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The Crystal and Molecular Structure of Quinone 4-Oxime

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The crystal structure of quinone 4-oxime $C_6H_5O_2N$, has been determined from three dimensional X-ray diffraction data and refined by least squares methods. The space group is $P2_1/c$, $a=7.209$ Å, $b=28.14$ Å, $c=6.671$ Å, $\beta=118.86°$. The final correlation factor was 4.7 % and the estimated standard deviation in bond lengths for non-hydrogen atoms was in the range 0.003 – 0.004 Å. The asymmetric unit contains two molecules which are nearly equal as to corresponding bond lengths and angles. Two hydrogen bonds of significantly different length and a close packing of molecules are characteristic for the crystal structure. The bond lengths indicate a considerable degree of π-resonance in the molecules.

The present structure determination of quinone 4-oxime (I) is a part of a series of structural investigations of monomeric C-nitroso compounds and oximes derived from these by protonation or tautomeric proton exchange.

Lüttke [1] has demonstrated the ability of *p*-substituted nitrosobenzenes in forming dimers of the azodioxy-type to be heavily dependent upon the electron donating ability of the *para* substituent. An intramolecular charge transfer from the *para* substituent to the nitroso-group is probably preventing dimerisation.

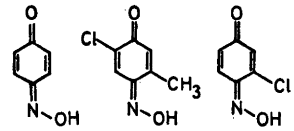
A comparison of the molecular structure of *these* nitrosobenzenes and their corresponding oximes might indicate to what degree this intramolecular charge transfer is present in the nitroso compounds.

So far the crystal and molecular structure of *N,N*-dimethyl-*p*-nitrosoaniline [2] and its hydrochloride,[3] have been investigated.

Spectroscopic investigations [4] of (I) indicate that only the oxime in the tautomeric equilibrium between the oxime and the nitroso compound is forming crystals. Structure determinations of 3-methyl-6-chloro- [5] (II) and 3-chloro-*p*-nitrosophenol [5] (III) have shown these compounds to occur in the quinone-oxime form in the crystal phase.

However, preliminary photographic investigations of crystals from diethyl ether solutions of (I), revealed a unit cell containing 8 molecules with the molecular weight of (I). Two of these molecules are thus constituting the asymmetric unit, as the space group is $P2_1/c$. (II) and (III) are shown to crystallize in the same space group, but with 1 molecule in the asymmetric unit.

The possibility of having both of the tautomeric forms in the unit cell was thus present. This possibility initiated the following structure determination.



(I) (II) (III)

EXPERIMENTAL

Yellow tabular crystals were grown by slow evaporation from a diethyl ether solution of commercially available *p*-nitrosophenol. From the systematic absences, *h0l* with *l* odd, *0k0* with *k* odd, the space group was determined to $P2_1/c$.

Three-dimensional data were collected, and unit cell parameters were determined on a SYNTEX-P1 computer controlled four-circle diffractometer with graphite monochromated Mo$K\alpha$ radiation. The unit cell parameters were obtained using a least squares treatment of measurements of twelve reflections.

All measurements were done using a crystal with approximate dimensions $0.40 \times 0.21 \times 0.09$ mm^3. The crystal was mounted with the c^*-axis nearly parallel to the goniometer head spindle axis.

The intensities were obtained using the $\omega - 2\theta$ scanning mode. Prior to each scan the intensity was measured with stationary crystal and

Table 1. Observed and calculated structure factors. The columns are: h, $10 \times F_{obs}$, $10 \times F_{calc}$.

H=	0,K=	0
4	1041	1056
6	320	337
H=	0,K=	1
-6	35	18
-5	35	28
-4	52	39
-3	73	72
-2	47	35
-1	60	60
1	54	60
2	46	35
3	69	72
4	49	39
H=	0,K=	2
-6	119	123
-5	72	83
-4	242	237
-3	91	88
-2	342	332
1	28	38
2	335	332
3	88	85
4	232	237
5	77	83
6	115	123
7	40	48
H=	0,K=	3
-3	75	73
-1	76	80
1	80	80
2	28	17
3	71	73
4	29	8
H=	0,K=	4
-7	39	42
-5	83	85
-4	57	47
-3	237	227
-2	86	84
-1	669	671
0	92	95
1	642	671
2	82	84
3	234	227
4	45	47
5	83	85
H=	0,K=	5
-5	46	42
-4	63	59
-3	121	119
-2	62	66
-1	104	105
1	107	105
2	63	66
3	118	119
4	63	59
5	39	42
H=	0,K=	6
-6	55	59
-4	122	120
-2	186	185
0	186	185
2	186	185
3	27	1
4	122	120
6	60	59
H=	0,K=	7
-4	51	50
-3	73	69
-2	73	73
-1	55	55
1	53	55
2	74	73
3	71	69
4	53	50
5	35	28
H=	0,K=	8
-6	75	77
-4	157	149
-3	121	122
-2	261	262
-1	321	320
0	337	338
1	320	320
2	256	262
3	126	122
4	148	149
6	72	77
H=	0,K=	9
-6	49	18
-5	38	42
-4	33	39
-3	72	71
-2	58	55
-1	39	46
1	42	46
2	53	55
3	75	71
4	38	39

5	39	42
H=	0,K=	10
-6	58	55
-5	93	90
-4	131	126
-3	294	291
-2	278	279
-1	580	578
0	393	399
1	595	578
2	286	279
3	286	291
4	123	126
5	88	90
6	54	55
H=	0,K=	11
-5	42	40
-4	55	55
-3	80	83
-2	85	86
1	86	86
2	83	86
3	83	83
4	55	55
5	41	40
H=	0,K=	12
-7	55	54
-6	36	17
-5	113	112
-4	88	84
-3	234	220
-2	267	266
-1	394	383
0	412	411
1	400	383
2	273	266
3	231	220
4	77	84
5	110	112
7	41	54
H=	0,K=	13
-2	42	40
2	31	40
4	33	29
5	32	6
H=	0,K=	14
-5	92	98
-4	32	31
-3	184	180
-2	151	153
-1	276	280
0	254	253
1	281	280
2	160	153
3	190	181
4	40	31
5	93	98
H=	0,K=	16
-6	37	27
-5	33	8
-4	69	71
-3	58	54
-2	176	177
-1	118	122
0	264	259
1	125	122
2	175	177
3	47	54
4	55	71
H=	0,K=	17
-6	45	36
-4	70	68
-2	74	73
2	80	73
4	78	68
6	39	36
H=	0,K=	18
-3	68	61
-2	56	56
-1	133	149
0	73	83
1	156	149
2	56	56
3	66	61
H=	0,K=	19
-5	81	74
-3	124	121
1	32	71
3	122	121
5	62	74
H=	0,K=	20
-6	49	43
-4	81	70
-3	106	104
-2	90	92
-1	158	177
0	100	100
1	179	177
2	88	92
3	102	104

