Acta Cryst. (1965). **18**, 259

The Crystal Structure of *N*-Phenyl-*N'*-benzoylselenourea*

By Håkon Hope†

Department of Chemistry, University of California at Los Angeles, Los Angeles 24, California, U.S.A.

(*Received* 27 *February* 1964)

The structure of phenylbenzoylselenourea, $C_6H_5.NH.CSe.NH.CO.C_6H_5$ (I) has been determined by three-dimensional Fourier and least-squares methods. (I) crystallizes in the monoclinic system, space group $P2_1/c$, $a=13{\cdot}16$ ($\sigma \sim 0{\cdot}005$), $b=5{\cdot}064$ ($\sigma \sim 0{\cdot}003$), $c=19{\cdot}94$ ($\sigma \sim 0{\cdot}005$) Å, $\beta=103{\cdot}65°$ ($\sigma \sim 0{\cdot}03°$), with four molecules in the unit cell. The molecule consists of three planar parts: $C_6H_5.NH.CSe\cdot$ (II), the carbonyl group with adjacent N and C (III), and the benzoyl phenyl group (IV). The major deviation from planarity of the molecule is caused by (IV) being twisted $\sim 30°$ out of plane with (III). The crystal is built up of centrosymmetric Se $\cdots$ H–N bonded dimers. Some of the interatomic distances observed are:

C–Se 1·82, C(at Se)–N (in II) 1·32, C(at Se)–N (in III) 1·40, N–C(phenyl) 1·43, N–C(in III) 1·39, C–C (in III) 1·48, C–O 1·22, O $\cdots$ (H)–N (in II) 2·59, Se $\cdots$ (H)'–N' (in III') 3·83 Å.

$\sigma \sim 0{\cdot}01$ Å for distances from Se, and $\sim 0{\cdot}015$ Å for other distances. The planarity of (II) results in a Se–(H)C distance of only 3·32 Å. (II) is highly strained with angle Se–C–N = 128·8°, angle C–N–C = 133·3° and angle N–C–C = 125·8°.

Introduction

The main purpose of the present investigation was to obtain information about the carbon–selenium double bond. Prior to this study the compounds O=C=Se (Strandberg, Wentink & Hill, 1949) and S=C=Se (Bak, Sloan & Williams, 1950) had been investigated by use of microwave methods. However, it appeared to be of interest to study the C–Se bond in a more typically organic molecule. It was therefore decided to investigate the crystal structure of a compound of the type RR'C=Se. Among these one finds that selenourea, and some *N*-substituted selenoureas are quite stable, crystalline compounds which can be synthesized with only moderate difficulty.

Work was first begun on selenourea but, as it turned out, this compound is rather complex crystallographically, with 27 formula units of $(NH_2)_2CSe$ in the trigonal unit cell. For this reason other compounds of this general type were taken into consideration, and when Prof. J. D. McCullough of these laboratories offered a gift of a number of substituted selenoureas this was gratefully accepted. Among the compounds received, *N*-phenyl-*N'*-benzoylselenourea,

$$C_6H_5.CO.NH.CSe.NH.C_6H_5\ ,$$

was found to be well suited for the present purpose, and the work on selenourea was therefore temporarily discontinued, while work on phenylbenzoylselenourea was started.

Experimental

The sample of *N*-phenyl-*N'*-benzoylselenourea had been prepared according to the procedure given by Douglass (1937). The crystals used in the X-ray study were long, thin, yellow needles grown by evaporation of an alcoholic solution. The crystals were studied partly by ordinary film techniques, and partly with a Picker diffractometer equipped with a General Electric goniostat.

Oscillation and Weissenberg photographs indicated a monoclinic unit cell with the crystallographic *b* axis along the needle axis. Based on the systematic absence of *h0l* reflexions with *l* odd, and the observation of 020 only of the 0*k*0 reflexions, the space group was taken to be $P2_1/c$. The choice of space group was confirmed through the successful determination and refinement of the structure.

Attempts to cut the crystals normal to the needle axis always resulted in a splitting of the ends into a brushlike bundle of thin fibers. The crystals used for intensity measurements were therefore long needles mounted along the *b* axis. The cross section was about $0{\cdot}05 \times 0{\cdot}02$ mm.

Integrated equi-inclination Weissenberg photographs of the layers $k=0$ through 4 were prepared with Cu $K\alpha$ radiation by use of the multiple-film technique. For the layers with $k=0$ and 1 a nickel filter was used; on higher levels the β reflexions were cut off by the layer line screen. For the purpose of interlayer scaling some 150 reflexions distributed over the five layers recorded were also measured with the diffractometer, using the $2\theta-\theta$ scan method. The reflexions recorded on film were measured with

---

* Contribution No. 1629 from the UCLA Dept. of Chemistry.

† Present address: Kjemisk Institutt, Universitetet i Oslo, Oslo 3, Norway.

a densitometer, except for the weakest ones, about one-quarter of all observed, which were estimated visually by use of a calibrated integrated comparison strip. Altogether 1432 reflexions were recorded. The intensities were corrected for Lorentz and polarization effects in the usual way. No absorption corrections were made.

Determination and refinement of the structure

The cell dimensions as determined from angles measured with the diffractometer are

$$a = 13{\cdot}16 \text{ (e.s.d. } 0{\cdot}005), \; b = 5{\cdot}064 \text{ (e.s.d. } 0{\cdot}003)\,,$$
$$c = 19{\cdot}94 \text{ (e.s.d. } 0{\cdot}005) \text{ Å}, \; \beta = 103{\cdot}65° \text{ (e.s.d. } 0{\cdot}03°).$$

The density calculated for $Z=4$ is 1·56 g.cm^{-3} while the density measured by flotation is 1·60 g.cm^{-3}.

The x and z coordinates for the Se atom were easily derived from a Patterson projection on (010). An electron-density projection calculated by use of the signs of the Se contribution to the structure factors showed all C, N and O atoms well resolved. The (x, z) coordinates found from this projection were refined through one cycle of Fourier refinement and three cycles of two-dimensional least-squares refinement. Individual isotropic temperature coefficients were also refined.

It was noted that on all layers the rows with l odd were systematically considerably weaker than those with l even. This indicates that the Se atoms are located near $y=\frac{1}{4}$ and $y=\frac{3}{4}$. At a stage before all the intensities had been collected, a generalized projection (Cochran & Dyer, 1952) was calculated from the $h2l$ data with l even. The signs used were those calculated for Se at $y=\frac{1}{4}$. Values for $\sigma_{i2}(x, z)$ were obtained from a 'calculated' generalized ($h2l$) projection with $y=0$ for all atoms, and the temperature factors from the two-dimensional least-squares refinement. With the aid of a model of the molecule approximate y parameters for the Se, C, N, and O atoms were derived.

