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The Crystal and Molecular Structure of 1-Thiacyclobutane-3-carboxylic Acid-1-oxide

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The high melting isomer of 1-thiacyclobutane-3-carboxylic acid-1-oxide ($C_4H_6O_3S$) is orthorhombic ($Pna2_1$) with $a = 9.89 \pm 0.05$, $b = 5.41 \pm 0.02$, and $c = 10.81 \pm 0.08$ Å. The molecule has the *trans* configuration and shows a puckered four membered ring (dihedral angle 153°). The molecules are held together by hydrogen bonds between the carboxyl and sulphoxide groups.

1-Thiacyclobutane-3-carboxylic acid-1-oxide ($C_4H_6O_3S$) was prepared by Allenmark.[1] He found that the synthetic product had a diffuse melting point and interpreted this as due to the presence of the geometric isomers which are possible because of the ring system. A separation of the two forms was possible by repeated recrystallization from ethyl acetate or acetone. One modification melted at 130.5 – 133.0°C whereas the other (isolated from the mother liquor) melted between 133°C and 138°C. Crystals from the high melting form were used for a crystal structure determination.

EXPERIMENTAL

Crystals of $C_4H_6O_3S$ are orthorhombic ($Pna2_1$) with the following unit cell dimensions: $a = 9.89 \pm 0.05$, $b = 5.41 \pm 0.02$, and $c = 10.81 \pm 0.08$ Å.

The intensity data were collected with the Weissenberg technique using Cu$K\alpha$ radiation. Rotation about the b-axis gave layers 0 – 4, and about the c-axis layers 0 – 7. The film intensities were measured on the automatic film scanner [2] developed at this institute. They were then scaled [3] together to a set of 532 independent reflexions. The intensities were corrected for the Lorentz and polarization factors but not for absorption.

STRUCTURE DETERMINATION

The sulphur atom was found from a sharpened Patterson series and the remaining atoms were then located from successive electron density and difference syntheses. The hydrogen atom of the carboxyl group was found at the expected position but was poorly defined. This has been the case in rather

Table 1. Observed and calculated structure factors. The phase angles are given as fractions of one revolution.