4	84	70
6	54	43
H=	0,K=	21
-5	49	59
-3	99	93
1	32	52
3	96	93
5	58	59
H=	0,K=	22
-5	36	25
-4	124	118
-2	174	172
0	189	193
2	187	172
4	119	118
H=	0,K=	23
-4	38	34
-3	51	53
3	51	53
4	39	34
5	47	36
H=	0,K=	24
-4	81	77
-2	157	162
0	200	214
2	158	162
4	79	77
H=	0,K=	25
-3	42	26
H=	0,K=	26
-4	102	95
-2	149	158
-1	32	36
0	185	189
1	39	36
2	158	158
4	98	95
H=	0,K=	28
-4	36	24
0	37	41
2	32	36
H=	0,K=	30
-3	41	38
-2	69	79
-1	46	42
0	95	101
2	81	79
3	48	35
H=	0,K=	32
-1	35	8
H=	1,K=	0
-6	207	218
-4	611	619
-2	1259	1243
0	972	999
2	248	247
4	40	40
H=	1,K=	1
-6	100	111
-4	263	271
-3	56	54
-2	474	494
0	309	321
1	165	169
3	148	150
5	84	92
H=	1,K=	2
-6	145	148
-4	442	447
-2	886	883
-1	126	129
0	701	718
1	226	238
2	216	218
3	115	116
4	45	42
5	38	35
H=	1,K=	3
-7	46	36
-6	114	110
-5	121	121
-4	248	237
-3	413	405
-2	446	446
-1	770	797
0	462	484
1	546	559
2	244	251
3	197	197
4	91	94
5	63	64
H=	1,K=	4
-7	87	87
-6	54	56
-5	167	161
-4	147	134
-3	349	343
-2	271	263
-1	380	394
0	288	288

1	118	123
2	160	158
4	61	57
H=	1,K=	5
-5	44	42
-4	36	30
-3	65	66
-2	76	80
-1	60	55
0	196	203
1	134	136
2	190	193
3	144	147
4	101	108
5	81	88
6	50	50
H=	1,K=	6
-6	47	46
-5	48	44
-4	104	95
-3	182	180
-2	242	230
-1	360	376
0	381	392
1	317	325
2	317	307
3	129	126
4	154	147
5	33	31
6	59	61
H=	1,K=	7
-4	43	47
-3	77	80
-2	105	108
-1	275	289
0	184	195
1	317	325
2	168	171
3	146	153
4	92	94
5	45	49
6	36	38
H=	1,K=	8
-6	55	52
-4	120	123
-3	48	40
-2	258	255
0	328	336
1	98	99
2	210	218
3	88	86
4	84	86
5	42	40
H=	1,K=	9
-5	32	33
-4	40	48
-2	99	101
-1	152	139
0	116	116
1	227	218
2	61	66
3	134	131
5	42	45
H=	1,K=	10
-6	43	43
-5	105	100
-4	124	121
-3	275	264
-2	229	234
-1	394	389
0	192	197
1	257	261
2	48	47
3	78	75
H=	1,K=	11
-6	43	37
-5	48	49
-3	129	126
-2	77	85
-1	221	221
0	138	141
1	172	169
2	49	65
3	82	77
5	35	33
6	42	27
H=	1,K=	12
-6	67	72
-4	184	186
-2	340	331
-1	34	36
0	305	283
2	102	97
H=	1,K=	13
-6	39	31
-4	97	88
-3	85	89
-2	235	228
-1	162	159
0	344	344

1	104	108
2	261	259
3	38	35
4	121	117
6	43	40
H=	1,K=	14
-4	78	72
-3	59	[illegible]
-2	122	112
-1	79	74
0	48	[illegible]
1	57	63
2	33	[illegible]
3	45	38
4	52	[illegible]
6	37	[illegible]
H=	1,K=	15
-6	59	52
-5	65	73
-4	157	154
-3	108	113
-2	325	311
-1	129	138
0	366	347
1	113	117
2	211	207
3	70	67
4	93	88
6	36	34
H=	1,K=	16
-7	86	49
-6	44	44
-5	143	144
-4	97	98
-3	315	311
-2	134	138
-1	456	435
0	96	97
1	332	342
2	38	46
3	172	164
5	64	58
H=	1,K=	17
-5	33	20
-4	61	54
-2	61	68
-1	48	46
0	77	81
2	76	72
4	39	42
H=	1,K=	18
-5	40	50
-4	37	37
-3	104	108
-1	197	196
0	28	28
1	211	209
2	35	38
3	139	134
5	60	62
H=	1,K=	19
-1	60	71
0	43	50
1	59	66
2	72	80
4	77	73
H=	1,K=	20
-4	84	88
-3	33	36
-2	165	166
-1	61	75
0	204	201
1	59	65
2	139	143
4	72	66
H=	1,K=	21
-3	47	42
-1	185	183
1	229	228
3	141	140
4	35	29
5	87	51
H=	1,K=	22
-2	39	40
0	89	98
2	116	116
3	67	70
4	76	75
5	59	57
H=	1,K=	23
-5	60	57
-4	60	43
-3	121	119
-2	87	86
-1	194	189
0	94	98
1	197	195
2	70	65
3	123	129
4	34	28

H=	1,K=	24
-5	66	56
-4	81	48
-3	88	93
-2	98	94
-1	87	90
0	135	134
1	49	45
2	123	118
4	69	62
H=	1,K=	25
-3	77	77
-1	96	95
0	35	35
1	64	64
H=	1,K=	26
-5	48	46
-3	59	55
-1	118	128
1	123	132
3	82	83
H=	1,K=	27
-3	88	84
-2	61	64
-1	81	97
0	56	61
1	90	103
2	52	42
3	69	70
H=	1,K=	28
-4	72	68
-2	69	80
0	72	78
2	62	67
H=	1,K=	29
-3	51	51
-1	83	60
1	85	84
H=	1,K=	30
-2	82	61
0	81	89
1	34	33
H=	1,K=	31
0	82	45
2	49	38
H=	1,K=	33
-1	61	63
0	64	59
H=	2,K=	0
-8	71	81
-6	191	197
-4	346	351
-2	361	366
0	150	153
2	31	31
H=	2,K=	1
-7	84	83
-6	36	58
-5	207	214
-3	437	440
-2	274	280
-1	536	545
0	388	392
1	359	369
2	144	148
3	166	173
5	66	74
H=	2,K=	2
-8	44	16
-3	66	69
-2	205	205
-1	71	70
0	285	285
2	136	143
4	38	40
H=	2,K=	3
-7	35	56
-5	115	114
-3	104	97
-1	138	136
0	43	39
1	219	223
3	120	122
5	46	41
H=	2,K=	4
-8	41	45
-6	121	127
-5	31	23
-4	305	302
-2	522	510
0	473	475
1	72	69
2	241	249
3	66	63
4	97	99
5	41	28
6	51	34
H=	2,K=	5
-8	47	39
-6	59	56

