Topochemistry. Part XIV.[1] The Crystal Structure of 2,3-Dimethyl-1,4-benzoquinone

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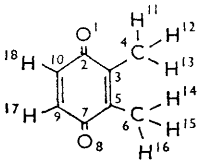
The crystal structure of 2,3-dimethyl-1,4-benzoquinone has been analysed from photographically recorded partial three-dimensional data. Comparison of the (chemically equivalent) bond lengths indicates an accuracy of 0·02 Å in C–C and C–O bond lengths.

THE structure analysis of 2,3-dimethyl-1,4-benzoquinone (I) forms part of our programme on the topochemical control of solid-state reactions. The interpretation of the photochemistry of *p*-quinones, including (I), in terms of the now available crystal structures will be given in Part XV.[2]



(I)

2,3-Dimethyl-1,4-benzoquinone (I). The numbering of atoms used in the present analysis.

EXPERIMENTAL

2,3-Dimethyl-1,4-benzoquinone (I) was prepared by oxidation of *vic*-xylenol (m. p. 75°) with Fremy's reagent,[3] and purified by sublimation at 30°/25 mm. Crystals were grown both by sublimation and by recrystallisation from slowly cooled solutions in methyl acetate. Powder patterns of crystalline materials obtained from thermally quenched solutions in methyl acetate or from rapidly evaporated solutions in diethyl ether were identical with those obtained from crushed single crystals. The cell dimensions determined from zero-level Weissenberg and precession photographs are listed in Table 1.

TABLE 1

Crystallographic constants of 2,3-dimethyl-1,4-benzoquinone. $C_8H_8O_2$, *M* 136·1; m. p. 55°

$a =$ 9·01	$\sigma(a) =$ 0·01	$\beta =$ 118·0°	$\sigma(\beta) =$ 0·2°
$b =$ 12·38	$\sigma(b) =$ 0·01		
$c =$ 7·36 Å	$\sigma(c) =$ 0·02 Å		

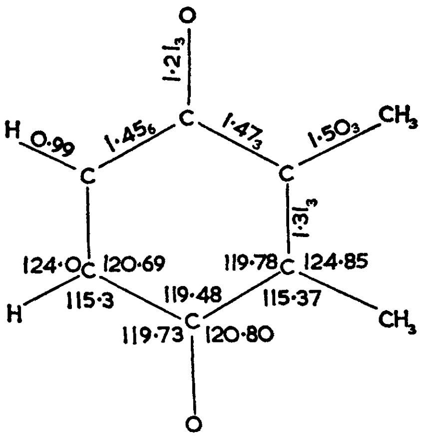
Systematic absences: $h0l$ absent for l odd; $0k0$ absent for k odd.

Space group: $P2_1/c$; $V =$ 724·9 Å^3; d (calc.) ($n = 4$) = 1·25 g./cm.^{3}. F (000) = 288.

The *hkl* ($l = 0, 1, 2, 3, 4$) intensities were recorded photographically with Ni-filtered Cu Kα radiation from a crystal sealed in a Lindemann-glass capillary, and processed as described previously.[4] The structure was solved from the sharpened Patterson projection ^{s}P (xy); [4] the z parameters were established from a trial model built from the x,y parameters after their refinement from the $hk0$ data to $r =$ 0·04. The *hkl* levels were assigned individual scale factors and the merged data refined by the full-matrix least-squares programme until the shifts in all parameters, including the five scale factors, had become smaller than one-sixth of their e.s.d.; at this stage $r[= \Sigma w(k^2F_o{}^2 - |F_c|^2)^2/\Sigma wk^4F_o{}^4]$ and $R[= \Sigma|kF_o - |F_c||/\Sigma kF_o]$ stood at 0·024 and 0·073, respectively. Hydrogen atoms which had been inserted in chemically reasonable positions were refined isotropically throughout. In view of the individual scale factors of the *hkl* levels the value of u_{33} includes an arbitrary constant. Observed and calculated structure factors are listed in Table 2. Standard deviations of all parameters were estimated as described in Part XII,[4] with n (= 771) the number of reflections included in the last refinement cycle, and s (= 127) the number of parameters adjusted. The following scattering-factor curves were used: $f_{C,O}$, Berghuis *et al.*,[5] f_H, McWeeny.[6]

DISCUSSION

Table 3 lists the co-ordinates, in Å, of all atoms in the asymmetric unit referred to the unit cell axes, together with their e.s.d. and the experimental atomic co-ordinates in the system of molecular axes L,M,N; these axes, which coincide with the principal axes of inertia of the heavy-atom skeleton of the molecule, have been computed by a modified Schomaker *et al.* procedure;[7] the components of the three unit vectors L,M,N, referred to the reciprocal cell edges a^*,b^*,c^* are listed in Table 3. The more conventional representation of the "best plane"



2,3-Dimethyl-1,4-benzoquinone. Bond lengths and angles averaged in accordance with molecular symmetry *mm*

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[1] Part XIII, D. Rabinovich, G. M. J. Schmidt, and E. Ubell, preceding Paper.

