

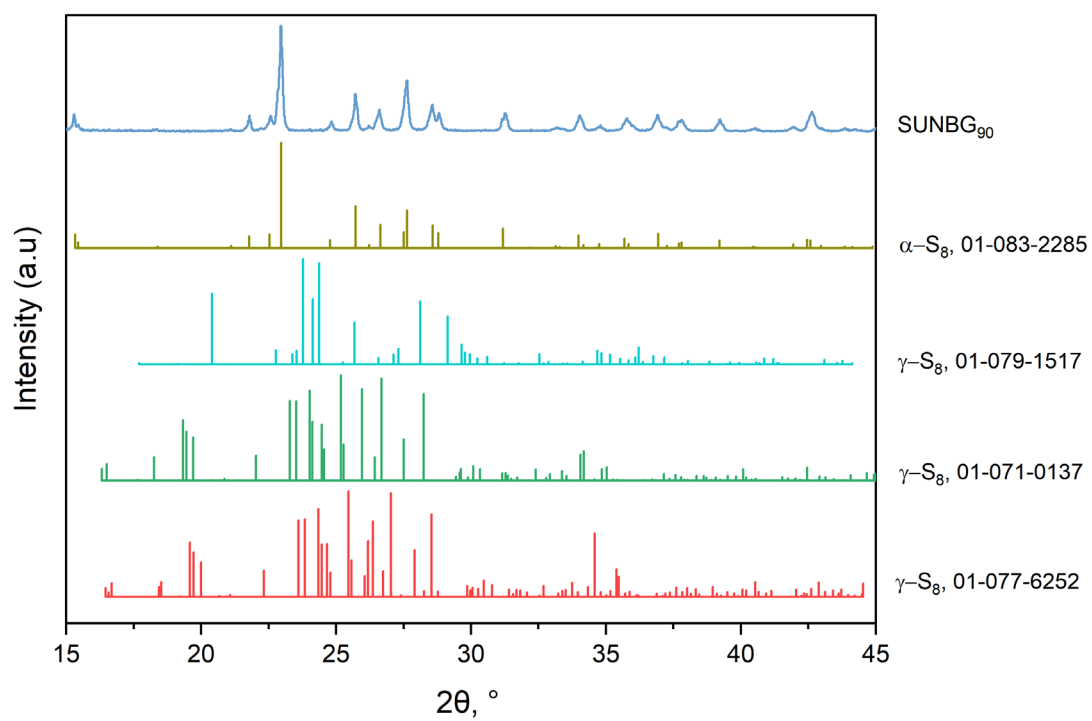
Supplemental Information for:

**Influence of Thermal and Chemical Stresses on Thermal Properties, Crystal Morphology, and Mechanical Strength Development of a Sulfur Polymer Composite**

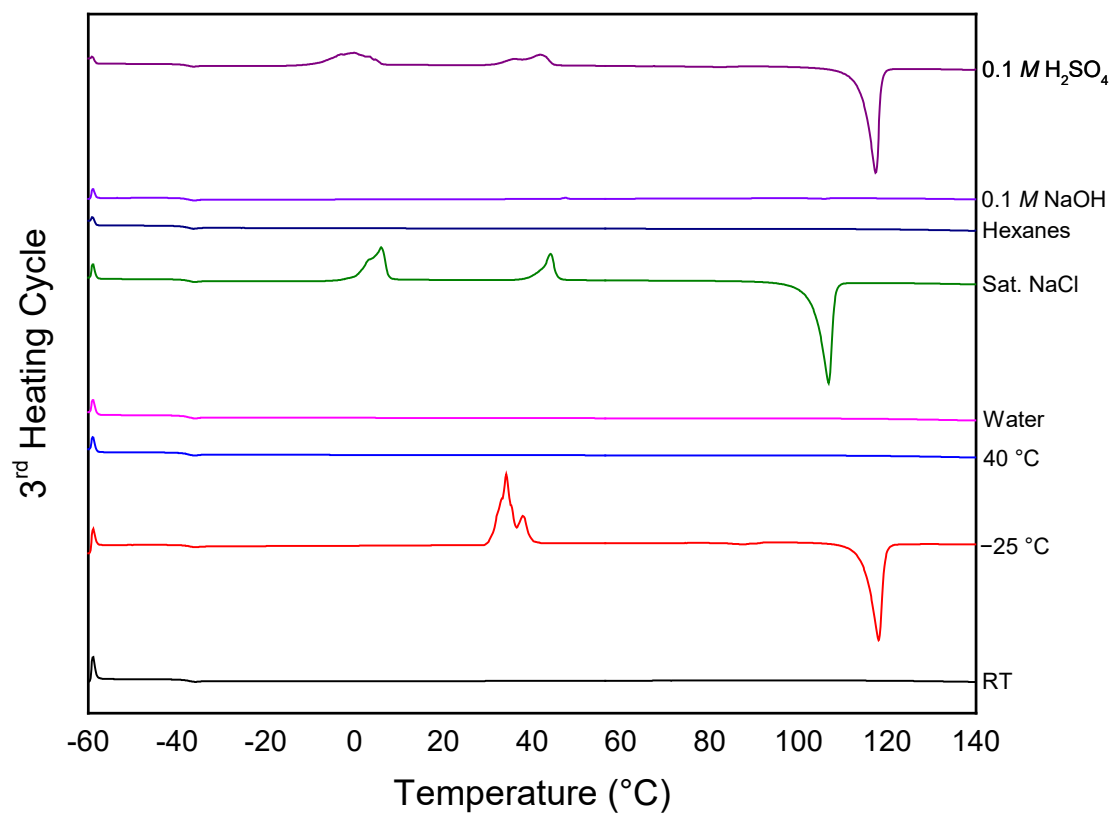
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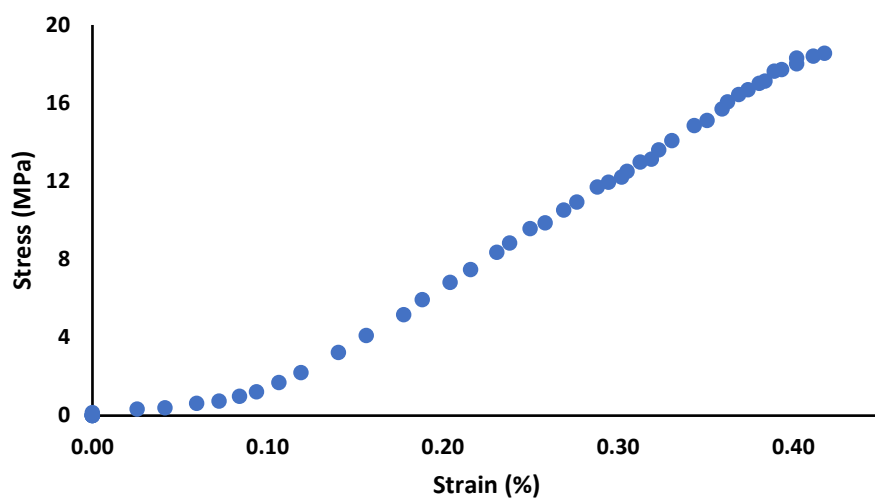
Correspondence to: Rhett C. Smith (E-mail: [rhett@clemson.edu](mailto:rhett@clemson.edu))



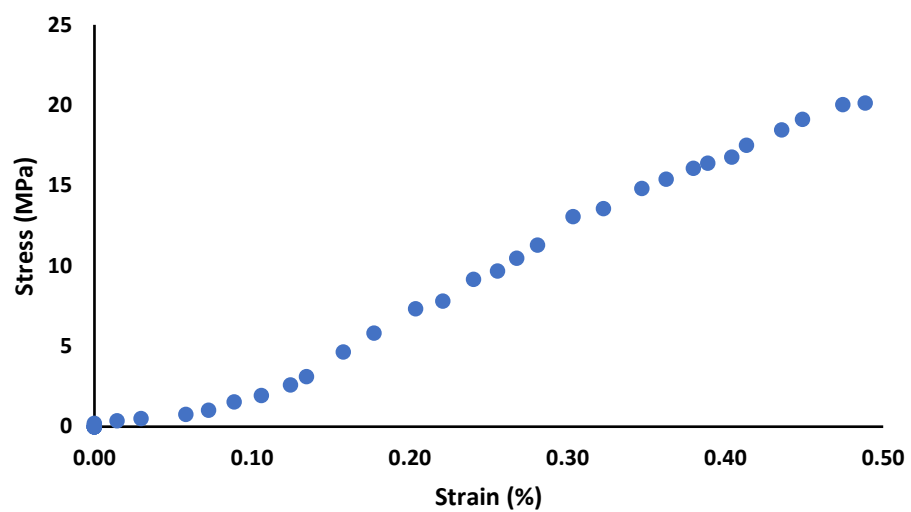
**Figure S1.** Powder-XRD traces for **SunBG<sub>90</sub>** structure, confirming the contribution of  $\gamma$ -sulfur after exposure to hexanes.



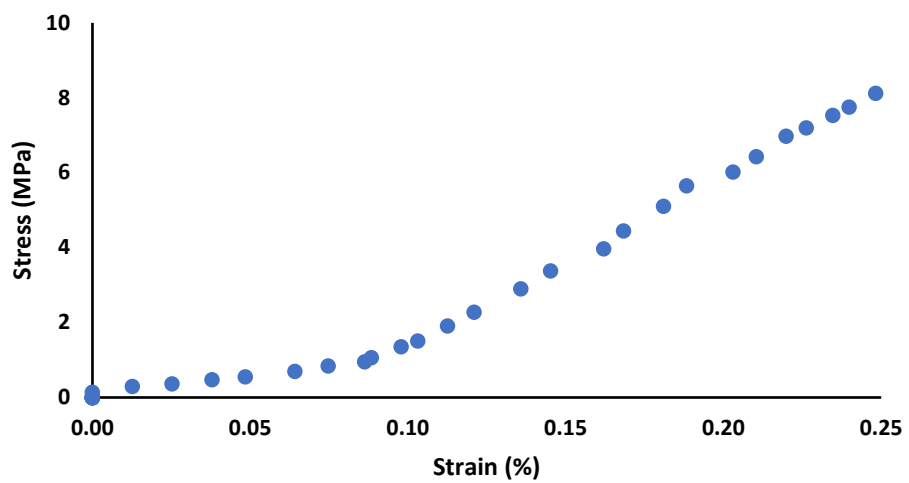
**Figure S2.** Differential scanning calorimetry (DSC) traces for SunBG<sub>90</sub> showing the third heating cycle after exposure to different environmental conditions.



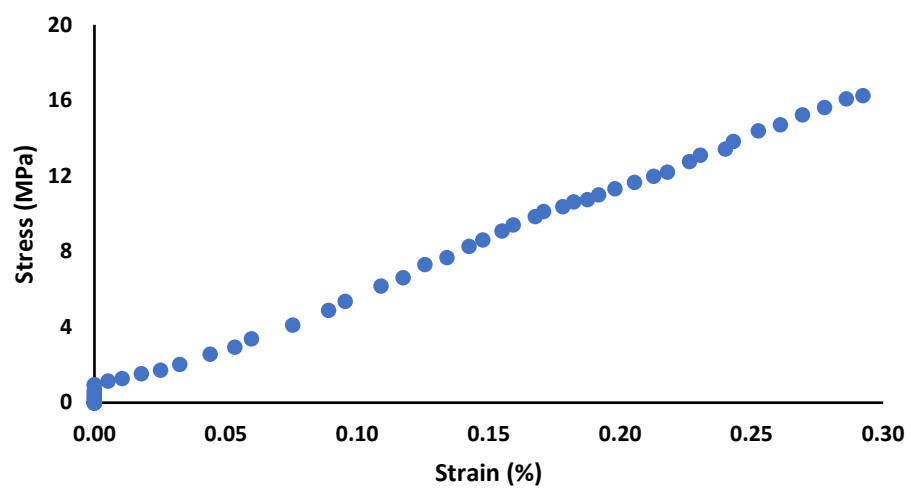
**Figure S3.** Stress-strain plots for measurements of the compressive strength of **SunBG<sub>90</sub>** after 4d at room temperature.



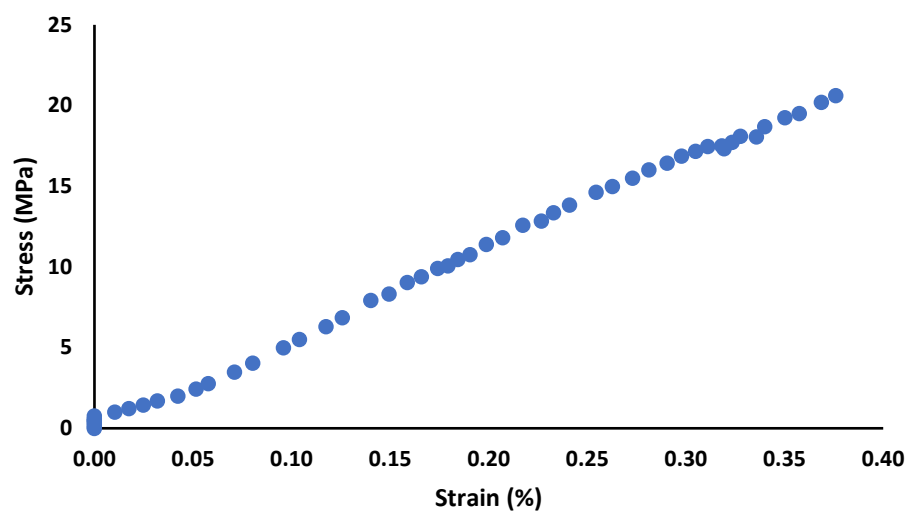
**Figure S4.** Stress-strain plots for measurements of the compressive strength of **SunBG<sub>90</sub>** after 4d exposure at  $-25\text{ }^{\circ}\text{C}$ .



**Figure S5.** Stress-strain plots for measurements of the compressive strength of **SunBG<sub>90</sub>** after 4d exposure at 40 °C.

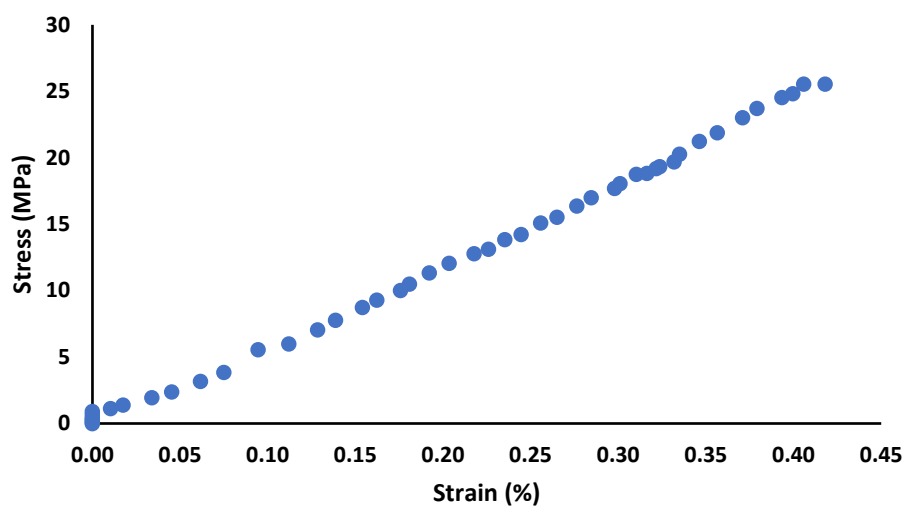


**Figure S6.** Stress-strain plots for measurements of the compressive strength of **SunBG<sub>90</sub>** after 4d exposure to water.

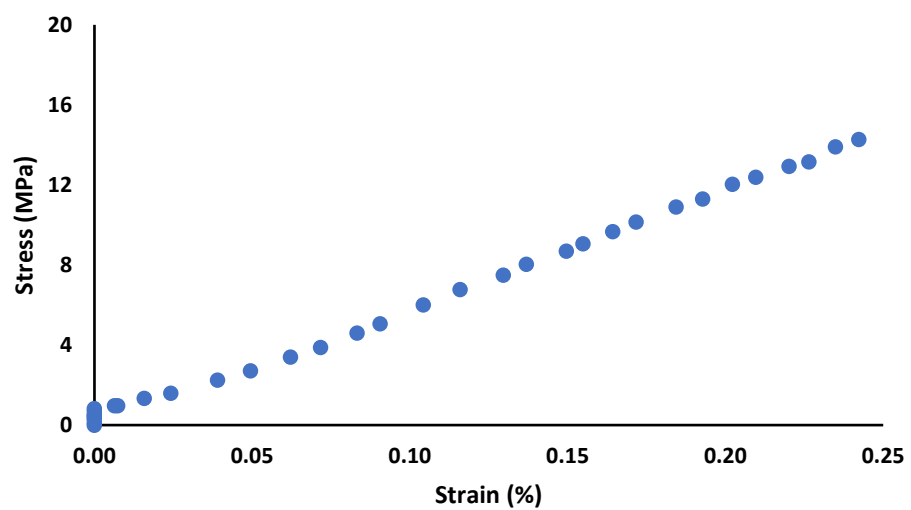


**Figure S7.** Stress-strain plots for measurements of the compressive strength of **SunBG<sub>90</sub>** after 4d exposure to saturated NaCl.

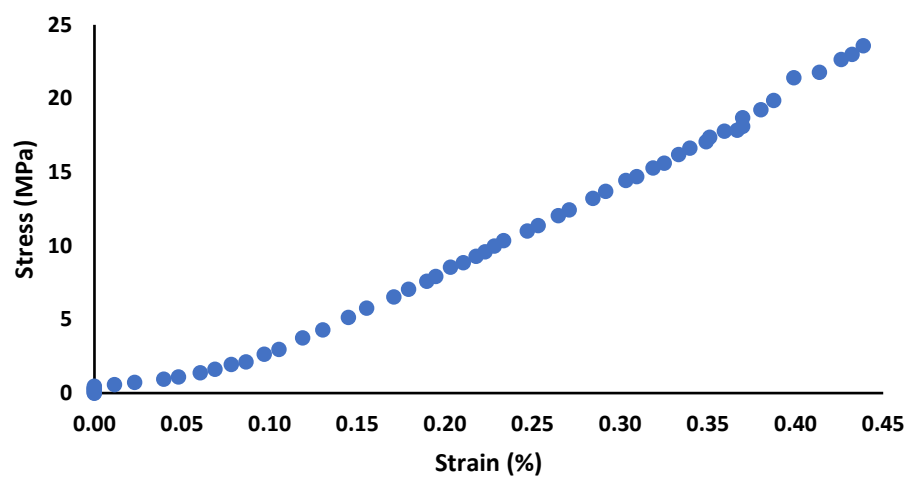




**Figure S8.** Stress-strain plots for measurements of the compressive strength of **SunBG<sub>90</sub>** after 4d exposure to 0.1 M NaOH.



