

Hypovalency – Kinetic-Energy Density Description of a 4c-2e Bond

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Supplementary Material

BH3

Optimized Geometry

B	0.000000	0.000000	0.000002
H	0.000000	0.000000	-1.200148
H	0.000000	1.039363	0.600069
H	0.000000	-1.039363	0.600069

(3,-3) attractors Xx: Cartesian coordinates and LOL values (for LOL < 0.99)

Xx	0.000000	0.000000	-0.793690	0.930790
Xx	0.000000	0.687360	0.396850	0.930790
Xx	0.000000	-0.687360	0.396850	0.930790

B2H6

Optimized Geometry

B	0.878548	0.000207	0.000184
B	-0.878468	0.000105	0.000127
H	-1.462236	-1.045511	-0.001057
H	-1.460440	1.046831	0.000041
H	0.000078	-0.001106	-0.986756
H	1.459843	1.047103	0.000080
H	1.462592	-1.045407	-0.001053
H	-0.000239	-0.003469	0.987189

(3,-3) attractors Xx: Cartesian coordinates and LOL values (for LOL < 0.99)

Xx	0.000080	-0.001090	-0.977180	0.989840
Xx	-0.000240	-0.003430	0.977610	0.989850
Xx	-1.267200	-0.701840	-0.000630	0.921140
Xx	-1.265930	0.702760	0.000150	0.921190
Xx	1.265610	0.702980	0.000210	0.921200
Xx	1.267450	-0.701700	-0.000590	0.921170
Xx	0.000070	-0.000850	-0.811430	0.847400
Xx	-0.000290	-0.002720	0.811870	0.847390
Xx	0.868210	0.000180	0.000200	0.786780

B4H4

Optimized Geometry

B	0.595842	0.595842	0.595842
H	1.284644	1.284644	1.284644
B	-0.595842	-0.595842	0.595842
H	-1.284644	-1.284644	1.284644
B	-0.595842	0.595842	-0.595842
H	-1.284644	1.284644	-1.284644
B	0.595842	-0.595842	-0.595842
H	1.284644	-1.284644	-1.284644

(3,-3) attractors Xx: Cartesian coordinates and LOL values (for LOL < 0.99)

Xx	1.054400	1.054400	1.054400	0.928800
Xx	-1.054400	-1.054400	1.054400	0.928800
Xx	-1.054400	1.054400	-1.054400	0.928800
Xx	1.054400	-1.054400	-1.054400	0.928800
Xx	0.437150	0.437150	-0.437150	0.682200
Xx	-0.437150	0.437150	0.437150	0.682200
Xx	-0.437150	-0.437150	-0.437150	0.682200
Xx	0.437150	-0.437150	0.437150	0.682200

B4H10

Optimized Geometry

B	0.856741	0.000000	-0.462357
B	0.000000	1.393395	0.382710
B	-0.856741	0.000000	-0.462357
B	0.000000	-1.393395	0.382710
H	0.000000	-2.431905	-0.215413
H	0.000000	-1.428183	1.587555
H	-1.376638	0.000000	-1.535086
H	-1.327627	-0.917849	0.280591
H	-1.327627	0.917849	0.280591
H	0.000000	1.428183	1.587555
H	0.000000	2.431905	-0.215413
H	1.327627	-0.917849	0.280591
H	1.327627	0.917849	0.280591
H	1.376638	0.000000	-1.535086

(3,-3) attractors Xx: Cartesian coordinates and LOL values (for LOL < 0.99)

Xx	-1.320320	-0.913600	0.276380	0.986320
Xx	-1.320320	0.913600	0.276380	0.986320
Xx	1.320320	-0.913600	0.276380	0.986320
Xx	1.320320	0.913600	0.276380	0.986320
Xx	0.000000	-2.089100	-0.023850	0.917490
Xx	0.000000	-1.411210	1.197090	0.910440
Xx	0.000000	2.089100	-0.023850	0.917490
Xx	1.209880	0.000000	-1.189390	0.912830
Xx	-1.209880	0.000000	-1.189390	0.912830
Xx	0.000000	1.411210	1.197090	0.910440
Xx	-1.204890	-0.825540	0.193760	0.840710
Xx	-1.204890	0.825540	0.193760	0.840710
Xx	1.204890	-0.825540	0.193760	0.840710
Xx	1.204890	0.825540	0.193760	0.840710
Xx	-1.133870	-0.693000	0.082630	0.825480
Xx	-1.133870	0.693000	0.082630	0.825480
Xx	1.133870	-0.693000	0.082630	0.825480
Xx	1.133870	0.693000	0.082630	0.825480
Xx	0.000000	0.000000	-0.462900	0.758510

B6H6 (2-)

