | 0.06005000 |
| B | 3.85034800 | 4.33082900 | 0.08568100 |
| B | -5.67611300 | 1.16871500 | 0.08696600 |
| B | 1.82573700 | -5.49955800 | 0.08741400 |
| B | 5.73103500 | 2.67091300 | 0.07728200 |
| B | -6.19072400 | -1.28625300 | 0.07777200 |
| N | 6.14674700 | 1.31198600 | 0.05202200 |
| N | -5.71120900 | -2.62398000 | 0.05166600 |
| N | -3.83132600 | -4.30952900 | 0.00729000 |
| N | 5.64815200 | -1.16308300 | 0.00861100 |
| N | 5.12812400 | -3.63377000 | 0.05408700 |

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|--|-------------|-------------|------------|
| N | -1.93691200 | -5.97879900 | 0.05232500 |
| B | 1.98144400 | 6.00396500 | 0.07767000 |
| B | -5.17881600 | 3.62724300 | 0.07926300 |
| B | 4.20923400 | -4.71785100 | 0.07970600 |
| B | -0.55213000 | -6.29822000 | 0.07826600 |
| N | -4.20973100 | 4.66675100 | 0.05400900 |
| N | -1.81678700 | 5.47252000 | 0.00935900 |
| N | 0.58309900 | 6.25759800 | 0.05266200 |
| H | 4.59442300 | -5.84288300 | 0.11679300 |
| H | 2.19999400 | -6.62725900 | 0.12817500 |
| H | -0.18815600 | -7.43030700 | 0.11501100 |
| H | 4.63977400 | 5.21885200 | 0.12607300 |
| H | 6.52952300 | 3.55210700 | 0.11372100 |
| H | 2.76302800 | 6.90021900 | 0.11392600 |
| H | -6.34118900 | 3.87810200 | 0.11595900 |
| H | -6.83986000 | 1.40830100 | 0.12764700 |
| H | -7.35765000 | -1.05747500 | 0.11452300 |
| H | 7.14157800 | 1.13230900 | 0.07489800 |
| H | 6.63851600 | -1.36690300 | 0.03813000 |
| H | 6.11299300 | -3.86173900 | 0.07726200 |
| H | -2.58991200 | -6.75052200 | 0.07493400 |
| H | -4.50316800 | -5.06518500 | 0.03637900 |
| H | -6.40113300 | -3.36290300 | 0.07433200 |
| H | -4.55161900 | 5.61811300 | 0.07690200 |
| H | -2.13534800 | 6.43215800 | 0.03872000 |
| H | 0.28834200 | 7.22460000 | 0.07550500 |
| Li ⁺ @Pristine <i>h</i> -BN (product) | | | |
| Li | -0.00081800 | 0.00166100 | 1.83017400 |

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|---|-------------|-------------|-------------|
| B | 0.69435000 | -1.30122900 | 0.03447000 |
| B | 0.77974800 | 1.25181700 | 0.03384900 |
| B | -1.47398500 | 0.04925200 | 0.03380400 |
| B | 2.91961900 | -0.09746800 | 0.06761800 |
| B | 2.99168900 | 2.41552600 | -0.01847300 |
| B | 0.84825200 | 3.75036100 | -0.01595000 |
| B | -1.37522600 | 2.57715100 | 0.06991100 |
| B | -3.58777700 | 1.38317800 | -0.01458300 |
| B | -3.67208100 | -1.14051900 | -0.01819700 |
| B | -1.54428200 | -2.47961200 | 0.06689300 |
| B | 0.59610800 | -3.79868400 | -0.01365400 |
| B | 2.82391300 | -2.60978800 | -0.01306900 |
| N | 1.36563400 | -2.55914500 | -0.00495200 |
| N | 1.44164300 | -0.04825900 | 0.14520000 |
| N | 3.57784700 | -1.37505800 | 0.02774600 |
| N | -0.84950300 | -3.73772500 | 0.02661800 |
| N | -0.76264800 | -1.22448000 | 0.14511000 |
| N | -2.97982200 | -2.41092000 | 0.02363800 |
| N | -2.89895400 | 0.09684600 | -0.00750700 |
| N | -0.67910700 | 1.27254200 | 0.14636400 |
| N | -2.81217900 | 2.60431100 | 0.02959300 |
| N | -0.59800700 | 3.78590500 | 0.02857000 |
| N | 1.53326600 | 2.46204300 | -0.00782400 |
| N | 3.66156900 | 1.13322700 | 0.02442000 |
| B | 5.04033900 | -1.42672700 | -0.01119300 |
| B | 5.12425900 | 1.08749400 | -0.01545400 |
| B | -1.28431500 | 5.07839100 | -0.00842800 |
| B | -3.50374400 | 3.89398100 | -0.00712300 |

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|---|-------------|-------------|-------------|
| B | -3.75593700 | -3.65139300 | -0.01694500 |
| B | -1.62056200 | -4.98135600 | -0.01314400 |
| N | 1.28572300 | -5.06662400 | -0.05530900 |
| N | 3.49329600 | -3.88852600 | -0.05461400 |
| N | 3.74483900 | 3.64654600 | -0.06416200 |
| N | 1.62092000 | 4.96924200 | -0.06097400 |
| N | -5.03059100 | 1.41979600 | -0.05842700 |
| N | -5.11413200 | -1.08090700 | -0.06305400 |
| B | 2.72841800 | -5.11252100 | -0.08126300 |
| B | 3.06334800 | 4.91888300 | -0.09123900 |
| B | -5.79167000 | 0.19353600 | -0.08901400 |
| B | 0.51949900 | -6.30130200 | -0.07493000 |
| B | 0.93893700 | 6.25243900 | -0.07882800 |
| N | -0.89935400 | -6.22028300 | -0.05212500 |
| N | -0.48207300 | 6.26629100 | -0.05025600 |
| N | -2.71481600 | 5.08722200 | -0.00250800 |
| N | -3.04846200 | -4.89472400 | -0.01262600 |
| N | -5.18583400 | -3.55065700 | -0.06028200 |
| N | -4.93725100 | 3.88884500 | -0.04737700 |
| B | 4.94560000 | -3.93927800 | -0.07339900 |
| B | 5.19724300 | 3.60053200 | -0.08551800 |
| B | -5.88431800 | -2.31304500 | -0.08512800 |
| B | -5.71680900 | 2.70072700 | -0.07541500 |
| N | 5.83653200 | 2.33136000 | -0.05916000 |
| N | 5.76323800 | -0.19235300 | -0.01020800 |
| N | 5.66808900 | -2.71551000 | -0.04995100 |
| H | -7.07306600 | -2.28433300 | -0.12339600 |
| H | -6.97911000 | 0.23345300 | -0.13085800 |

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|---|-------------|-------------|-------------|
| H | -6.90484000 | 2.75181500 | -0.11234100 |
| H | 3.28795000 | -6.16077800 | -0.11989200 |
| H | 1.06948700 | -7.35568100 | -0.10993600 |
| H | 5.51545700 | -4.98307500 | -0.10821300 |
| H | 5.83520800 | 4.60396600 | -0.12436200 |
| H | 3.69139400 | 5.92742400 | -0.13358100 |
| H | 1.55805100 | 7.26766700 | -0.11666600 |
| H | -1.41253500 | -7.09125400 | -0.07556700 |
| H | -3.58303000 | -5.75295600 | -0.04297700 |
| H | -5.74110200 | -4.39539100 | -0.08466200 |
| H | -5.43498200 | 4.76880500 | -0.06878600 |
| H | -3.19097100 | 5.97926400 | -0.03054500 |
| H | -0.93607600 | 7.16956400 | -0.07205500 |
| H | 6.84738500 | 2.32218700 | -0.08334200 |
| H | 6.77377900 | -0.22630500 | -0.04022700 |
| H | 6.67731900 | -2.77413300 | -0.07270100 |

Na⁺@ Pristine *h*-BN

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|----|-------------|-------------|-------------|
| Na | -0.79754900 | -0.15222300 | 0.32559400 |
| B | -2.48507500 | 0.47031400 | 1.74419000 |
| B | 0.60435900 | -1.73451600 | -0.64718900 |
| B | 1.35864200 | 0.86340700 | -0.69417700 |
| B | -2.89594500 | -1.48647100 | 0.86305700 |
| B | -1.25972100 | -3.51218700 | 0.19279300 |
| B | 1.39617200 | -3.59184200 | 0.05178100 |
| B | 2.72122700 | -1.42787200 | -0.45689000 |
| B | 3.89699300 | 0.78449200 | -0.44530000 |
| B | 2.58128900 | 2.91790200 | -0.21955100 |
| B | 0.05474200 | 2.78884800 | -0.11133100 |

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|---|-------------|-------------|-------------|
| B | -2.55876600 | 2.85136100 | 0.39802900 |
| B | -3.99445400 | 0.71188900 | 0.18013700 |
| N | -2.87788900 | 1.45756000 | 0.89013300 |
| N | -2.21068100 | -0.79838800 | 1.94654600 |
| N | -3.95952400 | -0.73526800 | 0.17202000 |
| N | -1.24396000 | 3.44342500 | 0.29128400 |
| N | 0.11990100 | 1.46204300 | -0.60786100 |
| N | 1.30432200 | 3.56479300 | -0.00534000 |
| N | 2.64158400 | 1.48473400 | -0.50775000 |
| N | 1.43453200 | -0.71069900 | -0.80218300 |
| N | 3.91752600 | -0.68660600 | -0.41905900 |
| N | 2.62516000 | -2.85221700 | -0.13952100 |
| N | 0.06201900 | -2.84128600 | -0.11881200 |
| N | -2.51836300 | -2.80540600 | 0.30594000 |
| B | -5.00283800 | -1.45379800 | -0.54451900 |
| B | -3.70173900 | -3.57919400 | -0.15900200 |
| B | 3.90019700 | -3.57322500 | 0.05969700 |
| B | 5.17725000 | -1.40362200 | -0.22459900 |
| B | 1.28872900 | 4.98855000 | 0.26551600 |
| B | -1.22794700 | 4.91729800 | 0.35076400 |
| N | -3.75966800 | 3.57796400 | 0.01361800 |
| N | -5.01094600 | 1.46148600 | -0.48042300 |
| N | -1.17983800 | -4.94845600 | 0.26133600 |
| N | 1.33851500 | -4.97727300 | 0.35218500 |
| N | 5.13523600 | 1.51254800 | -0.32846600 |
| N | 3.83465900 | 3.64845900 | -0.11073700 |
| B | -4.95722300 | 2.91387100 | -0.42945400 |
| B | 0.06616400 | -5.66974800 | 0.39595700 |

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|---|-------------|-------------|-------------|
| B | 5.09494100 | 2.96107400 | -0.20292100 |
| B | -3.71409500 | 5.03369200 | 0.01486400 |
| B | 2.60359500 | -5.69843300 | 0.50799300 |
| N | -2.47552000 | 5.64145500 | 0.31576900 |
| N | 3.81600100 | -4.97595700 | 0.36131700 |
| N | 5.11401300 | -2.83396900 | -0.04634200 |
| N | 0.01360500 | 5.62085900 | 0.41613000 |
| N | 2.53706800 | 5.70076700 | 0.33114600 |
| N | 6.37769400 | -0.63322900 | -0.20695500 |
| B | -6.09374800 | 0.73960800 | -1.13134800 |
| B | -2.41287700 | -5.72085200 | 0.11405400 |
| B | 3.80053100 | 5.07743800 | 0.15294000 |
| B | 6.39221200 | 0.79864300 | -0.24917200 |
| N | -3.59837600 | -5.01131700 | -0.19239200 |
| N | -4.88932600 | -2.88540100 | -0.55281500 |
| N | -6.05262200 | -0.68768400 | -1.14746600 |
| H | 4.80919200 | 5.70656200 | 0.22479200 |
| H | 6.11646900 | 3.56770900 | -0.14170900 |
| H | 7.42629700 | 1.38439100 | -0.19733000 |
| H | -5.89386500 | 3.54658300 | -0.79563200 |
| H | -4.69250500 | 5.67267300 | -0.20773500 |
| H | -6.98858200 | 1.32918900 | -1.64610700 |
| H | -2.39529300 | -6.90578200 | 0.19004900 |
| H | 0.05204900 | -6.84744700 | 0.53792600 |
| H | 2.59904800 | -6.86062200 | 0.75158000 |
| H | -2.44675100 | 6.65187300 | 0.34339800 |
| H | -0.01893400 | 6.62763400 | 0.50662000 |
| H | 2.53217600 | 6.69475300 | 0.51615500 |

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|---|-------------|-------------|-------------|
| H | 7.27163900 | -1.09652000 | -0.11333100 |
| H | 5.98527200 | -3.33071300 | 0.08974800 |
| H | 4.67320100 | -5.49824400 | 0.48932300 |
| H | -4.42690900 | -5.55565000 | -0.39381600 |
| H | -5.65057000 | -3.43414000 | -0.93105000 |
| H | -6.80784100 | -1.16150000 | -1.62510900 |

Na⁺@ Pristine *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Na | 0.00002300 | 0.00008700 | 0.00026000 |
| B | 0.00001200 | 0.00000000 | 2.39210515 |
| B | 1.82389622 | 0.00000000 | -1.62174487 |
| B | 0.51122333 | 2.36041451 | -1.38312304 |
| B | 0.51260753 | -1.91370573 | 1.41616946 |
| B | 2.31900908 | -2.41569674 | -0.51230258 |
| B | 3.74139083 | -0.75368835 | -2.01727744 |
| B | 2.82116831 | 1.62290301 | -2.52324375 |
| B | 2.07428720 | 4.01437285 | -2.52970858 |
| B | 0.12787348 | 4.74744466 | -1.10875710 |
| B | -1.12500576 | 3.00490620 | 0.23433702 |
| B | -2.32198083 | 1.40321710 | 1.99152627 |
| B | -1.86486224 | -1.14937433 | 1.99985038 |
| N | -1.33214620 | 0.26141409 | 2.17505653 |
| N | 1.03522009 | -0.72633428 | 2.06811256 |
| N | -0.93263134 | -2.18743309 | 1.58846476 |
| N | -2.03933150 | 2.68686112 | 1.39739152 |
| N | -0.53267325 | 2.00776646 | -0.56382392 |
| N | -0.86951940 | 4.41616022 | -0.10897584 |
| N | 0.91955662 | 3.68637617 | -1.73779686 |
| N | 1.48314375 | 1.24333929 | -1.93476515 |

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|---|-------------|-------------|-------------|
| N | 3.02426653 | 2.95922727 | -2.91587981 |
| N | 3.83365549 | 0.56806279 | -2.61265168 |
| N | 2.46008835 | -1.11362777 | -1.24890802 |
| N | 1.23148808 | -2.72108526 | 0.40162034 |
| B | -1.45720613 | -3.52113993 | 1.32345007 |
| B | 0.79864251 | -4.14836441 | 0.40271033 |
| B | 5.09480860 | 0.92031663 | -3.29670556 |
| B | 4.26804549 | 3.30219475 | -3.60069331 |
| B | -1.63962970 | 5.48378202 | 0.49159326 |
| B | -2.92729235 | 3.77567794 | 1.82251552 |
| N | -3.64670873 | 1.06195673 | 2.48945407 |
| N | -3.25383436 | -1.39333413 | 2.16538237 |
| N | 3.28745695 | -3.40707502 | -0.89844002 |
| N | 4.74057308 | -1.75138527 | -2.12218847 |
| N | 2.35202677 | 5.38266865 | -2.88257320 |
| N | 0.40796203 | 6.12617278 | -1.47522505 |
| B | -4.12482798 | -0.28772674 | 2.55661102 |
| B | 4.50188218 | -3.09066046 | -1.62250530 |
| B | 1.48467785 | 6.43363226 | -2.37385505 |
| B | -4.54709391 | 2.15079792 | 2.84316999 |
| B | 5.97260235 | -1.41002584 | -2.84602990 |
| N | -4.09310159 | 3.47020193 | 2.61635337 |
| N | 6.09481246 | -0.10611881 | -3.38597792 |
| N | 5.23329995 | 2.24913490 | -3.80321687 |
| N | -2.66103671 | 5.12562846 | 1.42691921 |
| N | -1.36669412 | 6.84411240 | 0.08963063 |
| N | 4.45165892 | 4.66140686 | -3.99275331 |
| B | -3.76210823 | -2.74754149 | 1.98258170 |

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|---|-------------|-------------|-------------|
| B | 3.00856010 | -4.81447347 | -0.60785646 |
| B | -0.37573172 | 7.18529904 | -0.86397123 |
| B | 3.53312300 | 5.70714574 | -3.65367745 |
| N | 1.73693087 | -5.13071421 | -0.06408231 |
| N | -0.50376133 | -4.49322426 | 0.86643330 |
| N | -2.84778332 | -3.75991251 | 1.55934669 |
| H | -0.18259099 | 8.32286518 | -1.15729652 |
| H | 1.69327468 | 7.56487198 | -2.69772061 |
| H | 3.75665602 | 6.82642712 | -3.98787123 |
| H | -5.23885835 | -0.51710184 | 2.89484017 |
| H | -5.60946729 | 1.92007234 | 3.33113687 |
| H | -4.90783912 | -2.99695264 | 2.16474159 |
| H | 3.80360133 | -5.65430640 | -0.87565991 |
| H | 5.30721449 | -3.93588224 | -1.82397550 |
| H | 6.84054642 | -2.21273323 | -2.95719575 |
| H | -4.70734217 | 4.22459710 | 2.89101755 |
| H | -3.26842848 | 5.85242378 | 1.77972094 |
| H | -1.89907751 | 7.59643833 | 0.50229627 |
| H | 5.28288103 | 4.93071442 | -4.50051623 |
| H | 6.09640096 | 2.48648004 | -4.27357312 |
| H | 6.96955478 | 0.10774836 | -3.86042242 |
| H | 1.51073963 | -6.11238199 | 0.04255636 |
| H | -0.79137756 | -5.45941465 | 0.79479105 |
| H | -3.22935647 | -4.69001858 | 1.42135834 |

Na⁺@ Pristine *h*-BN (Product)

| | | | |
|----|-------------|-------------|-------------|
| Na | -0.01512100 | 0.00985800 | 2.29969700 |
| B | -0.82812200 | -1.20947600 | -0.00299900 |
| B | 1.46205800 | -0.11368700 | -0.00152700 |

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|---|-------------|-------------|-------------|
| B | -0.63195400 | 1.32204300 | -0.00408900 |
| B | 1.25971000 | -2.63229000 | -0.00143200 |
| B | 3.52227000 | -1.53828400 | -0.06116900 |
| B | 3.71728200 | 0.97647900 | -0.05916700 |
| B | 1.65030500 | 2.40618600 | 0.00003900 |
| B | -0.42839100 | 3.81861500 | -0.06366600 |
| B | -2.70387300 | 2.73003500 | -0.06396900 |
| B | -2.90858000 | 0.22527500 | -0.00054300 |
| B | -3.09244000 | -2.28113900 | -0.05980100 |
| B | -1.01192700 | -3.70742100 | -0.06158900 |
| N | -1.63856900 | -2.39107000 | -0.03449700 |
| N | 0.62524200 | -1.30633000 | 0.07934600 |
| N | 0.43146600 | -3.80991100 | -0.03628100 |
| N | -3.70828800 | -0.97182700 | -0.03303800 |
| N | -1.44263300 | 0.11153600 | 0.07910000 |
| N | -3.51420300 | 1.53123300 | -0.03574500 |
| N | -1.25044100 | 2.61437200 | -0.03704800 |
| N | 0.81892000 | 1.19363900 | 0.07990400 |
| N | 1.01344100 | 3.69724400 | -0.03518300 |
| N | 3.08423100 | 2.27760300 | -0.03245000 |
| N | 2.89055400 | -0.22441400 | -0.03388300 |
| N | 2.69632200 | -2.72647000 | -0.03568600 |
| B | 1.05979400 | -5.12926100 | -0.08610900 |
| B | 3.32937400 | -4.04354200 | -0.08581200 |
| B | 3.91279900 | 3.48155000 | -0.08026300 |
| B | 1.83769600 | 4.90416200 | -0.08337700 |
| B | -4.97123400 | 1.64690600 | -0.08365600 |
| B | -5.16570400 | -0.86137700 | -0.08079100 |

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|---|-------------|-------------|-------------|
| N | -3.90082200 | -3.47891300 | -0.10297800 |
| N | -1.83782200 | -4.89325100 | -0.10511400 |
| N | 4.96387500 | -1.63951400 | -0.10468600 |
| N | 5.15722500 | 0.85423200 | -0.10211400 |
| N | -1.06157600 | 5.11737000 | -0.10915200 |
| N | -3.31791500 | 4.03794100 | -0.10928000 |
| B | -3.27626700 | -4.77964400 | -0.12873300 |
| B | 5.77811800 | -0.44824900 | -0.12826600 |
| B | -2.50033700 | 5.22693900 | -0.13531400 |
| B | -5.34907700 | -3.36881200 | -0.13352100 |
| B | 5.98032300 | 2.05092200 | -0.13265200 |
| N | -5.93300800 | -2.07301400 | -0.11861100 |
| N | 5.33773600 | 3.31866500 | -0.11789100 |
| N | 3.26100700 | 4.75553400 | -0.08578400 |
| N | -5.74865200 | 0.44546900 | -0.08615600 |
| N | -5.54255600 | 2.96223600 | -0.12428300 |
| N | 1.17198000 | 6.17441200 | -0.12442600 |
| B | -1.21302900 | -6.20434300 | -0.13824500 |
| B | 5.59266700 | -2.94867100 | -0.13803500 |
| B | -4.76585100 | 4.15253000 | -0.14092100 |
| B | -0.24217300 | 6.31665100 | -0.14111600 |
| N | 4.76234900 | -4.10225100 | -0.12501200 |
| N | 2.48897800 | -5.20186400 | -0.09152900 |
| N | 0.20615200 | -6.28177300 | -0.12521600 |
| H | -5.28902300 | 5.22069200 | -0.17926500 |
| H | -3.01325700 | 6.29909400 | -0.17492300 |
| H | -0.74558900 | 7.39427400 | -0.17961000 |
| H | -3.94858300 | -5.75981700 | -0.16661200 |

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|---|-------------|-------------|-------------|
| H | -6.03087000 | -4.34350600 | -0.16983100 |
| H | -1.87662200 | -7.19150500 | -0.17477600 |
| H | 6.77767000 | -3.05154600 | -0.17497900 |
| H | 6.96315800 | -0.53990100 | -0.16623500 |
| H | 7.16705500 | 1.97019000 | -0.16888600 |
| H | -6.94226800 | -2.01980000 | -0.14956600 |
| H | -6.75643500 | 0.52344600 | -0.12422600 |
| H | -6.54795300 | 3.06501400 | -0.15581000 |
| H | 1.72293600 | 7.02165500 | -0.15611800 |
| H | 3.83271300 | 5.58911100 | -0.12401100 |
| H | 5.92958600 | 4.13792200 | -0.14878300 |
| H | 5.22076900 | -5.00290600 | -0.15753200 |
| H | 2.92517000 | -6.11364800 | -0.13059200 |
| H | 0.61972000 | -7.20389500 | -0.15741200 |

Na@ V_B *h*-BN

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|----|-------------|-------------|-------------|
| Na | -1.67287500 | -0.11659700 | 0.30488300 |
| B | 0.97706700 | -1.20438800 | 0.27672900 |
| B | 0.67487300 | 1.35109700 | -0.16108200 |
| B | -1.07695600 | -2.65388800 | 0.50706400 |
| B | 1.20248600 | -3.67172200 | 0.08535700 |
| B | 3.24816700 | -2.19095300 | -0.08835000 |
| B | 2.94440000 | 0.31786200 | -0.03081200 |
| B | 2.68144700 | 2.83011700 | 0.03980200 |
| B | 0.35706400 | 3.82805900 | 0.02068900 |
| B | -1.67579700 | 2.33382100 | -0.15452500 |
| B | -3.94223100 | 0.82739000 | 0.28839900 |
| B | -3.65953700 | -1.63087900 | 0.49935600 |
| N | -3.50841200 | -0.31232000 | 1.01734700 |

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|---|-------------|-------------|-------------|
| N | -0.30664300 | -1.48815300 | 0.78445400 |
| N | -2.59487200 | -2.71301500 | 0.45013900 |
| N | -3.14237100 | 2.08604400 | 0.01955200 |
| N | -0.69100400 | 1.37204900 | -0.55233200 |
| N | -1.09308200 | 3.67055800 | -0.02429200 |
| N | 1.24830200 | 2.68353500 | -0.00565700 |
| N | 1.50157600 | 0.15400600 | 0.01722500 |
| N | 3.52420800 | 1.65333500 | -0.02290900 |
| N | 3.80749400 | -0.85195200 | -0.08559800 |
| N | 1.83079800 | -2.36340200 | 0.07063400 |
| N | -0.24307400 | -3.82950000 | 0.22553600 |
| B | -3.12689400 | -4.04939400 | 0.12734700 |
| B | -0.83538000 | -5.13871700 | 0.10435500 |
| B | 5.24699600 | -0.68644600 | -0.17015800 |
| B | 4.96734400 | 1.81357800 | -0.04208800 |
| B | -1.96419500 | 4.82640000 | -0.02403700 |
| B | -3.97224700 | 3.28045600 | -0.17640400 |
| N | -5.30497100 | 0.68372300 | -0.25353400 |
| N | -4.99466400 | -1.83222000 | -0.11280700 |
| N | 2.05322900 | -4.84122400 | -0.09528700 |
| N | 4.09223900 | -3.36811600 | -0.22252900 |
| N | 3.24812900 | 4.16824000 | 0.12227400 |
| N | 0.93519700 | 5.15903600 | 0.12887300 |
| B | -5.81244600 | -0.66845100 | -0.39996300 |
| B | 3.48483300 | -4.67904200 | -0.23045300 |
| B | 2.37322000 | 5.31535900 | 0.17525500 |
| B | -6.05282500 | 1.87563900 | -0.56000700 |
| B | 5.52513700 | -3.19266300 | -0.32424200 |

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|---|-------------|-------------|-------------|
| N | -5.39080100 | 3.12754700 | -0.40484200 |
| N | 6.05913900 | -1.87235000 | -0.28561600 |
| N | 5.79099700 | 0.64192600 | -0.13278900 |
| N | -3.37099300 | 4.59079700 | -0.15728100 |
| N | -1.35104400 | 6.12503800 | 0.08384700 |
| N | 5.50003300 | 3.15198300 | 0.02971100 |
| B | -5.45695900 | -3.17159300 | -0.36370400 |
| B | 1.45037400 | -6.15938500 | -0.13982000 |
| B | 0.05939200 | 6.31440900 | 0.16203500 |
| B | 4.68891400 | 4.31809900 | 0.12061300 |
| N | 0.03478800 | -6.27782300 | -0.04198800 |
| N | -2.26493500 | -5.20292900 | 0.10040600 |
| N | -4.53112200 | -4.22848200 | -0.15592700 |
| H | 0.51117100 | 7.41548900 | 0.24715400 |
| H | 2.84125400 | 6.40951500 | 0.25126700 |
| H | 5.19050900 | 5.39881700 | 0.18904600 |
| H | -6.91518900 | -0.82528600 | -0.82926500 |
| H | -7.19149100 | 1.82375600 | -0.91509000 |
| H | -6.57046300 | -3.39361500 | -0.73246500 |
| H | 2.12763000 | -7.13400400 | -0.26575300 |
| H | 4.17528600 | -5.64430600 | -0.35014000 |
| H | 6.25146100 | -4.13341300 | -0.43418000 |
| H | -5.93346900 | 3.96038400 | -0.58919100 |
| H | -3.98933500 | 5.38776800 | -0.23059500 |
| H | -1.93210100 | 6.95184300 | 0.10259000 |
| H | 6.50202900 | 3.28444800 | 0.02540100 |
| H | 6.79500500 | 0.75634400 | -0.16828500 |
| H | 7.06322600 | -1.77760100 | -0.35160500 |

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|---|-------------|-------------|-------------|
| H | -0.36006200 | -7.20650100 | -0.09775700 |
| H | -2.70492900 | -6.10193100 | -0.04642000 |
| H | -4.85714000 | -5.16726100 | -0.34148700 |

Na@ V_B *h*-BN (reactant)

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|----|-------------|-------------|-------------|
| Na | -1.35933800 | -0.63862300 | -2.12920800 |
| B | 1.33354800 | -0.79769800 | -0.30377400 |
| B | 0.11166300 | 1.36261100 | -0.13453900 |
| B | -0.09598600 | -2.79798700 | -0.23906300 |
| B | 2.42596000 | -2.99925300 | 0.00667800 |
| B | 3.81871500 | -0.90888300 | 0.02015100 |
| B | 2.64373800 | 1.30928800 | -0.05242000 |
| B | 1.46288500 | 3.50756300 | -0.01394600 |
| B | -1.04535300 | 3.61476000 | 0.02343300 |
| B | -2.44330300 | 1.48923700 | -0.02877100 |
| B | -3.90864600 | -0.53079300 | -0.10927800 |
| B | -2.67761100 | -2.66475300 | -0.14928600 |
| N | -2.79988800 | -1.29049800 | -0.51785500 |
| N | 0.12744100 | -1.43969400 | -0.63297100 |
| N | -1.42172400 | -3.42531400 | -0.14248700 |
| N | -3.76750600 | 0.90653600 | 0.03507300 |
| N | -1.20319100 | 0.76729100 | -0.19109400 |
| N | -2.33454300 | 2.95803800 | 0.04959200 |
| N | 0.17149300 | 2.83394600 | -0.05741700 |
| N | 1.36654500 | 0.64713100 | -0.16857700 |
| N | 2.69529000 | 2.75379500 | -0.00627000 |
| N | 3.87166400 | 0.53609600 | 0.00592500 |
| N | 2.54892400 | -1.56740900 | -0.10754400 |
| N | 1.11569800 | -3.61587700 | -0.01022300 |

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|---|-------------|-------------|------------|
| B | -1.48630000 | -4.86463100 | 0.10339400 |
| B | 1.02117300 | -5.04854400 | 0.15482500 |
| B | 5.15347200 | 1.20425500 | 0.10128700 |
| B | 3.98034800 | 3.42695800 | 0.05907700 |
| B | -3.54052500 | 3.76380100 | 0.20010200 |
| B | -4.95595200 | 1.70396600 | 0.24740400 |
| N | -5.19483500 | -1.18041900 | 0.15921300 |
| N | -3.95712500 | -3.35768100 | 0.15868700 |
| N | 3.63858400 | -3.79443900 | 0.17587400 |
| N | 5.02944900 | -1.70553600 | 0.16051400 |
| N | 1.52230600 | 4.96386300 | 0.03357800 |
| N | -0.96556300 | 5.07219800 | 0.08659400 |
| B | -5.18971400 | -2.61565600 | 0.26742400 |
| B | 4.92563000 | -3.14363200 | 0.23000900 |
| B | 0.31021800 | 5.73375500 | 0.07425700 |
| B | -6.37027200 | -0.37815400 | 0.38545200 |
| B | 6.30773100 | -1.03398800 | 0.23957100 |
| N | -6.22835500 | 1.03861300 | 0.38305400 |
| N | 6.33940200 | 0.38938300 | 0.19478400 |
| N | 5.17800800 | 2.63859500 | 0.10197800 |
| N | -4.81599800 | 3.12635000 | 0.30286700 |
| N | -3.41478400 | 5.19773700 | 0.24907600 |
| N | 3.99161100 | 4.86620700 | 0.08029700 |
| B | -3.99087000 | -4.78960500 | 0.31784300 |
| B | 3.52906600 | -5.23066700 | 0.30903600 |
| B | -2.16758200 | 5.86703200 | 0.18977400 |
| B | 2.80135400 | 5.64057100 | 0.07094100 |
| N | 2.23462500 | -5.81747000 | 0.29299400 |

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|---|-------------|-------------|------------|
| N | -0.28102100 | -5.63797900 | 0.17771100 |
| N | -2.76657900 | -5.50305600 | 0.25865300 |
| H | -2.11372700 | 7.05858100 | 0.23017100 |
| H | 0.36243600 | 6.92466200 | 0.10659500 |
| H | 2.85671700 | 6.83261800 | 0.09747400 |
| H | -6.21187000 | -3.19425200 | 0.48228700 |
| H | -7.43765000 | -0.88196600 | 0.57085500 |
| H | -5.02034500 | -5.36791600 | 0.49755300 |
| H | 4.50195900 | -5.91170300 | 0.43335500 |
| H | 5.91536800 | -3.80084200 | 0.34196100 |
| H | 7.32178400 | -1.65618500 | 0.34101100 |
| H | -7.05779600 | 1.59391200 | 0.54026600 |
| H | -5.63757300 | 3.69946900 | 0.43668100 |
| H | -4.24981100 | 5.75967800 | 0.33824600 |
| H | 4.87327800 | 5.35846300 | 0.11599900 |
| H | 6.06868000 | 3.11270400 | 0.16395700 |
| H | 7.24340400 | 0.83667400 | 0.25781200 |
| H | 2.17362900 | -6.82102100 | 0.39545400 |
| H | -0.36365200 | -6.63489400 | 0.32419700 |
| H | -2.79851200 | -6.50373800 | 0.39533300 |

Na@ V_B *h*-BN (product)

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|----|-------------|-------------|-------------|
| Na | 1.35940200 | 0.63974500 | 2.12877800 |
| B | -1.33423900 | 0.79654700 | 0.30365400 |
| B | -0.11035000 | -1.36272900 | 0.13464400 |
| B | 0.09339300 | 2.79815600 | 0.23971500 |
| B | -2.42866100 | 2.99719000 | -0.00622800 |
| B | -3.81943500 | 0.90551700 | -0.02088300 |
| B | -2.64244700 | -1.31157200 | 0.05178400 |

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|---|-------------|-------------|-------------|
| B | -1.45970000 | -3.50886300 | 0.01423900 |
| B | 1.04861700 | -3.61397500 | -0.02245500 |
| B | 2.44462400 | -1.48726100 | 0.02890300 |
| B | 3.90808100 | 0.53417700 | 0.10817200 |
| B | 2.67503800 | 2.66710000 | 0.14879100 |
| N | 2.79872900 | 1.29289500 | 0.51703600 |
| N | -0.12881800 | 1.43961000 | 0.63336100 |
| N | 1.41856500 | 3.42665800 | 0.14292100 |
| N | 3.76825800 | -0.90331600 | -0.03557600 |
| N | 1.20398600 | -0.76623400 | 0.19137700 |
| N | 2.33724900 | -2.95612500 | -0.04886700 |
| N | -0.16889400 | -2.83412600 | 0.05798300 |
| N | -1.36585200 | -0.64828800 | 0.16816700 |
| N | -2.69272800 | -2.75615000 | 0.00586500 |
| N | -3.87105500 | -0.53950100 | -0.00694400 |
| N | -2.55028200 | 1.56517500 | 0.10727500 |
| N | -1.11901900 | 3.61507700 | 0.01124500 |
| B | 1.48184000 | 4.86614200 | -0.10236800 |
| B | -1.02579300 | 5.04788500 | -0.15313500 |
| B | -5.15224600 | -1.20880500 | -0.10267100 |
| B | -3.97717100 | -3.43045400 | -0.05980700 |
| B | 3.54394800 | -3.76083200 | -0.19926800 |
| B | 4.95738700 | -1.69966900 | -0.24802200 |
| N | 5.19349000 | 1.18497100 | -0.16103200 |
| N | 3.95382700 | 3.36112600 | -0.15979100 |
| N | -3.64200800 | 3.79131400 | -0.17528000 |
| N | -5.03088500 | 1.70108600 | -0.16135400 |
| N | -1.51782200 | -4.96523300 | -0.03282200 |

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|---|-------------|-------------|-------------|
| N | 0.97014200 | -5.07147500 | -0.08501500 |
| B | 5.18700100 | 2.62020100 | -0.26927900 |
| B | -4.92840900 | 3.13929600 | -0.23021000 |
| B | -0.30508600 | -5.73412100 | -0.07277400 |
| B | 6.36961400 | 0.38375900 | -0.38750100 |
| B | -6.30852300 | 1.02838500 | -0.24093300 |
| N | 6.22908900 | -1.03313700 | -0.38449200 |
| N | -6.33889300 | -0.39502400 | -0.19648400 |
| N | -5.17550500 | -2.64316200 | -0.10334600 |
| N | 4.81878600 | -3.12223000 | -0.30272600 |
| N | 3.41948300 | -5.19491000 | -0.24746100 |
| N | -3.98718500 | -4.86972100 | -0.08063900 |
| B | 3.98632500 | 4.79314400 | -0.31839500 |
| B | -3.53382200 | 5.22771300 | -0.30757600 |
| B | 2.17288000 | -5.86528500 | -0.18779500 |
| B | -2.79627600 | -5.64305900 | -0.07050400 |
| N | -2.23994500 | 5.81576400 | -0.29097000 |
| N | 0.27588100 | 5.63850600 | -0.17577000 |
| N | 2.76153600 | 5.50563400 | -0.25795500 |
| H | 2.12008000 | -7.05690000 | -0.22761300 |
| H | -0.35627500 | -6.92508500 | -0.10461300 |
| H | -2.85061200 | -6.83516400 | -0.09662700 |
| H | 6.20850100 | 3.19967300 | -0.48488700 |
| H | 7.43641500 | 0.88855400 | -0.57354800 |
| H | 5.01521400 | 5.37233200 | -0.49864000 |
| H | -4.50732800 | 5.90790000 | -0.43178000 |
| H | -5.91874000 | 3.79563400 | -0.34206200 |
| H | -7.32311700 | 1.64965900 | -0.34261100 |

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|---|-------------|-------------|-------------|
| H | 7.05900300 | -1.58769400 | -0.54182200 |
| H | 5.64086100 | -3.69464400 | -0.43649700 |
| H | 4.25500200 | -5.75615000 | -0.33644300 |
| H | -4.86842000 | -5.36273300 | -0.11654800 |
| H | -6.06574400 | -3.11805600 | -0.16553300 |
| H | -7.24246100 | -0.84313700 | -0.25987500 |
| H | -2.17990100 | 6.81942200 | -0.39292100 |
| H | 0.35760100 | 6.63556700 | -0.32177800 |
| H | 2.79264400 | 6.50640100 | -0.39419900 |

Na⁺@ V_B *h*-BN

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|----|-------------|-------------|-------------|
| Na | -1.50254700 | -0.06118300 | -0.77491900 |
| B | 0.88929600 | -1.30928200 | -0.57927200 |
| B | 0.78909800 | 1.36496500 | -0.57309200 |
| B | -1.31637600 | -2.68369900 | -0.47449600 |
| B | 0.91518200 | -3.77006700 | -0.02703500 |
| B | 3.05550500 | -2.41735200 | -0.03345100 |
| B | 2.91988900 | 0.10482300 | -0.21320900 |
| B | 2.87091000 | 2.63072400 | -0.04137500 |
| B | 0.63791900 | 3.82450400 | -0.02673800 |
| B | -1.51242100 | 2.57926100 | -0.46008300 |
| B | -3.81772100 | 1.16365700 | -0.34778000 |
| B | -3.72185800 | -1.43166700 | -0.35549800 |
| N | -3.50212300 | -0.12170600 | -0.92199300 |
| N | -0.41196500 | -1.71788100 | -1.06723100 |
| N | -2.78519600 | -2.57228500 | -0.28361200 |
| N | -2.96824200 | 2.36816400 | -0.26820800 |
| N | -0.54345700 | 1.67724800 | -1.04793400 |
| N | -0.82446300 | 3.79140200 | -0.08214800 |

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|---|-------------|-------------|-------------|
| N | 1.42696000 | 2.60414200 | -0.19677000 |
| N | 1.45169300 | 0.05092200 | -0.48675600 |
| N | 3.59488600 | 1.38261400 | -0.09198600 |
| N | 3.68642200 | -1.11979000 | -0.08623600 |
| N | 1.61475900 | -2.49636800 | -0.19595600 |
| N | -0.54550900 | -3.84182500 | -0.08841500 |
| B | -3.43267000 | -3.85240300 | 0.12077300 |
| B | -1.22857300 | -5.09422400 | 0.20207400 |
| B | 5.14319900 | -1.06558500 | 0.05620400 |
| B | 5.05211800 | 1.43489800 | 0.04806200 |
| B | -1.59541700 | 4.99243500 | 0.20721200 |
| B | -3.70601900 | 3.59798200 | 0.13283100 |
| N | -5.17933500 | 1.08569800 | 0.17308100 |
| N | -5.08451300 | -1.45427400 | 0.16834000 |
| N | 1.67534400 | -4.96036900 | 0.25878700 |
| N | 3.80235800 | -3.63511300 | 0.18920100 |
| N | 3.52803600 | 3.90042300 | 0.17412500 |
| N | 1.31098300 | 5.06755800 | 0.25319000 |
| B | -5.80458300 | -0.20987900 | 0.38359100 |
| B | 3.12158400 | -4.89704900 | 0.32896800 |
| B | 2.75818400 | 5.10965200 | 0.31603900 |
| B | -5.86822300 | 2.32490200 | 0.48938900 |
| B | 5.25055100 | -3.57178600 | 0.28529800 |
| N | -5.11761900 | 3.52177700 | 0.39698300 |
| N | 5.86795900 | -2.29763800 | 0.19444100 |
| N | 5.78283900 | 0.20963700 | 0.06558200 |
| N | -3.01744300 | 4.84538400 | 0.25217700 |
| N | -0.88226800 | 6.20782400 | 0.44860800 |

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|---|-------------|-------------|------------|
| N | 5.68575600 | 2.71711400 | 0.17661800 |
| B | -5.68142100 | -2.74074500 | 0.48198900 |
| B | 0.99385500 | -6.22609400 | 0.47462900 |
| B | 0.54098600 | 6.28144400 | 0.46917800 |
| B | 4.97746800 | 3.94312400 | 0.26447600 |
| N | -0.43105900 | -6.25503100 | 0.44845200 |
| N | -2.65742900 | -5.04779500 | 0.24185900 |
| N | -4.84580300 | -3.87931100 | 0.38521400 |
| H | 1.08871000 | 7.31749100 | 0.67110800 |
| H | 3.30823900 | 6.14780700 | 0.49674000 |
| H | 5.54896300 | 4.97604500 | 0.41224200 |
| H | -6.91483200 | -0.25180400 | 0.80333100 |
| H | -7.00845300 | 2.32152500 | 0.82514500 |
| H | -6.81843600 | -2.82128000 | 0.81883100 |
| H | 1.61374700 | -7.21966600 | 0.68124200 |
| H | 3.74466900 | -5.89229700 | 0.51392900 |
| H | 5.89531700 | -4.55963600 | 0.43957600 |
| H | -5.59895500 | 4.37983800 | 0.63281700 |
| H | -3.57275000 | 5.65837100 | 0.48598400 |
| H | -1.39208100 | 7.06322900 | 0.62475500 |
| H | 6.69333400 | 2.75824600 | 0.25146800 |
| H | 6.78841400 | 0.24666100 | 0.16645000 |
| H | 6.87564000 | -2.26500400 | 0.27215400 |
| H | -0.87869500 | -7.14445600 | 0.62508100 |
| H | -3.15500300 | -5.89769300 | 0.47447600 |
| H | -5.26309500 | -4.77068700 | 0.61947300 |