**Figure S9.** Stress-strain plots for measurements of the compressive strength of **SunBG<sub>90</sub>** after 4d exposure to 0.1 M H<sub>2</sub>SO<sub>4</sub>.



**Figure S10.** Stress-strain plots for measurements of the compressive strength of **SunBG<sub>90</sub>** after 4d exposure to hexanes.

**Table S1.** Dimensional analysis and masses of samples before and after exposure to environmental factors. Samples were cylindrical in shape, so that L1 and L2 represent lengths (heights) of the cylinders measured at two positions with calipers, and D1–4 are diameters cross-section measured at four positions using calipers. The height and diameter used for volume calculations are the average of the individual caliper measurements for a given cylinder.

Room temperature							
	dimensions (cm)		Results		Property		Percentage of Initial
	Before	After	Initial Volume	2.45 cm <sup>3</sup>	Volume		99.83
L1	8.94	8.95	Final Volume	2.45 cm <sup>3</sup>	Density		100.17
L2	8.92	8.94	Initial Density	1.75 g/cm <sup>3</sup>			
D1	5.87	5.85	Final Density	1.75 g/cm <sup>3</sup>			
D2	5.89	5.86					
D3	5.94	5.95					
D4	5.94	5.94					
Mass (g)	0.43	0.43					
40 °C							
	dimensions (cm)		Results		Property		Percentage of Initial
	Before	After	Initial Volume	2.52 cm <sup>3</sup>	Volume		99.81
L1	9.36	9.34	Final Volume	2.51 cm <sup>3</sup>	Density		100.19
L2	9.34	9.34	Initial Density	1.79 g/cm <sup>3</sup>			
D1	5.88	5.86	Final Density	1.79 g/cm <sup>3</sup>			
D2	5.87	5.91					
D3	5.84	5.82					
D4	5.83	5.82					
Mass (g)	0.45	0.45					
Cold (–25 °C)							
	dimensions (cm)		Results		Property		Percentage of Initial
	Before	After	Initial Volume	2.61 cm <sup>3</sup>	Volume		99.45
L1	9.48	9.47	Final Volume	2.60 cm <sup>3</sup>	Density		100.55
L2	9.56	9.53	Initial Density	1.75 g/cm <sup>3</sup>			
D1	5.90	5.90	Final Density	1.76 g/cm <sup>3</sup>			
D2	5.89	5.91					
D3	5.92	5.89					
D4	5.92	5.89					
Mass (g)	0.46	0.46					
Sat. NaCl							
	dimensions (cm)		Results		Property		Percentage of Initial
	Before	After	Initial Volume	2.58 cm <sup>3</sup>	Volume		99.83
L1	9.46	9.50	Final Volume	2.58 cm <sup>3</sup>	Density		100.17
L2	9.47	9.43	Initial Density	1.80 g/cm <sup>3</sup>			
D1	5.92	5.90	Final Density	1.80 g/cm <sup>3</sup>			
D2	5.88	5.89					
D3	5.92	5.91					
D4	5.85	5.85					
Mass (g)	0.46	0.46					

(cont'd)

Water								
	dimensions (cm)			Results			Property	Percentage of Initial
	Before	After		Initial Volume	2.50 cm <sup>3</sup>		Volume	99.58
L1	9.51	9.48		Final Volume	2.49 cm <sup>3</sup>		Density	100.19
L2	9.49	9.49		Initial Density	1.73 g/cm <sup>3</sup>			
D1	5.85	5.85		Final Density	1.73 g/cm <sup>3</sup>			
D2	5.86	5.85						
D3	5.71	5.69						
D4	5.74	5.74						
Mass (g)	0.43	0.43						
NaOH								
	dimensions (cm)			Results			Property	Percentage of Initial
	Before	After		Initial Volume	2.57 cm <sup>3</sup>		Volume	99.66
L1	9.54	9.55		Final Volume	2.56 cm <sup>3</sup>		Density	100.57
L2	9.42	9.40		Initial Density	1.76 g/cm <sup>3</sup>			
D1	5.78	5.80		Final Density	1.77 g/cm <sup>3</sup>			
D2	5.80	5.76						
D3	5.79	5.82						
D4	5.80	5.74						
Mass (g)	0.44	0.44						
Sulfuric Acid								
	dimensions (cm)			Results			Property	Percentage of Initial
	Before	After		Initial Volume	2.50 cm <sup>3</sup>		Volume	99.52
L1	L1	9.54	9.55	Final Volume	2.49 cm <sup>3</sup>		Density	99.80
L2	L2	9.42	9.40	Initial Density	1.76 g/cm <sup>3</sup>			
D1	D1	5.78	5.80	Final Density	1.75 g/cm <sup>3</sup>			
D2	D2	5.80	5.76					
D3	D3	5.79	5.82					
D4	D4	5.80	5.74					
Mass (g)	Weight	0.44	0.44					
Hexanes								
	dimensions (cm)			Results			Property	Percentage of Initial
	Before	After		Initial Volume	2.59 cm <sup>3</sup>		Volume	103.05
L1	9.74	9.54		Final Volume	2.67 cm <sup>3</sup>		Density	95.14
L2	9.56	9.75		Initial Density	1.77 g/cm <sup>3</sup>			
D1	5.93	5.91		Final Density	1.69 g/cm <sup>3</sup>			
D2	5.83	5.91						
D3	5.77	5.89						
D4	5.85	6.03						
Mass (g)	0.46	0.45						

### **Supporting Information File S1:**

Modelling of  $\gamma$ -sulfur contribution to microstructure after exposure to hexanes at room temperature

## SUN-BG-90-WPPF report (SUN-BG-90)

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### General information

Analysis date	2023-08-04 12:14:46	Measurement start...	2023-08-04 09:46:33
Analyst	Administrator	Operator	Administrator
Sample name		Comment	
Measured data na...	C:\XRD Data\Kolis\Bhakti\SUN-BG-90.rasx	Memo	

### WPPF analysis results

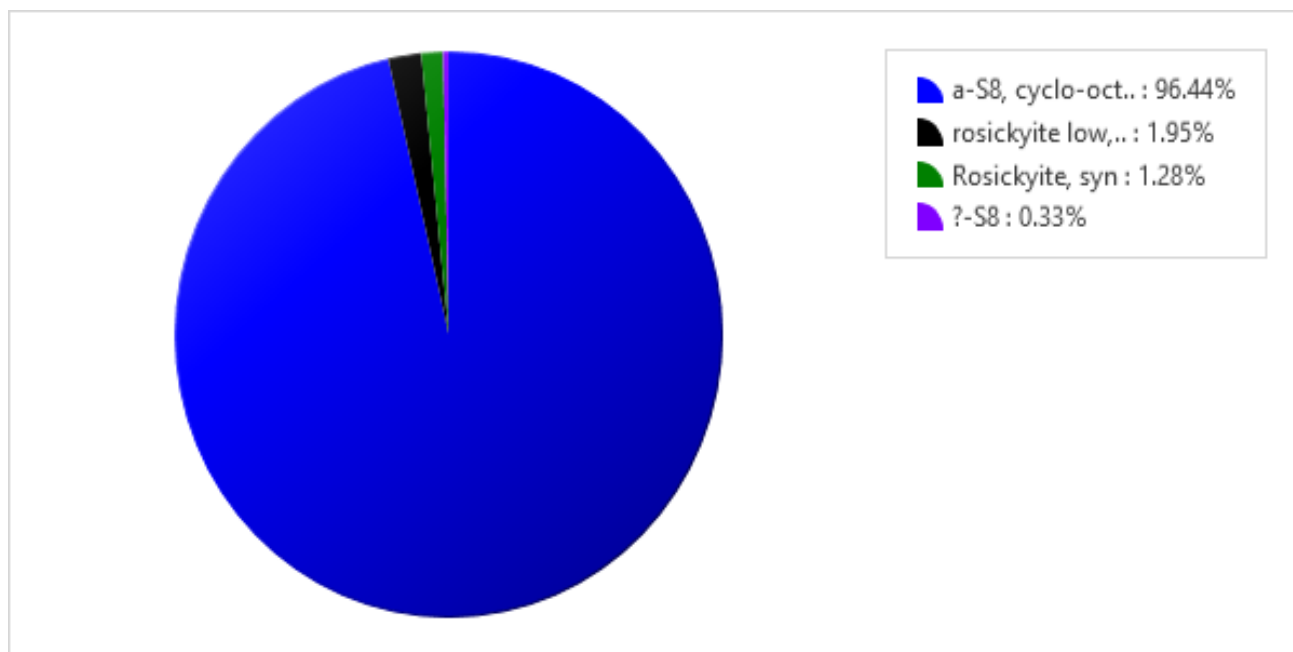
Phase / Dataset		SUN-BG-90
	Rwp, %	0.00
	Rp, %	0.00
	S	0.0000
	$\chi^2$	0.0000
▲	a-S8, cyclo-octasulfur, sulfur, syn	
	Weight fraction, wt%	96.44
	a, Å	10.48787
	b, Å	12.96149
	c, Å	24.54893
	$\alpha$ , °	90.000
	$\beta$ , °	90.000
	$\gamma$ , °	90.000
	Lattice volume, Å <sup>3</sup>	3337.143
	Size, Å	0.0
	Strain, %	0.02(6)
▲	rosickyite low, cyclo-octasulfur	
	Weight fraction, wt%	1.95
	a, Å	10.56488
	b, Å	10.58617
	c, Å	10.71125
	$\alpha$ , °	90.000
	$\beta$ , °	95.637
	$\gamma$ , °	90.000
	Lattice volume, Å <sup>3</sup>	1192.170
	Size, Å	0.0
	Strain, %	0.083(9)
▲	Rosickyite, syn	
	Weight fraction, wt%	1.28
	a, Å	8.31168
	b, Å	12.83076
	c, Å	9.10992
	$\alpha$ , °	90.000
	$\beta$ , °	124.890
	$\gamma$ , °	90.000
	Lattice volume, Å <sup>3</sup>	796.898
	Size, Å	0.0



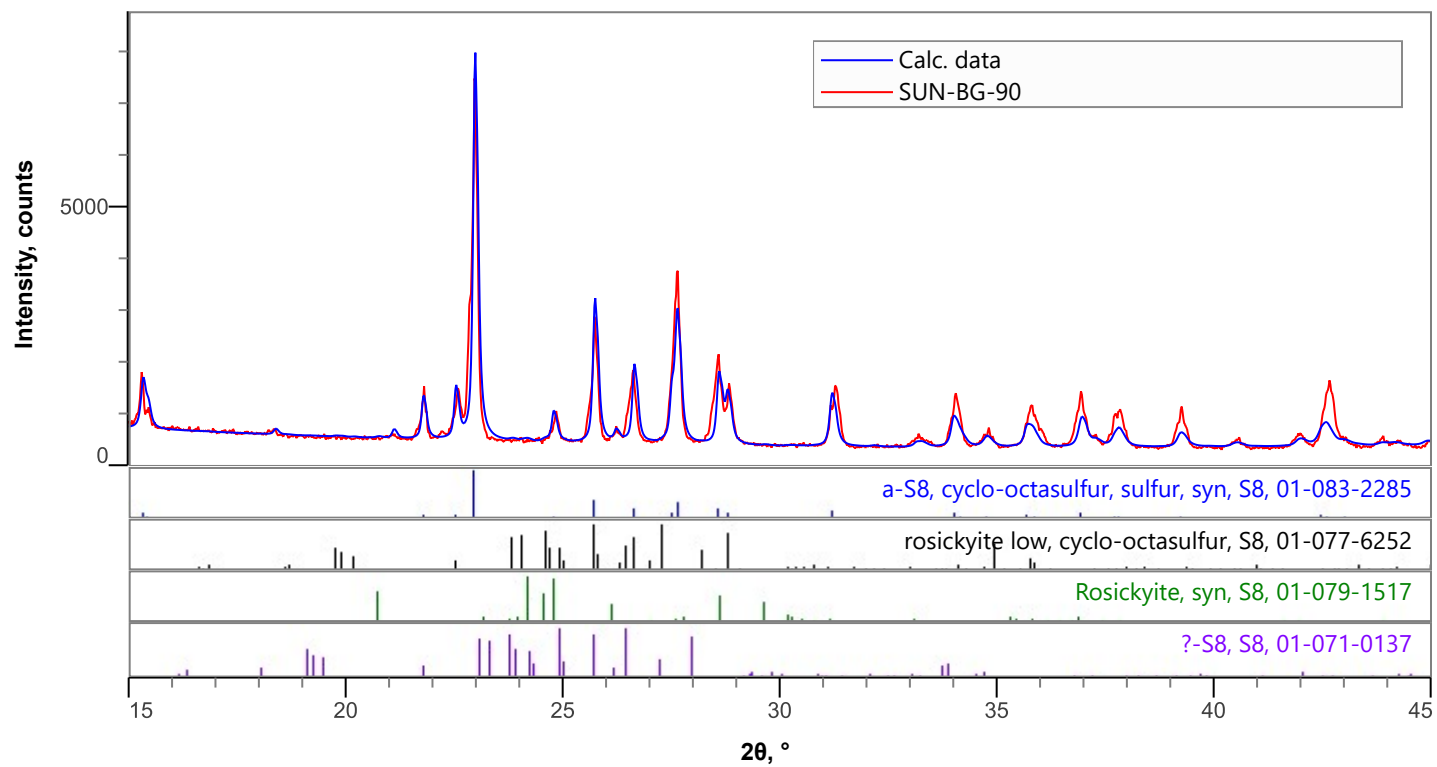
## WPPF analysis results

Phase / Dataset		SUN-BG-90
▲	Rosickyite, syn	
	Strain, %	0.083(9)
▲	?-S8	
	Weight fraction, wt%	0.33
	a, Å	11.02951
	b, Å	10.95784
	c, Å	10.89223
	$\alpha$ , °	90.000
	$\beta$ , °	95.920
	$\gamma$ , °	90.000
	Lattice volume, Å <sup>3</sup>	1309.410
	Size, Å	0.0
	Strain, %	0.10(3)

## WPPF weight fraction



### WPPF Profile View



### Lattice parameters

Phase name	a, Å	b, Å	c, Å	$\alpha$ , °	$\beta$ , °	$\gamma$ , °
a-S8, cyclo-octa...	10.48787	12.96149	24.54893	90.000	90.000	90.000
rosickyite low, c...	10.56488	10.58617	10.71125	90.000	95.637	90.000
Rosickyite, syn	8.31168	12.83076	9.10992	90.000	124.890	90.000
?-S8	11.02951	10.95784	10.89223	90.000	95.920	90.000

### d-I List

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**a-S8, cyclo-octasulfur, sulfur, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
1	15.32871	5.77565	1 1 3	13.00
2	15.44892	5.73098	0 2 2	5.40
3	18.38323	4.82229	2 0 2	1.50
4	21.10557	4.20602	1 1 5	2.30
5	21.78393	4.07655	2 2 0	11.10
6	22.53161	3.94294	1 3 1	12.90
7	22.96941	3.86877	2 2 2	100.00
8	24.78121	3.58987	1 3 3	7.70
9	25.72928	3.45970	0 2 6	39.60
10	26.22270	3.39571	2 2 4	3.20
11	26.63657	3.34388	3 1 1	22.20
12	27.50384	3.24037	0 4 0	15.00
13	27.63069	3.22578	2 0 6	35.80
14	27.66731	3.22160	1 1 7	0.00
15	28.58419	3.12031	3 1 3	21.70
16	28.78789	3.09869	1 3 5	14.30
17	29.07624	3.06862	0 0 8	0.00
18	30.94066	2.88782	2 2 6	0.00
19	31.18793	2.86549	0 4 4	18.80
20	32.15532	2.78146	3 1 5	0.40
21	33.13780	2.70120	3 3 1	1.80
22	33.28530	2.68957	2 4 2	1.30
23	33.98862	2.63550	1 3 7	12.20
24	34.16948	2.62197	4 0 0	3.00
25	34.64948	2.58674	1 1 9	0.70
26	34.75422	2.57918	3 3 3	4.00
27	35.67694	2.51456	2 4 4	9.10
28	35.84069	2.50345	1 5 1	4.20
29	36.62437	2.45166	2 2 8	0.00
30	36.93205	2.43193	3 1 7	13.70
31	37.26217	2.41114	4 0 4	2.50
32	37.35467	2.40539	1 5 3	0.00
33	37.69768	2.38428	4 2 2	4.60
34	37.80529	2.37774	3 3 5	5.60
35	39.21046	2.29571	0 2 10	7.40
36	39.38180	2.28611	2 4 6	0.10
37	39.85950	2.25981	4 2 4	0.20
38	39.99187	2.25264	1 3 9	0.00
39	40.23617	2.23952	1 5 5	0.00

**a-S8, cyclo-octasulfur, sulfur, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
40	40.45165	2.22809	0 4 8	1.50
41	40.54205	2.22333	2 0 10	0.90
42	41.93707	2.15254	1 1 11	3.60
43	42.02621	2.14818	3 3 7	0.60
44	42.45327	2.12755	0 6 2	8.20
45	42.57981	2.12152	3 1 9	7.30
46	42.97308	2.10301	2 2 10	2.30
47	43.26135	2.08966	4 2 6	0.30
48	43.58619	2.07484	3 5 1	0.00
49	43.84237	2.06331	5 1 1	1.60
50	44.12696	2.05066	2 4 8	1.40
51	44.23856	2.04574	0 0 12	0.00
52	44.26424	2.04462	1 5 7	0.30
53	44.40924	2.03828	4 4 0	0.00
54	44.88011	2.01798	3 5 3	2.80

