

Supporting information for
**Precise synthesis of schwarzites carbon:
hypothesis or reality?**

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1. Theoretical Calculations

The density functional theory (DFT) calculations were performed with the Gaussian 16 quantum chemistry package^[1] employing the M06-2X^[2] exchange-correlation functional and the def2-SVP^[3] basis set. The optimized structures were confirmed by harmonic frequency calculations, and there was no imaginary frequency.

The simulated absorption spectrum for **P192** was calculated employing the time-dependent DFT (TDDFT) linear response method under M06-2X/def2-SVP level and the lowest 50 states were computed at the optimized geometry. The calculated line spectra are represented by applying Gaussian broadening with a full width at half maximum (FWHM) of 0.15 eV. The simulated UV-vis spectrum was generated by Multiwfn 3.8 dev^[4].

Table S1. Calculated photophysical property data of the ground state of **P192** at the M06-2X/def2-SVP level.

Excited States	Energy [eV]	Wavelength [nm]	Oscillator Strength	Transitions
$S_0 \rightarrow S_{18}$				H-7 \rightarrow L+1 20.5%, H-3 \rightarrow L+4 16.6%, H-2 \rightarrow L+2 16.6%, H-1 \rightarrow L+7 8.7%, H \rightarrow L+7 8.2%, H-7 \rightarrow L 5.6%
$S_0 \rightarrow S_{19}$	2.9160	425	1.4459	H-5 \rightarrow L+1 18.6%, H-2 \rightarrow L+3 16.6%, H-4 \rightarrow L+4 16.6%, H-1 \rightarrow L+6 15.7%, H-5 \rightarrow L 7.5%
$S_0 \rightarrow S_{20}$				H-6 \rightarrow L 26.0%, H-3 \rightarrow L+3 16.6%, H-4 \rightarrow L+2 16.6%, H \rightarrow L+5 15.9%
$S_0 \rightarrow S_{36}$				H-3 \rightarrow L+4 30.4%, H-2 \rightarrow L+2 30.4%, H-7 \rightarrow L+1 13.8%
$S_0 \rightarrow S_{37}$	3.2692	379	0.1022	H-4 \rightarrow L+4 30.4%, H-2 \rightarrow L+3 30.4%, H-5 \rightarrow L+1 12.5%, H-5 \rightarrow L 5.0%
$S_0 \rightarrow S_{38}$				H-4 \rightarrow L+2 30.4%, H-3 \rightarrow L+3 30.4%, H-6 \rightarrow L 17.5%

Table S2. Frontier molecular orbital energies (eV)

	E_{LUMO} [eV]	E_{HOMO} [eV]	H-L Gap [eV]
P192	-2.45	-6.11	3.66
PL96	-3.23	-4.49	1.26

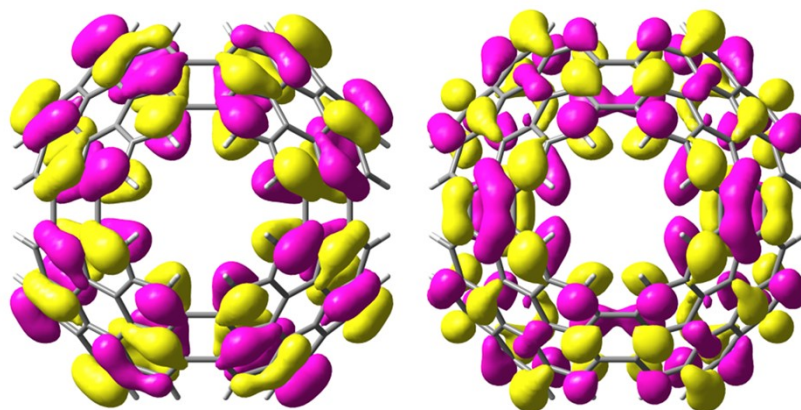


Figure 1. HOMO (left) and LUMO (right) orbital for **P192** (isovalue = 0.01).