Na⁺@ V_B *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Na | 1.42092300 | -0.49094200 | 2.26040500 |
| B | -1.17772300 | -0.94237000 | 0.24621500 |
| B | -0.31066800 | 1.43638000 | 0.20612700 |
| B | 0.48940600 | -2.86140700 | 0.15876100 |
| B | -1.98904400 | -3.30602500 | 0.00828900 |
| B | -3.62819200 | -1.38974900 | -0.00248400 |
| B | -2.77062900 | 0.97361800 | 0.02490300 |
| B | -1.93035600 | 3.34051600 | -0.00266300 |
| B | 0.54971900 | 3.79795300 | -0.00482800 |
| B | 2.20901600 | 1.90120400 | 0.11003100 |
| B | 3.87756500 | -0.00840600 | 0.08328900 |
| B | 3.00199500 | -2.39846200 | 0.09220100 |
| N | 2.92878300 | -1.01161500 | 0.50119900 |
| N | 0.09530500 | -1.53424000 | 0.60036000 |
| N | 1.86719000 | -3.28954300 | 0.00793900 |
| N | 3.55537500 | 1.39215500 | -0.03074800 |
| N | 1.06929200 | 1.09413700 | 0.51448100 |
| N | 1.92182200 | 3.31193000 | -0.01694500 |
| N | -0.55616300 | 2.85555700 | 0.08246200 |
| N | -1.39222000 | 0.48244200 | 0.14849200 |
| N | -3.01997600 | 2.39460600 | -0.01972000 |
| N | -3.86653600 | 0.03356300 | -0.01881900 |
| N | -2.26228700 | -1.88098500 | 0.10285800 |
| N | -0.61332900 | -3.78300100 | 0.00115100 |
| B | 2.12373300 | -4.71765800 | -0.23652100 |
| B | -0.34765900 | -5.20410300 | -0.19806100 |
| B | -5.24047500 | 0.52191100 | -0.10689000 |

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|---|-------------|-------------|-------------|
| B | -4.39368700 | 2.88699300 | -0.10168200 |
| B | 3.02163000 | 4.25754700 | -0.20043400 |
| B | 4.65219600 | 2.34149200 | -0.25442600 |
| N | 5.22873600 | -0.50711500 | -0.12008500 |
| N | 4.36622800 | -2.86691700 | -0.12238600 |
| N | -3.08567600 | -4.23645100 | -0.12169800 |
| N | -4.71777500 | -2.33783600 | -0.09647200 |
| N | -2.17837600 | 4.76486200 | -0.08088700 |
| N | 0.28098600 | 5.21292600 | -0.11346400 |
| B | 5.46475200 | -1.93014900 | -0.20797800 |
| B | -4.44959700 | -3.75219200 | -0.14631100 |
| B | -1.08212900 | 5.69601400 | -0.12652500 |
| B | 6.30849800 | 0.44332700 | -0.33498300 |
| B | -6.08412100 | -1.84863300 | -0.16717700 |
| N | 5.98647200 | 1.82403700 | -0.37993000 |
| N | -6.30124900 | -0.44479000 | -0.16120400 |
| N | -5.46024600 | 1.93476900 | -0.13553500 |
| N | 4.35065900 | 3.73573200 | -0.30711100 |
| N | 2.70758000 | 5.65237000 | -0.27665800 |
| N | -4.60353100 | 4.30664400 | -0.14469700 |
| B | 4.60380800 | -4.28619500 | -0.33276300 |
| B | -2.81837200 | -5.65688400 | -0.25535900 |
| B | 1.37767100 | 6.15588600 | -0.23238600 |
| B | -3.54565400 | 5.25334900 | -0.14312200 |
| N | -1.46446800 | -6.09531200 | -0.29383200 |
| N | 1.01884500 | -5.61972300 | -0.29830800 |
| N | 3.48449100 | -5.15463500 | -0.37278600 |
| H | 1.16972400 | 7.32530100 | -0.29940700 |

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|---|-------------|-------------|-------------|
| H | -1.29276700 | 6.86482700 | -0.18454100 |
| H | -3.76968600 | 6.42114100 | -0.19431900 |
| H | 6.56694900 | -2.33266500 | -0.39630000 |
| H | 7.42714300 | 0.06417900 | -0.47607400 |
| H | 5.71044000 | -4.69811300 | -0.47583500 |
| H | -3.71111300 | -6.43879700 | -0.33991900 |
| H | -5.34835300 | -4.52762900 | -0.21866200 |
| H | -6.99810100 | -2.60846100 | -0.23070300 |
| H | 6.74889100 | 2.47095400 | -0.53193300 |
| H | 5.11184300 | 4.38658500 | -0.44967000 |
| H | 3.45476100 | 6.32548600 | -0.38194100 |
| H | -5.54741100 | 4.66585800 | -0.19310300 |
| H | -6.41037000 | 2.27578600 | -0.19777100 |
| H | -7.25870000 | -0.12436700 | -0.21558500 |
| H | -1.30213300 | -7.08662900 | -0.40951800 |
| H | 1.21280300 | -6.60085900 | -0.45072000 |
| H | 3.66797700 | -6.13702200 | -0.52813500 |

Na⁺@ V_B *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Na | 1.41770400 | 0.50164100 | -2.26123400 |
| B | -0.30082300 | -1.43831400 | -0.20701900 |
| B | -1.18423200 | 0.93463400 | -0.24756900 |
| B | 2.22199900 | -1.88636400 | -0.11126000 |
| B | 0.57542800 | -3.79408000 | 0.00506600 |
| B | -1.90759700 | -3.35319900 | 0.00370400 |
| B | -2.76381300 | -0.99210200 | -0.02573400 |
| B | -3.63773500 | 1.36527900 | 0.00047900 |
| B | -2.01151500 | 3.29266600 | -0.00910600 |
| B | 0.46990900 | 2.86472100 | -0.15864200 |

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|---|-------------|-------------|-------------|
| B | 2.98547800 | 2.41833500 | -0.09145000 |
| B | 3.87767200 | 0.03445700 | -0.08404700 |
| N | 2.92171900 | 1.03116900 | -0.50132200 |
| N | 1.07687700 | -1.08688600 | -0.51549000 |
| N | 3.56490000 | -1.36830000 | 0.02920600 |
| N | 1.84476700 | 3.30174500 | -0.00687900 |
| N | 0.08481500 | 1.53528700 | -0.60126500 |
| N | -0.63901200 | 3.77880700 | -0.00087000 |
| N | -2.27515000 | 1.86583400 | -0.10446900 |
| N | -1.38877000 | -0.49165100 | -0.14974300 |
| N | -3.86624300 | -0.05957100 | 0.01730300 |
| N | -3.00365400 | -2.41468300 | 0.02010800 |
| N | -0.53674500 | -2.85904300 | -0.08247700 |
| N | 1.94429000 | -3.29895200 | 0.01597200 |
| B | 4.66821100 | -2.31025500 | 0.25195000 |
| B | 3.05051100 | -4.23710700 | 0.19917000 |
| B | -4.37394000 | -2.91638500 | 0.10281500 |
| B | -5.23686300 | -0.55724200 | 0.10554900 |
| B | -0.38295500 | 5.20144200 | 0.19997900 |
| B | 2.09163300 | 4.73135000 | 0.23887900 |
| N | 4.34646100 | 2.89581600 | 0.12364900 |
| N | 5.22539400 | 0.54216800 | 0.11934900 |
| N | 0.31624300 | -5.21062600 | 0.11531500 |
| N | -2.14602000 | -4.77909100 | 0.08380100 |
| N | -4.73376400 | 2.30603900 | 0.09396600 |
| N | -3.11444800 | 4.21556100 | 0.12077900 |
| B | 5.45148300 | 1.96669500 | 0.20850100 |
| B | -1.04359400 | -5.70283800 | 0.13002800 |

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|---|-------------|-------------|------------|
| B | -4.47512600 | 3.72207600 | 0.14438600 |
| B | 4.57450000 | 4.31647400 | 0.33543400 |
| B | -3.50991700 | -5.27679800 | 0.14710900 |
| N | 3.44937600 | 5.17734500 | 0.37597400 |
| N | -4.57420400 | -4.33731800 | 0.14777100 |
| N | -5.44704000 | -1.97147200 | 0.13545100 |
| N | 0.98072200 | 5.62597200 | 0.30124400 |
| N | -1.50577900 | 6.08502100 | 0.29610200 |
| N | -6.30422400 | 0.40223500 | 0.15885500 |
| B | 6.31173400 | -0.40104100 | 0.33306400 |
| B | 1.41924100 | -6.14625500 | 0.23424200 |
| B | -2.85670000 | 5.63761300 | 0.25611300 |
| B | -6.09676900 | 1.80750700 | 0.16425900 |
| N | 2.74579700 | -5.63393600 | 0.27667500 |
| N | 4.37615400 | -3.70649300 | 0.30450900 |
| N | 5.99908100 | -1.78389700 | 0.37682900 |
| H | -3.75472200 | 6.41344500 | 0.34072200 |
| H | -5.37908800 | 4.49150500 | 0.21614300 |
| H | -7.01598400 | 2.56105300 | 0.22718600 |
| H | 6.55086700 | 2.37668200 | 0.39717600 |
| H | 5.67831500 | 4.73564200 | 0.47912100 |
| H | 7.42776300 | -0.01432900 | 0.47424400 |
| H | 1.21894200 | -7.31692800 | 0.30264700 |
| H | -1.24629000 | -6.87297100 | 0.18963900 |
| H | -3.72598400 | -6.44600600 | 0.20004300 |
| H | 3.62625400 | 6.16079000 | 0.53231300 |
| H | 1.16824900 | 6.60821300 | 0.45460500 |
| H | -1.35015100 | 7.07728900 | 0.41285700 |

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|---|-------------|-------------|------------|
| H | -7.25948500 | 0.07531300 | 0.21314300 |
| H | -6.39481800 | -2.31890300 | 0.19794100 |
| H | -5.51563900 | -4.70277400 | 0.19692400 |
| H | 3.49752800 | -6.30196100 | 0.38196700 |
| H | 5.14172500 | -4.35223300 | 0.44682800 |
| H | 6.76587400 | -2.42579000 | 0.52814800 |

Na@ V_{BN} *h*-BN

| | | | |
|----|-------------|-------------|-------------|
| Na | -0.38018000 | 1.22280100 | 0.37657300 |
| B | 1.63969100 | 0.31637400 | 0.08375800 |
| B | -0.68472800 | -1.20810700 | 0.35698500 |
| B | 1.48694400 | 2.35745700 | -0.02310700 |
| B | -1.04496600 | 3.56227800 | 0.18522800 |
| B | -3.21397900 | 2.31411000 | 0.49105700 |
| B | -3.01308900 | -0.23284600 | 0.53304900 |
| B | -2.73134000 | -2.64024000 | -0.04518200 |
| B | -0.43986400 | -3.66637100 | -0.14236100 |
| B | 1.63912900 | -2.21437600 | 0.10652300 |
| B | 3.82635300 | -0.96480100 | 0.11409500 |
| B | 3.73910200 | 1.50737300 | -0.05253600 |
| N | 3.06301300 | 0.24245100 | 0.03332000 |
| N | 2.87983800 | 2.65428200 | -0.11930500 |
| N | 3.10345000 | -2.20120300 | 0.14849300 |
| N | 0.83520100 | -0.94571200 | 0.18495500 |
| N | 1.00159400 | -3.52207100 | -0.01622000 |
| N | -1.27062900 | -2.50610100 | 0.00776700 |
| N | -1.63553200 | -0.28625700 | 0.84558100 |
| N | -3.60922600 | -1.51294900 | 0.16272100 |
| N | -3.82302400 | 0.98769000 | 0.48687500 |

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|---|-------------|-------------|-------------|
| N | -1.85033400 | 2.55929200 | 0.75443500 |
| N | 0.48944200 | 3.47655300 | -0.02422600 |
| B | 3.45629300 | 3.97000500 | -0.22778200 |
| B | 1.09351500 | 4.81764500 | -0.27597400 |
| B | -5.24481000 | 0.87728100 | 0.22821100 |
| B | -5.04090100 | -1.62005900 | -0.01915000 |
| B | 1.79989100 | -4.74388100 | -0.04766300 |
| B | 3.89364700 | -3.42361800 | 0.18319700 |
| N | 5.28229200 | -0.87837200 | 0.13749900 |
| N | 5.17401800 | 1.61532700 | -0.05964600 |
| N | -1.81857800 | 4.75475200 | -0.21246200 |
| N | -3.99827300 | 3.50160700 | 0.11543400 |
| N | -3.32273500 | -3.93796400 | -0.35318700 |
| N | -1.05156100 | -4.96719500 | -0.38608500 |
| B | 5.94874500 | 0.39905900 | 0.04889800 |
| B | -3.27488000 | 4.70788700 | -0.19049100 |
| B | -2.48204000 | -5.08863500 | -0.51481000 |
| B | 6.04570000 | -2.10409300 | 0.23183400 |
| B | -5.43087800 | 3.38307300 | -0.03133900 |
| N | 5.33077600 | -3.32889800 | 0.26282100 |
| N | -6.01797500 | 2.09125800 | 0.08328500 |
| N | -5.83369100 | -0.42911200 | 0.08485600 |
| N | 3.21790600 | -4.67128800 | 0.11790700 |
| N | 1.15771300 | -6.01340000 | -0.25218900 |
| N | -5.58304600 | -2.92239600 | -0.31756600 |
| B | 5.75979900 | 2.94023000 | -0.15985900 |
| B | -1.15076300 | 5.98193900 | -0.53153900 |
| B | -0.23870900 | -6.15589200 | -0.44901300 |

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|---|-------------|-------------|-------------|
| B | -4.76142800 | -4.06982400 | -0.47864300 |
| N | 0.26774500 | 5.97345000 | -0.49606700 |
| N | 2.51911500 | 5.02988200 | -0.31665400 |
| N | 4.89478500 | 4.07205100 | -0.24746100 |
| H | -0.72118600 | -7.22830000 | -0.64970900 |
| H | -2.96364300 | -6.15456500 | -0.74712800 |
| H | -5.25038800 | -5.13138900 | -0.72286100 |
| H | 7.13945600 | 0.45300800 | 0.06256100 |
| H | 7.23761500 | -2.08762800 | 0.27515100 |
| H | 6.94407500 | 3.08222000 | -0.17027100 |
| H | -1.74835000 | 6.97767800 | -0.80494600 |
| H | -3.87680400 | 5.69851900 | -0.47635300 |
| H | -6.10878700 | 4.33972500 | -0.26251700 |
| H | 5.86856100 | -4.18324900 | 0.31126300 |
| H | 3.75386100 | -5.52797100 | 0.11290400 |
| H | 1.72808900 | -6.84668500 | -0.28625100 |
| H | -6.58054000 | -3.03861100 | -0.42968000 |
| H | -6.82868400 | -0.49319200 | -0.08271100 |
| H | -7.01630200 | 2.02190200 | -0.05822400 |
| H | 0.73715300 | 6.84559400 | -0.69800500 |
| H | 2.84049100 | 5.98059900 | -0.43893000 |
| H | 5.32920100 | 4.98196800 | -0.31769500 |

Na@ V_{BN} *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Na | 0.44253500 | -1.26184500 | -1.96889600 |
| B | -1.55529700 | -0.36292700 | -0.05541200 |
| B | 0.64112800 | 1.09507200 | -0.08712100 |
| B | -1.39854100 | -2.26126900 | 0.13991000 |
| B | 0.99840700 | -3.38211500 | 0.19095500 |

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|---|-------------|-------------|-------------|
| B | 3.12281100 | -2.25094900 | -0.39750700 |
| B | 2.93223900 | 0.18111200 | -0.42368800 |
| B | 2.69413000 | 2.58962900 | 0.10676700 |
| B | 0.42608800 | 3.58689400 | 0.37038700 |
| B | -1.64419400 | 2.17911400 | 0.02305000 |
| B | -3.77568400 | 0.92950800 | -0.29482300 |
| B | -3.67779100 | -1.52133900 | -0.15772800 |
| N | -2.99640700 | -0.26513400 | -0.21930200 |
| N | -2.80673000 | -2.62752900 | 0.07742700 |
| N | -3.09108800 | 2.17745200 | -0.15518400 |
| N | -0.84420600 | 0.92404200 | -0.03499200 |
| N | -1.01526100 | 3.47097900 | 0.25620100 |
| N | 1.24490100 | 2.42164600 | 0.16571900 |
| N | 1.51970600 | 0.07074100 | -0.49223000 |
| N | 3.55202100 | 1.47859000 | -0.20415200 |
| N | 3.78792600 | -0.98071400 | -0.53111900 |
| N | 1.70616500 | -2.34038600 | -0.44093100 |
| N | -0.48068600 | -3.38402300 | 0.36390900 |
| B | -3.38968200 | -3.92418300 | 0.29595600 |
| B | -1.06935200 | -4.69132800 | 0.74179000 |
| B | 5.22226300 | -0.87640100 | -0.48475800 |
| B | 4.99586600 | 1.60651600 | -0.21219500 |
| B | -1.81707800 | 4.68367800 | 0.35853600 |
| B | -3.88665400 | 3.39227000 | -0.13608300 |
| N | -5.22467900 | 0.83862200 | -0.46650400 |
| N | -5.10844200 | -1.64951100 | -0.29104200 |
| N | 1.80438400 | -4.57219600 | 0.56443400 |
| N | 3.92623500 | -3.45200300 | -0.15629600 |

| | | | |
|---|-------------|-------------|-------------|
| N | 3.30295500 | 3.89097200 | 0.37180900 |
| N | 1.04079400 | 4.88274000 | 0.64787700 |
| B | -5.88284700 | -0.44555000 | -0.47761600 |
| B | 3.23447900 | -4.60540400 | 0.33959000 |
| B | 2.47331900 | 5.02094200 | 0.66730600 |
| B | -5.99313400 | 2.06223500 | -0.53042900 |
| B | 5.36817400 | -3.37355200 | -0.23445900 |
| N | -5.30648500 | 3.29548200 | -0.37122500 |
| N | 5.98270900 | -2.10559000 | -0.45394500 |
| N | 5.80495600 | 0.43778500 | -0.42633700 |
| N | -3.22908300 | 4.62523600 | 0.13046300 |
| N | -1.17716100 | 5.93018100 | 0.67965200 |
| N | 5.55193000 | 2.91596600 | 0.02489500 |
| B | -5.68605800 | -2.97245300 | -0.15344100 |
| B | 1.18555300 | -5.75490600 | 1.09229700 |
| B | 0.22639100 | 6.05801400 | 0.83332900 |
| B | 4.74224000 | 4.04384000 | 0.32411600 |
| N | -0.22784500 | -5.77227600 | 1.17397600 |
| N | -2.48253700 | -4.94491300 | 0.67398800 |
| N | -4.81977500 | -4.06603900 | 0.13853300 |
| H | 0.71607100 | 7.11504100 | 1.09255100 |
| H | 2.96394200 | 6.08078600 | 0.91014900 |
| H | 5.24468600 | 5.10666900 | 0.53547300 |
| H | -7.06551400 | -0.51147800 | -0.61810200 |
| H | -7.17461700 | 2.03972100 | -0.69830800 |
| H | -6.86206900 | -3.14181800 | -0.26800100 |
| H | 1.82519200 | -6.70385800 | 1.43209100 |
| H | 3.84290300 | -5.60032400 | 0.59677700 |

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|---|-------------|-------------|-------------|
| H | 6.04133900 | -4.35204400 | -0.09703600 |
| H | -5.85598100 | 4.14339800 | -0.39039000 |
| H | -3.76756000 | 5.47891200 | 0.17990100 |
| H | -1.74399700 | 6.75972200 | 0.78569100 |
| H | 6.55401300 | 3.04513500 | 0.01488600 |
| H | 6.81082800 | 0.53009500 | -0.38596500 |
| H | 6.99261800 | -2.07157700 | -0.45794300 |
| H | -0.67089300 | -6.61967600 | 1.50042700 |
| H | -2.80969000 | -5.87581500 | 0.89227900 |
| H | -5.24313200 | -4.97566100 | 0.26036400 |

Na@ V_{BN} *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Na | 0.44376500 | -1.26171500 | 1.96976200 |
| B | -1.55534900 | -0.36312000 | 0.05518400 |
| B | 0.64096800 | 1.09522100 | 0.08730400 |
| B | -1.39832200 | -2.26147400 | -0.14007900 |
| B | 0.99883900 | -3.38207700 | -0.19033200 |
| B | 3.12308500 | -2.25046700 | 0.39778200 |
| B | 2.93225800 | 0.18161400 | 0.42350400 |
| B | 2.69375000 | 2.58998100 | -0.10729500 |
| B | 0.42550900 | 3.58701100 | -0.37019300 |
| B | -1.64449400 | 2.17892100 | -0.02251200 |
| B | -3.77592000 | 0.92903300 | 0.29447700 |
| B | -3.67777300 | -1.52178500 | 0.15642000 |
| N | -2.99655500 | -0.26551400 | 0.21833700 |
| N | -2.80653300 | -2.62786800 | -0.07844700 |
| N | -3.09137400 | 2.17710200 | 0.15574900 |
| N | -0.84434100 | 0.92391900 | 0.03523800 |
| N | -1.01575800 | 3.47094100 | -0.25551500 |

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|---|-------------|-------------|-------------|
| N | 1.24451400 | 2.42182500 | -0.16582800 |
| N | 1.51974500 | 0.07112000 | 0.49263100 |
| N | 3.55186100 | 1.47910200 | 0.20359500 |
| N | 3.78808700 | -0.98012300 | 0.53085500 |
| N | 1.70645000 | -2.34000000 | 0.44113100 |
| N | -0.48023200 | -3.38418900 | -0.36344400 |
| B | -3.38921600 | -3.92470900 | -0.29658800 |
| B | -1.06864700 | -4.69164900 | -0.74122800 |
| B | 5.22238900 | -0.87563900 | 0.48427100 |
| B | 4.99572500 | 1.60716400 | 0.21111400 |
| B | -1.81772700 | 4.68359700 | -0.35733100 |
| B | -3.88707200 | 3.39185100 | 0.13721800 |
| N | -5.22493500 | 0.83792400 | 0.46592200 |
| N | -5.10847500 | -1.65011700 | 0.28939000 |
| N | 1.80499500 | -4.57219900 | -0.56332500 |
| N | 3.92667600 | -3.45155400 | 0.15724500 |
| N | 3.30236000 | 3.89134100 | -0.37276400 |
| N | 1.04002800 | 4.88291400 | -0.64784600 |
| B | -5.88299500 | -0.44630300 | 0.47623900 |
| B | 3.23505500 | -4.60518100 | -0.33828700 |
| B | 2.47251600 | 5.02122000 | -0.66800600 |
| B | -5.99347500 | 2.06142900 | 0.53060700 |
| B | 5.36861600 | -3.37287700 | 0.23514400 |
| N | -5.30687700 | 3.29482900 | 0.37234100 |
| N | 5.98302200 | -2.10473200 | 0.45379700 |
| N | 5.80495400 | 0.43857600 | 0.42531800 |
| N | -3.22964500 | 4.62499500 | -0.12885600 |
| N | -1.17801100 | 5.93021100 | -0.67840000 |

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|----|-------------|-------------|-------------|
| N | 5.55155300 | 2.91660800 | -0.02648300 |
| B | -5.68586000 | -2.97314300 | 0.15175000 |
| B | 1.18641800 | -5.75504300 | -1.09118000 |
| B | 0.22545400 | 6.05816200 | -0.83273800 |
| B | 4.74163600 | 4.04434100 | -0.32563400 |
| N | -0.22693800 | -5.77258100 | -1.17314600 |
| N | -2.48176700 | -4.94553400 | -0.67357700 |
| N | -4.81935400 | -4.06667100 | -0.13974200 |
| H | 0.71492600 | 7.11526100 | -1.09205100 |
| H | 2.96295500 | 6.08110700 | -0.91103900 |
| H | 5.24393200 | 5.10715200 | -0.53745100 |
| H | -7.06568100 | -0.51237100 | 0.61654700 |
| H | -7.17496800 | 2.03876800 | 0.69840400 |
| H | -6.86189700 | -3.14265000 | 0.26589900 |
| H | 1.82627900 | -6.70390400 | -1.43081200 |
| H | 3.84357400 | -5.60017100 | -0.59500200 |
| H | 6.04185500 | -4.35138800 | 0.09816800 |
| H | -5.85646600 | 4.14267300 | 0.39200000 |
| H | -3.76820100 | 5.47864200 | -0.17790300 |
| H | -1.74492300 | 6.75974700 | -0.78408900 |
| H | 6.55362200 | 3.04593400 | -0.01694100 |
| H | 6.81081600 | 0.53090700 | 0.38475800 |
| H | 6.99292700 | -2.07057200 | 0.45762700 |
| H | -0.66984700 | -6.62002600 | -1.49968000 |
| H | -2.80867700 | -5.87657500 | -0.89163500 |
| H | -5.24261600 | -4.97635000 | -0.26147500 |
| Na | 0.16846400 | -1.19271200 | 0.53994700 |

Na@ V_N *h*-BN

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|---|-------------|-------------|-------------|
| B | -1.67383200 | -0.34098300 | -0.09966500 |
| B | 1.75854200 | -1.02712700 | 1.85268900 |
| B | 0.69429600 | 1.16343000 | 0.38489700 |
| B | -1.49340800 | -2.33107400 | -0.12945700 |
| B | 1.10773800 | -3.40422700 | 0.42325700 |
| B | 3.27616000 | -2.20035300 | 0.42230900 |
| B | 3.03882100 | 0.30513300 | 0.34194500 |
| B | 2.64541600 | 2.67773700 | -0.19298400 |
| B | 0.35889100 | 3.64105200 | 0.02077000 |
| B | -1.68085300 | 2.15440700 | 0.18802300 |
| B | -3.85949600 | 0.91686400 | -0.13643800 |
| B | -3.72655800 | -1.53704300 | -0.44669300 |
| N | -3.07622200 | -0.26171500 | -0.31685000 |
| N | -2.85134800 | -2.67257200 | -0.38416500 |
| N | -3.14780000 | 2.12836400 | 0.14107900 |
| N | -0.84989600 | 0.89337000 | 0.18316900 |
| N | -1.06625300 | 3.47294500 | 0.22765000 |
| N | 1.21271000 | 2.48037000 | 0.01516900 |
| N | 1.68402200 | 0.20395200 | 0.85962700 |
| N | 3.54927900 | 1.55961700 | -0.13206800 |
| N | 3.88206100 | -0.88364400 | 0.32340900 |
| N | 1.90938800 | -2.29264900 | 0.90761600 |
| N | -0.45082800 | -3.38877100 | 0.14569900 |
| B | -3.40187300 | -3.99945300 | -0.36162000 |
| B | -1.03522800 | -4.76645000 | 0.05527100 |
| B | 5.26778400 | -0.77051900 | -0.09845200 |
| B | 4.95971600 | 1.69943500 | -0.44179700 |
| B | -1.87852300 | 4.67732400 | 0.37921900 |

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|---|-------------|-------------|-------------|
| B | -3.95630600 | 3.32477500 | 0.32877200 |
| N | -5.31107500 | 0.81487700 | -0.22152300 |
| N | -5.15438700 | -1.66652100 | -0.55078300 |
| N | 1.85675600 | -4.63150700 | 0.12616200 |
| N | 4.02023000 | -3.38354500 | 0.05215300 |
| N | 3.18479100 | 3.99290500 | -0.50390900 |
| N | 0.93088300 | 4.97214300 | -0.15137200 |
| B | -5.95053500 | -0.46100500 | -0.45209700 |
| B | 3.30022500 | -4.62300500 | 0.00794100 |
| B | 2.32707700 | 5.14009900 | -0.45432400 |
| B | -6.09296700 | 2.01330600 | -0.00604100 |
| B | 5.43344000 | -3.27854600 | -0.23849900 |
| N | -5.39406600 | 3.21640400 | 0.27482000 |
| N | 6.02767600 | -1.98517600 | -0.26403700 |
| N | 5.79478700 | 0.53411800 | -0.38333300 |
| N | -3.29446400 | 4.56504000 | 0.53475800 |
| N | -1.25156900 | 5.96918300 | 0.34192000 |
| N | 5.43913600 | 3.00952600 | -0.79330200 |
| B | -5.70862900 | -3.00823000 | -0.62672900 |
| B | 1.20897400 | -5.91023200 | 0.05154500 |
| B | 0.11743000 | 6.14988700 | 0.02760900 |
| B | 4.59240100 | 4.15107700 | -0.80850000 |
| N | -0.20224400 | -5.93156500 | 0.13359100 |
| N | -2.44504400 | -5.02101100 | -0.13574100 |
| N | -4.82708800 | -4.13033900 | -0.54142100 |
| H | 0.58119500 | 7.24340800 | -0.07989700 |
| H | 2.76690000 | 6.22980100 | -0.65394000 |
| H | 5.03597500 | 5.22724600 | -1.07168300 |

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|---|-------------|-------------|-------------|
| H | -7.13777700 | -0.52521700 | -0.53597900 |
| H | -7.28431500 | 1.99311900 | -0.05908000 |
| H | -6.88439000 | -3.17380500 | -0.73974500 |
| H | 1.82800900 | -6.92168300 | -0.06819600 |
| H | 3.88014000 | -5.64821500 | -0.17334400 |
| H | 6.08491400 | -4.25193800 | -0.46843700 |
| H | -5.94427200 | 4.05232300 | 0.41674200 |
| H | -3.84039800 | 5.40856900 | 0.64265600 |
| H | -1.82412500 | 6.79329400 | 0.45925100 |
| H | 6.41697500 | 3.14617400 | -1.00808300 |
| H | 6.76705100 | 0.61976000 | -0.64684600 |
| H | 7.00588300 | -1.92742000 | -0.51129700 |
| H | -0.65355500 | -6.83425200 | 0.08067600 |
| H | -2.73224600 | -5.99048500 | -0.13540900 |
| H | -5.24863000 | -5.04883800 | -0.55979100 |

Na@ V_N *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Na | -1.05251600 | -3.10125300 | -1.89850600 |
| B | -1.20018100 | -0.83606500 | -0.40961000 |
| B | 1.21065800 | -0.89733100 | 0.38998700 |
| B | 0.05867500 | 1.32872400 | 0.01290900 |
| B | 0.00649500 | -2.19711500 | 0.09337900 |
| B | 2.35996700 | -2.75810100 | -0.59277600 |
| B | 3.73987600 | -0.79050800 | 0.00920000 |
| B | 2.49268800 | 1.28512100 | 0.50274700 |
| B | 1.31486500 | 3.48639700 | 0.34968600 |
| B | -1.09342500 | 3.54823200 | -0.30463600 |
| B | -2.37673200 | 1.40873700 | -0.49299500 |
| B | -3.73148000 | -0.60109800 | -0.02071000 |

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|---|-------------|-------------|-------------|
| B | -2.42493900 | -2.57158500 | 0.71501600 |
| N | -2.51355600 | -1.34920600 | -0.02246900 |
| N | -1.10052900 | -3.10487200 | 0.76877400 |
| N | -3.68142700 | 0.76955800 | -0.44010900 |
| N | -1.14015900 | 0.63134600 | -0.41554900 |
| N | -2.33723300 | 2.85728300 | -0.56050100 |
| N | 0.09178800 | 2.78799200 | 0.01833000 |
| N | 1.21784000 | 0.57220900 | 0.42957100 |
| N | 2.52329500 | 2.73437400 | 0.58749500 |
| N | 3.76108300 | 0.58517300 | 0.42147200 |
| N | 2.48298600 | -1.45851100 | -0.03343400 |
| N | 1.00416100 | -3.25008700 | -0.61465400 |
| B | -1.08892600 | -4.53560200 | 0.93685000 |
| B | 0.98886700 | -4.68820500 | -0.45039100 |
| B | 5.02663000 | 1.27723500 | 0.51479700 |
| B | 3.78326100 | 3.42943900 | 0.78749700 |
| B | -3.55961700 | 3.61710300 | -0.75837800 |
| B | -4.91077300 | 1.52916200 | -0.51429800 |
| N | -4.96302400 | -1.23637000 | 0.43080000 |
| N | -3.63164300 | -3.20825600 | 1.23040900 |
| N | 3.54878500 | -3.49737500 | -0.99908100 |
| N | 4.94999600 | -1.50731200 | -0.37774000 |
| N | 1.34091300 | 4.94438400 | 0.38579800 |
| N | -1.05093200 | 5.00585700 | -0.31988600 |
| B | -4.89915500 | -2.53940800 | 1.06384100 |
| B | 4.84077500 | -2.86092500 | -0.87859000 |
| B | 0.16239900 | 5.69282700 | 0.03990700 |
| B | -6.19795400 | -0.49844900 | 0.27598100 |

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|---|-------------|-------------|-------------|
| B | 6.21797700 | -0.83000100 | -0.21863600 |
| N | -6.14605600 | 0.82962800 | -0.24481500 |
| N | 6.22688300 | 0.51624200 | 0.25647500 |
| N | 5.00759200 | 2.67894800 | 0.81622800 |
| N | -4.82086300 | 2.92852500 | -0.80586000 |
| N | -3.45911800 | 5.05023600 | -0.86171000 |
| N | 3.75195500 | 4.86537500 | 0.91234000 |
| B | -3.47728500 | -4.53685900 | 1.78289100 |
| B | 3.37756600 | -4.90505200 | -1.26664700 |
| B | -2.24625500 | 5.75619000 | -0.63264400 |
| B | 2.57347600 | 5.63159400 | 0.70474400 |
| N | 2.09463300 | -5.46563600 | -0.99181800 |
| N | -0.08782300 | -5.32208700 | 0.26238800 |
| N | -2.21004500 | -5.16622400 | 1.62089900 |
| H | -2.22407700 | 6.94878900 | -0.68390400 |
| H | 0.18933800 | 6.88552100 | 0.04950100 |
| H | 2.60693900 | 6.82302200 | 0.77627200 |
| H | -5.90334800 | -3.06050600 | 1.44601400 |
| H | -7.24621400 | -0.98401800 | 0.57957100 |
| H | -4.38738900 | -5.10966700 | 2.30303100 |
| H | 4.27756700 | -5.59133100 | -1.64915200 |
| H | 5.82721500 | -3.46169100 | -1.18296400 |
| H | 7.24567900 | -1.37955300 | -0.48172900 |
| H | -7.02072300 | 1.33171100 | -0.31194400 |
| H | -5.66786000 | 3.47615300 | -0.87427000 |
| H | -4.29153700 | 5.59455800 | -1.04005600 |
| H | 4.61016400 | 5.36606900 | 1.09628000 |
| H | 5.88144800 | 3.18003700 | 0.90089900 |

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|---|-------------|-------------|-------------|
| H | 7.12595600 | 0.97120800 | 0.33481400 |
| H | 2.01349500 | -6.47298100 | -1.02145400 |
| H | -0.07699400 | -6.32594100 | 0.38464700 |
| H | -2.13577500 | -6.13823100 | 1.88895400 |

Na@ V_N *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Na | 1.05165300 | -3.10284400 | 1.89793100 |
| B | -1.21122000 | -0.89678500 | -0.38973000 |
| B | 1.20003800 | -0.83671900 | 0.41005000 |
| B | -0.05809400 | 1.32862500 | -0.01242100 |
| B | -0.00737900 | -2.19694400 | -0.09291100 |
| B | 2.42371100 | -2.57247700 | -0.71511600 |
| B | 3.73128100 | -0.60263100 | 0.02020000 |
| B | 2.37740900 | 1.40766500 | 0.49319600 |
| B | 1.09494900 | 3.54769100 | 0.30522100 |
| B | -1.31327300 | 3.48692800 | -0.34929100 |
| B | -2.49212500 | 1.28627500 | -0.50259100 |
| B | -3.74042700 | -0.78884400 | -0.00963000 |
| B | -2.36148400 | -2.75706900 | 0.59263900 |
| N | -2.48387000 | -1.45744900 | 0.03331200 |
| N | -1.00583500 | -3.24949000 | 0.61502700 |
| N | -3.76085300 | 0.58689500 | -0.42168900 |
| N | -1.21763400 | 0.57273700 | -0.42923200 |
| N | -2.52206000 | 2.73551900 | -0.58725800 |
| N | -0.09057600 | 2.78794800 | -0.01776600 |
| N | 1.14046500 | 0.63075500 | 0.41607600 |
| N | 2.33850100 | 2.85620900 | 0.56094700 |
| N | 3.68186500 | 0.76800900 | 0.43971400 |
| N | 2.51309700 | -1.35029000 | 0.02250300 |

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|---|-------------|-------------|-------------|
| N | 1.09903300 | -3.10522100 | -0.76855400 |
| B | -0.99079500 | -4.68766200 | 0.45144400 |
| B | 1.08722800 | -4.53606100 | -0.93571700 |
| B | 4.91151500 | 1.52711500 | 0.51365800 |
| B | 3.56122800 | 3.61550400 | 0.75866800 |
| B | -3.78164600 | 3.43118800 | -0.78750000 |
| B | -5.02608500 | 1.27952400 | -0.51523700 |
| N | -4.95094600 | -1.50520700 | 0.37688900 |
| N | -3.55071400 | -3.49593400 | 0.99847600 |
| N | 3.62997300 | -3.20960100 | -1.23100500 |
| N | 4.96241000 | -1.23824800 | -0.43188800 |
| N | 1.05312600 | 5.00533400 | 0.32056200 |
| N | -1.33864300 | 4.94493400 | -0.38544600 |
| B | -4.84241400 | -2.85890100 | 0.87765200 |
| B | 4.89783100 | -2.54126300 | -1.06494700 |
| B | -0.15987200 | 5.69285800 | -0.03931100 |
| B | -6.21859300 | -0.82733600 | 0.21749500 |
| B | 6.19766800 | -0.50079800 | -0.27744500 |
| N | -6.22674300 | 0.51900400 | -0.25737800 |
| N | 6.14646700 | 0.82721800 | 0.24358900 |
| N | 4.82222100 | 2.92644200 | 0.80562100 |
| N | -5.00635400 | 2.68128300 | -0.81640100 |
| N | -3.74965600 | 4.86709500 | -0.91240700 |
| N | 3.46133100 | 5.04865600 | 0.86235600 |
| B | -3.38006200 | -4.90361000 | 1.26629000 |
| B | 3.47510000 | -4.53831800 | -1.78299100 |
| B | -2.57083000 | 5.63273300 | -0.70457500 |
| B | 2.24875400 | 5.75514400 | 0.63340500 |

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|---|-------------|-------------|-------------|
| N | 2.20778500 | -5.16735100 | -1.62006300 |
| N | 0.08657700 | -5.32207600 | -0.25990000 |
| N | -2.09713600 | -5.46463300 | 0.99225100 |
| H | -2.60371000 | 6.82417600 | -0.77613000 |
| H | -0.18629700 | 6.88556300 | -0.04885700 |
| H | 2.22703800 | 6.94774400 | 0.68485700 |
| H | -5.82917600 | -3.45932800 | 1.18164300 |
| H | -7.24662100 | -1.37645100 | 0.48021200 |
| H | -4.28047100 | -5.58960600 | 1.64834400 |
| H | 4.38477900 | -5.11148500 | -2.30347000 |
| H | 5.90169000 | -3.06272600 | -1.44748000 |
| H | 7.24562300 | -0.98670500 | -0.58154700 |
| H | -7.12558700 | 0.97439700 | -0.33587600 |
| H | -5.87996900 | 3.18274600 | -0.90131400 |
| H | -4.60761100 | 5.36816300 | -1.09649100 |
| H | 4.29399600 | 5.59260800 | 1.04068400 |
| H | 5.66944400 | 3.47373500 | 0.87393000 |
| H | 7.02133000 | 1.32899200 | 0.31045700 |
| H | 2.13311900 | -6.13945900 | -1.88762700 |
| H | 0.07571500 | -6.32600700 | -0.38158100 |
| H | -2.01636400 | -6.47200300 | 1.02211000 |

Na⁺@ V_N *h*-BN

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|----|-------------|-------------|-------------|
| Na | -0.17803300 | -1.18876500 | -0.56146200 |
| B | -1.94267400 | -0.97558400 | -1.63249700 |
| B | 1.67100400 | -0.36512400 | 0.08119500 |
| B | -0.64144300 | 1.20690800 | -0.41074100 |
| B | 1.45410700 | -2.36901800 | 0.09708200 |
| B | 3.68580800 | -1.60591700 | 0.46833500 |

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|---|-------------|-------------|-------------|
| B | 3.87288200 | 0.85354300 | 0.16803500 |
| B | 1.73347600 | 2.14363300 | -0.21066600 |
| B | -0.27874600 | 3.66812700 | -0.08176600 |
| B | -2.58897500 | 2.74144300 | 0.17240700 |
| B | -3.05845200 | 0.37693200 | -0.29430700 |
| B | -3.34481100 | -2.15853300 | -0.38911900 |
| B | -1.14172500 | -3.41940200 | -0.48098500 |
| N | -1.97145900 | -2.26464900 | -0.93230000 |
| N | 0.38404400 | -3.40983300 | -0.21500200 |
| N | -3.89027300 | -0.81981600 | -0.25717000 |
| N | -1.69835900 | 0.24676400 | -0.86648000 |
| N | -3.51586300 | 1.63065700 | 0.16499900 |
| N | -1.15899300 | 2.50851300 | -0.06774400 |
| N | 0.86219700 | 0.88618000 | -0.22390700 |
| N | 1.13805700 | 3.46350900 | -0.27390100 |
| N | 3.18722700 | 2.07595900 | -0.13030700 |
| N | 3.05615600 | -0.31549500 | 0.32475500 |
| N | 2.78647600 | -2.73007000 | 0.37506500 |
| B | 0.95722000 | -4.80881700 | -0.12737800 |
| B | 3.32222500 | -4.07079000 | 0.36331600 |
| B | 4.02978400 | 3.26120100 | -0.30172400 |
| B | 1.98123900 | 4.65821600 | -0.42171200 |
| B | -4.92370300 | 1.79640800 | 0.51565900 |
| B | -5.28436100 | -0.68107700 | 0.19860900 |
| N | -4.07736400 | -3.32847000 | -0.03662900 |
| N | -1.92945200 | -4.60924000 | -0.22437400 |
| N | 5.09809200 | -1.76052000 | 0.60711000 |
| N | 5.31056200 | 0.71995900 | 0.28989400 |

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|---|-------------|-------------|-------------|
| N | -0.83568200 | 4.99849300 | 0.05965600 |
| N | -3.09942800 | 4.05799600 | 0.46249300 |
| B | -3.37389500 | -4.58382500 | -0.06306300 |
| B | 5.92344600 | -0.56671200 | 0.53674100 |
| B | -2.22521100 | 5.19848700 | 0.36977700 |
| B | -5.48712700 | -3.19759100 | 0.30592400 |
| B | 6.12686200 | 1.90527800 | 0.09630800 |
| N | -6.04399100 | -1.88920100 | 0.36909600 |
| N | 5.45751400 | 3.11987200 | -0.20641400 |
| N | 3.39402700 | 4.50949200 | -0.53629200 |
| N | -5.76610900 | 0.63100000 | 0.49311500 |
| N | -5.36331300 | 3.11412100 | 0.84991300 |
| N | 1.37001000 | 5.95461800 | -0.42103200 |
| B | -1.30357200 | -5.91500800 | -0.18550300 |
| B | 5.63197100 | -3.11320700 | 0.69724400 |
| B | -4.49803600 | 4.24620500 | 0.80773100 |
| B | 0.00130000 | 6.16669300 | -0.13354400 |
| N | 4.73170800 | -4.22118000 | 0.58110900 |
| N | 2.35014600 | -5.07358900 | 0.10129800 |
| N | 0.10296900 | -5.95225400 | -0.25616100 |
| H | -4.91532600 | 5.33217800 | 1.05532100 |
| H | -2.65107300 | 6.29436300 | 0.54337600 |
| H | -0.45191100 | 7.26368300 | -0.05589800 |
| H | -3.96338200 | -5.60184700 | 0.09553800 |
| H | -6.14495200 | -4.16049500 | 0.53686500 |
| H | -1.95060000 | -6.90788900 | -0.10906000 |
| H | 6.79796700 | -3.29639000 | 0.84374600 |
| H | 7.10316900 | -0.65515300 | 0.65434200 |

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|---|-------------|-------------|-------------|
| H | 7.31238800 | 1.85753400 | 0.18349000 |
| H | -7.01548500 | -1.82132500 | 0.64315100 |
| H | -6.73139700 | 0.73534600 | 0.77808300 |
| H | -6.33040700 | 3.27911700 | 1.09444000 |
| H | 1.95530200 | 6.76979300 | -0.54331900 |
| H | 3.96125700 | 5.33989300 | -0.64096600 |
| H | 6.03146200 | 3.94280100 | -0.33338900 |
| H | 5.14181200 | -5.14519900 | 0.61086800 |
| H | 2.62709700 | -6.04673000 | 0.10617700 |
| H | 0.53717500 | -6.86531800 | -0.22899600 |

