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The Crystal Structure of 2-Oxazolidinone

By June W. Turley

Chemical Physics Research Laboratory, The Dow Chemical Company, Midland, Michigan 48640, *U.S.A.*

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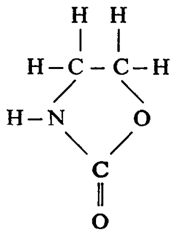
Crystals of 2-oxazolidinone, $C_3H_5NO_2$, are in monoclinic space group $P2_1/c$ with four molecules in a unit cell of dimensions $a=7·313$ (4), $b=5·672$ (5), $c=9·970$ (9) Å and $\beta=110·78$ (11)° measured at 24 °C; $D_x=1·50$ g.cm^{-3} and $D_m=1·42$ (2) g.cm^{-3}. Visual data, comprising 551 independent reflections above background, were collected with Cu $K\alpha$ radiation (1·5418 Å) and scaled from a Wilson plot. Iterative application of Sayre's equation in three dimensions led immediately to the solution of the structure. Refinement by full-matrix least-squares procedures gave a final residual index $R_1=0·132$ with hydrogen atoms included. The molecule is essentially planar with a root-mean-square deviation of 0·05 Å from the least-squares plane. There is one N–H···O hydrogen bond (2·858 Å) per molecule resulting in chains in the y direction, and no other close intermolecular distances. Bonds clockwise around the ring are C–C: 1·497 (10), C–O: 1·453 (8), O–C: 1·356 (10), C–N: 1·301 (8), and N–C: 1·466 (7) Å. The carbonyl C–O distance is 1·210 (8) Å. Angles in the ring are 100·3 (6), 106·0 (5), 108·6 (5), 110·2 (5), and 113·3 (6)° at C, C, O, C, and N respectively.

Introduction

Chemical studies (Walles, 1961) have shown that the ability of 2-oxazolidinone to form molecular complexes readily with materials such as phenols, aspirin, saccharin, iodine, *etc.*, can be attributed almost entirely to the oxazolidinone ring. The present investigation was undertaken to elucidate the molecular geometry as a basis for studying this complexing ability. Structures based on the oxazole ring system have not been studied previously, although a recent report has been made (Amirthalingam & Muralidharan, 1969) on a thiazole compound said to be a potential radioprotective agent.

Experimental

Crystals of 2-oxazolidinone, prepared by W. E. Walles,



are small, colorless prisms elongated along a. One such crystal, approximately 0·2 mm on a side and mounted on the b axis, gave equi-inclination Weissenberg photographs showing C_{2h} diffraction symmetry and extinctions for $h0l$ with $l=2n+1$ and $0k0$ with $k=2n+1$, thereby establishing space group $P2_1/c$.

Lattice parameters, initially measured from Weissenberg single-crystal photographs taken with Cu $K\alpha$ (1·5418 Å) radiation, were subsequently refined using X-ray powder-diffraction data, taken at 24 °C with crystal monochromatized Cu $K\alpha_1$ radiation (1·54050 Å) on an AEG* Guinier camera using Seeman–Bohlin focusing (Hofman & Jagodzinski, 1955). A 7·5 μ Al foil sample support was used to provide reference lines. Three cycles with the method of axial ratios (Frevel, 1964) gave $a=7·313\pm0·004$, $b=5·672\pm0·005$, $c=9·970\pm0·009$ Å, and $\beta=110·78\pm0·11°$. The crystal density measured by displacement in cyclohexane is 1·423 g.cm^{-3}, in fair agreement with the calculated density, 1·495 g.cm^{-3}, assuming four molecules per unit cell.

