

Structural, optical and electronic properties of single crystals of 4H lead-based hexagonal hybrid perovskite

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Figure S1: Picture of the harvested crystals under microscope.

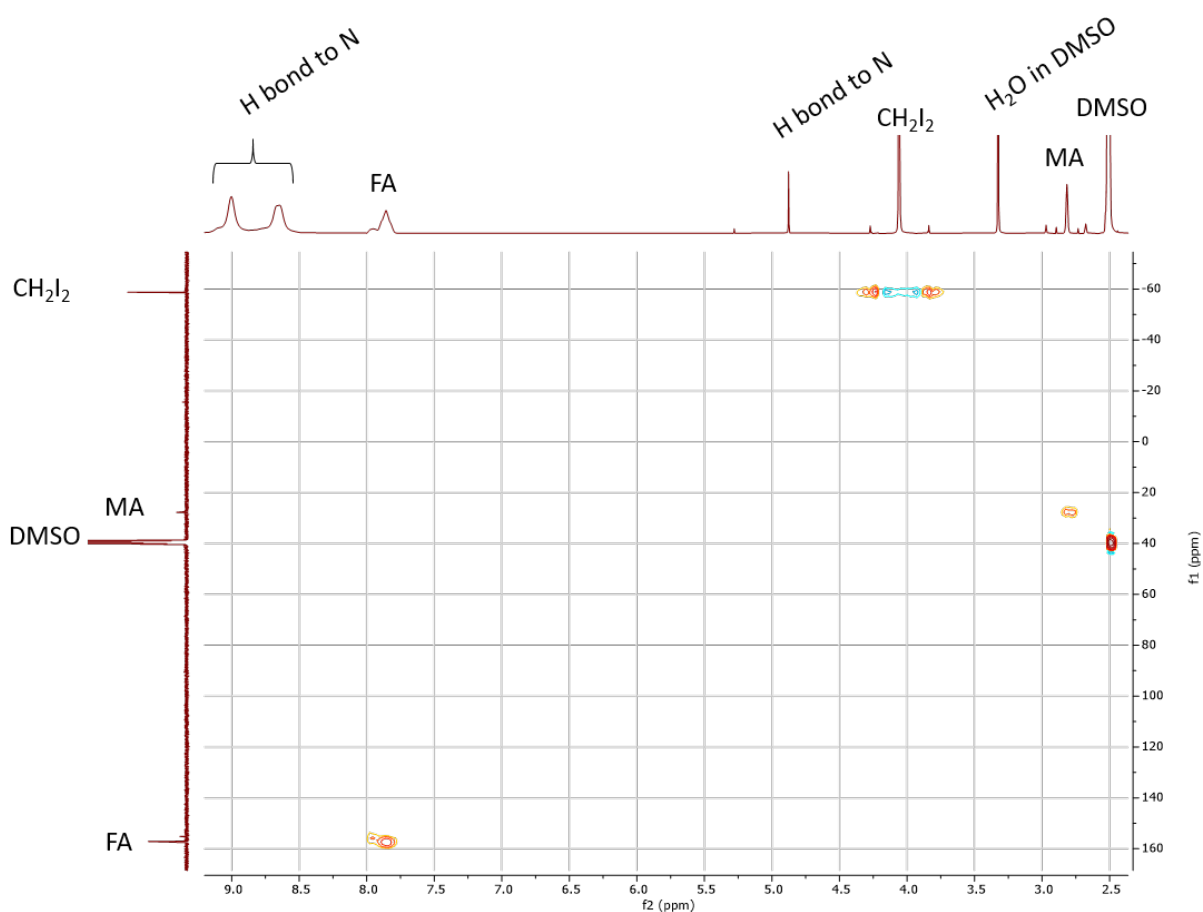


Figure S2: HSQC (heteronuclear single quantum correlation) plot of crystals dissolved in DMSO-d₆, here with the addition of CH₂I₂ for quantitative NMR. On the y axis is the ¹³C NMR spectra and on the x axis is the ¹H NMR spectra.

Table S1: Crystal data and structure refinement at 299 K. The organic cations amount has been calculated as a set, restricted by the BYPASS method. The final empirical amount of organic cations retained is FA_{0.9}MA_{0.1}, as extracted from quantitative NMR analysis (see Structural Analysis section in the manuscript).

Empirical formula	C _{0.96} H _{5.42} Br _{0.77} I _{2.23} N _{1.38} Pb
Formula weight	587.38
Temperature/K	299.08
Crystal system	hexagonal
Space group	P6 ₃ /mmc
a/Å	8.7964(6)
b/Å	8.7964(6)
c/Å	15.1514(12)
α/°	90
β/°	90
γ/°	120
Volume/Å ³	1015.30(16)
Z	4
ρ _{calc} /g/cm ³	3.845
μ/mm ⁻¹	26.361
F(000)	912.0
Crystal size/mm ³	0.05 × 0.01 × 0.005
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.348 to 52.444
Index ranges	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -18 ≤ l ≤ 18
Reflections collected	9464
Independent reflections	429 [R _{int} = 0.0358, R _{sigma} = 0.0124]
Data/restraints/parameters	429/0/14
Goodness-of-fit on F ²	1.159
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0293, wR ₂ = 0.0682
Final R indexes [all data]	R ₁ = 0.0417, wR ₂ = 0.0786
Largest diff. peak/hole / e Å ⁻³	0.71/-0.57