Na⁺@ V_N *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Na | 1.65714800 | -1.41948100 | -2.35154400 |
| B | -0.76277400 | -1.27340300 | -0.54141000 |
| B | 1.43327300 | -0.13898700 | 0.09696500 |
| B | -0.78333400 | 1.15773500 | -0.02877100 |
| B | 1.48756400 | -2.09605900 | 0.29591200 |
| B | 3.65068300 | -1.10999300 | -0.31745200 |
| B | 3.51305900 | 1.35079900 | -0.28128000 |
| B | 1.33311900 | 2.41019600 | 0.25631200 |
| B | -0.87399000 | 3.60899200 | 0.42711100 |
| B | -2.99218700 | 2.35824600 | -0.05565100 |
| B | -2.92381300 | -0.10019700 | -0.45634400 |
| B | -2.83870600 | -2.57745200 | -0.28571900 |
| B | -0.63559000 | -3.55466300 | 0.41326300 |
| N | -1.37361100 | -2.51040600 | -0.24729400 |
| N | 0.78160100 | -3.32807200 | 0.64509300 |
| N | -3.58669200 | -1.37660000 | -0.52677900 |
| N | -1.45477700 | -0.05180800 | -0.43993900 |

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|---|-------------|-------------|-------------|
| N | -3.67055000 | 1.11670500 | -0.35650700 |
| N | -1.54737000 | 2.36350700 | 0.12221700 |
| N | 0.65388300 | 1.09253700 | 0.18886000 |
| N | 0.57201700 | 3.61888300 | 0.47215600 |
| N | 2.76219400 | 2.51560100 | 0.05828900 |
| N | 2.82655600 | 0.06559100 | -0.31808600 |
| N | 2.89191600 | -2.30848900 | -0.08720600 |
| B | 1.54177900 | -4.54487200 | 1.00254600 |
| B | 3.65292100 | -3.53020200 | 0.17033600 |
| B | 3.44769300 | 3.80130900 | 0.16207100 |
| B | 1.25466000 | 4.89813100 | 0.65465700 |
| B | -5.12499200 | 1.07850100 | -0.46934900 |
| B | -5.04524200 | -1.43230400 | -0.57977200 |
| N | -3.49458500 | -3.83605600 | -0.03258800 |
| N | -1.32158100 | -4.77247600 | 0.77997700 |
| N | 5.06166500 | -1.09128600 | -0.56657400 |
| N | 4.94344000 | 1.39947100 | -0.53472000 |
| N | -1.64286000 | 4.82000400 | 0.62044400 |
| N | -3.74938100 | 3.58087200 | 0.09922400 |
| B | -2.73457500 | -4.93573300 | 0.50336800 |
| B | 5.71601900 | 0.19580100 | -0.70621300 |
| B | -3.07656100 | 4.80565500 | 0.45813500 |
| B | -4.93805200 | -3.91955300 | -0.20406400 |
| B | 5.61867000 | 2.68941300 | -0.47126800 |
| N | -5.65704000 | -2.73310900 | -0.52007100 |
| N | 4.85804900 | 3.83433700 | -0.12134400 |
| N | 2.68168800 | 4.94551200 | 0.52599200 |
| N | -5.76342100 | -0.19655300 | -0.64625200 |

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|---|-------------|-------------|-------------|
| N | -5.83132500 | 2.32259800 | -0.36944100 |
| N | 0.46312400 | 6.06255700 | 0.92911300 |
| B | -0.57562600 | -5.84907200 | 1.39572600 |
| B | 5.78307400 | -2.35265700 | -0.51699200 |
| B | -5.19056400 | 3.56028700 | -0.07642400 |
| B | -0.95839100 | 6.06461400 | 0.91109800 |
| N | 5.05232600 | -3.52615900 | -0.16692700 |
| N | 2.95648500 | -4.60212500 | 0.78398500 |
| N | 0.83148300 | -5.68704200 | 1.50039800 |
| H | -5.82782300 | 4.56021200 | 0.02989600 |
| H | -3.70211500 | 5.80592900 | 0.61108700 |
| H | -1.56928100 | 7.06629600 | 1.11192700 |
| H | -3.26643300 | -5.97184600 | 0.74350200 |
| H | -5.50279200 | -4.95834000 | -0.06713000 |
| H | -1.11168100 | -6.84328000 | 1.76792800 |
| H | 6.95023200 | -2.39991700 | -0.74136300 |
| H | 6.88248200 | 0.24699800 | -0.93046400 |
| H | 6.78456900 | 2.77148800 | -0.69608100 |
| H | -6.66231300 | -2.81231800 | -0.59659700 |
| H | -6.77371500 | -0.22494300 | -0.68834200 |
| H | -6.83783500 | 2.33506000 | -0.46426300 |
| H | 0.92598900 | 6.94489000 | 1.10063600 |
| H | 3.14698300 | 5.83791500 | 0.62473300 |
| H | 5.34854900 | 4.71724900 | -0.07116500 |
| H | 5.58299600 | -4.38112600 | -0.06251600 |
| H | 3.44754500 | -5.45467800 | 1.01835900 |
| H | 1.36279300 | -6.47388500 | 1.84875900 |

Na⁺@ V_N *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Na | -1.39811400 | -2.30879300 | 2.29740800 |
| B | -1.46165800 | -0.06485900 | -0.12197200 |
| B | 0.72371500 | -1.28278300 | 0.49886500 |
| B | 0.78596000 | 1.16804100 | 0.04952700 |
| B | -1.51497200 | -2.01844300 | -0.26148000 |
| B | 0.56213500 | -3.53805400 | -0.48569100 |
| B | 2.79078800 | -2.61090600 | 0.19090600 |
| B | 2.90334000 | -0.14218500 | 0.44872300 |
| B | 3.01687400 | 2.32785900 | 0.13715200 |
| B | 0.93212000 | 3.62808900 | -0.35909600 |
| B | -1.30023000 | 2.46991000 | -0.28175100 |
| B | -3.51303200 | 1.45083500 | 0.18167100 |
| B | -3.65727600 | -1.00256200 | 0.38232100 |
| N | -2.85316300 | 0.16161300 | 0.21988100 |
| N | -2.90122600 | -2.22734600 | 0.22248400 |
| N | -2.73334500 | 2.60120500 | -0.14552000 |
| N | -0.64533300 | 1.13978300 | -0.19684700 |
| N | -0.50947700 | 3.66696400 | -0.45639000 |
| N | 1.57555900 | 2.36343000 | -0.05929600 |
| N | 1.43375900 | -0.06992800 | 0.42857000 |
| N | 3.67195900 | 1.06393000 | 0.39968300 |
| N | 3.55264900 | -1.43052600 | 0.47005000 |
| N | 1.32842100 | -2.52223100 | 0.18072000 |
| N | -0.86090800 | -3.28433900 | -0.63581400 |
| B | -3.69760900 | -3.43504500 | -0.00671300 |
| B | -1.65598800 | -4.48634900 | -0.96425400 |
| B | 5.01020700 | -1.51086000 | 0.51454100 |

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|---|-------------|-------------|-------------|
| B | 5.12513700 | 0.99875200 | 0.51837400 |
| B | -1.16403400 | 4.95958200 | -0.65012800 |
| B | -3.39329400 | 3.89702700 | -0.26001600 |
| N | -4.94179400 | 1.52624000 | 0.43797800 |
| N | -5.06466500 | -0.95931000 | 0.65485600 |
| N | 1.21445400 | -4.75557100 | -0.90542900 |
| N | 3.42095200 | -3.87052300 | -0.12107500 |
| N | 3.79851500 | 3.54066100 | 0.03314000 |
| N | 1.72793300 | 4.82929600 | -0.50480800 |
| B | -5.71387700 | 0.33981200 | 0.69912300 |
| B | 2.63518300 | -4.94102600 | -0.67879800 |
| B | 3.15484000 | 4.78707000 | -0.30468600 |
| B | -5.59603200 | 2.82340900 | 0.33707200 |
| B | 4.86612400 | -3.97941000 | 0.02818000 |
| N | -4.81207300 | 3.95082500 | -0.02279900 |
| N | 5.60211800 | -2.81748100 | 0.39006200 |
| N | 5.74625100 | -0.29209000 | 0.63890800 |
| N | -2.59398600 | 5.03153700 | -0.58405900 |
| N | -0.34227300 | 6.11488900 | -0.87276000 |
| N | 5.85316200 | 2.23282500 | 0.47827500 |
| B | -5.79457900 | -2.21096700 | 0.69867300 |
| B | 0.42153400 | -5.80726400 | -1.50611800 |
| B | 1.07627200 | 6.09124100 | -0.79742500 |
| B | 5.23576900 | 3.49132600 | 0.22673400 |
| N | -0.98873900 | -5.62705800 | -1.52273300 |
| N | -3.05029400 | -4.52832100 | -0.64293400 |
| N | -5.08018000 | -3.40988500 | 0.38810800 |
| H | 1.71243200 | 7.08501600 | -0.95542300 |

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|---|-------------|-------------|-------------|
| H | 3.80128000 | 5.77989900 | -0.41321900 |
| H | 5.89030100 | 4.48391000 | 0.16693000 |
| H | -6.87967600 | 0.40858700 | 0.92427900 |
| H | -6.76364300 | 2.92918500 | 0.54410100 |
| H | -6.95570300 | -2.24216700 | 0.95515400 |
| H | 0.92183100 | -6.79875200 | -1.93115000 |
| H | 3.14719600 | -5.97407400 | -0.96995900 |
| H | 5.41527800 | -5.01837800 | -0.16079100 |
| H | -5.28768800 | 4.84055300 | -0.09142700 |
| H | -3.03811300 | 5.93409500 | -0.68755300 |
| H | -0.78322800 | 7.00772600 | -1.04744900 |
| H | 6.85861600 | 2.22403500 | 0.58368200 |
| H | 6.75605500 | -0.33564100 | 0.67904300 |
| H | 6.60689900 | -2.91287100 | 0.45438500 |
| H | -1.54891200 | -6.40000200 | -1.85711300 |
| H | -3.57479500 | -5.36526100 | -0.86106600 |
| H | -5.62389900 | -4.26046200 | 0.32165200 |

Na@ V_{N2B} *h*-BN

| | | | |
|----|-------------|-------------|-------------|
| Na | -0.04323000 | 1.29455800 | 0.25919300 |
| B | -1.38858100 | -0.53885800 | 0.10696900 |
| B | 1.43099300 | -0.43878400 | 0.11287800 |
| B | 0.09814600 | -2.61713900 | -0.18992600 |
| B | 2.59919900 | -2.71241000 | 0.05844800 |
| B | 3.83909800 | -0.59995200 | 0.37848600 |
| B | 2.42196100 | 1.34442500 | 0.17435800 |
| B | 1.05040000 | 3.67199200 | 0.08427100 |
| B | -1.29832900 | 3.59601000 | 0.17215700 |
| B | -2.50410500 | 1.17265800 | 0.26641200 |

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|---|-------------|-------------|-------------|
| B | -3.78303900 | -0.87616500 | 0.33189100 |
| B | -2.40125400 | -2.87477300 | -0.12195500 |
| N | -2.47614000 | -1.46508900 | 0.12040300 |
| N | 0.04273900 | -1.09655000 | 0.00315100 |
| N | -1.10133800 | -3.43649400 | -0.34424300 |
| N | -3.79298800 | 0.54147700 | 0.42269600 |
| N | -2.48064700 | 2.62731000 | 0.18053100 |
| N | -0.08845900 | 3.25677000 | 0.76288500 |
| N | 2.29327500 | 2.78796000 | 0.02725800 |
| N | 3.75511600 | 0.81700100 | 0.33907000 |
| N | 2.57537100 | -1.28868400 | 0.20887500 |
| N | 1.35289300 | -3.36458300 | -0.21854100 |
| B | -1.05003700 | -4.86571400 | -0.64365300 |
| B | 1.41347100 | -4.79930300 | -0.48810400 |
| B | 4.96801100 | 1.60081100 | 0.38595000 |
| B | 3.53968200 | 3.56226400 | -0.15774600 |
| B | -3.78504400 | 3.32099500 | 0.10070600 |
| B | -5.05564200 | 1.23292300 | 0.54888300 |
| N | -4.98728500 | -1.66462800 | 0.41285400 |
| N | -3.62192100 | -3.67122800 | -0.13713800 |
| N | 3.86443300 | -3.42861500 | 0.16199600 |
| N | 5.09060100 | -1.29631400 | 0.54064900 |
| N | 1.05404300 | 4.94900800 | -0.66688100 |
| N | -1.44093000 | 4.87761300 | -0.55752900 |
| B | -4.90178100 | -3.07713300 | 0.16594700 |
| B | 5.09636700 | -2.72929500 | 0.44030600 |
| B | -0.22521300 | 5.57231300 | -0.90262300 |
| B | -6.24743600 | -0.98249800 | 0.65486400 |

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|---|-------------|-------------|-------------|
| B | 6.30314400 | -0.51151600 | 0.70328100 |
| N | -6.24641600 | 0.43546600 | 0.73790500 |
| N | 6.21071800 | 0.90438100 | 0.63152200 |
| N | 4.82878200 | 2.98634600 | 0.13105300 |
| N | -5.01615000 | 2.64134300 | 0.41508500 |
| N | -3.85349500 | 4.69684000 | -0.30998200 |
| N | 3.48739500 | 4.91625200 | -0.63712500 |
| B | -3.55104200 | -5.07214900 | -0.47753200 |
| B | 3.89640800 | -4.85073200 | -0.08256700 |
| B | -2.73056000 | 5.45974100 | -0.74854500 |
| B | 2.28480800 | 5.59838900 | -0.98838000 |
| N | 2.67721700 | -5.48306600 | -0.43149800 |
| N | 0.21375400 | -5.49990800 | -0.78856200 |
| N | -2.27246800 | -5.61452500 | -0.75835600 |
| H | -2.88297900 | 6.54344200 | -1.22939500 |
| H | -0.27901100 | 6.65353900 | -1.41075500 |
| H | 2.32732900 | 6.67570900 | -1.50466100 |
| H | -5.88171400 | -3.75468200 | 0.19526700 |
| H | -7.26058900 | -1.60292400 | 0.76498800 |
| H | -4.53043200 | -5.75057700 | -0.52288700 |
| H | 4.91138400 | -5.47159300 | -0.00625200 |
| H | 6.11353200 | -3.33852700 | 0.56067000 |
| H | 7.35419800 | -1.04952100 | 0.87454900 |
| H | -7.13504900 | 0.89766000 | 0.87272100 |
| H | -5.87294500 | 3.17758400 | 0.41030400 |
| H | -4.76827400 | 5.11652200 | -0.40146900 |
| H | 4.36272200 | 5.38989700 | -0.81239000 |
| H | 5.64426000 | 3.57991800 | 0.06649400 |

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|---|-------------|-------------|-------------|
| H | 7.06741900 | 1.43431400 | 0.71313900 |
| H | 2.69542700 | -6.47752200 | -0.61002000 |
| H | 0.25177300 | -6.49239300 | -0.97423600 |
| H | -2.21633500 | -6.59804300 | -0.98359800 |

Na@ V_{N2B} *h*-BN (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Na | 0.00002500 | 0.00006700 | 0.00063000 |
| B | 0.00000000 | 0.00000000 | 2.42558799 |
| B | 2.29448667 | 0.00000000 | 0.79674153 |
| B | 2.24606720 | -1.03208340 | 3.15138617 |
| B | 4.43306245 | -0.85565306 | 1.91962986 |
| B | 4.43117699 | 0.11132149 | -0.35458783 |
| B | 2.21235750 | 0.58940655 | -1.15196444 |
| B | -0.15847680 | 1.25680100 | -2.26641509 |
| B | -2.06155629 | 1.34719853 | -0.88795874 |
| B | -1.78978077 | 0.68759239 | 1.72507446 |
| B | -1.79115780 | 0.08075838 | 4.05642711 |
| B | 0.31323913 | -1.01171128 | 4.75972471 |
| N | -0.42664476 | -0.30581486 | 3.75963029 |
| N | 1.45705122 | -0.33070998 | 2.04179023 |
| N | 1.64101308 | -1.43052307 | 4.42081303 |
| N | -2.51733690 | 0.62574872 | 2.96321115 |
| N | -2.55001588 | 1.02670930 | 0.52476831 |
| N | -0.74708367 | 1.74720574 | -1.10351577 |
| N | 1.32099466 | 0.87609520 | -2.27344223 |
| N | 3.61934893 | 0.53365706 | -1.44012700 |
| N | 3.70744820 | -0.23070486 | 0.85049886 |
| N | 3.67399133 | -1.32118756 | 3.04267401 |
| B | 2.36743188 | -2.18457569 | 5.44447100 |

| | | | |
|---|-------------|-------------|-------------|
| B | 4.41656431 | -2.04882756 | 4.07330132 |
| B | 4.23093928 | 0.78083328 | -2.72032916 |
| B | 1.91837534 | 0.90240828 | -3.63055230 |
| B | -4.01722424 | 1.16813476 | 0.66766431 |
| B | -3.91158357 | 0.95405198 | 3.13623662 |
| N | -2.37658387 | -0.10610439 | 5.35905452 |
| N | -0.29824753 | -1.28491931 | 6.05480383 |
| N | 5.87533851 | -1.02389785 | 1.81068538 |
| N | 5.86747458 | -0.00207164 | -0.46260117 |
| N | -0.96384249 | 0.94697889 | -3.48335545 |
| N | -2.97712669 | 1.05864304 | -2.02050821 |
| B | -1.61914007 | -0.79841703 | 6.36612271 |
| B | 6.59009842 | -0.56083353 | 0.64675342 |
| B | -2.39589232 | 0.92969561 | -3.32904102 |
| B | -3.74438986 | 0.35039835 | 5.57802335 |
| B | 6.50012065 | 0.37884752 | -1.71355836 |
| N | -4.46443148 | 0.88087801 | 4.47455148 |
| N | 5.67437544 | 0.76319640 | -2.80391472 |
| N | 3.34501189 | 0.96833905 | -3.81207574 |
| N | -4.63388030 | 1.25885365 | 1.96505744 |
| N | -4.86671605 | 1.21106095 | -0.49381630 |
| N | 1.08091781 | 0.87305036 | -4.80139455 |
| B | 0.41827354 | -2.06667095 | 7.02866868 |
| B | 6.59216852 | -1.72344629 | 2.85356545 |
| B | -4.39759639 | 1.04472513 | -1.82995581 |
| B | -0.34382148 | 0.79493122 | -4.75996197 |
| N | 5.83619818 | -2.22988180 | 3.93312613 |
| N | 3.72381808 | -2.54083084 | 5.21280941 |

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|---|-------------|-------------|-------------|
| N | 1.71538266 | -2.51557877 | 6.68280900 |
| H | -5.16972552 | 0.91959166 | -2.73175155 |
| H | -3.09582128 | 0.77670129 | -4.28619359 |
| H | -0.96776517 | 0.63889328 | -5.76317394 |
| H | -2.08190788 | -0.98766070 | 7.44759354 |
| H | -4.24947445 | 0.25638309 | 6.65343336 |
| H | -0.05610004 | -2.31986969 | 8.09315121 |
| H | 7.77392958 | -1.86957112 | 2.80388172 |
| H | 7.78071066 | -0.66874156 | 0.59196360 |
| H | 7.68523693 | 0.34152816 | -1.82620936 |
| H | -5.42327810 | 1.15354712 | 4.62918814 |
| H | -5.63688945 | 1.42248239 | 2.01142367 |
| H | -5.86495643 | 1.24654784 | -0.34561214 |
| H | 1.53204838 | 0.82246421 | -5.70501050 |
| H | 3.70207493 | 1.07118558 | -4.75313382 |
| H | 6.12610160 | 0.98376104 | -3.67941351 |
| H | 6.33316011 | -2.72328516 | 4.66350993 |
| H | 4.23494530 | -3.04064885 | 5.92885343 |
| H | 2.22958909 | -3.05028335 | 7.37151081 |

Na@ V_{N2B} *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Na | -0.46430200 | -3.29440100 | 2.71431500 |
| B | 1.32444000 | 0.49994500 | -0.17261800 |
| B | -1.35729000 | 0.33392300 | -0.09413300 |
| B | -0.13426600 | 2.53879700 | 0.25104900 |
| B | -2.59764900 | 2.51873900 | 0.57744200 |
| B | -3.76056000 | 0.56734500 | -0.32005200 |
| B | -2.21536700 | -1.19494300 | -0.59044100 |
| B | -0.92291900 | -3.26551900 | -0.00567900 |

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|---|-------------|-------------|-------------|
| B | 1.28556700 | -3.07980100 | 0.75214400 |
| B | 2.43249400 | -0.95477500 | 0.01315200 |
| B | 3.63306200 | 0.94421600 | -0.76959800 |
| B | 2.21070400 | 2.91002700 | -0.51230800 |
| N | 2.31931300 | 1.49341800 | -0.58578000 |
| N | -0.05172000 | 1.04469500 | 0.03097200 |
| N | 0.98864100 | 3.44300400 | 0.01357100 |
| N | 3.71617300 | -0.43820400 | -0.44332500 |
| N | 2.51173500 | -2.31425700 | 0.53087400 |
| N | 0.01936800 | -2.48617300 | 0.68101000 |
| N | -2.08192700 | -2.63740500 | -0.64749500 |
| N | -3.57663500 | -0.73670500 | -0.85083900 |
| N | -2.54106400 | 1.17475600 | 0.12779800 |
| N | -1.35192200 | 3.21260500 | 0.70366000 |
| B | 0.93122200 | 4.87044200 | 0.27852700 |
| B | -1.40668300 | 4.62103300 | 1.05053000 |
| B | -4.70137700 | -1.52281400 | -1.25525400 |
| B | -3.16303900 | -3.46518400 | -1.17309300 |
| B | 3.79931900 | -2.99561100 | 0.65124300 |
| B | 4.99603600 | -1.08012200 | -0.38078300 |
| N | 4.78504200 | 1.72920200 | -1.14858800 |
| N | 3.35294900 | 3.75263700 | -0.87249800 |
| N | -3.89647300 | 3.15680600 | 0.80905000 |
| N | -5.05849100 | 1.19466500 | -0.21253300 |
| N | -0.82594300 | -4.76570500 | -0.04214900 |
| N | 1.40768600 | -4.55346300 | 1.03263100 |
| B | 4.61853100 | 3.15856800 | -1.23883900 |
| B | -5.11886600 | 2.49478100 | 0.41024700 |

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|---|-------------|-------------|-------------|
| B | 0.32330500 | -5.38416500 | 0.55916700 |
| B | 6.06230500 | 1.04637400 | -1.23307900 |
| B | -6.19613900 | 0.44768100 | -0.71814900 |
| N | 6.13891600 | -0.33018700 | -0.86003500 |
| N | -5.99439100 | -0.86492500 | -1.24857200 |
| N | -4.43032800 | -2.89350900 | -1.55942000 |
| N | 5.01959500 | -2.38519900 | 0.19896600 |
| N | 3.83745500 | -4.32522600 | 1.23052000 |
| N | -2.96927200 | -4.89755300 | -1.23795000 |
| B | 3.24315800 | 5.18034400 | -0.68940700 |
| B | -3.91142400 | 4.50387500 | 1.32815700 |
| B | 2.68659200 | -5.14318000 | 1.35248500 |
| B | -1.84763600 | -5.56119600 | -0.67553200 |
| N | -2.66804800 | 5.17862400 | 1.47976000 |
| N | -0.23144700 | 5.41799400 | 0.90291300 |
| N | 2.05318800 | 5.69249500 | -0.10394200 |
| H | 2.78152900 | -6.28771400 | 1.69030100 |
| H | 0.39081300 | -6.57450200 | 0.66758100 |
| H | -1.77122700 | -6.75518300 | -0.71042000 |
| H | 5.53393600 | 3.85258900 | -1.56261500 |
| H | 7.04467800 | 1.63158000 | -1.57945800 |
| H | 4.13409300 | 5.91471200 | -0.99450700 |
| H | -4.93640800 | 5.05185600 | 1.60379600 |
| H | -6.17117200 | 3.03234100 | 0.58163900 |
| H | -7.29502700 | 0.91653600 | -0.68246700 |
| H | 7.05116900 | -0.76463300 | -0.88221400 |
| H | 5.88603700 | -2.89839200 | 0.28474000 |
| H | 4.73775300 | -4.75507800 | 1.39306100 |

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|---|-------------|-------------|-------------|
| H | -3.69571300 | -5.46894500 | -1.64680500 |
| H | -5.16998000 | -3.51351100 | -1.85991700 |
| H | -6.81557000 | -1.36525700 | -1.55992700 |
| H | -2.69493800 | 6.14153200 | 1.78534400 |
| H | -0.27378800 | 6.40927000 | 1.09454000 |
| H | 1.99673900 | 6.69056400 | 0.04377500 |

Na⁺@ V_{N2B} *h*-BN

| | | | |
|----|-------------|-------------|-------------|
| Na | -0.31007800 | 1.20903400 | -0.30925000 |
| B | -1.20990100 | -0.86222000 | 0.02330100 |
| B | 1.48955300 | -0.16037400 | -0.00056000 |
| B | 0.67684200 | -2.58298500 | -0.19785400 |
| B | 3.13556000 | -2.09473500 | -0.22518400 |
| B | 3.86490800 | 0.21983300 | 0.24596800 |
| B | 2.04626000 | 1.78352700 | 0.12835300 |
| B | 0.32455300 | 3.77902900 | -0.43213400 |
| B | -2.08380900 | 3.12688300 | -0.68739300 |
| B | -2.66724100 | 0.55858300 | -0.07804600 |
| B | -3.46140500 | -1.66350600 | 0.40432500 |
| B | -1.67588700 | -3.36184700 | 0.19908700 |
| N | -2.06080000 | -1.97417000 | 0.23993500 |
| N | 0.28904400 | -1.08584200 | -0.08118100 |
| N | -0.30708800 | -3.64555100 | -0.10783500 |
| N | -3.77908400 | -0.27311000 | 0.23771700 |
| N | -2.95941200 | 1.99718000 | -0.35459000 |
| N | -0.71356100 | 3.04735300 | -1.11563100 |
| N | 1.58297100 | 3.20024800 | 0.04809400 |
| N | 3.43152700 | 1.58056600 | 0.38408500 |
| N | 2.79307300 | -0.71807600 | 0.01454000 |

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|---|-------------|-------------|-------------|
| N | 2.05018000 | -3.01231700 | -0.38955000 |
| B | 0.04539600 | -5.05874200 | -0.29274700 |
| B | 2.40963500 | -4.41341700 | -0.63607000 |
| B | 4.42326500 | 2.59743900 | 0.67277200 |
| B | 2.58074800 | 4.25672100 | 0.43363000 |
| B | -4.39961100 | 2.42148800 | -0.27120200 |
| B | -5.16832100 | 0.13079000 | 0.33963200 |
| N | -4.45141800 | -2.65845000 | 0.68067100 |
| N | -2.67487200 | -4.38739700 | 0.42339000 |
| N | 4.53112500 | -2.48374500 | -0.27834000 |
| N | 5.24011300 | -0.16668700 | 0.31199000 |
| N | -0.06404400 | 5.17526700 | -0.29341200 |
| N | -2.47047500 | 4.53179900 | -0.62990500 |
| B | -4.04738300 | -4.04642600 | 0.70429400 |
| B | 5.58196900 | -1.54088100 | 0.01743500 |
| B | -1.45166500 | 5.54801000 | -0.47236700 |
| B | -5.83423200 | -2.24298300 | 0.84525900 |
| B | 6.23316500 | 0.84773700 | 0.62520000 |
| N | -6.14568800 | -0.86159700 | 0.67768100 |
| N | 5.78934800 | 2.18929000 | 0.82421000 |
| N | 3.92603800 | 3.92439900 | 0.76945600 |
| N | -5.42915900 | 1.50134800 | 0.07786700 |
| N | -4.77404900 | 3.78370000 | -0.54573400 |
| N | 2.20127100 | 5.64355000 | 0.44066600 |
| B | -2.29765200 | -5.78122600 | 0.28509200 |
| B | 4.86483800 | -3.85488800 | -0.61395800 |
| B | -3.87808700 | 4.86954800 | -0.65469100 |
| B | 0.92401800 | 6.15015200 | 0.11565900 |

| | | | |
|---|-------------|-------------|-------------|
| N | 3.79138700 | -4.75803900 | -0.81774300 |
| N | 1.37970400 | -5.39247400 | -0.65088200 |
| N | -0.96227300 | -6.06181900 | -0.09695600 |
| H | -4.24610200 | 5.99620500 | -0.74136000 |
| H | -1.76932500 | 6.69057700 | -0.40606800 |
| H | 0.66264500 | 7.30771800 | 0.18216900 |
| H | -4.84683300 | -4.89729200 | 0.92740400 |
| H | -6.68348500 | -3.03550300 | 1.10023200 |
| H | -3.08529400 | -6.65302000 | 0.47092000 |
| H | 5.99713100 | -4.20731700 | -0.70776800 |
| H | 6.71952800 | -1.88604200 | 0.01641200 |
| H | 7.38557600 | 0.56642000 | 0.71137800 |
| H | -7.11534400 | -0.59163100 | 0.77528900 |
| H | -6.37666100 | 1.85087600 | 0.13230200 |
| H | -5.76209500 | 4.00079600 | -0.54314000 |
| H | 2.90710100 | 6.31532300 | 0.71235800 |
| H | 4.55765900 | 4.68239400 | 0.99183200 |
| H | 6.49560800 | 2.88148300 | 1.03566100 |
| H | 4.02613300 | -5.71946700 | -1.02509200 |
| H | 1.62417900 | -6.36320600 | -0.79230900 |
| H | -0.70413600 | -7.03322200 | -0.20727100 |

Na⁺@ V_{N2B} *h*-BN (reactant)

| | | | |
|----|------------|-------------|-------------|
| Na | 0.00000000 | 0.00000000 | 0.00000000 |
| B | 0.00000000 | 0.00000000 | 2.39694422 |
| B | 2.25027086 | 0.00000000 | 0.76428286 |
| B | 2.07509004 | -1.43453272 | 2.88916282 |
| B | 4.16577586 | -1.51436961 | 1.50551978 |
| B | 4.35623622 | 0.05075047 | -0.39940997 |

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|---|-------------|-------------|-------------|
| B | 2.24329893 | 1.07170681 | -0.95458964 |
| B | -0.03281488 | 1.93804210 | -2.13162039 |
| B | -2.11986767 | 1.69097508 | -0.77598090 |
| B | -1.74376669 | 0.87449683 | 1.76842958 |
| B | -1.73487685 | 0.13471427 | 4.07274434 |
| B | 0.27350578 | -1.21225849 | 4.61912916 |
| N | -0.41651571 | -0.34289876 | 3.70135443 |
| N | 1.37503733 | -0.44866140 | 1.91676339 |
| N | 1.49143617 | -1.80891127 | 4.15694858 |
| N | -2.44094875 | 0.79981831 | 3.01736455 |
| N | -2.50786369 | 1.43291520 | 0.60854123 |
| N | -1.00971190 | 1.11157544 | -1.47501215 |
| N | 1.41845109 | 1.81403103 | -1.95963010 |
| N | 3.63504056 | 0.96343261 | -1.24317227 |
| N | 3.57640110 | -0.49488916 | 0.67966030 |
| N | 3.37128116 | -2.01137105 | 2.58779152 |
| B | 2.12657373 | -2.78957843 | 5.04925502 |
| B | 3.98968843 | -3.03745229 | 3.43950249 |
| B | 4.35499747 | 1.60402135 | -2.32699463 |
| B | 2.16199716 | 2.54939395 | -3.03643254 |
| B | -3.90829822 | 1.89098466 | 0.87967214 |
| B | -3.79249524 | 1.26045232 | 3.28997668 |
| N | -2.28549084 | -0.07447476 | 5.37611315 |
| N | -0.29096584 | -1.46351588 | 5.92747663 |
| N | 5.51548327 | -1.96771559 | 1.22921737 |
| N | 5.72509024 | -0.30911513 | -0.63084523 |
| N | -0.71629875 | 2.84393428 | -3.03739752 |
| N | -2.84367436 | 2.53599461 | -1.72066383 |

| | | | |
|---|-------------|-------------|-------------|
| B | -1.54764238 | -0.86824085 | 6.32978625 |
| B | 6.30725759 | -1.35182825 | 0.18789920 |
| B | -2.13631350 | 3.07636370 | -2.86789976 |
| B | -3.61134262 | 0.46004457 | 5.66657582 |
| B | 6.45038677 | 0.35750463 | -1.69559899 |
| N | -4.30965716 | 1.11862045 | 4.61544495 |
| N | 5.75367048 | 1.31683481 | -2.49162435 |
| N | 3.58516203 | 2.46114451 | -3.15927578 |
| N | -4.48627975 | 1.81070503 | 2.17689557 |
| N | -4.71149717 | 2.44842445 | -0.18106937 |
| N | 1.45179193 | 3.35225192 | -3.99178032 |
| B | 0.36961649 | -2.39731534 | 6.81888113 |
| B | 6.07421761 | -3.03764438 | 2.02400343 |
| B | -4.23049878 | 2.85089201 | -1.45257217 |
| B | 0.05229551 | 3.54853324 | -4.04109185 |
| N | 5.27842830 | -3.55891741 | 3.08140800 |
| N | 3.31255679 | -3.44507095 | 4.62054849 |
| N | 1.54383830 | -3.03866532 | 6.33699317 |
| H | -4.90460940 | 3.42484684 | -2.23998009 |
| H | -2.71739001 | 3.77591930 | -3.63030230 |
| H | -0.46318548 | 4.25937751 | -4.83678065 |
| H | -1.97821028 | -1.05204538 | 7.41938719 |
| H | -4.09013566 | 0.34719482 | 6.74758631 |
| H | -0.05418984 | -2.61874726 | 7.90679734 |
| H | 7.16438626 | -3.46360689 | 1.80802746 |
| H | 7.43009875 | -1.69763884 | 0.00653766 |
| H | 7.59762031 | 0.11669516 | -1.89370653 |
| H | -5.23602622 | 1.46265214 | 4.82382211 |

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|---|-------------|-------------|-------------|
| H | -5.43257298 | 2.15617843 | 2.30237201 |
| H | -5.67132871 | 2.67712212 | 0.03568489 |
| H | 2.00853775 | 3.83437731 | -4.69488404 |
| H | 4.02189727 | 2.96111597 | -3.91808879 |
| H | 6.27233013 | 1.76206823 | -3.23276313 |
| H | 5.67856449 | -4.28668555 | 3.64840797 |
| H | 3.74723983 | -4.12863010 | 5.22723245 |
| H | 1.99430286 | -3.69762254 | 6.95600862 |

Na⁺@ V_{N2B} *h*-BN (product)

| | | | |
|----|-------------|-------------|-------------|
| Na | -0.01770800 | -1.34769300 | -2.05293700 |
| B | -0.97163100 | 1.02922500 | -0.21867600 |
| B | 1.37557500 | -0.31117800 | -0.18092700 |
| B | 1.26359200 | 2.19064200 | -0.35188600 |
| B | 3.44692800 | 1.10710600 | -0.77023600 |
| B | 3.60555000 | -1.21589200 | 0.01464300 |
| B | 1.42829600 | -2.10041800 | 0.39847200 |
| B | -0.73489200 | -3.42697700 | 0.20711400 |
| B | -2.74130300 | -2.28068000 | -0.79189200 |
| B | -2.65858600 | 0.22667600 | -0.52398700 |
| B | -2.84562200 | 2.29324100 | 0.63399400 |
| B | -0.65414600 | 3.34503300 | 0.76032400 |
| N | -1.40812400 | 2.11642600 | 0.62028000 |
| N | 0.50171200 | 0.86478300 | -0.38840200 |
| N | 0.65538300 | 3.39264400 | 0.16622200 |
| N | -3.54078900 | 1.25417800 | -0.05541000 |
| N | -3.35261400 | -0.99508000 | -0.94028500 |
| N | -1.32468500 | -2.42045500 | -0.63982000 |
| N | 0.61311000 | -3.27622700 | 0.68472800 |

| | | | |
|---|-------------|-------------|-------------|
| N | 2.83916200 | -2.29903700 | 0.54921500 |
| N | 2.78432000 | -0.11304700 | -0.40890900 |
| N | 2.64128100 | 2.28820900 | -0.78279500 |
| B | 1.36548200 | 4.67337200 | 0.14565600 |
| B | 3.33325800 | 3.56911000 | -0.90151400 |
| B | 3.50979900 | -3.47162700 | 1.06083500 |
| B | 1.24307100 | -4.47818600 | 1.28194400 |
| B | -4.82699100 | -1.00322800 | -1.09152400 |
| B | -4.98291600 | 1.27996800 | -0.14203300 |
| N | -3.51111500 | 3.41888800 | 1.21553300 |
| N | -1.27536800 | 4.51076400 | 1.36206500 |
| N | 4.88228400 | 1.10989700 | -0.97937300 |
| N | 5.03178500 | -1.22510600 | -0.08220400 |
| N | -1.52466400 | -4.63380300 | 0.36568000 |
| N | -3.46927000 | -3.53891500 | -0.79462900 |
| B | -2.69275400 | 4.52803800 | 1.65677200 |
| B | 5.67880300 | -0.05287200 | -0.64508600 |
| B | -2.86523400 | -4.70330900 | -0.18678900 |
| B | -4.96411400 | 3.45584000 | 1.14461200 |
| B | 5.72122500 | -2.39703900 | 0.44191300 |
| N | -5.65069700 | 2.39788500 | 0.46733300 |
| N | 4.94860800 | -3.46220300 | 1.01024000 |
| N | 2.65426600 | -4.51933800 | 1.52540900 |
| N | -5.59155500 | 0.17158400 | -0.81391500 |
| N | -5.45293200 | -2.25167300 | -1.45557100 |
| N | 0.40181200 | -5.61862900 | 1.53663600 |
| B | -0.52084300 | 5.74903900 | 1.42984500 |
| B | 5.50909500 | 2.37051700 | -1.34399800 |

| | | | |
|---|-------------|-------------|-------------|
| B | -4.85236400 | -3.52037600 | -1.24496200 |
| B | -0.93381600 | -5.75490700 | 1.07807900 |
| N | 4.70694000 | 3.54717400 | -1.33209900 |
| N | 2.63213700 | 4.75033200 | -0.51596000 |
| N | 0.75742800 | 5.79267500 | 0.80737900 |
| H | -5.46042500 | -4.53177000 | -1.39597800 |
| H | -3.48776700 | -5.71234500 | -0.09843700 |
| H | -1.55251000 | -6.75457100 | 1.25991100 |
| H | -3.18829200 | 5.47106600 | 2.18525700 |
| H | -5.57223400 | 4.35915500 | 1.62537400 |
| H | -0.97347700 | 6.71307400 | 1.96122700 |
| H | 6.66802300 | 2.42378800 | -1.61039700 |
| H | 6.85837700 | -0.03630200 | -0.79796000 |
| H | 6.90863100 | -2.46988300 | 0.40293200 |
| H | -6.65966900 | 2.45876400 | 0.43460800 |
| H | -6.59821900 | 0.12522300 | -0.90158100 |
| H | -6.43911300 | -2.24761600 | -1.68191900 |
| H | 0.80888800 | -6.42179500 | 1.99796400 |
| H | 3.05163900 | -5.36978500 | 1.90244900 |
| H | 5.46689500 | -4.25667600 | 1.36137800 |
| H | 5.17887900 | 4.42382000 | -1.50986300 |
| H | 3.11307100 | 5.63953000 | -0.54544200 |
| H | 1.25586600 | 6.67188300 | 0.83991200 |

K⁺@Pristine *h*-BN

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|---|-------------|-------------|-------------|
| K | -0.30538100 | 0.03874400 | -1.47142000 |
| B | -1.41791400 | 2.18623800 | -1.62932300 |
| B | 0.16377800 | -2.43155700 | -1.47512300 |
| B | 1.18248000 | 2.00939300 | -1.79247200 |

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|---|-------------|-------------|-------------|
| B | -2.20948200 | -2.03754000 | -0.97476600 |
| B | -0.95755400 | -3.78937200 | 0.30792400 |
| B | 1.51755500 | -3.61295500 | 0.29585800 |
| B | 2.46104300 | -1.61741000 | -0.90606000 |
| B | 3.48256400 | 0.94167800 | -0.88159000 |
| B | 2.27543600 | 3.10098000 | -0.02525600 |
| B | -0.19034400 | 3.40826300 | -0.28135200 |
| B | -2.66477100 | 2.84246200 | -0.04805000 |
| B | -3.57935400 | 0.46873200 | -0.92298100 |
| N | -2.49972300 | 1.66803400 | -1.06090600 |
| N | -1.17797000 | -2.05211800 | -1.90083500 |
| N | -3.36919700 | -0.95002700 | -0.87539000 |
| N | -1.48687900 | 3.61148100 | 0.29499500 |
| N | -0.12833200 | 2.65824600 | -1.60257800 |
| N | 1.02509900 | 3.75618100 | 0.32471200 |
| N | 2.23526600 | 1.89555100 | -0.93321600 |
| N | 1.34714100 | -1.62779500 | -1.73872500 |
| N | 3.51860400 | -0.49055200 | -0.84585400 |
| N | 2.64203600 | -2.75048700 | 0.01647200 |
| N | 0.25358300 | -3.39265400 | -0.36400400 |
| N | -2.20827200 | -3.09654900 | 0.03569800 |
| B | -4.64339600 | -1.69030100 | -0.54866700 |
| B | -3.43049500 | -3.59537600 | 0.59674100 |
| B | 3.93888700 | -3.11857700 | 0.51260100 |
| B | 4.87631900 | -1.05608800 | -0.59019300 |
| B | 0.97340200 | 4.74519600 | 1.41218500 |
| B | -1.56697500 | 4.59329600 | 1.39881500 |
| N | -3.93785400 | 3.11167600 | 0.48053500 |

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|---|-------------|-------------|-------------|
| N | -4.87363900 | 1.09931500 | -0.70090000 |
| N | -0.89787300 | -4.81363900 | 1.33956900 |
| N | 1.60841000 | -4.66511400 | 1.30163900 |
| N | 4.69617400 | 1.74516800 | -0.71386800 |
| N | 3.50047800 | 3.59209900 | 0.48269200 |
| B | -5.07750000 | 2.34589100 | -0.02381200 |
| B | 0.39892600 | -5.29585400 | 1.77893900 |
| B | 4.73241200 | 3.00733100 | -0.04398000 |
| B | -4.06175600 | 4.18737100 | 1.46403000 |
| B | 2.91484600 | -5.00443800 | 1.82759500 |
| N | -2.88017200 | 4.85888500 | 1.90347200 |
| N | 4.04858500 | -4.25150800 | 1.38964300 |
| N | 5.04331800 | -2.31843600 | 0.04871500 |
| N | -0.33388800 | 5.16547000 | 1.85556300 |
| N | 2.23261800 | 5.18608200 | 1.91625100 |
| N | 6.03880200 | -0.27819800 | -0.95665400 |
| B | -6.08469900 | 0.29536500 | -0.91363200 |
| B | -2.13312000 | -5.29296900 | 1.91951300 |
| B | 3.49030700 | 4.68210100 | 1.44649900 |
| B | 6.00159700 | 1.12446400 | -0.95392200 |
| N | -3.37158400 | -4.69281300 | 1.51448700 |
| N | -4.63156200 | -2.93302800 | 0.14202100 |
| N | -5.91001700 | -1.09472100 | -0.91574600 |
| H | 4.50968100 | 5.13138700 | 1.85845500 |
| H | 5.76020900 | 3.57392300 | 0.13921900 |
| H | 6.97706900 | 1.79230900 | -1.08169600 |
| H | -6.17371900 | 2.74911900 | 0.18505800 |
| H | -5.12728800 | 4.47480200 | 1.90062100 |