Optimized Geometry

B	0.000000	0.000000	1.230160
B	0.000000	0.000000	-1.230160
B	0.000000	1.230160	0.000000
B	0.000000	-1.230160	0.000000
B	1.230160	0.000000	0.000000
B	-1.230160	0.000000	0.000000
H	2.453973	0.000000	0.000000
H	-2.453973	0.000000	0.000000
H	0.000000	2.453973	0.000000
H	0.000000	-2.453973	0.000000
H	0.000000	0.000000	2.453973
H	0.000000	0.000000	-2.453973

(3,-3) attractors Xx: Cartesian coordinates and LOL values (for LOL < 0.99)

Xx	2.055850	0.000000	0.000000	0.884590
Xx	-2.055850	0.000000	0.000000	0.884590
Xx	0.000000	2.055850	0.000000	0.884590
Xx	0.000000	-2.055850	0.000000	0.884590
Xx	0.000000	0.000000	2.055850	0.884600
Xx	0.000000	0.000000	-2.055850	0.884600
Xx	2.261710	0.000000	0.000000	0.864000
Xx	-2.261710	0.000000	0.000000	0.864000
Xx	0.000000	2.261710	0.000000	0.864000
Xx	0.000000	-2.261710	0.000000	0.864000
Xx	0.000000	0.000000	2.261710	0.864000
Xx	0.000000	0.000000	-2.261710	0.864000
Xx	-0.732120	0.000000	0.732120	0.690030
Xx	0.732120	0.000000	0.732120	0.690030
Xx	0.000000	-0.732120	0.732120	0.690030
Xx	0.000000	0.732120	0.732120	0.690030
Xx	0.732120	0.000000	-0.732120	0.690030
Xx	-0.732120	0.000000	-0.732120	0.690030
Xx	0.000000	-0.732120	-0.732120	0.690030
Xx	0.000000	0.732120	-0.732120	0.690030
Xx	-0.732120	0.732120	0.000000	0.690030
Xx	0.732120	0.732120	0.000010	0.690030
Xx	-0.732120	-0.732120	-0.000010	0.690030
Xx	0.732120	-0.732120	0.000000	0.690030
Xx	-0.572410	0.572380	0.572370	0.665660
Xx	0.572410	-0.572380	-0.572370	0.665660
Xx	0.572410	0.572400	0.572360	0.665660
Xx	-0.572410	-0.572400	-0.572360	0.665660

B6H7 (1-)

Optimized Geometry

B	0.045481	0.829243	0.934714
B	0.045481	-0.881045	-0.865497
B	0.045481	-0.881045	0.865497
B	0.045481	0.829243	-0.934714
B	-1.240858	-0.157277	0.000000
B	1.235283	0.029546	0.000000
H	-2.443119	-0.174676	0.000000
H	2.436013	0.122347	0.000000
H	0.044345	-1.708695	1.740326
H	-0.004496	1.689128	-1.773613
H	-0.004496	1.689128	1.773613
H	0.044345	-1.708695	-1.740326
H	-0.954339	1.248145	0.000000

(3,-3) attractors Xx: Cartesian coordinates and LOL values (for LOL < 0.99)

Xx	-0.949260	1.241560	0.000000	0.973460
Xx	-2.051910	-0.166350	0.000000	0.903870
Xx	2.045290	0.091440	0.000000	0.900810
Xx	0.045210	-1.439670	1.455280	0.900820
Xx	0.009690	1.410680	-1.499120	0.903830
Xx	0.009690	1.410680	1.499120	0.903830
Xx	0.045210	-1.439670	-1.455280	0.900820
Xx	-2.240790	-0.169280	0.000000	0.880660
Xx	2.236890	0.106990	0.000000	0.878110
Xx	0.044500	-1.571420	1.595270	0.878120
Xx	0.002070	1.545600	-1.631100	0.880640
Xx	0.002070	1.545600	1.631100	0.880640
Xx	0.044500	-1.571420	-1.595270	0.878120
Xx	-0.855280	1.120350	0.000000	0.794470
Xx	0.708320	0.528760	0.514920	0.702860
Xx	0.009460	-0.005670	1.022650	0.702890
Xx	-0.698960	-0.549100	-0.508420	0.703120
Xx	0.009460	-0.005670	-1.022650	0.702890
Xx	0.750690	-0.595660	-0.405750	0.688030
Xx	0.194960	-1.022100	0.000000	0.687800
Xx	-0.698960	-0.549100	0.508420	0.703120
Xx	0.750690	-0.595660	0.405750	0.688030
Xx	0.708320	0.528760	-0.514920	0.702860
Xx	0.616030	-0.804520	0.000000	0.684260
Xx	0.521940	0.834940	0.000000	0.687140
Xx	-0.577290	-0.006620	0.797720	0.687140
Xx	-0.577290	-0.006620	-0.797720	0.687140
Xx	0.038880	0.830380	0.926850	0.786600