-8	48	70
-3	194	188
-2	184	179
-1	378	373
0	330	319
1	347	343
2	211	204
3	174	171
4	74	73
5	62	59
H=	2,K=	6
-4	30	38
-3	82	82
-2	44	37
-1	94	92
0	33	27
1	27	20
H=	2,K=	7
-6	40	42
-5	112	102
-4	84	84
-3	319	298
-2	207	203
-1	486	443
0	278	262
1	283	282
2	162	163
3	104	103
4	66	74
H=	2,K=	8
-7	45	81
-5	138	140
-4	52	46
-3	283	280
-2	100	96
-1	319	305
0	85	82
1	151	147
2	30	14
3	40	36
H=	2,K=	9
-3	92	101
-2	36	48
-1	156	170
0	67	74
1	97	105
2	57	56
4	33	29
H=	2,K=	10
-5	56	51
-3	150	140
-2	165	161
-1	271	250
0	253	239
1	239	226
2	138	133
3	122	120
4	45	35
5	47	48
H=	2,K=	11
-7	68	68
-5	153	148
-4	52	45
-3	285	274
-2	111	108
-1	327	320
0	97	93
1	211	203
2	33	28
3	69	79
H=	2,K=	12
-6	48	47
-4	92	94
-2	53	37
0	108	106
1	37	50
2	126	128
4	67	75
H=	2,K=	13
-4	35	43
-3	63	68
-2	108	117
-1	123	128
0	111	118
1	110	111
2	46	45
3	54	54
H=	2,K=	14
-7	50	49
-5	134	131
-4	51	46
-3	246	246
-2	27	17
-1	251	262
1	144	149
3	55	53
H=	2,K=	15
-6	43	27
-4	48	41
-3	29	11

-1	30	
0	38	44
2	39	39
H=	2,K=	16
-3	73	77
-2	31	39
-1	105	108
1	76	83
2	38	33
3	39	39
4	46	40
H=	2,K=	17
-7	47	40
-6	38	3
-5	81	80
-3	107	111
-1	75	88
0	38	39
2	42	44
H=	2,K=	18
-6	47	89
-4	85	93
-2	109	113
0	96	104
2	71	80
4	52	51
H=	2,K=	19
-5	59	64
-4	56	46
-3	81	80
-2	57	61
-1	95	109
0	90	89
1	118	118
2	101	99
3	78	83
4	74	73
H=	2,K=	20
-6	62	61
-4	110	112
-3	32	23
-2	160	163
-1	35	37
0	170	170
1	105	114
2	122	123
3	118	116
4	67	66
H=	2,K=	21
-6	60	47
-5	102	95
-4	59	59
-3	173	181
-1	207	208
1	136	140
2	35	40
3	60	64
H=	2,K=	22
-6	127	126
-4	253	249
-3	35	43
-2	357	361
0	333	337
1	40	46
2	198	199
3	66	56
4	85	86
H=	2,K=	23
-6	47	43
-5	99	102
-4	80	74
-3	221	220
-2	127	121
-1	301	306
0	146	141
1	261	259
2	110	106
3	145	146
4	48	54
H=	2,K=	24
-5	45	45
-3	42	45
-2	65	68
-1	34	37
0	61	60
1	35	41
3	48	46
H=	2,K=	25
-5	81	83
-4	47	40
-3	123	127
-2	62	52
-1	131	138
0	52	50
1	113	112
2	41	39
3	77	72
H=	2,K=	26
-5	100	101
-3	156	164

counter, and the scan speed accordingly adjusted. The scan speed varied between 2.0 and 8.0 °/min. Background counts were measured at each end of the scan, the summarized counting times being equal to the scan time.

The scan range-limits were 1.0° below $2\theta(\alpha_1)$ and 1.0° above $2\theta(\alpha_2)$. Three test reflections were measured for every 50 reflections. The intensity of these showed no significant change during the measurements of 2547 reflections in

Table 1. Continued.