Intensity data for five levels along the b axis were read from equi-inclination Weissenberg multiple-film exposures made using Ni-filtered Cu $K\alpha$ (1·5418 Å) radiation. The films were read twice, independently by two different observers who compared them visually with a scale calibrated by a reflection from the same crystal. The data sets were then scaled internally using Wilson scale factors and were merged. The copper sphere allowed 883 reflections of which 551 were observed. The intensities were corrected for Lorentz and polarization effects, but no absorption correction was made ($\mu=10·46$ cm^{-1}). Assuming $\sigma(F^2)=0·10F^2$ for a given unique reflection, the expression $\sigma(F)=\sigma(F^2)/2F$ was used to estimate the σ's needed for computing the weights $w=4F^2/\sigma^2(F^2)$ used in the least-squares refinement (Gvildys, 1967), where the quantity $\sum w(F_o-F_c)^2$ was minimized. Reflections 011, $\bar{2}11$, and $\bar{2}12$ were excluded from least-squares refinements because of severe secondary extinction effects, seen as a factor-of-two difference between observed and calculated structure factors for these data.

Solution and refinement of the structure

Iterative application of Sayre's (1952) equation in three dimensions led immediately to the solution of the struc-

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* Allgemeine Elektrizitäts-Gesellschaft.

ture. The equation is:

$$s(E_a)=s\left(\sum_{\mathbf{a}=\mathbf{b}+\mathbf{c}} E_bE_c\right)$$

where s means 'sign of', **a**, **b**, **c** are the vectors (hkl) for the reflexions a, b, c, and E_a, E_b, & E_c are normalized structure factors for a, b, c. A set of 182 reflections having $|E|\geq 1{\cdot}5$, and a starting set comprising three origin-determining reflections assigned positive phases and four additional reflections with both positive and negative phases allowed, were used with a completely automated computer program (Long, 1965). E maps (Gvildys, 1965*a*) were calculated for the two unique solutions found, and the structure was clearly shown on one while the other gave a map with too few peaks and lower peak heights. An initial calculation with positions read from the E map gave a residual index $R=\sum||F_o|-|F_c||/\sum|F_o|$ of 0·334. Using a full-matrix least-squares program (Gvildys, 1967), refinement was carried out as described below. Four cycles of isotropic refinement defining all peaks as carbon atoms (Ibers, 1962) decreased R to 0·248. At this point, atoms were redefined as carbon, nitrogen, and oxygen based on refined thermal parameters and the known atomic sequence in the molecule. Next, three cycles of isotropic refinement, followed by three cycles of anisotropic refinement, gave $R=0{\cdot}155$, and a difference map showed positions for the five hydrogen atoms in the molecule.

Table 1. *Final fractional coordinates and anisotropic thermal displacement* ($\text{Å}\times 10^3$)* *for 2-oxazolidinone*

Fractional coordinates of non-hydrogen atoms are multiplied by 10^4 and those of the hydrogen atoms by 10^3. E.s.d.'s based on the least-squares refinement are given in parentheses.

	x	y	z	$U_{11}^{1/2}$	$U_{22}^{1/2}$	$U_{33}^{1/2}$	$U_{12}^{1/2}$	$U_{13}^{1/2}$	$U_{23}^{1/2}$
C(1)	2507 (12)	−3051 (13)	5530 (7)	254 (70)	153 (72)	196 (60)	35 (58)	190 (57)	100 (52)
C(2)	3619 (11)	−1133 (12)	6515 (7)	237 (66)	185 (68)	176 (56)	55 (56)	89 (54)	67 (51)
C(3)	2047 (9)	502 (13)	4312 (6)	181 (56)	191 (32)	162 (53)	47 (52)	75 (49)	25 (49)
N	1433 (9)	−1664 (12)	4251 (6)	234 (60)	181 (69)	171 (53)	34 (54)	77 (50)	25 (47)
O(1)	3406 (7)	952 (8)	5624 (4)	207 (50)	188 (54)	159 (45)	88 (44)	60 (42)	53 (41)
O(2)	1524 (8)	2034 (9)	3411 (5)	237 (55)	242 (62)	186 (49)	37 (49)	44 (46)	138 (47)
H(1)	364 (12)	−389 (13)	534 (8)	220	220	220	—	133	—
H(2)	191 (12)	−405 (15)	571 (9)	222	222	222	—	134	—
H(3)	507 (15)	−139 (17)	691 (11)	286	286	286	—	172	—
H(4)	313 (14)	−64 (15)	729 (10)	270	270	270	—	163	—
H(5)	95 (13)	−241 (16)	357 (10)	244	244	244	—	147	—