H	K	L	Fobs	Fcalc	FI
0	0	2	356	518	0.118
0	0	4	294	421	0.822
0	0	6	251	279	0.899
0	0	8	180	191	0.062
0	0	10	217	226	0.931
0	0	12	132	132	0.061
0	1	3	259	266	0.076
0	1	5	418	407	0.226
0	1	7	212	182	0.357
0	1	9	85	71	0.908
0	1	11	108	99	0.198
0	2	0	704	604	0.000
0	2	2	363	359	0.920
0	2	4	229	234	0.016
0	2	6	93	77	0.742
0	2	8	135	138	0.993
0	2	10	115	104	0.961
0	2	12	54	46	0.980
0	3	1	263	226	0.379
0	3	3	331	319	0.190
0	3	5	362	351	0.263
0	3	7	258	234	0.254
0	3	9	61	50	0.132
0	3	11	116	90	0.220
0	4	0	271	219	0.500
0	4	4	94	96	0.234
0	4	6	84	98	0.494
0	4	8	41	36	0.703
0	4	10	25	30	0.477
0	5	1	57	49	0.140
0	5	3	203	190	0.247
0	5	5	69	68	0.335
0	5	7	131	127	0.157
0	6	0	104	91	0.500
0	6	2	99	104	0.446
0	6	4	86	94	0.555
1	1	0	436	446	1.000
1	1	1	623	622	0.300
1	1	2	566	623	0.973
1	1	3	308	316	0.244
1	1	4	175	203	0.778
1	1	5	30	29	0.174
1	1	6	209	209	0.063
1	1	7	172	189	0.104
1	1	8	165	163	0.037
1	1	9	122	107	0.158
1	1	10	164	149	0.072
1	1	11	67	65	0.262
1	1	12	110	91	0.947
1	2	0	20	8	0.500
1	2	1	222	197	0.153
1	2	2	341	308	0.332
1	2	3	345	315	0.365
1	2	4	310	324	0.501
1	2	5	307	293	0.247
1	2	6	89	80	0.530
1	2	7	157	142	0.249
1	2	8	34	35	0.528
1	2	9	131	125	0.205
1	2	10	48	47	0.398
1	2	11	55	54	0.215
1	2	12	22	30	0.562
1	3	0	28	29	0.000
1	3	1	114	97	0.334
1	3	2	98	95	0.861
1	3	3	49	46	0.183
1	3	4	40	38	0.807
1	3	5	47	46	0.190
1	3	6	77	71	0.206
1	3	7	25	25	0.128
1	3	9	33	32	0.952
1	3	10	29	30	0.994
1	3	11	25	26	0.040
1	4	0	148	123	0.500
1	4	1	148	129	0.236
1	4	2	86	80	0.396
1	4	3	182	178	0.362
1	4	4	134	142	0.455
1	4	5	201	192	0.235
1	4	6	96	95	0.464
1	4	7	113	102	0.246
1	4	8	63	59	0.569
1	4	9	112	95	0.210
1	5	0	117	100	0.500
1	5	1	76	57	0.802
1	5	2	124	108	0.513
1	5	3	34	35	0.781
1	5	4	55	54	0.435
1	5	5	19	18	0.868
1	5	6	73	71	0.479
1	5	7	35	36	0.697
1	6	0	40	39	0.500
1	6	1	33	29	0.309
1	6	3	27	37	0.433
2	0	0	41	26	0.500
2	0	1	393	508	0.115
2	0	3	373	514	0.339
2	0	4	230	270	0.087
2	0	5	196	247	0.252
2	0	6	100	98	0.383
2	0	7	181	207	0.196
2	0	8	197	224	0.108
2	0	9	253	271	0.292
2	0	10	112	110	0.116
2	0	11	38	43	0.375
2	0	12	78	68	0.956
2	1	0	263	240	1.000
2	1	1	64	56	0.796
2	1	2	417	441	0.418
2	1	3	188	274	0.332
2	1	4	220	231	0.597
2	1	5	140	133	0.541
2	1	6	48	47	0.643
2	1	7	148	134	0.108
2	1	8	124	111	0.425
2	1	9	92	82	0.279
2	1	10	74	69	0.570
2	1	12	48	45	0.412
2	2	0	195	175	0.000
2	2	1	204	176	0.190
2	2	2	125	113	0.701
2	2	3	113	103	0.315
2	2	4	88	78	0.839
2	2	5	224	221	0.215
2	2	6	79	78	0.188
2	2	7	116	102	0.355
2	2	8	127	131	0.184
2	2	9	91	79	0.273
2	2	10	65	66	0.064