= 2	80	41	= 4	183	180	= 1	50	38	= 6	39	32	2	46	40	= 6	58	59	= 4	151	151		Me	6,Ke	10							
= 1	162	164	= 3	27	6	0	113	123	= 5	78	70		Me	4,Ke	17	= 5	57	70	= 2	149	155	= 8	40	52								
0	49	42	= 2	282	278	2	62	68	= 4	77	70	= 7	61	55	= 4	76	81	= 1	39	32	= 4	55	52								
1	131	131	= 1	43	35	Me	3,Ke	19	= 3	114	107	= 6	67	57	= 3	84	85	0	103	104	= 3	94	104								
3	70	61	0	241	230	= 6	65	64	= 2	109	106	= 5	98	99	= 2	67	67	Me	5,Ke	20	= 2	69	64								
Me	2,Ke	27	1	38	35	= 4	131	139	= 1	48	49	= 4	137	139	= 1	67	71	0	35	13	= 1	104	110								
= 4	82	87	2	100	100	= 2	225	229	0	98	96	= 3	130	130	0	37	35	Me	5,Ke	21	0	66	60								
= 2	86	84	Me	3,Ke	8	0	236	245	2	56	52	= 2	201	201	1	32	46	= 6	49	40	1	71	69								
0	90	90	= 8	46	46	2	159	163	Me	4,Ke	5	= 1	115	113	2	37	20	= 5	40	40	Me	6,Ke	11								
1	36	36	= 6	94	88	Me	3,Ke	20	= 6	41	50	0	162	164	Me	5,Ke	6	= 4	46	52	= 5	35	29								
2	79	71	= 5	40	44	= 5	160	149	= 6	105	109	1	67	69	= 8	80	75	= 2	49	39	= 4	40	33								
3	41	25	= 4	178	165	= 3	301	288	= 4	197	197	2	76	77	= 6	167	159	Me	5,Ke	22	= 3	59	48								
Me	2,Ke	28	= 3	60	58	= 2	44	34	= 3	68	73	Me	4,Ke	18	= 5	42	51	= 2	41	44	Me	6,Ke	12								
= 1	41	54	= 2	292	272	= 1	387	382	= 2	256	246	= 4	38	57	= 4	279	275	= 1	38	37	= 6	35	36								
Me	2,Ke	29	0	294	279	0	58	49	= 1	96	102	= 2	67	78	= 3	40	48	0	40	38	= 8	52	67								
= 1	38	36	2	177	175	1	324	316	0	194	191	0	72	83	= 2	334	326	Me	5,Ke	23	= 4	55	59								
1	40	36	4	84	83	3	176	175	1	83	80	1	64	61	0	241	240	= 3	45	39	= 3	47	62								
Me	2,Ke	30	Me	3,Ke	9	Me	3,Ke	21	2	111	110	2	62	63	2	119	119	= 1	35	38	= 2	58	62								
= 2	36	27	= 7	43	47	= 6	94	83	3	44	43	3	43	55	Me	5,Ke	7	Me	5,Ke	24	= 1	35	41								
0	62	53	= 6	119	120	= 3	144	143	4	53	53	Me	4,Ke	19	= 8	62	58	= 4	39	9	0	39	39								
Me	2,Ke	31	= 3	190	188	= 2	57	48	Me	4,Ke	6	= 6	170	170	= 7	39	34	= 3	48	42	Me	6,Ke	13								
= 2	76	80	= 2	28	11	= 1	144	159	= 5	73	70	= 4	87	81	= 6	121	116	= 1	40	34	= 6	42	53								
0	75	76	= 1	147	141	0	37	44	= 4	31	26	= 3	280	253	= 5	59	58	Me	5,Ke	25	Me	6,Ke	15								
Me	3,Ke	0	1	31	33	1	116	117	= 3	115	107	= 2	116	113	= 4	178	182	= 2	37	30	= 5	45	30								
= 6	32	28	2	35	38	3	69	60	= 1	79	77	= 1	258	260	= 3	87	81	Me	5,Ke	26	= 3	42	28								
= 4	158	162	Me	3,Ke	10	Me	3,Ke	22	0	61	66	0	86	90	= 2	200	200	= 3	49	32	= 2	39	43								
= 2	304	307	= 6	71	72	= 6	83	48	1	31	22	1	177	161	= 1	85	87	Me	6,Ke	9	Me	6,Ke	16								
0	276	277	= 5	78	84	= 5	110	110	2	58	67	2	44	42	0	149	145	= 8	63	76	= 2	39	28								
2	125	128	= 4	213	206	= 4	58	59	4	37	35	Me	4,Ke	20	1	84	66	= 6	109	109	Me	6,Ke	17								
4	44	41	= 3	191	206	= 3	116	112	Me	4,Ke	7	= 6	140	145	2	70	72	= 4	145	146	= 6	53	45								
Me	3,Ke	1	= 2	354	341	= 2	33	32	= 4	79	76	= 5	70	79	Me	5,Ke	8	= 2	167	166	Me	6,Ke	18								
= 6	73	78	= 1	254	270	= 1	84	71	= 3	37	42	= 4	217	226	= 6	56	57	0	149	142	= 5	56	54								
= 5	89	88	0	292	284	1	45	39	= 2	118	121	= 3	123	136	= 5	36	43	Me	6,Ke	1	= 3	70	71								
= 4	247	252	1	171	168	Me	3,Ke	23	= 1	45	47	= 2	230	242	= 4	70	68	= 8	45	42	= 1	51	59								
= 3	198	199	2	139	138	= 6	49	56	0	112	112	= 1	123	128	= 3	45	60	= 6	84	80	Me	6,Ke	19								
= 2	332	332	3	73	79	= 5	33	31	2	74	66	0	156	166	= 2	64	55	= 4	102	102	= 4	49	44								
= 1	260	265	4	49	51	= 4	89	95	Me	4,Ke	8	1	61	67	= 1	88	96	= 3	37	31	Me	6,Ke	20								
0	121	116	Me	3,Ke	11	= 3	36	35	= 7	41	43	2	81	80	0	49	41	= 2	86	85	= 4	68	57								
1	172	169	= 7	76	80	= 2	93	101	= 5	50	43	Me	4,Ke	21	1	98	99	= 1	42	40	= 2	73	61								
2	45	44	= 5	145	145	0	57	54	= 4	44	58	= 4	44	61	2	48	32	0	65	57	Me	6,Ke	21								
3	65	64	= 4	94	103	1	32	21	= 3	30	43	Me	5,Ke	9	1	46	39	= 4	83	73											
4	47	56	= 3	186	184	Me	3,Ke	24	= 2	44	46	= 2	50	57	= 6	39	35	Me	6,Ke	2	= 3	113	101								
Me	3,Ke	2	= 2	136	142	= 5	39	22	Me	4,Ke	9	= 1	57	64	= 5	72	79	= 8	69	71	= 2	93	77								
= 7	62	71	= 1	134	125	= 4	153	146	= 6	94	93	0	42	43	= 4	68	70	= 7	47	57	Me	7,Ke	0								
= 6	65	68	0	84	89	= 3	40	29	= 5	51	53	1	69	67	= 3	111	104	= 6	126	125	= 2	45	36								
= 5	117	114	1	36	34	= 3	154	150	= 4	153	156	Me	4,Ke	22	= 2	81	87	= 5	103	111	Me	7,Ke	1								
= 4	132	135	Me	3,Ke	12	0	93	87	= 3	104	109	= 6	73	77	= 1	88	85	= 4	152	155	= 4	43	37								
= 3	128	128	= 4	87	87	2	34	28	= 2	153	153	= 5	64	52	1	47	50	= 3	140	138	= 2	53	46								
= 2	166	170	= 2	163	156	Me	3,Ke	25	= 1	136	142	= 4	85	90	Me	5,Ke	10	= 2	128	126	Me	7,Ke	3								
= 1	92	98	0	120	116	= 3	45	52	0	80	86	= 3	97	90	= 5	50	61	= 1	102	106	= 1	67	55								
0	112	114	Me	3,Ke	13	= 2	36	24	1	79	84	= 2	82	85	= 3	54	59	0	67	77	Me	7,Ke	4								
1	88	83	= 7	55	48	= 1	35	43	2	34	34	= 1	99	88	Me	5,Ke	11	1	63	56	= 7	48	38								
2	33	34	= 6	94	94	Me	3,Ke	26	Me	4,Ke	10	0	69	71	= 6	85	83	Me	6,Ke	3	= 6	46	50								