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|---|-------------|-------------|-------------|
| H | -7.14643600 | 0.81661100 | -1.02279400 |
| H | -2.13287700 | -6.17091600 | 2.72517500 |
| H | 0.46071700 | -6.18056900 | 2.57441300 |
| H | 3.04799000 | -5.89129800 | 2.61288900 |
| H | -3.00308100 | 5.55931500 | 2.62373000 |
| H | -0.37951300 | 5.85148100 | 2.59901800 |
| H | 2.26971700 | 5.90286400 | 2.62934400 |
| H | 6.93963100 | -0.73457900 | -1.00961900 |
| H | 5.98734800 | -2.59881000 | 0.27912400 |
| H | 4.95201000 | -4.52105500 | 1.75450400 |
| H | -4.21872100 | -5.06018200 | 1.92596300 |
| H | -5.53094100 | -3.31383300 | 0.40611700 |
| H | -6.73255400 | -1.68217500 | -0.95466000 |

K⁺@Pristine *h*-BN (reactant)

| | | | |
|---|-------------|-------------|-------------|
| K | 0.00166800 | 0.00417700 | 2.69820500 |
| B | -1.28369100 | 0.69470200 | -0.10223300 |
| B | 0.03976700 | -1.45931100 | -0.10164100 |
| B | 1.24357500 | 0.76379300 | -0.10259000 |
| B | -2.48201300 | -1.52504800 | -0.10152900 |
| B | -1.16024500 | -3.66199000 | -0.13713500 |
| B | 1.35836900 | -3.59313800 | -0.13827800 |
| B | 2.56140800 | -1.38719100 | -0.10277900 |
| B | 3.75123800 | 0.82594500 | -0.13708000 |
| B | 2.43227400 | 2.97265200 | -0.13763500 |
| B | -0.07972600 | 2.91147800 | -0.10354400 |
| B | -2.59128400 | 2.83530600 | -0.13868300 |
| B | -3.79099200 | 0.61977600 | -0.13724600 |
| N | -2.54818400 | 1.37942800 | -0.11200200 |

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|---|-------------|-------------|-------------|
| N | -1.23370000 | -0.75812300 | -0.04117500 |
| N | -3.74335300 | -0.82650000 | -0.11962500 |
| N | -1.35406200 | 3.58593200 | -0.12209100 |
| N | -0.03965500 | 1.44702800 | -0.04239200 |
| N | 1.15591800 | 3.65454300 | -0.12139200 |
| N | 2.46881000 | 1.51657900 | -0.11177900 |
| N | 1.27311200 | -0.68960200 | -0.04184700 |
| N | 3.78273300 | -0.62078300 | -0.12054600 |
| N | 2.58715800 | -2.82875900 | -0.12150200 |
| N | 0.07910600 | -2.89672900 | -0.11150900 |
| N | -2.42892400 | -2.96588800 | -0.11962700 |
| B | -4.98898600 | -1.58889700 | -0.15900500 |
| B | -3.67199700 | -3.73244000 | -0.15905700 |
| B | 3.87022200 | -3.52621300 | -0.16188400 |
| B | 5.06813800 | -1.31395500 | -0.16036300 |
| B | 1.11841300 | 5.11441700 | -0.16143000 |
| B | -1.39643700 | 5.04568100 | -0.16241200 |
| N | -3.86814300 | 3.51598200 | -0.16863400 |
| N | -5.05887200 | 1.31705100 | -0.16714900 |
| N | -1.11122900 | -5.10810800 | -0.16728100 |
| N | 1.38854100 | -5.03976300 | -0.16869900 |
| N | 4.97916400 | 1.59145900 | -0.16585600 |
| N | 3.67008800 | 3.72205200 | -0.16645900 |
| B | -5.09644400 | 2.75922300 | -0.18647800 |
| B | 0.15831700 | -5.79342000 | -0.18671500 |
| B | 4.93785800 | 3.03353700 | -0.18414300 |
| B | -3.90963800 | 4.96728900 | -0.19793400 |
| B | 2.66446700 | -5.73266100 | -0.19822500 |

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|---|-------------|-------------|-------------|
| N | -2.68187200 | 5.68356800 | -0.19010100 |
| N | 3.85832100 | -4.96117200 | -0.19021700 |
| N | 5.06993000 | -2.74534600 | -0.16635000 |
| N | -0.15766000 | 5.76291100 | -0.16715200 |
| N | 2.36714400 | 5.82157000 | -0.18788100 |
| N | 6.26332100 | -0.51960900 | -0.18656800 |
| B | -6.29695600 | 0.55857900 | -0.19510500 |
| B | -2.34741400 | -5.86970400 | -0.19539400 |
| B | 3.63219500 | 5.17346500 | -0.19509900 |
| B | 6.25681100 | 0.90178000 | -0.19403800 |
| N | -3.58165800 | -5.16462800 | -0.18652600 |
| N | -4.91256600 | -3.01827900 | -0.16365300 |
| N | -6.22577400 | -0.86105000 | -0.18624900 |
| H | 4.63996800 | 5.80639000 | -0.22188900 |
| H | 5.95112100 | 3.65609200 | -0.21020100 |
| H | 7.27685400 | 1.51473200 | -0.22065800 |
| H | -6.14219500 | 3.32544800 | -0.21361600 |
| H | -4.95045100 | 5.54419200 | -0.22572600 |
| H | -7.34895200 | 1.11487500 | -0.22275400 |
| H | -2.32673600 | -7.05954000 | -0.22316800 |
| H | 0.19072700 | -6.98218300 | -0.21408700 |
| H | 2.70869200 | -6.92184800 | -0.22647600 |
| H | -2.73405400 | 6.69289700 | -0.21889200 |
| H | -0.18520700 | 6.77341800 | -0.20148600 |
| H | 2.36423700 | 6.83225300 | -0.21630800 |
| H | 7.16356300 | -0.97901200 | -0.21487100 |
| H | 5.95881300 | -3.22674800 | -0.20101700 |
| H | 4.73504200 | -5.46397100 | -0.21933000 |

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|---|-------------|-------------|-------------|
| H | -4.42961100 | -5.71460800 | -0.21486400 |
| H | -5.77388600 | -3.54745000 | -0.19799600 |
| H | -7.09960400 | -1.36891000 | -0.21444800 |

K@V_B h-BN

| | | | |
|---|-------------|-------------|-------------|
| K | -1.49474100 | 0.29423000 | 0.27588000 |
| B | 0.68606500 | -1.45390200 | 0.41573200 |
| B | 1.06488700 | 1.16989700 | -0.29462600 |
| B | -1.62281200 | -2.34366000 | 0.75512200 |
| B | 0.25307900 | -3.86366300 | 0.01583100 |
| B | 2.58961400 | -2.92957400 | -0.21824700 |
| B | 2.91574300 | -0.43014900 | 0.01026500 |
| B | 3.33874300 | 2.06316100 | 0.17406500 |
| B | 1.36593100 | 3.62885200 | 0.00987400 |
| B | -0.90551400 | 2.68877100 | -0.47247700 |
| B | -3.55274200 | 1.80790600 | 0.16109000 |
| B | -3.92776300 | -0.64788600 | 0.64202300 |
| N | -3.51176700 | 0.66769000 | 1.04391100 |
| N | -0.52025400 | -1.54262200 | 1.16672500 |
| N | -3.13446300 | -1.94898100 | 0.63524000 |
| N | -2.42755100 | 2.75501300 | -0.22404400 |
| N | -0.13445600 | 1.57912000 | -0.95703100 |
| N | -0.06746800 | 3.84216500 | -0.17272500 |
| N | 1.93097400 | 2.29470100 | 0.02335700 |
| N | 1.46517900 | -0.21935200 | 0.05848100 |
| N | 3.83386000 | 0.70425900 | 0.08365100 |
| N | 3.46368500 | -1.77534300 | -0.12309200 |
| N | 1.18388300 | -2.75500900 | 0.00205700 |
| N | -1.17277400 | -3.66178900 | 0.28561600 |

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|---|-------------|-------------|-------------|
| B | -4.00383000 | -3.12087700 | 0.39285500 |
| B | -2.09018600 | -4.76139600 | 0.14351400 |
| B | 4.89753300 | -1.97836800 | -0.21793300 |
| B | 5.26902400 | 0.48731900 | 0.09215000 |
| B | -0.63803300 | 5.16499000 | -0.14420500 |
| B | -2.93777000 | 4.12439500 | -0.43582400 |
| N | -4.90970800 | 1.95370500 | -0.38218400 |
| N | -5.28490800 | -0.53391900 | 0.06308500 |
| N | 0.75789500 | -5.18978500 | -0.30942100 |
| N | 3.09944100 | -4.26844700 | -0.47351400 |
| N | 4.22162000 | 3.20698700 | 0.35211500 |
| N | 2.24183000 | 4.76539600 | 0.23742300 |
| B | -5.75775900 | 0.77186000 | -0.37991000 |
| B | 2.17662300 | -5.37859300 | -0.53739900 |
| B | 3.66550600 | 4.54055000 | 0.40013600 |
| B | -5.31387800 | 3.27381000 | -0.80684900 |
| B | 4.52912000 | -4.45184700 | -0.60312600 |
| N | -4.34887000 | 4.31466400 | -0.70650100 |
| N | 5.37901600 | -3.31826800 | -0.45646700 |
| N | 5.76867600 | -0.84658700 | -0.07552700 |
| N | -2.05250700 | 5.26074900 | -0.38261700 |
| N | 0.26073000 | 6.26668200 | 0.08522400 |
| N | 6.12664700 | 1.63624300 | 0.26747600 |
| B | -6.08324400 | -1.73002600 | -0.05885200 |
| B | -0.16889600 | -6.30113000 | -0.38527200 |
| B | 1.66811900 | 6.09732600 | 0.27069000 |
| B | 5.64925200 | 2.97004700 | 0.41155500 |
| N | -1.55795600 | -6.06369400 | -0.16757800 |

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|---|-------------|-------------|-------------|
| N | -3.47944500 | -4.45842500 | 0.30381400 |
| N | -5.43360600 | -2.95776300 | 0.21276600 |
| H | 2.36202300 | 7.05158000 | 0.45064200 |
| H | 4.38955400 | 5.47413900 | 0.56482600 |
| H | 6.41505400 | 3.87284400 | 0.56508700 |
| H | -6.86220000 | 0.85936200 | -0.82133200 |
| H | -6.42140200 | 3.49011000 | -1.19471800 |
| H | -7.22991800 | -1.68877900 | -0.38593700 |
| H | 0.21840200 | -7.40207100 | -0.63540300 |
| H | 2.58985800 | -6.47268600 | -0.77304300 |
| H | 4.99298300 | -5.53060400 | -0.81844100 |
| H | -4.65845800 | 5.24900900 | -0.93821300 |
| H | -2.47075900 | 6.17755600 | -0.46895700 |
| H | -0.09788000 | 7.21104500 | 0.11970700 |
| H | 7.12762700 | 1.49921300 | 0.29798700 |
| H | 6.76842100 | -0.99339000 | -0.10659100 |
| H | 6.37414200 | -3.47336200 | -0.54173500 |
| H | -2.18239600 | -6.85431200 | -0.24778400 |
| H | -4.15120100 | -5.20157800 | 0.16410100 |
| H | -5.98175800 | -3.79924600 | 0.09547000 |

K@V_B *h*-BN (reactant)

| | | | |
|---|-------------|-------------|-------------|
| K | 1.40009200 | -0.58452500 | 2.53817900 |
| B | -1.33664000 | -0.82172600 | 0.22013700 |
| B | -0.17705400 | 1.36488300 | 0.06113700 |
| B | 0.14568300 | -2.77490400 | 0.15184400 |
| B | -2.37293100 | -3.05272500 | -0.07129000 |
| B | -3.82256400 | -1.00259300 | -0.08045100 |
| B | -2.71059600 | 1.24777400 | -0.00348400 |

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|---|-------------|-------------|-------------|
| B | -1.59082800 | 3.47597000 | -0.02694200 |
| B | 0.91098000 | 3.65407000 | -0.07589200 |
| B | 2.36441200 | 1.56411400 | -0.06728900 |
| B | 3.88226800 | -0.40683600 | -0.03857300 |
| B | 2.71258800 | -2.56899400 | 0.02526100 |
| N | 2.79713100 | -1.19038800 | 0.37101800 |
| N | -0.10996500 | -1.42208600 | 0.53006400 |
| N | 1.48436100 | -3.37239900 | 0.05005400 |
| N | 3.70686200 | 1.02909600 | -0.15419800 |
| N | 1.15098700 | 0.80027500 | 0.09530300 |
| N | 2.21625100 | 3.03330400 | -0.12134400 |
| N | -0.28141200 | 2.83762100 | 0.00300100 |
| N | -1.41610600 | 0.62261100 | 0.10073100 |
| N | -2.80347000 | 2.69065300 | -0.03731200 |
| N | -3.91720900 | 0.44074200 | -0.06074000 |
| N | -2.53500100 | -1.62505900 | 0.03603200 |
| N | -1.04687900 | -3.63245500 | -0.05519700 |
| B | 1.58740900 | -4.80983200 | -0.17773200 |
| B | -0.91346400 | -5.06292500 | -0.20600300 |
| B | -5.21692200 | 1.07291200 | -0.14763500 |
| B | -4.10668100 | 3.32757600 | -0.09331600 |
| B | 3.39715300 | 3.87492100 | -0.27190200 |
| B | 4.86932400 | 1.85938900 | -0.37103000 |
| N | 5.18487000 | -1.01952400 | -0.32630000 |
| N | 4.01073000 | -3.23023400 | -0.29147700 |
| N | -3.56570400 | -3.88270300 | -0.22633000 |
| N | -5.01283400 | -1.83227700 | -0.21289800 |
| N | -1.69248900 | 4.93127400 | -0.05535700 |

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|---|-------------|-------------|-------------|
| N | 0.79009200 | 5.11058500 | -0.11437600 |
| B | 5.21863700 | -2.45431500 | -0.42945500 |
| B | -4.86958100 | -3.26743600 | -0.27828800 |
| B | -0.50312500 | 5.73571800 | -0.08862500 |
| B | 6.33412700 | -0.18390100 | -0.55965700 |
| B | -6.30901500 | -1.19626500 | -0.28627700 |
| N | 6.15665700 | 1.22943600 | -0.53584900 |
| N | -6.38045400 | 0.22582400 | -0.24009000 |
| N | -5.28213300 | 2.50637800 | -0.13965100 |
| N | 4.69015200 | 3.27845200 | -0.39971000 |
| N | 3.23238900 | 5.30633700 | -0.29312700 |
| N | -4.15855200 | 4.76628600 | -0.10044700 |
| B | 4.08428300 | -4.66197400 | -0.43297200 |
| B | -3.41678600 | -5.31607200 | -0.34774300 |
| B | 1.96827800 | 5.94012400 | -0.21348200 |
| B | -2.98969600 | 5.57245800 | -0.08343000 |
| N | -2.10670800 | -5.86678600 | -0.33082300 |
| N | 0.40364200 | -5.61902200 | -0.22807900 |
| N | 2.88446600 | -5.41321800 | -0.34086500 |
| H | 1.88144200 | 7.13049700 | -0.23371900 |
| H | -0.58902400 | 6.92524400 | -0.10354300 |
| H | -3.07799600 | 6.76295400 | -0.09574800 |
| H | 6.25397400 | -3.00513500 | -0.65691900 |
| H | 7.41248000 | -0.65617300 | -0.76637900 |
| H | 5.12778500 | -5.21187200 | -0.62428500 |
| H | -4.37092800 | -6.02534400 | -0.46234300 |
| H | -5.84197300 | -3.95173600 | -0.38290100 |
| H | -7.30635300 | -1.84597700 | -0.38356800 |

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| H | 6.96881600 | 1.80777700 | -0.69981800 |
| H | 5.49232600 | 3.87758600 | -0.53697200 |
| H | 4.05123700 | 5.89174600 | -0.38113600 |
| H | -5.05362500 | 5.23405800 | -0.13015100 |
| H | -6.18604700 | 2.95549200 | -0.19554000 |
| H | -7.29674800 | 0.64789700 | -0.29908000 |
| H | -2.01811200 | -6.86897900 | -0.42609800 |
| H | 0.51224000 | -6.61440400 | -0.36759100 |
| H | 2.94477500 | -6.41374900 | -0.46838000 |

K⁺@V_B h-BN

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|---|-------------|-------------|-------------|
| K | 1.47513900 | 0.00231100 | 0.93993400 |
| B | -0.89119200 | -1.39244000 | 0.72303000 |
| B | -0.89551200 | 1.38967900 | 0.72309100 |
| B | 1.36296600 | -2.68540400 | 0.58012700 |
| B | -0.80764600 | -3.78813100 | -0.05632400 |
| B | -2.99499500 | -2.52139600 | 0.01488900 |
| B | -2.93631600 | -0.00454700 | 0.31211700 |
| B | -3.00294100 | 2.51216200 | 0.01546600 |
| B | -0.81957000 | 3.78569800 | -0.05602100 |
| B | 1.35457800 | 2.68965300 | 0.57987400 |
| B | 3.80501000 | 1.30346400 | 0.42639700 |
| B | 3.80911100 | -1.29163100 | 0.42677600 |
| N | 3.68639700 | 0.00581900 | 1.08358500 |
| N | 0.36649800 | -1.88236500 | 1.29407000 |
| N | 2.84648900 | -2.44933300 | 0.36850500 |
| N | 2.83876900 | 2.45815000 | 0.36794100 |
| N | 0.36074300 | 1.88345900 | 1.29394900 |
| N | 0.64321600 | 3.82095300 | 0.03872200 |

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|---|-------------|-------------|-------------|
| N | -1.56559900 | 2.54752900 | 0.18553200 |
| N | -1.45989800 | -0.00226200 | 0.64356100 |
| N | -3.66950300 | 1.24063800 | 0.15634400 |
| N | -3.66556300 | -1.25200500 | 0.15600400 |
| N | -1.55757400 | -2.55230600 | 0.18519200 |
| N | 0.65521000 | -3.81886700 | 0.03878200 |
| B | 3.52893600 | -3.69595600 | -0.11733500 |
| B | 1.38340100 | -5.02158300 | -0.32581400 |
| B | -5.12628600 | -1.25345600 | 0.03508700 |
| B | -5.13021800 | 1.23752500 | 0.03551200 |
| B | 1.36760400 | 5.02585900 | -0.32621900 |
| B | 3.51723700 | 3.70676500 | -0.11837500 |
| N | 5.09521400 | 1.28275600 | -0.25150900 |
| N | 5.09933100 | -1.26709300 | -0.25097900 |
| N | -1.51690800 | -4.97874200 | -0.45039600 |
| N | -3.69469100 | -3.74978800 | -0.28669700 |
| N | -3.70653600 | 3.73842500 | -0.28571200 |
| N | -1.53261300 | 4.97413900 | -0.44981000 |
| B | 5.74629800 | 0.00881800 | -0.52474000 |
| B | -2.96411000 | -4.96777700 | -0.52459800 |
| B | -2.97980100 | 4.95871100 | -0.52360300 |
| B | 5.71437600 | 2.54290500 | -0.61145200 |
| B | -5.14546900 | -3.74363400 | -0.34326800 |
| N | 4.92272900 | 3.70000600 | -0.42980900 |
| N | -5.80718300 | -2.50534500 | -0.14518300 |
| N | -5.81939600 | -0.00906400 | 0.07553400 |
| N | 2.79163200 | 4.92749700 | -0.29537000 |
| N | 0.61775200 | 6.18480500 | -0.69609900 |

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|---|-------------|-------------|-------------|
| N | -5.81509100 | 2.48731900 | -0.14424500 |
| B | 5.72256100 | -2.52543700 | -0.61023100 |
| B | -0.78692900 | -6.19838000 | -0.75503300 |
| B | -0.80647600 | 6.19600700 | -0.75467200 |
| B | -5.15729800 | 3.72774600 | -0.34202700 |
| N | 0.63723100 | -6.18281900 | -0.69593900 |
| N | 2.80711900 | -4.91892400 | -0.29437900 |
| N | 4.93451100 | -3.68495000 | -0.42829500 |
| H | -1.39007200 | 7.18669100 | -1.05814900 |
| H | -3.56554200 | 5.95847800 | -0.78896800 |
| H | -5.76932600 | 4.72661100 | -0.54942200 |
| H | 6.81218800 | 0.01042600 | -1.04850200 |
| H | 6.82020600 | 2.59122500 | -1.04387400 |
| H | 6.82864500 | -2.57045100 | -1.04236600 |
| H | -1.36738800 | -7.19084500 | -1.05871000 |
| H | -3.54667800 | -5.96932000 | -0.79025100 |
| H | -5.75432100 | -4.74435000 | -0.55107800 |
| H | 5.33974900 | 4.58188200 | -0.69807100 |
| H | 3.32980900 | 5.73699600 | -0.57646000 |
| H | 1.09814900 | 7.04270400 | -0.93209100 |
| H | -6.82475700 | 2.48393400 | -0.19947400 |
| H | -6.82660400 | -0.01063600 | -0.01410100 |
| H | -6.81684600 | -2.50511100 | -0.20057100 |
| H | 1.12034400 | -7.03925200 | -0.93171100 |
| H | 3.34785300 | -5.72681300 | -0.57519700 |
| H | 5.35434400 | -4.56562000 | -0.69613400 |

K⁺@V_B *h*-BN (reactant)

| | | | |
|---|-------------|-------------|-------------|
| K | 1.46617100 | -0.34745900 | 2.71310800 |
| B | -1.11344900 | -1.04051900 | 0.16019900 |
| B | -0.47547400 | 1.40261800 | 0.12588600 |
| B | 0.72769700 | -2.79002000 | 0.06456000 |
| B | -1.70001100 | -3.47054000 | -0.07754600 |
| B | -3.51336300 | -1.71956300 | -0.06868700 |
| B | -2.88553700 | 0.71438800 | -0.02422300 |
| B | -2.27151100 | 3.14898600 | -0.04103500 |
| B | 0.15264400 | 3.83874400 | -0.07772200 |
| B | 1.98528800 | 2.10421100 | 0.00474800 |
| B | 3.82474600 | 0.36836500 | -0.04391400 |
| B | 3.17938200 | -2.09132900 | -0.01981900 |
| N | 2.98574300 | -0.71868500 | 0.37745300 |
| N | 0.20624400 | -1.51127600 | 0.49805100 |
| N | 2.13806400 | -3.09117300 | -0.08543700 |
| N | 3.37439300 | 1.73339600 | -0.14750200 |
| N | 0.93105300 | 1.19509300 | 0.40589500 |
| N | 1.56324500 | 3.48526700 | -0.11016900 |
| N | -0.85714400 | 2.79643300 | 0.01974900 |
| N | -1.46760200 | 0.35631800 | 0.07778300 |
| N | -3.26906900 | 2.10582100 | -0.04989000 |
| N | -3.88790300 | -0.32532900 | -0.06578900 |
| N | -2.10720200 | -2.07941900 | 0.02104500 |
| N | -0.28605600 | -3.81485700 | -0.08529900 |
| B | 2.52762500 | -4.48824000 | -0.32173200 |
| B | 0.11313400 | -5.20436100 | -0.27761900 |
| B | -5.30206000 | 0.03083600 | -0.13467300 |

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|---|-------------|-------------|-------------|
| B | -4.68353000 | 2.46579200 | -0.10947600 |
| B | 2.56553700 | 4.53046600 | -0.30473200 |
| B | 4.37169100 | 2.78138700 | -0.38328100 |
| N | 5.21755200 | 0.00000000 | -0.26395600 |
| N | 4.58335000 | -2.42980600 | -0.24549000 |
| N | -2.70535600 | -4.50182400 | -0.20306500 |
| N | -4.50964200 | -2.76637000 | -0.16260000 |
| N | -2.65487800 | 4.54469000 | -0.10166800 |
| N | -0.25039200 | 5.22426100 | -0.17109300 |
| B | 5.58632000 | -1.39385200 | -0.35000200 |
| B | -4.10842700 | -4.14870100 | -0.22243400 |
| B | -1.65231800 | 5.57572000 | -0.15848900 |
| B | 6.19776500 | 1.04812500 | -0.49384900 |
| B | -5.91641500 | -2.40858000 | -0.21787800 |
| N | 5.74783500 | 2.39336700 | -0.52816400 |
| N | -6.26689800 | -1.03194300 | -0.19254100 |
| N | -5.65590100 | 1.41696900 | -0.14142100 |
| N | 3.93814200 | 4.14087900 | -0.42884300 |
| N | 2.12044100 | 5.89040400 | -0.37136500 |
| N | -5.02735300 | 3.85986700 | -0.13350300 |
| B | 4.95317200 | -3.82094200 | -0.44621100 |
| B | -2.30439400 | -5.88988800 | -0.33468800 |
| B | 0.74999400 | 6.26625900 | -0.30372100 |
| B | -4.06272100 | 4.90167200 | -0.13871500 |
| N | -0.91487500 | -6.19824900 | -0.37024500 |
| N | 1.51292000 | -5.49209100 | -0.37298900 |
| N | 3.92351200 | -4.79521800 | -0.46289000 |
| H | 0.43189400 | 7.41147900 | -0.36186700 |

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|---|-------------|-------------|-------------|
| H | -1.97459700 | 6.71971100 | -0.20386800 |
| H | -4.39748200 | 6.04351500 | -0.17502400 |
| H | 6.72045000 | -1.69116800 | -0.54676600 |
| H | 7.34534600 | 0.77696400 | -0.65383800 |
| H | 6.09299900 | -4.12611700 | -0.59931500 |
| H | -3.11866000 | -6.75373700 | -0.41811100 |
| H | -4.93061500 | -5.00516600 | -0.29593200 |
| H | -6.75500000 | -3.25105800 | -0.28336200 |
| H | 6.44299400 | 3.10940300 | -0.69164100 |
| H | 4.63070300 | 4.86198700 | -0.58214900 |
| H | 2.79958800 | 6.63048200 | -0.48696100 |
| H | -6.00136400 | 4.12890400 | -0.16683200 |
| H | -6.63468200 | 1.66663300 | -0.19126600 |
| H | -7.25091700 | -0.80378600 | -0.23642500 |
| H | -0.65897300 | -7.16971600 | -0.48501600 |
| H | 1.79763500 | -6.45106200 | -0.52339200 |
| H | 4.19891400 | -5.75638900 | -0.61444200 |

K@V_N *h*-BN

| | | | |
|---|-------------|-------------|-------------|
| K | 0.23106700 | -1.16504500 | 0.46909700 |
| B | -1.76683700 | -0.28542000 | -0.20363000 |
| B | 1.90469300 | -1.02729100 | 2.06230500 |
| B | 0.75864600 | 1.23424700 | 0.50556200 |
| B | -1.59128900 | -2.34389700 | -0.24832600 |
| B | 1.15865500 | -3.44119000 | 0.45727300 |
| B | 3.33413700 | -2.22665100 | 0.49613100 |
| B | 3.10602700 | 0.35484200 | 0.48687000 |
| B | 2.68901700 | 2.71294900 | -0.13189600 |
| B | 0.37014000 | 3.67803100 | 0.00555600 |

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|---|-------------|-------------|-------------|
| B | -1.69808800 | 2.20063600 | 0.14918900 |
| B | -3.91981500 | 0.97616200 | -0.14778000 |
| B | -3.81076200 | -1.50346000 | -0.46798200 |
| N | -3.16483100 | -0.21213200 | -0.38273000 |
| N | -2.95306700 | -2.66429200 | -0.45375100 |
| N | -3.17589100 | 2.18067400 | 0.09860800 |
| N | -0.89049800 | 0.94584400 | 0.16691000 |
| N | -1.06387700 | 3.51697400 | 0.17354200 |
| N | 1.24794700 | 2.53022900 | 0.08822600 |
| N | 1.79121300 | 0.32062400 | 1.08360900 |
| N | 3.59671000 | 1.59540700 | -0.05476600 |
| N | 3.91605500 | -0.87679200 | 0.41022600 |
| N | 2.01635200 | -2.38590800 | 1.05753200 |
| N | -0.50919300 | -3.40668400 | 0.07772900 |
| B | -3.49239600 | -3.99507200 | -0.37248400 |
| B | -1.08505200 | -4.76735300 | -0.04980000 |
| B | 5.28247100 | -0.75996000 | -0.08321500 |
| B | 4.99391600 | 1.72104300 | -0.41503000 |
| B | -1.87398400 | 4.72826800 | 0.27590800 |
| B | -3.96894800 | 3.38714800 | 0.28006800 |
| N | -5.37364500 | 0.87406400 | -0.15542900 |
| N | -5.24259400 | -1.62480100 | -0.46627200 |
| N | 1.86525900 | -4.64718700 | 0.05987300 |
| N | 4.04599200 | -3.38921500 | -0.00401400 |
| N | 3.21837900 | 4.01684300 | -0.49414300 |
| N | 0.94867200 | 4.99972900 | -0.21114000 |
| B | -6.02412300 | -0.40854200 | -0.33016000 |
| B | 3.31299700 | -4.62196000 | -0.10206200 |

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|---|-------------|-------------|-------------|
| B | 2.35116800 | 5.15957400 | -0.49466500 |
| B | -6.13425600 | 2.08541200 | 0.06771800 |
| B | 5.44302800 | -3.26573800 | -0.35471000 |
| N | -5.41026200 | 3.28918900 | 0.27747000 |
| N | 6.03194000 | -1.96971600 | -0.32846900 |
| N | 5.81461900 | 0.54492100 | -0.36995200 |
| N | -3.29170100 | 4.62829400 | 0.43210500 |
| N | -1.24296700 | 6.01706900 | 0.19674100 |
| N | 5.46908700 | 3.02399700 | -0.80029700 |
| B | -5.80279600 | -2.96966900 | -0.48343800 |
| B | 1.18228500 | -5.90370400 | -0.12187000 |
| B | 0.13123100 | 6.18437300 | -0.09953500 |
| B | 4.62291100 | 4.16618300 | -0.82311400 |
| N | -0.23172000 | -5.92717500 | -0.04775900 |
| N | -2.51190300 | -5.01398000 | -0.20226700 |
| N | -4.93047700 | -4.10585800 | -0.44724500 |
| H | 0.59793300 | 7.27223600 | -0.24445800 |
| H | 2.78930700 | 6.24335500 | -0.72706400 |
| H | 5.06202300 | 5.23589500 | -1.11792100 |
| H | -7.21464700 | -0.46972400 | -0.33786400 |
| H | -7.32701500 | 2.07689600 | 0.07479500 |
| H | -6.98491700 | -3.12835400 | -0.50783400 |
| H | 1.79233500 | -6.90906200 | -0.31932500 |
| H | 3.87864500 | -5.63409900 | -0.37781200 |
| H | 6.08543700 | -4.21970600 | -0.67471900 |
| H | -5.94725400 | 4.13355800 | 0.42072900 |
| H | -3.82975600 | 5.47894100 | 0.52312400 |
| H | -1.81559800 | 6.84605100 | 0.27226200 |

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|---|-------------|-------------|-------------|
| H | 6.44165500 | 3.15503200 | -1.04112000 |
| H | 6.77568600 | 0.61467300 | -0.67639100 |
| H | 6.99624900 | -1.89546000 | -0.62225600 |
| H | -0.67164700 | -6.83082500 | -0.15772700 |
| H | -2.79984500 | -5.98377000 | -0.19349700 |
| H | -5.37095000 | -5.01539400 | -0.42055100 |

K@V_N *h*-BN (reactant)

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|---|-------------|-------------|-------------|
| K | 2.33003800 | -1.05254100 | -2.21217600 |
| B | 1.11870200 | 0.07271000 | 0.13843300 |
| B | -0.21321100 | 1.24082300 | 0.53639200 |
| B | -1.19820600 | -0.80644400 | -0.19937500 |
| B | 2.03327000 | 1.52599800 | -0.55981300 |
| B | 0.54972600 | 3.54852100 | -0.14409700 |
| B | -1.77006300 | 3.24972500 | 0.66213300 |
| B | -2.76423600 | 1.01374600 | 0.38772800 |
| B | -3.65659100 | -1.23123100 | -0.24578700 |
| B | -2.02283100 | -3.09856100 | -0.55415000 |
| B | 0.40703300 | -2.54544900 | -0.11346800 |
| B | 2.62292400 | -2.04221800 | 0.92401800 |
| B | 3.60712500 | 0.09774100 | 0.54661200 |
| N | 2.39679000 | -0.63580300 | 0.75151900 |
| N | 3.44758600 | 1.25946500 | -0.27318300 |
| N | 1.66953100 | -3.02838100 | 0.42938200 |
| N | 0.19064400 | -1.14157300 | -0.35112900 |
| N | -0.65068700 | -3.53114100 | -0.38832300 |
| N | -2.30720400 | -1.70293800 | -0.42544500 |
| N | -1.43786200 | 0.50243600 | 0.29189000 |
| N | -3.89309400 | 0.14124400 | 0.13599000 |

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|---|-------------|-------------|-------------|
| N | -2.94278400 | 2.40073900 | 0.71423700 |
| N | -0.42574200 | 2.69778400 | 0.49393300 |
| N | 1.75377400 | 2.96472000 | -0.70321400 |
| B | 4.53684400 | 2.17510300 | -0.47920600 |
| B | 2.84070400 | 3.87923400 | -1.04528600 |
| B | -4.28371600 | 2.92988500 | 0.83906000 |
| B | -5.23561200 | 0.64691200 | 0.30622500 |
| B | -0.38797300 | -4.95000900 | -0.29079100 |
| B | 1.90166400 | -4.44930500 | 0.60585800 |
| N | 3.91549500 | -2.52637300 | 1.44999300 |
| N | 4.93055800 | -0.31514000 | 0.99652200 |
| N | 0.31594100 | 4.99417500 | -0.22313400 |
| N | -1.97596500 | 4.69393100 | 0.70016400 |
| N | -4.76590400 | -2.15640200 | -0.43746700 |
| N | -3.12146500 | -4.03722700 | -0.74188900 |
| B | 5.04490900 | -1.63259900 | 1.56047900 |
| B | -0.90829400 | 5.56095300 | 0.27954600 |
| B | -4.48467400 | -3.54737300 | -0.71414000 |
| B | 4.12031300 | -3.93887700 | 1.67273100 |
| B | -3.29391800 | 5.22963300 | 0.96969900 |
| N | 3.12094700 | -4.86189200 | 1.25202300 |
| N | -4.40894900 | 4.34611500 | 1.07264400 |
| N | -5.39971100 | 2.02704700 | 0.68613900 |
| N | 0.91582600 | -5.38150200 | 0.13204500 |
| N | -1.46549000 | -5.86413500 | -0.59476000 |
| N | -6.31835800 | -0.28208700 | 0.07328700 |
| B | 6.05226000 | 0.55754200 | 0.73158200 |
| B | 1.31072900 | 5.85424700 | -0.81402800 |

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|---|-------------|-------------|-------------|
| B | -2.81414800 | -5.44859100 | -0.80330900 |
| B | -6.11584600 | -1.64999700 | -0.28345300 |
| N | 2.53426400 | 5.27412400 | -1.24454100 |
| N | 4.20875800 | 3.41729100 | -1.11025600 |
| N | 5.84137300 | 1.76374600 | -0.00947200 |
| H | -3.66978700 | -6.25891200 | -0.99832800 |
| H | -5.38612700 | -4.30996600 | -0.89053800 |
| H | -7.05619800 | -2.36846600 | -0.44791600 |
| H | 6.07307100 | -2.00901300 | 2.03575800 |
| H | 5.12830000 | -4.33875500 | 2.17414900 |
| H | 7.14997600 | 0.27300900 | 1.10987900 |
| H | 1.12733800 | 7.02963500 | -0.92182600 |
| H | -1.05488600 | 6.74527200 | 0.29970800 |
| H | -3.45695300 | 6.40811500 | 1.07857400 |
| H | 3.29019100 | -5.84419000 | 1.41771900 |
| H | 1.08726300 | -6.37068000 | 0.25212600 |
| H | -1.28587400 | -6.85868900 | -0.58203100 |
| H | -7.27452400 | 0.02877300 | 0.17662300 |
| H | -6.33557900 | 2.39770800 | 0.78260700 |
| H | -5.31975200 | 4.75971900 | 1.21526300 |
| H | 3.26127600 | 5.89818400 | -1.56572300 |
| H | 4.93072700 | 4.10724900 | -1.26973700 |
| H | 6.63852400 | 2.37109600 | -0.14161400 |

K@V_N *h*-BN (product)

| | | | |
|---|-------------|-------------|-------------|
| K | -1.92428300 | -0.69589100 | 2.66318200 |
| B | -1.16138600 | 0.13467000 | -0.11298700 |
| B | 0.11081500 | -1.16823100 | 0.41275600 |
| B | 1.22021500 | 0.82857500 | -0.30401100 |

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|---|-------------|-------------|-------------|
| B | -2.06346100 | -1.27973300 | -0.83545800 |
| B | -0.72872500 | -3.40978100 | -0.40329400 |
| B | 1.55181200 | -3.27058200 | 0.52983800 |
| B | 2.66753500 | -1.08758700 | 0.29832400 |
| B | 3.69985900 | 1.10415100 | -0.31436400 |
| B | 2.18401000 | 3.05800700 | -0.69762300 |
| B | -0.29320100 | 2.66065500 | -0.35076000 |
| B | -2.59503800 | 2.33782700 | 0.52447600 |
| B | -3.66404000 | 0.25793200 | 0.07765300 |
| N | -2.43847100 | 0.89879400 | 0.46770300 |
| N | -3.47803000 | -0.96524700 | -0.62537700 |
| N | -1.53802400 | 3.23866500 | 0.13614300 |
| N | -0.13007500 | 1.24135000 | -0.47620100 |
| N | 0.83768800 | 3.57262400 | -0.59619000 |
| N | 2.38741600 | 1.65408700 | -0.50472600 |
| N | 1.37385900 | -0.50059500 | 0.18846500 |
| N | 3.84911400 | -0.28300400 | 0.07527000 |
| N | 2.76252700 | -2.48641700 | 0.62865800 |
| N | 0.23936200 | -2.64363200 | 0.34892000 |
| N | -1.85122100 | -2.73167600 | -1.01440800 |
| B | -4.59266900 | -1.77618600 | -1.02672500 |
| B | -2.95121200 | -3.56498500 | -1.50010100 |
| B | 4.07004100 | -3.09229600 | 0.76830800 |
| B | 5.15710400 | -0.86564000 | 0.26017500 |
| B | 0.65370900 | 5.00556600 | -0.56711300 |
| B | -1.70374400 | 4.67306400 | 0.22240600 |
| N | -3.90234200 | 2.90568500 | 0.92265800 |
| N | -5.00024200 | 0.75467400 | 0.37725500 |

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|---|-------------|-------------|-------------|
| N | -0.57093700 | -4.86370400 | -0.51957600 |
| N | 1.67404600 | -4.72481200 | 0.54386400 |
| N | 4.86730400 | 1.95559300 | -0.50051700 |
| N | 3.34431600 | 3.92327800 | -0.88253600 |
| B | -5.09455300 | 2.09742600 | 0.89002900 |
| B | 0.58578700 | -5.51668700 | 0.03489600 |
| B | 4.67265700 | 3.35677500 | -0.81160700 |
| B | -4.03933600 | 4.33796500 | 1.08594300 |
| B | 2.95311100 | -5.33709300 | 0.84072600 |
| N | -2.94547800 | 5.18168700 | 0.75670300 |
| N | 4.10908900 | -4.51683600 | 0.99250200 |
| N | 5.23630900 | -2.25535100 | 0.64172500 |
| N | -0.63536800 | 5.52946800 | -0.20906900 |
| N | 1.79502300 | 5.84601800 | -0.85795600 |
| N | 6.29607700 | -0.00508000 | 0.04342800 |
| B | -6.13705000 | -0.03864200 | -0.03822900 |
| B | -1.55848700 | -5.63797600 | -1.23223600 |
| B | 3.12113100 | 5.34705400 | -1.00882400 |
| B | 6.18019100 | 1.37143100 | -0.32631400 |
| N | -2.70509500 | -4.96806300 | -1.73292400 |
| N | -4.27871600 | -3.02367400 | -1.65267400 |
| N | -5.91560600 | -1.27334000 | -0.72369800 |
| H | 4.02931400 | 6.09792400 | -1.20685200 |
| H | 5.62335700 | 4.05912700 | -0.98156000 |
| H | 7.16577900 | 2.02857200 | -0.48262400 |
| H | -6.14730600 | 2.54676900 | 1.23087200 |
| H | -5.06722700 | 4.80938000 | 1.47353500 |
| H | -7.25181200 | 0.33125300 | 0.18506100 |

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|---|-------------|-------------|-------------|
| H | -1.43128600 | -6.81675500 | -1.37724200 |
| H | 0.66292200 | -6.70780000 | 0.02796700 |
| H | 3.04754200 | -6.52450400 | 0.93335100 |
| H | -3.07373400 | 6.17892900 | 0.85651500 |
| H | -0.76263600 | 6.53115200 | -0.16223500 |
| H | 1.67032800 | 6.84810600 | -0.89910700 |
| H | 7.23054400 | -0.37300500 | 0.15669500 |
| H | 6.14843000 | -2.68055800 | 0.74087200 |
| H | 4.99328000 | -4.98180700 | 1.14472100 |
| H | -3.43064500 | -5.53051200 | -2.15543000 |
| H | -5.01784900 | -3.64267500 | -1.95671100 |
| H | -6.73067500 | -1.80348500 | -0.99982400 |

$K^+@V_N$ *h*-BN

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|---|-------------|-------------|-------------|
| K | 0.20682500 | -1.16356700 | 0.44857200 |
| B | 2.06940300 | -1.00875000 | 1.74616700 |
| B | -1.78378600 | -0.29234800 | -0.21853500 |
| B | 0.69649300 | 1.25108100 | 0.48397600 |
| B | -1.59803700 | -2.35594900 | -0.25632400 |
| B | -3.81411900 | -1.52497800 | -0.46688500 |
| B | -3.93484100 | 0.96282000 | -0.14950300 |
| B | -1.72139600 | 2.20981100 | 0.14394600 |
| B | 0.34090100 | 3.68933000 | 0.01708800 |
| B | 2.67341500 | 2.73127500 | -0.11709400 |
| B | 3.13622300 | 0.38570400 | 0.45560000 |
| B | 3.37985100 | -2.22180500 | 0.47460700 |
| B | 1.11947700 | -3.45190000 | 0.45162700 |
| N | 2.04025200 | -2.35365100 | 1.05356400 |
| N | -0.47911700 | -3.41776600 | 0.09066100 |

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|---|-------------|-------------|-------------|
| N | 3.92881400 | -0.85978900 | 0.39078700 |
| N | 1.80671100 | 0.31215000 | 1.06889200 |
| N | 3.59767500 | 1.61734700 | -0.06335200 |
| N | 1.22599400 | 2.52548000 | 0.10698700 |
| N | -0.88781300 | 0.94892300 | 0.16674700 |
| N | -1.08773600 | 3.51798800 | 0.17307700 |
| N | -3.18907100 | 2.16779700 | 0.09451400 |
| N | -3.16876000 | -0.22663500 | -0.38611700 |
| N | -2.94312700 | -2.68563100 | -0.44779300 |
| B | -1.06420400 | -4.79141200 | -0.04294500 |
| B | -3.47998400 | -4.02390700 | -0.36066000 |
| B | -3.99575800 | 3.37599800 | 0.27093900 |
| B | -1.90898900 | 4.73352800 | 0.27092600 |
| B | 5.00350700 | 1.75410600 | -0.42350300 |
| B | 5.32014800 | -0.73425300 | -0.09092200 |
| N | 4.07276100 | -3.37961700 | 0.00719200 |
| N | 1.87467500 | -4.62524400 | 0.10239500 |
| N | -5.23480000 | -1.65436000 | -0.45499700 |
| N | -5.37915700 | 0.84734700 | -0.15214400 |
| N | 0.92177700 | 5.00256400 | -0.17915200 |
| N | 3.19401400 | 4.02909800 | -0.46198400 |
| B | 3.32905400 | -4.61232700 | -0.05791300 |
| B | -6.02718900 | -0.43833000 | -0.32218500 |
| B | 2.32289700 | 5.17601900 | -0.45298300 |
| B | 5.47984800 | -3.25130400 | -0.34255100 |
| B | -6.15191300 | 2.05761900 | 0.06781100 |
| N | 6.05633700 | -1.94900800 | -0.32035200 |
| N | -5.43122700 | 3.26444300 | 0.27066900 |