Table 1. *Positional parameters and isotropic temperature coefficients for atoms in one molecule*

(E.s.d. in parentheses)

The e.s.d. for the positional parameters have been multiplied by 10^4

Atom	x	y	z	B (Å^2)
Se(1)	0·1077 (1)	0·2808 (2)	0·5847 (5)	
C(2)	0·2096 (7)	0·3771 (17)	0·5416 (5)	
N(3)	0·3059 (6)	0·2864 (16)	0·5513 (4)	
C(4)	0·3630 (7)	0·0872 (19)	0·5952 (5)	2·94 (0·16)
C(5)	0·3250 (9)	−0·0692 (23)	0·6406 (6)	4·38 (0·22)
C(6)	0·3916 (10)	−0·2584 (25)	0·6793 (6)	5·29 (0·25)
C(7)	0·4901 (9)	−0·2926 (24)	0·6721 (6)	4·81 (0·23)
C(8)	0·5279 (11)	−0·1365 (28)	0·6253 (7)	5·83 (0·29)
C(9)	0·4632 (9)	0·0529 (24)	0·5876 (6)	4·54 (0·22)
N(10)	0·1818 (6)	0·5676 (15)	0·4897 (4)	
C(11)	0·2410 (9)	0·6517 (19)	0·4443 (5)	
C(12)	0·1880 (7)	0·8354 (19)	0·3893 (5)	3·02 (0·16)
C(13)	0·2188 (9)	0·8229 (23)	0·3270 (6)	4·32 (0·21)
C(14)	0·1765 (9)	0·9909 (24)	0·2741 (6)	4·60 (0·23)
C(15)	0·1011 (9)	1·1731 (24)	0·2814 (6)	4·71 (0·32)
C(16)	0·0688 (9)	1·1817 (22)	0·3427 (5)	4·05 (0·19)
C(17)	0·1127 (7)	1·0136 (20)	0·3966 (5)	3·31 (0·18)
O(18)	0·3295 (6)	0·5724 (17)	0·4485 (4)	

Table 2. *Anisotropic temperature coefficients for the six 'central' atoms*

(E.s.d. in parentheses)

All values have been multiplied by 10^5

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Se(1)	639	3850	228	312	334	417
	(7)	(60)	(3)	(36)	(7)	(22)
C(2)	573	1247	207	37	147	−380
	(68)	(389)	(25)	(229)	(64)	(138)
N(3)	546	2762	265	309	228	180
	(52)	(381)	(23)	(236)	(55)	(153)
N(10)	607	2004	219	−56	275	111
	(58)	(344)	(22)	(213)	(58)	(132)
C(11)	729	2349	288	−552	392	68
	(83)	(441)	(31)	(286)	(83)	(174)
O(18)	651	5570	445	941	638	1749
	(60)	(434)	(30)	(251)	(69)	(186)

The calculations carried out so far did not require a knowledge of the position of the molecule relative to the twofold screw axis. In order to determine the correct position, a comparison of F_o and F_c for the reflexions ($h2l$) with l odd was made for each of the two possible positions. The result of this test was an R value of about 0·35 for the position chosen for later refinement, whereas the other position gave R close to 0·60 for the reflexions included. As a further

Table 3. *Assumed and observed positional parameters for the hydrogen atoms*

	Assumed			Observed		
Atom	x	y	z	x	y	z
H(23)	—	—	—	0·3575	0·4028	0·5261
H(25)	0·2462	−0·0431	0·6475	0·2404	−0·0396	0·6426
H(26)	0·3633	−0·3794	0·7151	0·3573	−0·3828	0·7200
H(27)	0·5392	−0·4416	0·7021	0·5287	−0·4200	0·7150
H(28)	0·6076	−0·1578	0·6190	0·6024	−0·1532	0·5977
H(29)	0·4919	0·1763	0·5520	—	—	—
H(30)	—	—	—	0·1112	0·6700	0·4923
H(33)	0·2774	0·6847	0·3204	0·2771	0·7112	0·3225
H(34)	0·2013	0·9830	0·2266	0·2029	0·9388	0·2266
H(35)	0·0674	1·3925	0·2389	0·0831	1·2944	0·2395
H(36)	0·0093	1·3209	0·3483	0·0113	1·2540	0·3387
H(37)	0·0883	1·0212	0·4442	0·0903	1·0412	0·4366

Table 4. *Observed and calculated structure factors*

The data are separated into groups having common values of h and k.
The three columns in each group list values of l, $10F_o$ and $10F_c$, in that order