3	83	78	= 4	86	85	= 5	66	72	= 6	36	33	1	57	52	= 4	73	74	= 7	133	135	= 5	45	53								
5	58	56	= 3	148	138	= 3	80	75	= 5	48	34	2	60	49	= 3	135	136	= 5	232	229	= 4	44	43								
Me	3,Ke	3	= 2	133	129	= 2	34	17	= 4	84	85	Me	4,Ke	23	= 2	129	124	= 3	264	262	= 3	55	48								
= 7	38	43	= 1	137	136	1	37	24	= 3	88	77	= 5	40	35	= 1	112	125	= 1	195	186	Me	7,Ke	7								
= 6	71	73	0	98	91	Me	3,Ke	27	= 1	84	75	= 3	38	35	0	82	93	1	74	84	= 6	61	59								
= 5	53	58	1	94	98	= 5	37	27	4	36	21	Me	4,Ke	25	1	66	71	Me	6,Ke	4	= 5	43	27								
= 4	162	163	3	89	54	= 3	45	29	Me	4,Ke	11	= 3	42	34	Me	5,Ke	13	= 7	36	18	= 4	51	43								
= 3	51	57	Me	3,Ke	14	0	38	19	= 7	66	66	= 1	51	49	= 7	40	46	= 6	34	40	Me	7,Ke	8								
= 2	290	283	= 7	46	39	Me	3,Ke	29	= 5	100	101	Me	4,Ke	28	= 5	53	55	= 5	36	4	= 5	59	59								
= 1	63	59	= 6	36	37	= 4	41	42	= 3	94	89	= 2	59	37	= 4	53	51	= 4	66	62	Me	7,Ke	9								
0	307	297	= 6	68	62	= 2	61	56	= 2	71	68	= 1	38	6	= 3	41	34	= 2	63	69	= 6	49	36								
1	65	74	= 4	74	82	0	52	51	0	95	98	Me	5,Ke	0	= 2	79	78	= 1	39	39	= 4	40	38								
2	187	184	= 3	79	75	Me	3,Ke	30	2	61	67	= 4	58	51	0	62	58	1	36	46	= 3	37	44								
3	66	63	= 2	122	133	= 3	36	31	Me	4,Ke	12	= 2	70	68	Me	5,Ke	14	1	52	46	Me	7,Ke	10								
4	83	84	= 1	88	77	= 2	88	98	= 8	40	30	Me	4,Ke	1	= 4	36	54	Me	6,Ke	5	= 6	37	43								
5	58	58	0	117	130	= 1	60	62	= 8	82	69	= 6	55	50	= 2	63	64	= 7	77	85	= 5	36	36								
Me	3,Ke	4	1	70	64	0	105	102	= 5	48	63	= 4	81	83	= 1	37	46	= 6	71	68	= 4	39	33								
= 6	38	22	2	69	84	Me	4,Ke	0	= 4	111	115	= 3	104	101	0	74	84	= 5	117	120	= 3	40	42								
= 7	100	106	3	37	38	= 6	46	46	= 3	62	81	= 2	103	103	1	43	39	= 4	100	97	Me	7,Ke	11								
= 5	243	243	4	39	47	= 2	81	85	= 2	109	108	= 1	97	99	2	42	55	= 3	137	133	= 5	56	53								
= 4	59	61	Me	3,Ke	15	0	136	136	0	52	54	0	52	53	Me	5,Ke	15	= 2	68	73	= 3	48	48								
= 3	505	495	= 6	66	68	2	109	104	Me	4,Ke	13	1	50	49	= 7	52	48	= 1	115	121	= 2	34	20								
= 2	110	108	= 4	111	109	4	60	51	= 5	64	67	Me	5,Ke	2	= 6	41	34	1	98	88	Me	7,Ke	12								
= 1	629	605	= 3	43	33	Me	4,Ke	1	= 3	103	107	= 5	39	32	= 5	55	65	Me	6,Ke	6	= 4	78	81								
0	125	128	= 2	156	157	= 7	36	38	= 2	31	31	= 3	103	108	= 4	48	41	= 7	58	57	= 2	89	87								
1	372	369	= 1	73	70	= 6	46	41	= 1	110	110	= 2	80	92	= 3	54	41	= 6	49	57	Me	7,Ke	13								
2	85	90	0	174	174	= 5	60	63	0	66	64	= 1	149	151	= 1	43	41	= 5	103	105	= 4	49	63								
3	141	140	1	85	74	= 3	82	75	1	68	69	0	45	46	Me	5,Ke	16	= 4	71	73	= 2	57	60								
4	50	48	2	134	132	= 2	136	138	2	46	45	1	109	111	= 7	91	95	= 3	136	137	Me	8,Ke	0								
5	48	42	3	48	48	= 1	51	53	Me	4,Ke	14	3	52	50	= 6	59	67	= 2	41	50	8	106	112								
Me	3,Ke	5	4	77	72	0	190	189	= 4	36	34	Me	5,Ke	3	= 5	135	144	= 1	99	109	Me	8,Ke	2								
= 5	88	88	Me	3,Ke	16	2	116	115	= 2	48	41	= 8	73	80	= 4	75	85	1	52	54	= 8	41	52								
= 4	79	82	= 6	130	133	4	48	44	0	48	43	= 7	72	69	= 3	132	139	Me	6,Ke	7	8	56	52								
= 3	219	217	= 4	224	233	Me	4,Ke	2	2	39	40	= 6	169	172	= 2	67	79	= 7	39	23	Me	8,Ke	4								
= 2	158	148	= 2	326	332	= 5	77	79	Me	4,Ke	15	= 5	116	118	= 1	69	77	= 6	111	114	= 6	40	11								
= 1	291	283	0	305	325	= 3	81	80	= 7	36	27	= 4	283	289	0	85	86	= 5	34	37	Me	8,Ke	8								
0	125	119	2	214	221	= 2	50	48	= 6	46	44	= 3	159	164	Me	5,Ke	17	= 4	146	149	= 6	49	33								
1	173	178	4	119	118	0	47	47	= 5	74	69	= 2	320	329	= 7	59	51	= 2	129	130	Me	8,Ke	14								
2	33	32	Me	3,Ke	17	1	102	106	= 4	42	46	= 1	162	160	= 6	74	77	0	79	76	= 7	55	47								
3	62	67	= 6	56	49	2	35	30	= 3	103	105	0	235	239	= 5	89	86	Me	6,Ke	8	7	92	47								
Me	3,Ke	6	= 5	53	54	3	88	89	2	45	53	1	97	103	= 4	92	97	= 6	65	67	Me	8,Ke	22								
= 7	59	67	= 4	89	88	Me	4,Ke	3	= 1	80	84	2	120	123	= 3	95	106	= 4	87	91	= 6	66	60								
= 6	61	59	= 3	92	101	= 6	59	62	0	58	54	3	54	45	= 2	67	77	= 3	40	34	6	69	60								
= 5	164	169	= 2	92	93	= 5	69	72	2	41	37	Me	5,Ke	4	= 1	81	93	= 2	70	74	Me	8,Ke	24								
= 4	77	69	= 1	107	116	= 4	145	144	Me	4,Ke	16	= 8	78	79	0	33	37	Me	6,Ke	9	= 6	37	28								
= 3	265	254	0	43	46	= 3	126	131	= 7	63	54	= 6	135	133	1	55	61	= 7	51	50	Me	8,Ke	30								
= 2	83	87	1	68	70	= 2	226	230	= 6	84	79	= 4	179	174	Me	5,Ke	18	= 6	88	91	= 4	48	38								
= 1	197	190	Me	3,Ke	18	= 1	128	124	= 5	111	104	= 3	101	106	= 5	40	42	= 5	70	74	4	92	38								
0	75	67	= 7	44	50	0	210	207	= 4	134	124	= 2	173	169	= 4	44	47	= 4	111	120	Me	8,Ke	36								
1	85	84	= 6	99	101	1	69	66	= 3	160	155	= 1	152	148	= 3	66	68	= 3	80	82	= 1	71	47								
2	68	71	= 5	88	86	2	122	119	= 2	142	131	0	138	128	= 1	80	88	= 2	93	108	Me	1,Ke	0								
4	55	56	= 4	148	153	3	44	23	= 1	153	151	1	90	94	1	63	66	= 1	62	66	= 6	61	65								
Me	3,Ke	7	= 3	88	86	4	56	51	0	96	88	2	89	84	Me	5,Ke	19	0	48	69	Me	1,Ke	2								
= 6	68	87	= 2	157	168	Me	4,Ke	4	1	94	91	Me	5,Ke	5	= 6	97	97	1	43	38	= 8	53	40								

