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The Crystal Structure of Tellurium Di(morpholyldithiocarbamate)

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Tellurium di(morpholyldithiocarbamate), $Te[C_5H_8ONS_2]_2$, forms orange crystals with unit cell dimensions $a=11.242\pm0.005$ Å, $b=15.906\pm0.009$ Å, $c=9.150\pm0.004$ Å, $\beta=92.75\pm0.05°$ and $Z=4$. Density, calc. 1.84, found 1.82 g/cm³. The space group is C_{2h}^5-$P2_1/n$. 885 intensities above background were collected using Cu*K*α radiation and multiple film Weissenberg techniques. They were estimated visually. Full-matrix least squares refinement resulted in a conventional *R*-value of 6.4 %.

The molecules are essentially monomeric and the central tellurium atom is bonded to all four sulphur atoms of the molecule in a planar, but unsymmetric arrangement. All atoms in the molecule except for the outermost halves of the morpholyl groups and the hydrogen atoms, are roughly in one plane. The bond lengths and angles involving tellurium are: $Te-S_1=2.498\pm0.007$ Å, $Te-S_2=2.856\pm0.008$ Å, $Te-S_3=2.530\pm0.006$ Å, $Te-S_4=2.834\pm0.009$ Å, $\angle S_1-Te-S_2=66.8\pm0.2°$, $\angle S_1-Te-S_3=80.9\pm0.2°$, $\angle S_2-Te-S_4=145.7\pm0.2°$ and $\angle S_3-Te-S_4=66.6\pm0.2°$.

There are two short and two long C–S bonds, C_1-S_2 and C_6-S_4 the short ones with an average length of 1.68 Å, and C_1-S_1 and C_6-S_3 the long ones with an average length of 1.75 Å. There is considerable double bond character in the C_1-N_1 and C_6-N_2 bonds, both having a length of 1.33 Å.

Each tellurium atom is approached by a sulphur atom of a neighbouring molecule. This intermolecular contact distance is 3.68 Å.

Four-coordinate tellurium(II) compounds have been shown to prefer a planar configuration around the central atoms. With monodentate ligands as thiourea and halide ions, the complexes are square-planar, several of these are centrosymmetrical with tellurium in a center of symmetry.[1,2] The bonding in such square-planar tellurium complexes as *trans* $Te(etu)_2X_2$[3,4] where X is halogen and etu is ethylenethiourea, can be explained in terms of three-center four-electron bonding based on *p*-orbitals of the tellurium atom and the atoms bonded to it.[1,2] In analogy with the essentially isoelectronic ICl_4^-,[5] the Te–S and Te–X bonds are significantly longer than the respective single covalent bonds. If one assumes covalent single-bond radii for the ligand

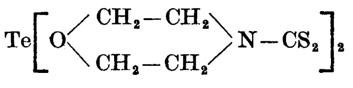
S and X atoms in such compounds, one arrives at a tellurium radius of 1.64 Å[1] which can be used to predict bond lengths in analogous compounds. It is found that with increasing asymmetry, the sum of two collinear *trans* bond lengths increases until the short one is close to a covalent bond length and the other becomes close to a van der Waals contact.[1]

Tellurium(II) and selenium(II) complexes with bidentate dithio or related ligands[6–12] have so far revealed a tendency to a planar configuration around the central tellurium and selenium atoms. Tellurium complexes with dimethyldithiophosphate and diethylthioselenophosphinate ions as ligands have shown a tendency toward square-planar configuration around tellurium;[8,11] however, two of the Te–S bonds are intermolecular and very weak, especially in the thioselenophosphinate.[11] The related compound, selenium bis-(diethyldiselenophosphinate)[12] is isomorphous with its tellurium analog. The two latter compounds according to Jørgensen[13] raise the classificatory question whether they can be considered to contain Se(II) and Te(II) central atoms or whether it is more sensible to consider them as catenated compounds like the polythionates. On the other hand, tellurium di(ethylxanthate)[8] is a planar complex where all four sulphur atoms in the molecule are bonded to the central tellurium atom in an asymmetric manner, having two short *cis* Te–S bond lengths near 2.49 Å at an interbond angle of 83.6°, and two long Te–S bond lengths near 2.88 Å at an interbond angle of 144.5°. Here, the average Te–S bond length is 2.68 Å, the same as in the centrosymmetrical *trans* complexes mentioned above.[1,2]

In order to extend the studies of divalent tellurium and selenium compounds with bidentate ligands to the dithiocarbamates of divalent tellurium, several of these were prepared. From preliminary investigations on unit cell and space group data, tellurium di(morpholyldithiocarbamate) was chosen for structure analysis.

EXPERIMENTAL

Tellurium di(morpholyldithiocarbamate),



$$\mathrm{Te}\left[\mathrm{O}\left\langle\begin{matrix}\mathrm{CH_2-CH_2}\\ \mathrm{CH_2-CH_2}\end{matrix}\right\rangle\mathrm{N-CS_2}\right]_2$$

was prepared by nucleophilic substitution on divalent tellurium.[14] An aqueous solution of sodium morpholyldithiocarbamate,[15] was added with stirring to an aqueous solution of potassium telluropentathionate. The resulting orange precipitate was washed with water and methanol and dried. Recrystallization of the microcrystalline powder was difficult due to decomposition and low solubility in most organic solvents; however, from a 1:1 mixture of alcohol and benzene, a few small orange-red prisms and needles were finally obtained. They decomposed above 200°C. (Found: Te 28.10. Calc. for $C_{10}H_{16}N_2O_2S_4Te$: Te 28.22). The crystals were elongated along the *c*-axis. Unit cell data were calculated from 22 high-order reflections read from NaCl-calibrated Weissenberg photographs, using a least squares program, "CELLDIM". This program and the other programs used in the computations were made available by the Weizmann Institute, Rehovoth, Israel, and modified for use on the University of Bergen's IBM 360–50H computer by Dr. Dove Rabinovich. The cell dimensions are $a = 11.242 \pm 0.005$ Å, $b = 15.906 \pm 0.009$ Å, $c = 9.150 \pm 0.004$ Å and $\beta = 92.75 \pm 0.05°$. There are four molecules per unit cell with density, calc. 1.84, found 1.82 g/cm^3. The space group, from systematic absences $h0l$ for $h+l=2n+1$, and $0k0$ for $k=2n+1$ found from Weissenberg films of the $hk0$, $h0l$, $h1l$ and $0kl$ layers, is C_{2h}^5-$P2_1/n$.

Using the multiple-film technique, integrated Weissenberg equi-inclination photographs were taken of the $0kl$, $hk0$, $hk1$, and $hk2$ layers using Ni-filtered CuK radiation. Reflection intensities were estimated visually, and out of the 1237 independent reflections read, 885 were observed and measured. The intensities were corrected in the usual way to give sets of relative structure factors. During refinement they were also corrected for absorption effects ($\mu = 197$ cm^{-1}). The crystals used for the intensity photographs exhibited (mainly) the crystal faces (011), $(0\bar{1}1)$, $(0\bar{1}\bar{1})$, $(01\bar{1})$, (100), $(\bar{1}10)$, and $(\bar{1}\bar{1}0)$. The distance of these faces from a common origin were 0.0030 cm for the first four, and 0.0081, 0.0083, and 0.0083 cm, respectively, for the others in the crystal used for the a axis photographs. The corresponding distances for the crystal used for the c axis photographs were 0.0034, 0.0059, 0.0068, and 0.0068 cm, respectively.

STRUCTURE ANALYSIS

Coordinates for the tellurium atom were found from Patterson projections along the a and c axes. Use of a model of the molecule based on assumed bond lengths and angles, and subsequent Fourier refinements of the two projections, gave the positions of the other atoms in the molecule; however, only tentative positions were found for the atoms in one of the morpholine rings.

All reflections were now scaled to the same scale, using reflections common to two layers. Full-matrix least squares refinement was then begun, using program "BDLS" from the set of programs made available by the Weizmann Institute. This program minimizes the expression $\sum w[|F_o| - k|F_c|]^2/\sum w|F_o|^2$, where k is the variable scale factor and w, the relative weight assigned to a reflection, is determined as the inverse of the square of the standard deviation of the reflection, $1/\sigma^2(F)$. $\sigma^2(F)$ is equal to $(ka_1)^2 + (a_2F_o)^2/4w_o$, where w_o is a variable related to the reliability with which the intensity of a given reflection is measured, and a_1 and a_2 are constants fixed at 2.0 and 1.0, respectively.