* These values are the square roots of the mean-square amplitude tensors, U_{ij}, based on the expression exp $-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+2hk\beta_{12}+2hl\beta_{13}+2kl\beta_{23})$ and relations such as $\beta_{12}=2\pi^2U_{12}a^*b^*$ (Cruickshank, 1965).

Table 2. *Observed and calculated structure factors for 2-oxazolidinone*

H	L	FOBS	FCALC
*** K = 0 ***			
2	0	4578	5598
3	0	1430	1126
4	0	2406	2255
5	0	458	382
6	0	1223	1159
7	0	397	313
8	0	168	139
0	2	4043	4281
0	4	2317	2524
0	6	1179	1002
0	8	2021	2110
0	10	1291	1437
1	2	443	479
1	4	1992	1777
1	6	807	775
1	8	559	440
1	10	301	239
2	2	3573	3762
2	4	1605	1568
2	6	1421	1220
2	8	1522	1505
2	10	301	323
3	2	856	679
3	4	884	811
3	6	443	97
3	8	260	172
3	10	30	106
4	2	2181	1832
4	4	0	15
4	6	727	709
4	8	0	46
5	2	0	117
5	4	207	67
5	6	0	35
6	2	316	297
6	4	0	102
6	6	0	76
7	2	0	138
8	2	254	288
−1	2	431	393
−1	4	553	514
−1	6	827	834
−1	8	263	308
−1	10	638	606
−1	12	0	110
−2	2	9933	10318
−2	4	1359	1260
−2	6	405	499
−2	8	567	553
−2	10	1687	1765
−2	12	709	762
−3	2	239	201
−3	4	505	497
−3	6	390	308
−3	8	358	253
−3	10	331	214
−3	12	290	412
−4	2	2967	2626
−4	4	2881	2564
−4	6	387	224
−4	8	375	276
−4	10	287	353
−4	12	887	924
−5	2	541	535
−5	4	337	322
−5	6	198	55
−5	8	228	211
−5	10	355	304
−5	12	130	180
−6	2	683	684
−6	4	872	794
−6	6	369	288
−6	8	0	1
−6	10	192	218
−7	2	491	492
−7	4	0	3
−7	6	0	141
−7	8	0	63
−7	10	275	268
−8	2	420	398
−8	4	0	68
−8	6	0	161
−9	2	222	348
−9	4	0	228
*** K = 1 ***			
1	0	893	907
2	0	381	366
3	0	379	252
4	0	252	211
5	0	694	659
6	0	0	29
7	0	427	493
8	0	0	83
0	1	2487	5184
0	2	1726	2246
0	3	1062	1072
0	4	2162	2455
0	5	878	959
0	6	568	452
0	7	945	969
0	8	1160	1308
0	9	986	1057
0	10	200	164
0	11	0	33
1	1	247	161
1	2	1396	1314
1	3	1136	1095
1	4	0	88
1	5	472	427
1	6	680	596
1	7	220	125
1	8	0	244
1	9	245	232
1	10	0	19
1	11	0	98
2	1	1432	1217
2	2	1284	1077
2	3	2240	2269
2	4	855	710
2	5	1133	1043
2	6	1805	1844
2	7	905	948
2	8	835	886
2	9	0	109
2	10	261	308
3	1	287	273
3	2	1127	975
3	3	730	607
3	4	121	37
3	5	218	280
3	6	225	263
3	7	0	36
3	8	193	235
3	9	0	98
4	1	2390	2049
4	2	568	477