h=0, k=0		
2	939	939
4	1028	-1117
6	987	-1075
8	636	-635
10	311	301
12	583	589
16	303	-329
22	221	223
24	125	144
h=1, k=0		
-24	136	128
-20	371	-382
-18	346	-322
-14	516	491
-12	516	507
-10	113	-123
-8	383	-400
-6	963	-1001
-4	749	735
-2	614	647
0	602	648
2	136	-125
4	688	-719
6	578	-579
8	331	315
10	836	858
12	411	436
16	516	-532
20	227	252
22	166	150
h=2, k=0		
-22	217	-240
-20	455	-422
-18	295	-218
-16	284	263
-14	387	348
-12	329	300
-10	351	-328
-8	468	-455
-6	171	-114
-4	636	658
-2	636	-596
0	380	-355
2	410	-442
4	1558	-1754
6	192	-166
8	525	499
10	852	833
12	385	330
14	158	-133
16	439	-422
20	219	172
22	177	163
h=3, k=0		
-22	210	-203
-16	516	476
-14	502	489
-12	208	-194
-10	1463	-1528
-8	963	-975
-6	439	419
-4	904	971
-2	808	865
0	963	-1017
2	836	-892
4	551	-595
6	311	288
8	499	512
10	237	243
12	435	-452
14	403	-373
16	166	-123
20	244	269
h=4, k=0		
-22	210	-180
-18	489	460
-16	571	565
-12	534	-524
-10	685	-667
-8	271	-257
-6	796	836
-4	636	229
-2	169	199
0	944	-964
2	761	-750
6	987	1045
8	418	406
10	493	-482
12	487	-450
14	268	-249
18	155	131
h=5, k=0		
-24	192	-206
-22	142	-116
-20	184	140
-18	450	406
-16	208	205
-14	381	-385
-12	473	-456
-10	125	87
-8	493	520
-6	1228	1287
-4	761	791
-2	802	-828
0	1005	-1025
4	551	549
6	599	609
8	342	311
10	297	-296
12	357	-356
14	166	-155
16	239	225
18	169	164
22	80	-77
h=6, k=0		
-24	158	-153
-20	273	243
-18	295	222
-14	542	-552
-12	423	-400
-10	306	318
-8	730	695
-6	458	460
-4	274	-275
-2	573	-590
2	583	552
4	671	669
6	326	309
10	502	-477
12	243	-261
14	166	165
16	231	245
h=7, k=0		
-22	171	162
-20	274	229
-16	294	-269
-14	439	-367
-12	221	-217
-10	504	472
-8	647	630
-4	405	-403
-2	535	-549
0	498	-482
2	498	519
4	492	494
6	166	-141
8	321	-311
10	187	-181
14	264	284
16	231	181
h=8, k=0		
-24	132	90
-22	264	248
-20	244	188
-18	257	-183
-16	551	-527
-14	431	-432
-12	381	341
-10	685	698
-8	208	210
-6	374	-341
-4	847	-836
-2	284	-276
0	212	170
2	291	307
6	379	-368
8	429	-444
12	241	232
14	225	180
18	132	-128
h=9, k=0		
-24	166	176
-22	227	221
-18	303	-302
-16	243	-273
-14	294	305
-12	474	429
-10	229	219
-8	489	-424
-6	779	-785
-4	498	-513
-2	399	391
0	614	606
2	380	316
6	375	-380
h=10, k=0		
-20	212	-184
-18	196	-160
-14	263	223
-12	294	269
-10	303	306
-8	329	-307
-6	484	-428
-2	357	317
0	528	538
4	189	-199
12	184	146
h=11, k=0		
-22	101	-90
-20	252	-258
-18	210	-186
-14	339	329
-12	166	142
-4	364	321
-2	410	395
0	189	172
2	244	-232
4	318	-315
6	283	-304
8	158	137
10	300	335
h=12, k=0		
-20	199	-195
-16	325	313
-14	299	302
-10	513	-497
-8	235	-206
-4	371	377
-2	166	129
2	243	-223
8	208	137
h=13, k=0		
-20	101	-72
-18	192	158
-16	292	295
-14	145	126
-12	152	-173
-10	467	-468
0	235	-177
6	158	200
h=14, k=0		
-18	125	112
-14	187	-158
-12	203	-139
-10	145	-132
-6	269	257
-4	196	166
0	259	-270
2	179	-128
6	145	170
h=15, k=0		
-14	152	-154
-12	117	-126
-8	184	140
-6	210	192
-2	129	-106
0	125	-103
h=16, k=0		
-10	160	158
-8	171	148
h=0, k=1		
2	970	-1054
3	1060	1013
4	1957	-2006
5	501	442
6	389	-342
7	129	-135
8	667	718
9	433	-395
10	581	567
12	133	-105
14	349	-331
16	224	-197
20	260	230
h=1, k=1		
-24	94	-94
-22	205	-250
-20	185	-178
-18	278	313
-17	253	-251
-16	478	475
-14	145	129
-13	139	177
-11	308	277
-10	653	-668
-8	235	-244
-7	157	-156
-6	676	699
-5	378	-370
-4	584	623
-3	129	-127
-2	467	467
-1	489	554
0	414	-474
2	1186	-1327
3	359	350
4	237	-211
5	342	-369
6	942	991
7	293	266
8	667	675
9	224	229
10	293	295
12	399	-421
14	405	-425
18	160	146
20	178	182
24	89	-124
h=2, k=1		
-24	199	-190
-22	187	-181
-19	129	-164
-18	321	343
-17	194	-181
-16	604	575
-13	111	125
-12	569	-578
-10	330	-340
-9	151	-135
-7	226	-212
-6	394	399
-5	296	278
-4	600	587
-3	129	130
-2	691	-747
-1	284	266
0	1129	-1223
1	1208	-1256
2	598	499
3	1005	-1025
4	241	203
5	122	-140
6	836	856
7	395	375
8	817	839
9	331	282
10	178	-158
12	450	-490
14	307	-332
18	248	275
20	173	181
h=3, k=1		
-24	142	-133
-20	218	194
-18	278	260
-14	508	-548
-12	711	-720
-11	214	-212
-10	165	-163
-8	520	538
-7	483	-454
-6	1018	1062
-5	205	-177
-4	441	422
-3	107	86
-2	643	-706
-1	210	207
0	1240	-1383
1	168	-178
2	98	98
3	299	-310
4	754	802
6	547	579
7	190	-171
10	480	-489
11	115	-128
12	367	-374
16	321	334
18	154	165
h=4, k=1		
-22	136	132
-20	307	294
-17	185	130
-16	272	-250
-14	513	-541
-12	515	-501
-11	103	-108
-10	258	283
-9	115	-132
-8	846	896
-6	570	572
-4	535	-528
-2	678	-706
-1	241	-206
0	791	-837
1	226	230
2	488	485
4	774	827
8	338	-339
10	467	-488
12	185	-168
13	157	-178
14	252	281
16	252	288
20	151	-125
h=5, k=1		
-22	187	200
-20	286	297
-16	397	-407
-14	384	-330
-12	194	186
-10	747	768
-9	307	301
-8	352	391
-7	481	492
-6	412	-383
-4	905	-953
-3	165	186
-2	311	-353
-1	94	65
2	498	501
4	687	691
5	231	219
6	122	-134
8	604	-604
10	348	-342
14	228	202
16	220	182
20	154	-166
h=6, k=1		
-22	243	254
-18	226	-225
-16	318	-346
-12	401	400
-10	717	743
-7	286	287
-6	444	-479
-5	270	216
-4	626	-628
0	844	859
2	511	525
3	296	313
5	180	190
6	500	-504
8	388	-395
9	148	-164
12	226	221
14	226	182
h=7, k=1		
-24	142	161
-22	126	118
-18	316	-311
-16	253	-274
-15	160	-175
-14	220	247
-12	424	443
-10	437	418
-9	133	183
-6	664	-691
-5	210	-186
-4	488	-453
-3	485	-471
-2	290	287
-1	119	-100
0	596	616
1	122	126
2	178	226
3	129	123
4	154	-150
6	443	-445
10	275	289
12	321	314
16	194	-156
18	157	-123
h=8, k=1		
-24	136	148
-20	244	-265
-18	311	-336
-14	354	463
-12	305	296
-8	424	-444
-6	588	-626
-3	185	-199
-2	346	385
0	441	469
3	142	-149
4	373	-394
6	262	-248
10	278	337
16	173	-210
h=9, k=1		
-22	154	-142
-20	268	-241
-16	194	122
-14	393	390
-10	647	-675
-8	504	-483
-7	145	-148
-5	142	-165
-4	484	458
-2	596	602
1	145	152
2	420	-410
3	151	140
4	218	-215
7	160	-155
10	194	185
h=10, k=1		
-22	165	-171
-20	154	-135
-16	268	269
-14	226	208
-13	278	281
-12	129	-137
-11	160	176