Table 1. Continued.

Hm	1,Km 3	-1	88	38	Hm	3,Km 16	Hm	4,Km 15	-1	48	51	-9	60	60	Hm	6,Km 24	-1	95	87					
-8	41	48	1	47	41	-8	60	68	-8	51	35	Hm	5,Km 3		Hm	6,Km 7	-4	68	75	Hm	6,Km 2			
Hm	1,Km 12	Hm	1,Km 36		Hm	3,Km 18	Hm	4,Km 19	4	92	51	-8	65	65	-2	94	88	-6	82	74				
-8	42	23	0	40	33	-8	42	51	-7	88	86	Hm	5,Km 4		Hm	6,Km 9	Hm	6,Km 25	-3	84	78				
Hm	1,Km 19	Hm	2,Km 22		Hm	3,Km 19	3	87	91	4	86	46	-8	43	49	-2	84	41	Hm	8,Km 3				
8	40	43	5	45	33	4	66	78	Hm	4,Km 21		Hm	5,Km 8		Hm	6,Km 18	Hm	7,Km 8	-6	86	88				
Hm	1,Km 23	Hm	2,Km 30		Hm	3,Km 20	3	53	51	3	73	66	-6	41	30	-7	43	44	-4	60	69				
8	69	62	2	69	58	-7	71	68	Hm	4,Km 29		Hm	5,Km 16		Hm	6,Km 21	Hm	7,Km 12	-2	53	61				
Hm	1,Km 26	Hm	2,Km 33		Hm	3,Km 22	-4	84	52	-8	42	38	-6	39	44	-6	38	54	Hm	8,Km 9				
8	82	31	-3	82	84	-7	78	69	-2	63	97	Hm	5,Km 24		-5	91	79	0	56	61	-3	46	27	
Hm	1,Km 33	-1	69	62	Hm	3,Km 24	Hm	4,Km 30	-6	54	28	-1	88	84	Hm	7,Km 13	Hm	8,Km 10						
-8	55	52	Hm	2,Km 34	-6	97	91	-4	81	71	Hm	5,Km 25		0	62	50	-6	39	40	-6	87	74		
1	81	70	-3	66	62	Hm	3,Km 30	-2	102	81	1	54	40	Hm	6,Km 23		Hm	8,Km 1	-4	113	98			
Hm	1,Km 34	-1	57	59	-4	59	66	-1	62	32	Hm	6,Km 0		-5	64	58	-7	99	92	-2	104	86		
-3	51	45	0	46	39	1	48	47	0	75	61	2	92	86	-3	74	62	-5	132	125	Hm	7,Km 13		
-1	64	56	1	49	42	2	63	66	Hm	4,Km 32		Hm	6,Km 3		-1	53	47	-3	135	123	-6	39	40	
Hm	1,Km 35																							

Table 2. Fractional atomic coordinates for non-hydrogen atoms, anisotropic thermal vibration parameters and their estimated standard deviations (multiplied by 10^5). The temperature factors are expressed as:
$\exp-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)$

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
O1A	34866	12195	23468	2947	96	4055	178	4271	70
	34	7	34	72	3	82	27	127	26
O4A	93700	−4462	23582	3030	90	3874	177	4008	−4
	41	7	36	81	3	83	27	136	26
O1B	68125	41747	24385	3645	99	3763	−207	4255	−10
	38	7	37	85	3	76	26	136	25
O4B	33424	21535	21341	3644	99	4609	−117	4199	47
	41	8	40	91	3	98	29	154	29
N4A	98096	311	24160	2570	108	2721	74	2807	33
	39	10	37	87	4	79	29	142	28
N4B	54777	22982	25803	3102	116	3325	−47	2948	53
	49	10	45	105	4	95	34	165	30
C1A	49883	9414	24594	2380	87	2257	−1	2511	−42
	48	10	46	102	4	90	34	163	31
C2A	47018	4269	25472	2420	96	3164	−110	3577	−28
	54	11	51	112	5	110	38	188	36
C3A	62275	1233	25468	2576	81	2829	−97	2864	−47
	50	11	51	113	4	99	36	175	33
C4A	82401	2917	24958	2017	91	2106	28	2222	35
	47	9	46	93	4	89	32	151	30
C5A	86005	8003	25286	2265	108	2849	−95	3052	73
	54	10	51	108	4	104	37	177	35
C6A	70876	11070	25350	2760	80	2964	−56	3189	68
	51	10	52	111	4	108	35	178	33
C1B	64877	37461	25279	2952	101	2482	−187	2984	−29
	51	10	48	107	4	96	40	166	35
C2B	42669	35650	21389	2897	107	3577	90	3701	107
	59	12	55	119	5	126	42	204	38
C3B	38615	31006	21485	2741	102	3439	−122	3339	6
	57	11	53	124	5	122	38	200	36
C4B	56484	27620	25724	3013	87	2640	−19	2748	39
	56	10	52	117	5	101	38	180	33
C5B	78674	29356	30182	2898	120	4447	116	3503	14
	64	13	62	128	5	152	45	228	42
C6B	82700	33983	30151	2416	122	4203	−117	3338	−45
	59	12	57	112	5	139	40	207	41

a quadrant with $2\theta < 55°$. 1504 unique reflections with intensities larger than $2.0 \times \sigma(I)$ were regarded as observed.

The intensity data were corrected for Lorentz and polarization effects. Atomic form factors were those of Doyle and Turner [6] for oxygen, nitrogen, and carbon, and of Stewart *et al.*[7] for hydrogen. All programs applied during the structure investigations are described in Ref. 8.

CRYSTAL DATA

1,4-Benzoquinone monoxime, $C_6H_5O_2N$, monoclinic, space group $P2_1/c$.
$a = 7.209(3)$ Å, $b = 28.14(1)$ Å, $c = 6.671(3)$ Å,
$\beta = 118.86(3)°$, $V = 1185$ Å^3, $M = 123.11$,
$F(000) = 512$,
$Z = 8$, D_{obs} (flotation) $= 1.37$ g/cm^3, $D_{calc} = 1.380$ g/cm^3.