4	3	943	880
4	4	1210	1228
4	5	413	480
4	6	1169	1236
4	7	112	149
4	8	225	245
5	1	610	548
5	2	458	536
5	3	415	419
5	4	312	224
5	5	0	174
5	6	189	261
6	1	611	565
6	2	514	407
6	3	0	89
6	4	839	859
6	5	0	101
7	1	357	384
7	2	197	202
7	3	0	141
8	1	0	18
−1	1	631	519
−1	2	1531	1634
−1	3	821	834
−1	4	947	849
−1	5	783	782
−1	6	958	901
−1	7	0	149
−1	8	390	372
−1	9	554	560
−1	10	211	55
−1	11	272	312
−2	1	2754	4536
−2	2	2707	3721
−2	3	2590	2951
−2	4	1179	1193
−2	5	296	236
−2	6	1890	2010
−2	7	0	51
−2	8	218	235
−2	9	640	711
−2	10	307	315
−2	11	646	766
−3	1	925	689
−3	2	783	541
−3	3	1087	955
−3	4	1210	897
−3	5	527	488
−3	6	110	119
−3	7	613	505
−3	8	624	625
−3	9	133	117
−3	10	0	63
−3	11	482	564
−4	1	171	127
−4	2	1347	1093
−4	3	2182	1909
−4	4	2867	2648
−4	5	1138	1133
−4	6	283	229
−4	7	379	382
−4	8	896	889
−4	9	133	155
−4	10	0	173
−4	11	400	420
−5	1	0	1
−5	2	516	447
−5	3	703	577
−5	4	234	338
−5	5	539	507
−5	6	249	187
−5	7	395	381
−5	8	317	303
−5	9	337	346
−5	10	0	125
−5	11	175	203
−6	1	990	917
−6	2	406	346
−6	3	130	99
−6	4	959	857
−6	5	635	591
−6	6	1107	1162
−6	7	224	248
−6	8	0	33
−6	9	207	212
−7	1	519	431
−7	2	132	152
−7	3	0	19
−7	4	290	322
−7	5	256	327
−7	6	0	98
−7	7	0	236
−7	8	0	91
−7	9	258	294
−8	1	177	228
−8	2	188	199
−8	3	224	237
−8	4	0	168
−8	5	0	120
−8	6	332	395
−8	7	0	128
−8	8	296	380
−8	9	189	7
*** K = 2 ***			
2	0	309	223
4	0	363	358
5	0	417	444
6	0	0	76
7	0	576	653
8	0	217	243
0	1	975	847
0	2	547	469
0	3	2602	2707
0	4	1080	807
0	5	3211	3082
0	6	863	766
0	7	233	97
0	8	0	137
0	9	632	590
0	10	202	202
0	11	0	60
1	0	1703	1912
1	1	2189	2313
1	2	1295	948
1	3	1008	811
1	4	1773	1613
1	5	592	442
1	6	294	314
1	7	986	1070
1	8	238	152
1	9	466	526
1	10	316	255
2	1	1188	1132
2	2	865	803
2	3	2680	2573
2	4	778	727
2	5	0	38
2	6	681	767
2	7	1078	1112
2	8	130	159
2	9	110	69
2	10	0	89
3	0	1672	1584
3	1	769	722
3	2	1237	1276
3	3	244	355
3	4	1109	1176
3	5	825	866
3	6	139	28
3	7	585	605
3	8	190	182
3	9	0	55
4	1	610	520
4	2	316	357
4	3	137	62
4	4	798	960
4	5	1020	1152
4	6	128	137
4	7	110	149
4	8	0	212
5	1	235	275
5	2	1033	1201
5	3	491	549
5	4	311	249
5	5	390	327
5	6	173	37
5	7	0	19
6	1	0	233