-10	427	-432
-9	157	-146
-8	220	-206
-6	154	153
-4	446	434
-2	216	200
2	314	-361
4	276	-287
6	160	154
8	194	175
h=11, k=1		
-22	160	-189
-18	212	221
-16	255	264
-10	228	-234
-6	318	326
-5	160	157
-4	194	201
-3	160	193
0	319	-330
1	160	-152
2	321	-351
6	314	357
8	183	178
h=12, k=1		
-20	162	158
-18	224	256
-16	136	123
-14	2.0	-207
-12	309	-333
-8	226	254
-6	299	284
-2	197	-181
0	226	-244
6	205	157
h=13, k=1		
-20	178	204
-18	126	149
-14	253	-280
-12	230	-213
-8	243	-231
-6	220	235
-2	154	-184
4	139	130
h=14, k=1		
-16	142	-141
-14	168	-159
-10	194	180
-8	173	174
-4	203	-200
-2	142	-169
h=15, k=1		
-16	145	-165
-12	151	139
-10	165	188
-4	122	-153
h=16, k=1		
-12	122	122
-10	122	144
-6	119	-153
0	78	114
h=0, k=2		
1	283	-305
2	98	-146
3	568	-568
4	468	470
5	468	-420
6	338	381
7	176	-147
8	582	570
9	138	-125
10	132	-117
12	435	-443
13	141	128
15	108	-114
16	154	122
18	203	188
19	102	96
20	96	116
22	75	-71
h=1, k=2		
-20	137	148
-18	213	239
-16	109	74
-15	322	305
-14	437	-428
-13	257	253
-12	389	-375
-11	125	-145
-9	296	-300
-8	582	571
-6	399	432
-5	410	395
-4	249	-223
-3	404	406
-2	692	-777
-1	230	209
0	517	-581
1	300	-298
2	106	104
4	968	981
5	131	88
6	859	911
7	100	106
8	152	-135
9	350	329
10	413	-430
12	362	-342
13	179	-180
15	152	-120
16	294	293
17	132	109
18	208	238
19	123	131
22	69	-98
h=2, k=2		
-23	98	-126
-22	100	87
-21	91	-84
-20	255	282
-19	104	93
-18	132	104
-17	153	132
-16	267	-289
-15	241	218
-14	622	-598
-13	138	139
-12	289	-270
-11	220	-188
-10	299	281
-9	109	-134
-8	736	718
-6	202	202
-5	158	140
-4	747	-752
-3	161	-167
-2	477	-545
-1	328	-372
0	318	-302
1	443	-455
2	695	716
3	204	173
4	692	698
5	845	825
6	323	-257
7	587	588
8	692	-701
10	293	-303
11	282	-282
14	296	302
16	287	318
17	108	94
20	87	-130
22	63	-89
h=3, k=2		
-22	128	161
-20	155	146
-19	129	118
-18	168	-141
-16	267	-250
-15	227	-208
-14	235	-249
-13	225	-237
-11	309	-295
-10	562	554
-9	113	88
-8	287	288
-7	383	378
-6	131	-172
-5	63	89
-4	854	-881
-3	321	-328
-2	575	-569
-1	129	68
0	239	230
2	665	725
3	222	-173
5	271	292
6	296	-282
8	547	-545
9	111	-99
10	324	-334
12	268	268
14	267	253
16	108	89
20	126	-157
h=4, k=2		
-24	113	151
-22	116	159
-19	128	132
-18	265	-281
-16	189	-216
-15	323	-326
-14	207	207
-13	318	-334
-12	408	408
-11	91	-81
-10	619	611
-9	82	114
-6	571	-593
-5	129	126
-4	814	-866
-3	173	-184
-2	164	-143
-1	257	-240
0	394	412
1	171	161
2	504	518
4	397	357
6	405	-428
7	121	-120
8	426	-407
9	247	-254
11	145	-147
12	299	317
14	153	162
18	177	-221
20	103	-124
h=5, k=2		
-24	160	192
-22	82	109
-20	120	-132
-18	243	-252
-16	216	-202
-14	367	375
-12	372	408
-9	214	214
-8	349	-339
-7	295	267
-6	405	-423
-5	147	-152
-4	203	149
-3	468	-479
-2	554	576
-1	272	-297
0	622	644
1	432	428
3	121	129
4	185	-187
5	194	-186
6	489	-514
7	229	-224
8	98	-101
9	157	-179
10	207	215
12	267	287
15	106	96
16	125	-142
18	120	-130
h=6, k=2		
-24	80	92
-21	89	102
-20	190	-205
-18	210	-246
-17	108	-60
-14	437	449
-13	104	86
-12	354	340
-11	265	255
-10	234	-239
-9	263	272
-8	493	-492
-6	346	-360
-5	200	-185
-4	481	442
-2	671	668
-1	80	-41
0	554	558
1	242	248
2	375	-365
3	151	155
4	484	-485
5	115	-115
6	167	-199
7	225	-205
8	126	134
9	148	-126
10	289	300
11	109	111
12	134	138
13	151	180
16	116	-108
17	106	-124
h=7, k=2		
-23	106	118
-22	170	-188
-20	245	-292
-17	132	-117
-16	268	269
-14	316	331
-13	263	265
-12	237	238
-11	251	276
-10	438	-443
-9	135	-129
-8	495	-511
-7	183	-173
-6	205	-186
-5	234	-206
-4	312	331
-2	412	388
-1	199	214
0	89	58
1	157	124
2	561	-564
4	365	-371
6	263	292
8	300	310
9	134	132
10	217	250
11	170	154
14	155	-181
16	120	-119
h=8, k=2		
-22	185	-192
-19	96	-86
-18	141	144
-17	106	-72
-16	244	245
-13	109	96
-12	244	-246
-11	165	165
-10	400	-403
-9	231	-210
-8	156	-140
-7	223	-219
-6	135	130
-4	405	390
-3	96	93
-2	116	130
0	335	-327
2	225	-246
4	253	-264
6	149	164
7	152	159
8	247	266
9	104	82
10	104	79
12	144	-158
14	158	-159
16	102	-47
h=9, k=2		
-22	106	-109
-20	82	66
-19	126	-104
-18	206	233
-16	182	214
-14	152	-148
-12	369	-338
-10	301	-291
-9	106	-124
-7	161	-162
-6	493	490
-4	263	263
-3	230	208
-1	287	304
0	254	-253
2	224	-229
3	211	-217
4	151	-141
5	246	-257
6	189	190
8	152	138
12	132	-124
14	123	-108
h=10, k=2		
-22	69	-79
-21	89	-110
-20	129	148
-18	238	256
-17	96	87
-15	181	181
-14	149	-161
-12	287	-296
-11	134	-115
-9	152	-147
-8	417	425
-7	151	-136
-6	378	372
-5	186	167
-3	212	188
-2	282	-295
0	361	-370
1	188	-202
4	329	324
6	151	146
10	148	-137
12	128	-89
h=11, k=2		
-21	82	-88
-20	148	165
-18	143	143
-17	123	116
-16	115	-97
-15	137	141
-14	249	-270
-12	106	-88
-10	188	219
-8	216	214
-7	153	153
-6	134	162
-4	109	-118
-3	153	-159
-2	288	-325
-1	189	-187
1	134	-136
2	188	205
4	211	230
5	100	87
10	116	-127
h=12, k=2		
-20	91	115
-19	85	50
-16	167	-179
-14	186	-193
-11	102	-82
-10	147	140
-8	185	171
-7	108	88
-5	132	124
-4	187	-168
-2	167	-159
1	106	-72
2	180	178
4	138	144
5	96	106
8	115	-118
h=13, k=2		
-18	144	-165
-16	143	-149
-13	137	-141
-12	128	138
-11	94	-80
-10	219	145
-6	200	-207
-4	201	-188
-2	109	-87
0	98	78
2	131	154
5	90	105
6	77	-84
8	77	-77
h=14, k=2		
-16	72	-77
-15	75	-73
-14	85	73
-12	135	156
-10	85	86
-9	108	109
-8	109	-104
-6	179	-182
-4	111	-83
0	85	77
6	75	-94
h=15, k=2		
-12	91	100
-9	98	94
-8	144	-172
-6	104	-91
-5	104	-110
-2	125	156
0	91	93
h=0, k=3		
1	404	-401
2	256	293
3	210	-155
4	331	313
5	358	328
6	242	-187
7	417	389
8	405	-380
10	235	-250
11	162	-151
12	148	-108
14	125	138
15	120	97
16	247	225
17	120	145
20	117	-124
21	112	-119
22	86	-102
h=1, k=3		
-22	90	125
-20	120	108
-19	132	106
-17	150	110
-16	125	-120
-13	173	-157
-12	114	87
-11	114	-108
-10	401	403
-8	334	279
-7	225	212
-6	266	-249
-5	426	350
-4	397	-399
-3	434	-398
-2	143	-141
-1	392	-430
0	423	487
1	93	49
2	632	749
3	227	249
4	355	329
5	345	345
6	203	-200
7	201	161
8	471	-443