After a few cycles of refinement using isotropic temperature factors, the reliability index $R = \sum||F_o| - |F_c||/\sum|F_o|$ reached a value of 0.12. Anomalous shifts in the atomic parameters of the morpholine ring bonded to C_1 indicated an error in its orientation. By rotating the ring 180° around the $C_1 - N_1$ bond the correct position was found. After further refinement, absorption correction using program "DATATO"[16] was applied to the reflections and all layers were then rescaled by comparison between observed and calculated structure factors. They were then given a common scale factor and anisotropic temperature factors were introduced for the heavy atoms. The final R value of 0.064 was reached after four additional refinement cycles.

Final observed and calculated structure factors are listed in Table 1. Atomic scattering factors for tellurium, sulphur, oxygen, nitrogen, and carbon listed in the *International Tables*[17] were used. The atomic scattering factors for tellurium and sulphur were corrected for anomalous dispersion according to Cromer,[18] using f' and f'' values from the *International Tables*.[17] The final positional parameters and their standard deviations are listed in Table 2. Components of atomic vibration tensors are given in Table 3 while interatomic distances and angles are given in Tables 4 to 6.

Table 1. Observed and calculated 0*kl*, *hk*0, *hk*1 and *hk*2 structure factors (×10) for tellurium di(morpholyldithiocarbamate). A minus sign in the F_o column indicates that the corresponding reflection is unobserved.

H	K	L	F(O)	F(C)
0	2	0	463	-532
0	4	0	930	-978
0	6	0	890	929
0	8	0	185	194
0	10	0	1082	-1127
0	12	0	327	281
0	14	0	130	124
0	16	0	-95	-39
0	18	0	152	-144
0	20	0	143	135
0	1	1	1132	1107
0	2	1	175	-129
0	3	1	2256	-2351
0	4	1	812	791
0	5	1	135	-137
0	6	1	418	382
0	7	1	961	966
0	8	1	314	-354
0	9	1	657	-687
0	10	1	114	-112
0	11	1	712	-725
0	12	1	-87	15
0	13	1	412	390
0	14	1	-95	43
0	15	1	183	172
0	16	1	171	-172
0	17	1	297	-280
0	18	1	-93	-6
0	19	1	84	79
0	20	1	-61	27
0	0	2	1238	1147
0	1	2	454	-391
0	2	2	-48	-6
0	3	2	591	-597
0	4	2	1340	-1454
0	5	2	271	269
0	6	2	1275	1142
0	7	2	1012	949
0	8	2	540	530
0	9	2	489	-490
0	10	2	382	-402
0	11	2	265	244
0	12	2	152	-134
0	13	2	442	438
0	14	2	603	593
0	15	2	273	-271
0	16	2	237	-218
0	17	2	123	-95
0	18	2	103	-83
0	19	2	192	165
0	1	3	644	600
0	2	3	1462	-1378
0	3	3	1274	-1199
0	4	3	346	-287
0	5	3	104	71
0	6	3	403	403
0	7	3	439	436
0	8	3	683	-675
0	9	3	187	-116
0	10	3	459	-455
0	11	3	279	-239
0	12	3	489	474
0	13	3	355	349
0	14	3	-97	1
0	15	3	-95	85
0	16	3	213	-213
0	17	3	147	-120
0	18	3	146	136
0	19	3	-71	-41
0	0	4	187	-127
0	1	4	1005	-989
0	2	4	-69	10
0	3	4	732	-741
0	4	4	293	-282
0	5	4	1270	1224
0	6	4	76	-82
0	7	4	602	-566
0	8	4	341	266
0	9	4	484	-440
0	10	4	227	-265
0	11	4	249	222
0	12	4	168	-151
0	13	4	309	300
0	14	4	226	224
0	15	4	194	-167
0	16	4	-91	-79
0	17	4	-89	-4
0	18	4	78	-76
0	19	4	110	127
0	1	5	263	226
0	2	5	1024	-938
0	3	5	634	623
0	4	5	583	517
0	5	5	129	-89
0	6	5	731	721
0	7	5	-97	45
0	8	5	612	-593
0	9	5	-93	-63
0	10	5	182	-176
0	11	5	107	-172
0	12	5	414	422
0	13	5	-95	8
0	14	5	160	-141
0	15	5	-91	22
0	16	5	107	-200
0	17	5	110	-99
0	18	5	75	96
0	0	6	-87	-36
0	1	6	757	-770
0	2	6	349	-327
0	3	6	196	174
0	4	6	255	264
0	5	6	917	929
0	6	6	136	-93
0	7	6	-93	12
0	8	6	171	-143
0	9	6	608	-592
0	10	6	-97	6
0	11	6	405	418
0	12	6	188	162
0	13	6	-92	-31
0	14	6	180	-182
0	15	6	196	-189
0	16	6	-78	58
0	17	6	-62	-34
0	1	7	362	-363
0	2	7	683	-672
0	3	7	172	179
0	4	7	675	476
0	5	7	207	192
0	6	7	467	412
0	7	7	158	-149
0	8	7	377	-309
0	9	7	-95	46
0	10	7	186	176
0	11	7	263	267
0	12	7	142	157
0	13	7	-88	-50
0	14	7	114	-90
0	15	7	-74	-76
0	16	7	-56	-75
0	0	8	371	-391
0	1	8	93	-104
0	2	8	242	212
0	3	8	293	-285
0	4	8	-94	63
0	5	8	156	175
0	6	8	140	-117
0	7	8	131	-138
0	8	8	299	-295
0	9	8	200	-213
0	10	8	210	247
0	11	8	130	108
0	12	8	-86	78
0	13	8	144	126
0	14	8	100	-100
0	1	9	-88	-56
0	2	9	-88	8
0	3	9	203	209
0	4	9	-87	-20
0	5	9	-88	126
0	6	9	98	53
0	7	9	286	-307
0	8	9	122	-123
0	9	9	-85	-62
0	10	9	106	-103
0	11	9	150	160
0	12	9	122	119
0	0	10	166	-180
0	1	10	-84	75
0	2	10	-83	86
0	3	10	-92	20
0	4	10	303	314
0	5	10	-81	22
0	6	10	175	-193
0	7	10	-75	17
0	8	10	-72	-73
0	9	10	-64	22
0	10	10	94	98
0	1	11	132	-159
0	2	11	-60	117
0	3	11	216	241
0	4	11	-63	-45
0	5	11	-59	-40
0	6	11	-52	-2
1	1	0	840	1021
1	2	0	1353	-1466
1	3	0	1373	-1526
1	4	0	159	91
1	5	0	279	228
1	6	0	623	549
1	7	0	1257	1242
1	8	0	509	-621
1	9	0	809	-311
1	10	0	180	130
1	11	0	472	-417
1	12	0	-122	73
1	13	0	314	323
1	14	0	166	-157
1	15	0	-123	88
1	16	0	-117	-65
1	17	0	197	-176
1	18	0	-108	75
1	19	0	-95	-23
1	20	0	-70	17
2	0	0	588	651
2	1	0	1938	-2164
2	2	0	277	-232
2	3	0	138	-110
2	4	0	1022	-1071
2	5	0	347	382
2	6	0	569	612
2	7	0	-104	-88
2	8	0	-111	-40
2	9	0	790	-813
2	10	0	375	-362
2	11	0	608	622
2	12	0	372	-397
2	13	0	301	308
2	14	0	222	206
2	15	0	212	-198
2	16	0	-116	-71
2	17	0	-114	-48
2	18	0	106	-94
2	19	0	205	182
2	20	0	77	76
3	1	0	913	855
3	2	0	1283	-1269
3	3	0	324	-312
3	4	0	114	17
3	5	0	353	309
3	6	0	995	1057
3	7	0	-107	-58
3	8	0	884	-930
3	9	0	375	-352
3	10	0	631	-642
3	11	0	272	-262
3	12	0	593	676
3	13	0	-129	14
3	14	0	-127	-77
3	15	0	-122	-3
3	16	0	259	-276
3	17	0	-113	27
3	18	0	222	206
3	19	0	-88	-35
4	0	0	304	305
4	1	0	572	-571
4	2	0	143	-156
4	3	0	777	-889
4	4	0	-86	16
4	5	0	1061	989
4	6	0	431	439
4	7	0	448	-409
4	8	0	456	-421
4	9	0	872	-823
4	10	0	157	140
4	11	0	193	166
4	12	0	248	237
4	13	0	551	536
4	14	0	229	-205
4	15	0	369	-366
4	16	0	-124	114
4	17	0	-117	24
4	18	0	136	95
4	19	0	150	158
5	1	0	126	60
5	2	0	1079	-1150
5	3	0	552	546
5	4	0	211	201
5	5	0	374	336
5	6	0	210	226
5	7	0	690	-667
5	8	0	719	-729
5	9	0	-134	-46
5	10	0	-137	-76
5	11	0	637	580
5	12	0	591	550
5	13	0	322	-320
5	14	0	-126	-67
5	15	0	-123	-97
5	16	0	-116	-96
5	17	0	187	186
5	18	0	117	82
6	0	0	1144	-1169
6	1	0	720	-736
6	2	0	-96	36
6	3	0	474	-419
6	4	0	817	841
6	5	0	-111	65
6	6	0	901	-791
6	7	0	-123	-23
6	8	0	303	-309
6	9	0	478	-455
6	10	0	624	614
6	11	0	264	209
6	12	0	-138	-1
6	13	0	-131	37
6	14	0	347	-365
6	15	0	-120	-39
6	16	0	159	157
6	17	0	-100	13
6	18	0	-76	91
7	1	0	872	-892
7	2	0	259	263
7	3	0	742	697
7	4	0	436	-425
7	5	0	133	82
7	6	0	-125	-20
7	7	0	720	-723
7	8	0	-138	25
7	9	0	249	202
7	10	0	163	-109
7	11	0	431	399
7	12	0	-137	60
7	13	0	256	-238
7	14	0	124	115
7	15	0	-116	-67
7	16	0	-102	-44
7	17	0	196	184
8	0	0	567	-551
8	1	0	611	595
8	2	0	201	185
8	3	0	-119	-65
8	4	0	334	289
8	5	0	589	-534
8	6	0	-130	-93
8	7	0	135	157
8	8	0	430	-419
8	9	0	248	193
8	10	0	515	504
8	11	0	268	-237
8	12	0	-134	75
8	13	0	-124	58
8	14	0	231	-211
8	15	0	-104	51
8	16	0	-86	63
9	1	0	390	-363
9	2	0	521	486
9	3	0	-126	100
9	4	0	453	-454
9	5	0	262	257
9	6	0	374	-385
9	7	0	255	-247
9	8	0	302	282
9	9	0	-139	26
9	10	0	-134	75
9	11	0	312	294
9	12	0	177	-152
9	13	0	-115	-46
9	14	0	-102	20
9	15	0	-85	-71
10	0	0	-128	-81
10	1	0	473	466
10	2	0	220	-185
10	3	0	184	172
10	4	0	160	126
10	5	0	398	-400
10	6	0	205	-161
10	7	0	-132	-24
10	8	0	132	103
10	9	0	401	356
10	10	0	-129	45
10	11	0	138	-126
10	12	0	113	90
10	13	0	100	-83
10	14	0	-78	-71
11	1	0	-127	-31
11	2	0	553	528
11	3	0	171	-158
11	4	0	207	-271
11	5	0	-129	-45
11	6	0	223	-195
11	7	0	147	136
11	8	0	364	313
11	9	0	-124	39
11	10	0	-117	22
11	11	0	-105	-13
11	12	0	165	-166
12	0	0	251	212
12	1	0	317	255
12	2	0	126	-108
12	3	0	177	149
12	4	0	345	-287
12	5	0	420	-380
12	6	0	232	191
12	7	0	259	205
12	8	0	115	104
12	9	0	107	101
12	10	0	109	-120
13	1	0	210	179
13	2	0	144	124
13	3	0	374	-319
13	4	0	-114	-48
13	5	0	-112	26
13	6	0	-106	-7
13	7	0	259	221
13	8	0	105	95
14	0	0	172	157
14	1	0	-91	1
14	2	0	-89	-63
14	3	0	-85	-33
14	4	0	199	-198
1	0	1	1185	1253
1	1	1	1020	-1235
1	2	1	749	750
1	3	1	1269	1235
1	4	1	1874	-1910
1	5	1	1759	1900
1	6	1	982	924
1	7	1	-83	57
1	8	1	-89	15
1	9	1	613	-563
1	10	1	552	-512
1	11	1	532	530
1	12	1	-103	-16
1	13	1	158	-147
1	14	1	341	327
1	15	1	136	-126
1	16	1	235	-242
1	17	1	-96	-106
1	18	1	-90	-53
1	19	1	-80	88
1	20	1	-57	55
2	1	1	979	1017
2	2	1	3036	-3277
2	3	1	441	396
2	4	1	1442	1337
2	5	1	-72	66
2	6	1	509	561
2	7	1	240	213
2	8	1	795	-805
2	9	1	203	188
2	10	1	122	130
2	11	1	378	-349
2	12	1	411	380
2	13	1	-107	107
2	14	1	130	-169
2	15	1	-103	62
2	16	1	175	-182
2	17	1	-95	-121
2	18	1	88	62
2	19	1	-77	-2
3	0	1	239	-244
3	1	1	585	-576
3	2	1	729	680
3	3	1	969	-996
3	4	1	594	575
3	5	1	1994	1985
3	6	1	409	-365
3	7	1	545	-551
3	8	1	131	-139
3	9	1	473	-483
3	10	1	-104	-87
3	11	1	331	334
3	12	1	257	-243
3	13	1	323	330
3	14	1	-107	71
3	15	1	371	-415
3	16	1	-98	32
3	17	1	-96	-55
3	18	1	-88	-1
3	19	1	125	140
4	1	1	240	-272
4	2	1	1191	-1111
4	3	1	603	615
4	4	1	847	892
4	5	1	-79	-40
4	6	1	697	754
4	7	1	333	-297
4	8	1	441	-391
4	9	1	-102	-56
4	10	1	303	-276
4	11	1	175	173
4	12	1	279	298
4	13	1	338	-365
4	14	1	-107	-50
4	15	1	143	-141
4	16	1	196	-223
4	17	1	122	110
4	18	1	-83	107
4	19	1	-64	26
5	0	1	442	-449
5	1	1	957	-949
5	2	1	127	-116
5	3	1	-77	-42