6	2	558	626
6	3	616	712
6	4	350	345
6	5	146	193
7	1	287	322
7	2	235	294
7	3	159	101
8	1	121	289
−1	1	1427	1798
−1	2	986	1056
−1	3	1589	1279
−1	4	811	620
−1	5	576	504
−1	6	981	828
−1	7	704	569
−1	8	540	474
−1	9	789	756
−1	10	215	201
−1	11	175	165
−2	1	1069	1052
−2	2	912	922
−2	3	1488	1399
−2	4	943	958
−2	5	2689	2029
−2	6	343	185
−2	7	2039	1766
−2	8	365	337
−2	9	139	37
−2	10	222	163
−2	11	110	75
−3	1	1490	1440
−3	2	1224	1197
−3	3	668	600
−3	4	345	365
−3	5	408	292
−3	6	908	937
−3	7	226	181
−3	8	139	54
−3	9	692	566
−3	10	612	611
−3	11	269	257
−4	1	0	44
−4	2	291	321
−4	3	1486	1500
−4	4	271	137
−4	5	894	978
−4	6	533	533
−4	7	829	829
−4	8	141	103
−4	9	580	621
−4	10	128	68
−4	11	0	84
−5	1	545	435
−5	2	798	815
−5	3	578	499
−5	4	585	590
−5	5	136	26
−5	6	616	641
−5	7	240	180
−5	8	513	553
−5	9	134	132
−5	10	206	227
−5	11	320	346
−6	1	437	436
−6	2	0	93
−6	3	139	111
−6	4	139	37
−6	5	715	904
−6	6	341	343
−6	7	607	506
−6	8	132	115
−6	9	211	191
−6	10	108	131
−6	11	0	128
−7	1	0	103
−7	2	134	115
−7	3	233	265
−7	4	233	238
−7	5	134	73
−7	6	224	268
−7	7	125	13
−7	8	388	422
−7	9	103	57
−7	10	0	193
−8	1	173	271
−8	2	0	33
−8	3	370	433
−8	4	112	86
−8	5	0	57
−8	6	199	176
−8	7	300	406
−8	8	150	161
*** K = 3 ***			
1	0	928	904
2	0	594	650
3	0	913	809
4	0	345	306
5	0	281	253
6	0	276	283
7	0	231	155
8	0	0	326
0	1	758	855
0	2	453	532
0	3	1525	1568
0	4	878	822
0	5	146	126
0	6	517	471
0	7	307	332
0	8	168	145
0	9	344	233
0	10	207	66
1	1	1295	1244
1	2	1840	1883
1	3	408	420
1	4	639	490
1	5	156	166
1	6	1829	1873
1	7	283	198
1	8	548	551
1	9	137	200
1	10	161	78
2	1	1753	1787
2	2	798	789
2	3	1326	1349
2	4	156	156
2	5	392	381
2	6	285	111
2	7	272	54
2	8	0	108
2	9	248	209
3	1	231	232
3	2	149	102
3	3	545	434
3	4	1541	1573
3	5	170	60
3	6	807	738
3	7	146	106
3	8	330	262
4	1	1468	1560
4	2	167	117
4	3	170	59
4	4	432	391
4	5	514	379
4	6	141	139
5	1	566	518
5	2	769	722
5	3	272	228
5	4	724	628
5	5	292	264
5	6	298	274
6	1	0	169
6	2	385	441
6	3	444	408
6	4	182	168
7	1	281	270
7	2	323	331
−1	1	370	304
−1	2	1486	1723
−1	3	717	767
−1	4	1600	1814
−1	5	316	385
−1	6	923	851
−1	7	521	573
−1	8	1248	1367
−1	9	267	34