9	270	-244
10	393	-361
11	206	-161
12	213	213
14	399	395
16	117	100
20	109	-132
21	86	-93
h=2, k=3		
-22	71	80
-21	109	111
-20	100	-80
-19	134	140
-18	204	-207
-16	200	-185
-15	156	-139
-14	125	117
-13	195	-225
-12	520	469
-11	288	-256
-10	383	365
-9	143	133
-7	90	80
-6	488	-488
-5	79	42
-4	520	-480
-3	112	-150
-2	164	136
-1	157	-159
0	574	549
1	206	188
2	187	212
3	327	342
5	122	117
6	311	-304
7	122	-123
8	183	-178
9	273	-253
10	378	382
11	239	-260
12	442	438
14	120	134
15	175	196
18	148	-154
20	79	-87
h=3, k=3		
-21	114	126
-20	137	-159
-18	233	-228
-17	122	-115
-16	125	-100
-15	311	-292
-14	219	206
-12	294	281
-11	257	232
-9	207	204
-8	469	-427
-7	114	-68
-6	450	-423
-5	209	-236
-4	79	42
-3	173	-197
-2	319	327
-1	139	-114
0	230	259
1	297	295
3	165	170
4	288	-305
6	300	-273
7	322	-313
9	201	-196
10	256	243
12	200	170
13	156	145
15	117	108
16	117	-127
18	100	-113
h=4, k=3		
-20	122	-151
-18	117	-102
-17	171	-143
-16	130	134
-15	251	-230
-14	235	241
-13	176	161
-11	446	433
-10	420	-411
-9	241	243
-8	561	-548
-7	100	-88
-6	253	-251
-5	488	-445
-4	150	158
-2	447	454
-1	143	115
0	464	426
1	276	262
2	176	-167
3	114	-95
4	511	-492
5	203	-166
6	150	-191
10	152	112
14	122	-133
16	156	-169
h=5, k=3		
-22	109	-123
-20	137	-139
-16	175	210
-15	125	-111
-14	176	174
-11	372	348
-10	201	-202
-8	242	-243
-7	145	-140
-5	219	-211
-4	455	423
-2	351	343
-1	266	254
0	238	-221
1	387	339
2	552	-547
3	143	-163
4	384	-377
5	411	-406
8	2.2	214
9	125	113
10	154	161
11	251	269
14	165	-173
16	143	-118
h=6, k=3		
-22	117	-153
-21	83	-57
-19	106	-95
-18	158	158
-16	213	229
-15	217	199
-14	176	166
-12	125	-106
-10	238	-236
-9	164	-144
-7	248	-261
-6	399	385
-5	148	-102
-4	444	442
-3	295	279
-1	279	260
0	378	-361
2	392	-363
4	114	-112
5	382	-371
6	210	194
8	344	329
9	176	186
11	175	156
12	150	-145
14	137	-128
15	103	-91
h=7, k=3		
-22	71	-53
-21	132	-144
-20	112	136
-19	100	-120
-18	268	286
-16	209	209
-15	215	268
-14	125	-128
-12	310	-324
-11	125	-107
-10	173	-183
-9	212	-235
-8	120	131
-7	164	-141
-6	359	354
-5	139	114
-4	158	141
-2	226	-199
0	160	-176
1	114	-114
3	145	144
4	241	257
6	329	365
8	156	142
9	125	101
10	125	-112
12	114	-137
13	109	-88
h=8, k=3		
-21	114	-115
-20	114	117
-18	127	122
-15	169	175
-14	246	-274
-12	220	-206
-11	251	-259
-9	175	-150
-8	276	280
-6	169	173
-5	209	228
-4	120	-84
-3	167	177
-2	148	-165
0	169	-163
1	342	-363
4	217	238
5	127	136
6	127	152
h=9, k=3		
-20	86	96
-17	103	104
-16	156	-167
-14	238	-288
-12	154	-147
-11	176	-163
-10	156	154
-8	219	221
-7	130	144
-6	176	156
-5	308	339
-2	350	-345
-1	154	-168
0	176	-200
1	249	-259
2	156	157
3	127	-126
4	127	146
5	125	160
8	117	-122
10	188	-167
h=10, k=3		
-20	79	102
-19	90	86
-17	93	88
-16	143	-169
-14	114	-118
-10	216	209
-9	125	110
-8	154	134
-7	127	82
-6	156	-146
-4	439	-407
-2	176	-171
-1	127	-133
2	217	216
5	148	155
6	117	-114
8	188	-191
h=11, k=3		
-19	83	108
-18	122	-135
-16	90	-85
-14	103	96
-13	109	-114
-12	196	203
-10	206	216
-9	120	116
-6	215	-233
-5	125	-101
-4	125	-114
-3	125	-128
1	120	115
2	120	85
3	117	124
h=12, k=3		
-17	86	-78
-15	103	-104
-14	90	72
-12	143	167
-10	109	90
-9	137	119
-6	114	-68
-5	143	-137
0	139	143
7	82	-89
h=13, k=3		
-15	100	-110
-14	127	151
-12	86	84
-11	90	90
-8	141	-172
-6	105	-138
-2	143	176
0	136	147
h=14, k=3		
-11	86	84
-10	93	-110
-8	100	-120
-4	106	102
-2	103	110
-1	79	80
h=0, k=4		
1	137	150
3	283	289
4	145	-130
5	248	212
6	272	-271
7	241	-226
8	202	-155
9	299	-296
10	172	148
11	141	-101
12	289	272
15	190	175
18	128	-109
19	120	-133
h=1, k=4		
-15	190	-169
-14	141	118
-11	369	326
-9	210	189
-7	166	-110
-6	289	-255
-5	202	-214
-2	325	306
-1	141	156
0	215	234
1	464	467
3	176	191
4	295	-285
5	185	-161
6	337	-291
7	120	-161
10	281	262
12	179	141
16	124	-126
18	137	-129
h=2, k=4		
-17	124	-126
-16	185	168
-15	133	-111
-14	141	125
-11	207	231
-10	193	-226
-9	148	143
-8	354	-343
-6	141	-110
-5	145	-161
-4	193	189
-3	124	-120
-2	279	303
-1	81	119
0	159	161
1	323	308
3	100	62
4	281	-233
5	244	-251
8	133	133
10	199	198
11	246	249
13	141	150
14	169	-169
16	148	-175
h=3, k=4		
-19	152	-160
-18	110	91
-17	120	-133
-16	225	224
-12	202	-161
-11	110	114
-10	279	-254
-8	128	-111
-7	300	-324
-6	202	187
-5	223	-250
-4	182	196
-3	141	146
-2	196	213
-1	166	224
0	100	-85
1	141	141
2	182	-169
5	410	-356
8	124	133
9	141	140
11	199	223
14	128	-144
17	115	-136
h=4, k=4		
-19	100	-105
-15	137	153
-13	179	164
-12	202	-207
-9	333	-319
-8	133	112
-7	337	-352
-6	404	388
-5	120	-99
-4	302	277
-3	273	251
-2	110	-77
-1	190	198
0	313	-317
1	162	-140
2	204	-207
5	133	-132
8	159	127
9	145	114
13	133	-152
15	141	-122
h=5, k=4		
-18	105	103
-15	188	190
-13	159	144
-12	202	-192
-9	196	-180
-8	152	132
-6	263	259
-5	159	169
-4	156	120
-3	196	186
-2	212	-221
0	348	-339
1	352	-322
2	338	-277
3	225	-245
4	137	151
6	241	255
7	141	132
8	196	142
9	141	131
12	128	-90
13	124	-116
h=6, k=4		
-18	124	132
-17	115	133
-15	128	127
-11	128	-136
-8	141	117
-7	193	178
-5	232	243
-3	133	125
-2	267	-257
0	169	-134
1	273	-275
3	196	-174
4	315	296
5	141	142
6	179	168
7	145	156
10	137	-142
12	120	-112
h=7, k=4		
-17	148	167
-16	166	-167
-15	105	108
-14	166	-178
-11	148	-177
-10	145	161
-8	145	130
-6	176	-124
-5	196	195
-4	141	-122
-3	124	103
0	124	111
2	199	188
3	115	110
4	115	105
5	196	167
7	141	92
11	120	-101
12	105	-95
h=8, k=4		
-18	105	-111
-16	152	-158
-14	100	-111
-13	105	-140
-12	169	143
-11	239	-206
-10	196	195
-8	141	119
-7	265	261
-5	137	82
-4	202	-181
-3	179	-163
-1	202	-186
0	141	101
2	141	139
3	199	165
5	196	190
h=9, k=4		
-16	74	-72
-15	152	-163
-12	159	140
-10	190	181
-9	172	195
-7	141	113
-6	176	-156
-5	141	-123
-4	179	-162
-3	199	-197
-1	124	-115
2	137	113
6	156	-161
h=10, k=4		
-15	115	-124
-8	133	-160
0	188	162
4	124	-90
6	110	-124
h=11, k=4		
-14	105	125
-11	133	151
-8	148	-149
1	166	171