Table 1. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
5	4	1	1317	1239	11	9	1	172	167	5	7	-1	287	-282	11	12	-1	-74	18	5	6	2	420	376
5	5	1	399	397	11	10	1	-93	-65	5	8	-1	158	143	12	1	-1	-104	130	5	7	2	721	-710
5	6	1	577	-576	11	11	1	-86	-24	5	9	-1	546	-482	12	2	-1	-106	358	5	8	2	126	88
5	7	1	426	-396	11	12	1	-71	-37	5	10	-1	354	311	12	3	-1	344	-115	5	9	2	322	332
5	8	1	692	-605	12	1	1	146	157	5	11	-1	281	245	12	4	-1	-106	-160	5	10	2	-95	-13
5	9	1	522	-691	12	2	1	147	156	5	12	-1	-114	20	12	5	-1	-104	-34	5	11	2	388	364
5	10	1	235	237	12	3	1	313	-308	5	13	-1	267	266	12	6	-1	173	-160	5	12	2	98	141
5	11	1	268	264	12	4	1	166	-163	5	14	-1	-105	-36	12	7	-1	208	195	5	13	2	283	-304
5	12	1	-114	45	12	5	1	-104	-64	5	15	-1	284	-289	12	8	-1	268	258	5	14	2	-93	-12
5	13	1	-111	-9	12	6	1	143	-135	5	16	-1	-97	44	12	9	-1	-90	-81	5	15	2	194	-190
5	14	1	383	-427	12	7	1	214	244	5	17	-1	-90	56	12	10	-1	-75	69	5	16	2	155	-160
5	15	1	-100	-24	12	8	1	130	97	5	18	-1	-77	10	13	0	-1	192	216	5	17	2	161	194
5	16	1	160	161	12	9	1	-84	-36	6	1	-1	934	-951	13	1	-1	-99	53	5	18	2	-67	68
5	17	1	-89	-31	12	10	1	-71	30	6	2	-1	493	-522	13	2	-1	-98	-50	6	0	2	1169	-1248
5	18	1	107	128	12	11	1	-50	-107	6	3	-1	1141	1169	13	3	-1	194	178	6	1	2	135	113
6	1	1	284	-231	13	2	1	136	-120	6	4	-1	329	300	13	4	-1	136	-147	6	2	2	765	811
6	2	1	405	-428	13	3	1	-95	-54	6	5	-1	236	-213	13	5	-1	-94	-101	6	3	2	248	245
6	3	1	1182	1179	13	4	1	300	-288	6	6	-1	524	481	13	6	-1	135	158	6	4	2	767	742
6	4	1	500	484	13	5	1	-89	7	6	7	-1	567	-554	13	7	-1	-81	29	6	5	2	232	196
6	5	1	-94	-8	13	6	1	224	219	6	8	-1	314	-332	13	8	-1	76	77	6	6	2	410	-390
6	6	1	-99	-17	13	7	1	-73	-60	6	9	-1	627	615	14	1	-1	139	133	6	7	2	103	75
6	7	1	1031	-999	1	1	-1	429	400	6	10	-1	200	-195	14	2	-1	-75	49	6	8	2	567	-543
6	8	1	415	-405	1	2	-1	565	-590	6	11	-1	293	261	14	3	-1	119	-127	6	9	2	-97	62
6	9	1	138	197	1	3	-1	387	-407	6	12	-1	344	384	1	1	2	95	-48	6	10	2	370	393
6	10	1	270	275	1	4	-1	674	-572	6	13	-1	198	-217	1	2	2	221	-183	6	11	2	-98	-78
6	11	1	387	386	1	5	-1	105	137	6	14	-1	-103	-49	1	3	2	720	-705	6	12	2	183	-154
6	12	1	-115	-92	1	6	-1	604	539	6	15	-1	-100	58	1	4	2	704	672	6	13	2	177	-162
6	13	1	357	-347	1	7	-1	250	-319	6	16	-1	169	-158	1	5	2	285	284	6	14	2	250	-273
6	14	1	-105	13	1	8	-1	1400	1410	6	17	-1	-83	55	1	6	2	1292	1203	6	15	2	-86	24
6	15	1	141	-105	1	9	-1	230	-292	6	18	-1	-63	73	1	7	2	924	965	6	16	2	-79	47
6	16	1	-93	51	1	10	-1	1076	-1076	7	0	-1	1162	-1216	1	8	2	697	-723	6	17	2	-69	23
6	17	1	235	244	1	11	-1	-109	82	7	1	-1	212	-223	1	9	2	227	-194	6	18	2	110	156
6	18	1	-61	-26	1	12	-1	-103	-29	7	2	-1	215	249	1	10	2	450	-436	7	1	2	458	-477
7	0	1	893	-910	1	13	-1	-105	77	7	3	-1	-92	-41	1	11	2	255	-258	7	2	2	573	606
7	1	1	-88	-12	1	14	-1	403	422	7	4	-1	743	811	1	12	2	562	586	7	3	2	778	820
7	2	1	632	654	1	15	-1	-103	-41	7	5	-1	241	-187	1	13	2	357	364	7	4	2	106	113
7	3	1	-93	-44	1	16	-1	-98	-142	7	6	-1	672	-706	1	14	2	132	-145	7	5	2	135	-144
7	4	1	692	753	1	17	-1	-96	113	7	7	-1	402	398	1	15	2	91	-75	7	6	2	459	-404
7	5	1	337	-323	1	18	-1	247	-256	7	8	-1	-116	-67	1	16	2	298	-331	7	7	2	654	-641
7	6	1	475	-458	1	19	-1	-80	14	7	9	-1	382	-358	1	17	2	-83	-73	7	8	2	234	254
7	7	1	208	-225	1	20	-1	137	177	7	10	-1	442	423	1	18	2	95	131	7	9	2	235	258
7	8	1	355	-351	2	1	-1	693	671	7	11	-1	-122	68	1	19	2	-67	-1	7	10	2	-99	55
7	9	1	276	267	2	2	-1	1012	-1004	7	12	-1	-115	90	2	0	2	614	-663	7	11	2	-98	60
7	10	1	530	538	2	3	-1	495	-445	7	13	-1	-106	97	2	1	2	1009	-1015	7	12	2	224	-239
7	11	1	-116	-125	2	4	-1	638	-643	7	14	-1	187	-186	2	2	2	691	-702	7	13	2	196	-198
7	12	1	113	-154	2	5	-1	580	-552	7	15	-1	-95	-58	2	3	2	608	-575	7	14	2	-88	-27
7	13	1	109	-106	2	6	-1	129	141	7	16	-1	-85	88	2	4	2	302	-283	7	15	2	-81	-45
7	14	1	194	-204	2	7	-1	903	872	7	17	-1	85	-85	2	5	2	2046	2158	7	16	2	114	113
7	15	1	136	131	2	8	-1	701	-694	8	1	-1	742	-742	2	6	2	445	-389	7	17	2	-53	71
7	16	1	-85	73	2	9	-1	153	171	8	2	-1	317	311	2	7	2	546	-490	8	0	2	238	-204
7	17	1	-67	16	2	10	-1	458	-478	8	3	-1	467	493	2	8	2	289	328	8	1	2	746	712
8	1	1	314	-288	2	11	-1	639	-596	8	4	-1	-103	-21	2	9	2	585	-550	8	2	2	305	325
8	2	1	509	512	2	12	-1	471	438	8	5	-1	-106	110	2	10	2	-88	115	8	3	2	142	126