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
1	16.61994	5.32973	0 0 2	8.60
2	16.73581	5.29309	0 2 0	4.30
3	16.85186	5.25689	2 0 0	13.10
4	17.89003	4.95411	1 0 -2	0.10
5	18.05236	4.90992	2 0 -1	0.10
6	18.62417	4.76044	0 1 2	9.50
7	18.70210	4.74078	0 2 1	14.10
8	18.75410	4.72775	1 2 0	0.00
9	18.83217	4.70833	2 1 0	0.00
10	19.38198	4.57599	1 0 2	0.80
11	19.53235	4.54110	2 0 1	0.00
12	19.76990	4.48707	1 1 -2	51.50
13	19.91746	4.45416	2 1 -1	42.40
14	20.19169	4.39428	1 2 -1	32.60
15	20.87136	4.25269	1 2 1	1.00
16	21.13432	4.20037	1 1 2	0.80
17	21.27280	4.17333	2 1 1	2.00
18	22.54160	3.94122	2 0 -2	25.00
19	23.67101	3.75566	0 2 2	0.00
20	23.83681	3.72992	2 2 0	72.60
21	24.07502	3.69355	2 1 -2	73.70

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
22	24.59250	3.61699	1 2 -2	83.40
23	24.71258	3.59968	2 2 -1	49.90
24	24.91146	3.57139	2 0 2	50.00
25	25.04142	3.55315	0 0 3	23.30
26	25.39411	3.50460	3 0 0	0.00
27	25.64313	3.47112	1 0 -3	0.00
28	25.71416	3.46170	1 2 2	100.00
29	25.82936	3.44652	2 2 1	34.90
30	25.95006	3.43076	3 0 -1	0.00
31	26.31499	3.38401	2 1 2	19.90
32	26.43851	3.36848	0 1 3	52.90
33	26.58750	3.34994	0 3 1	0.00
34	26.62478	3.34533	1 3 0	71.50
35	26.77403	3.32702	3 1 0	0.00
36	27.01121	3.29834	1 1 -3	24.60
37	27.24892	3.27011	1 0 3	0.00
38	27.30384	3.26365	3 1 -1	98.20
39	27.53922	3.23629	3 0 1	0.00
40	27.67498	3.22072	1 3 -1	1.90
41	28.18391	3.16371	1 3 1	44.60
42	28.20719	3.16115	2 2 -2	0.00
43	28.54568	3.12443	1 1 3	5.70
44	28.82395	3.09490	3 1 1	78.30
45	28.89096	3.08787	2 0 -3	0.00
46	29.06328	3.06996	3 0 -2	5.40
47	30.12284	2.96434	2 1 -3	0.00
48	30.16265	2.96052	2 2 2	10.60
49	30.27169	2.95010	0 2 3	6.30
50	30.28877	2.94848	3 1 -2	0.00
51	30.35405	2.94228	0 3 2	8.90
52	30.48594	2.92985	2 3 0	0.00
53	30.56846	2.92213	3 2 0	8.00
54	30.77875	2.90265	1 2 -3	15.50
55	31.03878	2.87892	3 2 -1	0.00
56	31.09146	2.87416	1 3 -2	11.50
57	31.18832	2.86546	2 3 -1	0.00
58	31.72538	2.81816	2 0 3	7.20
59	31.88378	2.80452	3 0 2	2.70
60	32.00269	2.79437	1 3 2	6.60

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
61	32.09708	2.78637	2 3 1	0.00
62	32.14886	2.78200	1 2 3	6.30
63	32.39900	2.76109	3 2 1	4.40
64	32.86105	2.72332	2 1 3	1.30
65	33.01458	2.71100	3 1 2	10.70
66	33.57284	2.66719	2 2 -3	3.50
67	33.60298	2.66486	0 0 4	0.00
68	33.72350	2.65561	3 2 -2	5.90
69	33.84257	2.64654	0 4 0	6.60
70	33.85217	2.64581	1 0 -4	0.00
71	34.07575	2.62896	2 3 -2	0.00
72	34.08265	2.62845	4 0 0	13.60
73	34.09561	2.62748	3 0 -3	0.00
74	34.29915	2.61235	4 0 -1	4.60
75	34.68399	2.58424	0 1 4	9.60
76	34.90252	2.56856	0 4 1	0.00
77	34.92638	2.56686	1 1 -4	0.00
78	34.93169	2.56648	1 4 0	60.00
79	35.15069	2.55099	4 1 0	4.60
80	35.16330	2.55010	3 1 -3	0.00
81	35.36145	2.53627	4 1 -1	1.60
82	35.52757	2.52479	1 0 4	5.60
83	35.74196	2.51013	2 3 2	26.30
84	35.76007	2.50890	1 4 -1	0.00
85	35.83580	2.50378	0 3 3	19.10
86	35.95631	2.49566	4 0 1	0.00
87	36.07752	2.48755	2 2 3	3.70
88	36.09167	2.48661	3 3 0	0.00
89	36.16598	2.48167	1 4 1	0.00
90	36.21904	2.47816	3 2 2	0.00
91	36.23575	2.47705	2 0 -4	5.10
92	36.27339	2.47457	1 3 -3	0.00
93	36.49855	2.45982	3 3 -1	1.70
94	36.55874	2.45591	1 1 4	1.60
95	36.57334	2.45496	4 0 -2	0.00
96	36.97713	2.42907	4 1 1	0.00
97	37.24997	2.41191	2 1 -4	3.30
98	37.46530	2.39854	1 3 3	1.10
99	37.57973	2.39150	4 1 -2	3.60

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
100	37.68434	2.38510	3 3 1	0.00
101	37.75281	2.38093	3 0 3	4.10
102	37.76445	2.38022	0 2 4	0.00
103	37.92705	2.37039	0 4 2	0.00
104	37.98980	2.36662	1 2 -4	8.80
105	38.03557	2.36388	2 4 0	0.00
106	38.19853	2.35417	4 2 0	0.00
107	38.21028	2.35347	3 2 -3	4.70
108	38.39484	2.34258	4 2 -1	8.60
109	38.53582	2.33433	1 4 -2	3.20
110	38.61615	2.32966	2 4 -1	0.00
111	38.71773	2.32378	2 3 -3	7.30
112	38.73299	2.32290	3 1 3	0.00
113	38.85100	2.31612	3 3 -2	2.50
114	39.29477	2.29098	1 4 2	0.00
115	39.34809	2.28800	2 0 4	9.60
116	39.37380	2.28656	2 4 1	0.00
117	39.51314	2.27882	1 2 4	3.30
118	39.66304	2.27055	4 0 2	1.40
119	39.90513	2.25733	4 2 1	4.60
120	40.16108	2.24353	2 2 -4	3.40
121	40.29551	2.23636	2 1 4	0.90
122	40.42687	2.22939	3 0 -4	0.00
123	40.47074	2.22708	4 2 -2	7.00
124	40.60433	2.22006	4 1 2	6.50
125	40.60676	2.21993	4 0 -3	0.00
126	40.95065	2.20208	2 3 3	14.10
127	41.04690	2.19714	2 4 -2	0.00
128	41.07786	2.19555	3 3 2	5.10
129	41.35372	2.18154	3 1 -4	3.50
130	41.53030	2.17267	4 1 -3	0.00
131	41.55647	2.17137	3 2 3	6.00
132	42.36268	2.13189	0 0 5	0.00
133	42.39112	2.13053	1 0 -5	0.00
134	42.47360	2.12658	0 3 4	0.00
135	42.47851	2.12634	2 4 2	7.00
136	42.55971	2.12248	0 4 3	0.00
137	42.67810	2.11686	1 3 -4	1.30
138	42.78141	2.11199	3 4 0	3.40



**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
139	42.86773	2.10794	4 3 0	0.00
140	42.87841	2.10744	3 3 -3	2.70
141	42.93912	2.10460	1 4 -3	0.00
142	42.97851	2.10276	5 0 0	0.00
143	42.98214	2.10259	5 0 -1	0.00
144	43.03382	2.10018	2 2 4	0.00
145	43.04626	2.09961	4 3 -1	8.00
146	43.13484	2.09550	3 4 -1	0.00
147	43.25551	2.08993	0 1 5	0.00
148	43.28348	2.08865	1 1 -5	0.00
149	43.32660	2.08667	4 2 2	13.70
150	43.54589	2.07667	0 5 1	0.00
151	43.57012	2.07557	1 5 0	5.10
152	43.86123	2.06246	5 1 0	6.40
153	43.86480	2.06230	5 1 -1	0.00
154	43.97881	2.05722	1 4 3	0.00
155	44.03816	2.05459	3 2 -4	0.00
156	44.06658	2.05333	1 3 4	3.40
157	44.13033	2.05051	1 0 5	0.00
158	44.17083	2.04872	3 4 1	7.10
159	44.20603	2.04717	4 2 -3	0.00
160	44.21287	2.04687	2 0 -5	0.00
161	44.26105	2.04476	1 5 -1	0.00
162	44.42551	2.03757	4 3 1	2.10
163	44.60155	2.02993	1 5 1	0.00
164	44.65845	2.02748	3 0 4	1.50
165	44.66021	2.02740	2 3 -4	0.00
166	44.70288	2.02557	5 0 1	0.00
167	44.71343	2.02511	5 0 -2	0.00
168	44.82448	2.02035	4 0 3	0.00
169	44.94454	2.01524	4 3 -2	2.90
170	44.99500	2.01309	1 1 5	12.90

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
1	18.00483	4.92278	1 2 -1	1.20
2	18.21081	4.86756	0 2 1	0.20
3	18.97952	4.67211	1 2 0	0.30
4	19.48075	4.55301	1 0 -2	0.50

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
5	20.68360	4.29087	1 1 -2	0.00
6	20.75181	4.27692	0 3 0	67.10
7	22.67439	3.91843	2 1 -1	0.30
8	23.15318	3.83848	2 0 -2	0.00
9	23.16754	3.83613	1 1 1	13.50
10	23.79594	3.73623	1 3 -1	9.90
11	23.79605	3.73621	0 0 2	0.00
12	23.94721	3.71297	1 2 -2	13.00
13	23.95411	3.71192	0 3 1	0.00
14	24.18204	3.67744	2 1 -2	100.00
15	24.55088	3.62302	1 3 0	61.90
16	24.79978	3.58722	0 1 2	95.80
17	25.69893	3.46372	2 2 -1	2.00
18	26.11992	3.40884	2 0 0	0.00
19	26.13833	3.40648	1 2 1	39.80
20	27.04293	3.29455	2 1 0	6.20
21	27.04833	3.29390	2 2 -2	0.00
22	27.60616	3.22859	0 2 2	9.40
23	27.78968	3.20769	0 4 0	14.70
24	28.61260	3.11728	1 3 -2	59.50
25	29.65263	3.01027	2 2 0	45.50
26	30.11239	2.96534	2 3 -1	0.00
27	30.17101	2.95972	1 4 -1	18.70
28	30.29815	2.94759	0 4 1	11.30
29	30.49304	2.92919	1 3 1	9.80
30	30.76412	2.90399	2 1 -3	6.10
31	30.78056	2.90248	1 4 0	0.00
32	31.13756	2.87001	1 1 -3	7.40
33	31.28652	2.85669	2 3 -2	0.00
34	31.77620	2.81377	0 3 2	1.30
35	32.31760	2.76786	3 0 -2	1.40
36	33.08211	2.70562	3 1 -2	0.00
37	33.10668	2.70367	2 2 -3	9.80
38	33.26332	2.69129	1 0 2	1.00
39	33.45667	2.67618	1 2 -3	2.30
40	33.59199	2.66571	2 3 0	0.00
41	34.00894	2.63398	1 1 2	0.80
42	34.16553	2.62226	1 4 -2	0.90
43	34.74442	2.57988	3 1 -1	2.80

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
44	34.93632	2.56615	0 5 0	0.00
45	35.28748	2.54142	3 2 -2	0.00
46	35.30218	2.54039	2 1 1	13.00
47	35.45376	2.52988	2 4 -1	10.80
48	35.75041	2.50956	3 1 -3	0.00
49	35.78355	2.50731	1 4 1	9.50
50	36.16461	2.48176	1 2 2	5.70
51	36.47446	2.46139	2 4 -2	4.20
52	36.71560	2.44577	2 3 -3	0.00
53	36.72513	2.44516	0 1 3	6.70
54	36.86254	2.43636	3 2 -1	16.30
55	36.90300	2.43378	1 5 -1	0.00
56	36.90307	2.43378	0 4 2	0.00
57	37.00948	2.42702	0 5 1	2.50
58	37.03566	2.42537	1 3 -3	0.00
59	37.39286	2.40302	2 2 1	0.00
60	37.41480	2.40166	1 5 0	8.10
61	37.81968	2.37687	3 2 -3	6.60
62	38.50631	2.33605	2 4 0	1.30
63	38.71912	2.32370	3 3 -2	3.30
64	38.74967	2.32194	0 2 3	0.00
65	39.53078	2.27784	1 3 2	2.80
66	39.55493	2.27651	2 0 -4	0.00
67	39.62655	2.27256	3 0 0	0.00
68	40.17879	2.24259	3 3 -1	0.60
69	40.19912	2.24150	2 1 -4	0.00
70	40.26978	2.23773	3 1 0	0.00
71	40.31114	2.23553	1 5 -2	2.10
72	40.67243	2.21650	2 3 1	1.50
73	41.07046	2.19593	3 3 -3	0.40
74	41.30958	2.18377	2 4 -3	2.20
75	41.41374	2.17852	3 0 -4	1.30
76	41.43492	2.17746	2 5 -1	0.00
77	41.59969	2.16921	1 4 -3	5.90
78	41.72431	2.16302	1 5 1	0.00
79	41.93993	2.15240	0 3 3	5.10
80	42.03430	2.14778	3 1 -4	0.00
81	42.08249	2.14543	2 2 -4	1.20
82	42.15055	2.14213	3 2 0	1.40

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
83	42.18217	2.14059	1 0 -4	0.00
84	42.22630	2.13846	0 6 0	0.00
85	42.33277	2.13333	2 5 -2	0.30
86	42.71166	2.11528	0 5 2	0.10
87	42.79365	2.11141	1 1 -4	0.00
88	43.13350	2.09556	3 4 -2	0.00
89	43.85308	2.06283	3 2 -4	0.00
90	43.87747	2.06174	1 4 2	4.60
91	43.91575	2.06003	1 6 -1	0.00
92	43.97230	2.05751	4 0 -2	0.00
93	44.00798	2.05593	0 6 1	0.00
94	44.13808	2.05017	2 5 0	0.30
95	44.35968	2.04044	1 6 0	1.80
96	44.47340	2.03549	3 4 -1	0.00
97	44.53710	2.03272	4 1 -3	0.00
98	44.56399	2.03156	4 1 -2	3.30
99	44.58745	2.03054	1 2 -4	0.00
100	44.92847	2.01592	2 4 1	1.40

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
1	16.14523	5.48535	2 0 0	0.00
2	16.16429	5.47892	0 2 0	11.20
3	16.35012	5.41707	0 0 2	15.80
4	17.48064	5.06920	1 0 -2	0.90
5	18.07028	4.90509	2 1 0	0.00
6	18.08310	4.90164	1 2 0	22.20
7	18.12921	4.88928	0 2 1	0.00
8	18.25418	4.85609	0 1 2	0.00
9	18.98913	4.66976	1 0 2	0.00
10	19.14603	4.63185	2 1 -1	57.10
11	19.27669	4.60075	1 1 -2	46.50
12	19.51454	4.54520	1 2 -1	41.00
13	20.20919	4.39051	1 2 1	0.80
14	20.53673	4.32122	2 1 1	0.60
15	20.65893	4.29594	1 1 2	2.20
16	21.81978	4.06994	2 0 -2	23.70
17	22.92327	3.87645	2 2 0	0.00
18	23.07000	3.85213	0 2 2	75.90

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
19	23.29594	3.81528	2 1 -2	75.30
20	23.78912	3.73728	2 2 -1	85.20
21	23.89548	3.72089	1 2 -2	55.90
22	24.23338	3.66977	2 0 2	53.20
23	24.31997	3.65690	3 0 0	29.90
24	24.93345	3.56829	2 2 1	100.00
25	25.03524	3.55401	1 2 2	34.30
26	25.57805	3.47981	2 1 2	0.00
27	25.66038	3.46883	3 1 0	0.00
28	25.68487	3.46558	1 3 0	0.00
29	25.71791	3.46120	0 3 1	86.70
30	25.95664	3.42991	0 1 3	0.00
31	26.17575	3.40169	3 1 -1	22.20
32	26.43446	3.36898	1 1 -3	96.70
33	26.72937	3.33248	1 3 -1	0.00
34	27.24941	3.27005	1 3 1	39.00
35	27.27404	3.26715	2 2 -2	0.00
36	27.73767	3.21359	3 1 1	0.00
37	27.97204	3.18719	3 0 -2	82.20
38	27.98300	3.18597	1 1 3	0.00
39	29.15636	3.06037	3 1 -2	3.90
40	29.26729	3.04902	2 2 2	0.00
41	29.30310	3.04537	2 1 -3	8.10
42	29.34003	3.04162	3 2 0	11.30
43	29.35355	3.04025	2 3 0	0.00
44	29.47028	3.02848	0 3 2	0.00
45	29.60219	3.01528	0 2 3	3.30
46	29.79651	2.99606	3 2 -1	13.80
47	30.02642	2.97364	1 2 -3	0.00
48	30.04637	2.97171	2 3 -1	11.10
49	30.13213	2.96345	1 3 -2	0.00
50	30.85568	2.89558	3 0 2	7.00
51	30.97608	2.88460	2 3 1	7.40
52	31.05951	2.87704	1 3 2	5.10
53	31.19180	2.86514	3 2 1	2.20
54	31.41247	2.84552	1 2 3	3.20
55	31.94258	2.79949	3 1 2	0.00
56	32.07776	2.78800	2 1 3	10.70
57	32.47306	2.75496	3 2 -2	2.70

