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 $a = 11.242 \pm 0.005$ Å, $b = 15.906 \pm 0.009$ Å, $c = 9.150 \pm 0.004$ Å, $\beta = 92.75 \pm 0.05°$ and $Z = 4$. Density, calc. 1.84, found 1.82 g/cm³. The space group is $C_{2h}{}^5\text{-}P2_1/n$. 885 intensities above background were collected using $CuK\alpha$ 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: $Te-S_1 = 2.498 \pm 0.007$ Å, $Te-S_2 = 2.856 \pm 0.008$ Å, $Te-S_3 = 2.530 \pm 0.006$ Å, $Te-S_4 = 2.834 \pm 0.009$ Å, $\angle S_1-Te-S_2 = 66.8 \pm 0.2°$, $\angle S_1-Te-S_3 = 80.9 \pm 0.2°$, $\angle S_2-Te-S_4 = 145.7 \pm 0.2°$ and $\angle S_3-Te-S_4 = 66.6 \pm 0.2°$.

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 dimethyl-dithiophosphate and diethylthioselenophosphinate ions as ligands have shown a tendency toward square-planar configuration around tellurium;[8,11] how-ever, two of the Te−S bonds are intermolecular and very weak, especially in the thioselenophosphinate.[11] The related compound, selenium bis-(diethyldi-selenophosphinate) [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 poly-thionates. 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 men-tioned above.[1,2]

In order to extend the studies of divalent tellurium and selenium com-pounds 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.

<div align="center">EXPERIMENTAL</div>

Tellurium di(morpholyldithiocarbamate),

$$Te\left[O\underset{CH_2-CH_2}{\overset{CH_2-CH_2}{<}}N-CS_2\right]_2$$
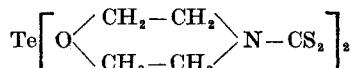
was prepared by nucleophilic substitution on divalent tellurium.[14] An aqueous solution of sodium morpholyldithiocarbamate,[15] was added with stirring to an aqueous solution of potassium telluropentathionate. The resulting orange precipitate was washed with water and methanol and dried. Recrystallization 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/cm³. 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 $0kl$, $hk0$, $hk1$ and $hk2$ structure factors ($\times 10$) for tellurium di(morpholyldithiocarbamate). A minus sign in the F_0 column indicates that the corresponding reflection is unobserved.

