

# Supplementary Materials

## Hydrogen vs. Halogen bonds in 1-halo-closoboranes

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**Table S1.** Electronic energy and optimized geometry of the isolated monomers at MP2/aug-cc-pVDZ/aug-cc-pVDZ-PP computational level.

| System                                                        | MP2 Energy<br>(Hartree) | Cartesian Coordinates<br>(Å)                |
|---------------------------------------------------------------|-------------------------|---------------------------------------------|
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F  | -429.97280638           | C,0.,0.7437835148,-1.3448219925             |
|                                                               |                         | C,0.,-0.8913918055,-1.2975714022            |
|                                                               |                         | B,1.4750655713,-0.0609198943,-0.9031926022  |
|                                                               |                         | B,0.9023475964,-1.4783116271,0.0295244619   |
|                                                               |                         | B,0.,-0.8719644622,1.4564406388             |
|                                                               |                         | B,-1.466031994,0.0064320412,0.8721568357    |
|                                                               |                         | B,0.,0.9283311444,1.3892937985              |
|                                                               |                         | B,-0.9073084557,1.4276030379,-0.0767096154  |
|                                                               |                         | B,0.9073084557,1.4276030379,-0.0767096154   |
|                                                               |                         | B,-0.9023475964,-1.4783116271,0.0295244619  |
|                                                               |                         | H,-1.4907074702,-2.5048024247,-0.1107071617 |
|                                                               |                         | H,1.4817000645,2.4442606183,-0.3104516857   |
|                                                               |                         | H,0.,-1.4817235357,2.4827742694             |
|                                                               |                         | H,1.4907074702,-2.5048024247,-0.1107071617  |
|                                                               |                         | H,-1.4817000645,2.4442606183,-0.3104516857  |
|                                                               |                         | H,0.,1.6199599405,2.3628451774              |
|                                                               |                         | H,2.3275071373,-0.0702282428,-1.7323145326  |
|                                                               |                         | H,-2.5003763979,0.0298427222,1.467516212    |
|                                                               |                         | H,0.,-1.3762303573,-2.2764449638            |
|                                                               |                         | B,1.466031994,0.0064320412,0.8721568357     |
|                                                               |                         | B,-1.4750655713,-0.0609198943,-0.9031926022 |
|                                                               |                         | H,2.5003763979,0.0298427222,1.467516212     |
|                                                               |                         | H,-2.3275071373,-0.0702282428,-1.7323145326 |
|                                                               |                         | F,0.,1.2887294666,-2.5925029374             |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl | -789.98805749           | C,0.,0.740953494,-1.3432106992              |
|                                                               |                         | C,0.,-0.9011357391,-1.2837970204            |
|                                                               |                         | B,1.4735261724,-0.06771899,-0.8915429021    |
|                                                               |                         | B,0.9012613534,-1.4847191909,0.04464192     |
|                                                               |                         | B,0.,-0.8803370807,1.4731665351             |
|                                                               |                         | B,-1.4650216558,-0.0007238683,0.885886224   |
|                                                               |                         | B,0.,0.9197482855,1.4057196932              |
|                                                               |                         | B,-0.9058363383,1.4204278544,-0.0613292762  |
|                                                               |                         | B,0.9058363383,1.4204278544,-0.0613292762   |
|                                                               |                         | B,-0.9012613534,-1.4847191909,0.04464192    |
|                                                               |                         | H,-1.4929350464,-2.5094247488,-0.0973200832 |
|                                                               |                         | H,1.4845115823,2.4358584017,-0.2904216892   |
|                                                               |                         | H,0.,-1.4914292115,2.4988770033             |
|                                                               |                         | H,1.4929350464,-2.5094247488,-0.0973200832  |
|                                                               |                         | H,-1.4845115823,2.4358584017,-0.2904216892  |
|                                                               |                         | H,0.,1.6121411359,2.3791093811              |
|                                                               |                         | H,2.3379406372,-0.0847394559,-1.707799601   |
|                                                               |                         | H,-2.5013729461,0.0235687388,1.4781044924   |
|                                                               |                         | H,0.,-1.3922985972,-2.2592250307            |
|                                                               |                         | B,1.4650216558,-0.0007238683,0.885886224    |
|                                                               |                         | B,-1.4735261724,-0.06771899,-0.8915429021   |
|                                                               |                         | H,2.5013729461,0.0235687388,1.4781044924    |

$\text{H}, -2.3379406372, -0.0847394559, -1.707799601$   
 $\text{Cl}, 0., 1.4745465887, -2.939421618$

$\text{C}, 0., 0.7581705491, -1.3326076784$   
 $\text{C}, 0., -0.8840491287, -1.2915461818$   
 $\text{B}, 1.4731549799, -0.0544826354, -0.8913205906$   
 $\text{B}, 0.9011554276, -1.4822634482, 0.0304385665$   
 $\text{B}, 0., -0.8941856755, 1.4659016939$   
 $\text{B}, -1.4649304125, -0.0079475873, 0.8879653826$   
 $\text{B}, 0., 0.9063162406, 1.4189430259$   
 $\text{B}, -0.9055171408, 1.4237624095, -0.0429583644$   
 $\text{B}, 0.9055171408, 1.4237624095, -0.0429583644$   
 $\text{B}, -0.9011554276, -1.4822634482, 0.0304385665$   
 $\text{H}, -1.4932244406, -2.5050981209, -0.123672175$   
 $\text{H}, 1.4858413893, 2.4415902717, -0.2572460359$   
 $\text{H}, 0., -1.5170399262, 2.4846940104$   
 $\text{H}, 1.4932244406, -2.5050981209, -0.123672175$   
 $\text{H}, -1.4858413893, 2.4415902717, -0.2572460359$   
 $\text{H}, 0., 1.5884695599, 2.3996874518$   
 $\text{H}, 2.342012414, -0.066197501, -1.7030253707$   
 $\text{H}, -2.5020227765, 0.0103453286, 1.4792367192$   
 $\text{H}, 0., -1.3679515763, -2.2707250054$   
 $\text{B}, 1.4649304125, -0.0079475873, 0.8879653826$   
 $\text{B}, -1.4731549799, -0.0544826354, -0.8913205906$   
 $\text{H}, 2.5020227765, 0.0103453286, 1.4792367192$   
 $\text{H}, -2.342012414, -0.066197501, -1.7030253707$   
 $\text{Br}, 0., 1.58165828, -3.0555662318$

$\text{o-B}_{10}\text{H}_{11}\text{C}_2\text{-1Br} \quad -2902.86986278$

$\text{C}, 0., 0.784976194, -1.3212264679$   
 $\text{C}, 0., -0.8597346966, -1.3023996169$   
 $\text{B}, 1.471731012, -0.0356377862, -0.8909451222$   
 $\text{B}, 0.9010091498, -1.4787677826, 0.0101359641$   
 $\text{B}, 0., -0.9141256924, 1.4552273117$   
 $\text{B}, -1.4647892202, -0.0185398966, 0.8905986007$   
 $\text{B}, 0., 0.886632695, 1.4373682622$   
 $\text{B}, -0.9047382841, 1.4276990644, -0.0169227321$   
 $\text{B}, 0.9047382841, 1.4276990644, -0.0169227321$   
 $\text{B}, -0.9010091498, -1.4787677826, 0.0101359641$   
 $\text{H}, -1.4936397615, -2.4987536309, -0.160780715$   
 $\text{H}, 1.4883051069, 2.4484172448, -0.2094757041$   
 $\text{H}, 0., -1.5535878377, 2.4639818528$   
 $\text{H}, 1.4936397615, -2.4987536309, -0.160780715$   
 $\text{H}, -1.4883051069, 2.4484172448, -0.2094757041$   
 $\text{H}, 0., 1.5535666444, 2.4286952856$   
 $\text{H}, 2.3465922167, -0.0394594201, -1.6966716751$   
 $\text{H}, -2.5026754337, -0.0089730265, 1.4809466278$   
 $\text{H}, 0., -1.3343852654, -2.2861432175$   
 $\text{B}, 1.4647892202, -0.0185398966, 0.8905986007$   
 $\text{B}, -1.471731012, -0.0356377862, -0.8909451222$   
 $\text{H}, 2.5026754337, -0.0089730265, 1.4809466278$   
 $\text{H}, -2.3465922167, -0.0394594201, -1.6966716751$

$\text{o-B}_{10}\text{H}_{11}\text{C}_2\text{-1I} \quad -625.12798071$

|                                                              |               |                                             |
|--------------------------------------------------------------|---------------|---------------------------------------------|
|                                                              |               | I,0.,1.7415532193,-3.2158974402             |
|                                                              |               | C,0.,-1.3089796983,-0.8043405428            |
|                                                              |               | B,0.9001214611,0.,-1.4225026712             |
|                                                              |               | B,-0.9001214611,0.,-1.4225026712            |
|                                                              |               | C,0.,1.3089796983,-0.8043405428             |
|                                                              |               | B,0.,1.4432576505,0.913493591               |
|                                                              |               | B,0.9047857162,0.,1.4742776087              |
|                                                              |               | B,-0.9047857162,0.,1.4742776087             |
|                                                              |               | B,0.,-1.4432576505,0.913493591              |
|                                                              |               | B,-1.4591403359,-0.892799674,0.018377352    |
|                                                              |               | B,1.4591403359,0.892799674,0.018377352      |
|                                                              |               | H,2.4142767602,1.5978903512,-0.0854170158   |
| <i>m</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub>     | -330.95472405 | H,-2.4142767602,-1.5978903512,-0.0854170158 |
|                                                              |               | H,0.,2.5284761086,1.4080335078              |
|                                                              |               | H,0.,2.229318079,-1.3928234482              |
|                                                              |               | H,0.,-2.5284761086,1.4080335078             |
|                                                              |               | H,-1.5450778069,0.,2.4821815724             |
|                                                              |               | H,-1.4337911734,0.,-2.4851121272            |
|                                                              |               | H,1.5450778069,0.,2.4821815724              |
|                                                              |               | H,1.4337911734,0.,-2.4851121272             |
|                                                              |               | B,-1.4591403359,0.892799674,0.018377352     |
|                                                              |               | B,1.4591403359,-0.892799674,0.018377352     |
|                                                              |               | H,-2.4142767602,1.5978903512,-0.0854170158  |
|                                                              |               | H,2.4142767602,-1.5978903512,-0.0854170158  |
|                                                              |               | H,0.,-2.229318079,-1.3928234482             |
|                                                              |               | C,1.3783749504,-1.2556751409,0.0000000021   |
|                                                              |               | B,1.2079924563,0.1755975877,0.9032589297    |
|                                                              |               | B,1.2079924562,0.1755975845,-0.9032589304   |
|                                                              |               | C,-0.0211819751,0.9474012657,-0.0000000017  |
|                                                              |               | B,-1.5447466111,0.1552016941,-0.0000000002  |
|                                                              |               | B,-1.2465243588,-1.3639453072,0.9054105703  |
|                                                              |               | B,-1.2465243589,-1.3639453104,-0.9054105653 |
|                                                              |               | B,-0.0025866796,-2.2853129248,0.0000000004  |
|                                                              |               | B,0.4595071158,-1.3456911967,-1.4605301297  |
|                                                              |               | B,-0.4914257754,0.162789393,1.4635942466    |
|                                                              |               | H,-0.7725593101,0.8420856121,2.4000374891   |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F | -429.99512783 | H,0.9252519171,-1.8859924979,-2.4143027769  |
|                                                              |               | H,-2.5250175409,0.8321305427,-0.0000000013  |
|                                                              |               | H,0.1595921572,-3.465649749,0.0000000061    |
|                                                              |               | H,-2.1012978898,-1.8985201353,-1.5440683779 |
|                                                              |               | H,2.0938218942,0.7676268666,-1.4283226152   |
|                                                              |               | H,-2.1012978896,-1.8985201298,1.5440683848  |
|                                                              |               | H,2.0938218944,0.7676268716,1.4283226122    |
|                                                              |               | B,-0.4914257755,0.1627893878,-1.4635942471  |
|                                                              |               | B,0.459507116,-1.3456911915,1.4605301344    |
|                                                              |               | H,-0.7725593103,0.8420856036,-2.400037492   |
|                                                              |               | H,0.9252519174,-1.8859924894,2.4143027835   |
|                                                              |               | H,2.3669157615,-1.7204112109,0.0000000029   |
|                                                              |               | F,-0.0061140675,2.3168059325,-0.0000000041  |