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
58	32.60628	2.74401	2 2 -3	6.30
59	32.62261	2.74267	4 0 0	0.00
60	32.66194	2.73946	0 4 0	0.00
61	32.92222	2.71839	2 3 -2	0.00
62	33.04551	2.70853	0 0 4	9.10
63	33.21552	2.69506	1 0 -4	4.50
64	33.65842	2.66060	4 1 0	0.00
65	33.69429	2.65785	1 4 0	0.00
66	33.72011	2.65587	0 4 1	24.70
67	33.85145	2.64587	4 1 -1	28.00
68	34.01190	2.63375	3 1 -3	0.00
69	34.06992	2.62940	0 1 4	0.00
70	34.23544	2.61707	1 1 -4	1.30
71	34.51693	2.59637	1 4 -1	11.10
72	34.62055	2.58883	2 3 2	0.00
73	34.68315	2.58430	3 3 0	12.80
74	34.90124	2.56865	1 0 4	0.00
75	34.90917	2.56809	0 3 3	1.50
76	34.93125	2.56651	1 4 1	0.00
77	35.02225	2.56005	3 2 2	0.00
78	35.07706	2.55618	3 3 -1	1.10
79	35.08746	2.55544	4 0 -2	0.00
80	35.14691	2.55126	2 2 3	0.00
81	35.27606	2.54221	1 3 -3	0.50
82	35.38553	2.53460	2 0 -4	0.40
83	35.51059	2.52596	4 1 1	0.30
84	35.87902	2.50086	1 1 4	0.00
85	36.06084	2.48867	4 1 -2	0.50
86	36.29087	2.47342	3 3 1	0.00
87	36.35197	2.46940	2 1 -4	1.20
88	36.48413	2.46076	1 3 3	0.50
89	36.61061	2.45255	4 2 0	0.00
90	36.63728	2.45082	2 4 0	0.00
91	36.73323	2.44464	0 4 2	0.00
92	36.79007	2.44099	4 2 -1	6.50
93	36.93937	2.43147	3 2 -3	0.00
94	36.99338	2.42804	0 2 4	2.10
95	37.14753	2.41832	1 2 -4	0.00
96	37.20868	2.41449	2 4 -1	5.60

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
97	37.27972	2.41005	1 4 -2	0.00
98	37.41759	2.40149	3 3 -2	3.60
99	37.53536	2.39422	2 3 -3	0.90
100	37.64132	2.38772	3 1 3	0.90
101	37.98237	2.36706	2 4 1	4.40
102	38.05218	2.36288	1 4 2	0.00
103	38.24947	2.35115	4 0 2	4.40
104	38.33860	2.34589	4 2 1	3.00
105	38.52640	2.33488	2 0 4	1.10
106	38.68383	2.32574	1 2 4	3.00
107	38.85438	2.31592	4 2 -2	1.10
108	39.12770	2.30037	2 2 -4	4.50
109	39.15510	2.29883	4 1 2	0.00
110	39.26634	2.29257	3 0 -4	0.00
111	39.42667	2.28362	2 1 4	4.30
112	39.62572	2.27260	2 4 -2	0.00
113	39.68978	2.26908	3 3 2	10.80
114	39.80185	2.26295	2 3 3	3.10
115	39.99684	2.25237	4 1 -3	1.40
116	40.15266	2.24398	3 1 -4	2.00
117	40.34148	2.23392	3 2 3	0.30
118	41.08368	2.19526	2 4 2	0.00
119	41.10557	2.19414	5 0 0	0.00
120	41.12371	2.19321	4 3 0	3.60
121	41.13782	2.19249	3 4 0	0.00
122	41.28653	2.18494	4 3 -1	0.00
123	41.33350	2.18256	0 4 3	2.30
124	41.42209	2.17810	3 3 -3	0.00
125	41.47115	2.17564	0 3 4	0.00
126	41.47906	2.17524	3 4 -1	0.00
127	41.61127	2.16863	1 3 -4	2.50
128	41.65186	2.16661	1 4 -3	0.00
129	41.77300	2.16061	4 2 2	1.10
130	41.94353	2.15222	5 1 -1	0.00
131	41.95961	2.15143	5 1 0	0.00
132	42.00718	2.14911	1 5 0	0.00
133	42.02859	2.14806	0 5 1	0.00
134	42.03050	2.14797	2 2 4	12.30
135	42.45557	2.12744	1 1 -5	0.00

**Supporting Information File S2:**

Modelling of  $\gamma$ -sulfur contribution to microstructure after exposure to hexanes at  $-25\text{ }^{\circ}\text{C}$



?-S8

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
136	42.49271	2.12567	0 1 5	4.30
137	42.53704	2.12355	3 4 1	0.00
138	42.57178	2.12190	4 2 -3	0.00
139	42.69191	2.11621	1 5 -1	0.00
140	42.69761	2.11594	4 3 1	0.00
141	42.70635	2.11553	1 4 3	3.50
142	42.71985	2.11489	3 2 -4	0.00
143	42.80636	2.11082	5 0 -2	0.00
144	43.01366	2.10112	1 3 4	1.80
145	43.03883	2.09995	1 5 1	0.00
146	43.16999	2.09387	4 3 -2	0.00
147	43.42076	2.08236	2 3 -4	0.80
148	43.52732	2.07751	3 4 -2	0.00
149	43.54921	2.07652	3 0 4	0.00
150	43.63127	2.07280	2 4 -3	5.40
151	43.63327	2.07271	5 1 -2	0.00
152	43.67999	2.07060	5 1 1	0.00
153	44.06768	2.05328	2 1 -5	0.00
154	44.17576	2.04851	1 1 5	0.00
155	44.22137	2.04650	4 1 3	7.30
156	44.36502	2.04021	3 1 4	0.00
157	44.42605	2.03755	5 2 -1	0.00
158	44.44141	2.03688	5 2 0	0.00
159	44.48116	2.03515	2 5 0	0.00
160	44.48530	2.03497	4 0 -4	6.00
161	44.53811	2.03268	3 3 3	6.20
162	44.56291	2.03160	0 5 2	0.00
163	44.91528	2.01648	1 2 -5	0.00
164	44.95079	2.01497	0 2 5	0.00
165	44.96895	2.01420	2 5 -1	3.00

SUNBG90\_hexanes\_-25C\_NEW-WPPF report (SUNBG90\_hexanes\_-25C\_NEW)

General information

Analysis date	2024-01-12 10:19:00	Measurement start...	2023-12-15 12:16:51
Analyst	Administrator	Operator	Administrator
Sample name		Comment	
Measured data na...	C:\XRD Data\Kolis\Bhakti\SUNBG90_hexa...	Memo	

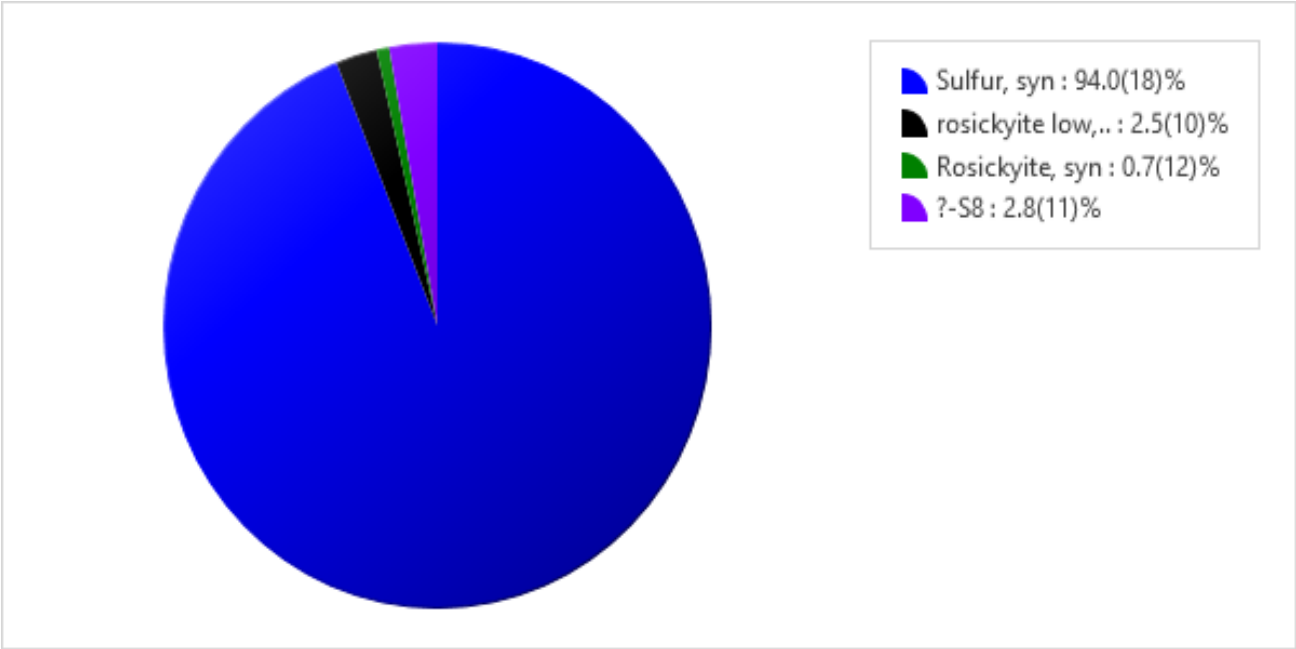
WPPF analysis results

Phase / Dataset		SUN
▲	Rwp, %	0.00
	Rp, %	0.00
	S	0.0000
	$\chi^2$	0.0000
▲	Sulfur, syn	
	Weight fraction, wt%	94.0(18)
	a, Å	10.48604
	b, Å	12.88756
	c, Å	24.55615
	$\alpha$ , °	90.000
	$\beta$ , °	90.000
	$\gamma$ , °	90.000
	Lattice volume, Å <sup>3</sup>	3318.503
	Size, Å	0.0
	Strain, %	0.074(5)
▲	rosickyite low, cyclo-octasulfur	
	Weight fraction, wt%	2.5(10)
	a, Å	10.88800
	b, Å	10.90994
	c, Å	11.03884
	$\alpha$ , °	90.000
	$\beta$ , °	95.637
	$\gamma$ , °	90.000
	Lattice volume, Å <sup>3</sup>	1304.934
	Size, Å	0.0
	Strain, %	0.034(3)
▲	Rosickyite, syn	
	Weight fraction, wt%	0.7(12)
	a, Å	8.30820
	b, Å	12.82538
	c, Å	9.10610
	$\alpha$ , °	90.000
	$\beta$ , °	124.890
	$\gamma$ , °	90.000
	Lattice volume, Å <sup>3</sup>	795.896
	Size, Å	0.0

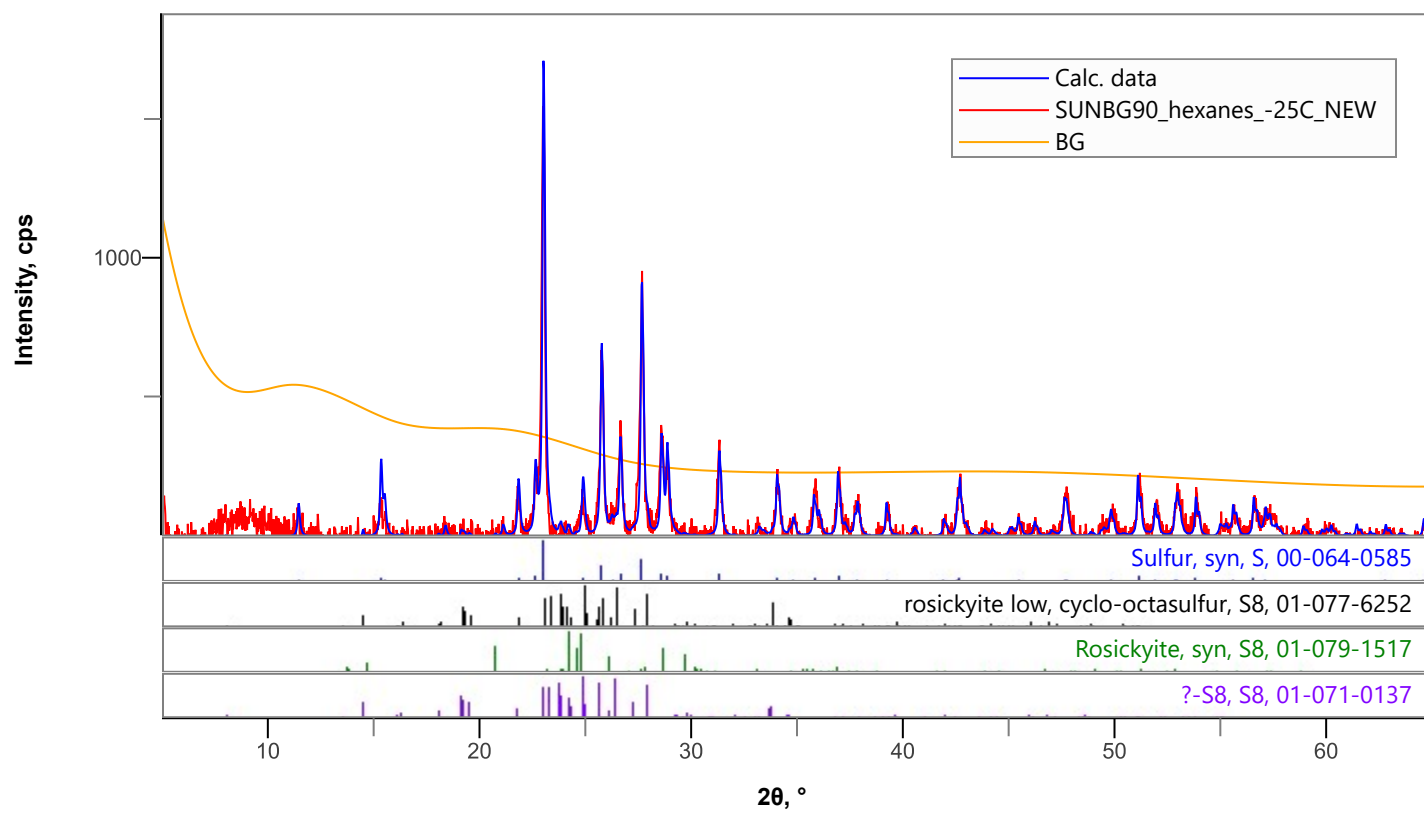
WPPF analysis results

Phase / Dataset		SUN
Rosickyite, syn		
Strain, %		0.034(3)
?-S8		
Weight fraction, wt%		2.8(11)
a, Å		11.04028
b, Å		10.96854
c, Å		10.90286
α, °		90.000
β, °		95.920
γ, °		90.000
Lattice volume, Å³		1313.250
Size, Å		0.0
Strain, %		0.034(3)

WPPF weight fraction



## WPPF Profile View



**Lattice parameters**

Phase name	a, Å	b, Å	c, Å	$\alpha$ , °	$\beta$ , °	$\gamma$ , °
Sulfur, syn	10.48604	12.88756	24.55615	90.000	90.000	90.000
rosickyite low, c...	10.88800	10.90994	11.03884	90.000	95.637	90.000
Rosickyite, syn	8.30820	12.82538	9.10610	90.000	124.890	90.000
?-S8	11.04028	10.96854	10.90286	90.000	95.920	90.000

**d-I List**

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**Sulfur, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
1	11.45112	7.72122	1 1 1	6.20
2	14.41639	6.13904	0 0 4	0.00
3	15.34488	5.76960	1 1 3	14.60
4	15.51770	5.70573	0 2 2	6.20
5	18.38513	4.82179	2 0 2	2.30
6	21.11450	4.20426	1 1 5	2.40
7	21.83640	4.06688	2 2 0	11.30
8	22.64113	3.92412	1 3 1	14.20
9	23.01863	3.86061	2 2 2	100.00
10	24.88011	3.57582	1 3 3	10.10
11	25.76667	3.45476	0 2 6	41.00
12	26.26438	3.39041	2 2 4	3.30
13	26.65114	3.34208	3 1 1	21.30
14	27.62741	3.22616	2 0 6	0.00
15	27.66476	3.22189	0 4 0	56.70
16	27.67080	3.22120	1 1 7	0.00
17	28.59674	3.11897	3 1 3	21.50
18	28.87182	3.08988	1 3 5	19.10
19	29.06750	3.06952	0 0 8	1.10
20	30.97391	2.88480	2 2 6	0.00
21	31.32949	2.85287	0 4 4	19.60
22	32.16461	2.78067	3 1 5	0.00
23	33.21783	2.69488	3 3 1	2.10
24	33.42191	2.67889	2 4 2	1.10
25	34.05810	2.63029	1 3 7	13.90
26	34.17563	2.62151	4 0 0	2.00
27	34.64861	2.58680	1 1 9	0.70
28	34.83004	2.57374	3 3 3	4.10
29	35.80417	2.50592	2 4 4	9.60
30	36.03931	2.49010	1 5 1	4.90
31	36.64992	2.45001	2 2 8	0.00
32	36.93763	2.43158	3 1 7	15.10
33	37.26613	2.41090	4 0 4	2.30
34	37.54552	2.39360	1 5 3	0.00
35	37.73335	2.38211	4 2 2	4.50
36	37.87408	2.37358	3 3 5	6.20
37	39.22943	2.29464	0 2 10	8.10
38	39.49670	2.27973	2 4 6	0.00
39	39.89230	2.25803	4 2 4	0.00

**Sulfur, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
40	40.04904	2.24955	1 3 9	0.00
41	40.41386	2.23008	1 5 5	0.50
42	40.53318	2.22379	2 0 10	0.00
43	40.55984	2.22239	0 4 8	2.00
44	41.93236	2.15277	1 1 11	3.90
45	42.08684	2.14522	3 3 7	0.60
46	42.58163	2.12143	3 1 9	7.80
47	42.70068	2.11579	0 6 2	9.00
48	42.99194	2.10213	2 2 10	2.20
49	43.29009	2.08834	4 2 6	0.00
50	43.75751	2.06711	3 5 1	0.00
51	43.85679	2.06266	5 1 1	1.50
52	44.22488	2.04635	0 0 12	0.00
53	44.22904	2.04616	2 4 8	1.70
54	44.42646	2.03753	1 5 7	0.00
55	44.52055	2.03344	4 4 0	0.00
56	45.04677	2.01090	3 5 3	1.80
57	45.14381	2.00680	5 1 3	0.00
58	45.16020	2.00611	4 4 2	1.00
59	45.46318	1.99345	4 0 8	4.60
60	45.60440	1.98760	2 6 0	0.00
61	46.23227	1.96206	2 6 2	3.70
62	46.62472	1.94645	1 3 11	0.00
63	47.03817	1.93030	4 4 4	1.40
64	47.22245	1.92320	3 3 9	0.00
65	47.54265	1.91099	3 5 5	1.90
66	47.63573	1.90747	5 1 5	7.00
67	47.71744	1.90440	4 2 8	4.50
68	47.78376	1.90191	0 6 6	0.00
69	48.07783	1.89096	2 6 4	0.00
70	48.40098	1.87909	5 3 1	0.00
71	48.88336	1.86167	3 1 11	0.90
72	49.36987	1.84446	1 5 9	1.30
73	49.49833	1.83997	1 1 13	1.20
74	49.59627	1.83656	5 3 3	0.40
75	49.78113	1.83018	2 4 10	2.40
76	49.84500	1.82798	2 2 12	5.10
77	50.04761	1.82105	4 4 6	0.00
78	50.42167	1.80842	1 7 1	0.50



