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

Supporting Information

Novel superconducting structures of BH_2 under high pressure

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Supporting Information Tables

Table S1. Detailed structural information of the predicted BH_2 compounds at selected pressures.

Phases	Pressure (GPa)	Lattice parameters (Å)	Atomic coordinates (fractional)
BH_2-Cmcm	50	a=10.668	H (8f) 0.000 -0.251 0.380
		b=3.094	H (8g) -0.395 -0.753 -1.250
		c=2.849	B (8g) -0.290 -0.655 -0.250
		α=β=γ=90.000	
BH_2-$P2_1/c$	50	a=4.527	H (4e) 0.390 -0.274 0.120
		b=2.938	H (4e) 0.768 -0.345 0.686
		c=4.842	B (4e) 0.925 -0.903 1.102
		α=γ=90.000	
		β=133.242	
BH_2-$P2_1/m$	50	a= 5.379	H (2e) -0.104 -0.250 -0.164
		b=2.864	H (2e) 0.889 0.250 -0.561
		c=3.068	H (2e) 0.727 0.250 -0.175
		α=γ=90.000	H (2e) 0.886 0.750 -0.929
		β=104.704	B (2e) 0.665 0.250 -0.610
			B (2e) 0.497 0.250 -0.169
BH_2-C2/c	250	a=2.474	H (4e) -1.000 -0.106 2.250
		b=6.979	H (4c) -1.250 0.250 0.500
		c=1.646	B (4e) -0.500 0.097 -0.250
		α=γ=90.000	
		β=81.610	
BH_2-$C222_1$	350	a=2.365	H (2a) 0.079 0.113 -0.080
		b=2.757	H (2a) 0.651 1.201 0.199
		c=4.042	H (2a) 0.453 1.201 0.594
		α=γ=90.000	H (2a) -0.501 0.788 1.080
		β=73.004	B (2a) 0.852 0.701 0.796
			B (2a) 0.055 0.701 0.390
BH_2-Cmcm	350	a=2.362	H (4c) -0.500 0.0460 0.250
		b=7.838	H (8g) 0.292 0.212 1.250
		c=2.728	H (4c) -0.500 0.149 -0.250
		α=β=γ=90.000	B (4c) 0.000 0.055 0.250
			B (4c) 0.000 -0.147 0.250

Table S2. **Detailed structural information of the predicted BH_4 and BH_5 compounds at selected pressures.**

Phases	Pressure (GPa)	Lattice parameters (Å)	Atomic coordinates (fractional)
BH_4-P_1	50	a=2.974	H(2i) 0.247 0.327 0.241
		b=4.948	H(2i) -0.250 0.043 0.594
		c=5.395	H(2i) -1.246 -0.873 1.226
		α=62.972	H(2i) -1.261 -0.464 1.065
		β=90.411	H(2i) -0.808 -0.289 1.227
		γ=91.189	H(2i) -1.737 -0.209 1.493
			H(2i) -1.731 -0.594 1.605
			H(2i) -1.755 -0.707 1.390
			B(2i) -0.786 -0.711 0.848
			B(2i) -1.705 -0.100 0.975
BH_4-C2/c	400	a=2.440	H(8f) -0.223 0.038 0.501
		b=9.266	H(4c) -0.750 0.250 0.000
		c=1.577	H(4e) -0.500 0.352 0.750
		α=γ=90.000	B(4e) 0.000 0.361 1.750
		β=105.531	
BH_5-P_1	50	a=3.201	H(2i) 0.168 0.174 -0.884
		b=3.366	H(2i) 0.261 -0.134 -0.401
		c=4.586	H(2i) 1.064 -0.187 -0.115
		α=68.122	H(2i) 0.797 -0.497 -0.345
		β=109.992	H(2i) 0.632 -0.214 0.155
		γ=89.212	B(2i) 0.612 -0.525 -0.630
BH_5-Cc	100	a=4.217	H(4a) 0.027 0.828 1.928
		b=7.333	H(4a) 0.261 -0.072 0.829
		c=2.963	H(4a) -0.419 0.053 -0.963
		α=γ=90.000	H(4a) 0.0291 -0.050 0.554
		β=133.772	H(4a) 0.175 0.315 1.173
			B(4a) 0.168 0.308 0.781
BH_5-P_1	400	a=2.415	H(2i) -0.264 0.379 -0.827
		b=2.426	H(2i) -0.202 0.126 -0.191
		c=3.818	H(2i) -0.395 0.674 -0.351
		α=98.024	H(2i) 0.277 0.327 -0.476
		β=108.282	H(1b) 0.000 0.000 -0.500
		γ=68.276	H(1c) 0.000 0.500 0.000
			B(2i) 0.284 0.121 -0.193

