The Luminescent Semiconductor $Pb_7I_6(CN_2)_4$

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Supporting Information:

Table S 1: Wyckoff position, site occupation factors and atomic coordinates of $Pb_7I_6(CN_2)_4$

Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c
Pb1	12k	.m.		-0.21139(2)	0.21139(2)	0.67292(2)
Pb2	4f	3m.		-2/3	-1/3	0.67125(2)
Pb3	12k	.m.		-0.41586(3)	-0.20793(2)	0.56014(2)
Pb4	4f	3m.		-1/3	1/3	0.55141(2)
Pb5	4e	3m.	0.75	0	0	0.61669(2)

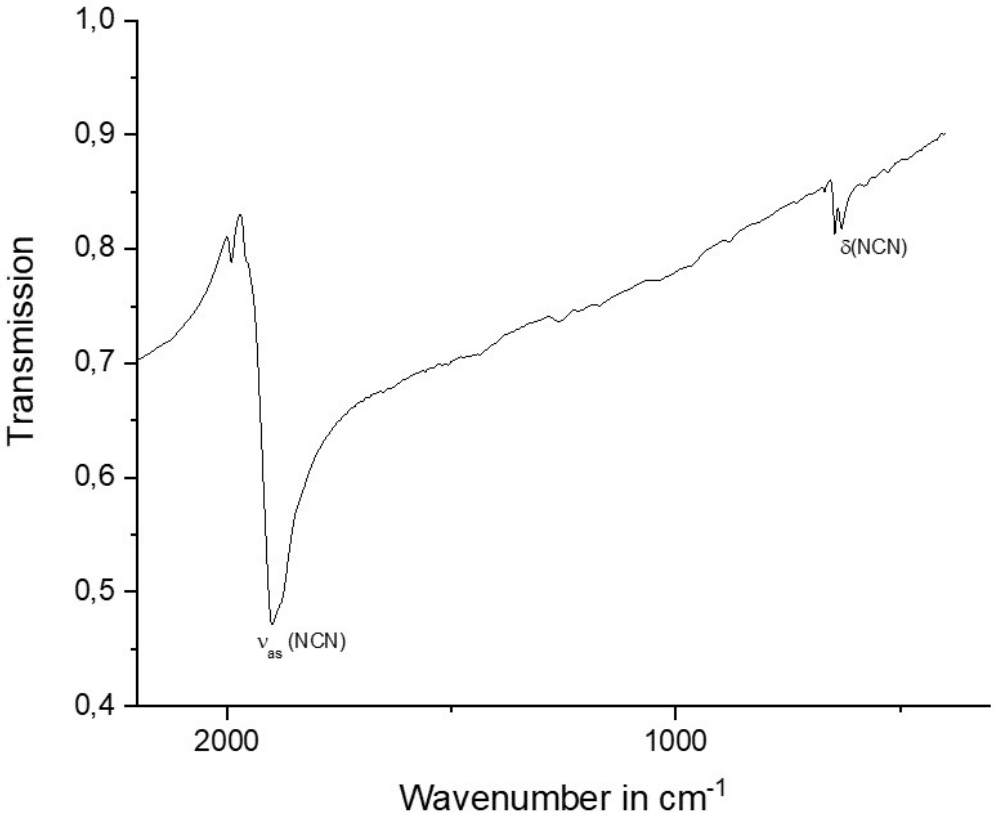