2	2	11	45	48	0.257
2	2	12	35	45	0.030
2	3	0	83	69	0.500
2	3	1	148	113	0.437
2	3	2	400	357	0.478
2	3	3	191	188	0.359
2	3	4	170	164	0.529
2	3	5	124	115	0.415
2	3	6	158	149	0.544
2	3	7	156	143	0.164
2	3	8	149	128	0.453
2	3	9	99	80	0.237
2	3	10	135	106	0.531
2	3	11	58	54	0.266
2	4	0	31	31	0.000
2	4	1	91	75	0.652
2	4	2	115	108	0.402
2	4	3	117	108	0.820
2	4	4	94	90	0.587
2	4	5	20	21	0.206
2	4	6	39	42	0.175
2	4	7	86	81	0.599
2	4	8	47	49	0.375
2	4	9	66	68	0.785
2	5	0	180	157	0.500
2	5	1	122	110	0.425
2	5	2	125	122	0.637
2	5	3	39	40	0.512
2	5	4	46	41	0.287
2	5	5	58	63	0.273
2	5	6	87	94	0.519
2	5	7	31	42	0.300
2	6	0	82	86	0.500
2	6	1	86	82	0.751
2	6	2	19	24	0.489
2	6	3	48	53	0.750
2	6	4	47	54	0.406
3	1	0	221	221	0.000
3	1	1	348	347	0.407
3	1	2	249	260	0.854
3	1	3	248	268	0.176
3	1	4	102	100	0.628
3	1	5	251	262	0.312
3	1	6	123	124	0.447
3	1	7	279	279	0.284
3	1	8	47	50	0.517
3	1	9	123	122	0.330
3	1	10	63	58	0.935
3	1	11	147	133	0.275
3	2	0	519	474	0.500
3	2	1	132	104	0.673
3	2	2	128	110	0.564
3	2	3	92	79	0.520
3	2	4	270	252	0.513
3	2	5	63	64	0.227
3	2	6	152	160	0.512
3	2	7	44	38	0.116
3	2	8	147	133	0.551
3	2	9	24	30	0.974
3	2	10	142	131	0.449
3	2	11	25	29	0.634
3	3	0	158	138	0.000
3	3	1	96	87	0.861
3	3	2	51	44	0.133
3	3	3	86	86	0.223
3	3	4	80	73	0.512
3	3	5	78	76	0.514
3	3	6	50	44	0.689
3	3	7	34	33	0.313
3	3	8	41	41	0.016
3	3	9	47	44	0.427
3	4	0	264	224	0.500
3	4	1	86	77	0.738
3	4	2	147	134	0.505
3	4	3	32	30	0.381
3	4	4	196	181	0.573
3	4	5	51	54	0.247
3	4	6	76	74	0.460
3	4	7	26	26	0.184
3	4	8	126	132	0.521
3	4	9	12	18	0.816
3	5	0	30	25	0.000
3	5	1	124	101	0.780
3	5	2	26	27	0.274
3	5	3	100	98	0.718
3	5	5	75	80	0.756
3	5	6	16	21	0.919
3	5	7	71	78	0.720
3	6	0	42	39	0.500
3	6	1	18	25	0.794
3	6	2	18	26	0.573
3	6	3	13	19	0.132
3	6	4	23	35	0.693
4	0	0	79	82	0.500
4	0	1	485	582	0.271
4	0	2	273	299	0.780
4	0	3	137	138	0.424
4	0	4	229	237	0.613
4	0	5	361	417	0.184
4	0	6	189	217	0.466
4	0	7	136	146	0.351
4	0	8	123	141	0.540
4	0	9	140	148	0.140
4	0	10	58	65	0.542
4	0	11	120	128	0.231
4	1	0	239	270	0.500
4	1	1	88	106	0.644
4	1	2	173	180	0.656
4	1	3	140	144	0.630
4	1	4	182	180	0.277
4	1	5	46	55	0.843
4	1	6	187	201	0.523
4	1	7	56	59	0.915
4	1	8	33	28	0.674
4	1	9	19	21	0.737
4	1	10	55	53	0.439
4	1	11	70	62	0.732
4	2	0	82	72	0.000
4	2	1	221	208	0.203
4	2	2	88	78	0.874
4	2	3	198	194	0.348
4	2	4	167	160	0.587
4	2	5	106	110	0.222
4	2	6	103	105	0.527
4	2	7	68	68	0.158
4	2	8	61	55	0.583
4	2	9	125	108	0.211
4	2	10	46	30	0.592
4	2	11	27	38	0.265
4	3	0	183	164	0.500
4	3	1	200	161	0.743
4	3	2	244	217	0.517