|                                                               |                |                                             |
|---------------------------------------------------------------|----------------|---------------------------------------------|
|                                                               |                | C,1.3774058236,-1.2730562059,0.000000003    |
|                                                               |                | B,1.2072250329,0.1607310836,0.9028857707    |
|                                                               |                | B,1.2072250339,0.1607310804,-0.9028857699   |
|                                                               |                | C,-0.0184094975,0.941090031,-0.0000000017   |
|                                                               |                | B,-1.5454343723,0.1384299816,-0.0000000011  |
|                                                               |                | B,-1.2462863135,-1.3814160685,0.9050025811  |
|                                                               |                | B,-1.2462863125,-1.3814160717,-0.9050025777 |
|                                                               |                | B,-0.0024913189,-2.3042183882,0.0000000041  |
|                                                               |                | B,0.4598955279,-1.3621618812,-1.4596709014  |
|                                                               |                | B,-0.4922458155,0.1470482606,1.4638496349   |
|                                                               |                | H,-0.7760872261,0.8180949942,2.4053085938   |
|                                                               |                | H,0.9255740725,-1.8989664147,-2.4157072706  |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl | -790.01122761  | H,-2.5295121461,0.8098727229,-0.0000000029  |
|                                                               |                | H,0.1593793506,-3.4847973455,0.0000000063   |
|                                                               |                | H,-2.1021219409,-1.9129202932,-1.5451747493 |
|                                                               |                | H,2.0968379733,0.7470114545,-1.4279700097   |
|                                                               |                | H,-2.1021219426,-1.9129202877,1.5451747536  |
|                                                               |                | H,2.0968379717,0.7470114595,1.4279700094    |
|                                                               |                | B,-0.4922458138,0.1470482554,-1.463849636   |
|                                                               |                | B,0.4598955262,-1.362161876,1.4596709068    |
|                                                               |                | H,-0.7760872234,0.8180949857,-2.4053085977  |
|                                                               |                | H,0.9255740698,-1.8989664061,2.4157072784   |
|                                                               |                | H,2.3673775627,-1.7350934175,0.0000000044   |
|                                                               |                | Cl,0.0008700754,2.7053214015,-0.0000000048  |
|                                                               |                | C,1.3771747105,-1.2788780584,0.0000000022   |
|                                                               |                | B,1.2068726453,0.1555618259,0.9026763479    |
|                                                               |                | B,1.2068726452,0.1555618227,-0.9026763486   |
|                                                               |                | C,-0.0181949208,0.9334050719,-0.0000000017  |
|                                                               |                | B,-1.5455626827,0.1326327342,-0.0000000002  |
|                                                               |                | B,-1.2461911362,-1.3872573705,0.904884649   |
|                                                               |                | B,-1.2461911363,-1.3872573738,-0.904884644  |
|                                                               |                | B,-0.0025432877,-2.309897235,0.0000000041   |
|                                                               |                | B,0.4599455856,-1.3678213313,-1.4595664097  |
|                                                               |                | B,-0.4925499383,0.1415762475,1.4638334826   |
|                                                               |                | H,-0.7773993821,0.8101803354,2.4069972218   |
|                                                               |                | H,0.9263041826,-1.9049153878,-2.4152731883  |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br | -2902.89327742 | H,-2.5316380742,0.8014701186,-0.0000000013  |
|                                                               |                | H,0.1597180497,-3.4906361083,0.0000000062   |
|                                                               |                | H,-2.1024391559,-1.9188842417,-1.5446916016 |
|                                                               |                | H,2.0980879999,0.7395328882,-1.4281060359   |
|                                                               |                | H,-2.1024391557,-1.9188842363,1.5446916086  |
|                                                               |                | H,2.098088,0.7395328932,1.428106033         |
|                                                               |                | B,-0.4925499384,0.1415762423,-1.4638334831  |
|                                                               |                | B,0.4599455857,-1.3678213261,1.4595664145   |
|                                                               |                | H,-0.7773993824,0.8101803268,-2.4069972246  |
|                                                               |                | H,0.9263041829,-1.9049153793,2.415273195    |
|                                                               |                | H,2.3670589012,-1.741481419,0.0000000003    |
|                                                               |                | Br,0.003493805,2.8498300095,-0.0000000051   |

|                                                              |               |                                             |
|--------------------------------------------------------------|---------------|---------------------------------------------|
|                                                              |               | C,1.3770969499,-1.2875448261,0.0000000016   |
|                                                              |               | B,1.2063661818,0.14831969,0.9021986099      |
|                                                              |               | B,1.2063661809,0.1483196868,-0.9021986117   |
|                                                              |               | C,-0.0176058831,0.928257338,-0.0000000017   |
|                                                              |               | B,-1.5451131302,0.1246926907,0.0000000005   |
|                                                              |               | B,-1.2461951891,-1.3957301308,0.9048970685  |
|                                                              |               | B,-1.24619519,-1.395730134,-0.9048970623    |
|                                                              |               | B,-0.0026158001,-2.3187866019,0.0000000041  |
|                                                              |               | B,0.4602119043,-1.3759370835,-1.4594084319  |
|                                                              |               | B,-0.4925084713,0.1339775846,1.463466572    |
|                                                              |               | H,-0.7790785812,0.7966299511,2.4107405396   |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I | -625.15158119 | H,0.9266703022,-1.9122555688,-2.4156122279  |
|                                                              |               | H,-2.5350298124,0.788572335,-0.0000000001   |
|                                                              |               | H,0.1595535514,-3.4997225434,0.0000000061   |
|                                                              |               | H,-2.1029500466,-1.9265140517,-1.5449440416 |
|                                                              |               | H,2.100493188,0.7269108861,-1.4294019772    |
|                                                              |               | H,-2.102950045,-1.9265140462,1.5449440506   |
|                                                              |               | H,2.1004931895,0.7269108912,1.4294019725    |
|                                                              |               | B,-0.4925084728,0.1339775794,-1.463466572   |
|                                                              |               | B,0.4602119058,-1.3759370782,1.4594084363   |
|                                                              |               | H,-0.7790785836,0.7966299425,-2.4107405417  |
|                                                              |               | H,0.9266703046,-1.9122555602,2.4156122337   |
|                                                              |               | H,2.3674248428,-1.7494298837,0.0000000019   |
|                                                              |               | I,0.0050388043,3.0555499888,-0.0000000055   |
|                                                              |               | C,-0.0000010904,0.0000007482,-1.5345747802  |
|                                                              |               | B,0.9009344047,1.240035756,-0.7548242928    |
|                                                              |               | B,-0.9009426412,1.2400358267,-0.7548261613  |
|                                                              |               | B,0.0000018809,1.5327653535,0.754822621     |
|                                                              |               | C,0.0000010903,-0.0000007481,1.5345747802   |
|                                                              |               | B,0.9009426411,-1.2400358266,0.7548261613   |
|                                                              |               | B,-0.9009344047,-1.2400357559,0.7548242928  |
|                                                              |               | B,-0.000001881,-1.5327653534,-0.754822621   |
|                                                              |               | B,-1.4577498289,-0.4736503151,-0.7548247095 |
|                                                              |               | B,1.4577498289,0.4736503152,0.7548247095    |
|                                                              |               | H,2.4145393239,0.7845329417,1.3924400058    |
| <i>p</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub>     | -330.96010003 | H,-2.414539324,-0.7845329416,-1.3924400058  |
|                                                              |               | H,-0.0000006979,0.0000022862,2.6271812622   |
|                                                              |               | H,0.0000053691,2.5388050818,1.3924384864    |
|                                                              |               | H,-0.0000053691,-2.5388050817,-1.3924384864 |
|                                                              |               | H,-1.4922668926,-2.0539373542,1.3924338579  |
|                                                              |               | H,-1.4922823742,2.0539505892,-1.3924501587  |
|                                                              |               | H,1.4922823741,-2.0539505892,1.3924501587   |
|                                                              |               | H,1.4922668925,2.0539373542,-1.3924338579   |
|                                                              |               | B,-1.4577434416,0.4736507068,0.7548218251   |
|                                                              |               | B,1.4577434415,-0.4736507068,-0.7548218251  |
|                                                              |               | H,-2.4145413244,0.7845344681,1.392436565    |
|                                                              |               | H,2.4145413243,-0.784534468,-1.392436565    |
|                                                              |               | H,0.0000006978,-0.0000022861,-2.6271812622  |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F | -430.00208655 | C,0.0000101879,-0.0002571098,-0.9976165119  |

|                                                               |                |                                             |
|---------------------------------------------------------------|----------------|---------------------------------------------|
|                                                               |                | B,-0.902919497,1.2427012313,-0.2236518133   |
|                                                               |                | B,-1.4609409098,-0.4747318049,-0.2231760566 |
|                                                               |                | B,-1.457502179,0.4739406045,1.2836192141    |
|                                                               |                | C,-0.0000290598,0.0006031588,2.0639749647   |
|                                                               |                | B,1.4574677933,0.4739499685,1.2836530407    |
|                                                               |                | B,0.9007598412,-1.2394267119,1.2841279011   |
|                                                               |                | B,1.4609434385,-0.4747213139,-0.2231382342  |
|                                                               |                | B,0.0000048962,-1.5361677585,-0.2228608094  |
|                                                               |                | B,-0.0000283171,1.5328743579,1.2833374307   |
|                                                               |                | H,-0.0000408873,2.5403322418,1.9177647754   |
|                                                               |                | H,0.0000172068,-2.5257639453,-0.8837556433  |
|                                                               |                | H,-0.0000495917,0.0009130687,3.1561141081   |
|                                                               |                | H,-2.4154969467,0.7853917479,1.9182351404   |
|                                                               |                | H,2.401942263,-0.7806527908,-0.8842075514   |
|                                                               |                | H,1.4928080998,-2.054151357,1.9190584053    |
|                                                               |                | H,-2.4019243386,-0.7806565776,-0.8842713151 |
|                                                               |                | H,2.4154402662,0.7853902536,1.9182821804    |
|                                                               |                | H,-1.4844808994,2.0429571168,-0.8850454538  |
|                                                               |                | B,-0.9007926257,-1.2394263766,1.2841072299  |
|                                                               |                | B,0.9029092934,1.2427211286,-0.2236339243   |
|                                                               |                | H,-1.4928714166,-2.0541552018,1.9190340211  |
|                                                               |                | H,1.4844716105,2.0429872193,-0.8850185771   |
|                                                               |                | F,0.0000283159,-0.0006433133,-2.3684338126  |
|                                                               |                | C,0.0000059954,-0.0002583929,-0.9900016244  |
|                                                               |                | B,-0.9034252633,1.2434322063,-0.2075209494  |
|                                                               |                | B,-1.4617930506,-0.4749962052,-0.207055202  |
|                                                               |                | B,-1.4569040643,0.4737532061,1.3003542842   |
|                                                               |                | C,-0.0000372169,0.0006109678,2.0818333657   |
|                                                               |                | B,1.4568619013,0.4737660251,1.300395973     |
|                                                               |                | B,0.9003813408,-1.2389043066,1.3008667236   |
|                                                               |                | B,1.4617778271,-0.475004203,-0.2070124397   |
|                                                               |                | B,-0.0000011563,-1.5370517887,-0.206743731  |
|                                                               |                | B,-0.0000189076,1.5322482751,1.3000748858   |
|                                                               |                | H,-0.0000385158,2.5412813183,1.9325081754   |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl | -790.01761467  | H,0.0000209647,-2.5299319498,-0.8624822595  |
|                                                               |                | H,-0.0000523831,0.0009089224,3.1741295873   |
|                                                               |                | H,-2.4164000432,0.7856930516,1.9329670349   |
|                                                               |                | H,2.4059010091,-0.7819553339,-0.8629454924  |
|                                                               |                | H,1.4933834423,-2.0549121018,1.9338064923   |
|                                                               |                | H,-2.405908008,-0.7819402234,-0.8630169187  |
|                                                               |                | H,2.4163268077,0.7856945125,1.9330310194    |
|                                                               |                | H,-1.4869049849,2.0463736104,-0.8637948344  |
|                                                               |                | B,-0.900423187,-1.2389210785,1.3008389423   |
|                                                               |                | B,0.9034323369,1.2434221797,-0.2074989614   |
|                                                               |                | H,-1.4934248348,-2.0549321462,1.9337763834  |
|                                                               |                | H,1.4869404063,2.046362515,-0.8637499694    |
|                                                               |                | Cl,0.0000299669,-0.0007400223,-2.7563257377 |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br | -2902.89950893 | C,0.000034925,-0.0002957799,-0.983180813    |
|                                                               |                | B,-0.9035228541,1.2435605163,-0.2028240022  |