STRUCTURE DETERMINATION

The structure was solved by the symbolic addition procedure. A preliminary scale factor and an overall isotropic thermal factor ($B = 3.0$ Å^2) were determined using the statistical methods of Wilson.[9] A U-map, computed with 400 reflections with $U \geq 0.110$ revealed the positions of all non-hydrogen atoms in two independent molecules of (I). Fourier and subsequent least-squares refinements of non-hydrogen atomic parameters reduced the conventional R-factor to 0.08. At this stage positional parameters for hydrogen atoms were calculated from stereochemical considerations. Least-squares full-matrix refinements of positional and thermal parameters of all atoms converged with a conventional R-factor of 0.047 and a weighted R-factor ($R_w = (\sum W\Delta^2/\sum WF_o^2)^{\frac{1}{2}}$ of 0.042. The goodness of fit, expressed by $\sum W\Delta^2/(M-n)$ where M is the number of reflections and n is the number of parameters refined, is 2.2.

Table 3. Fractional atomic coordinates ($\times 10^4$) and isotropic thermal parameters with estimated standard deviations for hydrogen atoms.

Atom	x	y	z	B
H2A	3362	326	2567	3.5
	47	9	41	7
H3A	5996	−191	2527	2.9
	43	10	37	6
H5A	9911	909	2531	2.4
	45	9	37	6
H6A	7242	1446	2419	3.5
	43	9	40	6
HOA	10729	−595	2454	4.7
	54	11	47	8
H2B	3137	3797	1826	3.8
	45	10	41	7
H3B	2375	2972	1849	4.2
	52	10	45	7
H5B	9001	2711	3280	5.3
	55	11	50	8
H6B	9737	3520	3328	5.4
	55	11	47	8
HOB	3412	1796	2045	12.8
	78	18	66	1.5

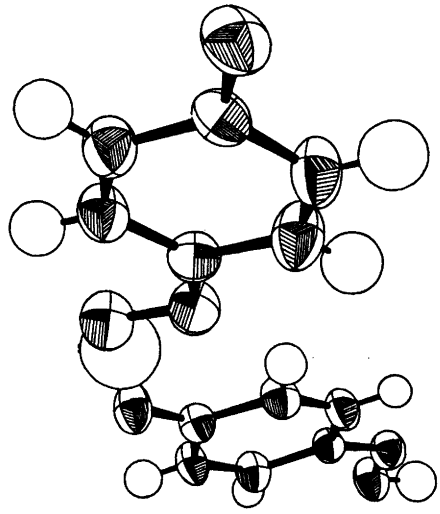


Fig. 1. 50 % probability ellipsoids.

A comparison of observed and calculated structure factors is given in Table 1. Final parameters are listed in Table 2 for non-hydrogen atoms, and in Table 3 for hydrogen atoms. Magnitudes and directions of the principal axes of the vibrational ellipsoids are given in Fig. 1.

The r.m.s. discrepancy between the atomic vibrational tensor components obtained in the structure determination and those calculated from a rigid-body analysis was 0.0028 Å^2 for molecule A and 0.0023 Å^2 for molecule B.

The translational r.m.s. amplitudes of vibration along the principal axes are 0.20, 0.19, and 0.19 Å for A and 0.21, 0.21, and 0.20 Å for B. The r.m.s. librational amplitudes are 6.8, 3.7, and 2.1° in A and 8.7, 3.5, and 2.5° in B. The coordinates were adjusted according to this

Table 4. Bond lengths (Å) and angles (°).

Bond lengths

Distance	(Å)	Distance	(Å)	Distance	(Å)
O1A–C1A	1.2428(31)	O4B–N4B	1.3623(34)	O1A–HOB	1.6356
O1B–C1B	1.2328(32)	C1A–C2A	1.4658(40)	N4A–C4A	1.3021(33)
O4A–N4A	1.3713(31)	C3A–C4A	1.4409(40)	C1A–C6A	1.4518(40)
N4B–C4B	1.3103(34)	C2B–C3B	1.3353(41)	C4A–C5A	1.4495(38)
C2A–C3A	1.3290(42)	O4B–HOB	1.0094	C1B–C2B	1.4601(43)
C5A–C6A	1.3297(40)			C4B–C5B	1.4401(46)
C1B–C6B	1.4466(42)				
C3B–C4B	1.4393(41)				
C5B–C6B	1.3296(45)				

Hydrogen bond lengths

O1A–O4B	2.6319(28)
O1B–O4A(a)	2.7000(32)

Bond angles

Angle	(°)	Angle	(°)
O1A–C1A–C6A	122.20(25)	O1A–C1A–C2A	120.48(25)
C1A–C2A–C3A	121.27(28)	C2A–C3A–C4A	120.79(27)
C3A–C4A–C5A	118.27(25)	C4A–C5A–C6A	121.37(28)
C5A–C6A–C1A	120.78(27)	C6A–C1A–C2A	117.31(25)
C3A–C4A–N4A	126.52(24)	N4A–C4A–C5A	115.22(25)
C4A–N4A–O4A	112.84(23)	O1B–C1B–C2B	121.25(28)
O1B–C1B–C6B	122.03(30)	C1B–C2B–C3B	121.97(33)
C2B–C3B–C4B	120.02(32)	C3B–C4B–C5B	118.66(29)
C4B–C5B–C6B	121.22(34)	C5B–C6B–C1B	121.34(34)
C6B–C1B–C2B	116.72(29)	C3B–C4B–N4B	126.57(32)
N4B–C4B–C5B	114.76(31)	C4B–N4B–O4B	112.30(23)

Dihedral angle	(°)	Dihedral angle	(°)
C3A–C4A–N4A–O4A	−.68(46)	C5A–C4A–N4A–O4A	179.14(23)
C4A–N4A–O4A–HOA	174.15	C2A–C1A–O1A–HOB	174.66
C3B–C4B–N4B–O4B	.21(48)	C5B–C4B–N4B–O4B	179.52(29)
C4B–N4B–O4B–HOB	−174.37	C2B–C1B–O4A–HOA	9.65(24)