8	3	1	339	392	2	13	-1	374	376	8	6	-1	-110	10	2	11	2	234	239	8	4	2	490	431
8	4	1	410	-423	2	14	-1	118	93	8	7	-1	453	-459	2	12	2	95	111	8	5	2	632	-601
8	5	1	-106	89	2	15	-1	281	305	8	8	-1	212	208	2	13	2	420	434	8	6	2	488	-487
8	6	1	496	-534	2	16	-1	225	-241	8	9	-1	263	246	2	14	2	-94	-2	8	7	2	177	181
8	7	1	481	-478	2	17	-1	271	-283	8	10	-1	-121	60	2	15	2	415	-473	8	8	2	-98	60
8	8	1	335	350	2	18	-1	221	214	8	11	-1	365	349	2	16	2	-85	-65	8	9	2	462	453
8	9	1	-116	72	2	19	-1	-78	43	8	12	-1	-110	-61	2	17	2	-82	27	8	10	2	-96	42
8	10	1	-114	-18	3	0	-1	168	222	8	13	-1	165	-158	2	18	2	-77	-24	8	11	2	282	-291
8	11	1	-110	146	3	1	-1	754	-679	8	14	-1	-96	60	2	19	2	-64	91	8	12	2	-89	-92
8	12	1	133	-269	3	2	-1	-55	-63	8	15	-1	145	-115	3	1	2	203	-155	8	13	2	99	-112
8	13	1	247	-153	3	3	-1	453	-445	8	16	-1	-72	-31	3	2	2	1131	-1077	8	14	2	-92	-69
8	14	1	136	80	3	4	-1	729	-733	9	0	-1	935	-998	3	3	2	1111	1195	8	15	2	160	157
8	15	1	-85	-76	3	5	-1	659	595	9	1	-1	357	369	3	4	2	627	639	8	16	2	-55	7
8	16	1	135	153	3	6	-1	486	508	9	2	-1	324	312	3	5	2	454	-439	9	1	2	-93	138
9	0	1	127	114	3	7	-1	405	367	9	3	-1	184	189	3	6	2	1206	1220	9	2	2	672	712
9	1	1	458	470	3	8	-1	213	201	9	4	-1	310	310	3	7	2	647	-678	9	3	2	224	194
9	2	1	182	-195	3	9	-1	1182	-1123	9	5	-1	-110	-162	3	8	2	608	-601	9	4	2	347	-371
9	3	1	150	151	3	10	-1	311	-344	9	6	-1	187	-203	3	9	2	274	255	9	5	2	-97	-4
9	4	1	187	171	3	11	-1	470	459	9	7	-1	-115	-10	3	10	2	90	-134	9	6	2	395	-375
9	5	1	518	-554	3	12	-1	-108	29	9	8	-1	209	-186	3	11	2	-94	-2	9	7	2	-97	55
9	6	1	137	-127	3	13	-1	475	478	9	9	-1	317	308	3	12	2	554	575	9	8	2	385	393
9	7	1	-114	-76	3	14	-1	407	409	9	10	-1	420	437	3	13	2	145	-128	9	9	2	-93	-86
9	8	1	139	-165	3	15	-1	283	-319	9	11	-1	-112	-67	3	14	2	200	-214	9	10	2	-91	5
9	9	1	359	378	3	16	-1	-98	-115	9	12	-1	-103	-59	3	15	2	-90	52	9	11	2	-88	-49
9	10	1	-107	11	3	17	-1	-94	-63	9	13	-1	119	-114	3	16	2	250	-264	9	12	2	283	-285
9	11	1	185	-175	3	18	-1	-86	-58	9	14	-1	102	-111	3	17	2	-83	-41	9	13	2	-81	-30
9	12	1	126	116	3	19	-1	175	219	9	15	-1	112	124	3	18	2	74	98	9	14	2	-71	57
9	13	1	180	-161	4	1	-1	-61	36	10	1	-1	260	-251	3	19	2	-59	30	9	15	2	-53	-8
9	14	1	170	-152	4	2	-1	1478	-1511	10	2	-1	487	492	4	0	2	1241	-1308	10	0	2	269	286
9	15	1	177	204	4	3	-1	655	-619	10	3	-1	401	430	4	1	2	616	-619	10	1	2	213	196
10	1	1	132	98	4	4	-1	217	260	10	4	-1	-110	-50	4	2	2	374	376	10	2	2	-95	40
10	2	1	229	214	4	5	-1	300	-305	10	5	-1	157	-157	4	3	2	271	218	10	3	2	234	207
10	3	1	133	-109	4	6	-1	517	548	10	6	-1	263	-257	4	4	2	1104	1133	10	4	2	256	-236
10	4	1	189	-188	4	7	-1	276	237	10	7	-1	201	-229	4	5	2	423	382	10	5	2	392	-402
10	5	1	-110	35	4	8	-1	946	-998	10	8	-1	352	374	4	6	2	889	-863	10	6	2	133	149
10	6	1	448	-448	4	9	-1	224	205	10	9	-1	196	219	4	7	2	625	659	10	7	2	-92	37
10	7	1	-110	55	4	10	-1	248	-238	10	10	-1	-109	61	4	8	2	204	201	10	8	2	-91	7
10	8	1	187	181	4	11	-1	-112	5	10	11	-1	-103	37	4	9	2	547	-550	10	9	2	165	192
10	9	1	130	-129	4	12	-1	676	715	10	12	-1	266	-263	4	10	2	323	308	10	10	2	155	-159
10	10	1	166	165	4	13	-1	165	131	10	13	-1	-83	-38	4	11	2	158	130	10	11	2	143	-125
10	11	1	-101	27	4	14	-1	-106	-82	10	14	-1	-65	15	4	12	2	-97	65	10	12	2	-76	-40
10	12	1	261	-261	4	15	-1	-101	-121	11	0	-1	-107	-46	4	13	2	154	148	10	13	2	140	-166
10	13	1	-81	-1	4	16	-1	240	-233	11	1	-1	488	546	4	14	2	244	-250	11	1	2	218	225
10	14	1	-62	37	4	17	-1	-92	-2	11	2	-1	-107	-54	4	15	2	208	-264	11	2	2	159	150
11	0	1	168	153	4	18	-1	162	155	11	3	-1	141	156	4	16	2	-86	55	11	3	2	183	-186
11	1	1	150	117	4	19	-1	-65	-16	11	4	-1	107	110	4	17	2	139	-131	11	4	2	-91	-62
11	2	1	-106	-70	5	0	-1	1512	-1531	11	5	-1	301	-316	4	18	2	-70	61	11	5	2	-89	-79
11	3	1	213	207	5	1	-1	954	-943	11	6	-1	-107	-112	4	19	2	110	169	11	6	2	191	-182
11	4	1	249	-220	5	2	-1	232	-169	11	7	-1	155	139	5	1	2	685	-663	11	7	2	187	171
11	5	1	373	-407	5	3	-1	870	-949	11	8	-1	146	134	5	2	2	141	102	11	8	2	-85	67
11	6	1	132	158	5	4	-1	463	478	11	9	-1	370	353	5	3	2	1048	961	11	9	2	-82	-84
11	7	1	-106	-64	5	5	-1	1133	1201	11	10	-1	-98	-46	5	4	2	-73	-49	11	10	2	-77	89
11	8	1	-103	69	5	6	-1	583	-514	11	11	-1	192	-207	5	5	2	394	363	11	11	2	226	-240