Figure S 1: Infrared spectrum of $Pb_7I_6(CN_2)_4$

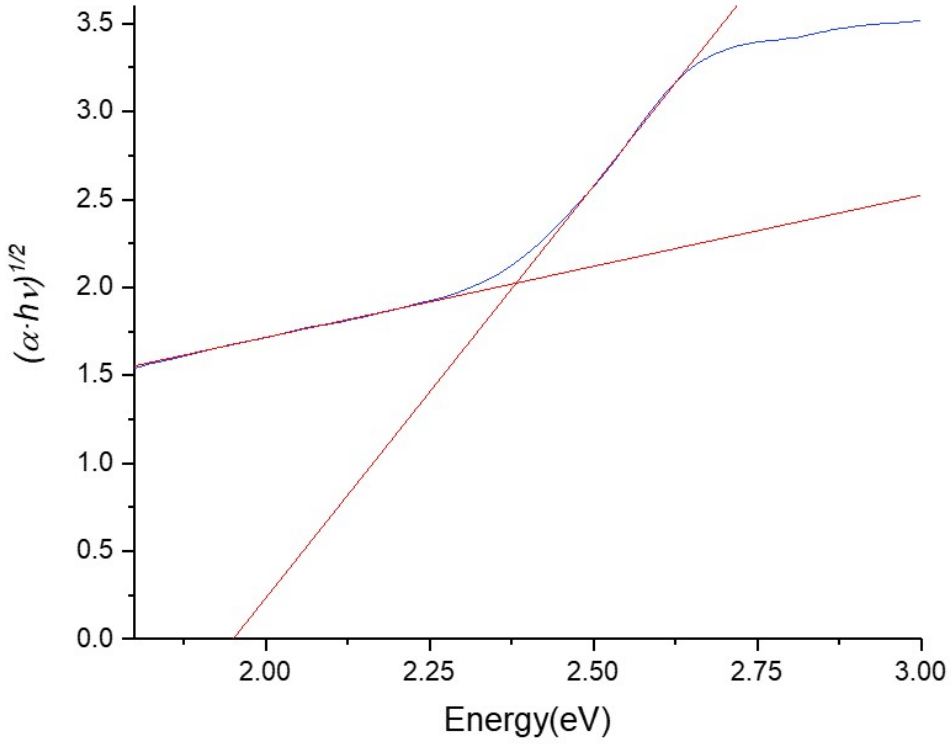

Figure S 2: Tauc plot for indirect allowed transition of $Pb_7I_6(CN_2)_4$

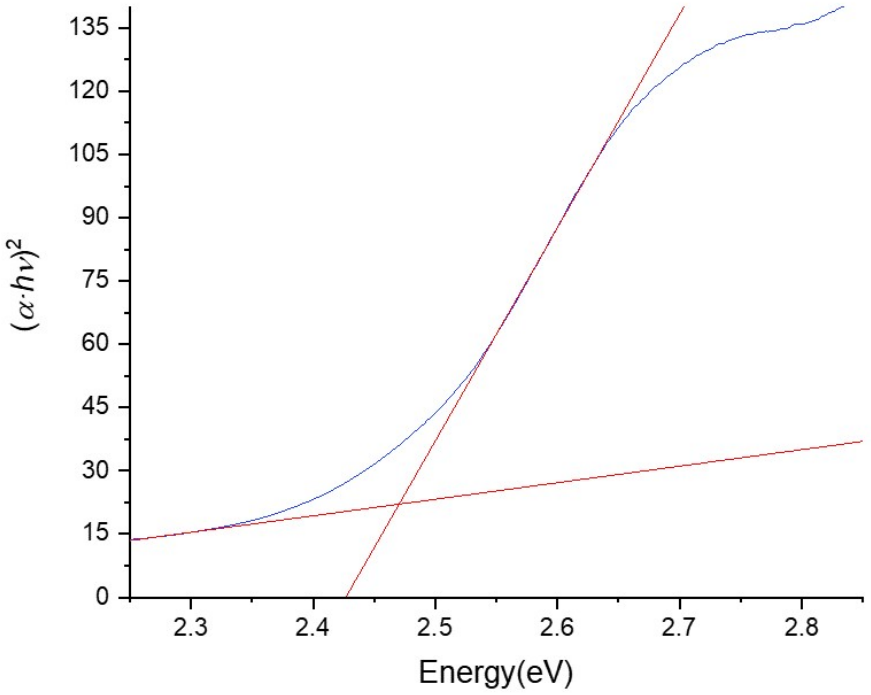

Figure S 3: Tauc plot for direct allowed transition of $Pb_7I_6(CN_2)_4$

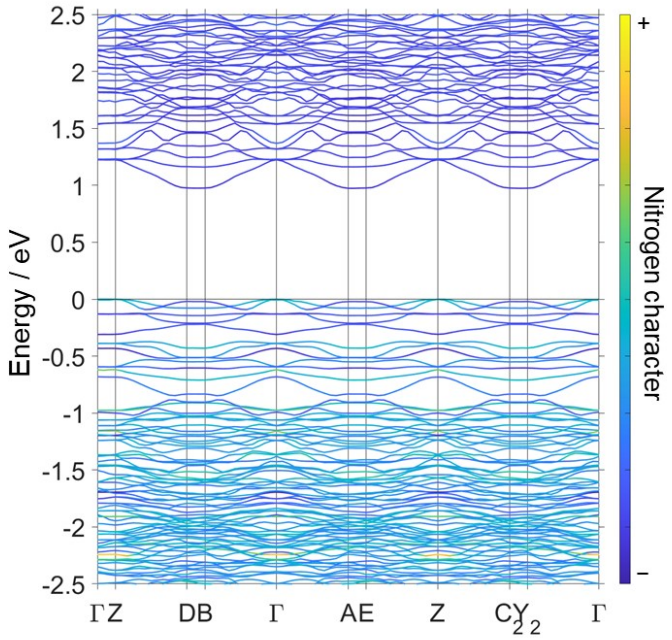

Figure S 4: The electronic band structure of $Pb_7I_6(CN_2)_4$, with bands coloured by their N character, on the same scale as Figure 5. Special points in and paths through the Brillouin Zone were chosen following literature.