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|---|-------------|-------------|-------------|
| N | -3.32261300 | 4.61899700 | 0.41691400 |
| N | 5.82473600 | 0.57329200 | -0.37648800 |
| N | 5.45846500 | 3.05744100 | -0.79339500 |
| N | -1.27730000 | 6.01836000 | 0.20149500 |
| B | 1.20929700 | -5.90596700 | -0.08663400 |
| B | -5.79175500 | -3.00453200 | -0.46681100 |
| B | 4.59947400 | 4.19496600 | -0.79719500 |
| B | 0.09833800 | 6.19263800 | -0.07312500 |
| N | -4.90983900 | -4.13750000 | -0.42753200 |
| N | -2.48348900 | -5.03207900 | -0.19142500 |
| N | -0.19995100 | -5.93934300 | -0.03774900 |
| H | 5.02528400 | 5.26912800 | -1.07915300 |
| H | 2.76152800 | 6.25900800 | -0.66935800 |
| H | 0.57080800 | 7.27611800 | -0.20513700 |
| H | 3.88735100 | -5.62990700 | -0.30651700 |
| H | 6.12054900 | -4.20455500 | -0.64971900 |
| H | 1.84335100 | -6.89562000 | -0.25837800 |
| H | -6.96990100 | -3.16787400 | -0.48690200 |
| H | -7.21418600 | -0.50787600 | -0.32670200 |
| H | -7.34148700 | 2.03804100 | 0.07720000 |
| H | 7.02400400 | -1.88018400 | -0.60798300 |
| H | 6.78755800 | 0.65460300 | -0.67746300 |
| H | 6.42782800 | 3.20812200 | -1.03818200 |
| H | -1.85021200 | 6.84809900 | 0.27440400 |
| H | -3.86758800 | 5.46582900 | 0.50766400 |
| H | -5.97587400 | 4.10531300 | 0.40941100 |
| H | -5.35043300 | -5.04756900 | -0.39896000 |
| H | -2.76836700 | -6.00348100 | -0.18681700 |

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|--|-------------|-------------|-------------|
| H | -0.62912900 | -6.84928500 | -0.14479600 |
| K ⁺ @V _N <i>h</i> -BN (reactant) | | | |
| K | 0.23489200 | -0.99809500 | -2.53289500 |
| B | 0.81339300 | -1.12794600 | 0.64806700 |
| B | -1.44027000 | -0.36797700 | 0.08287900 |
| B | 0.51035900 | 1.28297800 | 0.12013500 |
| B | -1.17190100 | -2.29753200 | -0.03632700 |
| B | -3.40042900 | -1.66203400 | 0.70170200 |
| B | -3.70050400 | 0.77338200 | 0.48824300 |
| B | -1.76744600 | 2.16393900 | -0.20037200 |
| B | 0.21339300 | 3.71124000 | -0.35314300 |
| B | 2.49501800 | 2.81839100 | 0.19803000 |
| B | 2.80378500 | 0.37500600 | 0.61487600 |
| B | 3.11602700 | -2.08368300 | 0.50418100 |
| B | 1.12051900 | -3.43042300 | -0.19893000 |
| N | 1.66475800 | -2.23825300 | 0.39206400 |
| N | -0.29757700 | -3.40746400 | -0.49442400 |
| N | 3.66140600 | -0.77516600 | 0.72691600 |
| N | 1.35118700 | 0.18080400 | 0.51867700 |
| N | 3.35081000 | 1.69660700 | 0.52295500 |
| N | 1.07804000 | 2.59174000 | -0.03289000 |
| N | -0.87615000 | 0.97551800 | -0.16331900 |
| N | -1.20949500 | 3.47978500 | -0.43510300 |
| N | -3.17905500 | 2.03621200 | 0.04320600 |
| N | -2.81513100 | -0.36700600 | 0.52552300 |
| N | -2.48869200 | -2.72359300 | 0.39244700 |
| B | -0.86971200 | -4.75118500 | -0.74303600 |
| B | -3.04568000 | -4.05223600 | 0.23233900 |

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|---|-------------|-------------|-------------|
| B | -4.06778500 | 3.18883200 | -0.04616200 |
| B | -2.09673900 | 4.62980400 | -0.60139500 |
| B | 4.78630600 | 1.89394800 | 0.70052900 |
| B | 5.10558700 | -0.59833200 | 0.84776200 |
| N | 3.96830400 | -3.23277700 | 0.31286900 |
| N | 1.99705300 | -4.53637800 | -0.51218000 |
| N | -4.77898100 | -1.86272900 | 1.04733000 |
| N | -5.10059700 | 0.60517800 | 0.83622000 |
| N | 0.78155800 | 5.03043900 | -0.53065100 |
| N | 3.04792200 | 4.14712700 | 0.06016600 |
| B | 3.40789500 | -4.46300700 | -0.19009300 |
| B | -5.63296000 | -0.70037100 | 1.15836800 |
| B | 2.19277400 | 5.24836300 | -0.32120600 |
| B | 5.39940800 | -3.08264600 | 0.54139300 |
| B | -5.98227700 | 1.75641100 | 0.75322700 |
| N | 5.91312200 | -1.78903700 | 0.84002300 |
| N | -5.44797600 | 2.99667800 | 0.30154000 |
| N | -3.50874200 | 4.43855400 | -0.46138300 |
| N | 5.61388000 | 0.73799100 | 0.91524600 |
| N | 5.28483200 | 3.23630200 | 0.61618500 |
| N | -1.49925900 | 5.90904200 | -0.87185700 |
| B | 1.42477800 | -5.73752800 | -1.08993100 |
| B | -5.27346000 | -3.22623700 | 1.09438900 |
| B | 4.46565200 | 4.35731400 | 0.29418800 |
| B | -0.09846900 | 6.14627700 | -0.82959300 |
| N | -4.39281500 | -4.27408600 | 0.68371800 |
| N | -2.23350900 | -5.02272100 | -0.43469800 |
| N | 0.01289900 | -5.78156200 | -1.23251000 |

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|---|-------------|-------------|-------------|
| H | 4.93903500 | 5.44614200 | 0.20863000 |
| H | 2.65293500 | 6.33700000 | -0.45710600 |
| H | 0.34224400 | 7.23604600 | -1.01820200 |
| H | 4.10554800 | -5.40826700 | -0.37495200 |
| H | 6.12455800 | -4.02282400 | 0.45923800 |
| H | 2.10949700 | -6.65562200 | -1.41252800 |
| H | -6.39197900 | -3.46515200 | 1.42409700 |
| H | -6.77537200 | -0.82464000 | 1.46633400 |
| H | -7.13311000 | 1.66262900 | 1.04381200 |
| H | 6.91364600 | -1.71146000 | 0.96570300 |
| H | 6.61172800 | 0.87367800 | 1.01169000 |
| H | 6.27008000 | 3.41290600 | 0.75944200 |
| H | -2.09796800 | 6.70734400 | -1.03522000 |
| H | -4.11637600 | 5.24317700 | -0.54057900 |
| H | -6.08324600 | 3.78198800 | 0.25594900 |
| H | -4.77669600 | -5.20922900 | 0.65485100 |
| H | -2.58711900 | -5.95956900 | -0.57696200 |
| H | -0.39122600 | -6.66251800 | -1.52229200 |

$K^+@V_N$ *h*-BN (product)

| | | | |
|---|-------------|-------------|-------------|
| K | -1.87898100 | -1.28518200 | 2.74261500 |
| B | 0.67787000 | -1.29418600 | 0.43268900 |
| B | -1.38100000 | -0.00839000 | -0.18885800 |
| B | 0.91763000 | 1.12442400 | -0.03883400 |
| B | -1.58774800 | -1.92823400 | -0.42725100 |
| B | -3.66992200 | -0.79729500 | 0.18312700 |
| B | -3.34213800 | 1.64026800 | 0.19093600 |
| B | -1.08788400 | 2.53520900 | -0.32702800 |
| B | 1.20609200 | 3.56356600 | -0.46806000 |

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|---|-------------|-------------|-------------|
| B | 3.21328900 | 2.14499300 | 0.02293900 |
| B | 2.94062000 | -0.30246400 | 0.41231300 |
| B | 2.65925500 | -2.76289400 | 0.23977500 |
| B | 0.40555800 | -3.55722100 | -0.51934900 |
| N | 1.20751100 | -2.57768900 | 0.16667900 |
| N | -0.97774600 | -3.21343100 | -0.78803100 |
| N | 3.49916200 | -1.62719900 | 0.49719300 |
| N | 1.48373400 | -0.13829200 | 0.36781800 |
| N | 3.78543600 | 0.85170500 | 0.32787600 |
| N | 1.77723100 | 2.26789100 | -0.16908100 |
| N | -0.51464600 | 1.17205000 | -0.26853000 |
| N | -0.23397400 | 3.68608400 | -0.52381900 |
| N | -2.50539900 | 2.75108100 | -0.13297600 |
| N | -2.75904900 | 0.30893600 | 0.22012100 |
| N | -3.01399200 | -2.04235700 | -0.08403500 |
| B | -1.82300700 | -4.35374500 | -1.19294600 |
| B | -3.86247700 | -3.18666800 | -0.39176100 |
| B | -3.08796800 | 4.08571300 | -0.22496700 |
| B | -0.81422600 | 5.01498500 | -0.69696800 |
| B | 5.22937800 | 0.69715200 | 0.46151400 |
| B | 4.94648200 | -1.79924200 | 0.57583400 |
| N | 3.21883300 | -4.07173100 | 0.00206400 |
| N | 1.00120100 | -4.82680500 | -0.87480000 |
| N | -5.07990000 | -0.67348100 | 0.43138900 |
| N | -4.76689100 | 1.79989800 | 0.44569800 |
| N | 2.06979200 | 4.71263600 | -0.64385500 |
| N | 4.06765200 | 3.30456600 | -0.11846000 |
| B | 2.38674100 | -5.10497800 | -0.56003500 |

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|---|-------------|-------------|-------------|
| B | -5.63163000 | 0.65741600 | 0.59307900 |
| B | 3.49669400 | 4.58166000 | -0.47315100 |
| B | 4.64639800 | -4.27059600 | 0.20291800 |
| B | -5.33924400 | 3.13842700 | 0.39507400 |
| N | 5.45333100 | -3.14518500 | 0.53113900 |
| N | -4.49246200 | 4.22566500 | 0.05855000 |
| N | -2.23448800 | 5.17174500 | -0.57522300 |
| N | 5.76089400 | -0.62460400 | 0.65164600 |
| N | 6.03535700 | 1.88043500 | 0.36914000 |
| N | 0.06803900 | 6.11763600 | -0.95357600 |
| B | 0.18930300 | -5.83016700 | -1.52922100 |
| B | -5.90058500 | -1.86838600 | 0.32142200 |
| B | 5.50021300 | 3.16642200 | 0.07084200 |
| B | 1.48557800 | 6.00889100 | -0.92643000 |
| N | -5.26434600 | -3.08245500 | -0.07010200 |
| N | -3.24495200 | -4.29707700 | -1.02316100 |
| N | -1.19344900 | -5.54729300 | -1.68378000 |
| H | 6.21836200 | 4.11114800 | -0.02693400 |
| H | 4.20160300 | 5.52985000 | -0.61413800 |
| H | 2.17346000 | 6.96260500 | -1.11276700 |
| H | 2.84012000 | -6.18045800 | -0.78985900 |
| H | 5.12857700 | -5.35206800 | 0.07913400 |
| H | 0.65257600 | -6.86364600 | -1.89361200 |
| H | -7.07085800 | -1.82954200 | 0.53505100 |
| H | -6.79170700 | 0.79665500 | 0.81706200 |
| H | -6.49584800 | 3.30882300 | 0.62070200 |
| H | 6.44737700 | -3.30475800 | 0.62610600 |
| H | 6.76492500 | -0.73407900 | 0.70809000 |

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|---|-------------|-------------|-------------|
| H | 7.03844100 | 1.81146800 | 0.47516300 |
| H | -0.32344500 | 7.03500900 | -1.11879400 |
| H | -2.62892800 | 6.09839900 | -0.66640100 |
| H | -4.91333400 | 5.14410600 | 0.01572600 |
| H | -5.86120100 | -3.88600600 | -0.21641900 |
| H | -3.79759800 | -5.10033400 | -1.29136000 |
| H | -1.77642300 | -6.28110200 | -2.06364900 |

K@V_{BN} *h*-BN

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|---|-------------|-------------|-------------|
| K | 1.28622000 | -0.06862800 | 0.25286800 |
| B | -0.39939400 | -1.62933100 | 1.15478500 |
| B | -1.42966500 | 0.80072200 | 0.80019400 |
| B | 3.03198200 | -1.64737200 | -0.37151700 |
| B | 3.86850200 | 0.93178000 | -0.63115000 |
| B | 2.50632900 | 2.87064700 | -0.27829000 |
| B | -0.11189600 | 2.81606100 | 0.40648800 |
| B | -2.62222500 | 2.87397800 | 0.15992500 |
| B | -3.88796300 | 0.71124800 | 0.11932800 |
| B | -2.64430500 | -1.45732000 | 0.33523300 |
| B | -1.31464400 | -3.61745700 | 0.14719900 |
| B | 1.19705700 | -3.54486200 | 0.23286200 |
| N | -0.06916500 | -2.88512300 | 0.47741100 |
| N | 2.53052000 | -2.85155500 | 0.00614300 |
| N | -2.56580000 | -2.91069300 | 0.11493500 |
| N | -1.46744600 | -0.76145000 | 0.83678300 |
| N | -3.87264200 | -0.75247900 | 0.09038100 |
| N | -2.68298200 | 1.43336100 | 0.37713000 |
| N | -0.25937200 | 1.52544900 | 0.96110100 |
| N | -1.36466800 | 3.57810300 | 0.15334800 |

| | | | |
|---|-------------|-------------|-------------|
| N | 1.20173900 | 3.49323600 | 0.07348900 |
| N | 2.67605100 | 1.55417700 | -0.79862700 |
| N | 3.92524300 | -0.68409100 | -0.57694300 |
| B | 3.84585400 | -3.61566900 | 0.05368800 |
| B | 5.19943100 | -1.41596100 | -0.30037700 |
| B | 1.17807300 | 4.94521000 | 0.07679000 |
| B | -1.34035100 | 5.00754600 | -0.00921700 |
| B | -5.08288000 | -1.48030300 | -0.22642200 |
| B | -3.78645900 | -3.63676700 | -0.21294300 |
| N | -1.24640100 | -5.04902200 | -0.09718800 |
| N | 1.24758000 | -4.98613000 | 0.12016300 |
| N | 5.15471500 | 1.54898700 | -0.32746300 |
| N | 3.77340200 | 3.65679000 | -0.08124900 |
| N | -3.87586500 | 3.59386000 | -0.09602100 |
| N | -5.12819400 | 1.42407800 | -0.16110400 |
| B | 0.00471000 | -5.73498100 | -0.02472100 |
| B | 5.04775800 | 3.00389300 | -0.13259800 |
| B | -5.10851300 | 2.87227200 | -0.22774100 |
| B | -2.47631400 | -5.78441000 | -0.36068400 |
| B | 3.70346000 | 5.08933700 | 0.09644700 |
| N | -3.69272100 | -5.06638200 | -0.41429800 |
| N | 2.42293900 | 5.69278100 | 0.09574600 |
| N | -0.07113200 | 5.66616500 | 0.05331100 |
| N | -5.01241000 | -2.91754600 | -0.32893200 |
| N | -6.29462800 | -0.73928500 | -0.43242600 |
| N | -2.59524400 | 5.70610200 | -0.19590400 |
| B | 2.49105300 | -5.72230600 | 0.15173500 |
| B | 6.37260100 | 0.82559700 | -0.19018000 |

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|---|-------------|-------------|-------------|
| B | -6.34093600 | 0.68919400 | -0.41224800 |
| B | -3.84384700 | 5.03435200 | -0.25650100 |
| N | 6.37231600 | -0.63525300 | -0.22645200 |
| N | 5.06773200 | -2.85814300 | -0.07903000 |
| N | 3.73931600 | -5.02203200 | 0.19994600 |
| H | -7.37468700 | 1.25198200 | -0.61388300 |
| H | -6.13087800 | 3.45867900 | -0.41990400 |
| H | -4.85392600 | 5.64732800 | -0.44038300 |
| H | 0.05514400 | -6.92036800 | -0.11449900 |
| H | -2.44592400 | -6.96412500 | -0.53187700 |
| H | 2.49151200 | -6.91172100 | 0.14593100 |
| H | 7.41889000 | 1.37190800 | -0.01579600 |
| H | 6.05839600 | 3.62480900 | 0.01427300 |
| H | 4.69304300 | 5.75291400 | 0.21108500 |
| H | -4.53469600 | -5.58799200 | -0.61625400 |
| H | -5.85588100 | -3.42667500 | -0.55588800 |
| H | -7.15483600 | -1.23075400 | -0.63086000 |
| H | -2.59476700 | 6.71009000 | -0.31028800 |
| H | -0.03734600 | 6.67533300 | 0.00551500 |
| H | 2.37801800 | 6.69999900 | 0.16457500 |
| H | 7.26384500 | -1.08519700 | -0.06774300 |
| H | 5.92815200 | -3.38302700 | 0.02475800 |
| H | 4.58050800 | -5.58207400 | 0.23656200 |

K@V_{BN} *h*-BN (reactant)

| | | | |
|---|-------------|-------------|-------------|
| K | 0.43291700 | -1.28236800 | -2.41377500 |
| B | -1.56070800 | -0.34587800 | 0.03245800 |
| B | 0.62857400 | 1.11434900 | -0.01645300 |
| B | -1.40090600 | -2.22070200 | 0.25043100 |

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|---|-------------|-------------|-------------|
| B | 0.99797500 | -3.32428300 | 0.32086200 |
| B | 3.11454500 | -2.20577600 | -0.28767800 |
| B | 2.91718700 | 0.21675000 | -0.35298900 |
| B | 2.67363100 | 2.62708300 | 0.15865800 |
| B | 0.40434100 | 3.61316800 | 0.42547700 |
| B | -1.65935300 | 2.19661100 | 0.08262700 |
| B | -3.78428000 | 0.94142500 | -0.25315300 |
| B | -3.68001100 | -1.50612000 | -0.09387100 |
| N | -3.00240300 | -0.24869300 | -0.16181800 |
| N | -2.80764600 | -2.60443500 | 0.16579900 |
| N | -3.10583900 | 2.19226400 | -0.10975600 |
| N | -0.85668800 | 0.94554800 | 0.04002100 |
| N | -1.03697100 | 3.49311400 | 0.31173300 |
| N | 1.22666900 | 2.45130200 | 0.22238300 |
| N | 1.50810900 | 0.09029400 | -0.41053500 |
| N | 3.53559800 | 1.51950000 | -0.15076700 |
| N | 3.78152600 | -0.93977800 | -0.46267700 |
| N | 1.70036300 | -2.28576500 | -0.31477300 |
| N | -0.48175500 | -3.33830400 | 0.49107000 |
| B | -3.38501400 | -3.90073700 | 0.39202700 |
| B | -1.06511700 | -4.64294200 | 0.87869900 |
| B | 5.21404900 | -0.83038600 | -0.42022100 |
| B | 4.97791500 | 1.65330200 | -0.16813800 |
| B | -1.84344900 | 4.70216600 | 0.40957400 |
| B | -3.90515900 | 3.40363200 | -0.09867600 |
| N | -5.23182500 | 0.84469600 | -0.44238900 |
| N | -5.10913000 | -1.64216200 | -0.24707000 |
| N | 1.80728200 | -4.51302200 | 0.70877300 |

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|---|-------------|-------------|-------------|
| N | 3.92483200 | -3.40149900 | -0.03217600 |
| N | 3.27861400 | 3.93348300 | 0.41419800 |
| N | 1.01334500 | 4.91393500 | 0.69871600 |
| B | -5.88497100 | -0.44241200 | -0.45248600 |
| B | 3.23622100 | -4.54755700 | 0.48498800 |
| B | 2.44506200 | 5.05963400 | 0.71162200 |
| B | -6.00311300 | 2.06567300 | -0.51557200 |
| B | 5.36501500 | -3.32165100 | -0.12126500 |
| N | -5.32261400 | 3.30165600 | -0.34931600 |
| N | 5.97772000 | -2.05763500 | -0.37226900 |
| N | 5.79245500 | 0.48720500 | -0.38075000 |
| N | -3.25459600 | 4.63915000 | 0.17437600 |
| N | -1.20940700 | 5.95172000 | 0.73182600 |
| N | 5.52994100 | 2.96708100 | 0.05782100 |
| B | -5.68071600 | -2.96696300 | -0.10214800 |
| B | 1.19279200 | -5.68860300 | 1.25510100 |
| B | 0.19389500 | 6.08514300 | 0.88455800 |
| B | 4.71651500 | 4.09224500 | 0.35790100 |
| N | -0.22103800 | -5.71307200 | 1.33359000 |
| N | -2.47664100 | -4.91002400 | 0.79718800 |
| N | -4.81286500 | -4.05295000 | 0.21326100 |
| H | 0.67893500 | 7.14489800 | 1.14246900 |
| H | 2.93143800 | 6.12279800 | 0.94975000 |
| H | 5.21583900 | 5.15826800 | 0.56209100 |
| H | -7.06583300 | -0.51335100 | -0.60781300 |
| H | -7.18283300 | 2.03964600 | -0.69679200 |
| H | -6.85442900 | -3.14450300 | -0.23088300 |
| H | 1.83554600 | -6.62985600 | 1.61187500 |

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|---|-------------|-------------|-------------|
| H | 3.84749700 | -5.53779500 | 0.75579400 |
| H | 6.04208700 | -4.29576200 | 0.03168000 |
| H | -5.87501800 | 4.14752100 | -0.37387600 |
| H | -3.79616000 | 5.49104500 | 0.22029800 |
| H | -1.77966300 | 6.77895800 | 0.83728000 |
| H | 6.53137100 | 3.10061700 | 0.04244400 |
| H | 6.79791700 | 0.58420500 | -0.34072800 |
| H | 6.98756700 | -2.02231500 | -0.37782700 |
| H | -0.66083000 | -6.55764800 | 1.67143400 |
| H | -2.79907700 | -5.83990900 | 1.02644500 |
| H | -5.23362000 | -4.96294000 | 0.34120900 |

K@V_{BN} *h*-BN (product)

| | | | |
|---|-------------|-------------|-------------|
| K | 0.43313600 | -1.28050000 | 2.41392200 |
| B | -1.56061800 | -0.34648900 | -0.03269700 |
| B | 0.62815700 | 1.11452100 | 0.01599300 |
| B | -1.40007700 | -2.22117800 | -0.25093200 |
| B | 0.99923600 | -3.32408400 | -0.31997000 |
| B | 3.11524300 | -2.20474800 | 0.28909700 |
| B | 2.91708500 | 0.21775900 | 0.35255400 |
| B | 2.67267700 | 2.62776000 | -0.16031900 |
| B | 0.40294600 | 3.61324600 | -0.42570200 |
| B | -1.66014500 | 2.19599700 | -0.08195100 |
| B | -3.78462500 | 0.93998200 | 0.25335600 |
| B | -3.67954700 | -1.50745100 | 0.09259600 |
| N | -3.00237800 | -0.24983300 | 0.16128700 |
| N | -2.80676000 | -2.60534400 | -0.16735900 |
| N | -3.10657600 | 2.19113400 | 0.11081200 |
| N | -0.85707400 | 0.94519100 | -0.03988900 |

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|---|-------------|-------------|-------------|
| N | -1.03822900 | 3.49278200 | -0.31081600 |
| N | 1.22572900 | 2.45157500 | -0.22330900 |
| N | 1.50807700 | 0.09077100 | 0.40986800 |
| N | 3.53503700 | 1.52059300 | 0.14946900 |
| N | 3.78177100 | -0.93841000 | 0.46334700 |
| N | 1.70106200 | -2.28524500 | 0.31579400 |
| N | -0.48041300 | -3.33853300 | -0.49097500 |
| B | -3.38362400 | -3.90178400 | -0.39406300 |
| B | -1.06317900 | -4.64335200 | -0.87886600 |
| B | 5.21426000 | -0.82854400 | 0.42093100 |
| B | 4.97732200 | 1.65483700 | 0.16656200 |
| B | -1.84508400 | 4.70167600 | -0.40758500 |
| B | -3.90625100 | 3.40227800 | 0.10064300 |
| N | -5.23215000 | 0.84267100 | 0.44249200 |
| N | -5.10865600 | -1.64401600 | 0.24547900 |
| N | 1.80913000 | -4.51262000 | -0.70725200 |
| N | 3.92599100 | -3.40036800 | 0.03455600 |
| N | 3.27717200 | 3.93419100 | -0.41681300 |
| N | 1.01144500 | 4.91416300 | -0.69934600 |
| B | -5.88488100 | -0.44465000 | 0.45161400 |
| B | 3.23794900 | -4.54670400 | -0.48270700 |
| B | 2.44312000 | 5.06010400 | -0.71375600 |
| B | -6.00378400 | 2.06336700 | 0.51660700 |
| B | 5.36613600 | -3.31996100 | 0.12392200 |
| N | -5.32365800 | 3.29968200 | 0.35127100 |
| N | 5.97835800 | -2.05557900 | 0.37418400 |
| N | 5.79222400 | 0.48920600 | 0.38026600 |
| N | -3.25606900 | 4.63818100 | -0.17157700 |

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|---|-------------|-------------|-------------|
| N | -1.21154400 | 5.95153100 | -0.72966800 |
| N | 5.52889300 | 2.96858100 | -0.06073300 |
| B | -5.67977600 | -2.96893900 | 0.09981100 |
| B | 1.19527100 | -5.68859000 | -1.25347600 |
| B | 0.19156000 | 6.08526800 | -0.88395300 |
| B | 4.71506800 | 4.09331500 | -0.36132000 |
| N | -0.21848500 | -5.71356400 | -1.33245700 |
| N | -2.47472800 | -4.91072900 | -0.79883700 |
| N | -4.81151000 | -4.05446900 | -0.21596800 |
| H | 0.67610700 | 7.14518900 | -1.14211100 |
| H | 2.92907600 | 6.12329300 | -0.95264600 |
| H | 5.21404000 | 5.15930300 | -0.56655300 |
| H | -7.06573400 | -0.51606300 | 0.60681400 |
| H | -7.18350600 | 2.03686600 | 0.69775800 |
| H | -6.85346800 | -3.14691200 | 0.22814200 |
| H | 1.83852100 | -6.62965900 | -1.60984600 |
| H | 3.84964400 | -5.53680400 | -0.75308100 |
| H | 6.04356700 | -4.29395800 | -0.02817500 |
| H | -5.87635100 | 4.14534200 | 0.37644700 |
| H | -3.79790200 | 5.48994000 | -0.21688600 |
| H | -1.78206900 | 6.77868800 | -0.83431300 |
| H | 6.53029200 | 3.10242200 | -0.04580200 |
| H | 6.79765500 | 0.58648800 | 0.34010300 |
| H | 6.98819500 | -2.01994100 | 0.37989600 |
| H | -0.65783200 | -6.55834000 | -1.67039300 |
| H | -2.79670500 | -5.84073400 | -1.02824300 |
| H | -5.23193400 | -4.96455100 | -0.34435800 |

$K^+@V_{BN} h\text{-BN}$

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|---|-------------|-------------|-------------|
| K | 1.24114900 | -0.14003800 | 0.09589600 |
| B | -0.61448700 | -1.70776800 | 0.62262900 |
| B | -1.40517400 | 0.91440500 | 0.68710900 |
| B | 3.08831400 | -1.70639300 | -0.40781400 |
| B | 3.91176300 | 0.91109500 | -0.48713900 |
| B | 2.55920800 | 2.87232400 | -0.18013900 |
| B | -0.05997900 | 2.87039600 | 0.35842600 |
| B | -2.58916700 | 2.94707900 | 0.10706200 |
| B | -3.89209500 | 0.78009800 | 0.12751800 |
| B | -2.72304300 | -1.43948100 | 0.34317600 |
| B | -1.39034600 | -3.65983900 | 0.12038200 |
| B | 1.22965600 | -3.59760400 | 0.06969400 |
| N | -0.05933000 | -2.90165100 | 0.28167700 |
| N | 2.53513800 | -2.91582000 | -0.11340900 |
| N | -2.61282900 | -2.89864600 | 0.15368200 |
| N | -1.46036600 | -0.70370600 | 0.71587100 |
| N | -3.90592500 | -0.70360300 | 0.15723400 |
| N | -2.66784500 | 1.49352800 | 0.31633100 |
| N | -0.21212700 | 1.53953400 | 0.85822700 |
| N | -1.31607500 | 3.62309100 | 0.11477300 |
| N | 1.24972500 | 3.52524700 | 0.08203400 |
| N | 2.71712700 | 1.52966500 | -0.64320100 |
| N | 3.95257400 | -0.71807300 | -0.50282300 |
| B | 3.85555700 | -3.70061400 | -0.02918000 |
| B | 5.22638400 | -1.47741400 | -0.22108900 |
| B | 1.24277000 | 4.98313800 | 0.05991500 |
| B | -1.27828400 | 5.05991700 | -0.06832300 |

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|---|-------------|-------------|-------------|
| B | -5.14780600 | -1.42967600 | -0.10053900 |
| B | -3.87894500 | -3.62641300 | -0.07749400 |
| N | -1.31770000 | -5.07271100 | -0.04743800 |
| N | 1.20693100 | -5.02400700 | 0.03301100 |
| N | 5.19184300 | 1.50641400 | -0.16748800 |
| N | 3.82464500 | 3.63619900 | 0.02698300 |
| N | -3.83523200 | 3.65941900 | -0.14467100 |
| N | -5.11775900 | 1.49296500 | -0.13709000 |
| B | -0.05568300 | -5.76380600 | -0.02864000 |
| B | 5.09561900 | 2.96947800 | 0.01922300 |
| B | -5.07826500 | 2.94954200 | -0.24448900 |
| B | -2.58560900 | -5.80198800 | -0.20642700 |
| B | 3.76872100 | 5.07899700 | 0.16726900 |
| N | -3.78920400 | -5.05885300 | -0.22099700 |
| N | 2.49682100 | 5.70172000 | 0.10850100 |
| N | -0.00384500 | 5.70375000 | -0.00971400 |
| N | -5.08287200 | -2.87533300 | -0.15527700 |
| N | -6.33441700 | -0.66695100 | -0.29310800 |
| N | -2.52863300 | 5.75659900 | -0.27085300 |
| B | 2.45261700 | -5.78976900 | 0.05127200 |
| B | 6.40040800 | 0.76700800 | -0.01675500 |
| B | -6.35273800 | 0.76943000 | -0.32452600 |
| B | -3.78732100 | 5.10531600 | -0.32280900 |
| N | 6.38518100 | -0.70046600 | -0.07710900 |
| N | 5.07181800 | -2.93579200 | -0.08152200 |
| N | 3.70653700 | -5.10652100 | 0.07849400 |
| H | -7.37900700 | 1.34026700 | -0.51566000 |
| H | -6.09585200 | 3.53641200 | -0.43703100 |

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|---|-------------|-------------|-------------|
| H | -4.78989800 | 5.72212100 | -0.51137900 |
| H | -0.02368500 | -6.94713000 | -0.08459400 |
| H | -2.57478200 | -6.98313900 | -0.32653300 |
| H | 2.42140400 | -6.97465600 | 0.06060000 |
| H | 7.44673000 | 1.29488000 | 0.18764000 |
| H | 6.10703000 | 3.57661200 | 0.18923200 |
| H | 4.76268300 | 5.72648500 | 0.29866100 |
| H | -4.64366100 | -5.58512700 | -0.35302500 |
| H | -5.94651300 | -3.37631600 | -0.32167300 |
| H | -7.21587900 | -1.13654200 | -0.45110500 |
| H | -2.52107400 | 6.75968200 | -0.39754800 |
| H | 0.03581700 | 6.71252600 | -0.06888400 |
| H | 2.47362500 | 6.71144200 | 0.15352300 |
| H | 7.27591400 | -1.15307300 | 0.08468000 |
| H | 5.93041200 | -3.46615400 | 0.02196500 |
| H | 4.53527700 | -5.68682800 | 0.12272800 |

$K^+@V_{BN}$ *h*-BN (reactant)

| | | | |
|---|-------------|-------------|-------------|
| K | 0.75988700 | -1.98808300 | -2.31335700 |
| B | -1.63477300 | -0.21759400 | -0.08818700 |
| B | 0.66723500 | 0.86704800 | 0.07815600 |
| B | -1.61528100 | -1.97406900 | -0.18407400 |
| B | 0.57697900 | -2.86517500 | 0.81006200 |
| B | 2.90954900 | -2.15585400 | 0.56988300 |
| B | 2.90891600 | -0.13452700 | -0.41273800 |
| B | 2.77358000 | 2.28048600 | -0.50397400 |
| B | 0.71221400 | 3.40955700 | 0.28277600 |
| B | -1.46954600 | 2.22316000 | 0.40780000 |
| B | -3.71914700 | 1.25194500 | -0.04387800 |

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|---|-------------|-------------|-------------|
| B | -3.76661400 | -1.13523800 | -0.64910300 |
| N | -3.02455900 | 0.04611900 | -0.34181600 |
| N | -2.93292400 | -2.30630800 | -0.66270900 |
| N | -2.91412800 | 2.35048500 | 0.39273000 |
| N | -0.78154700 | 0.91224100 | 0.20504800 |
| N | -0.69217800 | 3.41837300 | 0.60179300 |
| N | 1.38432000 | 2.14777500 | -0.06593000 |
| N | 1.49644100 | -0.37736200 | -0.09256800 |
| N | 3.52609500 | 1.08576800 | -0.76913400 |
| N | 3.70685900 | -1.27862200 | -0.19077800 |
| N | 1.49943800 | -1.74815100 | 0.54283700 |
| N | -0.76398600 | -3.05906200 | 0.25267100 |
| B | -3.55873200 | -3.59900200 | -0.66732800 |
| B | -1.43166600 | -4.39315700 | 0.36805900 |
| B | 5.14794700 | -1.27609000 | -0.17414300 |
| B | 4.98365900 | 1.10653800 | -0.93927400 |
| B | -1.35730200 | 4.67364700 | 0.96269900 |
| B | -3.59219300 | 3.59250100 | 0.72860600 |
| N | -5.16658700 | 1.28385500 | -0.16577400 |
| N | -5.18870800 | -1.15619700 | -0.79614100 |
| N | 1.17210300 | -3.97224100 | 1.58172000 |
| N | 3.50359700 | -3.25934100 | 1.25004700 |
| N | 3.44961300 | 3.55027600 | -0.63856500 |
| N | 1.44738100 | 4.66496200 | 0.28969300 |
| B | -5.89880100 | 0.09545200 | -0.56094500 |
| B | 2.57892500 | -4.13245800 | 1.90273500 |
| B | 2.79124100 | 4.75255000 | -0.20599600 |
| B | -5.83183000 | 2.52423400 | 0.19565200 |

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|---|-------------|-------------|-------------|
| B | 4.95824300 | -3.38132700 | 1.20411700 |
| N | -5.03022400 | 3.61763900 | 0.63839800 |
| N | 5.73670600 | -2.42008100 | 0.47648600 |
| N | 5.75709500 | -0.10084200 | -0.72612100 |
| N | -2.78182300 | 4.70599700 | 1.10152800 |
| N | -0.54917000 | 5.84604700 | 1.12947900 |
| N | 5.56372000 | 2.38336900 | -1.22851500 |
| B | -5.79762200 | -2.46163400 | -1.00880700 |
| B | 0.41528600 | -5.18282500 | 1.85290200 |
| B | 0.81735100 | 5.88573400 | 0.76112800 |
| B | 4.83734600 | 3.60025800 | -1.06155200 |
| N | -0.80577200 | -5.39260900 | 1.17242000 |
| N | -2.69700300 | -4.66752400 | -0.25845500 |
| N | -4.96720600 | -3.63607800 | -0.96900700 |
| H | 1.43774200 | 6.89962500 | 0.82460900 |
| H | 3.35572300 | 5.79810000 | -0.25140600 |
| H | 5.37653100 | 4.64730400 | -1.23384800 |
| H | -7.08371400 | 0.13160600 | -0.66741500 |
| H | -7.01654100 | 2.62700100 | 0.12886500 |
| H | -6.97074000 | -2.56876300 | -1.18241500 |
| H | 0.83996600 | -6.01066200 | 2.59239700 |
| H | 2.94749800 | -5.00386200 | 2.61971200 |
| H | 5.49389000 | -4.27989600 | 1.77223100 |
| H | -5.51775500 | 4.47098000 | 0.87693100 |
| H | -3.22260200 | 5.58504800 | 1.33711700 |
| H | -0.98154800 | 6.71117800 | 1.42331600 |
| H | 6.55048700 | 2.45994600 | -1.43501700 |
| H | 6.76537100 | -0.02129800 | -0.75567400 |

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|---|-------------|-------------|-------------|
| H | 6.74151000 | -2.52710100 | 0.52098800 |
| H | -1.29343200 | -6.26128000 | 1.34542700 |
| H | -3.07210200 | -5.60065000 | -0.14515500 |
| H | -5.44583500 | -4.52391300 | -1.04511000 |

$K^+@V_{BN}$ *h*-BN (product)

| | | | |
|---|-------------|-------------|-------------|
| K | 0.28260700 | -0.74405500 | 2.59831800 |
| B | -1.58962400 | -0.44000600 | 0.04961300 |
| B | 0.62373000 | 0.82668800 | -0.20574100 |
| B | -1.42714800 | -2.10678900 | -0.47949500 |
| B | 0.93604100 | -2.99000200 | -0.23672300 |
| B | 3.01078100 | -2.01350500 | 0.71646800 |
| B | 2.97662100 | 0.12465500 | 0.01951400 |
| B | 2.63938300 | 2.38046900 | -0.75874900 |
| B | 0.38664800 | 3.35411800 | -0.56108100 |
| B | -1.59185900 | 2.05625400 | 0.24884100 |
| B | -3.74006500 | 0.83316500 | 0.59860800 |
| B | -3.69343200 | -1.51981500 | -0.10603900 |
| N | -2.99276100 | -0.35023000 | 0.34463200 |
| N | -2.80143500 | -2.51260600 | -0.60936000 |
| N | -2.99397500 | 2.05843100 | 0.62848100 |
| N | -0.80769800 | 0.78015200 | 0.12271900 |
| N | -0.96883000 | 3.31580000 | -0.05817400 |
| N | 1.20678400 | 2.13850700 | -0.55298100 |
| N | 1.58214700 | -0.29846900 | -0.08354600 |
| N | 3.54616300 | 1.34435700 | -0.38818800 |
| N | 3.78887200 | -0.85121000 | 0.62430200 |
| N | 1.60639800 | -1.76602600 | 0.31055800 |
| N | -0.41746600 | -3.09748000 | -0.74999300 |

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|---|-------------|-------------|-------------|
| B | -3.31223000 | -3.72829900 | -1.16876000 |
| B | -0.90694600 | -4.38790800 | -1.31479600 |
| B | 5.22409600 | -0.78766800 | 0.70000200 |
| B | 4.99652700 | 1.50326000 | -0.32855900 |
| B | -1.74095100 | 4.55906000 | 0.05214300 |
| B | -3.75525300 | 3.29025800 | 0.79259700 |
| N | -5.18529900 | 0.74268000 | 0.71028600 |
| N | -5.11732700 | -1.63944300 | -0.10545200 |
| N | 1.70061600 | -4.24372800 | -0.09039000 |
| N | 3.64350400 | -3.24695300 | 1.06132900 |
| N | 3.19436700 | 3.62830400 | -1.22258200 |
| N | 0.93948400 | 4.61724100 | -1.02789600 |
| B | -5.87547900 | -0.49104400 | 0.36572300 |
| B | 2.95838900 | -4.41613500 | 0.60702500 |
| B | 2.31800100 | 4.74687200 | -1.42489900 |
| B | -5.90258000 | 1.96571000 | 1.02296800 |
| B | 5.08253300 | -3.21717300 | 1.34344300 |
| N | -5.15806700 | 3.18049900 | 1.10056000 |
| N | 5.83053100 | -2.00431900 | 1.18537500 |
| N | 5.80812400 | 0.43759300 | 0.23049900 |
| N | -3.06926800 | 4.52227400 | 0.58513000 |
| N | -1.14388500 | 5.77784000 | -0.40333700 |
| N | 5.49685200 | 2.74292000 | -0.84586600 |
| B | -5.65341200 | -2.87716200 | -0.66458500 |
| B | 1.26809100 | -5.44722000 | -0.79023100 |
| B | 0.14964000 | 5.83307800 | -0.97878400 |
| B | 4.63734400 | 3.78720800 | -1.30853400 |
| N | 0.04605900 | -5.44042400 | -1.49274300 |

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|---|-------------|-------------|-------------|
| N | -2.29416200 | -4.62690800 | -1.61520000 |
| N | -4.74912500 | -3.86875400 | -1.17884600 |
| H | 0.58875800 | 6.85926200 | -1.39133600 |
| H | 2.73177500 | 5.77447100 | -1.85616600 |
| H | 5.10190100 | 4.79881500 | -1.73067700 |
| H | -7.06218300 | -0.54593700 | 0.43791900 |
| H | -7.08141900 | 1.96345200 | 1.19114500 |
| H | -6.82890900 | -3.06458700 | -0.70320100 |
| H | 1.94468500 | -6.42481800 | -0.76978500 |
| H | 3.43269800 | -5.49582600 | 0.74769400 |
| H | 5.63572000 | -4.22183700 | 1.66322100 |
| H | -5.68604100 | 4.02647300 | 1.26928800 |
| H | -3.58311800 | 5.39084600 | 0.65095000 |
| H | -1.67625100 | 6.63617000 | -0.36266600 |
| H | 6.49205100 | 2.91736300 | -0.88367100 |
| H | 6.81285100 | 0.55536700 | 0.23802800 |
| H | 6.82975900 | -2.06826500 | 1.32839300 |
| H | -0.24155200 | -6.30276600 | -1.93503900 |
| H | -2.53582800 | -5.52858500 | -2.00474700 |
| H | -5.17288300 | -4.70323700 | -1.56244400 |

K@V_{N2B} *h*-BN

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|---|-------------|-------------|-------------|
| K | -0.00024900 | -1.42275800 | 0.30980100 |
| B | 1.43906700 | 0.57246000 | 0.07685300 |
| B | -1.43877200 | 0.57303500 | 0.07696800 |
| B | 0.00056500 | 2.69855800 | -0.15045100 |
| B | -2.52403000 | 2.87052300 | -0.06169500 |
| B | -3.84598900 | 0.78615500 | 0.24108100 |
| B | -2.50657100 | -1.22013600 | 0.22591400 |

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|---|-------------|-------------|-------------|
| B | -1.16371800 | -3.76268700 | 0.29470800 |
| B | 1.16222100 | -3.76314400 | 0.29447500 |
| B | 2.50612500 | -1.22112900 | 0.22551100 |
| B | 3.84635400 | 0.78461500 | 0.24107200 |
| B | 2.52520300 | 2.86957400 | -0.06110900 |
| N | 2.56263000 | 1.44573000 | 0.08815400 |
| N | 0.00027500 | 1.18022400 | 0.00056800 |
| N | 1.23716800 | 3.48536400 | -0.22288200 |
| N | 3.81533800 | -0.64009100 | 0.30748500 |
| N | 2.35665300 | -2.69822800 | 0.21239200 |
| N | -0.00063300 | -3.58379300 | 1.04231000 |
| N | -2.35772600 | -2.69729700 | 0.21282100 |
| N | -3.81553000 | -0.63854100 | 0.30787400 |
| N | -2.56201200 | 1.44672600 | 0.08796700 |
| N | -1.23573700 | 3.48579800 | -0.22335000 |
| B | 1.23838600 | 4.93201900 | -0.42786700 |
| B | -1.23637600 | 4.93242600 | -0.42855300 |
| B | -5.04625300 | -1.38541100 | 0.41154900 |
| B | -3.64442000 | -3.41965800 | 0.03538300 |
| B | 3.64301200 | -3.42112100 | 0.03463200 |
| B | 5.04575100 | -1.38748100 | 0.41094600 |
| N | 5.08385100 | 1.52099600 | 0.31017300 |
| N | 3.77687100 | 3.61725700 | -0.04784700 |
| N | -3.77542800 | 3.61867000 | -0.04885600 |
| N | -5.08321600 | 1.52304400 | 0.30995100 |
| N | -1.25287200 | -4.91201200 | -0.63586000 |
| N | 1.25071000 | -4.91249200 | -0.63614400 |
| B | 5.04153100 | 2.95101800 | 0.15803900 |