Table 1. Continued.

H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)	H	K	L	F(O)	F(C)
11	12	2	135	-163	2	15	-2	-90	-88	5	1	-2	323	-284	7	8	-2	163	-142	10	3	-2	233	250
12	2	2	-99	23	2	16	-2	91	-115	5	2	-2	1385	-1401	7	9	-2	-104	-12	10	4	-2	274	283
12	3	2	-90	-67	2	17	-2	-82	-64	5	3	-2	537	463	7	10	-2	-104	-49	10	5	-2	232	-260
12	4	2	238	-230	2	18	-2	190	-208	5	4	-2	1211	1227	7	11	-2	367	354	10	6	-2	155	-179
12	5	2	105	-75	2	19	-2	-65	60	5	5	-2	-76	-76	7	12	-2	188	194	10	7	-2	-98	74
12	6	2	102	94	3	1	-2	361	351	5	6	-2	758	711	7	13	-2	245	-258	10	8	-2	235	-256
12	7	2	113	-95	3	2	-2	1436	-1430	5	7	-2	152	-128	7	14	-2	-91	-29	10	9	-2	315	325
12	8	2	160	142	3	3	-2	1583	-1640	5	8	-2	688	-556	7	15	-2	155	-120	10	10	-2	258	239
12	9	2	-66	63	3	4	-2	713	731	5	9	-2	302	303	7	16	-2	128	-123	10	11	-2	170	-166
12	10	2	136	-211	3	5	-2	174	-164	5	10	-2	-99	2	7	17	-2	116	168	10	12	-2	115	-99
1	1	-2	258	-263	3	6	-2	675	686	5	11	-2	-101	-95	8	0	-2	365	-354	10	13	-2	131	-124
1	2	-2	137	-106	3	7	-2	1061	1028	5	12	-2	304	281	8	1	-2	456	-431	10	14	-2	93	-102
1	3	-2	1196	-1122	3	8	-2	714	-703	5	13	-2	-98	14	8	2	-2	-88	-80	11	1	-2	-94	-10
1	4	-2	284	253	3	9	-2	166	-152	5	14	-2	131	-149	8	3	-2	403	432	11	2	-2	413	423
1	5	-2	914	-841	3	10	-2	-93	10	5	15	-2	-88	52	8	4	-2	733	703	11	3	-2	-94	49
1	6	-2	291	-276	3	11	-2	152	-142	5	16	-2	174	-179	8	5	-2	237	234	11	4	-2	176	-198
1	7	-2	1392	1265	3	12	-2	228	207	5	17	-2	-77	11	8	6	-2	426	-385	11	5	-2	183	165
1	8	-2	138	121	3	13	-2	336	351	5	18	-2	-65	50	8	7	-2	-101	-44	11	6	-2	231	-244
1	9	-2	-93	50	3	14	-2	-94	-48	6	0	-2	787	-806	8	8	-2	265	-249	11	7	-2	129	-91
1	10	-2	166	160	3	15	-2	-99	51	6	1	-2	437	-448	8	9	-2	-103	-70	11	8	-2	269	308
1	11	-2	595	-552	3	16	-2	177	-206	6	2	-2	86	-71	8	10	-2	397	390	11	9	-2	-88	-50
1	12	-2	195	-201	3	17	-2	182	-188	6	3	-2	589	-541	8	11	-2	-98	69	11	10	-2	-83	28
1	13	-2	544	557	3	18	-2	-75	88	6	4	-2	548	559	8	12	-2	-96	86	11	11	-2	-77	51
1	14	-2	-93	-9	3	19	-2	-61	22	6	5	-2	1126	1140	8	13	-2	157	-152	11	12	-2	176	-207
1	15	-2	296	311	4	0	-2	132	83	6	6	-2	502	-539	8	14	-2	371	-372	12	0	-2	262	271
1	16	-2	186	203	4	1	-2	1584	-1644	6	7	-2	259	-222	8	15	-2	-76	49	12	1	-2	289	284
1	17	-2	327	-370	4	2	-2	159	-114	6	8	-2	-98	-38	8	16	-2	85	91	12	2	-2	-91	-69
1	18	-2	77	-95	4	3	-2	-61	-45	6	9	-2	213	-206	9	1	-2	329	-332	12	3	-2	129	141
1	19	-2	-68	29	4	4	-2	933	-961	6	10	-2	405	382	9	2	-2	105	71	12	4	-2	-91	-18
2	0	-2	1319	1395	4	5	-2	1617	1572	6	11	-2	145	148	9	3	-2	611	652	12	5	-2	230	-236
2	1	-2	242	-274	4	6	-2	653	638	6	12	-2	-102	-46	9	4	-2	108	94	12	6	-2	-89	99
2	2	-2	742	-701	4	7	-2	315	-304	6	13	-2	304	302	9	5	-2	98	46	12	7	-2	-97	-63
2	3	-2	113	112	4	8	-2	164	136	6	14	-2	119	-131	9	6	-2	-100	-56	12	8	-2	-81	-57
2	4	-2	977	-959	4	9	-2	540	-501	6	15	-2	231	-266	9	7	-2	599	-597	12	9	-2	246	250
2	5	-2	246	243	4	10	-2	-96	-38	6	16	-2	111	107	9	8	-2	-102	77	12	10	-2	90	-110
2	6	-2	348	335	4	11	-2	560	541	6	17	-2	-71	-73	9	9	-2	121	138	13	1	-2	167	167
2	7	-2	260	-180	4	12	-2	-99	-1	6	18	-2	-51	27	9	10	-2	202	195	13	2	-2	154	172
2	8	-2	872	948	4	13	-2	-98	-54	7	1	-2	377	-335	9	11	-2	244	250	13	3	-2	120	-130
2	9	-2	-96	-35	4	14	-2	208	224	7	2	-2	408	-401	9	12	-2	216	-231	13	4	-2	-83	-2
2	10	-2	753	-737	4	15	-2	202	-199	7	3	-2	677	640	9	13	-2	212	-211	13	5	-2	-79	11
2	11	-2	146	102	4	16	-2	-85	-82	7	4	-2	540	525	9	14	-2	-74	5	13	6	-2	182	-176
2	12	-2	-94	69	4	17	-2	-90	-41	7	5	-2	190	185	9	15	-2	-59	-72	13	7	-2	93	88
2	13	-2	196	106	4	18	-2	-72	-29	7	6	-2	513	482	10	0	-2	406	-431	14	0	-2	206	225
2	14	-2	408	410	4	19	-2	84	105	7	7	-2	450	-427	10	1	-2	231	251	14	1	-2	-65	35
															10	2	-2	381	390	14	2	-2	-62	-3