Table S3. Calculated the EPC parameter λ of the C2/c-BH_2 structure at the pressures of 250 GPa with the different k-point meshs and q-point meshs.

		Denser k-points				
		12×12×24	**16×16×32**	**18×18×36**	**20×20×40**	**24×24×48**
q-points	**2×2×4**	**0.814**	**0.770**		**0.814**	**0.833**
	3×3×6	**0.729**		**0.647**		**0.614**
	4×4×8		**0.748**			**0.593**
	6×6×12	**0.631**				**0.600**

Supporting Information Figures

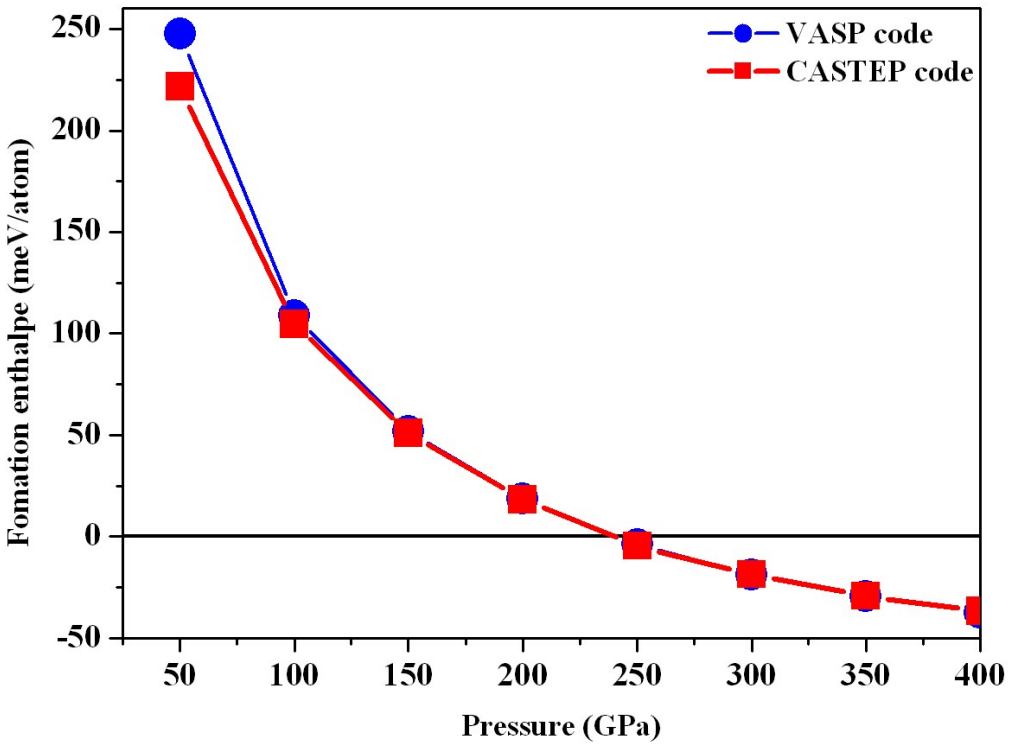

Fig. S1. Based on VASP and CASTEP codes, calculated formation enthalpies (in meV/atom) of C2/c-BH_2 with respect to B and H at the different pressures.