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)
0	2	0	463	-532	0	9	5	-93	-63	1	10	0	189	130	6	8	0	393	-309	12	12	0	139	-120
0	4	0	930	-073	0	10	5	192	-176	1	11	0	422	-417	6	9	0	478	-455	13	1	0	213	170
0	6	0	890	929	0	11	5	107	-172	1	12	0	-122	73	6	10	0	624	614	13	2	0	144	124
0	8	0	195	194	0	12	5	414	422	1	13	0	314	323	6	11	0	244	204	13	3	0	374	-319
0	10	0	1082	-1127	0	13	5	-95	8	1	14	0	166	-157	6	12	0	-138	-1	13	4	0	-114	-48
0	12	0	327	281	0	14	5	160	-141	1	15	0	-123	88	6	13	0	-131	39	13	5	0	-112	26
0	14	0	130	124	0	15	5	-91	22	1	16	0	-117	-65	6	14	0	347	-365	13	6	0	-106	-7
0	16	0	-95	-39	0	16	5	197	-201	1	17	0	197	-176	6	15	0	-170	-39	13	7	0	259	221
0	18	0	152	-144	0	17	5	113	-92	1	18	0	-198	75	6	16	0	159	157	13	8	0	195	95
0	20	0	143	145	0	18	5	75	96	1	19	0	-95	-23	6	17	0	-100	13	14	0	0	172	157
0	1	1	1132	1107	0	0	6	-87	-36	1	20	0	-70	17	6	18	0	-76	91	14	1	0	-91	1
0	2	1	175	-129	0	1	6	757	-770	2	0	0	588	651	7	1	0	872	-892	14	2	0	-89	-63
0	3	1	2256	-2351	0	2	6	348	-327	2	1	0	1938	-2164	7	2	0	259	263	14	3	0	-85	-33
0	4	1	832	791	0	3	6	196	174	2	2	0	277	-232	7	3	0	742	697	14	4	0	199	-198
0	5	1	135	-137	0	4	6	255	264	2	3	0	138	-119	7	4	0	436	-475	1	0	1	1195	1253
0	6	1	418	382	0	5	6	217	229	2	4	0	1022	-1071	7	5	0	133	82	1	1	1	1020	-1235
0	7	1	961	966	0	6	6	114	-93	2	5	0	347	382	7	6	0	-125	-20	1	2	1	749	750
0	8	1	314	-354	0	7	6	-93	12	2	6	0	568	612	7	7	0	720	-723	1	3	1	1269	1235
0	9	1	657	-687	0	8	6	171	-143	2	7	0	-104	-88	7	8	0	-138	25	1	4	1	1874	-1910
0	10	1	114	-112	0	9	6	608	-592	2	8	0	-111	-40	7	9	0	249	202	1	5	1	1759	1900
0	11	1	712	-725	0	10	6	-97	6	2	9	0	790	-813	7	10	0	163	-109	1	6	1	982	924
0	12	1	-87	15	0	11	6	405	418	2	10	0	375	-362	7	11	0	431	399	1	7	1	-83	57
0	13	1	412	309	0	12	6	188	167	2	11	0	608	622	7	12	0	-137	60	1	8	1	-89	15
0	14	1	-95	43	0	13	6	-92	-31	2	12	0	372	-397	7	13	0	256	-238	1	9	1	613	-563
0	15	1	183	172	0	14	6	180	-182	2	13	0	331	308	7	14	0	124	115	1	10	1	552	-512
0	16	1	171	-172	0	15	6	196	-189	2	14	0	222	206	7	15	0	-116	-67	1	11	1	532	530
0	17	1	297	-282	0	16	6	-78	58	2	15	0	212	-198	7	16	0	-102	-44	1	12	1	-103	-16
0	18	1	-93	-6	0	17	6	-52	-34	2	16	0	-116	-71	7	17	0	196	184	1	13	1	158	-147
0	19	1	84	79	0	1	7	362	-363	2	17	0	-114	-48	8	0	0	567	-551	1	14	1	341	-327
0	20	1	-61	27	0	2	7	683	-472	2	18	0	196	-94	8	1	0	611	595	1	15	1	136	-126
0	0	2	1238	1147	0	3	7	172	179	2	19	0	205	182	8	2	0	291	185	1	16	1	235	-242
0	1	2	454	-331	0	4	7	435	436	2	20	0	77	76	8	3	0	-119	-65	1	17	1	-96	-106
0	2	2	-48	-4	0	5	7	217	192	3	1	0	813	855	8	4	0	334	283	1	18	1	-90	-53
0	3	2	591	-597	0	6	7	467	412	3	2	0	1283	-1269	8	5	0	599	-534	1	19	1	-80	88
0	4	2	1340	-1454	0	7	7	158	-149	3	3	0	324	-312	8	6	0	-130	-93	1	20	1	-57	55
0	5	2	271	269	0	8	7	377	-399	3	4	0	114	17	8	7	0	135	157	2	1	1	979	1017
0	6	2	1275	1142	0	9	7	-95	46	3	5	0	353	309	8	8	0	430	-619	2	2	1	3036	-3277
0	7	2	1912	948	0	10	7	194	176	3	6	0	995	1057	8	9	0	248	193	2	3	1	441	396
0	8	2	540	530	0	11	7	263	247	3	7	0	-107	-58	8	10	0	515	504	2	4	1	1442	1337
0	9	2	489	-490	0	12	7	142	157	3	8	0	884	-930	8	11	0	268	-237	2	5	1	-72	66
0	10	2	382	-402	0	13	7	-88	-50	3	9	0	375	-352	8	12	0	-134	75	2	6	1	599	561
0	11	2	265	244	0	14	7	116	-90	3	10	0	631	-642	8	13	0	-124	58	2	7	1	240	213
0	12	2	152	-135	0	15	7	-74	-76	3	11	0	272	-262	8	14	0	231	-211	2	8	1	795	-805
0	13	2	442	438	0	16	7	-75	-75	3	12	0	593	676	8	15	0	-134	51	2	9	1	209	188
0	14	2	673	503	0	0	8	371	-391	3	13	0	-129	14	8	16	0	-86	63	2	10	1	122	130
0	15	2	273	-271	0	1	8	93	-134	3	14	0	-127	-77	9	1	0	390	-363	2	11	1	378	-349
0	16	2	237	-218	0	2	8	242	212	3	15	0	-122	-3	9	2	0	591	496	2	12	1	411	380
0	17	2	123	-95	0	3	8	203	-295	3	16	0	259	-276	9	3	0	-126	100	2	13	1	-107	107