Table 1. Continued.

H	K	L	Fobs	Fcalc	FI
4	3	3	152	127	0.670
4	3	4	168	159	0.387
4	3	5	44	42	0.880
4	3	6	213	222	0.526
4	3	7	68	74	0.854
4	3	8	84	75	0.513
4	3	9	79	66	0.777
4	3	10	88	74	0.516
4	4	0	120	99	0.000
4	4	1	84	72	0.864
4	4	2	59	57	0.108
4	4	3	44	40	0.356
4	4	4	23	12	0.779
4	4	5	96	93	0.683
4	4	6	46	47	0.904
4	4	7	60	64	0.938
4	4	8	42	41	0.954
4	4	9	35	20	0.461
4	5	0	35	33	0.000
4	5	1	75	78	0.792
4	5	2	147	145	0.410
4	5	3	34	21	0.794
4	5	4	81	93	0.528
4	5	5	23	22	0.162
4	5	6	38	46	0.541
4	5	7	28	31	0.773
4	6	4	42	56	0.017
5	1	0	109	114	0.500
5	1	1	121	125	0.244
5	1	2	318	383	0.567
5	1	3	238	261	0.206
5	1	4	212	217	0.556
5	1	5	87	95	0.315
5	1	6	184	193	0.482
5	1	7	110	121	0.138
5	1	8	134	183	0.383
5	1	9	30	33	0.185
5	1	10	98	94	0.503
5	1	11	43	40	0.115
5	2	0	175	177	0.500
5	2	1	269	271	0.626
5	2	2	101	106	0.476
5	2	3	237	240	0.709
5	2	4	90	79	0.585
5	2	5	139	143	0.734
5	2	6	90	101	0.268
5	2	7	64	70	0.803
5	2	8	124	119	0.507
5	2	9	120	110	0.776
5	3	0	68	61	0.500
5	3	1	126	123	0.361
5	3	2	100	98	0.689
5	3	3	23	22	0.760
5	3	5	59	63	0.127
5	3	6	48	52	0.470
5	3	7	17	23	0.208
5	3	9	30	30	0.998
5	4	0	134	133	0.500
5	4	1	164	170	0.685
5	4	2	48	45	0.152
5	4	3	114	116	0.679
5	4	4	109	99	0.433
5	4	5	127	139	0.702
5	4	6	52	58	0.479
5	4	7	81	88	0.841
5	4	8	28	29	0.573
5	4	9	41	70	0.807
5	5	0	60	58	0.000
5	5	1	28	23	0.791
5	5	2	72	74	0.031
5	5	3	35	34	0.678
5	5	4	39	51	0.030
5	5	5	23	26	0.819
5	5	6	21	56	0.005
6	0	0	171	159	0.500
6	0	1	245	267	0.845
6	0	2	234	231	0.453
6	0	3	76	69	0.207
6	0	4	430	475	0.550
6	0	5	73	69	0.424
6	0	6	169	186	0.433
6	0	7	45	50	0.524
6	0	8	173	185	0.454
6	0	10	75	76	0.441
6	1	1	141	147	0.721
6	1	2	44	39	0.573
6	1	3	176	172	0.711
6	1	4	73	71	0.891
6	1	5	28	24	0.970
6	1	6	50	53	0.096
6	1	7	92	95	0.653
6	1	8	23	26	0.402
6	1	9	87	83	0.807
6	1	10	21	23	0.666
6	2	0	171	175	0.500
6	2	1	75	77	0.758
6	2	2	107	98	0.563
6	2	3	26	22	0.803
6	2	4	196	198	0.520
6	2	5	15	26	0.227
6	2	6	125	137	0.435
6	2	7	35	44	0.444
6	2	8	84	75	0.468
6	2	10	42	45	0.386
6	3	0	37	28	0.500
6	3	1	230	237	0.749
6	3	2	39	42	0.678
6	3	3	238	227	0.691
6	3	4	84	81	0.924
6	3	5	72	66	0.763
6	3	6	45	45	0.077
6	3	7	129	129	0.711
6	3	9	108	94	0.797
6	4	0	25	22	0.500
6	4	1	53	54	0.427
6	4	2	72	73	0.868
6	4	3	39	39	0.724
6	4	4	68	69	0.094
6	4	5	21	20	0.042
6	4	7	23	21	0.315
6	4	8	25	39	0.978
6	5	0	28	31	0.500
6	5	1	91	103	0.783
6	5	2	13	24	0.781
6	5	3	67	74	0.641
6	5	5	9	58	0.724
7	1	0	56	54	0.000
7	1	1	149	146	0.741
7	1	2	129	119	0.580
7	1	3	159	152	0.689
7	1	4	181	179	0.477