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|---|-------------|-------------|-------------|
| B | -5.04034900 | 2.95298700 | 0.15723800 |
| B | -0.00124300 | -5.53375700 | -1.00561900 |
| B | 6.32290200 | 0.78134600 | 0.48966700 |
| B | -6.32255200 | 0.78393000 | 0.48968400 |
| N | 6.27348700 | -0.63894200 | 0.55084800 |
| N | -6.27368000 | -0.63636500 | 0.55131700 |
| N | -4.91901800 | -2.79224200 | 0.30656100 |
| N | 4.91794900 | -2.79422200 | 0.30561500 |
| N | 3.66678100 | -4.77576000 | -0.45333600 |
| N | -3.66883100 | -4.77434200 | -0.45245900 |
| B | 3.74933900 | 5.04500600 | -0.25938300 |
| B | -3.74735000 | 5.04632600 | -0.26096300 |
| B | 2.52429200 | -5.47891200 | -0.94106000 |
| B | -2.52674600 | -5.47795400 | -0.94046000 |
| N | -2.48277300 | 5.65095500 | -0.46549900 |
| N | 0.00115600 | 5.61538000 | -0.57724100 |
| N | 2.48502500 | 5.65015700 | -0.46399500 |
| H | 2.64907800 | -6.50199100 | -1.54654400 |
| H | -0.00151100 | -6.53902500 | -1.65283800 |
| H | -2.65207500 | -6.50100000 | -1.54588800 |
| H | 6.04856900 | 3.58760100 | 0.19259800 |
| H | 7.36348000 | 1.35896900 | 0.57460500 |
| H | 4.75048400 | 5.69256300 | -0.26534800 |
| H | -4.74827100 | 5.69422400 | -0.26742900 |
| H | -6.04715000 | 3.58996300 | 0.19148900 |
| H | -7.36290700 | 1.36198000 | 0.57443800 |
| H | 7.14933300 | -1.13240400 | 0.65506000 |
| H | 5.74425900 | -3.37491500 | 0.25953800 |

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|---|-------------|-------------|-------------|
| H | 4.57254900 | -5.19257100 | -0.61929800 |
| H | -4.57480500 | -5.19080700 | -0.61816100 |
| H | -5.74556400 | -3.37261400 | 0.26068800 |
| H | -7.14971700 | -1.12946400 | 0.65564900 |
| H | -2.45659400 | 6.65054400 | -0.61176300 |
| H | 0.00136200 | 6.61678600 | -0.71184700 |
| H | 2.45923600 | 6.64980300 | -0.60994000 |

K@V_{N2B} *h*-BN (reactant)

| | | | |
|---|-------------|-------------|-------------|
| K | 0.00112700 | -0.71999700 | 2.48802100 |
| B | -1.35584600 | 0.36332400 | -0.23225100 |
| B | 1.35668200 | 0.36024900 | -0.23201500 |
| B | 0.00279300 | 2.48128900 | 0.28676100 |
| B | 2.44699600 | 2.70575300 | -0.07824100 |
| B | 3.67429300 | 0.72422000 | -0.83691400 |
| B | 2.35676400 | -1.20117500 | -0.35373000 |
| B | 1.16615100 | -3.28542400 | 0.53306800 |
| B | -1.17366900 | -3.28203300 | 0.53864500 |
| B | -2.36048100 | -1.19576100 | -0.34848100 |
| B | -3.67195600 | 0.73187600 | -0.84012200 |
| B | -2.43952900 | 2.71236700 | -0.08749600 |
| N | -2.42398100 | 1.33418400 | -0.43980700 |
| N | 0.00112300 | 0.98030000 | 0.03275100 |
| N | -1.21795400 | 3.26689900 | 0.41751000 |
| N | -3.62777100 | -0.68326700 | -0.87237700 |
| N | -2.39175200 | -2.58891000 | 0.02936600 |
| N | -0.00219500 | -2.55612200 | 0.75075300 |
| N | 2.38443900 | -2.59544900 | 0.02004100 |
| N | 3.62535900 | -0.69055900 | -0.87649600 |

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|---|-------------|-------------|-------------|
| N | 2.42806500 | 1.32866100 | -0.43445800 |
| N | 1.22542800 | 3.26300300 | 0.42371800 |
| B | -1.22838100 | 4.65742400 | 0.84542500 |
| B | 1.23830600 | 4.65322600 | 0.85250000 |
| B | 4.83884200 | -1.43024100 | -1.08410600 |
| B | 3.59703000 | -3.39213600 | -0.20127300 |
| B | -3.60737100 | -3.38238200 | -0.18680900 |
| B | -4.84371500 | -1.41995000 | -1.07632400 |
| N | -4.87540100 | 1.49298300 | -1.08407900 |
| N | -3.66751800 | 3.49316900 | -0.21131000 |
| N | 3.67777600 | 3.48299800 | -0.19656400 |
| N | 4.88038500 | 1.48259900 | -1.07629000 |
| N | 1.23442300 | -4.75805600 | 0.73046300 |
| N | -1.24566500 | -4.75420900 | 0.73776400 |
| B | -4.86561600 | 2.89439400 | -0.76205800 |
| B | 4.87487000 | 2.88250400 | -0.74765100 |
| B | -0.00616000 | -5.45785400 | 0.92205800 |
| B | -6.06621000 | 0.75350000 | -1.47287100 |
| B | 6.06880100 | 0.74115200 | -1.46867100 |
| N | -6.01503300 | -0.66906700 | -1.49022800 |
| N | 6.01270500 | -0.68110900 | -1.49403700 |
| N | 4.78242200 | -2.81880400 | -0.79417200 |
| N | -4.79193600 | -2.80725400 | -0.77954500 |
| N | -3.63290200 | -4.76574900 | 0.20752000 |
| N | 3.61903200 | -4.77679400 | 0.18861600 |
| B | -3.67795300 | 4.84988800 | 0.27898200 |
| B | 3.69092700 | 4.83846000 | 0.29715100 |
| B | -2.47553100 | -5.47720900 | 0.63384600 |

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|---|-------------|-------------|-------------|
| B | 2.46129400 | -5.48503400 | 0.61922400 |
| N | 2.49103300 | 5.36367300 | 0.85468500 |
| N | 0.00498700 | 5.27724800 | 1.21437600 |
| N | -2.47855400 | 5.37228400 | 0.84018300 |
| H | -2.54565300 | -6.64708700 | 0.87654800 |
| H | -0.00725400 | -6.62717200 | 1.17730300 |
| H | 2.52862000 | -6.65554000 | 0.85967700 |
| H | -5.84567600 | 3.55778300 | -0.91282500 |
| H | -7.07683600 | 1.33003300 | -1.74283500 |
| H | -4.66327300 | 5.52110500 | 0.22440500 |
| H | 4.67867700 | 5.50651300 | 0.24789000 |
| H | 5.85741500 | 3.54325400 | -0.89380600 |
| H | 7.08150700 | 1.31567600 | -1.73510700 |
| H | -6.87088000 | -1.16098300 | -1.70747000 |
| H | -5.60740800 | -3.39360100 | -0.89229300 |
| H | -4.49084300 | -5.28703400 | 0.09315900 |
| H | 4.47482300 | -5.30064200 | 0.06994600 |
| H | 5.59595400 | -3.40728100 | -0.90980300 |
| H | 6.86696500 | -1.17472200 | -1.71366200 |
| H | 2.50573100 | 6.32355200 | 1.17051000 |
| H | 0.00588600 | 6.25266200 | 1.47964500 |
| H | -2.49143000 | 6.33271100 | 1.15441300 |

K@V_{N2B} *h*-BN (product)

| | | | |
|---|-------------|-------------|-------------|
| K | -0.00032700 | -1.42282700 | -0.30967500 |
| B | -1.43872200 | 0.57313600 | -0.07688800 |
| B | 1.43903100 | 0.57247000 | -0.07699200 |
| B | 0.00064600 | 2.69859100 | 0.15052200 |
| B | 2.52528200 | 2.86950800 | 0.06103300 |

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|---|-------------|-------------|-------------|
| B | 3.84633800 | 0.78450700 | -0.24133400 |
| B | 2.50607300 | -1.22120900 | -0.22562500 |
| B | 1.16214800 | -3.76322100 | -0.29431800 |
| B | -1.16380100 | -3.76272500 | -0.29474500 |
| B | -2.50660900 | -1.22005600 | -0.22596600 |
| B | -3.84594800 | 0.78628600 | -0.24108300 |
| B | -2.52393800 | 2.87062100 | 0.06176400 |
| N | -2.56195600 | 1.44683700 | -0.08790500 |
| N | 0.00029200 | 1.18026000 | -0.00056400 |
| N | -1.23562600 | 3.48585800 | 0.22346000 |
| N | -3.81554400 | -0.63842100 | -0.30795500 |
| N | -2.35781400 | -2.69723300 | -0.21290300 |
| N | -0.00066000 | -3.58383400 | -1.04223600 |
| N | 2.35660000 | -2.69830400 | -0.21227500 |
| N | 3.81528600 | -0.64020500 | -0.30766200 |
| N | 2.56264600 | 1.44567600 | -0.08834200 |
| N | 1.23728100 | 3.48533000 | 0.22298500 |
| B | -1.23621000 | 4.93247900 | 0.42867100 |
| B | 1.23855600 | 4.93196600 | 0.42809100 |
| B | 5.04569800 | -1.38764000 | -0.41101400 |
| B | 3.64294000 | -3.42119800 | -0.03443900 |
| B | -3.64453300 | -3.41957100 | -0.03552800 |
| B | -5.04629200 | -1.38524900 | -0.41165800 |
| N | -5.08314400 | 1.52321800 | -0.30997100 |
| N | -3.77530300 | 3.61881400 | 0.04888000 |
| N | 3.77697200 | 3.61715000 | 0.04770200 |
| N | 5.08386200 | 1.52085600 | -0.31052900 |
| N | 1.25056400 | -4.91253000 | 0.63632900 |

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|---|-------------|-------------|-------------|
| N | -1.25304100 | -4.91204700 | 0.63581400 |
| B | -5.04023900 | 2.95316600 | -0.15725200 |
| B | 5.04159300 | 2.95088000 | -0.15836600 |
| B | -0.00143600 | -5.53379400 | 1.00568900 |
| B | -6.32250200 | 0.78414900 | -0.48974400 |
| B | 6.32288800 | 0.78115200 | -0.48998400 |
| N | -6.27368900 | -0.63614800 | -0.55140200 |
| N | 6.27344000 | -0.63915200 | -0.55100900 |
| N | 4.91785700 | -2.79438400 | -0.30551200 |
| N | -4.91910400 | -2.79208900 | -0.30669800 |
| N | -3.66900500 | -4.77427100 | 0.45227900 |
| N | 3.66665800 | -4.77578900 | 0.45369900 |
| B | -3.74717100 | 5.04647500 | 0.26095000 |
| B | 3.74950800 | 5.04487300 | 0.25944200 |
| B | -2.52696600 | -5.47794900 | 0.94030500 |
| B | 2.52413900 | -5.47892200 | 0.94137900 |
| N | 2.48523500 | 5.65003700 | 0.46429600 |
| N | 0.00135000 | 5.61536500 | 0.57747700 |
| N | -2.48257500 | 5.65106100 | 0.46551700 |
| H | -2.65236900 | -6.50101800 | 1.54568000 |
| H | -0.00176700 | -6.53907300 | 1.65289000 |
| H | 2.64888100 | -6.50197400 | 1.54691800 |
| H | -6.04701900 | 3.59017100 | -0.19154900 |
| H | -7.36283400 | 1.36224100 | -0.57451100 |
| H | -4.74806200 | 5.69442000 | 0.26734800 |
| H | 4.75067500 | 5.69239500 | 0.26538500 |
| H | 6.04864400 | 3.58743800 | -0.19301600 |
| H | 7.36348100 | 1.35873700 | -0.57499600 |

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|---|-------------|-------------|-------------|
| H | -7.14974600 | -1.12920800 | -0.65574500 |
| H | -5.74567700 | -3.37242600 | -0.26085700 |
| H | -4.57500000 | -5.19070500 | 0.61794600 |
| H | 4.57241500 | -5.19259800 | 0.61972900 |
| H | 5.74415000 | -3.37509700 | -0.25939800 |
| H | 7.14927700 | -1.13264900 | -0.65512900 |
| H | 2.45949700 | 6.64966500 | 0.61037100 |
| H | 0.00158800 | 6.61676800 | 0.71211100 |
| H | -2.45636300 | 6.65065500 | 0.61174900 |

H₂O-Li@V_{N₂B} *h*-BN-H₂O

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.00864900 | -1.00756900 | -0.25465500 |
| B | -1.43452100 | 0.43161300 | 0.04073800 |
| B | 1.36912000 | 0.55957500 | 0.04307600 |
| B | -0.13624400 | 2.62329600 | -0.22335600 |
| B | 2.32659200 | 2.94060300 | 0.09686700 |
| B | 3.73412400 | 0.95419400 | 0.43099700 |
| B | 2.50414400 | -1.07463500 | 0.00847200 |
| B | 1.37617900 | -3.37520600 | -0.44707400 |
| B | -1.04185800 | -3.49595200 | -0.34101300 |
| B | -2.38265400 | -1.31733400 | 0.13070100 |
| B | -3.83053000 | 0.59156100 | 0.38486100 |
| B | -2.63582900 | 2.69129000 | -0.08326400 |
| N | -2.58857100 | 1.28063400 | 0.13370800 |
| N | -0.06333400 | 1.11050300 | -0.05391500 |
| N | -1.39703500 | 3.35341300 | -0.35482800 |
| N | -3.71422400 | -0.82282500 | 0.43349500 |
| N | -2.30145900 | -2.76728100 | -0.03983700 |
| N | 0.13317600 | -2.76688500 | -0.45485700 |

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|---|-------------|-------------|-------------|
| N | 2.57183400 | -2.52005400 | -0.21028500 |
| N | 3.78161600 | -0.46216700 | 0.32597100 |
| N | 2.42325700 | 1.52042500 | 0.22786300 |
| N | 1.04596800 | 3.48318600 | -0.23884700 |
| B | -1.46710700 | 4.77607400 | -0.66467500 |
| B | 0.98879300 | 4.91193100 | -0.52346300 |
| B | 5.05579200 | -1.13202300 | 0.43643100 |
| B | 3.85839100 | -3.22358300 | -0.14783200 |
| B | -3.49639900 | -3.59956800 | 0.13505400 |
| B | -4.90320700 | -1.61776900 | 0.62586900 |
| N | -5.09041600 | 1.27790900 | 0.54350500 |
| N | -3.91596000 | 3.39191800 | -0.03819700 |
| N | 3.51564200 | 3.77161100 | 0.26548100 |
| N | 4.90739200 | 1.75568200 | 0.68559100 |
| N | 1.49363800 | -4.83746500 | -0.59437700 |
| N | -1.01404700 | -4.96639300 | -0.46864700 |
| B | -5.12942700 | 2.69618800 | 0.31479300 |
| B | 4.78758000 | 3.18579900 | 0.60840800 |
| B | 0.26969400 | -5.60375600 | -0.63958200 |
| B | -6.27316100 | 0.48863000 | 0.83315400 |
| B | 6.17575300 | 1.08107000 | 0.88671900 |
| N | -6.14615900 | -0.92564100 | 0.89111700 |
| N | 6.21589200 | -0.33482200 | 0.76867500 |
| N | 5.07052100 | -2.52856100 | 0.19078600 |
| N | -4.76049700 | -3.02319100 | 0.50818400 |
| N | -3.41894900 | -5.02556800 | -0.06532800 |
| N | 3.91818400 | -4.63994900 | -0.40947300 |
| B | -3.96805500 | 4.79081000 | -0.38775200 |

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|---|-------------|-------------|-------------|
| B | 3.43440600 | 5.18744600 | -0.00226000 |
| B | -2.22013200 | -5.73325400 | -0.35752800 |
| B | 2.77942000 | -5.46923500 | -0.61640600 |
| N | 2.18794900 | 5.70391800 | -0.43668800 |
| N | -0.26058200 | 5.50573800 | -0.85758300 |
| N | -2.74927000 | 5.42766500 | -0.73347300 |
| H | -2.23393700 | -6.92164100 | -0.48865500 |
| H | 0.32451100 | -6.78990700 | -0.78367800 |
| H | 2.90945900 | -6.64599800 | -0.78283200 |
| H | -6.15839400 | 3.29308300 | 0.39830800 |
| H | -7.32991700 | 1.01668700 | 1.00485300 |
| H | -4.99787900 | 5.39301500 | -0.38926900 |
| H | 4.38423600 | 5.89832600 | 0.12273700 |
| H | 5.73759100 | 3.88183600 | 0.79468600 |
| H | 7.16474700 | 1.70374100 | 1.12956600 |
| H | -6.98374900 | -1.46444000 | 1.06270200 |
| H | -5.55882500 | -3.63224700 | 0.62168800 |
| H | -4.26763600 | -5.56542500 | 0.03271600 |
| H | 4.82435600 | -5.08723200 | -0.39577300 |
| H | 5.93482900 | -3.04996100 | 0.23919000 |
| H | 7.11125200 | -0.78961500 | 0.88190400 |
| H | 2.12765300 | 6.69357800 | -0.63139200 |
| H | -0.30429200 | 6.49684400 | -1.04886600 |
| H | -2.77834700 | 6.41127400 | -0.96290700 |
| O | -0.02477200 | -0.91490100 | -2.49570700 |
| H | 0.04735500 | -1.85280400 | -2.22303000 |
| H | -0.07744300 | -0.85467900 | -3.45518400 |
| O | 0.23296200 | -1.20950100 | 2.19762600 |

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|---|------------|-------------|------------|
| H | 0.15861800 | -1.12696300 | 3.15593300 |
| H | 0.65804500 | -2.06101200 | 2.02994700 |

H₂O-Li@V_{N2B} *h*-BN-H₂O (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Li | -0.22444100 | -0.83782600 | 1.08551400 |
| B | 1.42541300 | 0.43673200 | -0.22362700 |
| B | -1.26555800 | 0.17984200 | -0.65277800 |
| B | -0.07187200 | 2.40901100 | 0.20505300 |
| B | -2.42991300 | 2.56026800 | -0.69462500 |
| B | -3.71388900 | 0.56660100 | -0.80027600 |
| B | -2.38975900 | -1.20861800 | 0.07285100 |
| B | -1.08500600 | -3.32933700 | 0.44681400 |
| B | 1.34406300 | -3.28341300 | -0.17248600 |
| B | 2.47542500 | -1.05107800 | -0.60505800 |
| B | 3.80165700 | 0.89547600 | -0.35731300 |
| B | 2.38889800 | 2.70436200 | 0.50950500 |
| N | 2.50797200 | 1.39040100 | -0.01159400 |
| N | 0.04676500 | 0.93196900 | -0.04526900 |
| N | 1.06318100 | 3.20772300 | 0.70017000 |
| N | 3.78448600 | -0.46100300 | -0.80036000 |
| N | 2.48644900 | -2.51364700 | -0.61222300 |
| N | 0.06306200 | -2.64803700 | -0.08190400 |
| N | -2.33222900 | -2.61620300 | 0.50054000 |
| N | -3.71562200 | -0.76845600 | -0.26814000 |
| N | -2.42301800 | 1.16153200 | -0.90479300 |
| N | -1.27681300 | 3.18812000 | -0.07493300 |
| B | 0.94876000 | 4.59790600 | 1.10065900 |
| B | -1.37348900 | 4.60186400 | 0.25190600 |
| B | -4.93886000 | -1.49722400 | -0.07638500 |

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|---|-------------|-------------|-------------|
| B | -3.54746800 | -3.37552200 | 0.78731000 |
| B | 3.73684700 | -3.24406900 | -0.85954700 |
| B | 5.02246200 | -1.13732400 | -1.06108300 |
| N | 5.01312500 | 1.66375400 | -0.20817500 |
| N | 3.60167000 | 3.48145500 | 0.77742100 |
| N | -3.64934300 | 3.33704100 | -0.99481200 |
| N | -4.96464600 | 1.24044700 | -1.09846300 |
| N | -0.95299000 | -4.69803600 | 0.92100200 |
| N | 1.45015600 | -4.68563500 | 0.21212500 |
| B | 4.89994700 | 2.97042900 | 0.40004800 |
| B | -4.89281900 | 2.66664000 | -1.28457500 |
| B | 0.31058300 | -5.37568100 | 0.76731700 |
| B | 6.25401000 | 1.02563200 | -0.60474000 |
| B | -6.19694800 | 0.49687100 | -0.97807000 |
| N | 6.22608300 | -0.33351700 | -1.05106100 |
| N | -6.16087500 | -0.85044400 | -0.49053700 |
| N | -4.83354700 | -2.79581900 | 0.53108800 |
| N | 4.94580600 | -2.55632900 | -1.21914800 |
| N | 3.74266800 | -4.67587400 | -0.67005800 |
| N | -3.38923600 | -4.71710900 | 1.30668500 |
| B | 3.45126600 | 4.79490600 | 1.36120000 |
| B | -3.66337200 | 4.76049800 | -0.78291300 |
| B | 2.67550900 | -5.39679000 | -0.07449600 |
| B | -2.13873700 | -5.38961000 | 1.38273300 |
| N | -2.53305400 | 5.35145800 | -0.15860600 |
| N | -0.31369400 | 5.24197900 | 0.97382900 |
| N | 2.13374800 | 5.29302600 | 1.55231600 |
| H | 2.78624300 | -6.55941800 | 0.17181700 |

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|---|-------------|-------------|-------------|
| H | 0.41334300 | -6.51865900 | 1.09360000 |
| H | -2.07421600 | -6.50813200 | 1.79544100 |
| H | 5.87816000 | 3.62680000 | 0.59226900 |
| H | 7.29108100 | 1.61494400 | -0.54387400 |
| H | 4.40162300 | 5.45369900 | 1.65960900 |
| H | -4.60696300 | 5.42759800 | -1.08622700 |
| H | -5.86248400 | 3.29092600 | -1.59358300 |
| H | -7.24511400 | 0.99963300 | -1.25614300 |
| H | 7.11461600 | -0.75991700 | -1.27554000 |
| H | 5.78682700 | -3.10023700 | -1.35645500 |
| H | 4.59791100 | -5.18206800 | -0.85458400 |
| H | -4.21309200 | -5.23968600 | 1.57168400 |
| H | -5.66488000 | -3.34277100 | 0.70912100 |
| H | -7.04432300 | -1.33296900 | -0.40090600 |
| H | -2.55804400 | 6.34532700 | 0.02105900 |
| H | -0.39730500 | 6.22402100 | 1.19732000 |
| H | 2.03867200 | 6.23896700 | 1.89522800 |
| O | -0.07301100 | -0.71585300 | 2.99470100 |
| H | -0.64990600 | -1.21968200 | 3.58290700 |
| H | -0.02625000 | 0.18016000 | 3.35362900 |
| O | -0.73804000 | -0.48160300 | -1.87640400 |
| H | -1.46214000 | -0.70063300 | -2.47571800 |
| H | -0.11849800 | -1.91821400 | -0.78639800 |

H₂O-Li⁺@V_{N2B} *h*-BN-H₂O

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.25611000 | -1.10548900 | -0.08547900 |
| B | -1.46078700 | 0.18811900 | -0.05702200 |
| B | 1.23624200 | 0.78914800 | 0.02231000 |
| B | -0.57733700 | 2.58275400 | -0.07260600 |

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|---|-------------|-------------|-------------|
| B | 1.75891700 | 3.24819900 | 0.52533400 |
| B | 3.51746600 | 1.53639300 | 0.34192700 |
| B | 2.60137300 | -0.59711200 | -0.26973200 |
| B | 1.88126900 | -3.08330000 | -0.67928900 |
| B | -0.47999200 | -3.64032000 | -0.04810200 |
| B | -2.09302000 | -1.62296900 | 0.26429300 |
| B | -3.86846900 | -0.06170300 | -0.04272600 |
| B | -3.00222500 | 2.18232400 | -0.53749400 |
| N | -2.73630400 | 0.79715300 | -0.27516600 |
| N | -0.24455100 | 1.07826300 | -0.02914100 |
| N | -1.89235100 | 3.07840500 | -0.44479200 |
| N | -3.49844800 | -1.38296000 | 0.36108800 |
| N | -1.70372500 | -3.03706900 | 0.43638700 |
| N | 0.47361200 | -2.91764800 | -0.83518600 |
| N | 2.85264800 | -2.01506800 | -0.59840900 |
| N | 3.78123000 | 0.18235600 | -0.03701900 |
| N | 2.11472000 | 1.86763800 | 0.34448100 |
| N | 0.40029900 | 3.60398900 | 0.25490700 |
| B | -2.19189100 | 4.50597700 | -0.58179700 |
| B | 0.08386600 | 5.03474200 | 0.24307500 |
| B | 5.15853600 | -0.24800500 | -0.15927400 |
| B | 4.25757400 | -2.47883400 | -0.76989400 |
| B | -2.71942300 | -4.01494800 | 0.91720300 |
| B | -4.53206200 | -2.33023000 | 0.71715000 |
| N | -5.22912600 | 0.35679700 | -0.18780200 |
| N | -4.36368300 | 2.61194700 | -0.80639700 |
| N | 2.77918200 | 4.21284200 | 0.89331400 |
| N | 4.54937300 | 2.47351000 | 0.67110600 |

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|---|-------------|-------------|-------------|
| N | 2.20840900 | -4.51017000 | -0.64700400 |
| N | -0.11356100 | -5.03609800 | 0.14355900 |
| B | -5.47769500 | 1.70947900 | -0.63827500 |
| B | 4.16643700 | 3.82952700 | 0.99408100 |
| B | 1.21491900 | -5.47191600 | -0.22835900 |
| B | -6.27508600 | -0.59185700 | 0.15752600 |
| B | 5.93159800 | 2.03204900 | 0.59211200 |
| N | -5.89567100 | -1.88828300 | 0.62655700 |
| N | 6.19161000 | 0.69457400 | 0.16852000 |
| N | 5.35673600 | -1.58849100 | -0.59231500 |
| N | -4.07781000 | -3.62203200 | 1.11635900 |
| N | -2.32176100 | -5.38089100 | 1.13448000 |
| N | 4.51339500 | -3.85938900 | -1.09746700 |
| B | -4.60298500 | 4.00899400 | -1.11539100 |
| B | 2.40794500 | 5.60829400 | 1.02819800 |
| B | -1.07225100 | -5.93159800 | 0.75738800 |
| B | 3.56805500 | -4.90204900 | -0.96556400 |
| N | 1.07661200 | 5.96853500 | 0.69659400 |
| N | -1.18892100 | 5.45285200 | -0.23613300 |
| N | -3.50265600 | 4.89969700 | -1.02120000 |
| H | -0.81443600 | -7.07947200 | 0.93347000 |
| H | 1.51194100 | -6.61873100 | -0.12964900 |
| H | 3.86615100 | -6.04725300 | -1.08507300 |
| H | -6.58988200 | 2.07943600 | -0.84011200 |
| H | -7.42325300 | -0.29428900 | 0.06059000 |
| H | -5.68808800 | 4.39700000 | -1.41265100 |
| H | 3.19946900 | 6.42496100 | 1.37851800 |
| H | 4.99146300 | 4.62637400 | 1.30830900 |

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|---|-------------|-------------|-------------|
| H | 6.82428500 | 2.77080800 | 0.86324800 |
| H | -6.64416000 | -2.52537700 | 0.86447100 |
| H | -4.74408800 | -4.32799000 | 1.40038900 |
| H | -3.00841900 | -6.01893900 | 1.51479700 |
| H | 5.47039900 | -4.12753400 | -1.28582700 |
| H | 6.29370400 | -1.95327700 | -0.69968100 |
| H | 7.16055900 | 0.41243600 | 0.10440500 |
| H | 0.83373100 | 6.94881200 | 0.74530300 |
| H | -1.40179300 | 6.44004100 | -0.28163300 |
| H | -3.68432700 | 5.88076300 | -1.18529200 |
| O | 0.01912600 | -0.73983200 | -2.35347500 |
| H | -0.04032600 | -1.63301600 | -2.71915900 |
| H | -0.46437600 | -0.15072200 | -2.94678900 |
| O | 0.57054600 | -1.57431300 | 1.91051000 |
| H | -0.14899500 | -1.94978100 | 2.43569400 |
| H | 1.15509100 | -1.11362300 | 2.52622500 |

H₂O-Li⁺@V_{N2B} *h*-BN-H₂O (reactant)

| | | | |
|----|-------------|-------------|-------------|
| Li | 0.48228200 | -0.78262000 | -1.23653900 |
| B | 0.76572000 | 1.00895300 | 0.77722800 |
| B | -1.58529100 | -0.05302400 | 0.23646700 |
| B | -1.04974900 | 2.44072100 | -0.15216300 |
| B | -3.42157400 | 1.69078300 | -0.21626600 |
| B | -3.90441500 | -0.65143200 | 0.39588100 |
| B | -1.87215900 | -1.92567700 | 0.41675600 |
| B | 0.10331100 | -3.56294500 | -0.08233500 |
| B | 2.48436400 | -2.79519000 | -0.44549800 |
| B | 3.00787300 | -0.39276600 | -0.24150500 |
| B | 3.18838100 | 1.93381900 | 0.59903700 |

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|---|-------------|-------------|-------------|
| B | 1.24159400 | 3.41643400 | 0.29974600 |
| N | 1.73575400 | 2.08106300 | 0.60337500 |
| N | -0.56781700 | 1.04083200 | 0.16037900 |
| N | -0.13678900 | 3.57011500 | -0.10035500 |
| N | 3.78695900 | 0.65102400 | 0.28452600 |
| N | 3.44212100 | -1.72346100 | -0.37230500 |
| N | 1.08851800 | -2.49808900 | -0.15810000 |
| N | -1.26590200 | -3.26475500 | 0.31293800 |
| N | -3.29845400 | -1.92367400 | 0.63600000 |
| N | -2.94504800 | 0.38105200 | 0.11279800 |
| N | -2.43990000 | 2.71493900 | -0.43482300 |
| B | -0.61103300 | 4.92082100 | -0.42407100 |
| B | -2.92093100 | 4.05411600 | -0.76184300 |
| B | -4.15729100 | -3.05622200 | 0.88702900 |
| B | -2.14151500 | -4.45049800 | 0.52152200 |
| B | 4.88094200 | -1.99022400 | -0.31821600 |
| B | 5.23593300 | 0.41677000 | 0.37966500 |
| N | 4.06365100 | 3.05324800 | 0.83706700 |
| N | 2.13400400 | 4.55639500 | 0.40993800 |
| N | -4.85085700 | 1.92811700 | -0.31126100 |
| N | -5.31898000 | -0.42418700 | 0.40393800 |
| N | 0.56046300 | -4.89986000 | -0.42895500 |
| N | 2.92160800 | -4.12465300 | -0.75957800 |
| B | 3.51508200 | 4.38730100 | 0.77920500 |
| B | -5.79927300 | 0.88596500 | 0.02286300 |
| B | 1.93782700 | -5.18171800 | -0.76869900 |
| B | 5.49488700 | 2.84310100 | 0.97324200 |
| B | -6.17804500 | -1.54511200 | 0.75374600 |

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|---|-------------|-------------|-------------|
| N | 6.03332200 | 1.53267700 | 0.78578000 |
| N | -5.57100600 | -2.81165200 | 1.01206800 |
| N | -3.50746000 | -4.32103500 | 0.92494400 |
| N | 5.73347800 | -0.89004800 | 0.03475000 |
| N | 5.28056300 | -3.33319600 | -0.62561200 |
| N | -1.61557600 | -5.76555400 | 0.27108500 |
| B | 1.64287700 | 5.89049300 | 0.12167500 |
| B | -5.30827300 | 3.24160900 | -0.72049600 |
| B | 4.34966300 | -4.38885800 | -0.87894800 |
| B | -0.33085700 | -6.03098700 | -0.24950500 |
| N | -4.32968700 | 4.24531600 | -0.96576700 |
| N | -1.96670700 | 5.11014300 | -0.82755200 |
| N | 0.30153100 | 6.02331400 | -0.31248600 |
| H | 4.73780200 | -5.48049000 | -1.14948700 |
| H | 2.26718600 | -6.29340500 | -1.03165000 |
| H | 0.01694800 | -7.13773800 | -0.51247500 |
| H | 4.20982900 | 5.33083500 | 0.97952700 |
| H | 6.21444600 | 3.75525800 | 1.22937200 |
| H | 2.35152200 | 6.83972500 | 0.23545200 |
| H | -6.46855700 | 3.47763500 | -0.84376000 |
| H | -6.96780400 | 1.10566500 | -0.02138500 |
| H | -7.35986100 | -1.41300700 | 0.81128100 |
| H | 7.03456800 | 1.42940400 | 0.88457800 |
| H | 6.73273900 | -1.04493600 | 0.07476000 |
| H | 6.26265100 | -3.57327500 | -0.65852800 |
| H | -2.23213500 | -6.55563700 | 0.40642700 |
| H | -4.04635500 | -5.16576500 | 1.06149900 |
| H | -6.19144400 | -3.58103700 | 1.22591700 |

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|---|-------------|-------------|-------------|
| H | -4.66598500 | 5.16450800 | -1.21958900 |
| H | -2.28356000 | 6.04733600 | -1.03676100 |
| H | -0.03255000 | 6.95506700 | -0.51831000 |
| O | 1.00607900 | -0.06940400 | 1.62643000 |
| H | 0.95746500 | -1.77056600 | 0.54881500 |
| H | 1.83969700 | 0.01124400 | 2.10811000 |
| O | 0.06298500 | -0.71232700 | -3.07176700 |
| H | -0.02962500 | 0.08188100 | -3.61374400 |
| H | -0.06109100 | -1.46865000 | -3.65985900 |

H₂O-Na@V_{N2B} *h*-BN-H₂O

| | | | |
|----|-------------|-------------|-------------|
| Na | -0.03356900 | -1.22505700 | -0.34762400 |
| B | -1.38416700 | 0.60874900 | -0.10675000 |
| B | 1.42150400 | 0.52818100 | -0.10899600 |
| B | 0.07732200 | 2.68577300 | 0.24040000 |
| B | 2.57109500 | 2.81460100 | -0.02857900 |
| B | 3.81804600 | 0.72477300 | -0.41864100 |
| B | 2.40888000 | -1.20766300 | -0.19485900 |
| B | 1.07942700 | -3.56845900 | -0.04751500 |
| B | -1.26325400 | -3.50654000 | -0.13998500 |
| B | -2.46467500 | -1.07169300 | -0.30257900 |
| B | -3.77176900 | 0.94449000 | -0.38072900 |
| B | -2.41896400 | 2.93528300 | 0.15663700 |
| N | -2.47942800 | 1.53407300 | -0.12267400 |
| N | 0.03362900 | 1.17514600 | 0.01507200 |
| N | -1.12775900 | 3.49782600 | 0.41337000 |
| N | -3.76363500 | -0.47363000 | -0.50123500 |
| N | -2.43294400 | -2.53591000 | -0.20311900 |
| N | -0.05806200 | -3.26471900 | -0.80218900 |

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|---|-------------|-------------|-------------|
| N | 2.29413600 | -2.66174400 | -0.02615400 |
| N | 3.74219000 | -0.69476400 | -0.39184200 |
| N | 2.55658800 | 1.39708900 | -0.20900300 |
| N | 1.32445700 | 3.44813500 | 0.28377000 |
| B | -1.08780300 | 4.91624600 | 0.75334000 |
| B | 1.37480000 | 4.87305000 | 0.59312200 |
| B | 4.95449900 | -1.47098000 | -0.47057100 |
| B | 3.55129800 | -3.41962500 | 0.15589800 |
| B | -3.73610000 | -3.23236000 | -0.12237700 |
| B | -5.01331500 | -1.17604100 | -0.65936800 |
| N | -4.98317400 | 1.72106000 | -0.47261800 |
| N | -3.64816600 | 3.72230900 | 0.17069400 |
| N | 3.83058500 | 3.54386700 | -0.13592500 |
| N | 5.06302300 | 1.42976400 | -0.59649400 |
| N | 1.08429500 | -4.74724500 | 0.85420300 |
| N | -1.39995900 | -4.68527300 | 0.75119000 |
| B | -4.91478500 | 3.12816000 | -0.18022800 |
| B | 5.06043400 | 2.86125900 | -0.46009900 |
| B | -0.18782400 | -5.34914900 | 1.16132500 |
| B | -6.22576100 | 1.02873000 | -0.76284600 |
| B | 6.27147700 | 0.65099000 | -0.80159000 |
| N | -6.20623000 | -0.38983600 | -0.87496500 |
| N | 6.18662900 | -0.76842900 | -0.74636300 |
| N | 4.82702200 | -2.85805800 | -0.19876700 |
| N | -4.96096000 | -2.58650300 | -0.51455000 |
| N | -3.80292700 | -4.57861900 | 0.38626900 |
| N | 3.51400400 | -4.74597000 | 0.71933700 |
| B | -3.58978000 | 5.11183900 | 0.55838700 |

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|---|-------------|-------------|-------------|
| B | 3.85265400 | 4.95780900 | 0.15222800 |
| B | -2.69226300 | -5.26929100 | 0.95070000 |
| B | 2.32722100 | -5.37985900 | 1.18404200 |
| N | 2.63392600 | 5.56815400 | 0.54219200 |
| N | 0.17099500 | 5.55563000 | 0.92356100 |
| N | -2.31919500 | 5.65194700 | 0.87839700 |
| H | -2.84476100 | -6.29890100 | 1.53750000 |
| H | -0.24018100 | -6.37012800 | 1.78054700 |
| H | 2.37841700 | -6.40442300 | 1.79687600 |
| H | -5.90090500 | 3.79723000 | -0.21193200 |
| H | -7.24525700 | 1.63632400 | -0.88708000 |
| H | -4.57395900 | 5.78370900 | 0.60936300 |
| H | 4.86045700 | 5.59135400 | 0.07803600 |
| H | 6.07134800 | 3.48036700 | -0.58661400 |
| H | 7.31786700 | 1.19251400 | -0.99121400 |
| H | -7.08731100 | -0.85766200 | -1.03713500 |
| H | -5.81349100 | -3.12958600 | -0.50666100 |
| H | -4.71564800 | -5.00210600 | 0.48135700 |
| H | 4.39465900 | -5.20905900 | 0.89636200 |
| H | 5.64695400 | -3.44553800 | -0.13512900 |
| H | 7.04402400 | -1.29215500 | -0.85561500 |
| H | 2.64722700 | 6.55697300 | 0.74992400 |
| H | 0.20172200 | 6.54311200 | 1.13530400 |
| H | -2.27341600 | 6.62843800 | 1.13446000 |
| O | 0.15700500 | -1.39186600 | -2.76410900 |
| H | 0.07564500 | -2.25260700 | -2.25497100 |
| H | -0.59233700 | -1.38051900 | -3.37184300 |
| O | -0.09051800 | -1.71560000 | 2.17620200 |

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|---|-------------|-------------|------------|
| H | 0.68374200 | -2.28735300 | 2.28157900 |
| H | -0.84168100 | -2.31608700 | 2.28707900 |

H₂O-Na@V_{N2B} *h*-BN-H₂O (reactant)

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|----|-------------|-------------|-------------|
| Na | 0.19242400 | -0.86047500 | -1.55439700 |
| B | 1.27917000 | 0.23706700 | 0.65216500 |
| B | -1.39252000 | 0.55752300 | 0.21984600 |
| B | 0.14233300 | 2.49891900 | -0.21278900 |
| B | -2.31011100 | 2.84108200 | -0.53718200 |
| B | -3.76465300 | 1.06939400 | 0.33240400 |
| B | -2.48340400 | -0.90397500 | 0.65269900 |
| B | -1.40390500 | -3.19912600 | 0.38167200 |
| B | 1.00793100 | -3.31340300 | -0.25057600 |
| B | 2.36427900 | -1.19988500 | 0.00575700 |
| B | 3.74442100 | 0.56358600 | 0.79040300 |
| B | 2.51361100 | 2.59345800 | 0.65936800 |
| N | 2.47219200 | 1.19680400 | 0.87573900 |
| N | -0.00983000 | 1.02672300 | 0.03748800 |
| N | 1.36871900 | 3.25021800 | 0.05525100 |
| N | 3.70721000 | -0.79292100 | 0.31234900 |
| N | 2.26069800 | -2.62113800 | -0.38131400 |
| N | -0.09559500 | -2.64673600 | 0.35150300 |
| N | -2.53461800 | -2.36763200 | 0.73630000 |
| N | -3.78168000 | -0.27808600 | 0.80653500 |
| N | -2.46068900 | 1.52544900 | -0.02283700 |
| N | -0.97568000 | 3.32347100 | -0.70635800 |
| B | 1.49685300 | 4.66013800 | -0.27411200 |
| B | -0.82979000 | 4.70919000 | -1.11140000 |
| B | -5.03579000 | -0.90773600 | 1.10501600 |

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|---|-------------|-------------|-------------|
| B | -3.80717100 | -3.05312600 | 0.99765900 |
| B | 3.45156800 | -3.41116900 | -0.68691200 |
| B | 4.90693900 | -1.55651400 | 0.11947300 |
| N | 5.01751800 | 1.20854500 | 1.05863700 |
| N | 3.75811800 | 3.33950000 | 0.93977900 |
| N | -3.50531100 | 3.64277700 | -0.81642500 |
| N | -4.95823100 | 1.86454600 | 0.17552200 |
| N | -1.56477300 | -4.60009800 | -0.01534000 |
| N | 0.81561100 | -4.66397000 | -0.78730200 |
| B | 4.98666000 | 2.63967800 | 1.21993900 |
| B | -4.81481800 | 3.16391000 | -0.44345700 |
| B | -0.45706600 | -5.32153200 | -0.58436400 |
| B | 6.22714200 | 0.42848800 | 0.94554200 |
| B | -6.21268300 | 1.27182600 | 0.59397100 |
| N | 6.15107200 | -0.93184100 | 0.49671700 |
| N | -6.21827100 | -0.07554200 | 1.07600700 |
| N | -4.99877900 | -2.32149200 | 1.31913700 |
| N | 4.75579300 | -2.86590000 | -0.46028200 |
| N | 3.24815100 | -4.75419100 | -1.19703700 |
| N | -3.85491400 | -4.49253600 | 0.85922000 |
| B | 3.80545900 | 4.76198200 | 0.72488600 |
| B | -3.32455800 | 4.95462900 | -1.39679400 |
| B | 1.98144000 | -5.38862600 | -1.26646600 |
| B | -2.81521800 | -5.26361500 | 0.28078200 |
| N | -1.99726500 | 5.42851000 | -1.57204300 |
| N | 0.44475900 | 5.32712900 | -0.98239300 |
| N | 2.68040900 | 5.38135400 | 0.11992600 |
| H | 1.87425800 | -6.49877400 | -1.69249200 |

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|---|-------------|-------------|-------------|
| H | -0.59152900 | -6.46210800 | -0.90864200 |
| H | -2.96700800 | -6.42508600 | 0.05056600 |
| H | 5.97772400 | 3.24140600 | 1.50556600 |
| H | 7.29208100 | 0.90961300 | 1.19721200 |
| H | 4.77101300 | 5.40477500 | 1.01174100 |
| H | -4.26035600 | 5.63021700 | -1.70399900 |
| H | -5.77868700 | 3.83903300 | -0.64326700 |
| H | -7.23400400 | 1.88708000 | 0.52472800 |
| H | 7.02144000 | -1.43739000 | 0.40629600 |
| H | 5.56955900 | -3.43412400 | -0.65238300 |
| H | 4.05378300 | -5.29613700 | -1.47907200 |
| H | -4.72714800 | -4.96388500 | 1.05647600 |
| H | -5.85440100 | -2.83537400 | 1.47971600 |
| H | -7.11519000 | -0.47093800 | 1.32260700 |
| H | -1.87977800 | 6.37102200 | -1.91732400 |
| H | 0.55178500 | 6.30530900 | -1.21236900 |
| H | 2.72804100 | 6.37384400 | -0.06264000 |
| O | 0.73341900 | -0.34270700 | 1.91114100 |
| H | 0.09270500 | -1.81908600 | 0.93211700 |
| H | 1.45356600 | -0.55561700 | 2.51744100 |
| O | -0.27937800 | -2.53841400 | -3.05607500 |
| H | -1.17515000 | -2.77552900 | -3.32852800 |
| H | 0.09539700 | -3.35546000 | -2.68504700 |