|                                                              |               |                                             |
|--------------------------------------------------------------|---------------|---------------------------------------------|
|                                                              |               | B,-1.4619386447,-0.475072109,-0.2022935037  |
|                                                              |               | B,-1.4570160376,0.4738307153,1.305602907    |
|                                                              |               | C,-0.0000691836,0.0006886992,2.0869516272   |
|                                                              |               | B,1.4569321278,0.4738449847,1.3056969914    |
|                                                              |               | B,0.900422269,-1.2389364662,1.3062274617    |
|                                                              |               | B,1.4619494307,-0.4750585183,-0.2021976724  |
|                                                              |               | B,0.0000158986,-1.5372420186,-0.2019035349  |
|                                                              |               | B,-0.0000478056,1.5323936388,1.3053126474   |
|                                                              |               | H,-0.0000813047,2.5416423869,1.9375524531   |
|                                                              |               | H,0.0000513079,-2.5323978172,-0.8545330393  |
|                                                              |               | H,-0.0000957399,0.0010256277,3.1793311572   |
|                                                              |               | H,-2.4167017609,0.7858492188,1.9380146407   |
|                                                              |               | H,2.4082284433,-0.7827116543,-0.8550012353  |
|                                                              |               | H,1.4935038669,-2.0550511378,1.9390824135   |
|                                                              |               | H,-2.4081672768,-0.7827310921,-0.8551600606 |
|                                                              |               | H,2.4165629461,0.7858509807,1.9381988727    |
|                                                              |               | H,-1.4883185943,2.04826205,-0.8560379701    |
|                                                              |               | B,-0.9004962026,-1.2389441063,1.3061693894  |
|                                                              |               | B,0.9035437114,1.2435740776,-0.2027585237   |
|                                                              |               | H,-1.4936184522,-2.0550724332,1.9389665968  |
|                                                              |               | H,1.4883741138,2.0482909351,-0.8559427176   |
|                                                              |               | Br,0.0001005753,-0.0009076124,-2.9019796114 |
|                                                              |               | C,0.000036641,-0.0002855828,-0.9779512172   |
|                                                              |               | B,-0.9031167126,1.2429824877,-0.1954021268  |
|                                                              |               | B,-1.4612570424,-0.4748475923,-0.1948655376 |
|                                                              |               | B,-1.4573008328,0.4739229496,1.3138122861   |
|                                                              |               | C,-0.0000647218,0.0006848272,2.0945737308   |
|                                                              |               | B,1.457218297,0.4739295354,1.3139112152     |
|                                                              |               | B,0.9005920034,-1.239184517,1.3144432673    |
|                                                              |               | B,1.4612681769,-0.4748304892,-0.1947535668  |
|                                                              |               | B,0.0000079689,-1.5365092161,-0.1944598926  |
|                                                              |               | B,-0.0000560718,1.5326927549,1.313526911    |
|                                                              |               | H,-0.000076809,2.5417080038,1.946328127     |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I | -625.15763839 | H,0.0000407741,-2.5355773294,-0.8418870225  |
|                                                              |               | H,-0.0000928743,0.0010312671,3.1871908383   |
|                                                              |               | H,-2.4167719414,0.7858581917,1.946815661    |
|                                                              |               | H,2.4112761825,-0.7837015512,-0.8423923887  |
|                                                              |               | H,1.4935537606,-2.0551571172,1.9478723873   |
|                                                              |               | H,-2.4112105342,-0.7837257374,-0.842555544  |
|                                                              |               | H,2.4166393527,0.7858832244,1.9469720521    |
|                                                              |               | H,-1.4902325366,2.0508818892,-0.8434443337  |
|                                                              |               | B,-0.9006664229,-1.2391733645,1.3143768228  |
|                                                              |               | B,0.9031167203,1.2430013419,-0.1953224444   |
|                                                              |               | H,-1.493652242,-2.0551135117,1.9477573338   |
|                                                              |               | H,1.4902680981,2.0509025919,-0.8433225133   |
|                                                              |               | I,0.0001265251,-0.0009799702,-3.1079295711  |

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**Table S2.** Electronic energy and optimized geometry of the 1-halo-*closo*-carboranes:NCH complexes at MP2/aug-cc-pVDZ/aug-cc-pVDZ-PP computational level.

| System                                                                | MP2 Energy<br>(Hartree) | Cartesian Coordinates<br>(Å)                |
|-----------------------------------------------------------------------|-------------------------|---------------------------------------------|
| <i>o</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub> :NCH (HB)    | -424.12580502           | C,0.,0.3008301696,-1.4893367427             |
|                                                                       |                         | C,0.,-1.2771953985,-1.0727357017            |
|                                                                       |                         | B,1.4676947288,-0.3823578796,-0.8801684831  |
|                                                                       |                         | B,0.9009029751,-1.5588479005,0.3487564555   |
|                                                                       |                         | B,0.,-0.6559098517,1.6111423891             |
|                                                                       |                         | B,-1.4658216274,0.072682044,0.8436000788    |
|                                                                       |                         | B,0.,1.085301937,1.1514958666               |
|                                                                       |                         | B,-0.9009385149,1.2474193719,-0.3921030116  |
|                                                                       |                         | B,0.9009385149,1.2474193719,-0.3921030116   |
|                                                                       |                         | B,-0.9009029751,-1.5588479005,0.3487564555  |
|                                                                       |                         | H,-1.4887877695,-2.5919153269,0.4420975166  |
|                                                                       |                         | H,1.4888208961,2.1919524102,-0.8208248559   |
|                                                                       |                         | H,0.,-1.0267767044,2.7473221441             |
|                                                                       |                         | H,1.4887877695,-2.5919153269,0.4420975166   |
|                                                                       |                         | H,-1.4888208961,2.1919524102,-0.8208248559  |
|                                                                       |                         | H,0.,1.9686311257,1.9565872481              |
|                                                                       |                         | H,2.3408229941,-0.5887161224,-1.662134153   |
|                                                                       |                         | H,-2.5004223261,0.2251652971,1.4211104701   |
|                                                                       |                         | H,0.,-1.968384308,-1.9160371991             |
|                                                                       |                         | B,1.4658216274,0.072682044,0.8436000788     |
|                                                                       |                         | B,-1.4676947288,-0.3823578796,-0.8801684831 |
|                                                                       |                         | H,2.5004223261,0.2251652971,1.4211104701    |
|                                                                       |                         | H,-2.3408229941,-0.5887161224,-1.662134153  |
|                                                                       |                         | H,0.,0.485736981,-2.5639293735              |
|                                                                       |                         | N,0.,-1.2865514371,-4.3130047525            |
|                                                                       |                         | C,0.,-1.5852965335,-5.4563311366            |
|                                                                       |                         | H,0.,-1.8577164445,-6.4991842626            |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB) | -523.16656691           | C,0.,0.744747693,-1.3419371713              |
|                                                                       |                         | C,0.,-0.8893194779,-1.3009372604            |
|                                                                       |                         | B,1.47263989,-0.0595902891,-0.9033185625    |
|                                                                       |                         | B,0.9008519101,-1.4755852401,0.0268237816   |
|                                                                       |                         | B,0.,-0.8722044473,1.4560982627             |
|                                                                       |                         | B,-1.4658876322,0.006781369,0.8731567519    |
|                                                                       |                         | B,0.,0.9278828388,1.391793149               |
|                                                                       |                         | B,-0.9070677209,1.4285090219,-0.0734127791  |
|                                                                       |                         | B,0.9070677209,1.4285090219,-0.0734127791   |
|                                                                       |                         | B,-0.9008519101,-1.4755852401,0.0268237816  |
|                                                                       |                         | H,-1.490009912,-2.502020868,-0.1117696262   |
|                                                                       |                         | H,1.4803689658,2.4469199229,-0.303803571    |
|                                                                       |                         | H,0.,-1.4824649782,2.4824681823             |
|                                                                       |                         | H,1.490009912,-2.502020868,-0.1117696262    |
|                                                                       |                         | H,-1.4803689658,2.4469199229,-0.303803571   |
|                                                                       |                         | H,0.,1.6183442879,2.3667124701              |
|                                                                       |                         | H,2.3268003805,-0.0660570073,-1.7310595765  |
|                                                                       |                         | H,-2.499487631,0.0298520211,1.4706506514    |

|                                                                        |               |                                             |
|------------------------------------------------------------------------|---------------|---------------------------------------------|
|                                                                        |               | H,0.,-1.3720662386,-2.2826496611            |
|                                                                        |               | B,1.4658876322,0.006781369,0.8731567519     |
|                                                                        |               | B,-1.47263989,-0.0595902891,-0.9033185625   |
|                                                                        |               | H,2.499487631,0.0298520211,1.4706506514     |
|                                                                        |               | H,-2.3268003805,-0.0660570073,-1.7310595765 |
|                                                                        |               | F,0.,1.2980441504,-2.5864988285             |
|                                                                        |               | N,0.,-2.2659800405,-4.2573752124            |
|                                                                        |               | C,0.,-2.73957121,-5.3391412045              |
|                                                                        |               | H,0.,-3.1716052886,-6.3263846332            |
|                                                                        |               | C,0.,0.7383586098,-1.3423406042             |
|                                                                        |               | C,0.,-0.9023262277,-1.2863259725            |
|                                                                        |               | B,1.4711671942,-0.0694476224,-0.8927245613  |
|                                                                        |               | B,0.8998619306,-1.4837991602,0.0434005574   |
|                                                                        |               | B,0.,-0.8796023795,1.4733457214             |
|                                                                        |               | B,-1.4645428421,-0.0005810986,0.8857887277  |
|                                                                        |               | B,0.,0.9200617534,1.4058390675              |
|                                                                        |               | B,-0.9053807945,1.4197199235,-0.0610152128  |
|                                                                        |               | B,0.9053807945,1.4197199235,-0.0610152128   |
|                                                                        |               | B,-0.8998619306,-1.4837991602,0.0434005574  |
|                                                                        |               | H,-1.491968635,-2.5086732466,-0.0966347316  |
|                                                                        |               | H,1.4837087292,2.436192892,-0.2884778686    |
|                                                                        |               | H,0.,-1.4893612345,2.5003221638             |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (HB) | -883.18195058 | H,1.491968635,-2.5086732466,-0.0966347316   |
|                                                                        |               | H,-1.4837087292,2.436192892,-0.2884778686   |
|                                                                        |               | H,0.,1.6129258508,2.3794499511              |
|                                                                        |               | H,2.3365996396,-0.0859918264,-1.708291885   |
|                                                                        |               | H,-2.5007578399,0.0246494604,1.4792220813   |
|                                                                        |               | H,0.,-1.3931041977,-2.2637044749            |
|                                                                        |               | B,1.4645428421,-0.0005810986,0.8857887277   |
|                                                                        |               | B,-1.4711671942,-0.0694476224,-0.8927245613 |
|                                                                        |               | H,2.5007578399,0.0246494604,1.4792220813    |
|                                                                        |               | H,-2.3365996396,-0.0859918264,-1.708291885  |
|                                                                        |               | Cl,0.,1.4761555402,-2.9374636512            |
|                                                                        |               | N,0.,-2.2592865902,-4.2446336636            |
|                                                                        |               | C,0.,-2.7249450575,-5.3299513581            |
|                                                                        |               | H,0.,-3.1495895597,-6.3203891926            |
|                                                                        |               | C,-0.0005716255,0.7968612737,-1.2848217997  |
|                                                                        |               | C,0.008427416,-0.8468674735,-1.2683317022   |
|                                                                        |               | B,1.4750401946,-0.0183670592,-0.8486810706  |
|                                                                        |               | B,0.909125215,-1.4656237924,0.0442853619    |
|                                                                        |               | B,0.0007730719,-0.9084843961,1.4875877601   |
|                                                                        |               | B,-1.4668392674,-0.0202129984,0.921782976   |
|                                                                        |               | B,-0.009100171,0.892553451,1.4724354889     |
|                                                                        |               | B,-0.9126302855,1.4302912678,0.0173454316   |
|                                                                        |               | B,0.8968814653,1.4402483792,0.0225970289    |
|                                                                        |               | B,-0.8930002061,-1.4755426183,0.0390553691  |
|                                                                        |               | H,-1.4777985328,-2.4996561329,-0.1344811408 |
|                                                                        |               | H,1.4715964694,2.4653727285,-0.1718575527   |
|                                                                        |               | H,0.001385029,-1.5492332256,2.4955016491    |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (XB) | -883.17706351 |                                             |