**Sulfur, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
79	51.04127	1.78791	2 6 6	0.00
80	51.11132	1.78562	3 5 7	15.20
81	51.19956	1.78275	5 1 7	0.00
82	51.58239	1.77042	1 7 3	0.60
83	51.92580	1.75952	5 3 5	8.20
84	52.87205	1.73023	6 0 2	6.30
85	52.96612	1.72738	0 4 12	7.50
86	52.99108	1.72663	4 2 10	0.00
87	53.09903	1.72337	3 3 11	1.60
88	53.67890	1.70611	1 3 13	0.00
89	53.85005	1.70109	1 7 5	10.00
90	54.05228	1.69521	4 4 8	0.00
91	54.14814	1.69243	0 2 14	0.00
92	54.34601	1.68674	6 2 0	0.00
93	54.89919	1.67104	6 2 2	0.40
94	54.99441	1.66837	2 6 8	2.30
95	55.07852	1.66602	1 5 11	1.10
96	55.17292	1.66340	2 0 14	0.00
97	55.28816	1.66020	5 3 7	2.40
98	55.60929	1.65137	3 5 9	7.40
99	55.69253	1.64910	5 1 9	0.90
100	55.72746	1.64815	3 1 13	1.00
101	55.79011	1.64645	4 6 2	0.00
102	56.00524	1.64063	2 4 12	0.00
103	56.53683	1.62646	6 2 4	0.00
104	56.57861	1.62536	3 7 1	9.20
105	56.66091	1.62319	5 5 1	1.70
106	56.90844	1.61672	0 6 10	0.70
107	57.04860	1.61308	4 0 12	1.60
108	57.13118	1.61094	0 8 0	0.00
109	57.13452	1.61086	1 7 7	0.00
110	57.14455	1.61060	2 2 14	6.10
111	57.27408	1.60726	6 0 6	0.00
112	57.36658	1.60489	1 1 15	3.30
113	57.41092	1.60376	4 6 4	0.00
114	57.65281	1.59760	3 7 3	2.40
115	57.73412	1.59555	5 5 3	0.60
116	58.92238	1.56617	4 4 10	2.40
117	58.97933	1.56480	4 2 12	0.60

**Sulfur, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
118	59.20014	1.55948	6 2 6	0.00
119	59.25424	1.55819	0 8 4	0.00
120	59.57079	1.55066	5 3 9	0.00
121	59.60426	1.54987	3 3 13	0.00
122	59.76417	1.54611	3 7 5	0.00
123	59.81402	1.54494	2 6 10	1.80
124	59.84369	1.54424	5 5 5	0.00
125	60.04960	1.53944	4 6 6	1.50
126	60.25164	1.53476	0 0 16	2.20
127	60.54924	1.52793	2 8 2	0.00
128	60.70697	1.52433	6 4 2	0.00
129	60.91457	1.51963	3 5 11	0.50
130	60.99319	1.51786	5 1 11	0.40
131	61.17723	1.51374	1 3 15	0.00
132	61.33468	1.51023	1 7 9	0.00
133	61.44584	1.50776	1 5 13	3.20
134	62.09160	1.49362	2 8 4	1.30
135	62.24703	1.49027	6 4 4	0.00
136	62.48033	1.48526	7 1 1	0.00
137	62.81038	1.47825	6 2 8	0.00
138	62.82041	1.47804	2 4 14	3.10
139	62.84957	1.47742	3 7 7	0.00
140	62.92678	1.47579	5 5 7	0.00
141	63.06869	1.47282	3 1 15	0.00
142	63.49287	1.46399	7 1 3	0.80
143	63.63128	1.46114	4 6 8	0.40
144	64.55739	1.44240	4 4 12	0.00
145	64.61495	1.44125	2 8 6	4.00
146	64.67493	1.44006	5 3 11	0.90
147	64.76700	1.43824	6 4 6	1.30
148	64.88469	1.43591	2 2 16	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
1	8.04172	10.98546	0 0 1	7.20
2	8.15332	10.83534	1 0 0	0.00
3	10.88228	8.12351	1 0 -1	0.10
4	11.42168	7.74105	0 1 1	0.00
5	11.50079	7.68798	1 1 0	1.30

## rosickyite low, cyclo-octasulfur

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
6	12.01311	7.36124	1 0 1	0.00
7	13.57903	6.51567	1 1 -1	5.00
8	14.50407	6.10212	1 1 1	34.30
9	16.12339	5.49273	0 0 2	8.60
10	16.23575	5.45497	0 2 0	4.30
11	16.34828	5.41767	2 0 0	13.10
12	17.35495	5.10562	1 0 -2	0.10
13	17.51236	5.06008	2 0 -1	0.10
14	18.06677	4.90604	0 1 2	9.50
15	18.14234	4.88577	0 2 1	14.10
16	18.19275	4.87235	1 2 0	0.00
17	18.26844	4.85233	2 1 0	0.00
18	18.80150	4.71594	1 0 2	0.80
19	18.94728	4.67998	2 0 1	0.00
20	19.17758	4.62430	1 1 -2	51.50
21	19.32063	4.59038	2 1 -1	42.40
22	19.58648	4.52867	1 2 -1	32.60
23	20.24535	4.38275	1 2 1	1.00
24	20.50024	4.32883	1 1 2	0.80
25	20.63448	4.30097	2 1 1	2.00
26	21.86428	4.06175	2 0 -2	25.00
27	22.95884	3.87053	0 2 2	0.00
28	23.11951	3.84399	2 2 0	72.60
29	23.35034	3.80651	2 1 -2	73.70
30	23.85178	3.72761	1 2 -2	83.40
31	23.96814	3.70977	2 2 -1	49.90
32	24.16085	3.68062	2 0 2	50.00
33	24.28677	3.66182	0 0 3	23.30
34	24.62849	3.61178	3 0 0	0.00
35	24.86977	3.57729	1 0 -3	0.00
36	24.93858	3.56757	1 2 2	100.00
37	25.05019	3.55193	2 2 1	34.90
38	25.16713	3.53569	3 0 -1	0.00
39	25.52067	3.48750	2 1 2	19.90
40	25.64034	3.47150	0 1 3	52.90
41	25.78467	3.45239	0 3 1	0.00
42	25.82078	3.44764	1 3 0	71.50
43	25.96537	3.42877	3 1 0	0.00
44	26.19513	3.39922	1 1 -3	24.60

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
45	26.42539	3.37012	1 0 3	0.00
46	26.47859	3.36347	3 1 -1	98.20
47	26.70659	3.33527	3 0 1	0.00
48	26.83809	3.31922	1 3 -1	1.90
49	27.33103	3.26047	1 3 1	44.60
50	27.35357	3.25783	2 2 -2	0.00
51	27.68140	3.21999	1 1 3	5.70
52	27.95090	3.18955	3 1 1	78.30
53	28.01580	3.18231	2 0 -3	0.00
54	28.18267	3.16385	3 0 -2	5.40
55	29.20870	3.05500	2 1 -3	0.00
56	29.24725	3.05106	2 2 2	10.60
57	29.35283	3.04033	0 2 3	6.30
58	29.36937	3.03865	3 1 -2	0.00
59	29.43257	3.03227	0 3 2	8.90
60	29.56028	3.01946	2 3 0	0.00
61	29.64017	3.01150	3 2 0	8.00
62	29.84377	2.99142	1 2 -3	15.50
63	30.09552	2.96697	3 2 -1	0.00
64	30.14653	2.96206	1 3 -2	11.50
65	30.24030	2.95309	2 3 -1	0.00
66	30.76021	2.90435	2 0 3	7.20
67	30.91355	2.89030	3 0 2	2.70
68	31.02866	2.87984	1 3 2	6.60
69	31.12003	2.87159	2 3 1	0.00
70	31.17015	2.86708	1 2 3	6.30
71	31.41227	2.84554	3 2 1	4.40
72	31.85949	2.80661	2 1 3	1.30
73	32.00809	2.79391	3 1 2	10.70
74	32.54837	2.74876	2 2 -3	3.50
75	32.57754	2.74636	0 0 4	0.00
76	32.69417	2.73683	3 2 -2	5.90
77	32.80940	2.72748	0 4 0	6.60
78	32.81868	2.72673	1 0 -4	0.00
79	33.03504	2.70937	2 3 -2	0.00
80	33.04172	2.70884	4 0 0	13.60
81	33.05426	2.70784	3 0 -3	0.00
82	33.25122	2.69225	4 0 -1	4.60
83	33.62358	2.66328	0 1 4	9.60

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
84	33.83503	2.64712	0 4 1	0.00
85	33.85811	2.64536	1 1 -4	0.00
86	33.86325	2.64497	1 4 0	60.00
87	34.07513	2.62901	4 1 0	4.60
88	34.08734	2.62810	3 1 -3	0.00
89	34.27904	2.61384	4 1 -1	1.60
90	34.43975	2.60201	1 0 4	5.60
91	34.64715	2.58690	2 3 2	26.30
92	34.66467	2.58564	1 4 -1	0.00
93	34.73793	2.58035	0 3 3	19.10
94	34.85450	2.57199	4 0 1	0.00
95	34.97176	2.56363	2 2 3	3.70
96	34.98545	2.56266	3 3 0	0.00
97	35.05733	2.55757	1 4 1	0.00
98	35.10865	2.55395	3 2 2	0.00
99	35.12482	2.55281	2 0 -4	5.10
100	35.16123	2.55025	1 3 -3	0.00
101	35.37901	2.53505	3 3 -1	1.70
102	35.43723	2.53102	1 1 4	1.60
103	35.45136	2.53004	4 0 -2	0.00
104	35.84190	2.50336	4 1 1	0.00
105	36.10578	2.48567	2 1 -4	3.30
106	36.31402	2.47189	1 3 3	1.10
107	36.42468	2.46464	4 1 -2	3.60
108	36.52584	2.45804	3 3 1	0.00
109	36.59206	2.45375	3 0 3	4.10
110	36.60332	2.45302	0 2 4	0.00
111	36.76055	2.44289	0 4 2	0.00
112	36.82123	2.43900	1 2 -4	8.80
113	36.86549	2.43617	2 4 0	0.00
114	37.02306	2.42616	4 2 0	0.00
115	37.03442	2.42545	3 2 -3	4.70
116	37.21288	2.41422	4 2 -1	8.60
117	37.34919	2.40573	1 4 -2	3.20
118	37.42686	2.40091	2 4 -1	0.00
119	37.52507	2.39485	2 3 -3	7.30
120	37.53983	2.39395	3 1 3	0.00
121	37.65393	2.38695	3 3 -2	2.50
122	38.08295	2.36104	1 4 2	0.00

## rosickyite low, cyclo-octasulfur

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
123	38.13449	2.35797	2 0 4	9.60
124	38.15934	2.35649	2 4 1	0.00
125	38.29404	2.34851	1 2 4	3.30
126	38.43895	2.33999	4 0 2	1.40
127	38.67296	2.32637	4 2 1	4.60
128	38.92036	2.31215	2 2 -4	3.40
129	39.05029	2.30476	2 1 4	0.90
130	39.17725	2.29758	3 0 -4	0.00
131	39.21965	2.29519	4 2 -2	7.00
132	39.34876	2.28796	4 1 2	6.50
133	39.35111	2.28783	4 0 -3	0.00
134	39.68345	2.26943	2 3 3	14.10
135	39.77647	2.26434	2 4 -2	0.00
136	39.80639	2.26270	3 3 2	5.10
137	40.07296	2.24826	3 1 -4	3.50
138	40.24359	2.23912	4 1 -3	0.00
139	40.26888	2.23778	3 2 3	6.00
140	41.04782	2.19709	0 0 5	0.00
141	41.07530	2.19569	1 0 -5	0.00
142	41.15498	2.19162	0 3 4	0.00
143	41.15972	2.19138	2 4 2	7.00
144	41.23816	2.18739	0 4 3	0.00
145	41.35253	2.18160	1 3 -4	1.30
146	41.45233	2.17658	3 4 0	3.40
147	41.53572	2.17240	4 3 0	0.00
148	41.54603	2.17189	3 3 -3	2.70
149	41.60468	2.16896	1 4 -3	0.00
150	41.64273	2.16707	5 0 0	0.00
151	41.64624	2.16689	5 0 -1	0.00
152	41.69615	2.16442	2 2 4	0.00
153	41.70818	2.16382	4 3 -1	8.00
154	41.79373	2.15959	3 4 -1	0.00
155	41.91029	2.15385	0 1 5	0.00
156	41.93730	2.15253	1 1 -5	0.00
157	41.97896	2.15049	4 2 2	13.70
158	42.19076	2.14018	0 5 1	0.00
159	42.21416	2.13905	1 5 0	5.10
160	42.49531	2.12554	5 1 0	6.40
161	42.49876	2.12538	5 1 -1	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
162	42.60886	2.12014	1 4 3	0.00
163	42.66617	2.11743	3 2 -4	0.00
164	42.69362	2.11613	1 3 4	3.40
165	42.75519	2.11322	1 0 5	0.00
166	42.79430	2.11138	3 4 1	7.10
167	42.82829	2.10979	4 2 -3	0.00
168	42.83489	2.10948	2 0 -5	0.00
169	42.88142	2.10729	1 5 -1	0.00
170	43.04023	2.09989	4 3 1	2.10
171	43.21022	2.09202	1 5 1	0.00
172	43.26516	2.08949	3 0 4	1.50
173	43.26686	2.08941	2 3 -4	0.00
174	43.30805	2.08752	5 0 1	0.00
175	43.31824	2.08705	5 0 -2	0.00
176	43.42547	2.08215	4 0 3	0.00
177	43.54139	2.07687	4 3 -2	2.90
178	43.59011	2.07466	1 1 5	0.00
179	43.66859	2.07112	2 1 -5	0.00
180	43.67273	2.07093	2 4 -3	6.70
181	43.78644	2.06581	3 4 -2	6.20
182	44.09232	2.05219	3 1 4	0.00
183	44.13458	2.05032	5 1 1	0.00
184	44.14461	2.04988	5 1 -2	10.20
185	44.25024	2.04523	4 1 3	3.60
186	44.41568	2.03800	0 2 5	0.00
187	44.44146	2.03687	1 2 -5	0.00
188	44.50667	2.03404	3 3 3	4.80
189	44.57973	2.03088	4 0 -4	5.70
190	44.65005	2.02784	0 5 2	0.00
191	44.73946	2.02400	2 5 0	8.70
192	44.97444	2.01397	5 2 0	0.00
193	44.97774	2.01383	5 2 -1	4.10
194	45.15255	2.00644	1 5 -2	0.00
195	45.21903	2.00364	2 5 -1	6.00
196	45.38783	1.99658	4 1 -4	3.00
197	45.58960	1.98821	2 4 3	2.10
198	45.69953	1.98368	3 4 2	2.40
199	45.78224	1.98029	1 5 2	0.00
200	45.82661	1.97848	2 3 4	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
201	45.84800	1.97760	2 5 1	5.80
202	46.02213	1.97053	1 2 5	0.00
203	46.04092	1.96977	2 0 5	16.20
204	46.08903	1.96782	4 3 2	0.00
205	46.09733	1.96749	2 2 -5	0.00
206	46.16616	1.96471	3 0 -5	0.00
207	46.49776	1.95147	5 0 2	0.00
208	46.50359	1.95124	3 2 4	7.30
209	46.51382	1.95084	5 0 -3	0.00
210	46.54412	1.94964	5 2 1	0.00
211	46.55375	1.94926	5 2 -2	0.00
212	46.65509	1.94526	4 2 3	0.00
213	46.72788	1.94240	3 3 -4	3.60
214	46.82929	1.93843	2 1 5	0.00
215	46.87882	1.93649	4 3 -3	0.00
216	46.91040	1.93526	0 4 4	15.50
217	46.95291	1.93361	3 1 -5	0.00
218	47.08852	1.92836	1 4 -4	2.20
219	47.24888	1.92219	2 5 -2	0.00
220	47.25384	1.92200	4 4 0	0.00
221	47.26316	1.92164	3 4 -3	0.00
222	47.28027	1.92098	5 1 2	12.00
223	47.29612	1.92038	5 1 -3	0.00
224	47.40963	1.91604	4 4 -1	0.00
225	47.74790	1.90325	4 2 -4	1.70
226	48.30240	1.88269	1 4 4	0.00
227	48.36135	1.88054	0 3 5	0.00
228	48.38550	1.87965	1 3 -5	0.00
229	48.45971	1.87695	2 5 2	5.30
230	48.52871	1.87444	0 5 3	0.00
231	48.61743	1.87123	4 4 1	3.20
232	48.71725	1.86763	3 5 0	5.60
233	48.82369	1.86380	2 4 -4	0.00
234	48.85153	1.86281	1 5 -3	0.00
235	48.88508	1.86161	5 3 0	0.00
236	48.88817	1.86150	5 3 -1	13.60
237	49.01832	1.85686	3 5 -1	5.30
238	49.07383	1.85489	4 4 -2	0.00
239	49.13614	1.85268	2 2 5	0.00