−1	10	309	245
−1	11	246	280
−2	1	949	889
−2	2	321	287
−2	3	475	395
−2	4	212	168
−2	5	319	264
−2	6	529	510
−2	7	758	675
−2	8	436	499
−2	9	163	70
−2	10	144	166
−2	11	259	267
−3	1	602	483
−3	2	552	379
−3	3	335	269
−3	4	1328	1465
−3	5	149	67
−3	6	849	917
−3	7	281	260
−3	8	817	768
−3	9	470	434
−3	10	531	608
−3	11	189	95
−4	1	937	950
−4	2	331	392
−4	3	449	397
−4	4	345	326
−4	5	267	120
−4	6	278	222
−4	7	436	482
−4	8	281	216
−4	9	528	603
−4	10	233	246
−5	1	167	119
−5	2	165	57
−5	3	165	139
−5	4	278	84
−5	5	281	89
−5	6	750	732
−5	7	283	301
−5	8	272	202
−5	9	250	148
−5	10	413	421
−6	1	833	921
−6	2	170	70
−6	3	436	355
−6	4	170	120
−6	5	168	13
−6	6	371	388
−6	7	266	115
−6	8	248	263
−6	9	427	454
−7	1	330	322
−7	2	0	128
−7	3	0	257
−7	4	257	138
−7	5	0	152
−7	6	0	3
−7	7	229	224
−7	8	278	249
−7	9	170	208
−8	1	160	149
−8	2	243	261
−8	3	269	351
−8	4	0	153
−8	5	0	149
−8	6	0	90
*** K = 4 ***			
1	0	630	800
2	0	317	139
3	0	935	922
4	0	619	732
5	0	0	147
6	0	400	383
0	1	0	76
0	2	381	408
0	3	1018	945
0	4	383	179
0	5	1237	1014
0	6	448	207
0	7	445	124
0	8	411	337
0	9	201	301
1	1	690	526
1	2	959	841
1	3	217	23
1	4	242	280
1	5	1534	1507
1	6	264	137
1	7	809	686
1	8	375	347
1	9	279	277
2	1	345	266
2	2	697	624
2	3	877	929
2	4	441	428
2	5	449	277
2	6	433	276
2	7	0	201
3	1	408	320
3	2	0	36
3	3	1055	1265
3	4	264	125
3	5	841	973
3	6	227	235
3	7	312	312
4	1	446	424
4	2	547	500
4	3	443	506
4	4	245	95
4	5	219	25
5	1	476	608
5	2	247	212
5	3	637	757
5	4	197	47
6	1	373	378
6	2	196	31
−1	1	421	464
−1	2	821	919
−1	3	1431	1474
−1	4	564	369
−1	5	242	102
−1	6	441	359
−1	7	1020	979
−1	8	521	356
−1	9	373	256
−2	1	179	158
−2	2	653	875
−2	3	345	424
−2	4	381	476
−2	5	1211	1196
−2	6	441	202
−2	7	688	530
−2	8	254	4
−2	9	227	265
−3	1	377	409
−3	2	377	363
−3	3	595	661
−3	4	498	626
−3	5	1188	1332
−3	6	446	44
−3	7	0	120
−3	8	0	184
−3	9	385	331
−3	10	333	351
−4	1	430	163
−4	2	0	54
−4	3	0	203
−4	4	438	425
−4	5	483	601
−4	6	264	359
−4	7	723	730
−4	8	416	297
−4	9	216	102
−5	1	449	461
−5	2	635	634
−5	3	449	372
−5	4	0	21
−5	5	544	573
−5	6	257	305
−5	7	688	697
−6	1	0	62
−6	2	425	496
−6	3	250	142
−6	4	0	66
−6	5	244	184