0	18	2	133	-83	0	4	8	-94	63	3	17	0	-113	27	9	4	0	453	-456	2	14	1	130	-169
0	19	2	192	165	0	5	8	156	175	3	18	0	222	206	9	5	0	262	257	2	15	1	-103	62
0	1	3	644	600	0	6	8	140	-117	3	19	0	-88	-35	9	6	0	374	-385	2	16	1	175	-182
0	2	3	1462	-1378	0	7	8	131	-138	4	0	0	304	305	9	7	0	255	-247	2	17	1	-95	-121
0	3	3	1274	-1199	0	8	8	299	-295	4	1	0	572	-571	9	8	0	302	282	2	18	1	88	62
0	4	3	344	-287	0	9	8	209	-213	4	2	0	143	-156	9	9	0	-139	26	2	19	1	-77	-2
0	5	3	104	71	0	10	8	210	247	4	3	0	777	-888	9	10	0	-134	75	3	0	1	239	-244
0	6	3	403	433	0	11	8	130	108	4	4	0	-86	16	9	11	0	312	295	3	1	1	585	-574
0	7	3	439	436	0	12	8	-84	78	4	5	0	1061	989	9	12	0	177	-152	3	2	1	729	680
0	8	3	683	-675	0	13	8	144	126	4	6	0	431	439	9	13	0	-115	-44	3	3	1	969	-996
0	9	3	197	-116	0	14	8	192	-109	4	7	0	448	-409	9	14	0	-102	20	3	4	1	524	575
0	10	3	459	-455	0	1	9	-88	-56	4	8	0	456	-421	9	15	0	-85	-71	3	5	1	1994	1985
0	11	3	279	-239	0	2	9	-88	8	4	9	0	872	-823	10	0	0	-128	-81	3	6	1	409	-365
0	12	3	489	474	0	3	9	293	209	4	10	0	157	140	10	1	0	473	466	3	7	1	545	-551
0	13	3	355	349	0	4	9	-87	-20	4	11	0	193	166	10	2	0	220	-195	3	8	1	131	-139
0	14	3	-97	1	0	5	9	-88	126	4	12	0	248	237	10	3	0	194	172	3	9	1	473	-483
0	15	3	-95	85	0	6	9	98	53	4	13	0	551	536	10	4	0	160	126	3	10	1	-104	-87
0	16	3	213	-213	0	7	9	286	-307	4	14	0	229	-205	10	5	0	398	-400	3	11	1	331	334
0	17	3	147	-120	0	8	9	122	-123	4	15	0	367	-364	10	6	0	295	-181	3	12	1	257	-243
0	18	3	146	138	0	9	9	-85	-62	4	16	0	-124	114	10	7	0	-132	-24	3	13	1	323	330
0	19	3	-71	-41	0	10	9	106	-103	4	17	0	-117	24	10	8	0	132	103	3	14	1	-107	71
0	0	4	187	-127	0	11	9	150	160	4	18	0	136	95	10	9	0	451	356	3	15	1	371	-415
0	1	4	1095	-989	0	12	9	172	119	4	19	0	153	158	10	10	0	-129	45	3	16	1	-98	32
0	2	4	-69	19	0	0	10	166	-180	5	1	0	126	60	10	11	0	138	-126	3	17	1	-96	-55
0	3	4	732	-741	0	1	10	-84	75	5	2	0	1079	-1150	10	12	0	113	90	3	18	1	-88	-1
0	4	4	293	-282	0	2	10	-83	86	5	3	0	552	546	10	13	0	100	-83	3	19	1	125	140
0	5	4	1270	1274	0	3	10	-92	20	5	4	0	211	201	10	14	0	-78	-71	4	1	1	240	-272
0	6	4	76	-92	0	4	10	333	314	5	5	0	376	336	11	1	0	-127	-31	4	2	1	1191	-1111
0	7	4	602	-566	0	5	10	-81	-81	5	6	0	213	226	11	2	0	553	528	4	3	1	603	615
0	8	4	341	366	0	6	10	175	-193	5	7	0	693	-667	11	3	0	171	-158	4	4	1	847	892
0	9	4	484	-463	0	7	10	-75	17	5	8	0	710	-729	11	4	0	297	-371	4	5	1	-79	-40
0	10	4	277	-265	0	8	10	-72	-73	5	9	0	-134	-46	11	5	0	-129	-45	4	6	1	692	754
0	11	4	249	222	0	9	10	-64	22	5	10	0	-137	-76	11	6	0	223	-195	4	7	1	333	-297
0	12	4	168	-151	0	10	10	94	88	5	11	0	637	580	11	7	0	147	136	4	8	1	441	-391
0	13	4	309	309	0	1	11	132	-159	5	12	0	591	550	11	8	0	344	313	4	9	1	-102	-56
0	14	4	226	224	0	2	11	-60	117	5	13	0	322	-320	11	9	0	-128	30	4	10	1	303	-276
0	15	4	194	-167	0	3	11	216	241	5	14	0	-126	-67	11	10	0	-117	22	4	11	1	175	173
0	16	4	-91	-79	0	4	11	-63	-45	5	15	0	-123	-97	11	11	0	-105	-13	4	12	1	279	298
0	17	4	-89	-4	0	5	11	-59	-49	5	16	0	-116	-96	11	12	0	165	-166	4	13	1	338	-365
0	18	4	78	-75	0	6	11	-52	-2	5	17	0	197	186	12	0	0	251	212	4	14	1	-107	-50
0	19	4	113	127	1	1	0	860	1021	5	18	0	117	82	12	1	0	317	255	4	15	1	143	-141
0	1	5	263	224	1	2	0	1353	-1466	6	0	0	1144	-1163	12	2	0	126	-108	4	16	1	196	-223
0	2	5	1024	-938	1	3	0	1373	-1526	6	1	0	729	-736	12	3	0	177	149	4	17	1	122	110
0	3	5	434	623	1	4	0	158	91	6	2	0	-96	36	12	4	0	345	-287	4	18	1	-83	107
0	4	5	583	517	1	5	0	270	228	6	3	0	674	-619	12	5	0	420	-380	4	19	1	-64	26
0	5	5	129	-99	1	6	0	633	542	6	4	0	817	841	12	6	0	232	191	5	0	1	442	-449
0	6	5	731	721	1	7	0	1257	1742	6	5	0	-111	65	12	7	0	259	205	5	1	1	957	-949
0	7	5	-97	45	1	8	0	500	-421	6	6	0	901	-781	12	8	0	115	104	5	2	1	127	-316
0	8	5	612	-593	1	9	0	800	-911	6	7	0	-123	-23	12	9	0	107	101	5	3	1	-77	-42