check all the positional parameters, and individual isotropic temperature factors were refined through three least-squares cycles with all observed $h0l$, $h1l$ and $h2l$ reflexions included. The resulting positional parameters gave reasonable interatomic distances, the temperature coefficients were normal, and the R value was 0·13; the structure at this stage was taken to be sufficiently good to serve as initial input for least-squares refinements with the full set of intensity data.

The refinement was carried out in three steps. First all the positional parameters and temperature factors were refined through six least-squares cycles, the first three with isotropic temperature factors for all atoms, and the next three with an anisotropic temperature factor for selenium. Next a three-dimensional difference Fourier synthesis was calculated with all Se, C, N, O atoms subtracted. Except for some negative regions around the selenium position, there was no false detail in the map. Near all the expected hydrogen positions appeared rather convincing maxima, ranging from 0·4 to 0·7 e.Å^{-3}.

Positions for the ten phenyl hydrogen atoms were calculated from the positions of the carbon atoms, with an assumed C–H distance of 1·08 Å. The assumed H positions are given in Table 3. (The numbering of the 'heavy' atoms is shown in Fig. 2. The hydrogen atoms are given the numbers of the atoms to which they are attached +20). In the final three least-squares cycles these hydrogen atoms were included in the structure factor calculations with temperature coefficients of 4·5 Å^2, but no hydrogen parameters were refined. These cycles were carried out with anisotropic temperature factors for the six 'central' atoms Se(1), C(2), N(3), N(10), C(11), and O(18). The shifts in the final cycle were all less than 1/20 of the e.s.d.

In Table 1 are given the final positional parameters and isotropic temperature coefficients, B, together with their e.s.d. values. The temperature coefficients β_{ij} in the anisotropic temperature factors with their e.s.d. values are given in Table 2.

A comparison of observed and calculated structure factors is given in Table 4. The parameters used in the calculation of the F_c's are those listed in Tables 1 and 2, and the assumed H parameters. The R value is 0·071. As a final check of the structure a three-dimensional difference synthesis was calculated with all 'heavy' atoms subtracted. It shows a negative region with a minimum of about −0·8 e.Å^{-3} near the selenium position, and maxima of 0·4–0·6 e.Å^{-3} near the expected hydrogen positions. From this map the positions of all H atoms except H(29) were derived. The parameters found are listed in Table 3.

Computing procedures

The structure factors and all Fourier summations were calculated by use of a program written for the IBM 7090 computer by P. K. Gantzel and Håkon Hope in these laboratories. The least-squares refinement was carried out by use of ACA Computer program No. 317 (UCLALS-1) written by P. K. Gantzel, R. A. Sparks and K. N. Trueblood for the IBM 7090. This program minimizes the weighted sum of the squares of the quantity $(KF_o - G(F_c))$ by a full matrix routine. K and G are scale factors, G is one of the adjustable parameters. The weighting scheme used was that of Hughes (1941) with $4F_o(\text{min}) = 32$. The atomic form factors were taken from *International Tables for X-ray Crystallography* (1962); Se from Table 3·3·1B, and C, N, O, H from Table 3·3·1A. For carbon the C (valence) values were used. The f values for each reflexion were obtained by linear interpolation of $1/\sqrt{f}$ values.

