

Supporting Information

Correction to “Construction of 2-Arylbenzo[4,5]thieno[2,3-*d*]thiazole Skeleton *via* CuCl/S-Mediated Three-Component Reaction”

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1. X-ray Structure and Data of sublimed sulfur

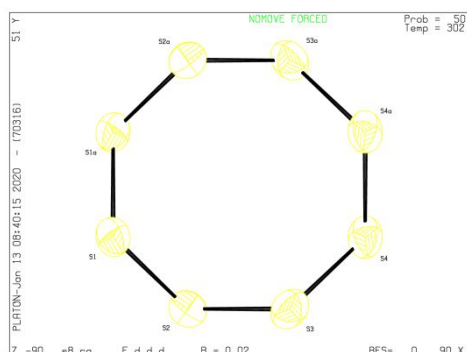


Table S1 Crystal data and structure refinement for **sublimed sulfur**.

Identification code	S8_Ra
Empirical formula	S ₈
Formula weight	256.48
Temperature/K	301.72(10)
Crystal system	orthorhombic
Space group	Fddd
a/Å	10.4623(4)
b/Å	12.8720(5)
c/Å	24.4788(9)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	3296.6(2)
Z	16
ρ _{calc} /cm ³	2.067
μ/mm ⁻¹	19.298
F(000)	2048.0
Crystal size/mm ³	0.1 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	11.484 to 144.488
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 15, -15 ≤ l ≤ 30
Reflections collected	2085
Independent reflections	785 [R _{int} = 0.0191, R _{sigma} = 0.0215]
Data/restraints/parameters	785/0/37
Goodness-of-fit on F ²	1.070
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0218, wR ₂ = 0.0562
Final R indexes [all data]	R ₁ = 0.0248, wR ₂ = 0.0573
Largest diff. peak/hole / e Å ⁻³	0.25/-0.23

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **sublimed sulfur**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
S2	2072.4(5)	2702.9(4)	7458.8(2)	49.28(17)
S4	2859.4(5)	3423.3(5)	6204.5(2)	47.67(17)
S1	3558.3(6)	2972.8(4)	7985.3(2)	48.87(16)
S3	2840.9(6)	2198.3(4)	6737.8(2)	50.24(17)

Table S3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **sublimed sulfur**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S2	49.3(3)	53.5(3)	44.9(3)	1.8(2)	4.9(2)	-9.8(2)
S4	38.5(3)	67.6(3)	36.9(3)	3.3(2)	-6.0(2)	1.4(2)
S1	65.5(3)	43.9(3)	37.2(3)	8.32(19)	-5.5(2)	-3.6(2)
S3	63.2(3)	41.5(3)	46.0(3)	-9.0(2)	-4.4(2)	-0.6(2)

Table S4 Bond Lengths for **sublimed sulfur**.

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA
S2	S1	2.0491(8)	S4	S3	2.0471(8)
S2	S3	2.0454(8)	S1	S1 ¹	2.0406(11)
S4	S4 ¹	2.0445(10)			

Table S5 Bond Angles for **sublimed sulfur**.

Atom	Atom	Atom	Angle/ $^\circ$	Atom	Atom	Atom	Angle/ $^\circ$
S3	S2	S1	107.36(3)	S1 ¹	S1	S2	108.38(4)
S4 ¹	S4	S3	109.00(3)	S2	S3	S4	108.03(3)