|                                                                        |                |                                             |
|------------------------------------------------------------------------|----------------|---------------------------------------------|
|                                                                        |                | H,1.5061723621,-2.4832306916,-0.125822492   |
|                                                                        |                | H,-1.4974468936,2.4490363125,-0.1804905388  |
|                                                                        |                | H,-0.0156254216,1.5553354298,2.4665773091   |
|                                                                        |                | H,2.3426754966,-0.0087017779,-1.6618225454  |
|                                                                        |                | H,-2.5048954617,-0.019130196,1.5123473441   |
|                                                                        |                | H,0.0138405734,-1.3092794867,-2.2578366628  |
|                                                                        |                | B,1.4617736769,-0.0040872127,0.9302801578   |
|                                                                        |                | B,-1.4696279583,-0.0345845931,-0.8572179466 |
|                                                                        |                | H,2.4963077052,0.0084138999,1.5268566438    |
|                                                                        |                | H,-2.3325802483,-0.0344607492,-1.6753782481 |
|                                                                        |                | Cl,-0.0002929093,1.5727654879,-2.8577677008 |
|                                                                        |                | N,-0.000462623,2.9129870684,-5.5487369998   |
|                                                                        |                | C,-0.0012013108,3.5021816262,-6.5736535388  |
|                                                                        |                | H,-0.0019257604,4.0402382048,-7.5069828542  |
|                                                                        |                | C,0.,0.755660033,-1.3315337279              |
|                                                                        |                | C,0.,-0.8850382831,-1.294055234             |
|                                                                        |                | B,1.4709155464,-0.0560986508,-0.8925124299  |
|                                                                        |                | B,0.8998113276,-1.481274859,0.0291284574    |
|                                                                        |                | B,0.,-0.8934979871,1.4659910034             |
|                                                                        |                | B,-1.4644974706,-0.0077998617,0.8878776354  |
|                                                                        |                | B,0.,0.9066087449,1.4190612047              |
|                                                                        |                | B,-0.9051420671,1.4231872295,-0.042680584   |
|                                                                        |                | B,0.9051420671,1.4231872295,-0.042680584    |
|                                                                        |                | B,-0.8998113276,-1.481274859,0.0291284574   |
|                                                                        |                | H,-1.4922177229,-2.5043686834,-0.1231175635 |
|                                                                        |                | H,1.4851255661,2.4420039507,-0.2553798033   |
|                                                                        |                | H,0.,-1.5151349675,2.4860139577             |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (HB) | -2996.06392077 | H,1.4922177229,-2.5043686834,-0.1231175635  |
|                                                                        |                | H,-1.4851255661,2.4420039507,-0.2553798033  |
|                                                                        |                | H,0.,1.5891593355,2.4000611894              |
|                                                                        |                | H,2.3407068588,-0.0673167509,-1.7035992742  |
|                                                                        |                | H,-2.5014157158,0.0113875502,1.4804512206   |
|                                                                        |                | H,0.,-1.3692323281,-2.2746909414            |
|                                                                        |                | B,1.4644974706,-0.0077998617,0.8878776354   |
|                                                                        |                | B,-1.4709155464,-0.0560986508,-0.8925124299 |
|                                                                        |                | H,2.5014157158,0.0113875502,1.4804512206    |
|                                                                        |                | H,-2.3407068588,-0.0673167509,-1.7035992742 |
|                                                                        |                | Br,0.,1.5828413569,-3.0535654194            |
|                                                                        |                | N,0.,-2.2756252172,-4.2340139382            |
|                                                                        |                | C,0.,-2.7737844464,-5.3048464997            |
|                                                                        |                | H,0.,-3.227970093,-6.2820749101             |
|                                                                        |                | C,-0.0011103478,0.781155444,-1.2716224966   |
|                                                                        |                | C,0.0084641829,-0.8622516032,-1.2484708104  |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (XB) | -2996.06104133 | B,1.4738458312,-0.0310297111,-0.8338209547  |
|                                                                        |                | B,0.9096086439,-1.4759311674,0.0662404794   |
|                                                                        |                | B,0.0015437061,-0.9143091051,1.508037559    |
|                                                                        |                | B,-1.4664892762,-0.028363766,0.9388080305   |
|                                                                        |                | B,-0.0089539354,0.8865174039,1.4868454906   |
|                                                                        |                | B,-0.9124192725,1.4189221732,0.0292292909   |

|                                                                       |               |                                             |
|-----------------------------------------------------------------------|---------------|---------------------------------------------|
|                                                                       |               | B,0.8958379232,1.4295251482,0.0339738927    |
|                                                                       |               | B,-0.8923066293,-1.4864927332,0.0615112213  |
|                                                                       |               | H,-1.4773491606,-2.5111856072,-0.1087342274 |
|                                                                       |               | H,1.4720456793,2.4540153655,-0.1605085777   |
|                                                                       |               | H,0.0026255775,-1.5518610784,2.518203757    |
|                                                                       |               | H,1.5075125685,-2.4936861907,-0.1008982098  |
|                                                                       |               | H,-1.499578151,2.436592511,-0.1683026863    |
|                                                                       |               | H,-0.0154620112,1.5531771974,2.4786042381   |
|                                                                       |               | H,2.346218012,-0.0279955567,-1.6421310245   |
|                                                                       |               | H,-2.5050831536,-0.0250651053,1.5285893825  |
|                                                                       |               | H,0.0138140505,-1.3323346927,-2.2344822533  |
|                                                                       |               | B,1.462054566,-0.0112054502,0.9464920906    |
|                                                                       |               | B,-1.4687157017,-0.0482754732,-0.8415454394 |
|                                                                       |               | H,2.4974339186,0.0042510504,1.5417109281    |
|                                                                       |               | H,-2.3368053859,-0.0554335501,-1.654435778  |
|                                                                       |               | Br,-0.0015769498,1.6269759122,-2.9833137161 |
|                                                                       |               | N,-0.0021795943,2.9806329285,-5.6406114332  |
|                                                                       |               | C,-0.0016884401,3.5680774776,-6.6660793655  |
|                                                                       |               | H,-0.0012886504,4.1044031787,-7.6005223881  |
|                                                                       |               | C,0.,0.7824180856,-1.3200752045             |
|                                                                       |               | C,0.,-0.8607517984,-1.3048410333            |
|                                                                       |               | B,1.4695223309,-0.0370924205,-0.8921790639  |
|                                                                       |               | B,0.8997474116,-1.4777012264,0.0087708535   |
|                                                                       |               | B,0.,-0.9134608,1.4553105313                |
|                                                                       |               | B,-1.4644180953,-0.0183214945,0.8904711238  |
|                                                                       |               | B,0.,0.8869129431,1.4375284729              |
|                                                                       |               | B,-0.9043587242,1.4272222325,-0.0165215644  |
|                                                                       |               | B,0.9043587242,1.4272222325,-0.0165215644   |
|                                                                       |               | B,-0.8997474116,-1.4777012264,0.0087708535  |
|                                                                       |               | H,-1.4926181155,-2.4980210351,-0.1604505586 |
|                                                                       |               | H,1.4874405358,2.4489090013,-0.207553462    |
|                                                                       |               | H,0.,-1.551785756,2.4652930512              |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (HB) | -718.32207036 | H,1.4926181155,-2.4980210351,-0.1604505586  |
|                                                                       |               | H,-1.4874405358,2.4489090013,-0.207553462   |
|                                                                       |               | H,0.,1.5541935487,2.4291203309              |
|                                                                       |               | H,2.3449028982,-0.0403207066,-1.697719448   |
|                                                                       |               | H,-2.5021481281,-0.0078630265,1.4820941352  |
|                                                                       |               | H,0.,-1.3369694056,-2.2892615995            |
|                                                                       |               | B,1.4644180953,-0.0183214945,0.8904711238   |
|                                                                       |               | B,-1.4695223309,-0.0370924205,-0.8921790639 |
|                                                                       |               | H,2.5021481281,-0.0078630265,1.4820941352   |
|                                                                       |               | H,-2.3449028982,-0.0403207066,-1.697719448  |
|                                                                       |               | I,0.,1.7426853267,-3.2135221254             |
|                                                                       |               | N,0.,-2.2864780059,-4.2281163793            |
|                                                                       |               | C,0.,-2.8444035352,-5.2691494425            |
|                                                                       |               | H,0.,-3.3525483404,-6.219423164             |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB) | -718.32129216 | C,-0.0007916369,0.7631048329,-1.2464174788  |
|                                                                       |               | C,0.0081217572,-0.8822296929,-1.2154249741  |
|                                                                       |               | B,1.4718924916,-0.0499947128,-0.8046013696  |

|                                                                    |                                             |
|--------------------------------------------------------------------|---------------------------------------------|
|                                                                    | B,0.9089453574,-1.4941168605,0.1005353852   |
|                                                                    | B,0.0013553512,-0.9301645853,1.5417821894   |
|                                                                    | B,-1.4661819207,-0.0443928446,0.9701571312  |
|                                                                    | B,-0.0084274531,0.8703357015,1.5179924385   |
|                                                                    | B,-0.9105730996,1.4006891423,0.0582773138   |
|                                                                    | B,0.8952824302,1.4105590507,0.0628913617    |
|                                                                    | B,-0.8926430167,-1.5039839653,0.0959370032  |
|                                                                    | H,-1.4785248193,-2.5286581097,-0.0727106904 |
|                                                                    | H,1.4754272349,2.4341428538,-0.1271098377   |
|                                                                    | H,0.0022593935,-1.5666049517,2.5530475963   |
|                                                                    | H,1.506862826,-2.5123057437,-0.0650937987   |
|                                                                    | H,-1.5008875568,2.4178821965,-0.1347179816  |
|                                                                    | H,-0.0145924518,1.5388753027,2.5087154215   |
|                                                                    | H,2.3511475218,-0.0543290638,-1.6059821538  |
|                                                                    | H,-2.5055725062,-0.0390010421,1.5588659563  |
|                                                                    | H,0.0132401188,-1.3608431815,-2.1973232091  |
|                                                                    | B,1.4620102091,-0.0283798735,0.9776209725   |
|                                                                    | B,-1.4667444942,-0.0660976205,-0.8120833166 |
|                                                                    | H,2.4982673582,-0.0116386766,1.571615783    |
|                                                                    | H,-2.3418107866,-0.0800253237,-1.6179426508 |
|                                                                    | I,-0.0011166172,1.7116985916,-3.1492492525  |
|                                                                    | N,-0.003384431,3.0946619871,-5.8336783801   |
|                                                                    | C,-0.0022041008,3.6817479942,-6.8587021345  |
|                                                                    | H,-0.0013591592,4.2178935952,-7.7936343246  |
|                                                                    | C,1.4237189644,-1.2056645654,-0.0065439747  |
|                                                                    | B,1.2139167312,0.2225300937,0.8969881133    |
|                                                                    | B,1.2103906182,0.2280282842,-0.9004884437   |
|                                                                    | C,-0.0293815246,0.9728671522,0.002985951    |
|                                                                    | B,-1.5335055369,0.1338456744,0.0033782237   |
|                                                                    | B,-1.1983707297,-1.3804827164,0.9027354955  |
|                                                                    | B,-1.2019215226,-1.3749562934,-0.9065146626 |
|                                                                    | B,0.067708018,-2.2673781893,-0.0071152211   |
|                                                                    | B,0.5045328734,-1.3099170978,-1.4626127498  |
|                                                                    | B,-0.4799985357,0.1669174621,1.460502166    |
|                                                                    | H,-0.7836930918,0.8107207861,2.4165466368   |
|                                                                    | H,0.9785811962,-1.8370412023,-2.4205862187  |
|                                                                    | H,-2.5458287795,0.7647063666,0.0072943498   |
|                                                                    | H,0.2566856752,-3.4449640191,-0.0110662352  |
|                                                                    | H,-2.0437222847,-1.9308408389,-1.5460300876 |
|                                                                    | H,2.0914062581,0.8210295571,-1.4352635708   |
|                                                                    | H,-2.0376492365,-1.9402801673,1.5421575154  |
|                                                                    | H,2.097058996,0.8122310315,1.4319214804     |
|                                                                    | B,-0.4857328423,0.1758392257,-1.4576381292  |
|                                                                    | B,0.5102601447,-1.3188140349,1.4524670285   |
|                                                                    | H,-0.7932152773,0.8254548579,-2.4085235156  |
|                                                                    | H,0.9880759196,-1.8518046879,2.4053240688   |
|                                                                    | H,2.4230288175,-1.6474978817,-0.009892383   |
|                                                                    | H,-0.0514471256,2.0649573559,0.0063634091   |
|                                                                    | N,4.4315364295,-2.6360252095,-0.0121224805  |
|                                                                    | C,5.411450677,-3.2958747567,-0.003394281    |
| <i>m</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub> :NCH (HB) | -424.14644076                               |

