

five, convergence was attained.

The agreement of calculated with observed structure amplitudes shows that the results are at least approximately correct. For the 429 observable data, the discrepancy factor is 0.16. Of the 436 data (not included among those systematically absent) below threshold, 388 have $|F_{\text{calc}}|$ below the minimum observable $|F_{\text{obs}}|$ and 48 have $|F_{\text{calc}}|$ greater than threshold values, in most cases, only slightly greater. For all the reflections systematically absent, the $|F_{\text{calc}}|$ was less than the minimum observable value. This overall agreement is satisfactory considering the nature of the crystals and the necessary idealization of the structure.

The structure of the helical molecule was given only one variable, namely, the radius, r , in the least-squares analysis. Because the final value of r , 0.95 Å, is very near that given by Prins et al.⁷ the structure of the molecule remains very much like the one they described: The S-S distance is 2.07 Å and the S-S-S bond angle, 106°; the shortest non-bonded S-S distance is 3.30 Å and the dihedral angle $S_1S_2S_3 - S_2S_3S_4$ is 95°.

None of the large number of intermolecular distances (Fig. 3) is significantly shorter than 3.37 Å, the shortest intermolecular distance

previously reported for sulfur.

We have indicated earlier that the pressure-induced fibrous modification of sulfur is identical with ψ -sulfur. The rotation photograph about the fiber axis of a crystal of the pressure-induced phase exactly matches that of a fiber pattern of ψ -sulfur. The literature¹² contains erroneous conclusions regarding the indexing of this pattern. For completeness, we give here (Table 1) our indexing based on the pseudo-orthorhombic cell and confirm that the data obtained by Tuinstra from the fiber pattern of ψ -sulfur agree with those from the pressure-induced phase. There is greater resolution in our data, however. (We hope to have a somewhat more detailed discussion of this indexing published elsewhere).

The crystals of the fibrous phase of sulfur have remained intact (at atmospheric pressure and room temperature), that is, with no apparent transformation to any other phase, for a period of approximately 3½ years.

With respect to phase (I), we have proposed that it is probable that the sulfur helical molecules lie in planes perpendicular to a 32.4 Å repeat distance as in the fibrous phase, but because it is lamellar, the helices are skew to each other in alternating planes. Phase I has

Table 1. Indexing of Rotation Photograph of Ψ -Sulfur

Tuinstra				Present Work				Tuinstra				Present Work				Tuinstra				Present Work									
Q _o	Q _o	Q _c	h k l	Q _o	Q _o	Q _c	h k l	Q _o	Q _o	Q _c	h k l	Q _o	Q _o	Q _c	h k l	Q _o	Q _o	Q _c	h k l	Q _o	Q _o	Q _c	h k l	Q _o	Q _o	Q _c	h k l		
473	478	467	002	*	2625	2634	2,12,3					3792	3774	3759	4,14,3														
613	613	610	080	*	3253	3284	245						3826	3800	425														
		620	042	*	3713	3701	2,16,3					4093	4036	4043	4,18,1														
1842	1847	1839	0,12,2	*	4092	4137	2,20,1					4751	4719	4715	4,10,5														
2050	2046	2022	044	*	4451	4501	2,12,5					*	5639	5629	4,14,5														
2431	2422	2439	0,16,0	*	5582	5570	2,16,5					*	6472	6503	4,22,3														
2470	2475	2480	084	*	5839	5814	2,24,1					*	6957	6910	467														
2868	2894	2906	0,16,2	*	6099	6089	247																						
3244	3234	3242	0,12,4	*	6610	6547	287					2250	2230	2233	660														
4265	4271	4208	006									2379	2372	2396	622														
		4278	0,20,2	946	950	939	370					2707	2706	2701	662														
4316	4345	4309	0,16,4	*	1032	1026	332					2800	2823	2843	6,10,0														
4845	4843	4817	086	1165	1160	1178	352				3284	3300	3311	6,10,2															
5449	5455	5487	0,24,0	1222	1224	1244	390				3797	3807	3798	624															
5618	5619	5579	0,12,6	1414	1414	1407	372				4172	4089	4103	664															
		5680	0,20,4	1691	1706	1712	392				*	4762	4712	6,10,4															
*	6631	6646	0,16,6	2104	2107	2093	3,11,2				*	4923	4977	6,18,0															
					2377	2352	314				*	5484	5444	6,18,2															
962	967	941	191		2431	2428	334				*	5640	5628	6,14,4															
1146	1133	1113	113	2500	2532	2550	3,13,2				*	6171	6136	626															
1300	1318	1322	1,11,1		2578	2581	354				*	6521	6501	6,22,0															
1361	1380	1342	153			2616	3,15,0				*	6952	6968	6,22,2															
1933	1934	1876	193	3110	3099	3083	3,15,2				*	7070	7050	6,10,6															
2250	2251	2257	1,11,3			3114	394																						
2978	2948	2922	1,17,1	*	3171	3226	3,17,0				2732	**	2699	711															
3113	3086	3060	135	3517	3489	3495	3,11,4				2808	**	2776	731															
3255	3233	3212	155	*	5547	5512	3,23,0				2950	**	2928	751															
		3248	1,15,3	*	6295	6290	3,13,6				3470	**	3461	791															
3470	3454	3441	175	*		7885	3,27,2				3712	**	3710	733															
3560	3548	3608	1,19,1	*	7916	7962	318				3867	**	3843	7,11,1															
3790	3750	3746	195	*	8263	8296	3,25,4					**	3863	753															
3860	3875	3857	1,17,3	*	8856	8881	3,21,6				4136	**	4092	773															
5130	5135	5118	1,15,5	*	9270	9287	3,27,4				4337	**	4397	793															
		5789	117																										
5900	5858	5865	137	1318	1316	1300	461				5414	**	5406	10,2,1															
		6123	1,25,1	1942	1936	1910	4,10,1				5550	**	5520	10,4,1															
6200	6096	6144	1,23,3			1930	423				6017	**	5978	10,8,1															
		6246	177	2250	2253	2235	463																						
*	7005	6932	1,11,7	2866	2856	2824	4,14,1																						
		7058	1,25,3			2844	4,10,3																						

* Not reported by Tuinstra.

** Not measured in present work.