**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
240	49.25537	1.84847	3 2 -5	1.10
241	49.48854	1.84031	4 0 4	0.00
242	49.57122	1.83743	5 2 2	3.10
243	49.58652	1.83690	5 2 -3	0.00
244	49.63636	1.83517	1 0 -6	0.00
245	49.73970	1.83160	1 5 3	1.60
246	49.75984	1.83091	0 0 6	0.00
247	49.86957	1.82714	1 3 5	0.00
248	49.90430	1.82595	3 5 1	2.40
249	49.94036	1.82471	2 3 -5	0.00
250	49.95584	1.82418	3 4 3	0.00
251	50.12798	1.81832	0 6 0	3.30
252	50.23577	1.81467	4 1 4	0.00
253	50.32304	1.81173	3 3 4	0.00
254	50.35464	1.81067	6 0 -1	0.00
255	50.36124	1.81045	5 3 1	10.00
256	50.37032	1.81014	5 3 -2	0.00
257	50.38197	1.80975	1 1 -6	0.00
258	50.46586	1.80694	4 3 3	0.00
259	50.49720	1.80589	6 0 0	0.00
260	50.50411	1.80566	0 1 6	6.70
261	50.66806	1.80020	3 0 5	0.00
262	50.68640	1.79959	2 5 -3	0.00
263	50.78791	1.79623	3 5 -2	0.00
264	50.83122	1.79480	4 0 -5	0.00
265	50.85823	1.79391	0 6 1	6.80
266	50.87849	1.79325	1 6 0	0.00
267	50.99248	1.78951	5 0 3	0.00
268	51.01347	1.78882	5 0 -4	0.00
269	51.01888	1.78864	2 0 -6	0.00
270	51.09259	1.78624	6 1 -1	6.60
271	51.16784	1.78378	2 4 4	8.40
272	51.23366	1.78165	6 1 0	0.00
273	51.38137	1.77687	1 0 6	0.00
274	51.40275	1.77618	3 1 5	0.00
275	51.40959	1.77596	4 4 2	0.00
276	51.45771	1.77442	1 6 -1	0.00
277	51.49791	1.77312	4 3 -4	0.00
278	51.56424	1.77100	4 1 -5	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
279	51.66307	1.76784	6 0 -2	0.00
280	51.72385	1.76591	5 1 3	0.00
281	51.74409	1.76527	1 6 1	0.00
282	51.74463	1.76525	5 1 -4	0.00
283	51.74999	1.76508	2 1 -6	0.00
284	51.99915	1.75721	3 4 -4	0.00
285	52.08215	1.75460	6 0 1	0.00
286	52.10884	1.75376	1 1 6	0.00
287	52.13866	1.75283	4 4 -3	0.00
288	52.38775	1.74508	6 1 -2	0.00
289	52.40603	1.74452	2 5 3	0.00
290	52.43077	1.74375	4 2 4	0.00
291	52.50516	1.74146	3 5 2	0.00
292	52.57258	1.73938	1 2 -6	0.00
293	52.69107	1.73575	0 2 6	0.00
294	52.80275	1.73234	6 1 1	0.00
295	52.81337	1.73202	2 3 5	0.00
296	52.92657	1.72858	3 3 -5	0.00
297	53.00532	1.72620	0 6 2	0.00
298	53.08401	1.72382	2 6 0	0.00
299	53.22661	1.71954	5 3 2	0.00
300	53.24115	1.71910	5 3 -3	0.00
301	53.26225	1.71847	6 2 -1	0.00
302	53.39925	1.71439	6 2 0	0.00
303	53.44814	1.71293	1 6 -2	0.00
304	53.50683	1.71119	2 6 -1	0.00
305	53.51306	1.71101	0 4 5	0.00
306	53.53551	1.71034	1 4 -5	0.00
307	53.56349	1.70952	3 2 5	0.00
308	53.60063	1.70842	0 5 4	0.00
309	53.72038	1.70489	4 2 -5	0.00
310	53.76231	1.70366	1 5 -4	0.00
311	53.82339	1.70187	3 0 -6	0.00
312	53.87550	1.70035	5 2 3	0.00
313	53.89569	1.69976	5 2 -4	0.00
314	53.90090	1.69961	2 2 -6	0.00
315	53.91249	1.69927	4 5 0	0.00
316	53.92095	1.69902	3 5 -3	0.00
317	54.00034	1.69671	5 4 0	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
318	54.00322	1.69663	5 4 -1	0.00
319	54.00492	1.69658	1 6 2	0.00
320	54.05411	1.69515	4 5 -1	0.00
321	54.06319	1.69489	2 6 1	0.00
322	54.24976	1.68950	1 2 6	0.00
323	54.34745	1.68669	6 0 -3	0.00
324	54.40454	1.68506	2 0 6	0.00
325	54.52103	1.68173	6 2 -2	0.00
326	54.52792	1.68154	3 1 -6	0.00
327	54.86760	1.67193	1 5 4	0.00
328	54.91866	1.67049	1 4 5	0.00
329	54.92485	1.67032	6 2 1	0.00
330	54.98480	1.66864	2 4 -5	0.00
331	55.02080	1.66763	6 0 2	0.00
332	55.04742	1.66689	6 1 -3	0.00
333	55.10402	1.66531	2 1 6	0.00
334	55.15541	1.66388	4 5 1	0.00
335	55.30948	1.65961	2 6 -2	0.00
336	55.34265	1.65870	3 4 4	0.00
337	55.34407	1.65866	2 5 -4	0.00
338	55.37839	1.65771	5 4 1	0.00
339	55.38689	1.65748	5 4 -2	0.00
340	55.47631	1.65502	4 4 3	0.00
341	55.57307	1.65236	4 5 -2	0.00
342	55.71507	1.64849	6 1 2	0.00
343	55.95327	1.64203	4 3 4	0.00
344	56.08895	1.63838	1 3 -6	0.00
345	56.20234	1.63535	0 3 6	0.00
346	56.38246	1.63055	3 5 3	0.00
347	56.39426	1.63023	2 6 2	0.00
348	56.40877	1.62985	4 0 5	0.00
349	56.44397	1.62892	4 4 -4	0.00
350	56.45628	1.62859	0 6 3	0.00
351	56.57844	1.62536	5 0 4	0.00
352	56.60356	1.62470	5 0 -5	0.00
353	56.60584	1.62464	3 2 -6	0.00
354	56.62586	1.62412	3 6 0	0.00
355	56.74673	1.62094	1 6 -3	0.00
356	56.74936	1.62087	6 3 -1	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
357	56.88066	1.61744	6 3 0	0.00
358	56.89698	1.61702	3 6 -1	0.00
359	57.03812	1.61335	3 3 5	0.00
360	57.09185	1.61196	4 1 5	0.00
361	57.11273	1.61142	6 2 -3	0.00
362	57.16797	1.61000	2 2 6	0.00
363	57.18858	1.60946	4 3 -5	0.00
364	57.26020	1.60762	5 1 4	0.00
365	57.28513	1.60698	5 1 -5	0.00
366	57.33739	1.60564	5 3 3	0.00
367	57.35676	1.60514	5 3 -4	0.00
368	57.36176	1.60502	2 3 -6	0.00
369	57.49930	1.60150	2 5 4	0.00
370	57.54822	1.60026	1 6 3	0.00
371	57.68170	1.59687	2 4 5	0.00
372	57.69661	1.59649	1 3 6	0.00
373	57.69713	1.59648	3 6 1	0.00
374	57.72269	1.59584	4 5 2	0.00
375	57.76464	1.59478	6 2 2	0.00
376	57.78843	1.59418	3 4 -5	0.00
377	57.90853	1.59116	4 0 -6	0.00
378	57.95714	1.58994	6 3 -2	0.00
379	58.07149	1.58708	5 4 2	0.00
380	58.08522	1.58674	5 4 -3	0.00
381	58.26833	1.58218	3 5 -4	0.00
382	58.27888	1.58192	6 0 -4	0.00
383	58.34524	1.58028	6 3 1	0.00
384	58.39762	1.57899	4 5 -3	0.00
385	58.40625	1.57878	2 6 -3	0.00
386	58.49848	1.57651	3 6 -2	0.00
387	58.54967	1.57525	1 0 -7	0.00
388	58.58035	1.57450	4 1 -6	0.00
389	58.68333	1.57198	3 0 6	0.00
390	58.79129	1.56935	0 0 7	0.00
391	58.94805	1.56555	6 1 -4	0.00
392	59.11053	1.56163	4 2 5	0.00
393	59.17885	1.55999	6 0 3	0.00
394	59.21693	1.55908	1 1 -7	0.00
395	59.27525	1.55769	5 2 4	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
396	59.29964	1.55711	5 2 -5	0.00
397	59.34966	1.55591	3 1 6	0.00
398	59.43005	1.55400	7 0 -1	0.00
399	59.45686	1.55336	0 1 7	0.00
400	59.65899	1.54858	2 0 -7	0.00
401	59.67474	1.54821	0 5 5	0.00
402	59.68767	1.54791	7 0 0	0.00
403	59.69565	1.54772	1 5 -5	0.00
404	59.84177	1.54429	6 1 3	0.00
405	59.89213	1.54311	0 7 1	0.00
406	59.91030	1.54269	1 7 0	0.00
407	59.96394	1.54143	3 3 -6	0.00
408	59.97418	1.54119	2 6 3	0.00
409	60.06492	1.53908	3 6 2	0.00
410	60.09128	1.53847	7 1 -1	0.00
411	60.12898	1.53760	5 5 0	0.00
412	60.13167	1.53753	5 5 -1	0.00
413	60.31868	1.53321	2 1 -7	0.00
414	60.34718	1.53256	7 1 0	0.00
415	60.37382	1.53195	1 0 7	0.00
416	60.43041	1.53065	1 7 -1	0.00
417	60.45301	1.53013	6 3 -3	0.00
418	60.47526	1.52962	7 0 -2	0.00
419	60.50634	1.52891	2 3 6	0.00
420	60.56789	1.52750	4 2 -6	0.00
421	60.65430	1.52553	4 4 4	0.00
422	60.68813	1.52476	1 7 1	0.00
423	60.78329	1.52260	1 4 -6	0.00
424	60.89113	1.52016	0 4 6	0.00
425	60.92824	1.51933	6 2 -4	0.00
426	60.98704	1.51800	1 5 5	0.00
427	61.02886	1.51706	1 1 7	0.00
428	61.04894	1.51661	2 5 -5	0.00
429	61.07015	1.51614	0 6 4	0.00
430	61.08264	1.51586	6 3 2	0.00
431	61.12966	1.51480	7 1 -2	0.00
432	61.19183	1.51341	1 2 -7	0.00
433	61.21888	1.51281	1 6 -4	0.00
434	61.23817	1.51238	7 0 1	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
435	61.32197	1.51051	3 2 6	0.00
436	61.35713	1.50973	4 6 0	0.00
437	61.36492	1.50956	3 6 -3	0.00
438	61.38406	1.50913	3 5 4	0.00
439	61.41176	1.50852	6 4 -1	0.00
440	61.41755	1.50839	5 5 1	0.00
441	61.42551	1.50821	5 5 -2	0.00
442	61.42710	1.50818	0 2 7	0.00
443	61.48757	1.50684	4 6 -1	0.00
444	61.50933	1.50636	4 5 3	0.00
445	61.53683	1.50575	6 4 0	0.00
446	61.68687	1.50245	3 4 5	0.00
447	61.80465	1.49987	6 2 3	0.00
448	61.82742	1.49937	0 7 2	0.00
449	61.83029	1.49931	4 4 -5	0.00
450	61.88780	1.49805	7 1 1	0.00
451	61.89872	1.49781	2 7 0	0.00
452	61.97219	1.49622	5 4 3	0.00
453	61.99066	1.49581	5 4 -4	0.00
454	61.99543	1.49571	2 4 -6	0.00
455	62.04945	1.49454	7 2 -1	0.00
456	62.07495	1.49398	3 0 -7	0.00
457	62.22904	1.49066	1 7 -2	0.00
458	62.23823	1.49046	1 6 4	0.00
459	62.27263	1.48972	2 2 -7	0.00
460	62.28232	1.48951	2 7 -1	0.00
461	62.30060	1.48911	7 2 0	0.00
462	62.31493	1.48881	1 4 6	0.00
463	62.38469	1.48731	4 3 5	0.00
464	62.41778	1.48660	4 5 -4	0.00
465	62.50438	1.48475	4 6 1	0.00
466	62.54424	1.48390	5 3 4	0.00
467	62.56368	1.48348	6 4 -2	0.00
468	62.56787	1.48339	5 3 -5	0.00
469	62.67898	1.48103	2 6 -4	0.00
470	62.71957	1.48017	3 1 -7	0.00
471	62.73517	1.47984	1 7 2	0.00
472	62.78430	1.47880	7 0 -3	0.00
473	62.78821	1.47872	2 7 1	0.00

**rosickyite low, cyclo-octasulfur**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
474	62.89110	1.47655	4 6 -2	0.00
475	62.93450	1.47563	6 4 1	0.00
476	62.96989	1.47489	1 2 7	0.00
477	63.06890	1.47281	7 2 -2	0.00
478	63.09579	1.47225	5 0 5	0.00
479	63.12453	1.47165	5 0 -6	0.00
480	63.23671	1.46931	2 0 7	0.00
481	63.31822	1.46761	6 0 -5	0.00
482	63.42483	1.46540	7 1 -3	0.00
483	63.58364	1.46212	2 5 5	0.00
484	63.64222	1.46092	3 6 3	0.00
485	63.68436	1.46005	3 5 -5	0.00
486	63.73458	1.45902	5 1 5	0.00
487	63.76316	1.45844	5 1 -6	0.00
488	63.79774	1.45773	4 3 -6	0.00
489	63.81383	1.45740	7 2 1	0.00
490	63.87472	1.45616	2 1 7	0.00
491	63.92599	1.45512	2 7 -2	0.00
492	63.95165	1.45459	5 5 2	0.00
493	63.95578	1.45451	6 1 -5	0.00
494	63.96462	1.45433	5 5 -3	0.00
495	64.02626	1.45308	7 0 2	0.00
496	64.07075	1.45218	4 0 6	0.00
497	64.14762	1.45062	6 3 -4	0.00
498	64.40367	1.44547	1 3 -7	0.00
499	64.41982	1.44515	6 0 4	0.00
500	64.48458	1.44385	3 4 -6	0.00
501	64.53013	1.44294	3 3 6	0.00
502	64.63168	1.44092	3 2 -7	0.00
503	64.63230	1.44091	0 3 7	0.00
504	64.65999	1.44036	7 1 2	0.00
505	64.68222	1.43992	2 6 4	0.00
506	64.70425	1.43948	4 1 6	0.00
507	64.89073	1.43579	4 6 2	0.00
508	64.92127	1.43519	2 7 2	0.00
509	64.95397	1.43455	6 4 -3	0.00
510	64.97831	1.43407	0 7 3	0.00
511	64.99935	1.43366	6 3 3	0.00

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
1	6.88655	12.82538	0 1 0	0.50
2	12.98033	6.81481	1 0 0	0.10
3	13.43531	6.58504	1 1 -1	0.00
4	13.70836	6.45448	0 1 1	18.20
5	13.79813	6.41269	0 2 0	10.80
6	14.70791	6.01801	1 1 0	27.50
7	18.01244	4.92071	1 2 -1	1.20
8	18.21851	4.86551	0 2 1	0.20
9	18.98756	4.67015	1 2 0	0.30
10	19.48900	4.55110	1 0 -2	0.50
11	20.69237	4.28907	1 1 -2	0.00
12	20.76061	4.27513	0 3 0	67.10
13	22.68403	3.91679	2 1 -1	0.30
14	23.16302	3.83687	2 0 -2	0.00
15	23.17739	3.83452	1 1 1	13.50
16	23.80606	3.73466	1 3 -1	9.90
17	23.80617	3.73465	0 0 2	0.00
18	23.95740	3.71141	1 2 -2	13.00
19	23.96431	3.71036	0 3 1	0.00
20	24.19234	3.67590	2 1 -2	100.00
21	24.56133	3.62150	1 3 0	61.90
22	24.81035	3.58572	0 1 2	95.80
23	25.70989	3.46226	2 2 -1	2.00
24	26.13107	3.40741	2 0 0	0.00
25	26.14949	3.40505	1 2 1	39.80
26	27.05449	3.29316	2 1 0	6.20
27	27.05990	3.29252	2 2 -2	0.00
28	27.61797	3.22724	0 2 2	9.40
29	27.80157	3.20634	0 4 0	14.70
30	28.62486	3.11597	1 3 -2	59.50
31	29.66536	3.00900	2 2 0	45.50
32	30.12532	2.96410	2 3 -1	0.00
33	30.18397	2.95848	1 4 -1	18.70
34	30.31116	2.94635	0 4 1	11.30
35	30.50614	2.92796	1 3 1	9.80
36	30.77735	2.90278	2 1 -3	6.10
37	30.79379	2.90126	1 4 0	0.00
38	31.15096	2.86881	1 1 -3	7.40
39	31.29998	2.85549	2 3 -2	0.00



**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
40	31.78988	2.81259	0 3 2	1.30
41	32.33153	2.76670	3 0 -2	1.40
42	33.09638	2.70449	3 1 -2	0.00
43	33.12097	2.70254	2 2 -3	9.80
44	33.27767	2.69017	1 0 2	1.00
45	33.47112	2.67506	1 2 -3	2.30
46	33.60650	2.66459	2 3 0	0.00
47	34.02364	2.63287	1 1 2	0.80
48	34.18030	2.62116	1 4 -2	0.90
49	34.75946	2.57880	3 1 -1	2.80
50	34.95145	2.56508	0 5 0	0.00
51	35.30276	2.54035	3 2 -2	0.00
52	35.31748	2.53933	2 1 1	13.00
53	35.46913	2.52881	2 4 -1	10.80
54	35.76592	2.50851	3 1 -3	0.00
55	35.79907	2.50626	1 4 1	9.50
56	36.18031	2.48072	1 2 2	5.70
57	36.49030	2.46036	2 4 -2	4.20
58	36.73156	2.44475	2 3 -3	0.00
59	36.74108	2.44414	0 1 3	6.70
60	36.87856	2.43534	3 2 -1	16.30
61	36.91904	2.43276	1 5 -1	0.00
62	36.91911	2.43276	0 4 2	0.00
63	37.02557	2.42601	0 5 1	2.50
64	37.05176	2.42435	1 3 -3	0.00
65	37.40913	2.40201	2 2 1	0.00
66	37.43108	2.40065	1 5 0	8.10
67	37.83615	2.37588	3 2 -3	6.60
68	38.52310	2.33507	2 4 0	1.30
69	38.73601	2.32273	3 3 -2	3.30
70	38.76657	2.32097	0 2 3	0.00
71	39.54805	2.27689	1 3 2	2.80
72	39.57222	2.27555	2 0 -4	0.00
73	39.64387	2.27160	3 0 0	0.00
74	40.19637	2.24165	3 3 -1	0.60
75	40.21671	2.24056	2 1 -4	0.00
76	40.28740	2.23679	3 1 0	0.00
77	40.32878	2.23459	1 5 -2	2.10
78	40.69024	2.21557	2 3 1	1.50