Table 1. Continued.

H	K	L	F(O)	F(C)
5	4	1	1317	1239
5	5	1	399	387
5	6	1	577	-576
5	7	1	426	-396
5	8	1	682	-605
5	9	1	522	-541
5	10	1	215	237
5	11	1	268	264
5	12	1	-114	45
5	13	1	-111	-7
5	14	1	383	-427
5	15	8	-100	-74
5	16	1	160	141
5	17	1	-89	-91
5	18	1	107	125
6	1	1	286	-731
6	2	1	405	-428
6	3	1	1182	1179
6	4	1	500	484
6	5	1	-94	-8
6	6	1	-99	-17
6	7	1	1031	-991
6	8	1	415	-405
6	9	1	118	197
6	10	1	270	275
6	11	1	367	386
6	12	1	-115	-92
6	13	1	357	-347
6	14	1	-105	13
6	15	1	141	-105
6	16	1	-93	51
6	17	1	215	244
6	18	1	-61	-26
7	0	1	893	-910
7	1	1	-88	-12
7	2	1	692	654
7	3	1	-93	-44
7	4	1	692	753
7	5	1	337	-323
7	6	1	475	-458
7	7	1	208	-225
7	8	1	355	-351
7	9	1	276	267
7	10	1	530	538
7	11	1	-116	-125
7	12	1	113	-154
7	13	1	109	-106
7	14	1	194	-204
7	15	1	136	131
7	16	1	-95	73
7	17	1	-67	16
8	1	1	314	-288
8	2	1	509	512
8	3	1	339	392
8	4	1	410	-423
8	5	1	-136	89
8	6	1	496	-534
8	7	1	441	-478
8	8	1	335	359
8	9	1	-118	72
8	10	1	-114	-18
8	11	1	-110	146
8	12	1	133	-249
8	13	1	247	-153
8	14	1	136	80
8	15	1	-85	-76
8	16	1	135	153
9	0	1	127	114
9	1	1	454	470
9	2	1	182	-195
9	3	1	150	151
9	4	1	187	171
9	5	1	518	-554
9	6	1	137	-127
9	7	1	-114	-76
9	8	1	139	-165
9	9	1	359	378
9	10	1	-107	11
9	11	1	185	-175
9	12	1	126	116
9	13	1	180	-161
9	14	1	170	-152
9	15	1	177	204
10	1	1	132	98
10	2	1	229	214
10	3	1	133	-109
10	4	1	189	-188
10	5	1	-110	35
10	6	1	448	-448
10	7	1	-110	55
10	8	1	187	181
10	9	1	130	-129
10	10	1	166	165
10	11	1	-101	27
10	12	1	261	-280
10	13	1	-81	-1
10	14	1	-62	37
11	0	1	158	153
11	1	1	150	117
11	2	1	-106	-70
11	3	1	213	207
11	4	1	249	-229
11	5	1	373	-407
11	6	1	132	158
11	7	1	-106	-64
11	8	1	-103	68
11	9	1	172	167
11	10	1	-93	-65
11	11	1	-86	-24
11	12	1	-71	-37
12	1	1	146	157
12	2	1	147	156
12	3	1	313	-308
12	4	1	166	-163
12	5	1	-106	-44
12	6	1	143	-135
12	7	1	214	244
12	8	1	130	97
12	9	1	-84	-36
12	10	1	-71	30
12	11	1	-50	-107
13	2	1	136	-120
13	3	1	-95	-54
13	4	1	300	-288
13	5	1	-89	7
13	6	1	224	219
13	7	1	-73	-62
1	1	-1	429	400
1	2	-1	545	-590
1	3	-1	387	-407
1	4	-1	674	-572
1	5	-1	135	137
1	6	-1	604	539
1	7	-1	250	-319
1	8	-1	1400	1419
1	9	-1	230	-292
1	10	-1	1076	-1076
1	11	-1	-107	82
1	12	-1	-103	-29
1	13	-1	-115	77
1	14	-1	403	427
1	15	-1	-103	-41
1	16	-1	-98	-142
1	17	-1	-96	113
1	18	-1	247	-256
1	19	-1	-80	14
1	23	-1	137	177
2	1	-1	693	671
2	2	-1	1012	-1004
2	3	-1	495	-445
2	4	-1	638	-643
2	5	-1	580	-552
2	6	-1	129	141
2	7	-1	903	872
2	8	-1	701	-694
2	9	-1	153	171
2	10	-1	458	-478
2	11	-1	639	-596
2	12	-1	471	438
2	13	-1	374	376
2	14	-1	118	91
2	15	-1	281	305
2	16	-1	225	-241
2	17	-1	271	-283
2	18	-1	221	214
2	19	-1	-78	63
3	0	-1	168	222
3	1	-1	754	-679
3	2	-1	-55	-63
3	3	-1	453	-445
3	4	-1	729	-733
3	5	-1	659	595
3	6	-1	486	502
3	7	-1	405	367
3	8	-1	213	201
3	9	-1	1182	-1123
3	10	-1	311	-344
3	11	-1	470	459
3	12	-1	-109	29
3	13	-1	475	478
3	14	-1	437	409
3	15	-1	283	-319
3	16	-1	-98	-115
3	17	-1	-94	-63
3	18	-1	-86	-58
3	19	-1	175	210
4	1	-1	-61	36
4	2	-1	1478	-1511
4	3	-1	655	-619
4	4	-1	217	260
4	5	-1	300	-305
4	6	-1	517	548
4	7	-1	276	237
4	8	-1	946	-898
4	9	-1	224	205
4	10	-1	248	-238
4	11	-1	-112	5
4	12	-1	676	715
4	13	-1	165	131
4	14	-1	-106	-82
4	15	-1	-101	-121
4	16	-1	240	-233
4	17	-1	-92	-2
4	18	-1	152	155
4	19	-1	-65	-16
5	0	-1	1512	-1531
5	1	-1	954	-943
5	2	-1	232	-169
5	3	-1	870	-849
5	4	-1	463	478
5	5	-1	1133	1201
5	6	-1	583	-514
5	7	-1	287	-282
5	8	-1	158	143
5	9	-1	546	-482
5	10	-1	354	311
5	11	-1	281	245
5	12	-1	-114	29
5	13	-1	267	266
5	14	-1	-105	-36
5	15	-1	284	-289
5	16	-1	-97	44
5	17	-1	-90	56
5	18	-1	-77	10
6	1	-1	934	-951
6	2	-1	493	-522
6	3	-1	1141	1169
6	4	-1	329	300
6	5	-1	236	-213
6	6	-1	524	481
6	7	-1	567	-554
6	8	-1	314	-332
6	9	-1	677	615
6	10	-1	200	-195
6	11	-1	293	261
6	12	-1	344	384
6	13	-1	198	-217
6	14	-1	-103	-49
6	15	-1	-100	58
6	16	-1	169	-158
6	17	-1	-83	55
6	18	-1	-63	77
7	0	-1	1162	-1216
7	1	-1	212	-223
7	2	-1	215	249
7	3	-1	-92	-41
7	4	-1	743	811
7	5	-1	741	-187
7	6	-1	672	-706
7	7	-1	402	398
7	8	-1	-116	-67
7	9	-1	382	-358
7	10	-1	442	423
7	11	-1	-122	68
7	12	-1	-115	90
7	13	-1	-106	97
7	14	-1	187	-186
7	15	-1	-95	-58
7	16	-1	-85	88
7	17	-1	85	-85
8	1	-1	742	-742
8	2	-1	317	311
8	3	-1	467	493
8	4	-1	-103	-21
8	5	-1	-106	110
8	6	-1	-110	10
8	7	-1	453	-459
8	8	-1	212	208
8	9	-1	263	246
8	10	-1	-121	60
8	11	-1	365	349
8	12	-1	-110	-61
8	13	-1	165	-158
8	14	-1	-96	60
8	15	-1	145	-115
8	16	-1	-77	-31
9	0	-1	935	-998
9	1	-1	357	369
9	2	-1	324	312
9	3	-1	146	189
9	4	-1	310	310
9	5	-1	-110	-162
9	6	-1	187	-203
9	7	-1	-115	-10
9	8	-1	209	-186
9	9	-1	317	308
9	10	-1	420	437
9	11	-1	-112	-67
9	12	-1	-103	-59
9	13	-1	119	-114
9	14	-1	102	-111
9	15	-1	112	124
10	1	-1	260	-251
10	2	-1	487	492
10	3	-1	401	430
10	4	-1	-110	-50
10	5	-1	157	-157
10	6	-1	263	-257
10	7	-1	201	-229
10	8	-1	352	374
10	9	-1	196	219
10	10	-1	-109	61
10	11	-1	-103	37
10	12	-1	266	-263
10	13	-1	-83	-38
11	0	-1	-65	15
11	1	-1	-107	-46
11	2	-1	488	546
11	3	-1	141	156
11	4	-1	107	110
11	5	-1	301	-316
11	6	-1	-107	-112
11	7	-1	155	139
11	8	-1	146	134
11	9	-1	370	353
11	10	-1	-98	-46
11	11	-1	192	-207
11	12	-1	-74	18
12	1	-1	-104	130
12	2	-1	-106	358
