

Supplementary Information

A C₂₀-based 3D carbon allotrope with high thermal conductivity

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1. Atomic Wyckoff positions of optimized HSP3-C₃₄

Table S1. Atomic Wyckoff positions of HSP3-C₃₄

Wyckoff positions	<i>x</i>	<i>y</i>	<i>z</i>
12o	0.79044	0.20956	0.72560
6m	0.13091	0.86909	0.50000
4h	0.66667	0.33333	0.63712
12n	0.61404	0.00000	0.86032