RESULTS AND DISCUSSION

The crystals consist of tellurium di(morpholyldithiocarbamate) molecules as shown in Fig. 1, which is a representation of the packing of the molecules

Table 2. Atomic coordinates for tellurium di(morpholyldithiocarbamate) in fractions of cell edges. Origin at a center of symmetry.

	x	y	z
Te	0.0727(1)	0.1456(1)	0.0490(2)
S_1	0.2329(4)	0.1712(3)	−0.1257(9)
S_2	0.0468(5)	0.0464(4)	−0.2108(9)
S_3	0.1914(5)	0.2555(3)	0.1928(10)
S_4	−0.0171(5)	0.1797(3)	0.3270(10)
O_1	0.3724(14)	0.0297(10)	−0.6019(27)
O_2	0.1090(14)	0.4425(9)	0.6110(27)
N_1	0.2429(15)	0.0729(10)	−0.3600(30)
N_2	0.1263(17)	0.2920(12)	0.4577(33)
C_1	0.1772(17)	0.0933(12)	−0.2478(34)
C_2	0.3750(22)	0.0995(15)	−0.3718(46)
C_3	0.3934(25)	0.1093(19)	−0.5217(47)
C_4	0.2454(24)	0.0092(16)	−0.6007(52)
C_5	0.2160(23)	−0.0070(16)	−0.4461(41)
C_6	0.0988(16)	0.2457(12)	0.3393(35)
C_7	0.0464(21)	0.2969(15)	0.5891(40)
C_8	0.0056(20)	0.3881(14)	0.5952(37)
C_9	0.1817(22)	0.4398(15)	0.4863(40)
C_{10}	0.2313(19)	0.3511(14)	0.4863(39)

Table 3. Components of atomic vibration tensors, $U \times 10^3$, in Å^2 with standard deviations, referred to crystallographic axes. For Te and S, the expression is $\exp\{-2\pi^2[U_{11}(ha^{-1})^2+U_{22}(kb^{-1})^2+U_{33}(lc^{-1})^2+2U_{12}a^{-1}b^{-1}hk+2U_{23}b^{-1}c^{-1}kl+2U_{13}a^{-1}c^{-1}hl]\}$. For the O, N, and C atoms, the expression is $\exp[-8\pi^2U(\sin^2\theta/\lambda^2)]$.

	$U_{11}(U)$	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
Te	46.50 (0.60)	58.27 (0.65)	54.56 (1.43)	1.73 (0.61)	−6.91 (1.00)	6.39 (1.13)
S_1	58.07 (2.46)	60.77 (2.59)	46.71 (5.20)	−8.78 (2.19)	−8.39 (3.52)	8.02 (4.93)
S_2	60.13 (2.73)	86.18 (3.56)	56.51 (6.09)	−18.90 (2.62)	−19.34 (4.28)	5.40 (5.32)
S_3	63.84 (2.77)	66.79 (2.87)	58.00 (5.60)	−9.32 (2.46)	−10.79 (3.83)	12.46 (5.41)
S_4	67.75 (2.94)	61.68 (2.74)	76.81 (7.06)	−6.78 (2.46)	−15.01 (4.25)	24.69 (5.71)
O_1	86.67 (5.24)					
O_2	85.22 (5.31)					
N_1	65.89 (5.02)					
N_2	79.63 (5.98)					
C_1	56.50 (5.44)					
C_2	85.76 (8.66)					
C_3	110.70 (11.40)					
C_4	98.53 (9.36)					
C_5	94.72 (9.99)					
C_6	56.08 (5.45)					
C_7	72.16 (7.76)					
C_8	77.61 (7.20)					
C_9	84.51 (7.92)					
C_{10}	75.82 (6.95)					

in the unit cell viewed down the c axis. As may be seen from this figure, the molecules are linked together in pairs across centers of symmetry by short intermolecular Te···S_2 contacts. These have a length of 3.68 Å as compared

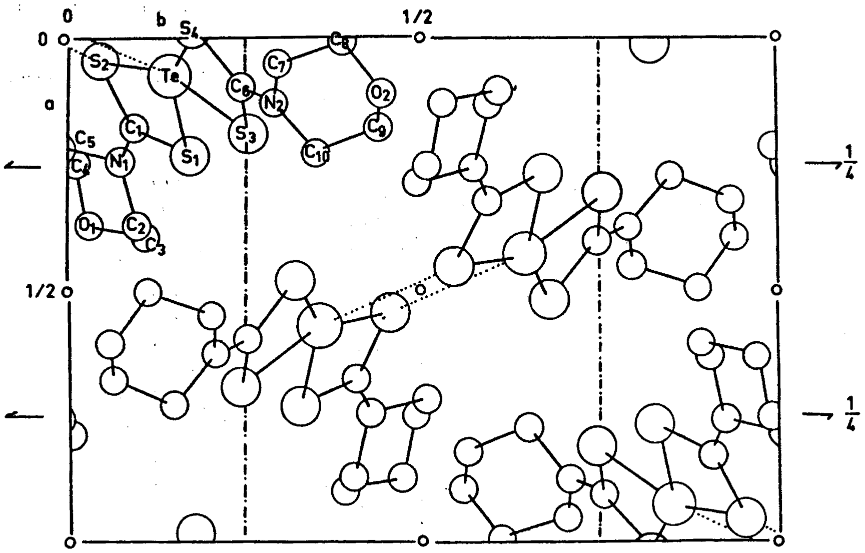


Fig. 1. The arrangement of molecules in the unit cell as seen along the c axis. Dotted lines indicate short, intermolecular Te···S contacts.

to the corresponding length of 3.61 Å found in tellurium di(ethylxanthate)[10] and the sum of van der Waals radii which is 4.05 Å.[19] Other short intermolecular approaches are listed in Table 6.