|                                                                         |               |                                             |
|-------------------------------------------------------------------------|---------------|---------------------------------------------|
|                                                                         |               | H,6.305468168,-3.8974291867,0.0044145153    |
|                                                                         |               | C,1.407673552,-1.2547220497,-0.0032301608   |
|                                                                         |               | B,1.226214898,0.1727826606,0.9018046138     |
|                                                                         |               | B,1.2253901535,0.1769748335,-0.9013952861   |
|                                                                         |               | C,-0.0095597651,0.9397761882,0.0025362238   |
|                                                                         |               | B,-1.5277088101,0.13780508,0.0013584767     |
|                                                                         |               | B,-1.218640145,-1.38104277,0.9029319955     |
|                                                                         |               | B,-1.2194792338,-1.3768243966,-0.9075515338 |
|                                                                         |               | B,0.0327392714,-2.2904184035,-0.0050033496  |
|                                                                         |               | B,0.4872919045,-1.3457529972,-1.4617211783  |
|                                                                         |               | B,-0.4734890241,0.1491034216,1.4641600905   |
|                                                                         |               | H,-0.7599318654,0.8251097087,2.4017581678   |
|                                                                         |               | H,0.9533527171,-1.8806559091,-2.4186294532  |
|                                                                         |               | H,-2.512833721,0.8082437147,0.0033649525    |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB)   | -523.18760279 | H,0.1997784961,-3.4702157774,-0.0078355741  |
|                                                                         |               | H,-2.0720523854,-1.9152924115,-1.5466786543 |
|                                                                         |               | H,2.1046733832,0.7791972555,-1.426171182    |
|                                                                         |               | H,-2.070628846,-1.922488017,1.5403231561    |
|                                                                         |               | H,2.1059802775,0.7725471564,1.4285992774    |
|                                                                         |               | B,-0.4748286621,0.1559145108,-1.4623270015  |
|                                                                         |               | B,0.4886444296,-1.3525370038,1.4556762425   |
|                                                                         |               | H,-0.7621150048,0.836270888,-2.3965165782   |
|                                                                         |               | H,0.9555836163,-1.8918847732,2.4096560953   |
|                                                                         |               | H,2.4002690387,-1.712073697,-0.0047414318   |
|                                                                         |               | F,-0.0054305729,2.3104323447,0.0057238585   |
|                                                                         |               | N,4.4203147482,-2.6348765589,-0.0069896351  |
|                                                                         |               | C,5.4460858617,-3.2206074114,-0.0103810282  |
|                                                                         |               | H,6.3820611128,-3.7546086332,-0.0134345314  |
|                                                                         |               | C,1.405849264,-1.2719694069,-0.0022996454   |
|                                                                         |               | B,1.2255627383,0.1590578655,0.9001975793    |
|                                                                         |               | B,1.2238588818,0.1602489923,-0.9026691012   |
|                                                                         |               | C,-0.0073393361,0.9328946128,0.0004392283   |
|                                                                         |               | B,-1.5289484899,0.121576005,0.0012662012    |
|                                                                         |               | B,-1.2185721966,-1.3962382244,0.9046283019  |
|                                                                         |               | B,-1.2201784172,-1.3950896735,-0.9045811658 |
|                                                                         |               | B,0.0316877299,-2.308922995,-0.0016387228   |
|                                                                         |               | B,0.4861683445,-1.3648132054,-1.4590556414  |
|                                                                         |               | B,-0.4740542291,0.1359586241,1.4639421814   |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl: NCH (HB) | -883.20365011 | H,-0.7626435733,0.8064619866,2.4048086126   |
|                                                                         |               | H,0.9524293065,-1.8986820532,-2.416722668   |
|                                                                         |               | H,-2.5173950223,0.7873231611,0.0026469251   |
|                                                                         |               | H,0.1986203204,-3.4890416558,-0.0026193217  |
|                                                                         |               | H,-2.0744818271,-1.9316569996,-1.5434967574 |
|                                                                         |               | H,2.1066916547,0.7557669749,-1.4291781524   |
|                                                                         |               | H,-2.0717211785,-1.9336437208,1.5443607797  |
|                                                                         |               | H,2.1093644469,0.7539288624,1.4258565968    |
|                                                                         |               | B,-0.4767497505,0.1378678281,-1.4633549516  |
|                                                                         |               | B,0.4888540223,-1.3666400737,1.456077051    |
|                                                                         |               | H,-0.7671083189,0.8096080769,-2.4027823746  |

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|-------------------------------------------------------------------------|----------------|---------------------------------------------|
|                                                                         |                | H,0.9568617158,-1.9017892874,2.4121811635   |
|                                                                         |                | H,2.3994392545,-1.727674991,-0.0036241283   |
|                                                                         |                | Cl,-0.0010608252,2.6984391324,0.0015946812  |
|                                                                         |                | N,4.4224334961,-2.6413207488,-0.0072023507  |
|                                                                         |                | C,5.4513935896,-3.2213799033,-0.0138075315  |
|                                                                         |                | H,6.3903938242,-3.7501122301,-0.0196802173  |
|                                                                         |                | C,1.3747234115,-1.3135122724,0.0021585903   |
|                                                                         |                | B,1.2121620985,0.1220279852,0.9042144682    |
|                                                                         |                | B,1.2151909098,0.1223850787,-0.8998554756   |
|                                                                         |                | C,-0.0055484936,0.9137533983,0.0002982169   |
|                                                                         |                | B,-1.5367862977,0.1178597874,-0.0024251937  |
|                                                                         |                | B,-1.2501170545,-1.404344962,0.9023811263   |
|                                                                         |                | B,-1.2470988804,-1.4039801879,-0.9068813003 |
|                                                                         |                | B,-0.0115242908,-2.3352649795,-0.0003719178 |
|                                                                         |                | B,0.4593596858,-1.3958672011,-1.4585747898  |
|                                                                         |                | B,-0.4870786958,0.1191872314,1.4621667949   |
|                                                                         |                | H,-0.7687565355,0.7907020733,2.4041301091   |
|                                                                         |                | H,0.9236662827,-1.9374686957,-2.4129411751  |
|                                                                         |                | H,-2.5176939888,0.7942628778,-0.0039418577  |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl: NCH (XB) | -883.19916280  | H,0.1428443629,-3.5171877193,-0.0003535965  |
|                                                                         |                | H,-2.1052949669,-1.9315483253,-1.5478793976 |
|                                                                         |                | H,2.1107515559,0.7005510998,-1.4241368985   |
|                                                                         |                | H,-2.110452136,-1.9321854809,1.5402827559   |
|                                                                         |                | H,2.1059499364,0.6999904484,1.4317346284    |
|                                                                         |                | B,-0.4821696305,0.1197856886,-1.4634879302  |
|                                                                         |                | B,0.4544744909,-1.3964556429,1.4597739515   |
|                                                                         |                | H,-0.7607098107,0.7916745293,-2.4061231501  |
|                                                                         |                | H,0.9155814228,-1.9384392992,2.4154721809   |
|                                                                         |                | H,2.3610137554,-1.7833394111,0.0037221119   |
|                                                                         |                | Cl,0.025055398,2.6759150823,0.0007387583    |
|                                                                         |                | N,0.0605740047,5.7127665037,0.00124527      |
|                                                                         |                | C,0.02869511,6.8947783072,0.000463815       |
|                                                                         |                | H,-0.0011554184,7.971582383,-0.0002634818   |
|                                                                         |                | C,1.4053162035,-1.278482521,-0.0043631047   |
|                                                                         |                | B,1.2260464856,0.1532250435,0.89862781      |
|                                                                         |                | B,1.2228056678,0.1551337403,-0.9037181961   |
|                                                                         |                | C,-0.0071673662,0.9256657945,0.0005026501   |
|                                                                         |                | B,-1.5292294551,0.1163117151,0.0023919156   |
|                                                                         |                | B,-1.218350078,-1.4023821085,0.9049344883   |
|                                                                         |                | B,-1.2216022076,-1.400453465,-0.9044896073  |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br: NCH (HB) | -2996.08571144 | B,0.0308375982,-2.3150506558,-0.0029976621  |
|                                                                         |                | B,0.4845224491,-1.3700937391,-1.4603587265  |
|                                                                         |                | B,-0.4730183859,0.130127949,1.4642318393    |
|                                                                         |                | H,-0.7614881408,0.7967599916,2.4080580479   |
|                                                                         |                | H,0.9497969212,-1.9029396393,-2.4191774453  |
|                                                                         |                | H,-2.519737126,0.7791979173,0.0048721838    |
|                                                                         |                | H,0.197314745,-3.4953969813,-0.0045580967   |
|                                                                         |                | H,-2.0769950997,-1.9358137859,-1.5430998652 |
|                                                                         |                | H,2.1069482076,0.7480847875,-1.4312766652   |