12	3	-1	344	-115
12	4	-1	-106	-160
12	5	-1	-104	-34
12	6	-1	173	-160
12	7	-1	208	195
12	8	-1	268	258
12	9	-1	-90	-81
12	10	-1	-75	69
13	0	-1	192	216
13	1	-1	-99	53
13	2	-1	-98	-50
13	3	-1	194	178
13	4	-1	136	-147
13	5	-1	-94	-101
13	6	-1	135	158
13	7	-1	-81	29
13	8	-1	76	77
14	1	-1	139	133
14	2	-1	-75	49
14	3	-1	119	-127
1	1	2	95	-44
1	2	2	221	-183
1	3	2	720	-705
1	4	2	704	672
1	5	2	285	284
1	6	2	1292	1203
1	7	2	924	965
1	8	2	697	-723
1	9	2	227	-194
1	10	2	450	-438
1	11	2	255	-258
1	12	2	562	586
1	13	2	357	344
1	14	2	132	-145
1	15	2	91	-75
1	16	2	298	-331
1	17	2	-83	-73
1	18	2	95	131
1	19	2	-67	-1
2	0	2	614	-663
2	1	2	1000	-1015
2	2	2	691	-702
2	3	2	608	-575
2	4	2	302	-283
2	5	2	2046	2158
2	6	2	445	-389
2	7	2	546	-490
2	8	2	289	328
2	9	2	565	-550
2	10	2	-88	115
2	11	2	234	239
2	12	2	95	111
2	13	2	420	434
2	14	2	-94	-2
2	15	2	473	-473
2	16	2	-85	-65
2	17	2	-82	27
2	18	2	-77	-24
2	19	2	-64	91
3	1	2	203	-155
3	2	2	1131	-1077
3	3	2	1111	1195
3	4	2	627	639
3	5	2	454	-439
3	6	2	1206	1220
3	7	2	647	-578
3	8	2	608	-601
3	9	2	274	255
3	10	2	90	-134
3	11	2	-94	-2
3	12	2	554	575
3	13	2	145	-128
3	14	2	200	-214
3	15	2	-90	52
3	16	2	250	-264
3	17	2	-83	-41
3	18	2	74	98
3	19	2	-59	30
4	0	2	1241	-1308
4	1	2	616	-619
4	2	2	374	376
4	3	2	271	218
4	4	2	1104	1133
4	5	2	423	382
4	6	2	889	-863
4	7	2	625	659
4	8	2	204	201
4	9	2	547	-550
4	10	2	323	308
4	11	2	158	130
4	12	2	-97	65
4	13	2	154	149
4	14	2	244	-250
4	15	2	208	-264
4	16	2	-86	55
4	17	2	139	-131
4	18	2	-70	61
4	19	2	110	169
5	1	2	685	-663
5	2	2	141	102
5	3	2	1048	961
5	4	2	-73	-49
5	5	2	394	363
5	6	2	420	376
5	7	2	721	-719
5	8	2	126	88
5	9	2	322	332
5	10	2	-95	-13
5	11	2	388	364
5	12	2	98	141
5	13	2	283	-304
5	14	2	-93	-12
5	15	2	194	-190
5	16	2	155	-160
5	17	2	161	194
5	18	2	-67	68
6	0	2	1169	-1248
6	1	2	135	113
6	2	2	765	811
6	3	2	248	245
6	4	2	767	742
6	5	2	232	196
6	6	2	410	-390
6	7	2	103	75
6	8	2	567	-543
6	9	2	-97	62
6	10	2	370	393
6	11	2	-98	-78
6	12	2	183	-154
6	13	2	177	-162
6	14	2	250	-273
6	15	2	-86	24
6	16	2	-79	47
6	17	2	-69	23
6	18	2	110	156
7	1	2	458	-477
7	2	2	573	606
7	3	2	778	820
7	4	2	106	113
7	5	2	135	-144
7	6	2	459	-404
7	7	2	654	-641
7	8	2	234	254
7	9	2	235	258
7	10	2	-99	55
7	11	2	-98	60
7	12	2	224	-239
7	13	2	196	-198
7	14	2	-81	-27
7	15	2	-81	-45
7	16	2	114	113
7	17	2	-53	71
8	0	2	238	-204
8	1	2	746	712
8	2	2	305	325
8	3	2	142	126
8	4	2	490	431
8	5	2	632	-601
8	6	2	488	-487
8	7	2	177	181
8	8	2	-98	60
8	9	2	462	453
8	10	2	-96	42
8	11	2	282	-291
8	12	2	-89	-92
8	13	2	99	-112
8	14	2	-92	-69
8	15	2	160	157
8	16	2	-55	7
9	1	2	-93	138
9	2	2	672	712
9	3	2	224	194
9	4	2	347	-371
9	5	2	-97	-4
9	6	2	395	-375
9	7	2	-97	55
9	8	2	385	393
9	9	2	-93	-86
9	10	2	-91	5
9	11	2	-88	-49
9	12	2	283	-285
9	13	2	-81	30
9	14	2	-71	57
9	15	2	-53	-8
10	0	2	269	286
10	1	2	213	196
10	2	2	-95	40
10	3	2	234	207
10	4	2	256	-236
10	5	2	392	-402
10	6	2	133	149
10	7	2	-92	37
10	8	2	-91	7
10	9	2	165	192
10	10	2	155	-159
10	11	2	143	-125
10	12	2	-76	-40
10	13	2	140	-166
11	1	2	218	225
11	2	2	159	150
11	3	2	183	-146
11	4	2	-91	-62
11	5	2	-89	-79
11	6	2	191	-182
11	7	2	187	171
11	8	2	-85	67
11	9	2	-67	-84
11	10	2	-77	89
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	-87	-64	5	3	-2	537	463	7	10	-2	-104	-49	10	5	-2	232	-260
12	4	2	238	-230	2	18	-2	197	-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	189	196	10	7	-2	-98	74
12	6	2	112	96	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	140	142	3	3	-2	1583	-1649	5	8	-2	688	-556	7	15	-2	155	-120	10	10	-2	258	239
12	9	2	-56	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	1029	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	1245	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	-83	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	162	3	15	-2	-99	51	6	1	-2	437	-448	8	9	-2	-103	-70	11	8	-2	269	308
1	11	-2	585	-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	25
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	-51	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	-94	-38	8	16	-2	85	91	12	2	-2	-91	-69
1	18	-2	77	-95	4	3	-2	-61	-45	6	9	-2	713	-206	9	1	-2	329	-332	12	3	-2	129	141
1	19	-2	-68	25	4	4	-2	933	-861	6	10	-2	405	382	9	2	-2	105	71	12	4	-2	-91	-18
2	0	-2	1319	1385	4	5	-2	1517	1572	6	11	-2	145	168	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	96	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	184	136	6	14	-2	119	-131	9	6	-2	-100	-56	12	8	-2	-91	-57
2	4	-2	977	-950	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	540	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	22	9	10	-2	202	195	13	2	-2	154	172
2	8	-2	872	848	4	13	-2	-98	-54	7	1	-2	377	-335	9	11	-2	244	253	13	3	-2	129	-130
2	9	-2	-96	-35	4	14	-2	208	224	7	2	-2	409	-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	19
2	11	-2	146	192	4	16	-2	-85	-52	7	4	-2	560	525	9	14	-2	-74	5	13	6	-2	182	-176
2	12	-2	-94	62	4	17	-2	-90	-41	7	5	-2	207	185	9	15	-2	-59	-72	13	7	-2	-81	77
2	13	-2	136	106	4	18	-2	-72	-29	7	6	-2	513	492	13	0	-2	406	-431	14	0	-2	296	225
2	14	-2	438	410	4	19	-2	86	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 $\exp[-8\pi^2 U(\sin^2\theta/\lambda^2)]$.