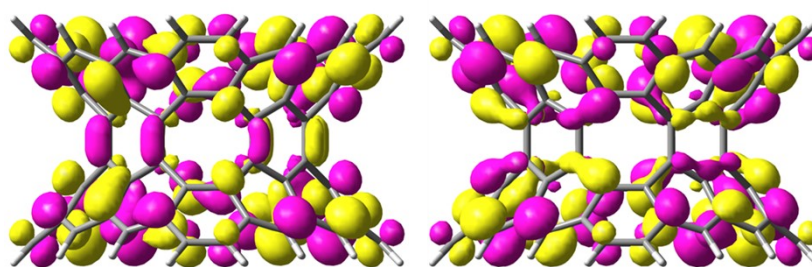


Figure 2. HOMO (left) and LUMO (right) orbital for **PL96** (isovalue = 0.02).

Table S3. The cartesian coordinates of optimized structures for **P192** and **PL96** are listed as follows:

P192

C	1.45051500	3.18094600	6.60395500
C	2.73219400	2.73219400	6.19300100
C	3.18094600	1.45051500	6.60395500
C	0.74358200	4.12418200	5.88676500
C	1.43351300	4.88006000	4.88006000
C	2.76380200	4.51971200	4.51971200
C	3.37870300	3.37870300	5.11841100
C	4.51971200	2.76380200	4.51971200
C	4.88006000	1.43351300	4.88006000
C	4.12418200	0.74358200	5.88676500
C	-3.18094600	1.45051500	6.60395500
C	-2.73219400	2.73219400	6.19300100
C	-1.45051500	3.18094600	6.60395500
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C	-4.51971200	2.76380200	4.51971200
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C	-2.76380200	4.51971200	4.51971200
C	-1.43351300	4.88006000	4.88006000

C	-0.74358200	4.12418200	5.88676500
C	-1.45051500	-3.18094600	6.60395500
C	-2.73219400	-2.73219400	6.19300100
C	-3.18094600	-1.45051500	6.60395500
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C	5.11841100	-3.37870300	-3.37870300
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H	7.37955200	-0.95755200	2.59628100
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H	7.37955200	0.95755200	2.59628100

H	7.37955200	2.59628100	0.95755200
PL96			
C	2.43017000	4.39522300	2.63019000
C	2.43617000	3.41732800	1.56279400
C	1.23643100	3.41803700	0.69830400
C	0.00000000	3.70920000	1.34473300
C	0.00000000	4.55000700	2.50509800
C	1.23704100	4.98954500	3.02145100
C	-1.23643100	3.41803700	0.69830400
C	-2.43617000	3.41732800	1.56279400
C	-2.43017000	4.39522300	2.63019000
C	-1.23704100	4.98954500	3.02145100
C	1.23643100	3.41803700	-0.69830400
C	0.00000000	3.70920000	-1.34473300
C	-1.23643100	3.41803700	-0.69830400
C	2.43617000	3.41732800	-1.56279400
C	2.43017000	4.39522300	-2.63019000
C	1.23704100	4.98954500	-3.02145100
C	0.00000000	4.55000700	-2.50509800
C	-1.23704100	4.98954500	-3.02145100
C	-2.43017000	4.39522300	-2.63019000
C	-2.43617000	3.41732800	-1.56279400
C	-3.62743600	4.58687500	3.40068300
C	3.62743600	4.58687500	3.40068300
C	3.62743600	4.58687500	-3.40068300
C	3.62743600	-4.58687500	3.40068300
C	4.39522300	-2.43017000	2.63019000
C	3.41732800	-2.43617000	1.56279400
C	3.41803700	-1.23643100	0.69830400
C	3.70920000	0.00000000	1.34473300
C	4.55000700	0.00000000	2.50509800
C	4.98954500	-1.23704100	3.02145100
C	3.41803700	1.23643100	0.69830400
C	3.41732800	2.43617000	1.56279400
C	4.39522300	2.43017000	2.63019000
C	4.98954500	1.23704100	3.02145100
C	3.41803700	-1.23643100	-0.69830400
C	3.70920000	0.00000000	-1.34473300
C	3.41803700	1.23643100	-0.69830400
C	3.41732800	-2.43617000	-1.56279400
C	4.39522300	-2.43017000	-2.63019000
C	4.98954500	-1.23704100	-3.02145100
C	4.55000700	0.00000000	-2.50509800
C	4.98954500	1.23704100	-3.02145100