7	1	5	86	80	0.696
7	1	6	238	251	0.554
7	1	7	90	94	0.736
7	1	8	41	46	0.521
7	1	9	27	35	0.770
7	2	0	112	109	0.000
7	2	1	267	260	0.778
7	2	2	110	103	0.014
7	2	3	43	37	0.996
7	2	4	87	76	0.048
7	2	5	113	115	0.633
7	2	6	78	79	0.907
7	2	7	75	76	0.845
7	2	8	63	66	0.004
7	2	9	103	87	0.735
7	3	0	67	70	0.000
7	3	1	27	26	0.795
7	3	2	36	37	0.483
7	3	3	39	39	0.582
7	3	4	56	53	0.705
7	3	5	20	22	0.713
7	3	6	18	20	0.279
7	3	8	52	49	0.500
7	4	0	98	94	0.000
7	4	1	137	141	0.695
7	4	2	63	60	0.022
7	4	3	105	98	0.800
7	4	4	58	65	0.004
7	4	5	30	34	0.784
7	4	6	52	53	0.961
7	4	7	25	34	0.752
7	5	0	24	21	1.000
7	5	1	41	40	0.268
7	5	2	17	57	0.967
7	5	3	19	31	0.250
8	0	0	71	63	0.500
8	0	1	130	136	0.664
8	0	2	101	98	0.786
8	0	3	111	136	0.710
8	0	4	125	128	0.562
8	0	5	196	206	0.752
8	0	6	87	92	0.519
8	0	7	116	126	0.876
8	0	8	43	44	0.506
8	0	9	81	83	0.793
8	1	0	131	113	0.000
8	1	1	103	89	0.839
8	1	2	108	100	0.101
8	1	3	32	29	0.442
8	1	4	25	26	0.981
8	1	5	23	27	0.598
8	1	6	73	69	0.990
8	1	7	39	38	0.819
8	1	8	47	52	0.974
8	2	0	25	19	0.500
8	2	1	75	68	0.655
8	2	2	65	57	0.733
8	2	3	68	53	0.745
8	2	4	80	77	0.623
8	2	5	85	82	0.759
8	2	6	34	29	0.466
8	2	7	57	63	0.852
8	2	8	37	39	0.462
8	3	0	154	136	0.000
8	3	1	98	83	0.794
8	3	2	172	150	0.074
8	3	3	66	61	0.576
8	3	4	75	66	0.031
8	3	5	26	32	0.745
8	3	6	106	95	0.009
8	3	7	52	52	0.828
8	4	0	28	28	0.000
8	4	1	42	35	0.239
8	4	3	49	46	0.194
8	4	4	18	29	0.858
8	4	5	47	51	0.241
9	1	0	40	35	1.000
9	1	1	144	128	0.758
9	1	2	51	54	0.641
9	1	3	168	161	0.732
9	1	4	46	52	0.746
9	1	5	91	87	0.869
9	1	6	61	58	0.255
9	1	7	87	86	0.742
9	2	0	122	104	0.000
9	2	1	85	78	0.469
9	2	2	104	93	0.992
9	2	3	42	45	0.621
9	2	4	119	120	0.053
9	2	5	42	41	0.287
9	2	6	74	75	0.946
9	2	7	11	12	0.310
9	3	0	59	43	0.500
9	3	1	81	69	0.875
9	3	2	25	30	0.776
9	3	3	29	30	0.148
9	3	4	29	35	0.371
9	3	6	20	31	0.504
9	4	0	88	80	0.000
9	4	2	55	51	0.988
9	4	3	33	42	0.441
10	0	0	115	115	0.000
10	0	1	152	160	0.688
10	0	2	100	100	0.937
10	0	3	136	140	0.756
10	0	4	40	48	0.052
10	0	5	78	87	0.723
10	0	6	27	24	0.139
10	1	0	23	24	1.000
10	1	1	33	29	0.332
10	1	2	73	63	0.989
10	1	3	50	39	0.362
10	1	4	36	39	0.011
10	1	5	25	29	0.232
10	1	6	36	39	0.974
10	2	0	100	85	0.000
10	2	1	115	99	0.721
10	2	2	42	38	0.005
10	2	3	71	62	0.760
10	2	5	62	53	0.687
10	3	0	53	47	0.000
10	3	1	28	29	0.345
10	3	2	99	98	0.992
10	3	3	35	56	0.302
10	3	4	75	69	0.983
11	1	0	138	118	0.000
11	1	1	57	53	0.795
11	1	2	127	135	0.957
11	1	3	61	56	0.572
11	1	4	96	79	0.934
11	2	0	67	75	0.000
11	2	1	75	76	0.275
11	2	4	26	38	0.923
11	14	4	102	1	0.951