	$U_{11}(U)$		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$\cdots$S$_2$ contacts. These have a length of 3.68 Å as compared
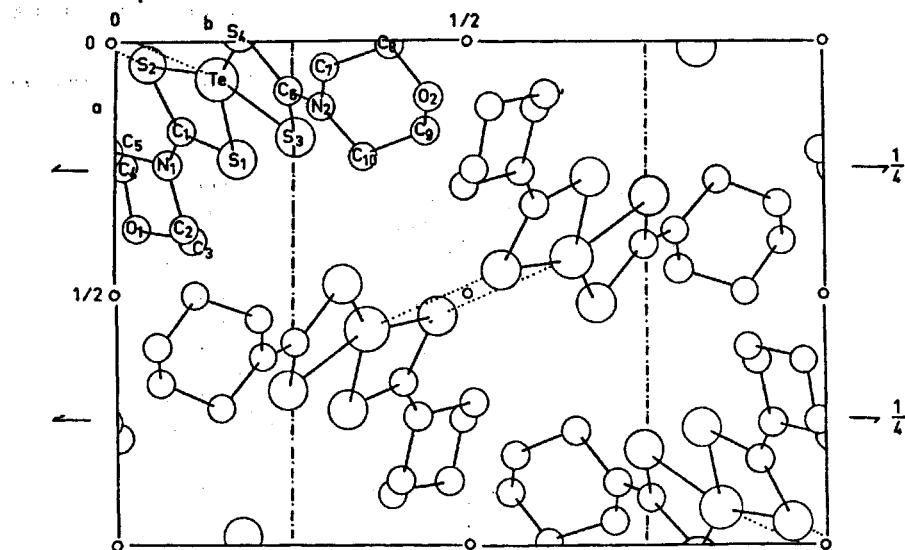
Fig. 1. The arrangement of molecules in the unit cell as seen along the c axis. Dotted lines indicate short, intermolecular Te$\cdots$S contacts.