C	4.39522300	2.43017000	-2.63019000
C	3.41732800	2.43617000	-1.56279400
C	4.58687500	-3.62743600	3.40068300
C	4.58687500	-3.62743600	-3.40068300
C	4.58687500	3.62743600	3.40068300
C	4.58687500	3.62743600	-3.40068300
C	1.23643100	-3.41803700	0.69830400
C	2.43617000	-3.41732800	1.56279400
C	2.43017000	-4.39522300	2.63019000
C	-1.23643100	-3.41803700	-0.69830400
C	0.00000000	-3.70920000	-1.34473300
C	1.23643100	-3.41803700	-0.69830400
C	-1.23704100	-4.98954500	-3.02145100
C	0.00000000	-4.55000700	-2.50509800
C	1.23704100	-4.98954500	-3.02145100
C	2.43017000	-4.39522300	-2.63019000
C	2.43617000	-3.41732800	-1.56279400
C	3.62743600	-4.58687500	-3.40068300
C	0.00000000	-3.70920000	1.34473300
C	0.00000000	-4.55000700	2.50509800
C	1.23704100	-4.98954500	3.02145100
C	-2.43617000	-3.41732800	-1.56279400
C	-2.43017000	-4.39522300	-2.63019000
C	-3.62743600	-4.58687500	-3.40068300
C	-3.62743600	-4.58687500	3.40068300
C	-2.43617000	-3.41732800	1.56279400
C	-1.23643100	-3.41803700	0.69830400
C	-1.23704100	-4.98954500	3.02145100
C	-2.43017000	-4.39522300	2.63019000
C	-3.62743600	4.58687500	-3.40068300
C	-3.41803700	1.23643100	-0.69830400
C	-3.41732800	2.43617000	-1.56279400
C	-4.39522300	2.43017000	-2.63019000
C	-4.58687500	3.62743600	-3.40068300
C	-4.39522300	2.43017000	2.63019000
C	-3.41732800	2.43617000	1.56279400
C	-3.41803700	1.23643100	0.69830400
C	-3.70920000	0.00000000	1.34473300
C	-4.55000700	0.00000000	2.50509800
C	-4.98954500	1.23704100	3.02145100
C	-3.41803700	-1.23643100	0.69830400
C	-4.98954500	-1.23704100	3.02145100
C	-3.70920000	0.00000000	-1.34473300
C	-3.41803700	-1.23643100	-0.69830400

C	-4.98954500	1.23704100	-3.02145100
C	-4.55000700	0.00000000	-2.50509800
C	-4.98954500	-1.23704100	-3.02145100
C	-4.39522300	-2.43017000	-2.63019000
C	-3.41732800	-2.43617000	-1.56279400
C	-4.58687500	3.62743600	3.40068300
C	-4.58687500	-3.62743600	-3.40068300
C	-4.58687500	-3.62743600	3.40068300
C	-4.39522300	-2.43017000	2.63019000
C	-3.41732800	-2.43617000	1.56279400
H	1.24395200	5.71528500	3.83787200
H	-1.24395200	5.71528500	3.83787200
H	1.24395200	5.71528500	-3.83787200
H	-1.24395200	5.71528500	-3.83787200
H	-3.68558300	5.44306500	4.07548500
H	3.68558300	5.44306500	4.07548500
H	3.68558300	5.44306500	-4.07548500
H	3.68558300	-5.44306500	4.07548500
H	5.71528500	-1.24395200	3.83787200
H	5.71528500	1.24395200	3.83787200
H	5.71528500	-1.24395200	-3.83787200
H	5.71528500	1.24395200	-3.83787200
H	5.44306500	-3.68558300	4.07548500
H	5.44306500	-3.68558300	-4.07548500
H	5.44306500	3.68558300	4.07548500
H	5.44306500	3.68558300	-4.07548500
H	-1.24395200	-5.71528500	-3.83787200
H	1.24395200	-5.71528500	-3.83787200
H	3.68558300	-5.44306500	-4.07548500
H	1.24395200	-5.71528500	3.83787200
H	-3.68558300	-5.44306500	-4.07548500
H	-3.68558300	-5.44306500	4.07548500
H	-1.24395200	-5.71528500	3.83787200
H	-3.68558300	5.44306500	-4.07548500
H	-5.44306500	3.68558300	-4.07548500
H	-5.71528500	1.24395200	3.83787200
H	-5.71528500	-1.24395200	3.83787200
H	-5.71528500	1.24395200	-3.83787200
H	-5.71528500	-1.24395200	-3.83787200
H	-5.44306500	3.68558300	4.07548500
H	-5.44306500	-3.68558300	-4.07548500
H	-5.44306500	-3.68558300	4.07548500

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