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
79	41.08846	2.19501	3 3 -3	0.40
80	41.32770	2.18286	2 4 -3	2.20
81	41.43191	2.17761	3 0 -4	1.30
82	41.45310	2.17654	2 5 -1	0.00
83	41.61795	2.16830	1 4 -3	5.90
84	41.74263	2.16211	1 5 1	0.00
85	41.95835	2.15149	0 3 3	5.10
86	42.05277	2.14688	3 1 -4	0.00
87	42.10099	2.14453	2 2 -4	1.20
88	42.16908	2.14123	3 2 0	1.40
89	42.20071	2.13970	1 0 -4	0.00
90	42.24486	2.13756	0 6 0	0.00
91	42.35139	2.13243	2 5 -2	0.30
92	42.73046	2.11439	0 5 2	0.10
93	42.81249	2.11053	1 1 -4	0.00
94	43.15250	2.09468	3 4 -2	0.00
95	43.87243	2.06196	3 2 -4	0.00
96	43.89684	2.06087	1 4 2	4.60
97	43.93514	2.05917	1 6 -1	0.00
98	43.99170	2.05665	4 0 -2	0.00
99	44.02740	2.05506	0 6 1	0.00
100	44.15757	2.04931	2 5 0	0.30
101	44.37928	2.03958	1 6 0	1.80
102	44.49305	2.03463	3 4 -1	0.00
103	44.55679	2.03187	4 1 -3	0.00
104	44.58369	2.03071	4 1 -2	3.30
105	44.60716	2.02969	1 2 -4	0.00
106	44.94835	2.01507	2 4 1	0.30
107	45.08793	2.00916	2 0 2	0.00
108	45.09836	2.00872	2 3 -4	1.10
109	45.16281	2.00600	3 3 0	0.00
110	45.31615	1.99957	3 4 -3	1.00
111	45.66869	1.98495	2 1 2	2.60
112	45.91052	1.97506	1 1 3	0.90
113	46.12164	1.96651	0 4 3	0.80
114	46.29766	1.95944	4 2 -3	1.20
115	46.32377	1.95840	4 2 -2	0.00
116	46.68455	1.94410	2 5 -3	10.10
117	46.77915	1.94039	3 3 -4	0.00

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
118	46.92274	1.93478	1 6 -2	0.00
119	46.94817	1.93379	1 5 -3	1.70
120	47.34692	1.91843	4 0 -4	0.60
121	47.37767	1.91726	2 2 2	0.00
122	47.47858	1.91342	1 3 -4	0.00
123	47.61280	1.90834	1 2 3	0.20
124	47.90645	1.89733	4 1 -4	0.00
125	47.92224	1.89674	2 6 -1	4.20
126	47.98274	1.89449	4 1 -1	0.00
127	48.18070	1.88716	1 6 1	3.90
128	48.34794	1.88103	3 5 -2	2.10
129	48.58362	1.87245	3 1 1	2.10
130	48.72546	1.86733	2 6 -2	0.60
131	48.72569	1.86732	0 0 4	0.00
132	49.03036	1.85643	1 5 2	0.00
133	49.05074	1.85571	2 4 -4	9.70
134	49.06559	1.85518	0 6 2	0.00
135	49.09252	1.85422	4 3 -3	0.00
136	49.11119	1.85356	3 4 0	0.00
137	49.11750	1.85334	4 3 -2	0.00
138	49.27341	1.84784	0 1 4	1.00
139	49.55637	1.83795	4 2 -4	0.00
140	49.57854	1.83718	3 5 -1	2.20
141	49.63076	1.83537	4 2 -1	2.00
142	49.72251	1.83220	0 7 0	0.00
143	49.99806	1.82274	2 5 1	0.00
144	50.12683	1.81836	2 3 2	7.30
145	50.21692	1.81531	3 2 1	4.30
146	50.33751	1.81124	3 5 -3	0.00
147	50.35215	1.81075	2 6 0	4.90
148	50.35232	1.81075	1 3 3	0.00
149	50.63111	1.80143	3 4 -4	0.90
150	50.86846	1.79358	3 1 -5	2.60
151	50.89033	1.79286	0 2 4	0.00
152	51.08261	1.78656	0 5 3	0.00
153	51.21958	1.78210	1 7 -1	0.00
154	51.28027	1.78014	2 1 -5	0.00
155	51.29106	1.77979	1 4 -4	8.00
156	51.30173	1.77944	0 7 1	0.00

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
157	51.61539	1.76936	1 7 0	0.30
158	52.22029	1.75028	4 3 -4	0.00
159	52.29193	1.74805	4 3 -1	3.60
160	52.44958	1.74317	3 2 -5	5.70
161	52.65196	1.73695	2 6 -3	0.00
162	52.81877	1.73185	4 4 -3	9.30
163	52.84247	1.73113	4 4 -2	0.00
164	52.85258	1.73082	2 2 -5	0.00
165	52.85671	1.73070	3 3 1	0.00
166	52.89337	1.72959	1 6 -3	0.00
167	53.50631	1.71121	0 3 4	0.30
168	53.76095	1.70370	4 0 0	0.00
169	53.80119	1.70252	2 4 2	0.00
170	53.81034	1.70226	2 5 -4	0.00
171	53.86692	1.70060	3 5 0	1.90
172	53.90005	1.69963	1 7 -2	0.00
173	54.01570	1.69627	1 4 3	0.60
174	54.15540	1.69222	4 1 -5	1.50
175	54.17962	1.69152	3 6 -2	0.00
176	54.27179	1.68887	4 1 0	0.00
177	54.80576	1.67367	2 7 -1	4.50
178	54.80930	1.67357	1 6 2	0.00
179	55.01325	1.66785	3 3 -5	0.00
180	55.04064	1.66708	1 7 1	1.70
181	55.29296	1.66007	3 5 -4	0.00
182	55.31629	1.65942	3 6 -1	0.00
183	55.33242	1.65898	1 1 -5	0.70
184	55.40336	1.65702	2 3 -5	0.60
185	55.53662	1.65336	2 7 -2	0.70
186	55.67091	1.64969	4 2 -5	0.00
187	55.70499	1.64876	2 6 1	0.00
188	55.76464	1.64714	5 1 -3	5.40
189	55.78516	1.64658	4 2 0	0.00
190	55.79706	1.64626	4 4 -4	0.00
191	55.84690	1.64491	0 7 2	0.00
192	55.86553	1.64440	4 4 -1	0.00
193	55.91418	1.64309	1 5 -4	0.00
194	56.01993	1.64024	3 6 -3	0.00
195	56.33977	1.63168	5 0 -4	0.50

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
196	56.40568	1.62993	3 4 1	0.00
197	56.71254	1.62184	0 6 3	0.60
198	56.82687	1.61885	1 2 -5	0.50
199	56.83497	1.61864	5 1 -4	0.00
200	57.02460	1.61370	2 7 0	0.00
201	57.02774	1.61362	0 4 4	2.70
202	57.12504	1.61110	5 0 -2	1.60
203	57.25165	1.60784	5 2 -3	4.00
204	57.35667	1.60515	4 5 -3	6.50
205	57.37698	1.60463	2 1 3	0.00
206	57.37909	1.60457	4 5 -2	0.00
207	57.43387	1.60317	0 8 0	0.00
208	57.61586	1.59854	5 1 -2	0.60
209	58.13815	1.58542	4 3 -5	0.00
210	58.16819	1.58467	1 0 4	1.50
211	58.24925	1.58266	4 3 0	0.00
212	58.28742	1.58171	2 5 2	0.00
213	58.30422	1.58130	5 2 -4	0.00
214	58.33750	1.58047	3 0 2	2.70
215	58.47399	1.57711	3 4 -5	0.00
216	58.49096	1.57669	1 5 3	2.20
217	58.65345	1.57271	1 1 4	0.80
218	58.79377	1.56929	1 8 -1	0.00
219	58.82189	1.56861	3 1 2	0.00
220	58.83758	1.56823	2 2 3	3.90
221	58.84909	1.56795	2 4 -5	0.00
222	58.86865	1.56747	0 8 1	0.00
223	59.07273	1.56254	5 2 -2	0.00
224	59.14502	1.56081	2 7 -3	0.50
225	59.15482	1.56057	1 8 0	0.00
226	59.26283	1.55798	2 6 -4	0.00
227	59.26298	1.55798	1 3 -5	0.70
228	59.31596	1.55672	3 6 0	0.00
229	59.36867	1.55546	1 7 -3	0.00
230	59.67676	1.54816	5 3 -3	0.10
231	60.09459	1.53839	1 2 4	0.00
232	60.18538	1.53629	4 5 -4	0.00
233	60.25065	1.53478	4 5 -1	0.00
234	60.26055	1.53455	3 2 2	1.00

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
235	60.56356	1.52760	3 7 -2	0.20
236	60.65803	1.52545	3 6 -4	0.00
237	60.70302	1.52442	5 3 -4	0.00
238	60.72715	1.52388	5 1 -5	0.00
239	60.76594	1.52300	3 5 1	0.30
240	61.03010	1.51703	3 0 -6	0.00
241	61.15045	1.51434	1 7 2	1.50
242	61.22356	1.51270	2 3 3	0.00
243	61.24439	1.51224	1 6 -4	0.00
244	61.25068	1.51210	1 8 -2	0.00
245	61.36014	1.50966	0 5 4	2.90
246	61.45315	1.50760	5 3 -2	0.00
247	61.48613	1.50687	4 4 -5	0.00
248	61.50151	1.50653	3 1 -6	1.60
249	61.59352	1.50450	4 4 0	2.30
250	61.62389	1.50383	3 7 -1	0.00
251	61.98739	1.49588	2 7 1	0.10
252	62.08684	1.49373	2 8 -1	0.00
253	62.13916	1.49260	5 2 -5	0.00
254	62.22177	1.49081	5 1 -1	0.00
255	62.25695	1.49005	4 0 -6	0.00
256	62.28226	1.48951	3 7 -3	0.00
257	62.30415	1.48904	1 8 1	0.20
258	62.45164	1.48588	1 3 4	0.90
259	62.54760	1.48383	0 1 5	0.00
260	62.57437	1.48326	1 4 -5	1.90
261	62.60977	1.48250	4 6 -3	0.00
262	62.61391	1.48241	3 3 2	0.00
263	62.63104	1.48205	4 6 -2	0.00
264	62.72301	1.48010	4 1 -6	0.00
265	62.74477	1.47964	3 5 -5	0.00
266	62.76365	1.47924	2 8 -2	1.50
267	62.87162	1.47696	4 1 1	0.00
268	62.90340	1.47629	3 2 -6	0.00
269	62.93175	1.47569	0 7 3	0.90
270	62.97519	1.47478	5 4 -3	0.00
271	63.05153	1.47317	0 8 2	0.70
272	63.10457	1.47206	2 5 -5	0.00
273	63.12231	1.47169	2 0 -6	0.00

**Rosickyite, syn**

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
274	63.49351	1.46398	2 6 2	0.00
275	63.58479	1.46210	2 1 -6	0.00
276	63.61459	1.46149	5 2 -1	0.00
277	63.68705	1.46000	1 6 3	0.00
278	63.93643	1.45490	0 2 5	0.00
279	63.97042	1.45421	5 4 -4	0.00
280	64.10972	1.45139	4 2 -6	0.00
281	64.14713	1.45063	2 8 0	0.00
282	64.25655	1.44843	4 2 1	0.00
283	64.45288	1.44449	5 3 -5	0.00
284	64.47582	1.44403	2 4 3	0.00
285	64.69887	1.43959	5 4 -2	0.00
286	64.96135	1.43440	2 2 -6	0.00

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
1	8.04469	10.98141	1 0 0	9.30
2	11.39300	7.76047	1 1 0	1.00
3	11.46518	7.71178	0 1 1	0.00
4	13.52684	6.54068	1 1 -1	6.50
5	14.49961	6.10399	1 1 1	42.20
6	16.12938	5.49070	2 0 0	0.00
7	16.14842	5.48427	0 2 0	11.20
8	16.33406	5.42236	0 0 2	15.80
9	17.46345	5.07415	1 0 -2	0.90
10	18.05250	4.90988	2 1 0	0.00
11	18.06531	4.90643	1 2 0	22.20
12	18.11138	4.89405	0 2 1	0.00
13	18.23622	4.86083	0 1 2	0.00
14	18.97044	4.67432	1 0 2	0.00
15	19.12718	4.63637	2 1 -1	57.10
16	19.25770	4.60524	1 1 -2	46.50
17	19.49532	4.54964	1 2 -1	41.00
18	20.18926	4.39480	1 2 1	0.80
19	20.51647	4.32544	2 1 1	0.60
20	20.63856	4.30013	1 1 2	2.20
21	21.79823	4.07391	2 0 -2	23.70
22	22.90060	3.88024	2 2 0	0.00
23	23.04719	3.85589	0 2 2	75.90

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
24	23.27289	3.81900	2 1 -2	75.30
25	23.76558	3.74093	2 2 -1	85.20
26	23.87183	3.72452	1 2 -2	55.90
27	24.20938	3.67335	2 0 2	53.20
28	24.29588	3.66047	3 0 0	29.90
29	24.90874	3.57178	2 2 1	100.00
30	25.01042	3.55748	1 2 2	34.30
31	25.55268	3.48321	2 1 2	0.00
32	25.63492	3.47222	3 1 0	0.00
33	25.65938	3.46896	1 3 0	0.00
34	25.69239	3.46458	0 3 1	86.70
35	25.93087	3.43326	0 1 3	0.00
36	26.14976	3.40501	3 1 -1	22.20
37	26.40820	3.37227	1 1 -3	96.70
38	26.70281	3.33573	1 3 -1	0.00
39	27.22232	3.27324	1 3 1	39.00
40	27.24692	3.27034	2 2 -2	0.00
41	27.71006	3.21672	3 1 1	0.00
42	27.94420	3.19030	3 0 -2	82.20
43	27.95514	3.18908	1 1 3	0.00
44	29.12728	3.06335	3 1 -2	3.90
45	29.23810	3.05200	2 2 2	0.00
46	29.27387	3.04835	2 1 -3	8.10
47	29.31076	3.04459	3 2 0	11.30
48	29.32427	3.04322	2 3 0	0.00
49	29.44088	3.03143	0 3 2	0.00
50	29.57265	3.01823	0 2 3	3.30
51	29.76677	2.99898	3 2 -1	13.80
52	29.99644	2.97654	1 2 -3	0.00
53	30.01637	2.97461	2 3 -1	11.10
54	30.10203	2.96634	1 3 -2	0.00
55	30.82482	2.89841	3 0 2	7.00
56	30.94510	2.88742	2 3 1	7.40
57	31.02845	2.87985	1 3 2	5.10
58	31.16060	2.86794	3 2 1	2.20
59	31.38103	2.84830	1 2 3	3.20
60	31.91058	2.80223	3 1 2	0.00
61	32.04562	2.79073	2 1 3	10.70
62	32.44051	2.75765	3 2 -2	2.70



## ?-S8

No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
63	32.57358	2.74669	2 2 -3	6.30
64	32.58990	2.74535	4 0 0	0.00
65	32.62919	2.74214	0 4 0	0.00
66	32.88919	2.72105	2 3 -2	0.00
67	33.01234	2.71118	0 0 4	9.10
68	33.18218	2.69769	1 0 -4	4.50
69	33.62461	2.66320	4 1 0	0.00
70	33.66044	2.66045	1 4 0	0.00
71	33.68623	2.65847	0 4 1	24.70
72	33.81743	2.64845	4 1 -1	28.00
73	33.97771	2.63633	3 1 -3	0.00
74	34.03567	2.63197	0 1 4	0.00
75	34.20101	2.61962	1 1 -4	1.30
76	34.48220	2.59890	1 4 -1	11.10
77	34.58570	2.59136	2 3 2	0.00
78	34.64825	2.58682	3 3 0	12.80
79	34.86610	2.57116	1 0 4	0.00
80	34.87402	2.57059	0 3 3	1.50
81	34.89607	2.56902	1 4 1	0.00
82	34.98697	2.56255	3 2 2	0.00
83	35.04173	2.55867	3 3 -1	1.10
84	35.05212	2.55794	4 0 -2	0.00
85	35.11150	2.55375	2 2 3	0.00
86	35.24052	2.54469	1 3 -3	0.50
87	35.34987	2.53707	2 0 -4	0.40
88	35.47480	2.52842	4 1 1	0.30
89	35.84282	2.50330	1 1 4	0.00
90	36.02445	2.49110	4 1 -2	0.50
91	36.25424	2.47583	3 3 1	0.00
92	36.31527	2.47181	2 1 -4	1.20
93	36.44728	2.46316	1 3 3	0.50
94	36.57363	2.45494	4 2 0	0.00
95	36.60027	2.45322	2 4 0	0.00
96	36.69612	2.44703	0 4 2	0.00
97	36.75290	2.44338	4 2 -1	6.50
98	36.90203	2.43384	3 2 -3	0.00
99	36.95598	2.43041	0 2 4	2.10
100	37.10996	2.42068	1 2 -4	0.00
101	37.17105	2.41685	2 4 -1	5.60

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
102	37.24201	2.41240	1 4 -2	0.00
103	37.37973	2.40383	3 3 -2	3.60
104	37.49737	2.39656	2 3 -3	0.90
105	37.60322	2.39006	3 1 3	0.90
106	37.94390	2.36938	2 4 1	4.40
107	38.01363	2.36519	1 4 2	0.00
108	38.21070	2.35344	4 0 2	4.40
109	38.29973	2.34818	4 2 1	3.00
110	38.48734	2.33716	2 0 4	1.10
111	38.64459	2.32801	1 2 4	3.00
112	38.81495	2.31819	4 2 -2	1.10
113	39.08797	2.30262	2 2 -4	4.50
114	39.11535	2.30107	4 1 2	0.00
115	39.22646	2.29481	3 0 -4	0.00
116	39.38661	2.28585	2 1 4	4.30
117	39.58545	2.27482	2 4 -2	0.00
118	39.64943	2.27130	3 3 2	10.80
119	39.76138	2.26516	2 3 3	3.10
120	39.95615	2.25457	4 1 -3	1.40
121	40.11180	2.24618	3 1 -4	2.00
122	40.30041	2.23610	3 2 3	0.30
123	41.04179	2.19740	2 4 2	0.00
124	41.06365	2.19628	5 0 0	0.00
125	41.08178	2.19535	4 3 0	3.60
126	41.09587	2.19463	3 4 0	0.00
127	41.24441	2.18707	4 3 -1	0.00
128	41.29133	2.18470	0 4 3	2.30
129	41.37982	2.18023	3 3 -3	0.00
130	41.42883	2.17776	0 3 4	0.00
131	41.43674	2.17736	3 4 -1	0.00
132	41.56879	2.17075	1 3 -4	2.50
133	41.60934	2.16873	1 4 -3	0.00
134	41.73034	2.16272	4 2 2	1.10
135	41.90068	2.15432	5 1 -1	0.00
136	41.91674	2.15353	5 1 0	0.00
137	41.96426	2.15120	1 5 0	0.00
138	41.98565	2.15016	0 5 1	0.00
139	41.98755	2.15007	2 2 4	12.30
140	42.41214	2.12952	1 1 -5	0.00