any structures with hydrogen bonding both with film scanner and diffractometer data. All hydrogen atoms were, however, included in the following structure factor calculations at their calculated positions with isotropic temperature factors corresponding to those of the parent atom. The refinement was performed by least-squares using anisotropic thermal parameters for all non-hydrogen atoms. The hydrogen parameters were not varied. The final R-value is 0.097 for all observed independent reflexions. In the refinement the residual $\sum w\,(|F_o| - |k|F_c|)^2$ was minimized where the weight w was

$$\frac{1}{1+\left(\frac{|F_o| - 4.42|F_{min}|}{6.19|F_{min}|}\right)^2}$$

The form factors of the International Tables for X-Ray Crystallography [4] were used. The calculations were performed with the program system of Abrahamsson *et al.*[5]

RESULTS

A list of the final set of observed and calculated structure factors is given in Table 1, the atomic parameters in Tables 2 and 3. The interatomic distances and angles are shown in Fig. 1, and with standard deviations in Table 4. There are no unexpected features in these values.

Table 2. Fractional coordinates for the atoms of the structure. The standard deviations (within brackets) are multiplied by 10^4 for x, y, and z, respectively.

	x	$\sigma(x)$	y	$\sigma(y)$	z	$\sigma(z)$	B (Å^2)
S (1)	0.08491	(2)	1.07513	(4)	0.00041	(0)	
C (1)	0.26706	(13)	1.03379	(27)	−0.03464	(12)	
C (2)	0.29227	(11)	0.94342	(19)	0.09476	(14)	
C (3)	0.14365	(11)	0.87000	(22)	0.12383	(14)	
C (4)	0.33843	(11)	1.14552	(22)	0.18207	(11)	
O (1)	−0.00559	(9)	0.93981	(15)	−0.09174	(11)	
O (2)	0.42151	(9)	1.06842	(18)	0.27195	(12)	
O (3)	0.30000	(11)	1.35747	(16)	0.17275	(11)	
H(11)	0.29060		0.88400		−0.10610		4.07
H(12)	0.32570		1.19440		−0.06200		4.07
H(21)	0.37100		0.80740		0.10340		3.17
H(31)	0.12250		0.67040		0.10820		3.65
H(32)	0.10930		0.91590		0.21710		3.65
H(24)	0.46140		1.20030		0.33960		4.65

Table 3. Anisotropic thermal parameters $\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{23}klb^*c^* + 2U_{31}lhc^*a^* + 2U_{12}hka^*b^*)]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12}
S(1)	0.03491	0.04201	0.03670	−0.00296	0.00085	0.00291
C(1)	0.04208	0.07829	0.03735	−0.02307	0.00522	−0.00529
C(2)	0.03381	0.03960	0.05260	−0.00706	0.00351	0.00145
C(3)	0.03776	0.04641	0.05848	0.00060	−0.00309	−0.00084
C(4)	0.03748	0.04711	0.03179	−0.00663	−0.00362	0.00374
O(1)	0.03306	0.06287	0.06432	−0.01514	−0.00061	−0.00235
O(2)	0.05733	0.05710	0.06293	−0.00645	−0.01754	0.00870
O(3)	0.07737	0.03495	0.06616	−0.00076	−0.02431	0.01350

Table 4. Interatomic distances and angles with e.s.d.'s.

S(1) – C(1)	= 1.854 Å	(0.012)
– C(3)	= 1.830	(0.013)
– O(1)	= 1.526	(0.010)
C(1) – C(2)	= 1.503	(0.017)
C(2) – C(3)	= 1.555	(0.014)
– C(4)	= 1.515	(0.015)
C(4) – O(2)	= 1.339	(0.015)
– O(3)	= 1.212	(0.014)
O(1) – S(1) – C(1)	= 112.2°	(0.6)
O(1) – S(1) – C(3)	= 111.8	(0.5)
C(1) – S(1) – C(3)	= 76.6	(0.5)
S(1) – C(1) – C(2)	= 90.6	(0.7)
C(1) – C(2) – C(3)	= 96.6	(0.9)
C(1) – C(2) – C(4)	= 113.3	(0.9)
C(3) – C(2) – C(4)	= 110.1	(0.9)
S(1) – C(3) – C(2)	= 89.8	
C(2) – C(4) – O(3)	= 122.4	(1.0)
C(2) – C(4) – O(2)	= 114.3	(0.9)
O(2) – C(4) – O(3)	= 123.2	(1.1)

From the stereoscopic drawing given in Fig. 2 it is obvious that the high melting form of $C_4H_6O_3S$ has the *trans* configuration.