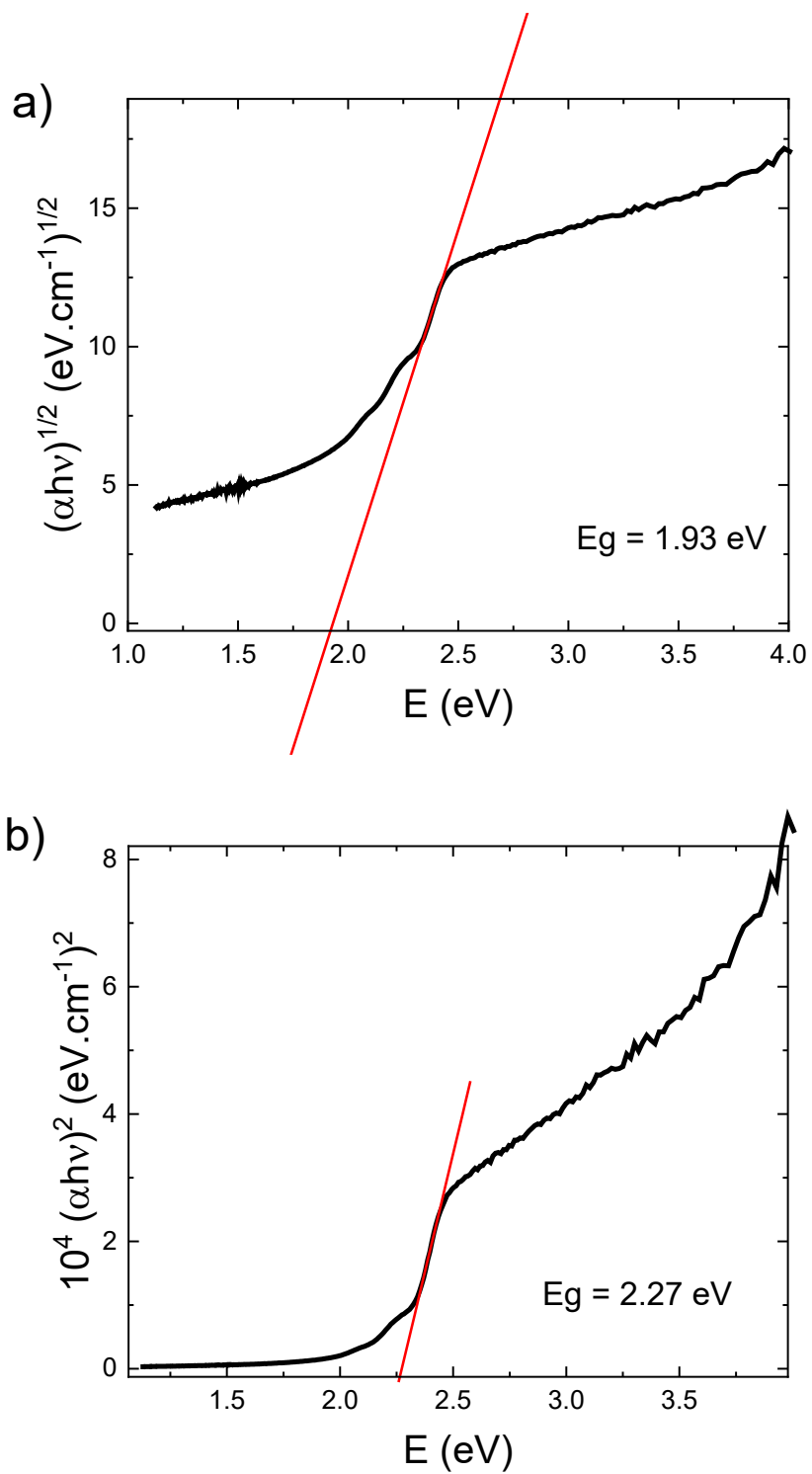


Figure S3: Tauc plots for (a) indirect allowed transition ($n=2$) with linear fit ($R = 0.99964$) and for (b) direct allowed transition ($n = 1/2$) with linear fit ($R = 0.99938$).

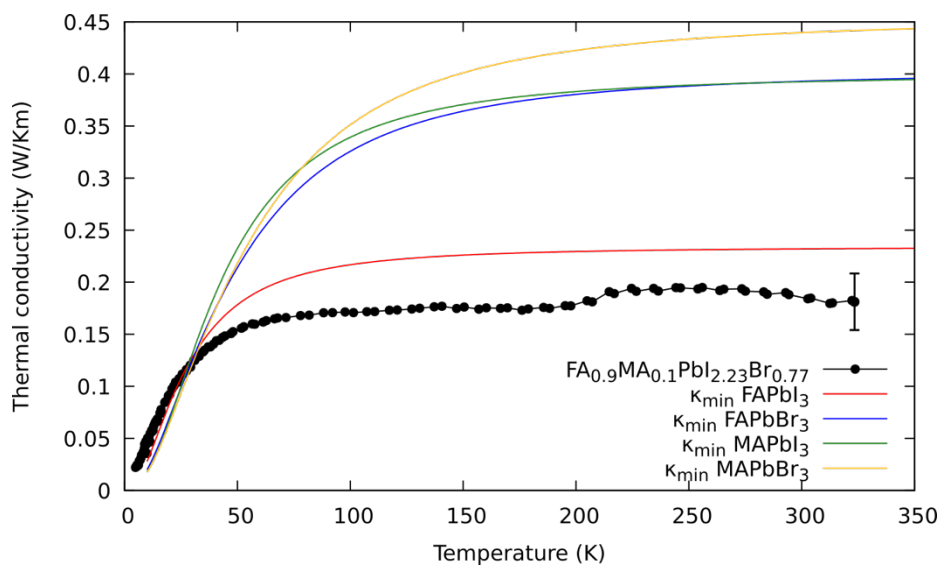


Figure S4: Minimum thermal conductivity curves as for **Figure 6** but with additional calculated curves for MAPbI₃ and MAPbBr₃. The sound velocities for all except FAPbI₃ are quite similar, leading to similar magnitudes of κ_{\min} .