The isotropic temperature factors are of the form $\exp(-B\sin^2\theta/\lambda^2)$, and the anisotropic of the form $\exp[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})]$.

The R index is defined by $R=\Sigma||F_o|-|F_c||/\Sigma F_o$.

The standard deviations were estimated from the inverse matrix of the normal equations.

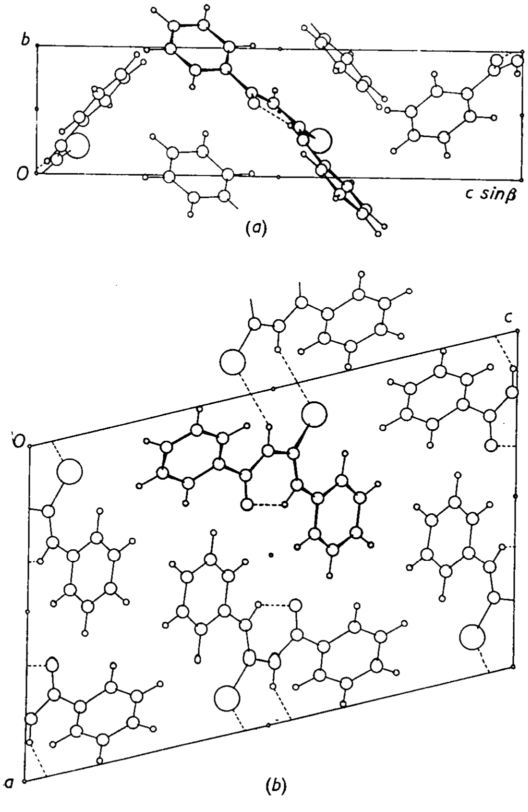


Fig. 1. (*a*) Projection of the structure along the *a* axis. Only one layer of molecules, related through the *c* glide, is shown. The heavily outlined molecule corresponds to the positional parameters given in Table 1. (*b*) Projection of the structure along the *b* axis. The assumed hydrogen bonds are indicated by broken lines. For identification of the atoms compare with Fig. 2.

Description of the structure

In Figs. 1(*a*) and 1(*b*) are shown two projections of the structure, along the *a* axis and the *b* axis respectively. Bond distances are given in Table 5 and Fig. 2(*a*), and bond angles in Table 6 and Fig. 2(*b*). Some dihedral angles are also indicated in Fig. 2(*b*).

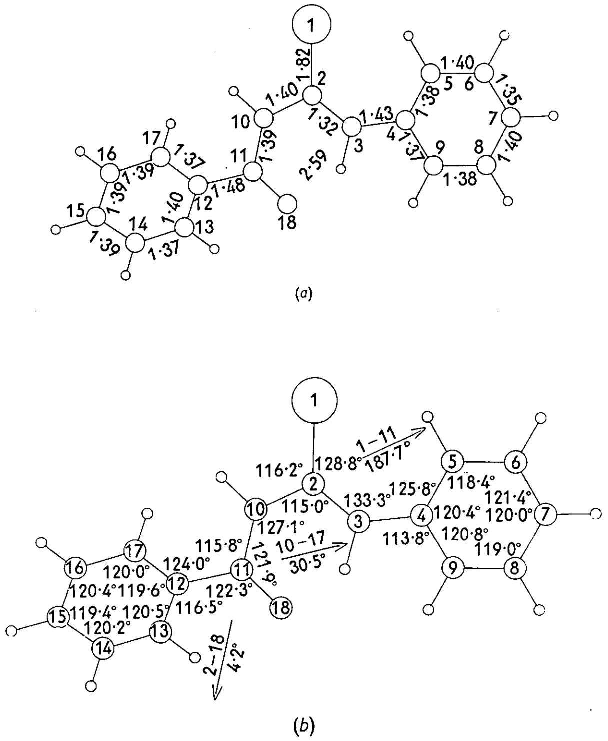
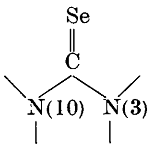


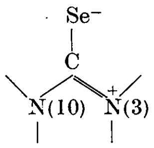
Fig. 2. (*a*) Interatomic distances in phenylbenzoylselenourea, with indication of the numbering system adopted. 1 = Se, 3 and 10 = N, 18 = O, and the remaining numbered atoms = C. Hydrogen atoms are given the numbers of the atoms to which they are attached + 20. The drawing represents a projection of the molecule on the plane defined by atoms 1 through 9. (*b*) Bond angles, and some dihedral angles. The dihedral angles are given with arrows which indicate the direction of positive rotation in a right-handed reference system.

The molecule consists of three planar portions, of which one is made up of the atoms Se(1) through C(9), the next of N(10), C(11), C(12), O(18), and the last of the phenyl group C(12)–C(17). The parameters defining the three least-squares planes are given in Table 7, together with individual deviations from the planes. It is noted that the major deviation from planarity of the molecule as a whole is caused by the phenyl group C(12)–C(17) being twisted about 31° at the C(11)–C(12) bond.

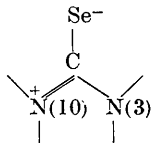
It seems reasonable to assume that the most important contributions to the actual structure of the central part of the molecule could be represented by the formulae (I), (II), and (III).



(I)



(II)



(III)

The sum of the covalent bond radii for Se and C is 1·94 Å for the single bond, and 1·74 Å for the

Table 5. *Interatomic distances*

(E.s.d. in parentheses)

Atoms	Distance
Se(1)–C(2)	1·82 (0·010) Å
C(2)–N(3)	1·32 (0·013)
N(3)–C(4)	1·43 (0·012)
C(4)–C(5)	1·38 (0·015)
C(5)–C(6)	1·40 (0·017)
C(6)–C(7)	1·35 (0·018)
C(7)–C(8)	1·40 (0·018)
C(8)–C(9)	1·38 (0·018)
C(9)–C(4)	1·37 (0·015)
C(2)–N(10)	1·40 (0·013)
N(10)–C(11)	1·39 (0·014)
C(11)–C(12)	1·48 (0·014)
C(11)–O(18)	1·22 (0·014)
C(12)–C(13)	1·40 (0·014)
C(13)–C(14)	1·37 (0·016)
C(14)–C(15)	1·39 (0·017)
C(15)–C(16)	1·39 (0·016)
C(16)–C(17)	1·39 (0·015)
C(17)–C(12)	1·37 (0·014)
N(3) · · · O(18)	2·59 (0·012)
N(3)–H(23)	1·11
H(23) · · · O(18)	1·73
Se(1)′ · · · N(10)	3·83 (0·008)
N(10)–H(30)	1·08
Se(1)′ · · · H(30)	2·94

Table 6. *Bond angles*

(E.s.d. in parentheses)