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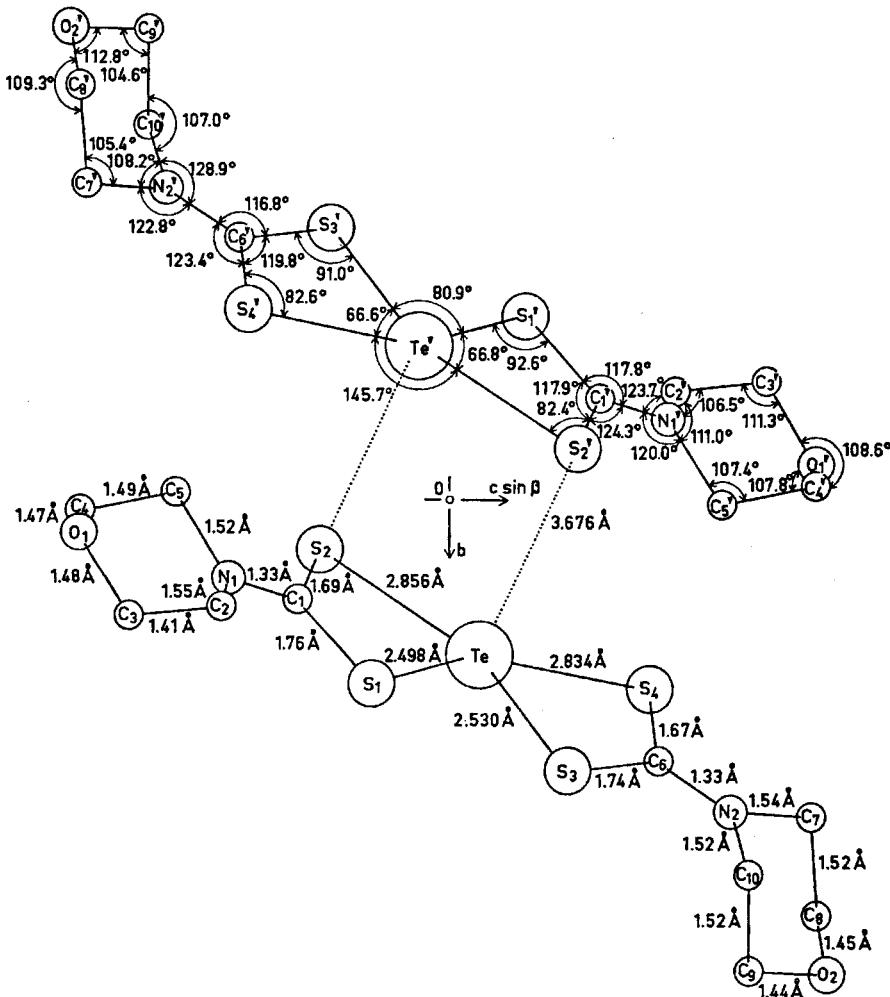
Fig. 2. A pair of tellurium di(morpholyldithiocarbamate) molecules related by a center of symmetry as seen in the projection along the *a* axis.