In Fig. 2, a pair of molecules as mentioned above, is shown, with bond lengths and angles indicated. The molecules are roughly planar, except for the hydrogen atoms and the outermost halves of the morpholyl groups. The configuration around the central tellurium atom is indicated in Fig. 3, which shows the planar part of the molecule projected into the least squares plane

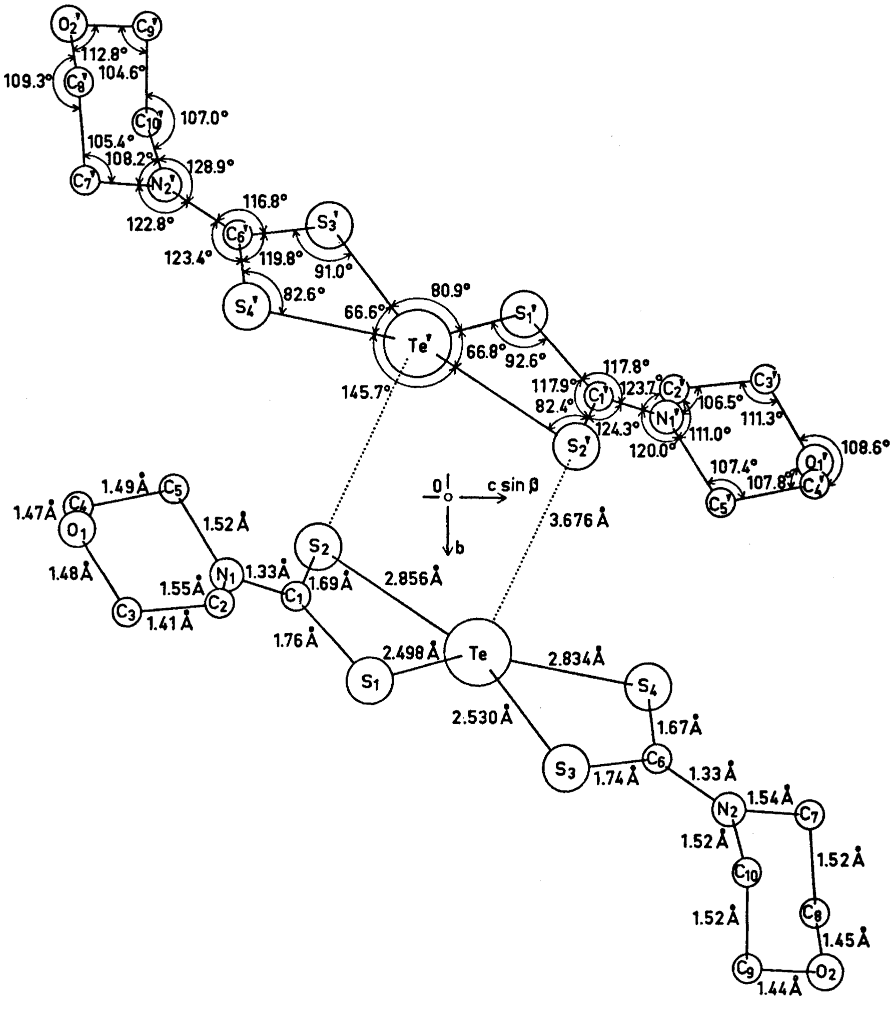

O2'
C9'
112.8°
109.3°
C8'
104.6°
C10'
107.0°
105.4°
108.2°
128.9°
C7'
N2'
116.8°
122.8°
C6'
S3'
123.4°
119.8°
91.0°
S4'
82.6°
80.9°
66.6°
S1'
Te'
66.8°
92.6°
117.8°
145.7°
117.9°
C1'
123.7°
C2'
C3'
82.4°
N1'
106.5°
124.3°
111.3°
S2'
111.0°
120.0°
108.6°
107.4°
O1'
107.8°
C4'
C5'
O
c sin β
b
1.49 Å
C5
1.47 Å
C4
O1
1.52 Å
1.48 Å
1.55 Å
N1
1.33 Å
S2
1.69 Å
2.856 Å
3.676 Å
C2
C1
C3
1.41 Å
1.76 Å
2.498 Å
Te
2.834 Å
S1
S4
2.530 Å
1.67 Å
S3
C6
1.74 Å
1.33 Å
N2
1.54 Å
C7
1.52 Å
C10
1.52 Å
1.52 Å
C8
1.45 Å
C9
O2
1.44 Å

Fig. 2. A pair of tellurium di(morpholyldithiocarbamate) molecules related by a center of symmetry as seen in the projection along the *a* axis.

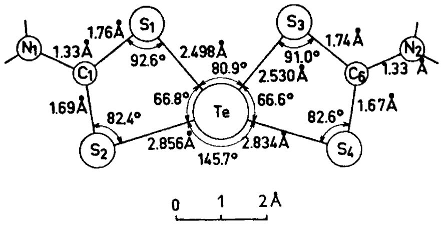


Fig. 3. The projection of the central part of the molecule as seen along the normal to the least squares plane through the nearly planar TeS_4 group.

through tellurium and the four ligand sulphur atoms bonded to it. The equation of the vector normal to this plane with all atoms given equal weight is $0.574\ x - 0.717\ y + 0.425\ z = 0$ referred to the crystal axes. The plane's distance from the origin is -0.996 Å. The distances from the plane are -0.033, 0.037, -0.008, -0.025, and 0.029 Å for Te, S_1, S_2, S_3, and S_4, respectively (S_2' is 2.0 Å above the plane). The least squares plane through the whole molecule except for the hydrogen atoms and the outer halves of the morpholyl groups, makes an angle of 6.6° with the TeS_4 plane. All thirteen atoms defining the plane are within a distance of 0.36 Å from it, thus the planarity is less pro-

Table 4. Bond lengths and angles with standard deviations.

$Te-S_1$	2.498(7) Å	$\angle S_1-Te-S_2$	66.8(2)°
$Te-S_2$	2.856(8)	$\angle S_2-Te-S_3$	80.9(2)
$Te-S_3$	2.530(6)	$\angle S_1-Te-S_4$	147.5(2)
$Te-S_4$	2.834(9)	$\angle S_2-Te-S_3$	147.6(2)
S_1-C_1	1.76(3)	$\angle S_2-Te-S_4$	145.7(2)
S_2-C_1	1.69(2)	$\angle S_3-Te-S_4$	66.6(2)
S_3-C_6	1.74(3)	$\angle Te-S_1-C_1$	92.6(8)
S_4-C_6	1.67(2)	$\angle Te-S_2-C_1$	82.4(10)
C_1-N_1	1.33(4)	$\angle Te-S_3-C_6$	91.0(8)
C_6-N_2	1.33(4)	$\angle Te-S_4-C_6$	82.6(11)
N_1-C_2	1.55(4)	$\angle S_1-C_1-S_2$	117.9(16)
C_2-C_3	1.41(6)	$\angle S_1-C_1-N_1$	117.8(15)
C_3-O_1	1.48(4)	$\angle S_2-C_1-N_1$	124.3(18)
O_1-C_4	1.47(3)	$\angle S_3-C_6-S_4$	119.8(17)
C_4-C_5	1.49(6)	$\angle S_3-C_6-N_2$	116.8(16)
C_5-N_1	1.52(3)	$\angle S_4-C_6-N_2$	123.4(21)
N_2-C_7	1.54(4)	$\angle C_1-N_1-C_2$	123.7(23)
C_7-C_8	1.52(3)	$\angle C_1-N_1-C_5$	120.0(19)
C_8-O_2	1.45(3)	$\angle C_2-N_1-C_5$	111.0(20)
O_2-C_9	1.44(4)	$\angle N_1-C_2-C_3$	106.5(26)
C_9-C_{10}	1.52(3)	$\angle C_2-C_3-O_1$	111.3(25)
$C_{10}-N_2$	1.52(3)	$\angle C_3-O_1-C_4$	108.6(21)
		$\angle O_1-C_4-C_5$	107.8(29)
		$\angle C_4-C_5-N_1$	107.4(22)
		$\angle C_6-N_2-C_7$	122.8(19)
		$\angle C_6-N_2-C_{10}$	128.9(25)
		$\angle C_7-N_2-C_{10}$	108.2(23)
		$\angle N_2-C_7-C_8$	105.4(22)
		$\angle C_7-C_8-O_2$	109.3(17)
		$\angle C_8-O_2-C_9$	112.8(22)
		$\angle O_2-C_9-C_{10}$	104.6(23)
		$\angle C_9-C_{10}-N_2$	107.0(18)

nounced than in tellurium di(ethylxanthate).[10] This deviation from planarity is probably due to packing effects resulting from the large morpholyl groups.

From the figures and from bond lengths and angles listed in Table 4, it is seen that the configuration around the tellurium atom closely resembles that of tellurium di(ethylxanthate).[10] There are two short Te – S bond lengths: $\mathrm{Te}-\mathrm{S}_1=2.498\pm0.007$ and $\mathrm{Te}-\mathrm{S}_3=2.530\pm0.006$ Å at an interbond angle of 80.9±0.2°, and two long ones, $\mathrm{Te}-\mathrm{S}_2=2.856\pm0.008$ and $\mathrm{Te}-\mathrm{S}_4=2.834\pm0.009$ Å at an interbond angle of 145.7±0.2°. Each of the short bonds are *trans* to a long one, the bond angles being $\angle\mathrm{Se}_1-\mathrm{Te}-\mathrm{S}_4=147.5\pm0.2$ and $\angle\mathrm{S}_2-\mathrm{Te}-\mathrm{S}_3=147.6\pm0.2°$. The average length of these two three-center systems are 5.36 Å, corresponding to an average Te – S bond length of 2.68 Å which is the same as found in centrosymmetrical square-planar complexes and in tellurium di(ethylxanthate).[10] Bonding in linear three-center systems is explained on basis of three-center four-electron bonds based on *p*-orbitals of the respective atoms.[1,2]

Table 5. Intramolecular distances in tellurium di(morpholyldithiocarbamate).