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|-------------------------------------------------------------------------|----------------|---------------------------------------------|
|                                                                         |                | H,-2.0714426778,-1.9390955173,1.5454705663  |
|                                                                         |                | H,2.1120679571,0.7450573896,1.4242765432    |
|                                                                         |                | B,-0.4782979734,0.1332423482,-1.4632082571  |
|                                                                         |                | B,0.4897626448,-1.373191935,1.454731378     |
|                                                                         |                | H,-0.7701677707,0.8018657421,-2.4045788344  |
|                                                                         |                | H,0.9584791027,-1.9080663413,2.410740528    |
|                                                                         |                | H,2.3990843261,-1.7339289611,-0.0065866957  |
|                                                                         |                | Br,0.0015046423,2.8429071913,0.0025249327   |
|                                                                         |                | N,4.4240932484,-2.6430545891,-0.0062833877  |
|                                                                         |                | C,5.4541534655,-3.2212637949,-0.0093477021  |
|                                                                         |                | H,6.394118041,-3.7482086222,-0.0120320652   |
|                                                                         |                | C,1.3746404336,-1.3333352341,0.0003350692   |
|                                                                         |                | B,1.2126398142,0.1037727973,0.9018907847    |
|                                                                         |                | B,1.213296984,0.1039212612,-0.9010833376    |
|                                                                         |                | C,-0.0055685395,0.8935793344,0.0000311096   |
|                                                                         |                | B,-1.5367715945,0.098488994,-0.0006001346   |
|                                                                         |                | B,-1.2489581698,-1.4241562417,0.9040211185  |
|                                                                         |                | B,-1.2482922977,-1.4240088687,-0.9052598518 |
|                                                                         |                | B,-0.0114586967,-2.3552000889,-0.0002418353 |
|                                                                         |                | B,0.457678392,-1.4154752153,-1.459067378    |
|                                                                         |                | B,-0.4853742055,0.1005514352,1.4621321735   |
|                                                                         |                | H,-0.767083543,0.768256188,2.4071429829     |
|                                                                         |                | H,0.9208691854,-1.9565607539,-2.4144037022  |
|                                                                         |                | H,-2.5203473419,0.7714252772,-0.0009096054  |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br: NCH (XB) | -2996.08327217 | H,0.1429575201,-3.5372995761,-0.0002838878  |
|                                                                         |                | H,-2.1074954903,-1.9513831358,-1.5452771915 |
|                                                                         |                | H,2.1100282962,0.6789937468,-1.4273255141   |
|                                                                         |                | H,-2.1086191873,-1.9516388792,1.5433328611  |
|                                                                         |                | H,2.1089880604,0.6787510397,1.4288843272    |
|                                                                         |                | B,-0.4843098008,0.1007917571,-1.4625652437  |
|                                                                         |                | B,0.4566194033,-1.4157074728,1.4590662391   |
|                                                                         |                | H,-0.7653374018,0.768658804,-2.4076639335   |
|                                                                         |                | H,0.9191158536,-1.9569631935,2.4146436244   |
|                                                                         |                | H,2.3612472261,-1.8026718333,0.0006578111   |
|                                                                         |                | Br,0.0286366624,2.8098092612,0.000210967    |
|                                                                         |                | N,0.0598704138,5.8216051763,0.0008303182    |
|                                                                         |                | C,0.0287859025,7.0032505573,0.0013649361    |
|                                                                         |                | H,-0.0001016529,8.080173161,0.0016839058    |
|                                                                         |                | C,1.4081940349,-1.2800393581,-0.0034918208  |
|                                                                         |                | B,1.2232730479,0.1528403005,0.8987764732    |
|                                                                         |                | B,1.2207133803,0.1543948532,-0.9026842165   |
|                                                                         |                | C,-0.0117217301,0.9226224067,0.0004905227   |
|                                                                         |                | B,-1.5309376294,0.1050510808,0.001956475    |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I: NCH (HB)  | -718.34395097  | B,-1.2151044991,-1.412958793,0.9048417148   |
|                                                                         |                | B,-1.2177177711,-1.4113651737,-0.9044885113 |
|                                                                         |                | B,0.0374855568,-2.3216733461,-0.0024336006  |
|                                                                         |                | B,0.4886826213,-1.3745763374,-1.4595253965  |
|                                                                         |                | B,-0.4754938893,0.1233887164,1.4638358854   |
|                                                                         |                | H,-0.7684286184,0.7829945916,2.4116558461   |

|                                                                       |               |                                             |
|-----------------------------------------------------------------------|---------------|---------------------------------------------|
|                                                                       |               | H,0.9563221127,-1.9049843044,-2.418670509   |
|                                                                       |               | H,-2.5275727599,0.7593899752,0.0039283714   |
|                                                                       |               | H,0.2081134975,-3.50159939,-0.003694833     |
|                                                                       |               | H,-2.0714496839,-1.9489355498,-1.5436804839 |
|                                                                       |               | H,2.1057841615,0.7451139565,-1.4319639344   |
|                                                                       |               | H,-2.0670100314,-1.951637542,1.5455261578   |
|                                                                       |               | H,2.1099108439,0.7426066535,1.4265083907    |
|                                                                       |               | B,-0.4796836867,0.1259400554,-1.4629061058  |
|                                                                       |               | B,0.4928745407,-1.3771345555,1.4550075238   |
|                                                                       |               | H,-0.7752979087,0.7872369768,-2.4087146377  |
|                                                                       |               | H,0.9632859567,-1.9091953905,2.4118770203   |
|                                                                       |               | H,2.4038517396,-1.7314463548,-0.0053054073  |
|                                                                       |               | I,-0.0112943399,3.0505631286,0.0023311403   |
|                                                                       |               | N,4.4255624873,-2.6526488356,-0.008983322   |
|                                                                       |               | C,5.4507534392,-3.2394963207,-0.0113766203  |
|                                                                       |               | H,6.3862605523,-3.7742944906,-0.0136145404  |
|                                                                       |               | C,1.3739218226,-1.372277324,-0.0058675405   |
|                                                                       |               | B,1.2167112339,0.0670184796,0.8955379301    |
|                                                                       |               | B,1.209429143,0.0673075584,-0.9055006485    |
|                                                                       |               | C,-0.0033230088,0.8606501352,0.0000842117   |
|                                                                       |               | B,-1.5350499269,0.0634318875,0.0061147834   |
|                                                                       |               | B,-1.2455029814,-1.460219027,0.9093234712   |
|                                                                       |               | B,-1.2528054361,-1.4599449604,-0.8998732465 |
|                                                                       |               | B,-0.0130520245,-2.3927576447,-0.0004105779 |
|                                                                       |               | B,0.451027976,-1.45252788,-1.4609038511     |
|                                                                       |               | B,-0.4778066151,0.0649752185,1.4632825512   |
|                                                                       |               | H,-0.7567215923,0.725913339,2.4143840787    |
|                                                                       |               | H,0.9095114793,-1.9932231551,-2.418890306   |
|                                                                       |               | H,-2.5224678661,0.7315643795,0.0101892362   |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB) | -718.34362739 | H,0.140100601,-3.5752991221,-0.0012140665   |
|                                                                       |               | H,-2.1156306202,-1.9857629951,-1.5365335074 |
|                                                                       |               | H,2.1076875314,0.6351925701,-1.4378828134   |
|                                                                       |               | H,-2.1031771358,-1.9862215712,1.5527696038  |
|                                                                       |               | H,2.1192546541,0.6347107447,1.4208125394    |
|                                                                       |               | B,-0.4896247359,0.0654195722,-1.4595358908  |
|                                                                       |               | B,0.4628090444,-1.4529951478,1.4565728937   |
|                                                                       |               | H,-0.7761907251,0.7267028545,-2.4081304324  |
|                                                                       |               | H,0.9290274355,-1.9939901287,2.4106529731   |
|                                                                       |               | H,2.3604237563,-1.8420413497,-0.009220987   |
|                                                                       |               | I,0.0349187578,2.9917207665,0.0000727369    |
|                                                                       |               | N,0.0580304391,6.0502709519,0.0019985886    |
|                                                                       |               | C,0.0265410998,7.2313908609,0.0020061288    |
|                                                                       |               | H,-0.00238608,8.3086192848,0.0024098658     |
|                                                                       |               | C,0.0002095158,0.0001128112,-1.0186816208   |
|                                                                       |               | B,-0.9007934185,1.239906048,-0.2388091951   |
| <i>p</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub> :NCH (HB)    | -424.15127447 | B,-1.457545477,-0.4735828608,-0.2391488039  |
|                                                                       |               | B,-1.4561994292,0.4728866085,1.2714880294   |
|                                                                       |               | C,-0.0004798181,-0.0002396106,2.0530023808  |
|                                                                       |               | B,1.4555973794,0.4728996962,1.272134252     |

|                                                                        |               |                                             |
|------------------------------------------------------------------------|---------------|---------------------------------------------|
|                                                                        |               | B,0.8994783584,-1.238617939,1.2718227843    |
|                                                                        |               | B,1.4576009399,-0.4735788993,-0.2384869618  |
|                                                                        |               | B,0.0000376683,-1.5325599646,-0.2389473669  |
|                                                                        |               | B,-0.0002947518,1.5306677174,1.2719312765   |
|                                                                        |               | H,-0.0004463461,2.5379160901,1.9081892205   |
|                                                                        |               | H,0.000187182,-2.5374032133,-0.8793105518   |
|                                                                        |               | H,-0.0007576011,-0.0003921352,3.1457801432  |
|                                                                        |               | H,-2.4143626063,0.784082244,1.907437221     |
|                                                                        |               | H,2.4134709693,-0.7840331634,-0.8785419245  |
|                                                                        |               | H,1.4914514832,-2.0536575892,1.9079813468   |
|                                                                        |               | H,-2.4131279894,-0.7840490904,-0.8796415473 |
|                                                                        |               | H,2.41348459,0.7841008926,1.9085153543      |
|                                                                        |               | H,-1.4913273165,2.0529866075,-0.8790892008  |
|                                                                        |               | B,-0.9001035433,-1.2386151477,1.2714126847  |
|                                                                        |               | B,0.9008601859,1.2399107056,-0.2384022809   |
|                                                                        |               | H,-1.4923331844,-2.0536290829,1.9073111768  |
|                                                                        |               | H,1.4916744184,2.0529725862,-0.8784051171   |
|                                                                        |               | H,0.0004601632,0.000243605,-2.111317005     |
|                                                                        |               | N,0.0004995598,0.0003188632,5.4005557988    |
|                                                                        |               | C,0.0011006206,0.0006274828,6.58206864      |
|                                                                        |               | H,0.0016584473,0.0007267383,7.6595335606    |
|                                                                        |               | C,0.0005201514,0.0000011389,-0.9959567457   |
|                                                                        |               | B,-0.9026539807,1.2425172725,-0.2217833214  |
|                                                                        |               | B,-1.4605798214,-0.4746048532,-0.2221030514 |
|                                                                        |               | B,-1.4562007843,0.4728912121,1.2860563046   |
|                                                                        |               | C,-0.0012021085,-0.00000105,2.0691357887    |
|                                                                        |               | B,1.4546755528,0.4728936713,1.2876742052    |
|                                                                        |               | B,0.8987441126,-1.2380583665,1.2873721898   |
|                                                                        |               | B,1.4607543111,-0.4745939293,-0.2204581916  |
|                                                                        |               | B,0.0000837666,-1.5358312205,-0.2212801862  |
|                                                                        |               | B,-0.0007507305,1.5303242847,1.2868682371   |
|                                                                        |               | H,-0.0010984009,2.5395253277,1.9189818138   |
|                                                                        |               | H,0.0004510285,-2.5245480744,-0.8841049762  |
|                                                                        |               | H,-0.0017690792,-0.0000334932,3.1617040793  |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB)  | -523.19391774 | H,-2.4163691072,0.7847538907,1.9176140821   |
|                                                                        |               | H,2.4014484451,-0.7801308533,-0.8827608278  |
|                                                                        |               | H,1.4915808737,-2.0545251447,1.9198042505   |
|                                                                        |               | H,-2.4005283678,-0.7801281927,-0.8854641597 |
|                                                                        |               | H,2.4141199166,0.7847488963,1.9203270611    |
|                                                                        |               | H,-1.4834282306,2.0424124489,-0.8849334898  |
|                                                                        |               | B,-0.9002694131,-1.2380693606,1.2863612968  |
|                                                                        |               | B,0.9028295314,1.2425173225,-0.2207754581   |
|                                                                        |               | H,-1.4938168749,-2.0545468921,1.9181217866  |
|                                                                        |               | H,1.4843522272,2.0424054631,-0.8832693001   |
|                                                                        |               | F,0.0012826771,0.0000045597,-2.3680950498   |
|                                                                        |               | N,0.0010778873,0.0000339818,5.40362567      |
|                                                                        |               | C,0.002578585,-0.0000068494,6.5850936927    |
|                                                                        |               | H,0.0041678326,0.0000488098,7.6626265934    |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (HB) | -883.20942082 | C,0.0000077556,-0.0002550938,-0.9900636968  |

B,-0.9031859244,1.2430899952,-0.2075318463  
 B,-1.4613865385,-0.4748668117,-0.2070673322  
 B,-1.4550885671,0.4731670143,1.3016405301  
 C,-0.0000363834,0.0006122421,2.0844779952  
 B,1.4550415023,0.473179658,1.3016729593  
 B,0.8992453982,-1.2373536502,1.3021640949  
 B,1.461380234,-0.4748585849,-0.2070006008  
 B,-0.000048457,-1.5366119802,-0.2067348915  
 B,-0.0000171393,1.5303399322,1.3013566466  
 H,-0.000033963,2.5407040672,1.9320654422  
 H,0.0000120002,-2.528872473,-0.8641743793  
 H,0.0000078131,0.0008429857,3.1772707836  
 H,-2.4158528284,0.7855166806,1.9325147106  
 H,2.4049060416,-0.7816231881,-0.864631625  
 H,1.49302108,-2.05445064,1.9333582879  
 H,-2.4048884302,-0.7816274807,-0.8647236267  
 H,2.4157921504,0.7855234221,1.9325808577  
 H,-1.4862922036,2.0455079362,-0.8654972968  
 B,-0.8993138241,-1.2373604123,1.302126209  
 B,0.9031759287,1.2430902945,-0.207511952  
 H,-1.4931036191,-2.0544505557,1.9333222478  
 H,1.486303852,2.0455110784,-0.8654570377  
 Cl,0.0000408932,-0.0007553978,-2.7577217327  
 N,0.0000417368,-0.0005482369,5.4178772656  
 C,0.000083075,-0.0013701898,6.5992750156  
 H,0.0001448058,-0.0020806114,7.6767952656  
  