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
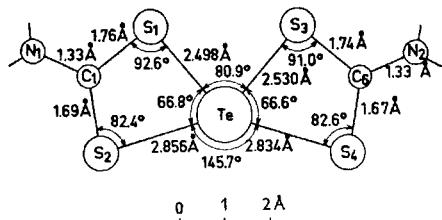
Fig. 3. The projection of the central part of the molecule as seen along the normal to the least squares plane through the nearly planar TeS$_4$ group.

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: $Te-S_1 = 2.498 \pm 0.007$ and $Te-S_3 = 2.530 \pm 0.006$ Å at an interbond angle of $80.9 \pm 0.2°$, and two long ones, $Te-S_2 = 2.856 \pm 0.008$ and $Te-S_4 = 2.834 \pm 0.009$ Å at an interbond angle of $145.7 \pm 0.2°$. Each of the short bonds are *trans* to a long one, the bond angles being $\angle S_1 - Te - S_4 = 147.5 \pm 0.2$ and $\angle S_2 - Te - S_3 = 147.6 \pm 0.2°$. The average length of these two three-center

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

$Te-C_1$	3.12 Å	C_6-C_{10}	2.58 Å
$Te-C_6$	3.10	N_1-O_1	2.79
S_1-S_2	2.96	N_1-C_3	2.37
S_1-S_3	3.26	N_1-C_4	2.43
S_1-N_1	2.66	N_2-O_2	2.79
S_1-C_2	3.04	N_2-C_8	2.43
S_2-N_1	2.68	N_2-C_9	2.44
S_2-C_5	3.06	C_2-O_1	2.38
S_3-S_4	2.96	C_2-C_4	2.88
S_3-N_2	2.63	C_2-C_5	2.53
S_3-C_{10}	3.10	C_3-C_4	2.39
S_4-N_2	2.65	C_3-C_5	2.83
S_4-C_7	3.09	C_7-O_2	2.43
C_1-C_2	2.55	C_7-C_9	2.92
C_1-C_3	3.58	C_7-C_{10}	2.48
C_1-C_4	3.61	C_8-C_9	2.41
C_1-C_5	2.47	C_8-C_{10}	2.83
C_6-C_7	2.52	O_1-C_5	2.39
C_6-C_8	3.46	O_2-C_{10}	2.34
C_6-C_9	3.48		

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]

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: $S_1-C_1 = 1.76 \pm 0.03$ Å and $S_3-C_6 = 1.74 \pm 0.03$ 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 $S_2-C_1 = 1.69 \pm 0.02$ Å and $S_4-C_6 = 1.67 \pm 0.02$ 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
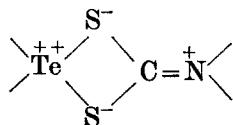
This is also supported by the planarity of the molecule and the values of the bond angles at C_1, C_2, N_1, and N_2 which are consistent with sp^2 hybridization of these atoms. The short $C - S$ bond lengths imply that canonical forms of the type
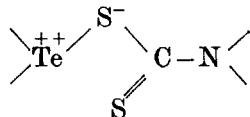
contribute to the overall structure.

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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