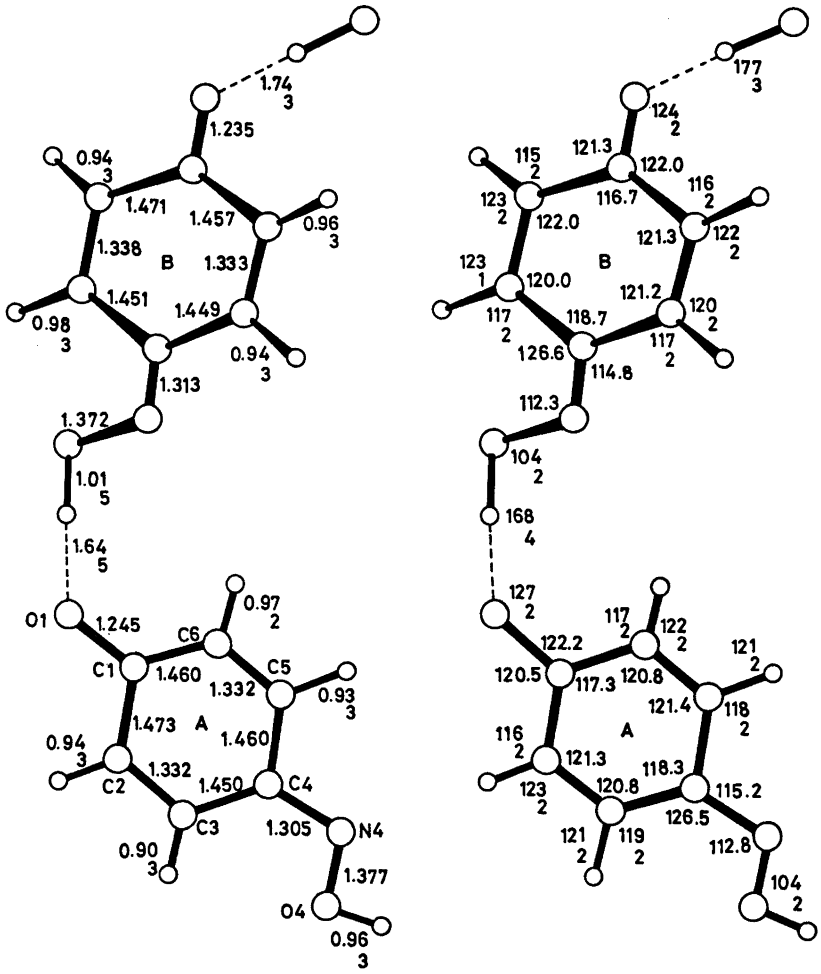


Fig. 2. Bond angles and bond lengths (corrected).

libration. Uncorrected bond lengths and angles are given in Table 4. The bond lengths corrected for the librational effects and angles may be found in Fig. 2. Estimated standard deviations were calculated from the correlation matrix. Standard deviations are 0.004 Å in carbon–carbon bond lengths, 0.003 Å in carbon–nitrogen, carbon–oxygen and nitrogen–oxygen bond lengths, and 0.3° in angles involving non-hydrogen atoms. Deviations from least-squares planes are given in Table 5.

DISCUSSION

The packing of molecules in the crystal is shown in Fig. 3.

Refining of hydrogen atom parameters and the final bond lengths involving non-hydrogen atoms showed that the two independent molecules both were oximes. All A-molecules are situated near planes parallel to the ab planes at $Z = 1/4$, 3/4 whereas the B-molecules have a tilt of 12° to these planes.

Owing to two O4H···O1 hydrogen bonds, the molecules are forming chains along the screw axes. The repeating unit along these chains is one A- and one B-molecule. Close-packing and normal van der Waals contacts are found in the direction of the a and c^* axes.

The hydrogen bond lengths are quite normal. Interestingly, the hydrogen bond crossing the screw axes is substantially longer (0.07 Å) than

Table 5. Deviations (in Å) of atoms from least-squares planes through the atoms C1A, C2A, C3A, C4A, C5A, C6A, and C1B, C2B, C3B, C4B, C5B, C6B.

Plane A				Plane B			
C1A	−0.0301	O1A	−0.095	C1B	−0.0164	O1B	−0.0613
C2A	−0.0166			C2B	0.0087		
C3A	0.0094			C3B	0.0048		
C4A	−0.0219	O4A	−0.123	C4B	−0.0108	O4B	−0.0710
C5A	0.0075	O4A	−0.078	C5B	0.0025	N4B	−0.0496
C6A	0.0185			C6B	0.0111		

The angle between planes A and B is 12.6°.

the other hydrogen bond. Hadzi (1956)[10] observed a splitting of the νOH band of about 150 cm^{-1} in IR spectra from (I) in the solid state. Probably this splitting is explained by the presence of two different hydrogen bonds in the structure. Packing effects are probably causing the difference between the two bonds. According to investigations by Craven *et al.*[11] of hydrogen bonding effects on the molecular structure, the hydrogen bonds are probably causing the slight difference between the two C1 – O1 and the two N4 – O4 bond lengths. These differences are significant while other differences between corresponding bond lengths are not significant.

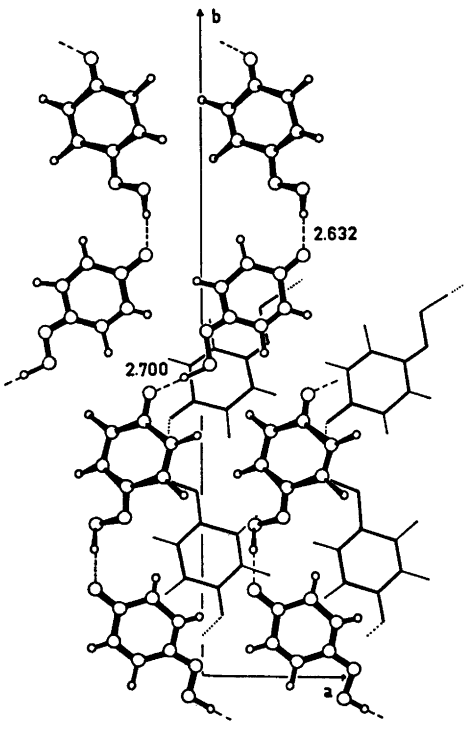


Fig. 3. Packing of molecules. The view is down c^*.

The bond lengths and angles in (I) are of the same order as corresponding bond lengths and angles in (II) and (III), and the similarity between (I) and the cation of *N,N*-dimethyl-*p*-nitrosoaniline hydrochloride [3] is remarkable. No significant differences are found between corresponding bond lengths and angles in (I) and this last oxime. Even the slight (but significant) difference between the C1 – C2 and the C1 – C6 bond lengths is found in both structures.

A comparison of (I) and 1,4-benzoquinone [12] shows that the C=O and the C=C double bonds are possibly slightly (but not significantly) longer, and the C – C single bonds significantly shorter in (I) than those in 1,4-benzoquinone.

The CN bond lengths [1.302(3) Å and 1.310(3) Å] are significantly longer than the corresponding bond lengths in formaldehyde oxime [13] [1.276(5) Å] and 1,4-cyclohexandione dioxime [14] [1.276(3) Å]. Accordingly the NO bond lengths [1.362(3) and 1.373(3) Å] are significantly shorter than those of formaldehyde oxime and 1,4-cyclohexandione dioxime [1.408(5) and 1.411(3) Å, respectively]. The CN and NO bond lengths in these last two oximes are pure double and single-bond bond lengths.[15]

Thus, the difference between (I) and 1,4-benzoquinone and the last two oximes indicates that the following structure contributes considerably to resonance in (I):

CNDO/2 [16] calculations indicate a considerable degree of delocalisation of π-bonds in (I).

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