$\mathrm{Te}-\mathrm{C}_1$	3.12 Å	$\mathrm{C}_6-\mathrm{C}_{10}$	2.58 Å
$\mathrm{Te}-\mathrm{C}_6$	3.10	$\mathrm{N}_1-\mathrm{O}_1$	2.79
$\mathrm{S}_1-\mathrm{S}_2$	2.96	$\mathrm{N}_1-\mathrm{C}_3$	2.37
$\mathrm{S}_1-\mathrm{S}_3$	3.26	$\mathrm{N}_1-\mathrm{C}_4$	2.43
$\mathrm{S}_1-\mathrm{N}_1$	2.66	$\mathrm{N}_2-\mathrm{O}_2$	2.79
$\mathrm{S}_1-\mathrm{C}_2$	3.04	$\mathrm{N}_2-\mathrm{C}_8$	2.43
$\mathrm{S}_2-\mathrm{N}_1$	2.68	$\mathrm{N}_2-\mathrm{C}_9$	2.44
$\mathrm{S}_2-\mathrm{C}_5$	3.06	$\mathrm{C}_2-\mathrm{O}_1$	2.38
$\mathrm{S}_3-\mathrm{S}_4$	2.96	$\mathrm{C}_2-\mathrm{C}_4$	2.88
$\mathrm{S}_3-\mathrm{N}_2$	2.63	$\mathrm{C}_2-\mathrm{C}_5$	2.53
$\mathrm{S}_3-\mathrm{C}_{10}$	3.10	$\mathrm{C}_3-\mathrm{C}_4$	2.39
$\mathrm{S}_4-\mathrm{N}_2$	2.65	$\mathrm{C}_3-\mathrm{C}_5$	2.83
$\mathrm{S}_4-\mathrm{C}_7$	3.09	$\mathrm{C}_7-\mathrm{O}_2$	2.43
$\mathrm{C}_1-\mathrm{C}_2$	2.55	$\mathrm{C}_7-\mathrm{C}_9$	2.92
$\mathrm{C}_1-\mathrm{C}_3$	3.58	$\mathrm{C}_7-\mathrm{C}_{10}$	2.48
$\mathrm{C}_1-\mathrm{C}_4$	3.61	$\mathrm{C}_8-\mathrm{C}_9$	2.41
$\mathrm{C}_1-\mathrm{C}_5$	2.47	$\mathrm{C}_8-\mathrm{C}_{10}$	2.83
$\mathrm{C}_6-\mathrm{C}_7$	2.52	$\mathrm{O}_1-\mathrm{C}_5$	2.39
$\mathrm{C}_6-\mathrm{C}_8$	3.46	$\mathrm{O}_2-\mathrm{C}_{10}$	2.34
$\mathrm{C}_6-\mathrm{C}_9$	3.48		

The deviation from linearity in the present case and in the xanthate [10] makes such bonding less evident here. Geometrical considerations involving the size of the tellurium atom (radius of 1.37 Å [19]) relative to the S – S spacing in each ligand and the size of the sulphur atom, lead to the conclusion that formation of a mononuclear, planar complex with Te – S bond angles of 90 and 180° is prohibited.

To each short Te – S bond, there corresponds a long S – C bond, the lengths being: $\mathrm{S}_1-\mathrm{C}_1=1.76\pm0.03$ Å and $\mathrm{S}_3-\mathrm{C}_6=1.74\pm0.03$ Å. These lengths are shorter, but not significantly different from the single bond length of 1.81 Å.[19] The two other S – C bonds however, corresponding to the long Te – S bonds have lengths which are $\mathrm{S}_2-\mathrm{C}_1=1.69\pm0.02$ Å and $\mathrm{S}_4-\mathrm{C}_6=1.67\pm0.02$ Å, indicating a considerable amount of double bond character.

Table 6. Intermolecular distances and angles.

Te$-$C$_{10}$	$-1/2+x,\ 1/2-y,\ -1/2+z$	3.85 Å
C$_4-$C$_9$	$1/2-x,\ -1/2+y,\ 3/2-z$	3.82
C$_1-$O$_2$	$1/2-x,\ 1/2+y,\ 1/2-z$	3.58
C$_1-$C$_9$	»	3.72
N$_1-$O$_2$	»	3.45
C$_2-$O$_2$	»	3.45
C$_5-$O$_2$	»	3.65
C$_2-$C$_8$	$1/2+x,\ 1/2-y,\ -3/2+z$	3.78
O$_1-$C$_8$	»	3.47
S$_2-$C$_4$	$-x,\ -y,\ 1-z$	3.74
S$_1-$S$_4$	$1/2+x,\ 1/2-y,\ -1/2+z$	3.72
S$_1-$C$_8$	»	3.71
S$_2-$S$_4$	$-x,\ -y,\ -z$	3.76
S$_4-$C$_5$	»	3.74
C$_8-$C$_8$	$-x,\ -1\ -y,\ -1\ -z$	3.96
C$_8-$O$_2$	»	3.50
C$_8-$C$_9$	»	3.51
O$_2-$O$_2$	»	3.61
O$_2-$C$_9$	»	3.83
C$_2-$O$_1$	$-1\ -x,\ -y,\ 1-z$	3.52
C$_3-$O$_1$	»	3.58
O$_1-$O$_1$	»	3.48

The left column represents distances from an atom in the original molecule (Table 2) to an atom in a molecule whose transformation from the original one is listed in the next column.

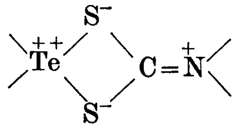
Te$-$S$_2'$=3.676 (7) Å $\angle$S$_2'-$Te$-$S$_2$=81.5 (2)°
$\angle$S$_2'-$Te$-$S$_4$=69.2 (2)

S$_2'$ represents S$_2$ transformed by a center of symmetry in (0, 0, 0).

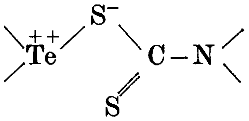
Since the Te$-$S bonds are all significantly longer than single bonds, π-bonding orbitals are probably not much involved in these bonds. Assuming the ligand S$_1$ and S$_3$ sulphur atoms to bond to tellurium through a σp orbital, the C$-$S$-$Te angles close to 90° are accounted for. Use by tellurium of its σp orbitals for overlap is in accord with the planarity of the complex as the other ends of the p-orbitals of tellurium would point towards the lone pair p orbitals of the partly double-bonded S$_2$ and S$_4$ atoms and overlap with these to form a bent bond. However, from decrease in overlap on this basis as compared to linear overlap and also because of asymmetry [1,2] one would expect an elongation of this three-center system as compared to a linear one. This is, however, not found. Contribution from s orbitals might account for the observed bond lengths, and together with steric factors, for the observed bond angles.

The structure of selenium bis(diethyldithiocarbamate) [20] is being determined in this laboratory. The structure is analogous to that found for tellurium di(morpholyldithiocarbamate). The average length of the corresponding S$-$Se$-$S three-center system is 5.07 Å corresponding to a Se$-$S average bond length of 2.53 Å. The compound phenylarsenic bis(diethyldithiocarbamate) [21] is isoelectronic with selenium bis(diethyldithiocarbamate), the Ph$-$As group corresponding to a selenium atom. It is not surprising that its structure, apart from the phenyl group is very similar to that of the selenium complex.

In tellurium di(morpholyldithiocarbamate), both C_1-N_1 and C_6-N_2 bonds have lengths of 1.33 Å which seems to be normal for most dithiocarbamates whose structures are known.[20-38] It clearly demonstrates the importance of the canonical form



This is also supported by the planarity of the molecule and the values of the bond angles at C_1, C_2, N_1, and N_2 which are consistent with sp^2 hybridization of these atoms. The short $C-S$ bond lengths imply that canonical forms of the type



contribute to the overall structure.

Transfer of charge from nitrogen to sulphur makes the ligand a very good donor. A corresponding effect is found in tellurium di(ethylxanthate)[10] where charge is transferred from oxygen to sulphur. These excellent donor properties may be part of the explanation of the unexpected short average $Te-S$ bond length found in tellurium complexes with these ligands.

Both morpholyl groups have the chair form, and bond lengths and angles seem to be normal within error limits.

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