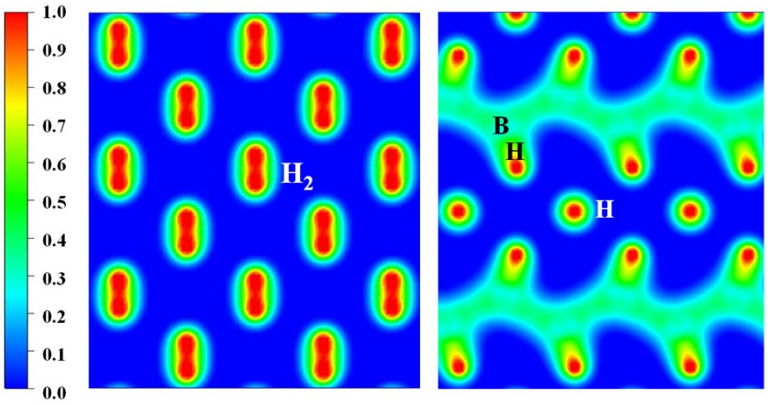

Fig. S2 2D-ELF of Cmcm-BH_2 on the (1,0,0) and (0,0,1) planes, respectively.

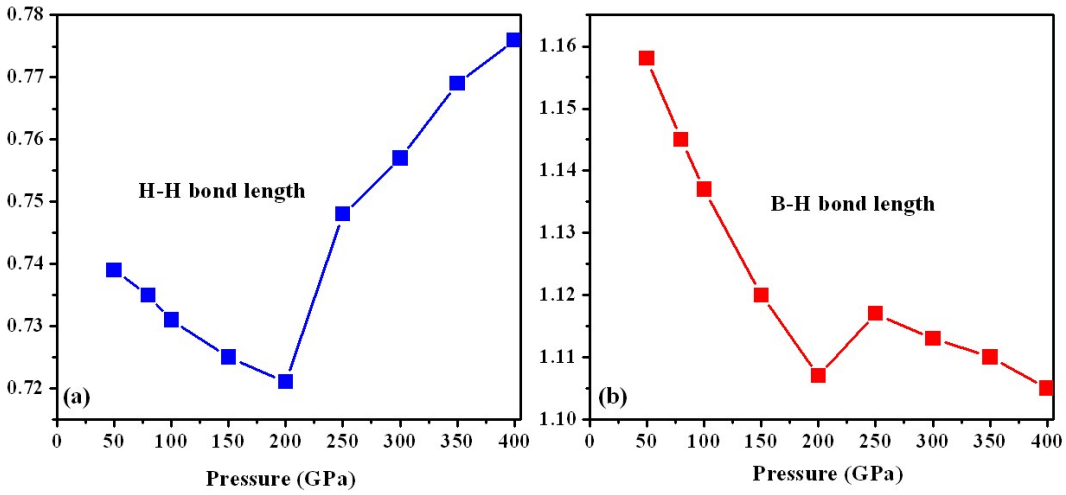

Fig. S3 Bond lengths (Å) of H-H in H_2 unit and B-H for the Cmcm-BH_2 as function of the pressure.

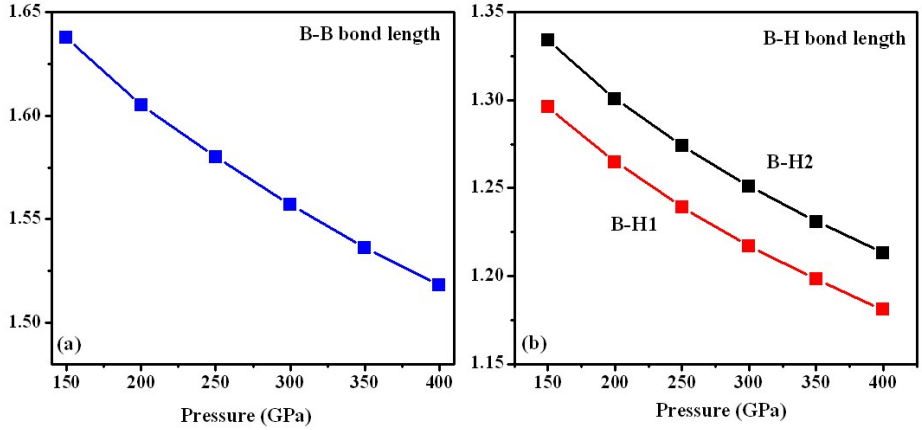

Fig. S4 Bond lengths (Å) of B-B and B-H for the C2/c-BH_2 as function of the pressure.