H₂O-Na⁺@V_{N2B} *h*-BN-H₂O

| | | | |
|----|-------------|-------------|-------------|
| Na | -0.34250100 | -1.17498700 | -0.27169300 |
| B | -1.16441200 | 0.96119900 | -0.01683200 |
| B | 1.51843000 | 0.16389700 | -0.03718800 |
| B | 0.78833700 | 2.61472200 | 0.07303300 |

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|---|-------------|-------------|-------------|
| B | 3.19988900 | 2.06835600 | -0.35634800 |
| B | 3.89238700 | -0.28857500 | -0.17569200 |
| B | 2.02273000 | -1.74863600 | 0.11558200 |
| B | 0.20118100 | -3.72729300 | -0.02139800 |
| B | -2.15309900 | -3.02640400 | -0.48184900 |
| B | -2.64703700 | -0.36797000 | -0.32456300 |
| B | -3.40749700 | 1.87834000 | 0.05295400 |
| B | -1.54617000 | 3.44554600 | 0.46267700 |
| N | -1.98990000 | 2.10416100 | 0.19274800 |
| N | 0.34607000 | 1.13724000 | 0.00463200 |
| N | -0.13945200 | 3.69126200 | 0.38573200 |
| N | -3.75870400 | 0.52771800 | -0.28068300 |
| N | -2.98523600 | -1.81744100 | -0.48728500 |
| N | -0.78426300 | -3.14180800 | -0.89792500 |
| N | 1.50586000 | -3.14129400 | 0.28231000 |
| N | 3.44250900 | -1.62227000 | 0.09042800 |
| N | 2.83257500 | 0.68827200 | -0.21277900 |
| N | 2.15945500 | 3.03378200 | -0.17506900 |
| B | 0.28654500 | 5.08719600 | 0.52669900 |
| B | 2.57440800 | 4.43925800 | -0.16210200 |
| B | 4.42302400 | -2.66844500 | 0.27855600 |
| B | 2.49533300 | -4.18699600 | 0.69539300 |
| B | -4.43661500 | -2.17214700 | -0.60717400 |
| B | -5.15751900 | 0.20162200 | -0.46502700 |
| N | -4.38726400 | 2.90762500 | 0.23818100 |
| N | -2.52443500 | 4.48229200 | 0.74027300 |
| N | 4.58554100 | 2.41828500 | -0.61677200 |
| N | 5.27354300 | 0.03557900 | -0.37193400 |

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|---|-------------|-------------|-------------|
| N | -0.26682400 | -5.01515900 | 0.48044400 |
| N | -2.62379600 | -4.35271000 | -0.08148300 |
| B | -3.93718500 | 4.22372400 | 0.63058000 |
| B | 5.61972200 | 1.41311800 | -0.64030500 |
| B | -1.67375800 | -5.33825600 | 0.38731900 |
| B | -5.78688900 | 2.58915700 | 0.01926800 |
| B | 6.25822400 | -1.02570300 | -0.24934000 |
| N | -6.12547500 | 1.25439200 | -0.35181000 |
| N | 5.80645100 | -2.33736300 | 0.09043400 |
| N | 3.89920300 | -3.93435500 | 0.66459400 |
| N | -5.44482200 | -1.16879500 | -0.70577800 |
| N | -4.85261300 | -3.55261700 | -0.60216200 |
| N | 2.03306400 | -5.48714600 | 1.10914100 |
| B | -2.06527800 | 5.82687300 | 1.02948600 |
| B | 4.94349400 | 3.81690600 | -0.74774600 |
| B | -4.03354600 | -4.64131100 | -0.22378000 |
| B | 0.69160600 | -5.93145200 | 1.05870900 |
| N | 3.92409000 | 4.77540300 | -0.52107800 |
| N | 1.63330200 | 5.42920500 | 0.23027800 |
| N | -0.67458300 | 6.07655200 | 0.92842500 |
| H | -4.46901500 | -5.73124900 | -0.03256700 |
| H | -2.06319800 | -6.40057900 | 0.75177100 |
| H | 0.36222800 | -7.00171500 | 1.45966400 |
| H | -4.72740200 | 5.08671900 | 0.84311700 |
| H | -6.62911200 | 3.41994100 | 0.14662700 |
| H | -2.83095000 | 6.69077200 | 1.31864400 |
| H | 6.05574000 | 4.14703600 | -1.01269000 |
| H | 6.75000100 | 1.71571800 | -0.85341400 |

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|---|-------------|-------------|-------------|
| H | 7.41592800 | -0.80467200 | -0.41377100 |
| H | -7.10532900 | 1.04770100 | -0.49182200 |
| H | -6.40557800 | -1.46978200 | -0.80108100 |
| H | -5.84124700 | -3.73710700 | -0.71026500 |
| H | 2.72457400 | -6.14028000 | 1.45312000 |
| H | 4.52563000 | -4.69841900 | 0.88033600 |
| H | 6.51100300 | -3.05542300 | 0.19265800 |
| H | 4.18262100 | 5.75169700 | -0.56823800 |
| H | 1.92248400 | 6.39639300 | 0.28183500 |
| H | -0.35719600 | 7.02372700 | 1.08439300 |
| O | 0.10175300 | -1.06375700 | -2.59078600 |
| H | -0.15832300 | -1.93702900 | -2.91642200 |
| H | -0.03732500 | -0.44300300 | -3.31674700 |
| O | -0.75209800 | -1.72405600 | 2.02368700 |
| H | -1.50527700 | -1.51491500 | 2.59066900 |
| H | -0.07158900 | -2.08746700 | 2.60498400 |

H₂O-Na⁺@V_{N2B} *h*-BN-H₂O (reactant)

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|----|-------------|-------------|-------------|
| Na | -0.00140600 | -0.55926400 | -2.16323900 |
| B | 1.36814500 | 0.29324200 | 0.17705600 |
| B | -1.29335400 | 0.42355900 | 0.19679400 |
| B | 0.14248600 | 2.47283300 | -0.37911000 |
| B | -2.26368000 | 2.81329600 | 0.12300300 |
| B | -3.55866400 | 0.87432300 | 0.89432300 |
| B | -2.35455200 | -1.08187400 | 0.31477100 |
| B | -1.36581900 | -3.19424700 | -0.70563500 |
| B | 1.07228400 | -3.33473300 | -0.58339600 |
| B | 2.24395700 | -1.31358500 | 0.42167400 |
| B | 3.68064700 | 0.52212100 | 0.82284600 |

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|---|-------------|-------------|-------------|
| B | 2.59838500 | 2.54898300 | -0.05459400 |
| N | 2.49570500 | 1.18029100 | 0.34068000 |
| N | 0.06701600 | 0.96185500 | -0.14547600 |
| N | 1.40362700 | 3.17043900 | -0.54343000 |
| N | 3.50754400 | -0.88743900 | 0.96976400 |
| N | 2.18207100 | -2.73612500 | 0.09756800 |
| N | -0.09097700 | -2.56348900 | -0.97666500 |
| N | -2.44973800 | -2.48080900 | -0.09578600 |
| N | -3.56518500 | -0.55415300 | 0.89492300 |
| N | -2.30258700 | 1.42549200 | 0.46272900 |
| N | -1.03820400 | 3.31264000 | -0.42719200 |
| B | 1.48176600 | 4.57419400 | -0.93866900 |
| B | -0.98566200 | 4.72020400 | -0.81383400 |
| B | -4.80843500 | -1.24757200 | 1.12333700 |
| B | -3.71305900 | -3.23152500 | 0.10474500 |
| B | 3.33589600 | -3.61635900 | 0.40446800 |
| B | 4.65369500 | -1.70408100 | 1.28066200 |
| N | 4.92847600 | 1.19521600 | 1.03629700 |
| N | 3.87446600 | 3.23717300 | 0.04499600 |
| N | -3.44511400 | 3.63924200 | 0.31383900 |
| N | -4.71606800 | 1.67012300 | 1.18566400 |
| N | -1.45463300 | -4.58803200 | -1.11120700 |
| N | 1.02804100 | -4.74038600 | -0.95595500 |
| B | 5.02694100 | 2.57954500 | 0.62720800 |
| B | -4.65251100 | 3.08502900 | 0.88984600 |
| B | -0.23816200 | -5.34500400 | -1.30015700 |
| B | 6.04199700 | 0.39315100 | 1.52278500 |
| B | -5.92422300 | 0.96902400 | 1.59411900 |

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|---|-------------|-------------|-------------|
| N | 5.86306500 | -1.01913900 | 1.66386600 |
| N | -5.92518500 | -0.46148900 | 1.58425900 |
| N | -4.82095000 | -2.63606200 | 0.78599600 |
| N | 4.48829200 | -3.11002000 | 1.08477200 |
| N | 3.28934900 | -4.98379100 | -0.04350400 |
| N | -3.80865800 | -4.56322500 | -0.43409100 |
| B | 3.96076300 | 4.59353800 | -0.45855100 |
| B | -3.40130900 | 5.01551800 | -0.13897000 |
| B | 2.19568100 | -5.56976200 | -0.72668700 |
| B | -2.73485200 | -5.26502500 | -1.03620200 |
| N | -2.19524300 | 5.49276100 | -0.72561200 |
| N | 0.26816500 | 5.27492400 | -1.21705100 |
| N | 2.77842400 | 5.19523700 | -0.97698500 |
| H | 2.21554300 | -6.70790100 | -1.07442300 |
| H | -0.28764600 | -6.48314100 | -1.64069700 |
| H | -2.86399500 | -6.37908000 | -1.43465600 |
| H | 6.05381600 | 3.16936400 | 0.74683100 |
| H | 7.09177100 | 0.89736400 | 1.77216100 |
| H | 4.98961100 | 5.19288900 | -0.43787600 |
| H | -4.34854700 | 5.72878000 | -0.02857000 |
| H | -5.59651600 | 3.78240800 | 1.08743200 |
| H | -6.90402100 | 1.57210000 | 1.90174200 |
| H | 6.67323900 | -1.55324700 | 1.94860400 |
| H | 5.25912300 | -3.74116600 | 1.25918700 |
| H | 4.09205000 | -5.57316100 | 0.13356300 |
| H | -4.68994100 | -5.05243200 | -0.34994800 |
| H | -5.66789600 | -3.17810200 | 0.89451000 |
| H | -6.79810600 | -0.91732600 | 1.81451600 |

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|---|-------------|-------------|-------------|
| H | -2.17571900 | 6.46281300 | -1.01034700 |
| H | 0.31364600 | 6.25522100 | -1.46142700 |
| H | 2.84985000 | 6.15586200 | -1.28451000 |
| O | -0.35269200 | -0.23245400 | 2.76757600 |
| H | -0.71070800 | -0.92215400 | 3.34167200 |
| H | -0.49587600 | 0.58806500 | 3.25738900 |
| O | -0.11725800 | 0.04954000 | -4.31534000 |
| H | 0.58211100 | 0.44747100 | -4.85002100 |
| H | -0.88044600 | -0.02199900 | -4.90334100 |

H₂O-K@V_{N₂B} *h*-BN-H₂O

| | | | |
|---|-------------|-------------|-------------|
| K | -0.00494000 | -1.29561300 | -0.29407100 |
| B | -1.43755800 | 0.68814700 | -0.05438800 |
| B | 1.44032800 | 0.67919400 | -0.05546300 |
| B | 0.00946500 | 2.80481900 | 0.18678000 |
| B | 2.53347500 | 2.97344800 | 0.09236100 |
| B | 3.84378500 | 0.88960000 | -0.24012200 |
| B | 2.48938600 | -1.09743000 | -0.22017400 |
| B | 1.15497800 | -3.63261900 | -0.25872100 |
| B | -1.18578200 | -3.62563100 | -0.25542100 |
| B | -2.49932500 | -1.08102400 | -0.21259400 |
| B | -3.83845200 | 0.91567700 | -0.24145900 |
| B | -2.51282400 | 2.99142800 | 0.08217000 |
| N | -2.55632000 | 1.56972800 | -0.07228900 |
| N | 0.00450700 | 1.29030200 | 0.02885700 |
| N | -1.22368900 | 3.59945100 | 0.25941000 |
| N | -3.81079000 | -0.51126200 | -0.30789600 |
| N | -2.36117200 | -2.57291500 | -0.19542900 |
| N | -0.01543900 | -3.49484400 | -1.02249700 |

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|---|-------------|-------------|-------------|
| N | 2.34139000 | -2.58862100 | -0.20772000 |
| N | 3.80537400 | -0.53709200 | -0.31713500 |
| N | 2.56676000 | 1.55205600 | -0.06975700 |
| N | 1.24864200 | 3.59025800 | 0.26660500 |
| B | -1.21969000 | 5.04324400 | 0.47624500 |
| B | 1.25422000 | 5.03377000 | 0.48572100 |
| B | 5.03064100 | -1.28790800 | -0.43448800 |
| B | 3.62550200 | -3.31366400 | -0.04384100 |
| B | -3.65062700 | -3.28885100 | -0.03216000 |
| B | -5.04098100 | -1.25359800 | -0.42637300 |
| N | -5.07359500 | 1.65506500 | -0.32249300 |
| N | -3.76214300 | 3.74499200 | 0.06005400 |
| N | 3.78893400 | 3.71730900 | 0.07849000 |
| N | 5.08499100 | 1.61961400 | -0.31372000 |
| N | 1.23150400 | -4.75595000 | 0.71135900 |
| N | -1.26630100 | -4.75147600 | 0.71153400 |
| B | -5.02649400 | 3.08524000 | -0.16388800 |
| B | 5.04855700 | 3.04941100 | -0.14525400 |
| B | -0.01912600 | -5.38093100 | 1.07963600 |
| B | -6.31088000 | 0.91888900 | -0.51793100 |
| B | 6.31706500 | 0.87547700 | -0.50998100 |
| N | -6.26469500 | -0.50288100 | -0.57978700 |
| N | 6.26019000 | -0.54570000 | -0.58178800 |
| N | 4.89888400 | -2.69709500 | -0.33082300 |
| N | -4.91967800 | -2.66304600 | -0.31565500 |
| N | -3.67868000 | -4.64576400 | 0.46333900 |
| N | 3.64435400 | -4.66948500 | 0.45357300 |
| B | -3.72894900 | 5.17078900 | 0.28289100 |

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|---|-------------|-------------|-------------|
| B | 3.76563800 | 5.14255100 | 0.30792700 |
| B | -2.54671300 | -5.33251600 | 0.98619500 |
| B | 2.50823300 | -5.34545500 | 0.98302200 |
| N | 2.50413100 | 5.74789600 | 0.52740600 |
| N | 0.01944600 | 5.72046300 | 0.64145100 |
| N | -2.46384100 | 5.76736600 | 0.50721100 |
| H | -2.67065800 | -6.35102000 | 1.59868300 |
| H | -0.02051600 | -6.38297400 | 1.73105300 |
| H | 2.62730600 | -6.36293600 | 1.59809000 |
| H | -6.03110000 | 3.72555700 | -0.20704800 |
| H | -7.35007200 | 1.49744200 | -0.61441700 |
| H | -4.72665100 | 5.82415900 | 0.28258500 |
| H | 4.76858700 | 5.78779200 | 0.31589400 |
| H | 6.05851900 | 3.68168300 | -0.18120900 |
| H | 7.36105500 | 1.44636100 | -0.59965400 |
| H | -7.14079100 | -0.99316300 | -0.69588500 |
| H | -5.74896600 | -3.23975500 | -0.27428300 |
| H | -4.58582100 | -5.06626800 | 0.61181300 |
| H | 4.54847800 | -5.09648500 | 0.60202700 |
| H | 5.72436600 | -3.27907200 | -0.28598300 |
| H | 7.13324000 | -1.04185700 | -0.69595600 |
| H | 2.48144700 | 6.74586200 | 0.68480600 |
| H | 0.02267400 | 6.72071800 | 0.78408700 |
| H | -2.43442000 | 6.76567700 | 0.66121800 |
| O | -0.04161300 | -1.58055200 | -2.99331000 |
| H | -0.02731200 | -2.43178600 | -2.46790400 |
| H | 0.52202600 | -1.73258700 | -3.76012300 |
| O | -0.01008200 | -2.23347300 | 2.42466900 |

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|---|-------------|-------------|------------|
| H | -0.78039800 | -2.81936900 | 2.39406700 |
| H | 0.73772600 | -2.84801300 | 2.39507100 |

H₂O-K@V_{N2B} *h*-BN-H₂O (reactant)

| | | | |
|---|-------------|-------------|-------------|
| K | 0.14352200 | 0.78312600 | -2.07621600 |
| B | -1.36511600 | -0.63201700 | 0.26393300 |
| B | 1.28589200 | -0.23332500 | 0.69670300 |
| B | 0.21707100 | -2.53811700 | -0.13132300 |
| B | 2.59022000 | -2.55988700 | 0.73703700 |
| B | 3.76456300 | -0.49352500 | 0.80166300 |
| B | 2.31563200 | 1.22461600 | 0.03998900 |
| B | 0.89948200 | 3.30419000 | -0.16079000 |
| B | -1.48674900 | 3.11826700 | 0.53143500 |
| B | -2.50035700 | 0.78610100 | 0.72598400 |
| B | -3.72997300 | -1.20261500 | 0.30866000 |
| B | -2.21681400 | -2.93071700 | -0.54149100 |
| N | -2.40970700 | -1.61643100 | -0.03866100 |
| N | 0.02547600 | -1.07404600 | 0.10606600 |
| N | -0.86870000 | -3.39176800 | -0.65509600 |
| N | -3.78766300 | 0.12496900 | 0.83160300 |
| N | -2.59230200 | 2.24461100 | 0.86750300 |
| N | -0.17502900 | 2.59361600 | 0.43001300 |
| N | 2.16732100 | 2.64673500 | -0.34500100 |
| N | 3.68027300 | 0.85865100 | 0.31341600 |
| N | 2.51473700 | -1.16106400 | 0.91291200 |
| N | 1.45682900 | -3.26084300 | 0.16037000 |
| B | -0.68420500 | -4.77982500 | -1.03500600 |
| B | 1.61981900 | -4.67283900 | -0.13648400 |
| B | 4.85419700 | 1.65536000 | 0.10396400 |

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|---|-------------|-------------|-------------|
| B | 3.33090100 | 3.47985100 | -0.63887000 |
| B | -3.87864000 | 2.88511400 | 1.16584300 |
| B | -5.05899700 | 0.71029200 | 1.14483000 |
| N | -4.90232600 | -2.02133800 | 0.10935500 |
| N | -3.38628300 | -3.75643600 | -0.86193700 |
| N | 3.85792100 | -3.26688600 | 1.01980000 |
| N | 5.06088300 | -1.09967200 | 1.05633500 |
| N | 0.67224600 | 4.68514200 | -0.61261700 |
| N | -1.68269900 | 4.54005600 | 0.22759000 |
| B | -4.71578400 | -3.30759600 | -0.52401600 |
| B | 5.07166800 | -2.52649900 | 1.25548900 |
| B | -0.60157000 | 5.31095000 | -0.32358400 |
| B | -6.17683200 | -1.47303200 | 0.52747300 |
| B | 6.24544500 | -0.28767300 | 0.91486000 |
| N | -6.22219000 | -0.14578900 | 1.05944500 |
| N | 6.12323100 | 1.06594900 | 0.45564100 |
| N | 4.65526700 | 2.96531000 | -0.45983200 |
| N | -5.05690100 | 2.11075500 | 1.43444100 |
| N | -3.95826100 | 4.32972200 | 1.11897700 |
| N | 3.08842900 | 4.83948800 | -1.08703200 |
| B | -3.16048600 | -5.06940600 | -1.42271600 |
| B | 3.93427200 | -4.69420300 | 0.85362200 |
| B | -2.93953900 | 5.15828100 | 0.58461700 |
| B | 1.81209900 | 5.45681200 | -1.07888600 |
| N | 2.81656600 | -5.35838100 | 0.28237500 |
| N | 0.59278800 | -5.37683700 | -0.84678300 |
| N | -1.81962600 | -5.52293100 | -1.53807200 |
| H | -3.11634600 | 6.32972600 | 0.43445300 |

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|---|-------------|-------------|-------------|
| H | -0.75793700 | 6.46870800 | -0.57021900 |
| H | 1.67594700 | 6.58866100 | -1.43524700 |
| H | -5.65950200 | -3.99970400 | -0.75968600 |
| H | -7.18187200 | -2.10956400 | 0.41944300 |
| H | -4.07155900 | -5.76354000 | -1.76204000 |
| H | 4.91701400 | -5.30625400 | 1.15018200 |
| H | 6.08428400 | -3.09350100 | 1.53787100 |
| H | 7.32818400 | -0.73555000 | 1.15281500 |
| H | -7.13138000 | 0.21809900 | 1.30952400 |
| H | -5.92464000 | 2.59576100 | 1.61794100 |
| H | -4.83824800 | 4.76861100 | 1.35316900 |
| H | 3.87770500 | 5.41139600 | -1.35587200 |
| H | 5.44746200 | 3.56560200 | -0.64465300 |
| H | 6.97674400 | 1.59663300 | 0.34989900 |
| H | 2.88587400 | -6.35447900 | 0.12875600 |
| H | 0.72372200 | -6.35653300 | -1.05699200 |
| H | -1.67267700 | -6.46733700 | -1.86651900 |
| O | 0.73151000 | 0.31473600 | 1.96820900 |
| H | 0.03695100 | 1.73272000 | 0.94869100 |
| H | 1.44791400 | 0.61914800 | 2.53904400 |
| O | -0.52690700 | 3.17439000 | -3.10542500 |
| H | -1.39435400 | 3.54735800 | -3.30650900 |
| H | -0.09998100 | 3.84074600 | -2.53856500 |

H₂O-Li@V_B *h*-BN-H₂O

| | | | |
|---|-------------|-------------|-------------|
| B | -1.19377600 | -1.01242300 | -0.34997900 |
| B | -0.47209700 | 1.40194900 | -0.02691600 |
| B | -2.91567100 | 0.77111000 | -0.09848900 |

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|---|-------------|-------------|-------------|
| B | -2.24794100 | 3.19142100 | -0.07037100 |
| B | 0.18804900 | 3.83292500 | 0.01249100 |
| B | 1.98693700 | 2.05595900 | 0.17902500 |
| B | 3.89019100 | 0.33660800 | 0.35047400 |
| B | 3.20000900 | -2.06932800 | 0.22425700 |
| B | 0.62152600 | -2.72571200 | -0.24035900 |
| B | -1.79869600 | -3.41249100 | -0.08861900 |
| B | -3.59406800 | -1.65291600 | -0.04621600 |
| N | -2.21193300 | -2.03222900 | -0.16425900 |
| N | -1.51790700 | 0.39425500 | -0.17665200 |
| N | -3.94815500 | -0.25085100 | -0.05922600 |
| N | -0.38430300 | -3.76658000 | -0.10827300 |
| N | 0.10084200 | -1.45961000 | -0.70791600 |
| N | 2.06922300 | -3.00383900 | -0.02679100 |
| N | 3.07793500 | -0.74554300 | 0.74734600 |
| N | 0.89497700 | 1.13563500 | 0.26585000 |
| N | 3.41034500 | 1.70660800 | 0.21359600 |
| N | 1.59206000 | 3.46872300 | 0.09498400 |
| N | -0.84804400 | 2.82004800 | -0.04633400 |
| N | -3.27758400 | 2.17330300 | -0.06638900 |
| B | -5.34626500 | 0.12913700 | 0.01082700 |
| B | -4.67922400 | 2.55426200 | -0.03843100 |
| B | 2.61132800 | 4.50422600 | 0.06599100 |
| B | 4.41214500 | 2.74976000 | 0.08699400 |
| B | 2.43975600 | -4.42140600 | -0.04180800 |
| B | 0.01753300 | -5.15599400 | -0.03895000 |
| N | -2.81078200 | -4.44853800 | 0.03930000 |
| N | -4.60749500 | -2.69218300 | 0.06526000 |

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|---|-------------|-------------|-------------|
| N | -2.61461000 | 4.60098900 | -0.07637700 |
| N | -0.19597900 | 5.23971000 | -0.03047500 |
| N | 5.29598900 | -0.02498300 | 0.09263100 |
| N | 4.59941600 | -2.45718500 | 0.00127900 |
| B | -4.20843500 | -4.07807600 | 0.10191600 |
| B | -1.58774300 | 5.61040100 | -0.07138100 |
| B | 5.62206900 | -1.42420900 | -0.04653100 |
| B | -2.40261400 | -5.83709200 | 0.10099400 |
| B | 0.82228700 | 6.26831800 | -0.01829400 |
| N | -1.01395500 | -6.15524400 | 0.05030800 |
| N | 2.18728300 | 5.87988300 | 0.02185000 |
| N | 3.98989100 | 4.11970200 | 0.05463400 |
| N | 1.42195600 | -5.43687400 | -0.07033500 |
| N | 3.83550400 | -4.78969400 | -0.04332800 |
| N | 5.80599200 | 2.37888900 | -0.00413300 |
| B | -6.00165200 | -2.30528700 | 0.12872100 |
| B | -4.01193100 | 4.97870900 | -0.07030800 |
| B | 4.91332600 | -3.86369500 | -0.08856300 |
| B | 6.26538400 | 1.03533900 | -0.06163900 |
| N | -5.00087600 | 3.95756000 | -0.04647000 |
| N | -5.67777500 | 1.52413600 | -0.00052800 |
| N | -6.33141500 | -0.92111700 | 0.09035000 |
| H | 6.04118000 | -4.24027900 | -0.18885200 |
| H | 6.75301200 | -1.74630000 | -0.24969600 |
| H | 7.42203600 | 0.78976400 | -0.23001300 |
| H | -5.03838000 | -4.93015200 | 0.18747200 |
| H | -3.21407700 | -6.70717000 | 0.19056600 |
| H | -6.86130900 | -3.12910700 | 0.21079800 |

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|----|-------------|-------------|-------------|
| H | -4.33207900 | 6.12830700 | -0.08152000 |
| H | -1.89209300 | 6.76310900 | -0.09364100 |
| H | 0.52265100 | 7.42310900 | -0.04438700 |
| H | -0.75904700 | -7.13178200 | 0.10435900 |
| H | 1.72258000 | -6.40250300 | -0.06653600 |
| H | 4.07067900 | -5.77240000 | -0.07124400 |
| H | 6.49623200 | 3.11046300 | -0.10295800 |
| H | 4.69334200 | 4.84149000 | -0.02441900 |
| H | 2.88408000 | 6.61180400 | 0.01809000 |
| H | -5.96950400 | 4.24534700 | -0.03577500 |
| H | -6.65122600 | 1.79456600 | 0.03718400 |
| H | -7.31074300 | -0.67622500 | 0.13926200 |
| Li | 1.48599800 | -0.70704300 | 0.03522700 |
| O | 0.76855100 | -0.96414100 | 2.48265700 |
| H | 1.73758800 | -0.97206200 | 2.41198600 |
| H | 0.56015500 | -0.07485900 | 2.15357500 |
| O | 2.14904600 | -0.48575500 | -2.40898300 |
| H | 2.53771900 | -1.22808300 | -2.88869700 |
| H | 1.25211100 | -0.78898200 | -2.16412200 |

H₂O-Li@V_B *h*-BN-H₂O (reactant)

| | | | |
|---|-------------|-------------|-------------|
| B | 1.39005000 | -0.73809500 | -0.34015800 |
| B | 0.08042800 | 1.37952600 | -0.09274700 |
| B | 2.61413000 | 1.41934400 | -0.06001600 |
| B | 1.35242900 | 3.57368700 | 0.00655000 |
| B | -1.15604800 | 3.59327800 | 0.06824700 |
| B | -2.47360100 | 1.42847400 | 0.02434900 |
| B | -3.84780500 | -0.64010600 | -0.14105700 |
| B | -2.52144300 | -2.73550800 | -0.18332600 |

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|---|-------------|-------------|-------------|
| B | 0.05195200 | -2.78910400 | -0.27971000 |
| B | 2.57028500 | -2.89471000 | -0.02168000 |
| B | 3.87767600 | -0.75187600 | -0.00702100 |
| N | 2.63435800 | -1.45758000 | -0.13495600 |
| N | 1.36028600 | 0.70794800 | -0.17308000 |
| N | 3.87208500 | 0.69463900 | -0.01706700 |
| N | 1.28620100 | -3.56012500 | -0.03447800 |
| N | 0.20729500 | -1.42165800 | -0.67540500 |
| N | -1.25120200 | -3.45991500 | -0.20006800 |
| N | -2.68268700 | -1.34396800 | -0.51686000 |
| N | -1.21344600 | 0.72889300 | -0.04734000 |
| N | -3.77391100 | 0.79413800 | 0.03700100 |
| N | -2.42221300 | 2.89583100 | 0.09293300 |
| N | 0.08650600 | 2.85267700 | -0.02484800 |
| N | 2.61140100 | 2.86469200 | -0.00297700 |
| B | 5.12870300 | 1.41095000 | 0.07391600 |
| B | 3.87126600 | 3.58628500 | 0.05327200 |
| B | -3.65865000 | 3.65434500 | 0.23771900 |
| B | -4.99824200 | 1.54174000 | 0.22955400 |
| B | -1.26938200 | -4.90178200 | 0.03812500 |
| B | 1.24289000 | -4.99563900 | 0.12592300 |
| N | 3.81176500 | -3.64223500 | 0.14840900 |
| N | 5.11887200 | -1.50069000 | 0.12795200 |
| N | 1.35963100 | 5.03115000 | 0.05819800 |
| N | -1.12886600 | 5.05204500 | 0.13343800 |
| N | -5.11124000 | -1.34738800 | 0.05295600 |
| N | -3.78606200 | -3.47150000 | 0.05838900 |
| B | 5.07238700 | -2.94235000 | 0.19858500 |

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|---|-------------|-------------|------------|
| B | 0.12202000 | 5.75848800 | 0.11425700 |
| B | -5.05011300 | -2.78281800 | 0.13914900 |
| B | 3.75533400 | -5.08219100 | 0.28563900 |
| B | -2.35890900 | 5.80271000 | 0.24563500 |
| N | 2.48416900 | -5.71764200 | 0.27059600 |
| N | -3.58300900 | 5.09096200 | 0.29987900 |
| N | -4.91055900 | 2.96709700 | 0.31582400 |
| N | -0.03774700 | -5.63068400 | 0.13254700 |
| N | -2.53011400 | -5.58217300 | 0.16130100 |
| N | -6.24417300 | 0.82201900 | 0.30828000 |
| B | 6.37046300 | -0.78052300 | 0.20155600 |
| B | 2.61285500 | 5.75482100 | 0.08690400 |
| B | -3.77684000 | -4.90840600 | 0.18932500 |
| B | -6.32599500 | -0.59900300 | 0.26079900 |
| N | 3.83022700 | 5.02449300 | 0.08134900 |
| N | 5.09818400 | 2.84465200 | 0.08033100 |
| N | 6.34571100 | 0.64306300 | 0.15751900 |
| H | -4.79294100 | -5.52083500 | 0.32251300 |
| H | -6.05391800 | -3.40459300 | 0.31161600 |
| H | -7.37655700 | -1.15180600 | 0.39099400 |
| H | 6.08766900 | -3.55943600 | 0.30865300 |
| H | 4.75353700 | -5.72497200 | 0.41207000 |
| H | 7.40843700 | -1.36249800 | 0.29774200 |
| H | 2.62446600 | 6.94781600 | 0.11793000 |
| H | 0.13306900 | 6.95017900 | 0.15184500 |
| H | -2.34612800 | 6.99496800 | 0.29490000 |
| H | 2.46185400 | -6.72288100 | 0.37226700 |
| H | -0.08703600 | -6.63079300 | 0.27228700 |

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|----|-------------|-------------|-------------|
| H | -2.53484200 | -6.58486700 | 0.28639700 |
| H | -7.10150500 | 1.33658700 | 0.45417100 |
| H | -5.75591200 | 3.50757300 | 0.43717200 |
| H | -4.43621100 | 5.62409500 | 0.39401400 |
| H | 4.69379700 | 5.54818300 | 0.11207000 |
| H | 5.97027800 | 3.35255100 | 0.13902000 |
| H | 7.23160700 | 1.12563000 | 0.21746900 |
| Li | -1.26655400 | -0.65686400 | -1.65567800 |
| O | -1.10151700 | -0.09813600 | -3.51156400 |
| H | -1.58197200 | 0.65446500 | -3.87853100 |
| H | -0.19289600 | -0.02557800 | -3.83116000 |
| O | -1.07869400 | -1.19195000 | 2.40851400 |
| H | -0.13285300 | -1.34042000 | 2.52693600 |
| H | -1.13002100 | -0.68093500 | 1.58336300 |

H₂O-Li⁺@V_B *h*-BN-H₂O

| | | | |
|---|-------------|-------------|-------------|
| B | -0.51167700 | 1.41998400 | -0.36185400 |
| B | 1.62916600 | -0.06801300 | -0.29934600 |
| B | 1.76060100 | 2.42767300 | -0.07751100 |
| B | 3.86830700 | 1.02938500 | -0.14170100 |
| B | 3.68879900 | -1.49591100 | -0.15614100 |
| B | 1.45219900 | -2.63577800 | -0.20020500 |
| B | -0.87328700 | -3.82600300 | -0.16435800 |
| B | -2.99942900 | -2.37301700 | -0.21514600 |
| B | -2.81983700 | 0.28675100 | -0.33974300 |
| B | -2.58843400 | 2.76623200 | 0.05671600 |
| B | -0.30688900 | 3.86659000 | 0.09951600 |
| N | -1.13467000 | 2.68595200 | -0.06492900 |
| N | 0.93581400 | 1.21639100 | -0.24430900 |

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|---|-------------|-------------|-------------|
| N | 1.13094000 | 3.72518200 | 0.05527000 |
| N | -3.41084500 | 1.56327300 | -0.00892600 |
| N | -1.47662300 | 0.46991800 | -0.85333500 |
| N | -3.51127800 | -1.00204900 | -0.12393000 |
| N | -1.70760800 | -2.78974000 | -0.70053200 |
| N | 0.91449300 | -1.31826500 | -0.47087600 |
| N | 0.58559800 | -3.80613500 | -0.06152400 |
| N | 2.88531200 | -2.71780500 | -0.11464700 |
| N | 3.05940400 | -0.17608800 | -0.21198600 |
| N | 3.20563700 | 2.31306600 | -0.06885600 |
| B | 1.95258200 | 4.92655200 | 0.18020300 |
| B | 4.02881300 | 3.52017300 | 0.02482600 |
| B | 3.52860300 | -4.01511900 | 0.04612200 |
| B | 1.24107900 | -5.09610200 | 0.20418400 |
| B | -4.95606300 | -0.88253200 | 0.17102200 |
| B | -4.84601900 | 1.64409300 | 0.21568700 |
| N | -3.20318400 | 4.04844500 | 0.30242500 |
| N | -0.94577900 | 5.14783500 | 0.30815700 |
| N | 5.31046700 | 0.91453100 | -0.11627700 |
| N | 5.12669100 | -1.58803600 | -0.10041000 |
| N | -1.67813900 | -4.98372100 | 0.21193000 |
| N | -3.77600200 | -3.55541700 | 0.15509200 |
| B | -2.38270900 | 5.23886100 | 0.40180500 |
| B | 5.93539700 | -0.38323600 | -0.11046200 |
| B | -3.11645300 | -4.83802100 | 0.34114500 |
| B | -4.64753300 | 4.13787800 | 0.45074100 |
| B | 5.77081000 | -2.89062300 | -0.01603900 |
| N | -5.42140000 | 2.94270100 | 0.40624100 |

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|---|-------------|-------------|-------------|
| N | 4.96001600 | -4.05909100 | 0.06114800 |
| N | 2.67340900 | -5.15526700 | 0.20952500 |
| N | -5.56357100 | 0.40749900 | 0.28407200 |
| N | -5.73192300 | -2.08344100 | 0.34747100 |
| N | 0.42066800 | -6.25499700 | 0.43397300 |
| B | -0.12107100 | 6.33820200 | 0.42417200 |
| B | 6.12093500 | 2.11893200 | -0.05966100 |
| B | -5.20261800 | -3.39726200 | 0.38267500 |
| B | -0.99867400 | -6.24015600 | 0.48267400 |
| N | 5.45731300 | 3.37320300 | 0.00326800 |
| N | 3.37548600 | 4.78642100 | 0.13883000 |
| N | 1.29010200 | 6.19076500 | 0.34364900 |
| H | -5.89092400 | -4.34057300 | 0.60931100 |
| H | -3.76806900 | -5.77849800 | 0.66359600 |
| H | -1.61945700 | -7.22108500 | 0.74293400 |
| H | -2.90010800 | 6.29646200 | 0.56975600 |
| H | -5.17323300 | 5.19211800 | 0.61838400 |
| H | -0.61625800 | 7.40874500 | 0.58323100 |
| H | 7.30920300 | 2.05392100 | -0.05808800 |
| H | 7.12093400 | -0.47308100 | -0.09869100 |
| H | 6.95709700 | -2.97694300 | 0.00021100 |
| H | -6.42010700 | 3.03468000 | 0.53522700 |
| H | -6.55921700 | 0.44079900 | 0.46050300 |
| H | -6.72365900 | -1.98705800 | 0.52226800 |
| H | 0.87382000 | -7.14096400 | 0.61551300 |
| H | 3.10630100 | -6.05798200 | 0.35914300 |
| H | 5.43677000 | -4.94734400 | 0.13974300 |
| H | 6.03673000 | 4.20058300 | 0.05042400 |

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|----|-------------|-------------|-------------|
| H | 3.94570800 | 5.61832500 | 0.21563100 |
| H | 1.84719200 | 7.03058000 | 0.42645700 |
| Li | -0.87929800 | -1.19376100 | -0.56841000 |
| O | -0.97069700 | -1.11500800 | 1.67800600 |
| H | -1.78948900 | -0.93892800 | 2.16063400 |
| H | -0.25137800 | -0.87269000 | 2.27517300 |
| O | -4.02127200 | 0.41555900 | -2.95077500 |
| H | -4.29165500 | -0.31013000 | -3.52758000 |
| H | -3.48186700 | 0.98237600 | -3.51658900 |

H₂O-Li⁺@V_B *h*-BN-H₂O (reactant)

| | | | |
|---|-------------|-------------|-------------|
| B | -1.11453200 | 0.99597600 | -0.24383000 |
| B | -0.43266300 | -1.43924000 | -0.18272100 |
| B | -2.85192700 | -0.79417100 | -0.03031800 |
| B | -2.19457600 | -3.21816100 | -0.01651200 |
| B | 0.24144400 | -3.86230400 | 0.01093100 |
| B | 2.03566800 | -2.09804500 | -0.06858000 |
| B | 3.83388300 | -0.32433700 | -0.06126300 |
| B | 3.13886200 | 2.11931800 | -0.10293800 |
| B | 0.67567700 | 2.77045100 | -0.16995900 |
| B | -1.75359400 | 3.41041900 | -0.03953500 |
| B | -3.53014900 | 1.62554800 | -0.02046900 |
| N | -2.13202900 | 2.00979100 | -0.11938300 |
| N | -1.44113400 | -0.40791700 | -0.12637700 |
| N | -3.87679900 | 0.22463000 | 0.00156500 |
| N | -0.34767700 | 3.78214600 | -0.03345100 |
| N | 0.20433500 | 1.46910700 | -0.62361200 |
| N | 2.08135600 | 3.09946800 | -0.01775400 |
| N | 2.93652300 | 0.73148800 | -0.46956100 |

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|---|-------------|-------------|-------------|
| N | 0.97288900 | -1.18923100 | -0.46953400 |
| N | 3.41632500 | -1.69599400 | 0.07843500 |
| N | 1.64560700 | -3.48368600 | 0.04534000 |
| N | -0.78821700 | -2.83729000 | -0.07794000 |
| N | -3.21038800 | -2.19305200 | 0.00090300 |
| B | -5.28380300 | -0.15845700 | 0.06863800 |
| B | -4.61768200 | -2.58036600 | 0.05709900 |
| B | 2.66892700 | -4.50897600 | 0.23572500 |
| B | 4.43886300 | -2.72196300 | 0.29760400 |
| B | 2.45004700 | 4.50647000 | 0.18445800 |
| B | 0.02444500 | 5.17991400 | 0.14329600 |
| N | -2.77833800 | 4.42338700 | 0.07535500 |
| N | -4.54800400 | 2.65322700 | 0.06022100 |
| N | -2.55177300 | -4.62103500 | 0.04104300 |
| N | -0.13444900 | -5.25458100 | 0.10297800 |
| N | 5.22322000 | 0.07164900 | 0.09951600 |
| N | 4.53988500 | 2.48884300 | 0.06560700 |
| B | -4.17447400 | 4.04372400 | 0.09847400 |
| B | -1.52968300 | -5.63296900 | 0.09069600 |
| B | 5.56721600 | 1.47419600 | 0.14541900 |
| B | -2.40439200 | 5.82113800 | 0.18767000 |
| B | 0.88672000 | -6.27794800 | 0.23065800 |
| N | -1.02153700 | 6.15671900 | 0.22343000 |
| N | 2.24996500 | -5.87737200 | 0.30049700 |
| N | 4.03302100 | -4.09009000 | 0.35871400 |
| N | 1.41843700 | 5.49340900 | 0.23991000 |
| N | 3.84277500 | 4.84171500 | 0.28990300 |
| N | 5.80978500 | -2.30403900 | 0.40528700 |

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|----|-------------|-------------|-------------|
| B | -5.94725800 | 2.26881400 | 0.11944300 |
| B | -3.95217300 | -5.00463700 | 0.07922900 |
| B | 4.89100500 | 3.88873500 | 0.23617600 |
| B | 6.23195500 | -0.95203800 | 0.31980400 |
| N | -4.93569300 | -3.98053100 | 0.07999500 |
| N | -5.61051300 | -1.55083100 | 0.08772000 |
| N | -6.27007700 | 0.88527800 | 0.11330300 |
| H | 6.02942700 | 4.21885300 | 0.33979500 |
| H | 6.70137100 | 1.79688500 | 0.29677300 |
| H | 7.37884100 | -0.65575100 | 0.43310100 |
| H | -5.01315700 | 4.88509200 | 0.16009100 |
| H | -3.23582800 | 6.66976900 | 0.25809300 |
| H | -6.80251900 | 3.09526700 | 0.17338200 |
| H | -4.26588900 | -6.15254100 | 0.11270400 |
| H | -1.82982100 | -6.78307500 | 0.13257300 |
| H | 0.58984100 | -7.42903400 | 0.28473200 |
| H | -0.78419600 | 7.13459400 | 0.32217600 |
| H | 1.68798400 | 6.46050400 | 0.36401700 |
| H | 4.10424200 | 5.81064400 | 0.41446100 |
| H | 6.52458800 | -3.00303500 | 0.55747900 |
| H | 4.74255300 | -4.79707400 | 0.49993700 |
| H | 2.94267800 | -6.60554400 | 0.41087300 |
| H | -5.90466000 | -4.26749800 | 0.11069300 |
| H | -6.58443700 | -1.81962600 | 0.13290600 |
| H | -7.24943800 | 0.63771500 | 0.15604100 |
| Li | 1.41375200 | 0.32898800 | -1.80748900 |
| O | 1.44417400 | 0.34388700 | -3.71778600 |
| H | 0.82197000 | 0.81596000 | -4.28524500 |

