

Supporting Information
Crystal structure and physical properties of the cage compound
Hf₂B_{2-2δ}Ir_{5+δ}

Olga Sichevych¹, Sever Flipo^{1,2}, Alim Ormeci¹, Matej Bobnar¹, Lev Akselrud¹, Yurii Prots¹,
 Ulrich Burkhardt¹, Roman Gumeniuk^{1,2}, Andreas Leithe-Jasper^{1*}, Yuri Grin¹

¹ *Max-Planck- Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187
 Dresden, Germany*

² *Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09599
 Freiberg, Germany*

*email: jasper@cpfs.mpg.de

Table S1. Selected interatomic distances (in Å) in Hf₂B_{2-2δ}Ir_{5+δ}

Hf -	4B	2.67(2) – 2.82(2)	4Ir3	2.718(7) – 2.735(7)
	2Ir1	2.823(5)	4Hf	2.828(7) – 2.840(7)
	4Ir2	2.828(7) – 2.840(7)	Ir3- 2B	2.289(13)
	4Ir3	2.769(10) – 2.876(10)	4Ir1	2.718(5)
	3Hf	3.472(9) – 3.8328(2)	4Ir2	2.718(7) – 2.735(7)
	2Ir4	2.589(8)	1Ir4	2.865(7)
Ir1-	2B	2.33(2)	4Hf	2.769(10) – 2.876(10)
	2Ir2	2.782(6)	B- B	1.85(3)
	4Ir3	2.718(5)	2Ir1	2.33(2)
	2Hf	2.823(5)	1Ir2	2.18(2)
	2Ir4	2.815(4)	2Ir3	2.289(13)
Ir2-	B	2.18(2)	4Hf	2.67(2) – 2.82(2)
	2Ir1	2.782(6)	1Ir4	1.09(3)
	2Ir2	2.816(12)		

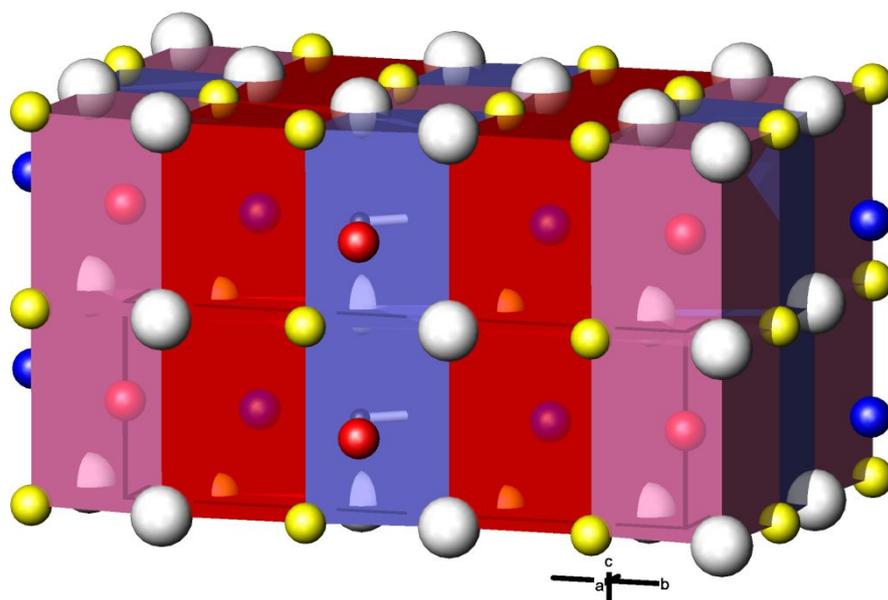


Figure S1. 3-D representation of the crystal structure of Hf₂B₂Ir₅. Hf (white spheres) and Ir₃ (yellow spheres) form cuboids which are centered by Ir₁ (red spheres), or Ir₂ (blue spheres). Boron dumbbells (B (black spheres)) reside in fused trigonal prisms.

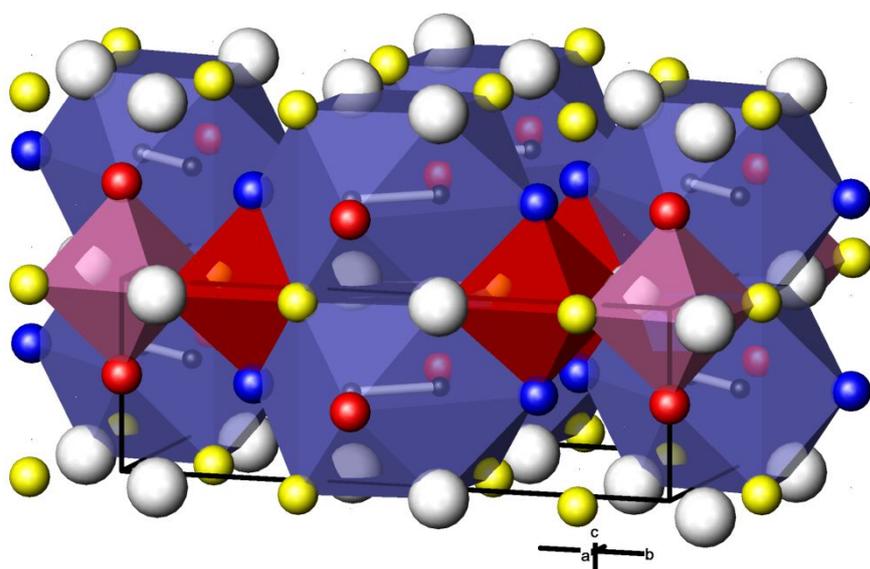


Figure S2. Alternative 3-D representation of the crystal structure of Hf₂B₂Ir₅. Emphasis is laid on octahedrons formed by Hf (white spheres) and Ir₃ (yellow spheres) and Ir₁ (red spheres), as well as Ir₂ (blue spheres). Boron dumbbells (B (black spheres)) center distorted cuboctahedrons accordingly.

Microhardness

The small size and number of samples hampered detailed hardness measurements. Nevertheless, preliminary hardness tests could be carried out using a Paar Physica MHT-10 micro hardness tester with a Zeiss Axioplan 2 light-optical microscope. An average of 15 indents was taken for each measurement with a force of 0.9807 N and a 10 seconds dwell time. Hardness values $HV(0.1) = 13(1)$ GPa and $HV(0.1) = 11(1)$ GPa for $Hf_2B_{2-2\delta}Ir_{5+\delta}$ and $Zr_2B_{2-2\delta}Ir_{5+\delta}$, respectively, point towards moderate hardness of these metal-rich borides.