Revision #1

SUPPLEMENTAL

Table S1. Unit-cell parameters indexed for the 6 grains of *C*23 Fe_2S analyzed in this study.

Pnma Fe_2S grains indexed	**Grain 1: C132, 90 GPa, Map 16**	**Grain 2: C132, 90 GPa, Map 23**	**Grain 3: C132, 90 GPa, Map 31**	**Grain 4: C132, 90 GPa, Map 32**	**Grain 5: C132, 90 GPa, Map 32**	**Grain 6: C132, 90 GPa, S1**
a (Å)	5.066(2),	5.066 (2),	5.07 (2),	5.089 (1),	5.06 (2),	5.078 (3),
b (Å)	3.286 (2),	3.285 (2),	3.279 (1),	3.27 (1),	3.283 (1),	3.289 (2),
c (Å)	6.124 (2)	6.125 (2)	6.140 (1)	6.105 (1)	6.148 (2)	6.123 (3)
V (Å^3), (*Z*=4)	101.9 (1)	101.9 (1)	102.0 (3)	101.6 (3)	102.2 (4)	102.3 (1)
μ (mm^{-1})	2.49	2.49	2.49	2.5	2.49	2.48

Table S2. Reduction and refinement parameters for the 6 grains of *C*23 Fe_2S analyzed in this study.

Sample Name	**Grain 1: C132, 90 GPa, Map 16**	**Grain 2: C132, 90 GPa, Map 23**	**Grain 3: C132, 90 GPa, Map 31**	**Grain 4: C132, 90 GPa, Map 32**	**Grain 5: C132, 90 GPa, Map 32**	**Grain 6: C132, 90 GPa, S1**
Reduction						
No. of measured, independent and observed [I > 2σ(I)] reflections	220, 116, 110	231, 119, 114	214, 82, 76	206, 98, 91	193, 81, 68	260, 147, 134
R_{int}, R_{sigma}	0.0147, 0.0188	0.0127, 0.0162	0.0221, 0.0213	0.0423, 0.0488	0.0679, 0.0460	0.0096, 0.0116
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.877	0.877	0.852	0.856	0.851	0.862
Refinement						
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.069, 1.15	0.028, 0.076, 1.14	0.033, 0.087, 1.10	0.060, 0.168, 1.18	0.055, 0.148, 1.11	0.080, 0.189, 1.06
No. of reflections	116	119	82	98	81	147
omitted reflections	(525)			(218), (802), (801), (811)	(243)	(444), (443)
No. of parameters	10	15	10	10	10	10
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.10, −1.25	1.28, −1.15	0.73, −1.44	1.60, −1.68	1.90, −2.10	5.12, −3.36

Table S3. Atomic fractional coordinates and thermal parameters refined for 6 grains of *C*23 Fe_2S.

Grain 1: C132, Map 16

Atom		**x**	**y**	**z**	**U11**	**U22**	**U33**	**U23**	**U13**	**U12**	**Ueq**
Fe1	coordinate	0.9698	0.25	0.6738	0.0054						
	error	0.0002		0.0002	0.0003						
Fe2	coordinate	0.8530	0.25	0.0662	0.0049						
	error	0.0002		0.0001	0.0003						
S3	coordinate	0.7518	0.25	0.3808	0.0049						
	error	0.0002		0.0002	0.0004						

Grain 2: C132, Map 23

Atom		**x**	**y**	**z**	**U11**	**U22**	**U33**	**U23**	**U13**	**U12**	**Ueq**
Fe1	coordinate	0.9700	0.25	0.6740	0.0074	0.0032	0.0055	0	0.0004	0	0.0054

Revision #1

	error	0.0002		0.0002	0.0005	0.0008	0.0003		0.0003		0.0002
Fe2	coordinate	0.8529	0.25	0.0661	0.0056	0.0048	0.0047	0	0.0002	0	0.0050
	error	0.0002		0.0001	0.0006	0.0009	0.0004		0.0003		0.0002
S3	coordinate	0.7518	0.25	0.3806	0.0053						
	error	0.0003		0.0002	0.0000						

Grain 3: C132, Map 31

Atom		x	y	z	U11	U22	U33	U23	U13	U12	Ueq
Fe1	coordinate	0.9699	0.25	0.6736	0.0043						
	error	0.0007		0.0002	0.0004						
Fe2	coordinate	0.8529	0.25	0.0666	0.0035						
	error	0.0009		0.0002	0.0005						
S3	coordinate	0.753	0.25	0.3811	0.0036						
	error	0.001		0.0004	0.0005						

Grain 4: C132, Map 32

Atom		x	y	z	U11	U22	U33	U23	U13	U12	Ueq
Fe1	coordinate	0.9705	0.25	0.6719	0.0115						
	error	0.0003		0.0002	0.0008						
Fe2	coordinate	0.8538	0.25	0.0660	0.013						
	error	0.0003		0.0002	0.001						
S3	coordinate	0.7500	0.25	0.3807	0.0125						
	error	0.0005		0.0004	0.0009						

Grain 5: C132, Map 32

Atom		x	y	z	U11	U22	U33	U23	U13	U12	Ueq
Fe1	coordinate	0.968	0.25	0.6733	0.0034						
	error	0.001		0.0004	0.0007						
Fe2	coordinate	0.854	0.25	0.0665	0.0040						
	error	0.001		0.0004	0.0008						
S3	coordinate	0.754	0.25	0.3807	0.0027						
	error	0.002		0.0006	0.0009						

Grain 6: C132, S1

Atom		x	y	z	U11	U22	U33	U23	U13	U12	Ueq
Fe1	coordinate	0.9704	0.25	0.6725	0.0091						
	error	0.0003		0.0002	0.0007						
Fe2	coordinate	0.8539	0.25	0.0662	0.0087						
	error	0.0003		0.0002	0.0007						
S3	coordinate	0.7511	0.25	0.3810	0.0091						
	error	0.0004		0.0005	0.0007						