Atoms	Angle
Se(1)–C(2)–N(3)	128·8° (0·4°)
Se(1)–C(2)–N(10)	116·2 (0·4)
N(3)–C(2)–N(10)	115·0 (0·6)
C(2)–N(3)–C(4)	133·3 (0·6)
N(3)–C(4)–C(5)	125·8 (0·7)
N(3)–C(4)–C(9)	113·8 (0·7)
C(5)–C(4)–C(9)	120·4 (0·8)
C(4)–C(5)–C(6)	118·4 (0·8)
C(5)–C(6)–C(7)	121·4 (0·8)
C(6)–C(7)–C(8)	120·0 (0·9)
C(7)–C(8) C(9)	119·0 (0·9)
C(4)–C(9)–C(8)	120·8 (0·8)
C(2)–N(10)–C(11)	127·1 (0·7)
N(10)–C(11)–C(12)	115·8 (0·7)
N(10)–C(11)–O(18)	121·9 (0·7)
C(12)–C(11)–O(18)	122·3 (0·7)
C(11)–C(12)–C(13)	116·5 (0·8)
C(11)–C(12)–C(17)	124·0 (0·8)
C(13)–C(12)–C(17)	119·6 (0·8)
C(12)–C(13)–C(14)	120·5 (0·8)
C(13)–C(14)–C(15)	120·2 (0·8)
C(14)–C(15)–C(16)	119·4 (0·8)
C(15)–C(16)–C(17)	120·4 (0·8)
C(12)–C(17)–C(16)	120·0 (0·7)
C(2)–N(3)–O(18)	88·9 (0·7)
N(3)–O(18)–C(11)	87·0 (0·7)

Table 7. *Least-squares planes and distances from planes*

I. Plane defined by Se(1) through C(9):
$(0{\cdot}02537\mathbf{a}+0{\cdot}13383\mathbf{b}+0{\cdot}03707\mathbf{c}).\mathbf{r}-8{\cdot}8821=0$
II. Plane defined by N(10), C(11), C(12), O(18):
$(0{\cdot}02734\mathbf{a}+0{\cdot}15254\mathbf{b}+0{\cdot}03089\mathbf{c}).\mathbf{r}-7{\cdot}9189=0$
III. Plane defined by phenyl group C(12)–C(17):
$(0{\cdot}05584\mathbf{a}+0{\cdot}13311\mathbf{b}+0{\cdot}01826\mathbf{c}).\mathbf{r}-5{\cdot}9253=0$

Atom	Deviation	from plane
Se(1)	0·006 Å	I
C(2)	−0·018	I
N(3)	0·001	I
C(4)	0·017	I
C(5)	−0·001	I
C(6)	0·000	I
C(7)	−0·006	I
C(8)	−0·008	I
C(9)	0·009	I
N(10)	−0·107	I
N(10)	−0·003	II
C(11)	0·011	II
C(12)	−0·003	II
O(18)	−0·004	II
C(11)	0·044	III
C(12)	0·008	III
C(13)	−0·009	III
C(14)	0·002	III
C(15)	0·006	III
C(16)	−0·007	III
C(17)	0·000	III

double bond. The observed value 1·82 Å for the C–Se bond indicates a considerable contribution from structure (I). Likewise the C(2)–N(3) distance of 1·32 Å indicates a substantial contribution from (II), whereas (III) probably is of less significance.

The unusually short N(3)–H · · · O(18) hydrogen bond (2·59 Å) is consistent with the assumption of a positive charge placed on the NH group, leading to retraction of much of the H electron. It is suggested that the possibility of the NH group thus being able to form a strong hydrogen bond may be part of the cause for the difference between the bond distances C(2)–N(3) and C(2)–N(10).

Selenium normally does not form hydrogen bonds; however, the rather short Se(1′)–H(30)–N(10) distance of 3·83 Å, in a grouping with N(10)–H(30) = 1·08 Å, Se(1′)–H(30) = 2·94 Å, and the angle N(10)–H(30)–Se(1′) = 140°, is taken to indicate that a hydrogen bond Se · · · H–N exists, so that phenylbenzoylselenourea crystallizes as a centrosymmetric hydrogen-bonded dimer. This increased hydrogen bonding ability is thought to be caused by a partial negative charge on the selenium atom.

A striking feature of the structure is the planarity of the group formed by Se(1), C(2), N(3) and the phenyl group C(4)–C(9). It is interesting to compare this with the structure of acetanilide (Brown & Corbridge, 1954), where the phenyl group is twisted 38° out of plane, to avoid an 'impossibly' close CH–O contact. All the angles Se(1)–C(2)–N(3), C(2)–N(3)–C(4) and N(3)–C(4)–C(5) are highly strained, but even so a remarkably short distance of 3·32 Å between Se(1) and C(5) is observed, or, based on the assumed H(25) position, a Se(1)–H(25) distance of only 2·55 Å is found. This is over 0·6 Å less than the accepted sum of van der Waals radii. The angle C(2)–Se(1)–H(25) is 83°. To achieve a Se–H distance of about 3 Å by bending the H atom out of plane would require a bending angle of nearly 60°, which is very unlikely. In any event, something quite unusual seems to take place in this region, and the idea of some kind of bond between Se and H(25) comes close. With the estimated standard deviations for bond lengths in mind the irregularities observed in the phenyl groups are not of sufficient magnitude to warrant discussion.

A point of interest is the location of the hydrogen atoms. With the observed H positions, C–H distances were calculated. The average value found is 1·06 Å, with individual values ranging from 0·83 to 1·24 Å. It is evident that even in the presence of an atom as heavy as selenium, hydrogen atoms can be successfully located, provided that sufficient care is exercized when intensity data are collected.

Except for the Se–HN distance, all other intermolecular distances are normal. Some of the shorter intermolecular distances are Se(1′) (at $-x, 1-y, 1-z$)–C(17) = 3·93, Se(1′) (same)–H(36′) (at $x, y-1, z$) = 3·25, O(18)–H(29′) (at $1-x, 1-y, 1-z$) = 2·67 Å.

The author considers it a pleasant duty to thank Prof. J. D. McCullough for the gift of a sample of phenylbenzoylselenourea, for his steady interest in this study, and for many inspiring discussions.

The author also wishes to thank the National Science Foundation for their financial support of this research under Grant NSF-G 24997, the Numerical Analysis Project of the UCLA Department of Mathematics for the use of their computing facilities, and the Fulbright Foundation for a travel grant.

References

Bak, B., Sloan, R. & Williams, D. (1950). *Phys. Rev.* **80**, 101.

Brown, C. J. & Corbridge, D. E. C. (1954). *Acta Cryst.* **7**, 711.

Cochran, W. & Dyer, H. B. (1952). *Acta Cryst.* **5**, 634.

Douglass, I. B. (1937). *J. Amer. Chem. Soc.* **59**, 740.

Hughes, E. W. (1941). *J. Amer. Chem. Soc.* **63**, 1737.

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.

Strandberg, M. W. P., Wentink, T. & Hill, A. G. (1949). *Phys. Rev.* **75**, 827.