 C,0.0001817779,0.0002198809,-0.8630032971  
 B,-0.9024284032,1.2424004158,-0.0761327554  
 B,-1.4602714831,-0.4743814449,-0.0763550297  
 B,-1.4567298678,0.4733195949,1.4321417026  
 C,-0.0001062127,-0.0000710725,2.2137095911  
 B,1.4566766624,0.4732937349,1.4324385949  
 B,0.900247151,-1.2391498936,1.4322194397  
 B,1.4604886247,-0.4743813506,-0.0760644102  
 B,0.000116357,-1.5353740278,-0.0763150799  
 B,-0.0000028558,1.5316572638,1.4323798383  
 H,-0.0000629279,2.5395099991,2.0672253891  
 H,0.0001817236,-2.5296962687,-0.7301926378  
 H,-0.0002174005,-0.0001771564,3.3060250825  
 H,-2.4153934057,0.7847480457,2.0668441019  
 H,2.4062898018,-0.7816182766,-0.7298035743  
 H,1.492624031,-2.0546287906,2.0669543698  
 H,-2.4059520407,-0.7815961152,-0.7302728398  
 H,2.4152080065,0.7846944297,2.0673278503  
 H,-1.4868414958,2.0469670081,-0.7298949447  
 B,-0.9003249924,-1.2391386629,1.4320314455  
 B,0.9026927289,1.2423827448,-0.0759697513  
 H,-1.4928270951,-2.0546223969,2.066659699  
 H,1.487257077,2.0469285169,-0.7296317116  
 Cl,0.0003741553,0.0004195716,-2.6271345421

*p*-B<sub>10</sub>H<sub>11</sub>C<sub>2</sub>-1Cl:NCH (XB)      -883.20517392

|                                                                        |                                                          |
|------------------------------------------------------------------------|----------------------------------------------------------|
|                                                                        | N,-0.0002006394,-0.0004257421,-5.6775363205              |
|                                                                        | C,-0.0003888851,-0.0006355035,-6.8600498475              |
|                                                                        | H,-0.0005903821,-0.000644504,-7.9372179379               |
|                                                                        | C,0.0000431711,-0.0002980943,-0.9831602998               |
|                                                                        | B,-0.9032756744,1.2432422072,-0.2028169834               |
|                                                                        | B,-1.4615644438,-0.4749514815,-0.2022953364              |
|                                                                        | B,-1.4551810198,0.4732302125,1.3068797742                |
|                                                                        | C,-0.0000742852,0.0006921232,2.0895851874                |
|                                                                        | B,1.4550962803,0.4732591994,1.3069618911                 |
|                                                                        | B,0.8992907056,-1.2373685489,1.3074917747                |
|                                                                        | B,1.461564194,-0.4749392942,-0.2021906908                |
|                                                                        | B,0.000011224,-1.5368545624,-0.2018908413                |
|                                                                        | B,-0.0000430784,1.5304635603,1.306587988                 |
|                                                                        | H,-0.0000832101,2.5411017878,1.9370245874                |
|                                                                        | H,0.0000362524,-2.5313527168,-0.8562394255               |
|                                                                        | H,-0.0000758429,0.0009880766,3.1824292762                |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (HB) | -2996.09134178 H,-2.4162069234,0.7856880389,1.9374552965 |
|                                                                        | H,2.4072206627,-0.7823913994,-0.8567281667               |
|                                                                        | H,1.493195507,-2.054612448,1.9385531533                  |
|                                                                        | H,-2.4071744653,-0.7824003624,-0.8569058599              |
|                                                                        | H,2.4160588909,0.7856988725,1.9376570171                 |
|                                                                        | H,-1.4876928143,2.0474183936,-0.8577666092               |
|                                                                        | B,-0.8993585893,-1.2373843974,1.3074634468               |
|                                                                        | B,0.9033118951,1.24326678,-0.202748924                   |
|                                                                        | H,-1.493309972,-2.0546527292,1.9384485963                |
|                                                                        | H,1.4877522618,2.047457021,-0.8576687245                 |
|                                                                        | Br,0.0001050328,-0.0009071528,-2.9028316536              |
|                                                                        | N,0.0000282814,-0.0005053036,5.422254555                 |
|                                                                        | C,0.0001405736,-0.0014937028,6.6036544129                |
|                                                                        | H,0.0001853861,-0.0023940791,7.6811788209                |
|                                                                        | C,0.0000032275,0.0000082533,-0.8428913305                |
|                                                                        | B,-0.9024991613,1.2420332435,-0.0578037312               |
|                                                                        | B,-1.4601230378,-0.4744934225,-0.0577098812              |
|                                                                        | B,-1.4567737823,0.4733429253,1.4513702597                |
|                                                                        | C,0.0000192871,0.0001759871,2.232770861                  |
|                                                                        | B,1.4567423834,0.4736005844,1.4514112021                 |
|                                                                        | B,0.9004475046,-1.2390005317,1.4514972187                |
|                                                                        | B,1.4601850013,-0.4742499127,-0.0577079471               |
|                                                                        | B,0.0001425831,-1.535203689,-0.0576389556                |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (XB) | -2996.08909232 B,-0.000110026,1.5318602128,1.4513254382  |
|                                                                        | H,-0.0002298596,2.5400076107,2.0859368579                |
|                                                                        | H,0.0002346592,-2.5322586267,-0.7079579699               |
|                                                                        | H,0.000001468,0.0002402689,3.3251964324                  |
|                                                                        | H,-2.4155696815,0.7848418649,2.0860100193                |
|                                                                        | H,2.4084306814,-0.7823281842,-0.7080695442               |
|                                                                        | H,1.4930703399,-2.0544999834,2.0862040187                |
|                                                                        | H,-2.4083111081,-0.7827013176,-0.7081026885              |
|                                                                        | H,2.4154824219,0.7852330925,2.086061036                  |
|                                                                        | H,-1.4885888842,2.0485710676,-0.7082276897               |

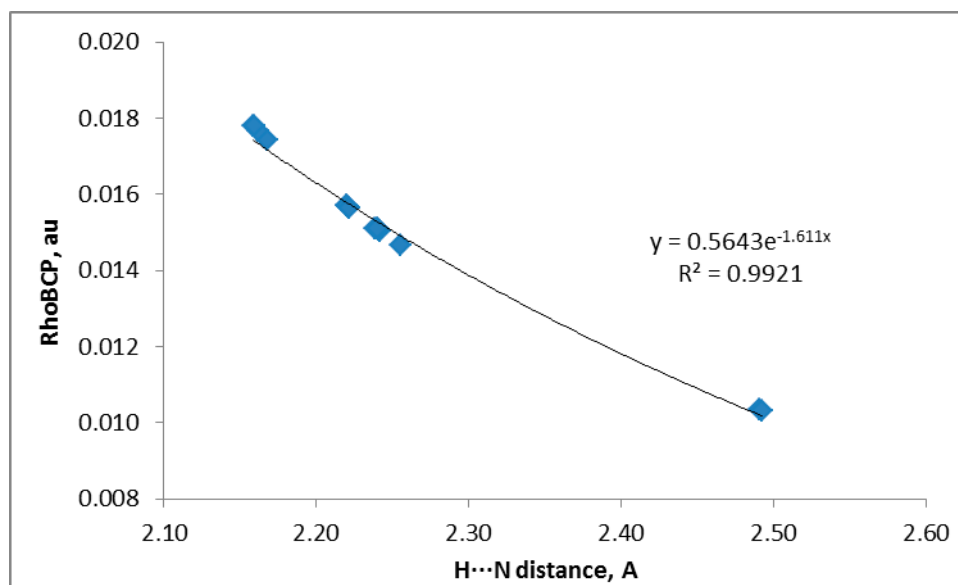
|                                                                       |               |                                             |
|-----------------------------------------------------------------------|---------------|---------------------------------------------|
|                                                                       |               | B,-0.9002073023,-1.239137979,1.4514733011   |
|                                                                       |               | B,0.9023105839,1.2422002622,-0.0577891943   |
|                                                                       |               | H,-1.4926754099,-2.0547433092,2.0861858313  |
|                                                                       |               | H,1.4882812648,2.0488157681,-0.7082174078   |
|                                                                       |               | Br,0.0000430694,-0.0001011582,-2.7612209809 |
|                                                                       |               | N,-0.0001092262,-0.0005829033,-5.7833974895 |
|                                                                       |               | C,-0.0000998437,-0.000738143,-6.9655281886  |
|                                                                       |               | H,-0.0000971599,-0.0008919807,-8.0427970098 |
|                                                                       |               | C,0.0001622558,-0.0006655717,-0.9778812878  |
|                                                                       |               | B,-0.9031783217,1.2431151471,-0.1968477183  |
|                                                                       |               | B,-1.4614909194,-0.4749240145,-0.1956877091 |
|                                                                       |               | B,-1.4554903489,0.4739324066,1.3138914363   |
|                                                                       |               | C,-0.0004054442,0.0016434839,2.0967275566   |
|                                                                       |               | B,1.455046775,0.4738765485,1.314353145      |
|                                                                       |               | B,0.8991139624,-1.2368990363,1.3155696611   |
|                                                                       |               | B,1.4615515389,-0.4749651438,-0.1951436148  |
|                                                                       |               | B,-0.0000080579,-1.536788156,-0.194558469   |
|                                                                       |               | B,-0.0001595747,1.5311632732,1.3132944787   |
|                                                                       |               | H,-0.0003051338,2.5422834873,1.9431741841   |
|                                                                       |               | H,0.0000725335,-2.5354092423,-0.8432536257  |
|                                                                       |               | H,-0.0005681226,0.0023755506,3.1895952876   |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (HB) | -718.34943470 | H,-2.4168043191,0.7867860992,1.9440330929   |
|                                                                       |               | H,2.410953908,-0.7839551001,-0.8441887867   |
|                                                                       |               | H,1.4930298871,-2.0540585988,1.9468550031   |
|                                                                       |               | H,-2.4106486236,-0.7838662737,-0.8450863062 |
|                                                                       |               | H,2.4160980909,0.7866084248,1.9449462216    |
|                                                                       |               | H,-1.4897477232,2.0501332719,-0.8469918593  |
|                                                                       |               | B,-0.8997367674,-1.2368454197,1.3152667457  |
|                                                                       |               | B,0.9033432421,1.2432179497,-0.1965451306   |
|                                                                       |               | H,-1.4939097151,-2.0540059193,1.9463689944  |
|                                                                       |               | H,1.490144507,2.050218771,-0.8464995236     |
|                                                                       |               | I,0.0005174705,-0.0022938596,-3.1096779692  |
|                                                                       |               | N,0.0002538318,-0.0014078433,5.4294172077   |
|                                                                       |               | C,0.0007524133,-0.00366902,6.6108525551     |
|                                                                       |               | H,0.0014126552,-0.0056012146,7.6883986932   |
|                                                                       |               | C,-0.0002198849,-0.0001971865,-0.8092056817 |
|                                                                       |               | B,-0.9018861363,1.2416129434,-0.0216388424  |
|                                                                       |               | B,-1.4597133207,-0.473987838,-0.0212891855  |
|                                                                       |               | B,-1.4567060935,0.4738467048,1.4886096886   |
|                                                                       |               | C,0.0001227068,0.0003400039,2.2697443944    |
|                                                                       |               | B,1.4569790556,0.4732651078,1.488329821     |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB) | -718.34920760 | B,0.900161815,-1.2392536676,1.4886730201    |
|                                                                       |               | B,1.4592401084,-0.4745783865,-0.0215770694  |
|                                                                       |               | B,-0.0004349908,-1.5346401358,-0.0212594497 |
|                                                                       |               | B,0.0003394938,1.5320222617,1.4882776427    |
|                                                                       |               | H,0.0005943956,2.5402714858,2.1229487866    |
|                                                                       |               | H,-0.0006951841,-2.5361336178,-0.6655262452 |
|                                                                       |               | H,0.0002309638,0.0005278989,3.3623059304    |
|                                                                       |               | H,-2.4153783901,0.785705735,2.1234948896    |