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
141	42.44925	2.12774	0 1 5	4.30
142	42.49352	2.12563	3 4 1	0.00
143	42.52822	2.12397	4 2 -3	0.00
144	42.64822	2.11828	1 5 -1	0.00
145	42.65392	2.11801	4 3 1	0.00
146	42.66264	2.11759	1 4 3	3.50
147	42.67613	2.11695	3 2 -4	0.00
148	42.76254	2.11288	5 0 -2	0.00
149	42.96961	2.10317	1 3 4	1.80
150	42.99476	2.10200	1 5 1	0.00
151	43.12576	2.09592	4 3 -2	0.00
152	43.37625	2.08439	2 3 -4	0.80
153	43.48269	2.07954	3 4 -2	0.00
154	43.50456	2.07854	3 0 4	0.00
155	43.58652	2.07482	2 4 -3	5.40
156	43.58852	2.07473	5 1 -2	0.00
157	43.63518	2.07262	5 1 1	0.00
158	44.02244	2.05529	2 1 -5	0.00
159	44.13040	2.05051	1 1 5	0.00
160	44.17595	2.04850	4 1 3	7.30
161	44.31944	2.04220	3 1 4	0.00
162	44.38040	2.03953	5 2 -1	0.00
163	44.39574	2.03887	5 2 0	0.00
164	44.43545	2.03714	2 5 0	0.00
165	44.43958	2.03696	4 0 -4	6.00
166	44.49233	2.03466	3 3 3	6.20
167	44.51711	2.03359	0 5 2	0.00
168	44.86907	2.01845	1 2 -5	0.00
169	44.90454	2.01694	0 2 5	0.00
170	44.92268	2.01617	2 5 -1	3.00
171	44.98341	2.01359	1 5 -2	0.00
172	45.24108	2.00271	4 1 -4	1.30
173	45.49948	1.99194	3 4 2	0.00
174	45.58598	1.98836	2 5 1	0.00
175	45.59966	1.98780	2 4 3	0.00
176	45.64602	1.98589	1 5 2	1.20
177	45.81588	1.97892	4 3 2	1.90
178	45.99522	1.97162	5 2 -2	8.40
179	46.03995	1.96981	5 2 1	0.00

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
180	46.05474	1.96921	2 3 4	0.00
181	46.12692	1.96629	5 0 2	8.30
182	46.41135	1.95490	2 2 -5	1.60
183	46.51494	1.95079	1 2 5	0.00
184	46.55760	1.94910	4 3 -3	0.00
185	46.55866	1.94906	4 2 3	2.90
186	46.69534	1.94367	3 3 -4	0.00
187	46.69640	1.94363	3 2 4	0.00
188	46.78600	1.94012	4 4 0	13.30
189	46.83233	1.93831	5 1 -3	0.00
190	46.90585	1.93544	5 1 2	0.00
191	46.93270	1.93440	4 4 -1	0.00
192	47.00769	1.93148	2 5 -2	0.00
193	47.05494	1.92966	3 4 -3	0.00
194	47.09920	1.92794	0 4 4	0.00
195	47.14530	1.92617	3 1 -5	4.20
196	47.22568	1.92308	1 4 -4	0.00
197	47.31580	1.91962	2 1 5	2.80
198	47.58205	1.90950	4 2 -4	0.30
199	48.20921	1.88611	4 4 1	0.00
200	48.28269	1.88342	2 5 2	0.00
201	48.28755	1.88324	5 3 -1	0.00
202	48.30192	1.88271	5 3 0	0.00
203	48.33027	1.88167	3 5 0	4.80
204	48.49632	1.87562	1 4 4	0.00
205	48.50237	1.87540	0 5 3	5.40
206	48.63054	1.87075	3 5 -1	0.00
207	48.63849	1.87047	4 4 -2	9.50
208	48.74577	1.86660	1 3 -5	0.00
209	48.77906	1.86540	0 3 5	0.00
210	48.78283	1.86527	1 5 -3	4.70
211	48.86677	1.86226	2 4 -4	0.00
212	49.11492	1.85343	5 2 -3	0.00
213	49.18584	1.85092	5 2 2	0.60
214	49.41693	1.84281	3 2 -5	0.50
215	49.56547	1.83763	3 5 1	0.00
216	49.58153	1.83708	2 2 5	2.30
217	49.59307	1.83668	4 0 4	0.00
218	49.71564	1.83243	1 5 3	1.50

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
219	49.77945	1.83023	6 0 0	0.00
220	49.80440	1.82938	5 3 -2	0.00
221	49.84181	1.82809	0 6 0	2.90
222	49.84653	1.82793	5 3 1	0.00
223	49.88701	1.82654	3 4 3	0.00
224	50.19650	1.81600	2 3 -5	0.00
225	50.26504	1.81369	1 0 -6	0.00
226	50.29418	1.81270	1 3 5	6.20
227	50.33125	1.81145	4 1 4	0.00
228	50.33542	1.81131	4 3 3	0.00
229	50.34893	1.81086	6 1 -1	0.00
230	50.44584	1.80761	3 5 -2	0.00
231	50.45049	1.80745	0 0 6	0.00
232	50.46536	1.80696	3 3 4	0.00
233	50.51563	1.80527	6 1 0	5.90
234	50.53853	1.80451	2 5 -3	0.00
235	50.57561	1.80327	1 6 0	0.00
236	50.59413	1.80266	0 6 1	0.00
237	50.68050	1.79979	5 0 -4	1.90
238	50.94720	1.79099	6 0 -2	3.70
239	50.99610	1.78939	1 1 -6	0.00
240	51.10323	1.78589	4 4 2	5.30
241	51.16907	1.78374	1 6 -1	6.70
242	51.17963	1.78340	0 1 6	0.00
243	51.30209	1.77943	4 3 -4	0.00
244	51.32342	1.77874	2 4 4	0.00
245	51.40728	1.77604	5 1 -4	0.00
246	51.47080	1.77399	1 6 1	3.10
247	51.50331	1.77295	5 1 3	0.00
248	51.53415	1.77196	2 0 -6	0.00
249	51.57178	1.77076	4 1 -5	0.00
250	51.67127	1.76758	6 1 -2	0.00
251	51.78765	1.76388	4 4 -3	0.00
252	51.79512	1.76365	3 1 5	2.20
253	51.91496	1.75986	3 4 -4	0.60
254	52.07927	1.75469	1 0 6	0.00
255	52.16105	1.75213	6 1 1	3.20
256	52.25240	1.74928	2 1 -6	0.00
257	52.25554	1.74919	3 5 2	0.00

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
258	52.34592	1.74638	2 5 3	3.20
259	52.50036	1.74160	4 2 4	2.30
260	52.51752	1.74108	6 2 -1	0.00
261	52.67928	1.73611	6 2 0	0.00
262	52.73251	1.73448	2 6 0	0.00
263	52.75500	1.73380	5 3 -3	2.10
264	52.79225	1.73266	1 1 6	0.00
265	52.80437	1.73229	0 6 2	0.00
266	52.82236	1.73174	5 3 2	0.00
267	53.04193	1.72509	3 3 -5	2.20
268	53.14574	1.72197	1 2 -6	0.00
269	53.16178	1.72148	2 6 -1	0.00
270	53.19841	1.72038	2 3 5	0.00
271	53.21537	1.71988	1 6 -2	7.60
272	53.32401	1.71663	0 2 6	3.50
273	53.39140	1.71462	5 4 -1	0.00
274	53.40477	1.71422	5 4 0	0.00
275	53.41960	1.71378	4 5 0	4.00
276	53.54518	1.71006	5 2 -4	6.20
277	53.55279	1.70983	4 5 -1	0.00
278	53.63851	1.70730	5 2 3	0.00
279	53.66383	1.70656	3 5 -3	0.00
280	53.70406	1.70537	0 5 4	0.00
281	53.70506	1.70534	4 2 -5	0.00
282	53.74817	1.70408	2 6 1	0.00
283	53.80136	1.70252	1 6 2	0.00
284	53.80177	1.70251	6 2 -2	0.00
285	53.81786	1.70204	1 4 -5	0.00
286	53.81904	1.70200	1 5 -4	4.60
287	53.84887	1.70113	0 4 5	0.00
288	53.92217	1.69899	3 2 5	0.00
289	54.18448	1.69138	3 0 -6	1.60
290	54.27804	1.68869	6 2 1	2.40
291	54.36691	1.68614	2 2 -6	2.20
292	54.40489	1.68505	6 1 -3	0.00
293	54.49997	1.68233	6 0 2	1.30
294	54.71544	1.67622	4 5 1	0.00
295	54.80565	1.67367	5 4 -2	0.00
296	54.84503	1.67256	5 4 1	0.00

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
297	54.87842	1.67162	3 1 -6	4.70
298	54.89230	1.67123	1 2 6	0.00
299	54.97785	1.66884	1 5 4	0.00
300	55.01252	1.66787	2 6 -2	7.60
301	55.06022	1.66653	2 0 6	0.00
302	55.10790	1.66520	4 5 -2	4.10
303	55.17237	1.66341	2 4 -5	0.00
304	55.19121	1.66289	6 1 2	0.00
305	55.26381	1.66088	1 4 5	0.00
306	55.30241	1.65981	4 4 3	0.00
307	55.31688	1.65941	2 5 -4	2.10
308	55.42410	1.65645	3 4 4	0.00
309	55.74679	1.64762	2 1 6	0.00
310	55.98313	1.64123	4 3 4	0.00
311	55.99955	1.64079	6 3 -1	0.00
312	56.15441	1.63663	6 3 0	0.00
313	56.15465	1.63662	2 6 2	0.00
314	56.19742	1.63548	3 6 0	0.00
315	56.20887	1.63517	4 4 -4	0.00
316	56.25332	1.63398	3 5 3	0.00
317	56.35220	1.63135	0 6 3	0.00
318	56.46393	1.62839	6 2 -3	0.00
319	56.46755	1.62829	3 6 -1	0.00
320	56.53533	1.62650	5 0 4	0.00
321	56.60127	1.62476	1 3 -6	0.00
322	56.60471	1.62467	1 6 -3	0.00
323	56.77216	1.62028	0 3 6	0.00
324	56.92600	1.61626	3 2 -6	0.00
325	56.98427	1.61475	5 3 -4	0.00
326	57.07380	1.61243	5 3 3	0.00
327	57.09524	1.61187	5 1 -5	0.00
328	57.13765	1.61078	4 3 -5	0.00
329	57.21018	1.60891	5 1 4	0.00
330	57.23045	1.60839	6 3 -2	0.00
331	57.23137	1.60836	6 2 2	0.00
332	57.31119	1.60631	3 6 1	0.00
333	57.34602	1.60542	3 3 5	0.00
334	57.36318	1.60498	4 1 5	0.00
335	57.37460	1.60469	4 5 2	0.00

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
336	57.44704	1.60284	1 6 3	0.00
337	57.57621	1.59955	5 4 -3	0.00
338	57.57816	1.59950	2 5 4	0.00
339	57.63974	1.59793	5 4 2	0.00
340	57.68776	1.59672	6 3 1	0.00
341	57.74978	1.59515	6 0 -4	0.00
342	57.77313	1.59456	2 3 -6	0.00
343	57.77404	1.59454	2 2 6	0.00
344	57.84692	1.59270	3 4 -5	0.00
345	57.99463	1.58900	2 4 5	0.00
346	58.00786	1.58867	4 5 -3	0.00
347	58.08740	1.58668	4 0 -6	0.00
348	58.10903	1.58614	3 6 -2	0.00
349	58.12584	1.58572	3 5 -4	0.00
350	58.19322	1.58405	2 6 -3	0.00
351	58.27817	1.58194	1 3 6	0.00
352	58.41561	1.57855	6 1 -4	0.00
353	58.75081	1.57034	4 1 -6	0.00
354	58.81512	1.56877	7 0 0	0.00
355	59.09257	1.56207	5 2 -5	0.00
356	59.18713	1.55980	7 1 -1	0.00
357	59.20505	1.55937	5 2 4	0.00
358	59.25768	1.55811	3 0 6	0.00
359	59.35479	1.55579	4 2 5	0.00
360	59.46570	1.55315	6 1 3	0.00
361	59.47346	1.55297	7 1 0	0.00
362	59.49787	1.55239	5 5 -1	0.00
363	59.51032	1.55209	5 5 0	0.00
364	59.54717	1.55122	1 7 0	0.00
365	59.56376	1.55083	0 7 1	0.00
366	59.58782	1.55026	7 0 -2	0.00
367	59.75901	1.54623	3 6 2	0.00
368	59.79188	1.54546	6 3 -3	0.00
369	59.84176	1.54429	2 6 3	0.00
370	59.89547	1.54303	1 5 -5	0.00
371	59.91303	1.54262	3 1 6	0.00
372	59.92440	1.54236	0 5 5	0.00
373	59.98324	1.54098	1 1 -7	0.00
374	60.07976	1.53874	1 7 -1	0.00



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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
375	60.23774	1.53508	3 3 -6	0.00
376	60.24098	1.53501	7 1 -2	0.00
377	60.28373	1.53402	0 1 7	0.00
378	60.35116	1.53247	1 7 1	0.00
379	60.38548	1.53168	6 2 -4	0.00
380	60.53259	1.52831	6 3 2	0.00
381	60.63380	1.52600	4 4 4	0.00
382	60.64941	1.52564	6 4 -1	0.00
383	60.71399	1.52417	4 2 -6	0.00
384	60.79674	1.52230	6 4 0	0.00
385	60.81856	1.52180	5 5 -2	0.00
386	60.82705	1.52161	4 6 0	0.00
387	60.85543	1.52097	5 5 1	0.00
388	60.94957	1.51885	4 6 -1	0.00
389	60.97969	1.51817	2 1 -7	0.00
390	61.05178	1.51655	3 6 -3	0.00
391	61.05694	1.51643	2 3 6	0.00
392	61.08849	1.51572	7 1 1	0.00
393	61.08881	1.51572	0 6 4	0.00
394	61.14177	1.51453	7 2 -1	0.00
395	61.16202	1.51408	2 5 -5	0.00
396	61.19470	1.51335	1 6 -4	0.00
397	61.22214	1.51274	1 4 -6	0.00
398	61.24771	1.51217	1 5 5	0.00
399	61.28390	1.51136	4 5 3	0.00
400	61.38494	1.50911	0 4 6	0.00
401	61.39800	1.50882	3 5 4	0.00
402	61.41497	1.50845	6 2 3	0.00
403	61.42258	1.50828	7 2 0	0.00
404	61.49037	1.50678	2 7 0	0.00
405	61.55546	1.50534	0 7 2	0.00
406	61.58711	1.50464	5 4 -4	0.00
407	61.67247	1.50277	5 4 3	0.00
408	61.73337	1.50143	4 4 -5	0.00
409	61.82188	1.49949	6 4 -2	0.00
410	61.85384	1.49879	3 2 6	0.00
411	61.86987	1.49844	1 1 7	0.00
412	61.87952	1.49823	2 7 -1	0.00
413	61.92275	1.49729	1 2 -7	0.00

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
414	61.92816	1.49717	1 7 -2	0.00
415	61.93214	1.49709	3 4 5	0.00
416	62.02184	1.49514	4 6 1	0.00
417	62.13486	1.49269	4 5 -4	0.00
418	62.17571	1.49181	7 2 -2	0.00
419	62.21768	1.49090	0 2 7	0.00
420	62.25834	1.49002	6 4 1	0.00
421	62.26451	1.48989	1 6 4	0.00
422	62.33293	1.48842	5 3 -5	0.00
423	62.33987	1.48827	2 4 -6	0.00
424	62.38487	1.48731	4 6 -2	0.00
425	62.41235	1.48672	2 7 1	0.00
426	62.44191	1.48608	5 3 4	0.00
427	62.46076	1.48568	1 7 2	0.00
428	62.57840	1.48317	2 6 -4	0.00
429	62.58701	1.48299	4 3 5	0.00
430	62.59418	1.48283	7 1 -3	0.00
431	62.82251	1.47799	1 4 6	0.00
432	62.90109	1.47634	2 2 -7	0.00
433	63.00797	1.47409	7 2 1	0.00
434	63.10280	1.47210	5 0 -6	0.00
435	63.23678	1.46930	3 1 -7	0.00
436	63.34213	1.46711	7 0 2	0.00
437	63.42286	1.46544	5 5 -3	0.00
438	63.44739	1.46493	3 6 3	0.00
439	63.48283	1.46420	5 5 2	0.00
440	63.55918	1.46263	6 1 -5	0.00
441	63.56598	1.46249	2 7 -2	0.00
442	63.58672	1.46206	6 3 -4	0.00
443	63.67846	1.46017	3 5 -5	0.00
444	63.73476	1.45902	5 1 -6	0.00
445	63.77584	1.45818	1 2 7	0.00
446	63.81802	1.45732	2 5 5	0.00
447	63.86630	1.45633	5 1 5	0.00
448	63.90569	1.45553	4 3 -6	0.00
449	63.97278	1.45416	7 1 2	0.00
450	64.21777	1.44921	6 0 4	0.00
451	64.27226	1.44811	6 4 -3	0.00
452	64.32126	1.44712	7 3 -1	0.00

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No.	2 $\theta$ , °	d, Å	h k l	Norm. I.
453	64.48812	1.44378	7 2 -3	0.00
454	64.49172	1.44371	4 6 2	0.00
455	64.53503	1.44285	4 0 6	0.00
456	64.58681	1.44181	6 3 3	0.00
457	64.59422	1.44167	7 3 0	0.00
458	64.61348	1.44128	2 7 2	0.00
459	64.65280	1.44050	3 7 0	0.00
460	64.68175	1.43993	2 6 4	0.00
461	64.68690	1.43982	2 1 7	0.00
462	64.70017	1.43956	3 4 -6	0.00
463	64.79516	1.43768	0 7 3	0.00
464	64.84377	1.43672	6 1 4	0.00
465	64.90131	1.43559	3 7 -1	0.00
466	64.98337	1.43397	6 4 2	0.00