Finally, three cycles with all atoms anisotropic except the hydrogen (Stewart, Davidson & Simpson, 1965) gave an R value of 0·132. Reasonable convergence was indicated by a maximum coordinate shift of 0·04σ for non-hydrogen atoms and 0·17σ for hydrogen atoms, and a value of 1·97 for the indicator $[\sum(w\Delta F^2)/(NO-NV)]^{\frac{1}{2}}$, where NO is the number of observations and NV is the number of parameters varied. The refined atomic parameters are listed in Table 1, and the observed and calculated structure factors are compared in Table 2.

Discussion

Fig. 1 shows the molecular structure (Johnson, 1965). The molecule is approximately planar with a root-mean-square deviation of 0·05 Å from the least-squares plane of all atoms (Gvildys, 1965*b*), plane 1 in Table 3, from which atoms C(1) and C(2) show the largest deviation. Plane 2 is fitted to atoms C(3), O(1), N, and O(2), and plane 3 to atoms C(1), C(2), O(1), and N; the dihedral angle between them is 2° 33′, showing a significant deviation from planarity when compared with the estimated errors of 0·6° in the bond angles.

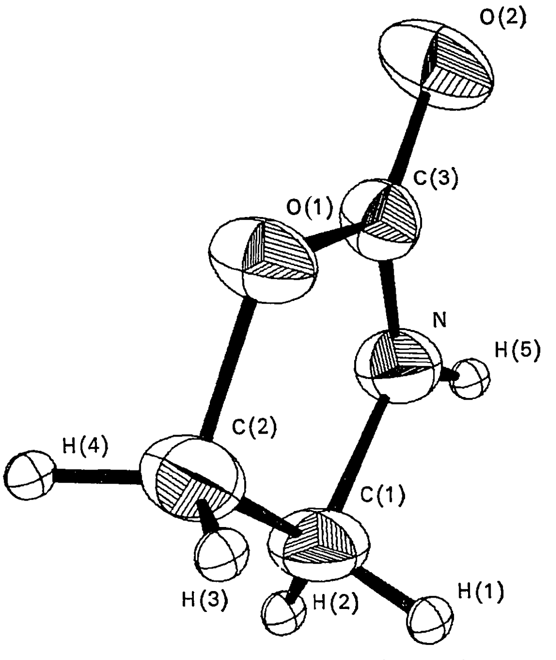
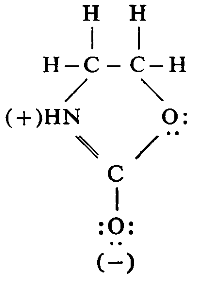


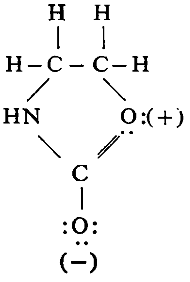
Fig. 1. Molecular structure of 2-oxazolidinone with atoms represented as 50% probability thermal-motion ellipsoids.

Although the bond distances and angles, given in Table 4 (Gvildys, 1964), show some differences from expected values (Sutton, 1965) they agree well with values found in other lactone structures (Koenig, Chiu, Krebs & Walter, 1969; Kalyani & Vijayan, 1969). The C(1)–C(2) distance is 0·04 Å less than the expected value of 1·537 Å for a simple C–C bond, C(2)–O(1) is 0·02 Å longer than the expected C–O single bond length of 1·435 Å, and C(3)–O(1) is 0·04 Å longer than the analogous C–O bond (1·312 Å) in organic acids but much shorter than a C–O single bond distance. Also, the C(3)–N distance of 1·301 Å is much shorter than expected (1·333 Å) for an N–C=O group, and the C(1)–N distance of 1·466 Å is shorter than the value of 1·472 Å usually observed for trivalent nitrogen. Although these observed bond distances have moderately high estimated errors, the differences discussed above are large enough to suggest that the major resonance forms for the structure are:



(I)

and



(II)

Here, the N=C–O portion of the molecule can act as a dipole on a polarizable molecule, suggesting an explanation for the unusual complexing ability of this ring system.

The molecular packing is shown in Fig. 2. Hydrogen-bonded chains are formed in the **y** direction by the 2·862 Å N–H···O(2) interaction, resulting in planar strips slightly more than two molecules wide and aligned to suggest some dipole-dipole interaction between them in the **x** direction. Only van der Waals approaches of CH_3 groups occur in the **z** direction.