H,2.4114839546,-0.7843166248,-0.666058864  
H,1.4926430459,-2.0548919338,2.1235953425  
H,-2.412231113,-0.7833653092,-0.6655672913  
H,2.4159189312,0.7847121215,2.123032363  
H,-1.4904103959,2.0517708785,-0.6661689153  
B,-0.9005878175,-1.2388814798,1.4888495716  
B,0.902124329,1.2412480023,-0.0218157137  
H,-1.4932725873,-2.0542772334,2.1238971578  
H,1.4908323548,2.0511690621,-0.6664745289  
I,-0.0003957429,-0.0005444473,-2.9425527414  
N,0.0002085483,-0.0005240421,-6.013799653  
C,0.000437651,-0.0004855667,-7.1954396618  
H,0.000614296,-0.0004147362,-8.2730022974

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**Table S3.**  $q_{\text{BCP}}$ ,  $V2q_{\text{BCP}}$  and  $H_{\text{BCP}}$  (au) of the intermolecular BCPs in the 1-halo-*closo*-carboranes:NCH complexes.

|                                                                        | Atoms    | $q_{\text{BCP}}$ | $V2q_{\text{BCP}}$ | $H_{\text{BCP}}$ |
|------------------------------------------------------------------------|----------|------------------|--------------------|------------------|
| <i>o</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub> :NCH (HB)     | N25-H24  | 0.0103           | 0.0336             | 0.0009           |
|                                                                        | H19-N25  | 0.0103           | 0.0335             | 0.0009           |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB)  | N25-H19  | 0.0174           | 0.0534             | 0.0011           |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (HB) | N25-H19  | 0.0177           | 0.0543             | 0.0011           |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (HB) | H19-N25  | 0.0178           | 0.0548             | 0.0011           |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (HB)  | H19-N25  | 0.0178           | 0.0548             | 0.0011           |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> :NCH (HB)     | N25-H23  | 0.0151           | 0.0458             | 0.0009           |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB)  | H23-N25  | 0.0157           | 0.0476             | 0.0009           |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (HB) | N25-H23  | 0.0157           | 0.0477             | 0.0009           |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (HB) | N25-H23  | 0.0157           | 0.0477             | 0.0009           |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (HB)  | N25-H23  | 0.0156           | 0.0475             | 0.0009           |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> :NCH (HB)     | H13-N25  | 0.0147           | 0.0443             | 0.0008           |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB)  | H13-N25  | 0.0150           | 0.0455             | 0.0009           |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (HB) | N25-H13  | 0.0151           | 0.0456             | 0.0009           |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (HB) | N25-H13  | 0.0151           | 0.0457             | 0.0009           |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (HB)  | N25-H13  | 0.0151           | 0.0457             | 0.0009           |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (XB) | N25-Cl24 | 0.0107           | 0.0406             | 0.0016           |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (XB) | Cl24-N25 | 0.0101           | 0.0380             | 0.0015           |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (XB) | Cl24-N25 | 0.0099           | 0.0369             | 0.0015           |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (XB) | N25-Br24 | 0.0133           | 0.0472             | 0.0016           |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (XB) | N25-Br24 | 0.0126           | 0.0444             | 0.0016           |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (XB) | N25-Br24 | 0.0123           | 0.0435             | 0.0015           |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB)  | I24-N25  | 0.0156           | 0.0493             | 0.0011           |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB)  | I24-N25  | 0.0145           | 0.0459             | 0.0011           |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB)  | I24-N25  | 0.0142           | 0.0449             | 0.0011           |



**Figure S1.**  $\rho_{\text{BCP}}$  (au) vs. the interatomic N...H distance (Å) in the 1-halo-*closo*-carboranes:NCH (HB) complexes.

**Table S4.** NEDA partition terms, kJ mol<sup>-1</sup>, of the 1-halo-*closo*-carboranes:NCH complexes.

|                                                                        | Charge Transfer | Electrostatic | Polarization | Exchange Correlation | DEF<br>1-halcarborane | DEF<br>NCH |
|------------------------------------------------------------------------|-----------------|---------------|--------------|----------------------|-----------------------|------------|
| <i>o</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub> :NCH (HB)     | -39.6           | -23.3         | -34.8        | -23.9                | 29.0                  | 77.9       |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB)  | -57.3           | -23.5         | -29.2        | -16.9                | 22.0                  | 91.1       |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (HB) | -59.1           | -23.3         | -30.5        | -18.0                | 25.3                  | 92.9       |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (HB) | -59.8           | -23.2         | -31.5        | -18.5                | 26.5                  | 94.0       |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (HB)  | -59.8           | -23.1         | -32.7        | -19.2                | 28.4                  | 94.3       |
| <i>m</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub> :NCH (HB)     | -46.6           | -17.7         | -23.2        | -14.4                | 17.7                  | 74.7       |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB)  | -48.8           | -19.6         | -24.4        | -14.9                | 18.4                  | 78.1       |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (HB) | -48.9           | -19.5         | -24.5        | -14.9                | 18.4                  | 78.4       |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (HB) | -48.9           | -19.5         | -24.5        | -14.9                | 18.5                  | 78.4       |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (HB)  | -48.7           | -19.2         | -24.3        | -14.8                | 18.3                  | 78.0       |
| <i>p</i> -B <sub>10</sub> H <sub>12</sub> C <sub>2</sub> :NCH (HB)     | -45.6           | -16.2         | -22.6        | -14.1                | 17.2                  | 72.9       |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1F:NCH (HB)  | -46.9           | -17.8         | -23.5        | -14.4                | 17.5                  | 75.3       |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (HB) | -47.0           | -17.8         | -23.5        | -14.4                | 17.6                  | 75.4       |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (HB) | -47.1           | -17.8         | -23.6        | -14.4                | 17.6                  | 75.6       |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (HB)  | -47.1           | -17.6         | -23.5        | -14.4                | 17.6                  | 75.5       |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (XB) | -17.8           | -11.4         | -49.7        | -16.4                | 39.2                  | 50.9       |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (XB) | -28.2           | -18.3         | -81.7        | -22.8                | 56.2                  | 86.2       |
| <i>o</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB)  | -44.0           | -27.1         | -64.3        | -27.8                | 75.4                  | 73.0       |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (XB) | -16.2           | -8.1          | -44.7        | -15.2                | 36.4                  | 45.3       |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (XB) | -25.6           | -14.6         | -74.5        | -21.3                | 52.5                  | 78.0       |
| <i>m</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB)  | -40.0           | -22.6         | -58.0        | -25.7                | 69.2                  | 65.8       |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Cl:NCH (XB) | -15.6           | -7.0          | -43.3        | -14.8                | 35.2                  | 43.8       |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1Br:NCH (XB) | -24.9           | -13.5         | -72.8        | -20.8                | 51.3                  | 76.1       |
| <i>p</i> -B <sub>10</sub> H <sub>11</sub> C <sub>2</sub> -1I:NCH (XB)  | -39.0           | -21.2         | -56.6        | -25.2                | 67.5                  | 64.2       |

**Table S5.** CH...N distances (Å) in the CSD search between carboranes and N-bases.

| o-carboranes |        | m-carboranes |        | p-carboranes |        |
|--------------|--------|--------------|--------|--------------|--------|
| Refcode      | CH...N | Refcode      | CH...N | Refcode      | CH...N |
| MOYHEQ       | 2.394  | DOVXOE       | 2.814  | IDIHOT       | 2.404  |
| MOYHEQ       | 2.717  | DOVXOE       | 2.649  | IMEQIB       | 2.79   |
| MOYHEQ       | 2.111  | DOVYIZ       | 2.793  | JABGIF       | 2.603  |
| VOZZAO       | 2.507  | DOVYIZ       | 2.61   | JABGIF       | 2.331  |
| XUHZEI       | 2.164  | DOVYOF       | 2.363  | MIFJUH       | 2.82   |
| BOKKOB       | 2.533  | DOVYOF       | 2.713  | MIFJUH       | 2.455  |
| BOVQUY       | 2.891  | DOWMIO       | 2.389  | MIFKES       | 2.76   |
| BOVQUY       | 2.279  | FEZJUR       | 2.281  | MIFKES       | 2.79   |
| BOVQUY       | 2.502  | FEZJUR       | 2.373  |              |        |
| BOZXAR       | 2.6    | FEZJUR       | 2.915  |              |        |
| BOZXAR       | 2.864  | FEZJUR       | 2.863  |              |        |
| BUQXEQ       | 2.816  | GISFUM       | 2.456  |              |        |
| COXPEM       | 2.492  | GISGAT       | 2.841  |              |        |
| COXPEM       | 2.603  | GISGAT       | 2.933  |              |        |
| ECIRIS       | 2.905  | IDIGUY       | 2.442  |              |        |
| GAFFEB       | 2.683  | IDIGUY       | 2.327  |              |        |
| GAFFEB       | 2.986  | IMEMAQ       | 2.472  |              |        |
| GAFFEB       | 2.856  | IMEMAQ       | 2.51   |              |        |
| GAFFEB       | 2.732  | IMEMAQ       | 2.891  |              |        |
| HIYGEE       | 2.218  | IZAHUN       | 2.616  |              |        |
| ICUSAD       | 2.907  | IZAJAV       | 2.156  |              |        |
| JABGOL       | 2.887  | IZAJAV       | 2.295  |              |        |
| JABGOL       | 2.48   | MATLAX       | 2.514  |              |        |
| LAQGIW       | 2.315  | OWITEV       | 2.253  |              |        |
| LUTGAI       | 2.526  | OWITEV       | 2.765  |              |        |
| NACGIH       | 2.498  | OWITOF       | 2.218  |              |        |
| NACGIH01     | 2.498  | OWITOF       | 2.188  |              |        |
| NEQXOZ       | 2.246  | QUKHOU       | 2.663  |              |        |
| NEQXOZ       | 2.776  | QUKHUA       | 2.672  |              |        |
| NEQXOZ       | 2.816  | RECYUV       | 2.709  |              |        |
| NEQXOZ       | 2.754  | TAVXIY       | 2.99   |              |        |
| NEQXOZ       | 2.448  | TIWCIO       | 2.648  |              |        |
| NURLER       | 2.468  | TIWCUA       | 2.374  |              |        |
| PECHEM       | 2.69   | TIWCUA       | 2.419  |              |        |
| POVVAZ       | 2.601  | TOKMAK       | 2.721  |              |        |
| POVVAZ       | 2.278  | TOKMAK       | 2.575  |              |        |
| QUKHIO       | 2.276  | TOKMEO       | 2.65   |              |        |
| RASYIV       | 2.891  | TOKMEO       | 2.935  |              |        |
| RASYIV       | 2.447  | TOKMIS       | 2.766  |              |        |
| REJMUO01     | 2.402  | TOKMOY       | 2.71   |              |        |
| RINQUD       | 2.988  | TOKMUE       | 2.51   |              |        |
| ROHWAM       | 2.865  | TOKNAL       | 2.472  |              |        |
| TELLAX       | 2.844  | TOKNAL       | 2.535  |              |        |
| TULQIC       | 2.954  | UDOSUE       | 2.546  |              |        |
| VEPVET       | 2.462  | UDOSUE       | 2.613  |              |        |
| VEPVET       | 2.804  | VEPVIX       | 2.955  |              |        |
| WADPID       | 2.388  | VEPVIX       | 2.68   |              |        |

|        |       |        |       |
|--------|-------|--------|-------|
| XARCIC | 2.517 | VEPVIX | 2.766 |
| XARCIC | 2.617 | VEPVIX | 2.493 |
| YADJAP | 2.721 | YIZXUB | 2.413 |
| YADJET | 2.775 | YIZYAI | 2.334 |
| YADJET | 2.836 | YIZYIQ | 2.868 |
|        |       | YIZYOW | 2.848 |

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