The four membered ring is non-planar. The dihedral angle between the planes defined by C(1), S(1), C(3) and C(1), C(2), C(3) is 153°, which agrees well with the values usually found in puckered cyclobutane rings.[6] The carboxyl group is roughly perpendicular to the four membered ring. The angle between the planes C(1), C(2), C(3) and O(2), C(4), O(3) is 98°.

The packing of the molecules is shown in Fig. 3. The molecules are linked together by hydrogen bonds between the carboxyl and the sulphoxide group. The I O(1) and III O(2) distance is 2.63 Å. The other intermolecular contacts

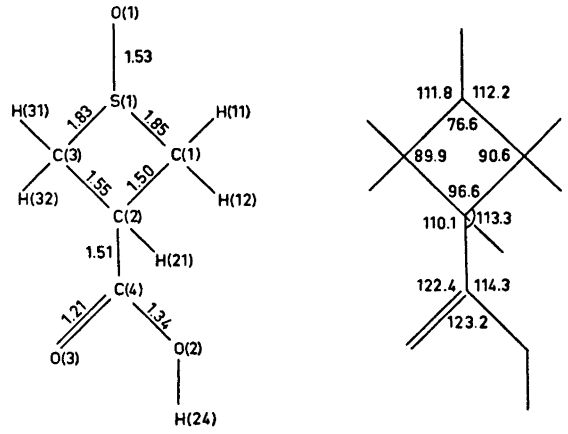

Fig. 1. Interatomic distances and angles of $C_4H_6O_3S$. The atomic numbering is also indicated.

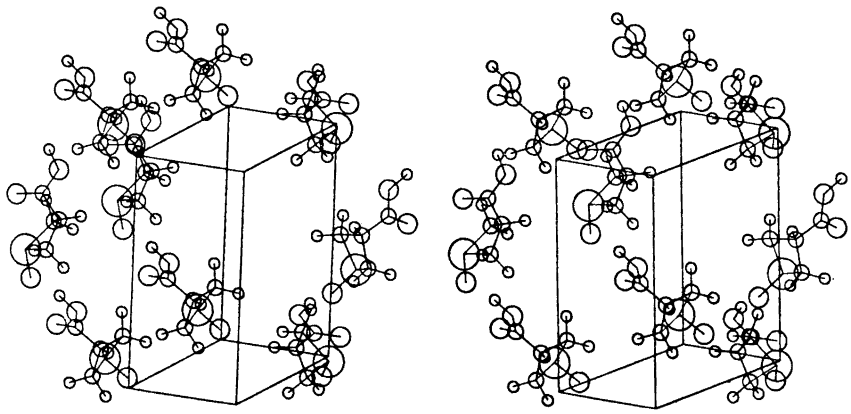

Fig. 2. Stereoscopic pair of $C_4H_6O_3S$.

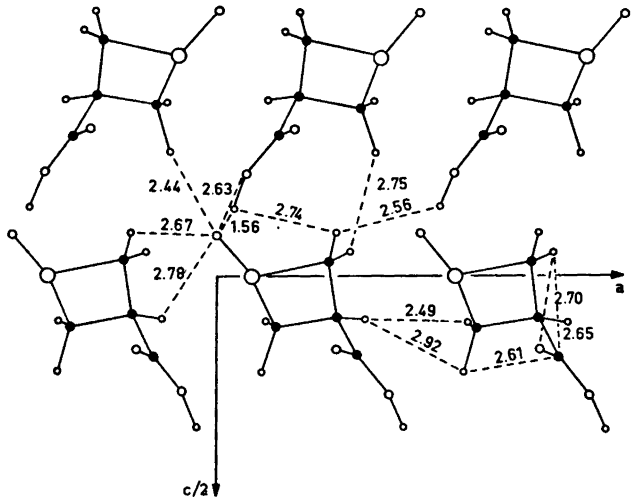

Fig. 3. Molecular packing of $C_4H_6O_3S$. Some short intra- and intermolecular contacts are shown.

as well as the nonbonded intramolecular distances indicate normal packing conditions.

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