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Table 3. *Molecular planes in 2-oxazolidinone*

Equation of the plane is $M1x+M2y+M3z=D$, where D is the origin-to-plane distance and x,y,z are fractional coordinates in the crystal system. The Δ's are the distances of the atoms from the fitted plane.

Plane	$M1$	$M2$	$M3$	D	ΔC(1)	ΔC(2)	ΔO(1)	ΔC(3)	ΔN	ΔO(2)
1	6·687	−1·428	−6·189	−1·381	0·071 Å	−0·069 Å	0·042 Å	0·010 Å	−0·054 Å	−0·001 Å
2	6·554	−1·606	−6·354	−1·490	0·110†	−0·095†	−0·003	0·012	−0·004	−0·005
3	6·684	−1·406	−6·228	−1·409	0·069	−0·071	0·049	0·021†	−0·047	0·017†

† These atoms were not included when fitting the plane.

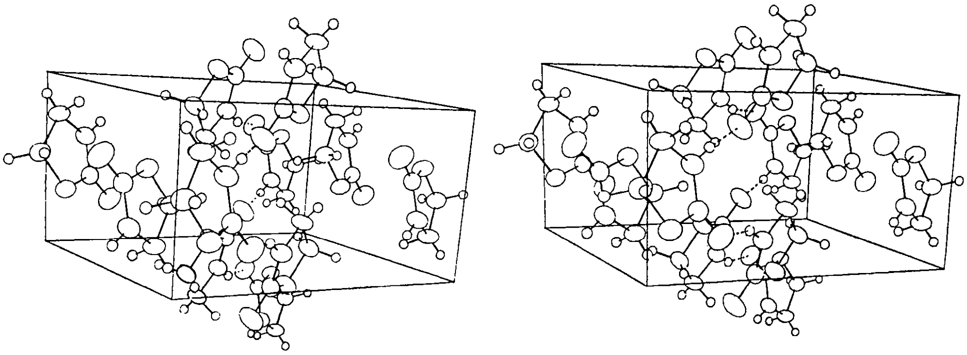

Fig. 2. Stereo view of molecular packing in 2-oxazolidinone with one unit cell outlined.

Table 4. *Interatomic distances and angles in 2-oxazolidinone*

Errors given in parentheses are in the last one or two significant figures.

C(1)–C(2)	1·497 (10) Å
C(2)–O(1)	1·453 (8)
O(1)–C(3)	1·356 (10)
C(3)–N	1·301 (8)
N——C(1)	1·466 (7)
C(3)–O(2)	1·210 (8)
C(1)–H(1)	1·03 (8)
C(1)–H(2)	0·77 (8)
C(2)–H(3)	1·00 (10)
C(2)–H(4)	1·00 (9)
N——H(5)	0·77 (9)
N.....O(2)	2·862 (7)
H(5)...O(2)	2·18 (9)

N——C(1)–C(2)	100·3 (6)°
H(1)–C(1)–N	108·0 (43)
H(1)–C(1)–C(2)	99·9 (43)
H(1)–C(1)–H(2)	104·8 (82)
H(2)–C(1)–N	115·2 (61)
H(2)–C(1)–C(2)	126·7 (61)
C(1)–C(2)–O(1)	106·0 (5)
H(3)–C(2)–C(1)	113·8 (58)
H(3)–C(2)–O(1)	103·1 (56)
H(3)–C(2)–H(4)	111·0 (79)
H(4)–C(2)–O(1)	104·8 (50)
H(4)–C(2)–C(1)	116·6 (53)
C(2)–O(1)–C(3)	108·6 (5)
O(1)–C(3)–N	110·2 (5)
O(1)–C(3)–O(2)	120·7 (6)
N——C(3)–O(2)	129·0 (6)
C(3)–N——C(1)	113·3 (6)
H(5)–N——C(1)	114·2 (70)
H(5)–N——C(3)	127·0 (70)

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