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|---|-------------|-------------|-------------|
| H | 2.08905100 | -0.07442700 | -4.30174200 |
| O | 0.50025200 | 1.14727900 | 2.45163300 |
| H | 0.88668900 | 1.81837900 | 3.02868200 |
| H | -0.20742600 | 0.75572700 | 2.97942700 |

H₂O-Na@V_B h-BN-H₂O

| | | | |
|---|-------------|-------------|-------------|
| B | 0.85549800 | 1.27572900 | -0.23747200 |
| B | 0.91240300 | -1.31464900 | 0.31227400 |
| B | 3.00332400 | 0.02354200 | -0.05939500 |
| B | 3.06901800 | -2.49968900 | -0.15883400 |
| B | 0.90644500 | -3.78527300 | 0.07571100 |
| B | -1.23431300 | -2.55980100 | 0.61640700 |
| B | -3.67533100 | -1.29053900 | 0.53453800 |
| B | -3.71551100 | 1.19445000 | 0.18284100 |
| B | -1.35053900 | 2.48453000 | -0.29880600 |
| B | 0.78522600 | 3.77223300 | -0.01057100 |
| B | 2.99310700 | 2.54884200 | 0.04110900 |
| N | 1.55397900 | 2.54095800 | -0.02517300 |
| N | 1.54738100 | -0.00116100 | 0.00543500 |
| N | 3.71404500 | 1.29582800 | -0.03807000 |
| N | -0.66683200 | 3.75819500 | -0.10403700 |
| N | -0.47231700 | 1.43917500 | -0.74279800 |
| N | -2.83270300 | 2.36789600 | -0.12411500 |
| N | -3.40008500 | 0.04359000 | 0.95218900 |
| N | -0.35850700 | -1.47418300 | 0.92096700 |
| N | -2.75245600 | -2.47662600 | 0.57943200 |
| N | -0.53673300 | -3.80612600 | 0.27696100 |
| N | 1.64842500 | -2.53854900 | 0.04370600 |
| N | 3.75306400 | -1.21979600 | -0.14154200 |

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|---|-------------|-------------|-------------|
| B | 5.16642500 | 1.31638700 | -0.06316500 |
| B | 5.20053600 | -1.19240200 | -0.24836300 |
| B | -1.25200100 | -5.05276000 | 0.17683700 |
| B | -3.42241800 | -3.75808700 | 0.30194900 |
| B | -3.56084600 | 3.63106400 | -0.27865900 |
| B | -1.42851700 | 4.98603500 | -0.07516800 |
| N | 1.48589000 | 5.03754600 | 0.14211400 |
| N | 3.68739300 | 3.82345100 | 0.15210100 |
| N | 3.79616200 | -3.74724700 | -0.33518200 |
| N | 1.63701200 | -5.02610400 | -0.15119400 |
| N | -5.04879000 | -1.37322100 | -0.02905300 |
| N | -5.10636500 | 1.14911400 | -0.31165900 |
| B | 2.93053700 | 5.05118000 | 0.21644800 |
| B | 3.07001600 | -4.99631900 | -0.34066800 |
| B | -5.74623500 | -0.15298700 | -0.37552400 |
| B | 0.72156800 | 6.26963900 | 0.19064300 |
| B | 0.91218500 | -6.28130900 | -0.18471000 |
| N | -0.69921600 | 6.21778900 | 0.08363300 |
| N | -0.50179600 | -6.26713900 | -0.02199000 |
| N | -2.67943600 | -4.98883900 | 0.25926900 |
| N | -2.84999400 | 4.88325900 | -0.24112200 |
| N | -4.99194400 | 3.59404000 | -0.48602100 |
| N | -4.84965800 | -3.80417200 | 0.07820000 |
| B | 5.13585500 | 3.83191900 | 0.15476700 |
| B | 5.23602900 | -3.70766400 | -0.46710400 |
| B | -5.75865700 | 2.40113300 | -0.60885500 |
| B | -5.66277200 | -2.66963900 | -0.16860200 |
| N | 5.89423600 | -2.44557800 | -0.40850600 |

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|----|-------------|-------------|-------------|
| N | 5.87246000 | 0.07482300 | -0.18701700 |
| N | 5.82781200 | 2.59429000 | 0.03672200 |
| H | -6.90731200 | 2.43854100 | -0.93169600 |
| H | -6.86536400 | -0.21900000 | -0.78541100 |
| H | -6.80787600 | -2.78659100 | -0.48497800 |
| H | 3.50333900 | 6.09161100 | 0.32308300 |
| H | 1.27394100 | 7.32016300 | 0.31369300 |
| H | 5.74070100 | 4.85652900 | 0.24670300 |
| H | 5.86652000 | -4.71022000 | -0.61516500 |
| H | 3.66318300 | -6.01887300 | -0.50013900 |
| H | 1.48861400 | -7.31283400 | -0.35304400 |
| H | -1.19910700 | 7.09544700 | 0.11987300 |
| H | -3.39575700 | 5.73325800 | -0.29055400 |
| H | -5.47092900 | 4.46848000 | -0.65357600 |
| H | -5.27694400 | -4.71161300 | -0.04825200 |
| H | -3.20751100 | -5.84290600 | 0.13733600 |
| H | -0.98568900 | -7.15320400 | -0.06764700 |
| H | 6.90123900 | -2.44386600 | -0.49447900 |
| H | 6.88234400 | 0.09202300 | -0.23280100 |
| H | 6.83798800 | 2.62688000 | 0.03241000 |
| Na | -1.51588800 | 0.05401600 | 0.27716000 |
| O | -0.52194600 | 0.83178100 | 2.63254200 |
| H | -0.42986300 | -0.10570500 | 2.36054000 |
| H | 0.38626700 | 1.15909400 | 2.65690900 |
| O | -2.01916100 | -0.41401300 | -2.19349600 |
| H | -2.77752100 | -0.01080900 | -2.63452600 |
| H | -1.36899200 | 0.31094700 | -2.08031400 |

H₂O-Na@V_B *h*-BN-H₂O (reactant)

| | | | |
|---|-------------|-------------|-------------|
| B | 0.83791400 | -0.87784100 | 0.00892900 |
| B | -1.48491800 | -0.11418900 | 0.71351100 |
| B | -1.15904200 | -2.45875200 | -0.15039300 |
| B | -3.49395700 | -1.61083300 | 0.25374400 |
| B | -3.79785600 | 0.80366900 | 0.67019900 |
| B | -1.71230900 | 2.11109800 | 0.62663600 |
| B | 0.32558800 | 2.98037900 | -0.64155100 |
| B | 2.73296300 | 2.49205900 | -0.27468600 |
| B | 3.01005900 | 0.33253000 | 0.28335500 |
| B | 3.14991100 | -2.08745700 | 0.18838200 |
| B | 1.13446600 | -3.40130700 | -0.35725100 |
| N | 1.71705100 | -2.08957200 | -0.05974800 |
| N | -0.58562600 | -1.14270300 | 0.13540700 |
| N | -0.29050600 | -3.56835200 | -0.48347700 |
| N | 3.79295300 | -0.83928100 | 0.46869800 |
| N | 1.58362000 | 0.43940600 | 0.01405300 |
| N | 3.65769500 | 1.58993700 | 0.30345400 |
| N | 1.38464100 | 1.93464200 | -0.33095600 |
| N | -0.96409300 | 1.08287800 | 1.22658000 |
| N | -1.04215100 | 3.14577600 | -0.18658700 |
| N | -3.18173800 | 2.09519400 | 0.60790000 |
| N | -2.93528100 | -0.34789100 | 0.59619300 |
| N | -2.59432700 | -2.69004200 | -0.09475300 |
| B | -0.85812800 | -4.86640900 | -0.82086000 |
| B | -3.16294100 | -3.97631600 | -0.44298600 |
| B | -3.97065700 | 3.24291600 | 0.28112800 |
| B | -1.88110500 | 4.26084600 | -0.63436100 |
| B | 5.08064400 | 1.77425900 | 0.32958100 |

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|---|-------------|-------------|-------------|
| B | 5.23476500 | -0.70649700 | 0.63864700 |
| N | 3.97767300 | -3.28179100 | 0.16272600 |
| N | 1.99229000 | -4.57745600 | -0.52565100 |
| N | -4.94530500 | -1.78875900 | 0.24773800 |
| N | -5.24723000 | 0.66377300 | 0.63403100 |
| N | 0.88368400 | 4.12708600 | -1.42254800 |
| N | 3.21986200 | 3.75260400 | -0.75640200 |
| B | 3.39537700 | -4.52848000 | -0.24030500 |
| B | -5.81082500 | -0.65215500 | 0.47259000 |
| B | 2.26486100 | 4.51116400 | -1.50571700 |
| B | 5.39022400 | -3.19973300 | 0.46469500 |
| B | -6.05476400 | 1.86541600 | 0.55638900 |
| N | 5.98215100 | -1.93015900 | 0.72746800 |
| N | -5.40812200 | 3.12700200 | 0.38812800 |
| N | -3.25120000 | 4.38544500 | -0.20507600 |
| N | 5.85071300 | 0.60333300 | 0.64411100 |
| N | 5.52989800 | 3.09009000 | -0.04941400 |
| N | -1.33414500 | 5.21676700 | -1.55366600 |
| B | 1.43406700 | -5.84832500 | -0.93888100 |
| B | -5.49174400 | -3.08848700 | -0.05891600 |
| B | 4.63494600 | 4.04810400 | -0.63476100 |
| B | 0.01121200 | 5.15718500 | -1.96459700 |
| N | -4.59281200 | -4.14292700 | -0.38699200 |
| N | -2.27684300 | -5.03154100 | -0.83031200 |
| N | 0.03435900 | -5.95560300 | -1.11258200 |
| H | 5.06280500 | 5.08730900 | -1.03653400 |
| H | 2.60999600 | 5.45505400 | -2.14370500 |
| H | 0.43982700 | 5.96866800 | -2.72577300 |

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|----|-------------|-------------|-------------|
| H | 4.06967100 | -5.50672300 | -0.33284900 |
| H | 6.06236100 | -4.18553500 | 0.47957200 |
| H | 2.14268900 | -6.79090300 | -1.12070000 |
| H | -6.67015600 | -3.28214200 | -0.04846600 |
| H | -6.99518400 | -0.80233800 | 0.47997000 |
| H | -7.24761400 | 1.80167000 | 0.58625100 |
| H | 6.97955400 | -1.90413600 | 0.88734600 |
| H | 6.86004300 | 0.65429300 | 0.67629700 |
| H | 6.51229400 | 3.32688900 | -0.03793700 |
| H | -1.92120400 | 5.94614300 | -1.93254800 |
| H | -3.76455700 | 5.19826300 | -0.51814700 |
| H | -5.99556100 | 3.93710800 | 0.24755800 |
| H | -4.99164400 | -5.04317600 | -0.61401000 |
| H | -2.66078900 | -5.93564500 | -1.06822200 |
| H | -0.34554800 | -6.85332300 | -1.37777800 |
| Na | 1.04945100 | 1.58549200 | 2.15854100 |
| O | -0.36917700 | 1.34378800 | 3.88516800 |
| H | -0.92697700 | 1.16900000 | 3.07619300 |
| H | -0.57555500 | 0.64506600 | 4.51649900 |
| O | -1.20930000 | 0.72731400 | -2.50244900 |
| H | -1.95357400 | 1.22277200 | -2.13831400 |
| H | -1.10124800 | -0.00674100 | -1.88125500 |

H₂O-Na⁺@V_B *h*-BN-H₂O

| | | | |
|---|------------|-------------|-------------|
| B | 0.94351600 | 1.32174300 | 0.57380700 |
| B | 0.90644100 | -1.34814500 | 0.55516100 |
| B | 3.00986600 | -0.04123500 | 0.21872000 |
| B | 3.01739100 | -2.56429200 | 0.01255600 |
| B | 0.81307900 | -3.80623900 | -0.02092700 |

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|---|-------------|-------------|-------------|
| B | -1.37025200 | -2.61681000 | 0.43624400 |
| B | -3.70955900 | -1.25975400 | 0.29316500 |
| B | -3.67502400 | 1.32431500 | 0.29281800 |
| B | -1.28945400 | 2.63784400 | 0.45582400 |
| B | 0.91371100 | 3.77394900 | -0.02029100 |
| B | 3.08365000 | 2.47792300 | 0.00917000 |
| N | 1.64147000 | 2.52152500 | 0.16198200 |
| N | 1.54569300 | -0.02020600 | 0.49525900 |
| N | 3.75007800 | 1.20036100 | 0.08603700 |
| N | -0.54856800 | 3.81123500 | 0.04132400 |
| N | -0.35509900 | 1.72396200 | 1.07767100 |
| N | -2.75802000 | 2.49041900 | 0.24766400 |
| N | -3.48301200 | 0.03167800 | 0.90212200 |
| N | -0.41209400 | -1.70521400 | 1.00178200 |
| N | -2.83407800 | -2.44779800 | 0.25149800 |
| N | -0.64869800 | -3.81041400 | 0.03633000 |
| N | 1.57435700 | -2.56984400 | 0.15275500 |
| N | 3.71616000 | -1.30204900 | 0.08736700 |
| B | 5.20696900 | 1.18021800 | -0.04759000 |
| B | 5.17337800 | -1.32050300 | -0.04288400 |
| B | -1.38785800 | -5.03188500 | -0.23807800 |
| B | -3.53281000 | -3.69473900 | -0.15682900 |
| B | -3.42928700 | 3.75511100 | -0.16500400 |
| B | -1.25785800 | 5.04667200 | -0.24827100 |
| N | 1.64513800 | 4.98224100 | -0.31748800 |
| N | 3.80297200 | 3.71211800 | -0.22490100 |
| N | 3.70646700 | -3.81689200 | -0.21233000 |
| N | 1.51786900 | -5.03446800 | -0.30542900 |

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|---|-------------|-------------|-------------|
| N | -5.04147900 | -1.21733300 | -0.31299800 |
| N | -5.00355800 | 1.32017000 | -0.31963900 |
| B | 3.09215200 | 4.95397400 | -0.38373900 |
| B | 2.96422400 | -5.04211800 | -0.36647000 |
| B | -5.68366300 | 0.05843400 | -0.56560900 |
| B | 0.93512600 | 6.22872000 | -0.54195000 |
| B | 0.77851600 | -6.26617800 | -0.51893000 |
| N | -0.49003000 | 6.22480300 | -0.50921100 |
| N | -0.64578600 | -6.22957200 | -0.48785700 |
| N | -2.81437800 | -4.92718800 | -0.26414100 |
| N | -2.68565800 | 4.97216900 | -0.27262700 |
| N | -4.83475400 | 3.75184000 | -0.47175400 |
| N | -4.93948700 | -3.65594600 | -0.46023500 |
| B | 5.25289800 | 3.68474900 | -0.30657600 |
| B | 5.15617000 | -3.82666700 | -0.28946600 |
| B | -5.62563600 | 2.58931000 | -0.63987700 |
| B | -5.69730900 | -2.47258400 | -0.62904200 |
| N | 5.83750700 | -2.58672900 | -0.18106300 |
| N | 5.87795200 | -0.07888700 | -0.04544200 |
| N | 5.90279400 | 2.42908600 | -0.19306000 |
| H | -6.74526500 | 2.64326800 | -1.03661200 |
| H | -6.77293500 | 0.07526200 | -1.04046700 |
| H | -6.81938200 | -2.49519100 | -1.02261500 |
| H | 3.69075700 | 5.96243200 | -0.58030800 |
| H | 1.53022000 | 7.23533000 | -0.76020900 |
| H | 5.87342300 | 4.68731900 | -0.46821400 |
| H | 5.75244300 | -4.84494300 | -0.44413700 |
| H | 3.53954100 | -6.06557100 | -0.55549900 |

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|----|-------------|-------------|-------------|
| H | 1.35081200 | -7.28815500 | -0.72751000 |
| H | -0.96010300 | 7.10192700 | -0.68853300 |
| H | -3.20287700 | 5.80857100 | -0.51070100 |
| H | -5.26539800 | 4.63555800 | -0.71024900 |
| H | -5.39514600 | -4.52796400 | -0.69504200 |
| H | -3.34865800 | -5.75458700 | -0.49569900 |
| H | -1.13540300 | -7.09791500 | -0.65732400 |
| H | 6.84621500 | -2.60460000 | -0.24830000 |
| H | 6.88461500 | -0.09277200 | -0.14036100 |
| H | 6.91145200 | 2.42091800 | -0.26319100 |
| Na | -1.44272700 | 0.02726700 | 0.75524000 |
| O | -1.70214800 | 0.08397000 | 3.14127900 |
| H | -2.63217300 | 0.19636300 | 3.37949000 |
| H | -1.24152000 | 0.85698700 | 3.49466000 |
| O | -1.35086000 | 0.10353600 | -1.61777600 |
| H | -1.64617900 | 0.83289300 | -2.17794100 |
| H | -1.02857000 | -0.57763600 | -2.22188600 |

H₂O-Na⁺@V_B *h*-BN-H₂O (reactant)

| | | | |
|---|-------------|-------------|-------------|
| B | -0.79480600 | -1.31454200 | 0.14879900 |
| B | -1.00475900 | 1.19977800 | 0.17992400 |
| B | -3.04792900 | -0.22603600 | -0.03430100 |
| B | -3.25134100 | 2.27878700 | -0.06414000 |
| B | -1.16477800 | 3.69291500 | -0.04810800 |
| B | 1.11193100 | 2.60530600 | 0.09576700 |
| B | 3.41505200 | 1.50292000 | 0.04616000 |
| B | 3.62910600 | -1.00814700 | 0.03347400 |
| B | 1.51542700 | -2.41168200 | 0.04965800 |
| B | -0.58254100 | -3.81637400 | -0.05603400 |

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|---|-------------|-------------|-------------|
| B | -2.85684700 | -2.72934900 | -0.05447000 |
| N | -1.40580000 | -2.62138500 | 0.03190800 |
| N | -1.59257300 | -0.11446100 | 0.08614600 |
| N | -3.66282800 | -1.53187200 | -0.07476500 |
| N | 0.86783500 | -3.70282800 | -0.07421900 |
| N | 0.62323200 | -1.34076500 | 0.45030900 |
| N | 2.94809500 | -2.27509800 | -0.09675800 |
| N | 2.99377000 | 0.19712700 | 0.50654800 |
| N | 0.37777900 | 1.43138600 | 0.52465800 |
| N | 2.55325400 | 2.66196500 | -0.05052300 |
| N | 0.28735000 | 3.78905000 | -0.05463400 |
| N | -1.80599100 | 2.39277400 | 0.04222400 |
| N | -3.85884000 | 0.96933400 | -0.08026000 |
| B | -5.11587500 | -1.64584500 | -0.15844400 |
| B | -5.31115500 | 0.85932700 | -0.17009400 |
| B | 0.91667500 | 5.09039900 | -0.24187200 |
| B | 3.17317700 | 3.97285100 | -0.28166400 |
| B | 3.75331400 | -3.47773700 | -0.32737500 |
| B | 1.68021300 | -4.90131100 | -0.26153100 |
| N | -1.21234300 | -5.11448600 | -0.16125100 |
| N | -3.47012100 | -4.03997900 | -0.13053300 |
| N | -4.05394200 | 3.48105000 | -0.15866300 |
| N | -1.97876600 | 4.88197400 | -0.17273100 |
| N | 4.85578300 | 1.60897400 | -0.17242700 |
| N | 5.06489200 | -0.89164000 | -0.18719000 |
| B | -2.65365800 | -5.22460300 | -0.17404300 |
| B | -3.42121500 | 4.77439600 | -0.20233800 |
| B | 5.66704500 | 0.41794200 | -0.27123300 |

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|---|-------------|-------------|-------------|
| B | -0.39957500 | -6.30953500 | -0.28224300 |
| B | -1.34643500 | 6.18157900 | -0.29547500 |
| N | 1.01495800 | -6.16854100 | -0.33321500 |
| N | 0.07494100 | 6.24728700 | -0.33007000 |
| N | 2.34403700 | 5.13502000 | -0.34148900 |
| N | 3.09835300 | -4.74588600 | -0.37995200 |
| N | 5.17691400 | -3.33527400 | -0.46538200 |
| N | 4.60170100 | 4.04555500 | -0.41483600 |
| B | -4.91685300 | -4.15228300 | -0.19477000 |
| B | -5.49985600 | 3.36860700 | -0.23355400 |
| B | 5.85237700 | -2.08850000 | -0.41780600 |
| B | 5.45564500 | 2.91416400 | -0.37654100 |
| N | -6.08036600 | 2.07171100 | -0.22816800 |
| N | -5.89558000 | -0.44648000 | -0.19611000 |
| N | -5.69082400 | -2.96154400 | -0.19926200 |
| H | 7.03074700 | -2.01955900 | -0.57189400 |
| H | 6.83638000 | 0.51658000 | -0.46617100 |
| H | 6.63207600 | 3.02608700 | -0.51941600 |
| H | -3.16268600 | -6.29825100 | -0.23126500 |
| H | -0.90413600 | -7.38553100 | -0.34679500 |
| H | -5.44032600 | -5.22049100 | -0.24526400 |
| H | -6.18201300 | 4.34230800 | -0.29915000 |
| H | -4.08397200 | 5.75984400 | -0.27322000 |
| H | -2.00073600 | 7.17270300 | -0.37460600 |
| H | 1.56219200 | -7.01183500 | -0.44105600 |
| H | 3.66246000 | -5.57280000 | -0.52507700 |
| H | 5.73790700 | -4.16188700 | -0.62189200 |
| H | 5.03357200 | 4.94841100 | -0.55927800 |

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|----|-------------|-------------|-------------|
| H | 2.78930600 | 6.03214500 | -0.48327500 |
| H | 0.49448800 | 7.16086500 | -0.43779700 |
| H | -7.08821700 | 2.01507000 | -0.28502300 |
| H | -6.90176100 | -0.52575300 | -0.26018000 |
| H | -6.69562500 | -3.06127800 | -0.25000600 |
| Na | 1.37049800 | 0.08817300 | 2.25702300 |
| O | 1.45658300 | 0.09445300 | 4.50570200 |
| H | 2.24796400 | 0.00509100 | 5.05217100 |
| H | 0.72641200 | 0.20959600 | 5.12728000 |
| O | 2.52343900 | 0.31178400 | -2.62090000 |
| H | 2.86359600 | -0.39565000 | -3.18347600 |
| H | 2.69056600 | 1.11864100 | -3.12451100 |

H₂O-K@V_B *h*-BN-H₂O

| | | | |
|---|-------------|-------------|-------------|
| B | -1.16672200 | -1.09426400 | -0.32887400 |
| B | -0.65889500 | 1.50808300 | 0.41799700 |
| B | -2.92930600 | 0.60567900 | -0.03784600 |
| B | -2.46471800 | 3.08085100 | -0.26185600 |
| B | -0.09108700 | 3.88938700 | 0.04025300 |
| B | 1.67827200 | 2.26702700 | 0.81885000 |
| B | 3.88255600 | 0.46407000 | 0.65935600 |
| B | 3.37826400 | -1.97069000 | 0.10020700 |
| B | 0.70242800 | -2.70993100 | -0.52581900 |
| B | -1.59864300 | -3.52848900 | 0.00140300 |
| B | -3.48449000 | -1.85926400 | 0.15117100 |
| N | -2.08888800 | -2.16419800 | 0.01950900 |
| N | -1.49361300 | 0.31732100 | 0.03331500 |
| N | -3.90745200 | -0.47758000 | 0.03732700 |
| N | -0.18374200 | -3.81705200 | -0.20087800 |

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|---|-------------|-------------|-------------|
| N | -0.00522300 | -1.56012400 | -1.02954300 |
| N | 2.21925200 | -2.85593800 | -0.29198300 |
| N | 3.40907800 | -0.84820500 | 1.00777800 |
| N | 0.52451300 | 1.52144900 | 1.22346600 |
| N | 3.16864700 | 1.79821700 | 0.71718300 |
| N | 1.31177600 | 3.60947800 | 0.35149900 |
| N | -1.07732400 | 2.83138700 | -0.00384900 |
| N | -3.40271400 | 1.97626300 | -0.18404500 |
| B | -5.32894100 | -0.18454300 | 0.02574800 |
| B | -4.82177500 | 2.25517500 | -0.30197200 |
| B | 2.28899300 | 4.66007700 | 0.23911900 |
| B | 4.10497600 | 2.92304600 | 0.51532900 |
| B | 2.66409900 | -4.24847500 | -0.48439800 |
| B | 0.31933800 | -5.16565500 | -0.15916200 |
| N | -2.53380000 | -4.61459200 | 0.24052000 |
| N | -4.42837800 | -2.95245200 | 0.33276800 |
| N | -2.89767400 | 4.44432300 | -0.52754900 |
| N | -0.51690100 | 5.24063800 | -0.29430900 |
| N | 5.24302100 | 0.28183100 | 0.10313400 |
| N | 4.73827300 | -2.17002600 | -0.42201500 |
| B | -3.94337800 | -4.31368400 | 0.39789400 |
| B | -1.91587400 | 5.50430900 | -0.56366300 |
| B | 5.64496200 | -1.03261400 | -0.38302700 |
| B | -2.02839100 | -5.97412200 | 0.28532900 |
| B | 0.46882100 | 6.30195200 | -0.33839000 |
| N | -0.63297400 | -6.21717100 | 0.09317200 |
| N | 1.83537000 | 5.99026100 | -0.07954100 |
| N | 3.65593400 | 4.28761600 | 0.43946600 |

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|---|-------------|-------------|-------------|
| N | 1.72435700 | -5.33869400 | -0.41602500 |
| N | 4.06689000 | -4.50371500 | -0.75266200 |
| N | 5.52873700 | 2.68460800 | 0.36263400 |
| B | -5.84210500 | -2.63984600 | 0.37235600 |
| B | -4.31234800 | 4.70322600 | -0.68744700 |
| B | 5.08102300 | -3.50974900 | -0.84297800 |
| B | 6.11263300 | 1.43407300 | 0.05219900 |
| N | -5.22564400 | 3.61760700 | -0.55503300 |
| N | -5.75427900 | 1.17217800 | -0.16402400 |
| N | -6.24748800 | -1.28458700 | 0.20643000 |
| H | 6.18111100 | -3.77802000 | -1.21984600 |
| H | 6.74525900 | -1.16451200 | -0.82371300 |
| H | 7.26215900 | 1.33764200 | -0.25258200 |
| H | -4.71689100 | -5.20531300 | 0.57024100 |
| H | -2.76958400 | -6.88934000 | 0.47951900 |
| H | -6.65616500 | -3.49901900 | 0.52776000 |
| H | -4.71344100 | 5.80460400 | -0.91412100 |
| H | -2.26416100 | 6.61878800 | -0.80866100 |
| H | 0.14755400 | 7.42244300 | -0.59540700 |
| H | -0.32281500 | -7.17810200 | 0.13801600 |
| H | 2.09501800 | -6.27694800 | -0.48780500 |
| H | 4.33587900 | -5.45255100 | -0.97602600 |
| H | 6.12557100 | 3.49718500 | 0.28600100 |
| H | 4.36815400 | 4.99594200 | 0.32150000 |
| H | 2.50349200 | 6.74629200 | -0.13782000 |
| H | -6.20904000 | 3.82648500 | -0.65932900 |
| H | -6.74424400 | 1.37189100 | -0.21001300 |
| H | -7.24025600 | -1.09534000 | 0.22338600 |

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|---|-------------|-------------|-------------|
| K | 1.41153300 | -0.35028800 | 0.26272500 |
| O | 0.10169600 | -0.93308000 | 2.68828000 |
| H | 0.17879500 | 0.03474700 | 2.55785900 |
| H | -0.84725900 | -1.10622300 | 2.64311000 |
| O | 1.73189500 | 0.13707600 | -2.39854200 |
| H | 2.14894200 | -0.09101500 | -3.23722200 |
| H | 0.99732900 | -0.50619000 | -2.27062300 |

H₂O-K@V_B *h*-BN-H₂O (reactant)

| | | | |
|---|-------------|-------------|-------------|
| B | 1.51449600 | 0.13492300 | 0.62759300 |
| B | -0.79020900 | 0.93917400 | -0.03527100 |
| B | 1.22201300 | 2.48956800 | -0.21428000 |
| B | -1.05900700 | 3.47375200 | -0.32322300 |
| B | -3.08091000 | 2.16799100 | 0.22271100 |
| B | -2.96557900 | -0.25696000 | 0.20508700 |
| B | -2.71412900 | -2.38767800 | -0.46222700 |
| B | -0.31051000 | -2.91958200 | -0.74292500 |
| B | 1.70590100 | -2.08826700 | 0.57093900 |
| B | 3.81061800 | -0.81795900 | 0.60520700 |
| B | 3.54396100 | 1.59641400 | 0.15197700 |
| N | 2.96887700 | 0.34693000 | 0.51454800 |
| N | 0.63413800 | 1.18165200 | 0.05748000 |
| N | 2.66072000 | 2.69347600 | -0.18792100 |
| N | 3.17634400 | -2.10332600 | 0.59091400 |
| N | 0.96092500 | -1.04501400 | 1.14212400 |
| N | 1.02599300 | -3.12830500 | -0.23079900 |
| N | -1.35949200 | -1.84129900 | -0.49390700 |
| N | -1.54701200 | -0.36728700 | -0.07620000 |
| N | -3.63053900 | -1.50703600 | 0.16158900 |

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|---|-------------|-------------|-------------|
| N | -3.73590300 | 0.91370400 | 0.45169300 |
| N | -1.65507600 | 2.16306200 | -0.04844500 |
| N | 0.36236700 | 3.62096300 | -0.49678400 |
| B | 3.24256000 | 3.97191200 | -0.53798400 |
| B | 0.94341000 | 4.91518100 | -0.82118600 |
| B | -5.17848400 | 0.79159600 | 0.61420600 |
| B | -5.05629900 | -1.67105100 | 0.16773700 |
| B | 1.85950000 | -4.25158600 | -0.66667200 |
| B | 3.94713800 | -3.26399400 | 0.27357800 |
| N | 5.26342000 | -0.69975800 | 0.55615100 |
| N | 4.99816100 | 1.75093100 | 0.12399900 |
| N | -1.90297800 | 4.66808100 | -0.42396500 |
| N | -3.89262700 | 3.37325500 | 0.26155400 |
| N | -3.21364900 | -3.62125700 | -0.99897300 |
| N | -0.86308100 | -4.03495200 | -1.57734200 |
| B | 5.84595100 | 0.60275000 | 0.35770800 |
| B | -3.29809200 | 4.62813800 | -0.10137000 |
| B | -2.24662800 | -4.38296100 | -1.73157000 |
| B | 6.05301600 | -1.91358400 | 0.50049900 |
| B | -5.30271500 | 3.29335900 | 0.57201400 |
| N | 5.38731600 | -3.17012200 | 0.37370400 |
| N | -5.90968400 | 2.01809800 | 0.77178300 |
| N | -5.81200200 | -0.50965700 | 0.54690700 |
| N | 3.21272100 | -4.40575500 | -0.19667300 |
| N | 1.32383600 | -5.19209100 | -1.60990500 |
| N | -5.52121300 | -2.95818900 | -0.28536100 |
| B | 5.56116800 | 3.03779300 | -0.20461500 |
| B | -1.33427800 | 5.94127200 | -0.81759500 |

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|---|-------------|-------------|-------------|
| B | 0.00758900 | -5.08164300 | -2.09352900 |
| B | -4.63346400 | -3.90028300 | -0.90773400 |
| N | 0.05948800 | 6.02873300 | -1.04435100 |
| N | 2.36437800 | 5.05022300 | -0.88439400 |
| N | 4.67662500 | 4.10924000 | -0.51990700 |
| H | -0.40486600 | -5.86474200 | -2.89279700 |
| H | -2.58749800 | -5.30073800 | -2.40888800 |
| H | -5.07209400 | -4.91387200 | -1.36072000 |
| H | 7.03307400 | 0.73247700 | 0.34651000 |
| H | 7.24729800 | -1.86669900 | 0.51702400 |
| H | 6.74320500 | 3.20978300 | -0.21993000 |
| H | -2.03087700 | 6.90232100 | -0.94172000 |
| H | -3.95939300 | 5.61920300 | -0.13526700 |
| H | -5.96342400 | 4.28449800 | 0.64361700 |
| H | 5.96157700 | -3.99070200 | 0.23978000 |
| H | 3.72184800 | -5.21980700 | -0.51388400 |
| H | 1.91227300 | -5.92523700 | -1.97926600 |
| H | -6.50723700 | -3.17954300 | -0.29748900 |
| H | -6.82224500 | -0.54764300 | 0.56859000 |
| H | -6.90687000 | 1.99680000 | 0.93377200 |
| H | 0.44489600 | 6.92784400 | -1.29667800 |
| H | 2.75882400 | 5.95142300 | -1.11617700 |
| H | 5.08894800 | 5.00089500 | -0.75640000 |
| K | -1.20207700 | -1.79076600 | 2.50092800 |
| O | 0.59567200 | -0.62405000 | -2.74389100 |
| H | -0.31686500 | -0.83683200 | -2.50967900 |
| H | 0.86502000 | -0.00731700 | -2.04883000 |
| O | 0.91095900 | -1.26597400 | 3.86630600 |

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|---|-------------|-------------|-------------|
| H | 1.70242200 | -1.31047200 | 4.41311000 |
| H | 1.21896500 | -1.09835800 | 2.93037600 |
| H ₂ O-K ⁺ @V _B h-BN-H ₂ O | | | |
| B | -0.42577700 | -1.58879400 | 0.39219700 |
| B | -1.32177900 | 0.91901900 | -0.35265500 |
| B | -2.79935300 | -1.03290800 | -0.04145400 |
| B | -3.72604400 | 1.32694300 | 0.07250200 |
| B | -2.11589700 | 3.27847200 | -0.07237600 |
| B | 0.32004000 | 2.86922000 | -0.49214000 |
| B | 3.01882300 | 2.46533000 | 0.07509000 |
| B | 3.89373300 | 0.09132400 | 0.58023000 |
| B | 2.08303800 | -2.02941200 | 0.75024400 |
| B | 0.50281100 | -3.88750400 | 0.08855400 |
| B | -1.97910900 | -3.42787800 | -0.18657200 |
| N | -0.63035400 | -2.96912900 | 0.06267700 |
| N | -1.39328200 | -0.52167900 | 0.00819000 |
| N | -3.05254100 | -2.45833500 | -0.14124000 |
| N | 1.86286200 | -3.40121200 | 0.34435600 |
| N | 0.79417800 | -1.50338500 | 1.20657500 |
| N | 3.41898700 | -1.33432600 | 0.63890200 |
| N | 3.20606700 | 1.31862800 | 0.95545200 |
| N | -0.24882100 | 1.63849900 | -1.05219400 |
| N | 1.75847400 | 3.19531100 | -0.25980400 |
| N | -0.75247100 | 3.78664200 | -0.21979400 |
| N | -2.38913700 | 1.84455500 | -0.10218200 |
| N | -3.91632400 | -0.10657600 | 0.00668200 |
| B | -4.42446900 | -2.95337300 | -0.24470700 |
| B | -5.28773700 | -0.61222200 | 0.02397200 |

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|---|-------------|-------------|-------------|
| B | -0.46522600 | 5.20691100 | -0.15117700 |
| B | 2.00482900 | 4.65705400 | -0.42064700 |
| B | 4.53099900 | -2.30553000 | 0.40897800 |
| B | 2.98833400 | -4.30693600 | 0.21439000 |
| N | 0.27057700 | -5.27921400 | -0.20997200 |
| N | -2.20054400 | -4.83660700 | -0.41841100 |
| N | -4.81379400 | 2.26175200 | 0.25611500 |
| N | -3.20138500 | 4.19622100 | 0.16239000 |
| N | 4.33167500 | 2.86918200 | -0.39856300 |
| N | 5.19145800 | 0.50445300 | 0.04507000 |
| B | -1.08263400 | -5.75162600 | -0.44500600 |
| B | -4.55254700 | 3.68294600 | 0.31270100 |
| B | 5.40751300 | 1.88598200 | -0.37919700 |
| B | 1.39781800 | -6.19611600 | -0.26408700 |
| B | -2.92002600 | 5.62266500 | 0.22983500 |
| N | 2.71534500 | -5.68630400 | -0.06042100 |
| N | -1.57446500 | 6.08493700 | 0.07584500 |
| N | 0.90884600 | 5.58355200 | -0.34768500 |
| N | 4.28453300 | -3.71770200 | 0.34836400 |
| N | 5.87824800 | -1.82904400 | 0.22578900 |
| N | 3.35494800 | 5.10431300 | -0.65682200 |
| B | -3.56665300 | -5.30973300 | -0.56763700 |
| B | -6.16848900 | 1.73986200 | 0.32600900 |
| B | 6.24350500 | -0.48824800 | -0.04752200 |
| B | 4.49957400 | 4.26447500 | -0.76387100 |
| N | -6.35645700 | 0.33655700 | 0.19032100 |
| N | -5.50045400 | -2.01846500 | -0.12757900 |
| N | -4.62133900 | -4.36227600 | -0.45867900 |

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|---|-------------|-------------|-------------|
| H | 7.35319100 | -0.18971500 | -0.35367900 |
| H | 6.48371500 | 2.20336500 | -0.77111300 |
| H | 5.55638100 | 4.68988600 | -1.10554600 |
| H | -1.26960600 | -6.90691600 | -0.65716900 |
| H | 1.22789500 | -7.35238200 | -0.48740400 |
| H | -3.79542600 | -6.46114400 | -0.76410700 |
| H | -7.09625200 | 2.46944500 | 0.48022700 |
| H | -5.45195100 | 4.44336500 | 0.47896300 |
| H | -3.80037000 | 6.40198200 | 0.41354200 |
| H | 3.47889900 | -6.34574500 | -0.12902800 |
| H | 5.09345800 | -4.31465900 | 0.23301900 |
| H | 6.60811200 | -2.52374400 | 0.13538000 |
| H | 3.49872200 | 6.08891200 | -0.84041300 |
| H | 1.13350200 | 6.56842800 | -0.40929200 |
| H | -1.42638500 | 7.08372200 | 0.13268600 |
| H | -7.30839400 | -0.00302800 | 0.22539800 |
| H | -6.44997200 | -2.36553300 | -0.15649800 |
| H | -5.56489400 | -4.71427700 | -0.55088400 |
| K | 1.22120500 | 0.49727800 | 0.26354000 |
| O | 0.13106900 | 1.30299600 | 2.59427400 |
| H | 0.45960200 | 1.96770800 | 3.21290500 |
| H | -0.02480400 | 0.51076100 | 3.12580000 |
| O | 1.57607400 | -0.26728600 | -2.25921900 |
| H | 1.97469400 | -0.78640300 | -2.96819500 |
| H | 0.90965800 | 0.29996400 | -2.67427300 |

H₂O-K⁺@V_B *h*-BN-H₂O (reactant)

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|---|------------|-------------|-------------|
| B | 0.99941600 | 1.15873700 | -0.10088700 |
| B | 0.68281500 | -1.36470800 | -0.09690300 |

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|---|-------------|-------------|-------------|
| B | 2.98024800 | -0.36951400 | 0.02335600 |
| B | 2.68842300 | -2.86650600 | 0.10464300 |
| B | 0.38189700 | -3.86090800 | 0.17731000 |
| B | -1.63463800 | -2.38221400 | 0.04703300 |
| B | -3.62750000 | -0.84313300 | 0.19465700 |
| B | -3.30547100 | 1.71100600 | 0.21457800 |
| B | -0.99614700 | 2.71361100 | 0.06448900 |
| B | 1.32222700 | 3.65366300 | 0.16348200 |
| B | 3.31328000 | 2.12306400 | 0.07499400 |
| N | 1.87247100 | 2.31333000 | 0.03778500 |
| N | 1.52806000 | -0.18862700 | -0.07561800 |
| N | 3.85367500 | 0.78453500 | 0.04827800 |
| N | -0.11617900 | 3.84963900 | 0.20851200 |
| N | -0.36894100 | 1.51220600 | -0.41803500 |
| N | -2.42364500 | 2.84436900 | 0.27024800 |
| N | -2.91238600 | 0.36624900 | -0.09652000 |
| N | -0.72842400 | -1.36943500 | -0.42730500 |
| N | -3.05301900 | -2.15966300 | 0.23924900 |
| N | -1.06126400 | -3.69875600 | 0.19899600 |
| N | 1.24509200 | -2.69664100 | 0.05474700 |
| N | 3.54236900 | -1.70289600 | 0.06502200 |
| B | 5.30138100 | 0.60381500 | 0.08120200 |
| B | 4.98983400 | -1.88455800 | 0.10374500 |
| B | -1.92793700 | -4.84888100 | 0.41441800 |
| B | -3.92418300 | -3.31550400 | 0.45859800 |
| B | -2.98194700 | 4.17793900 | 0.50393600 |
| B | -0.67167200 | 5.17589000 | 0.43538400 |
| N | 2.20385400 | 4.79568200 | 0.27772600 |

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|---|-------------|-------------|------------|
| N | 4.18584700 | 3.28075800 | 0.14700700 |
| N | 3.24959200 | -4.20169400 | 0.19965000 |
| N | 0.95567000 | -5.18296500 | 0.31058900 |
| N | -5.06452200 | -0.63144300 | 0.38563800 |
| N | -4.74989700 | 1.85869400 | 0.40929100 |
| B | 3.63557800 | 4.60694800 | 0.24367000 |
| B | 2.39010000 | -5.35134400 | 0.30028300 |
| B | -5.60909100 | 0.70144800 | 0.48205500 |
| B | 1.65175200 | 6.12574000 | 0.44973700 |
| B | 0.09277900 | -6.33733000 | 0.47233500 |
| N | 0.23811100 | 6.27871900 | 0.53250400 |
| N | -1.31670600 | -6.14049300 | 0.52374500 |
| N | -3.34061100 | -4.61859900 | 0.51140100 |
| N | -2.09642500 | 5.29790200 | 0.55366300 |
| N | -4.40735300 | 4.29573000 | 0.64979500 |
| N | -5.33661100 | -3.08027600 | 0.59024800 |
| B | 5.62538500 | 3.09571900 | 0.15189000 |
| B | 4.69010300 | -4.37749900 | 0.21797000 |
| B | -5.29598600 | 3.19136400 | 0.61385600 |
| B | -5.92482200 | -1.79034100 | 0.56590800 |
| N | 5.51159200 | -3.22213300 | 0.15775500 |
| N | 5.82633300 | -0.72566700 | 0.08809600 |
| N | 6.13647600 | 1.77253800 | 0.10819200 |
| H | -6.46809800 | 3.34208700 | 0.75707200 |
| H | -6.77657200 | 0.84741400 | 0.65498000 |
| H | -7.09903600 | -1.64789100 | 0.70078200 |
| H | 4.35805900 | 5.55050700 | 0.30356400 |
| H | 2.36656300 | 7.07454000 | 0.52908600 |

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|---|-------------|-------------|-------------|
| H | 6.35855600 | 4.03321300 | 0.19455300 |
| H | 5.16862600 | -5.46601800 | 0.28290700 |
| H | 2.85827600 | -6.44216700 | 0.38105700 |
| H | 0.55313100 | -7.43102500 | 0.56787700 |
| H | -0.11993800 | 7.21335100 | 0.67502100 |
| H | -2.49031000 | 6.21589300 | 0.71255600 |
| H | -4.81192200 | 5.20942300 | 0.80488400 |
| H | -5.95514000 | -3.86762900 | 0.73154300 |
| H | -3.94915300 | -5.41245000 | 0.66158200 |
| H | -1.89463100 | -6.95887000 | 0.65935700 |
| H | 6.51283500 | -3.36047900 | 0.17843500 |
| H | 6.82935000 | -0.85091000 | 0.11720500 |
| H | 7.14116700 | 1.66087600 | 0.12140200 |
| K | -1.50818700 | 0.20733700 | -2.63667000 |
| O | -0.70246700 | 0.05176200 | 2.39496700 |
| H | -0.54979800 | 0.02227800 | 3.34839800 |
| H | -1.65606400 | 0.16325200 | 2.29840900 |
| O | -1.40300800 | 0.11414300 | -5.32276400 |
| H | -1.64507300 | 0.80067700 | -5.95793700 |
| H | -1.07269900 | -0.61269100 | -5.86693300 |