[2] D. Rabinovich and G. M. J. Schmidt, following Paper.

[3] H.-J. Teuber and W. Rau, *Chem. Ber.*, 1953, **86**, 1036.

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[5] J. Berghuis, IJ. M. Haanappel, M. Potters, B. O. Loopstra, C. H. MacGillavry, and A. L. Veenendaal, *Acta Cryst.*, 1955, **8**, 478.

[6] R. McWeeny, *Acta Cryst.*, 1951, **4**, 513.

[7] V. Schomaker, J. Waser, R. E. Marsh, and G. Bergman, *Acta Cryst.*, 1959, **12**, 600.

TABLE 2

Structure factors

Total number of reflections estimated, 1021; number of unobserved reflections, 256; unobserved reflections included in refinement, 10; zero-weighted reflections, 4; total number of reflections included in refinement, 771; " u " = unobserved; " z " = assigned zero weight.

h	*k*	*l*	F_o	F_c
0	2	0	37·31z	47·37
	4		20·91	−23·04
	6		3·71	−3·74
	8		4·22	−4·31
	10		5·03	5·18
	12		1·68	−1·22
	14		1·39	1·09
1	1		57·51z	65·20
	2		17·89	−17·63
	3		28·13	−27·98
	4		12·11	12·38
	5		14·16	15·00
	6		7·54	7·22
	7		4·94	−4·94
	8		2·85	2·29
	9		1·89	1·98
	10		1·64u	−0·70
	11		2·08	2·40
	12		4·57	−4·63
	13		1·57	1·01
	14		1·37	0·82
	15		2·30	1·73
2	0		27·78	−24·90
	1		5·05	−5·02
	2		34·62	−33·91
	3		1·74	1·34
	4		3·97	3·53
	5		10·68	−10·77
	6		1·52	−1·32
	7		10·33	−10·22
	8		2·34	1·91
	9		6·14	5·99
	10		7·81	8·42
	11		1·69	0·74
	12		1·65u	1·55
	13		1·52u	−1·69
	14		1·60	1·56
	15		1·86	1·52
3	1		16·95	15·55
	2		5·37	−5·31
	3		1·72	0·87
	4		16·24	−16·36
	5		20·51	−19·69
	6		6·77	−6·47
	7		8·57	−8·67
	8		9·23	9·35
	9		10·39	10·12
	10		5·07	5·11
	11		3·14	3·52
	12		1·59u	−0·83
	13		1·43	−1·22
	14		1·46u	−0·28
	15		0·98	0·19
4	0		9·31	9·66
	1		3·55	−3·29
	2		10·13	10·90
	3		12·78	−12·96
	4		1·63	−0·54
	5		3·44	3·72
	6		13·39	−13·37
	7		21·73	20·76
	8		7·88	−8·07
	9		5·20	5·23
	10		1·69u	−0·66
	11		3·04	−2·23
	12		1·49	−0·70
	13		1·29u	−0·24
	14		1·22u	−0·03
5	1		7·27	−7·12
	2		1·99	1·99
	3		3·97	−3·99
	4		1·50	−0·93
	5		1·56	0·87
	6		8·85	8·86
	7		9·92	−10·11
	8		2·08	2·43
	9		7·52	−7·60
	10		3·44	−3·47
	11		1·50u	−0·17
	12		1·32u	0·85
	13		1·30	−0·04
	14		0·59u	−0·51
6	0		5·07	5·05
	1		4·16	−4·13
	2		8·26	−8·92
	3		8·07	−8·39
	4		5·81	−5·28
	5		3·35	−3·51
	6		1·69u	0·00
	7		2·93	−2·48
	8		3·10	−3·32
	9		4·04	−3·96
	10		1·79	1·11
	11		1·29u	0·53
	12		1·27	−0·56
	13		0·63	0·48
7	1		1·69u	1·02
	2		13·48	−13·94
	3		5·08	−4·91
7	4	0	5·98	−6·14
	5		2·91	3·37
	6		1·64u	0·94
	7		1·58u	−0·68
	8		1·49u	0·16
	9		1·36u	0·13
	10		1·45	0·50
	11		1·14u	−0·01
8	0		2·02	−0·54
	1		2·32	−2·49
	2		1·63	−1·92
	3		1·60u	−1·25
	4		2·22	2·48
	5		2·14	1·88
	6		1·43	0·15
	7		1·62	1·54
	8		2·50	−2·25
	9		2·30	1·78
	10		0·70u	−0·14
9	1		1·38	1·13
	2		2·14	2·10
	3		1·31u	0·60
	4		1·76	0·90
	5		1·42u	0·29
	6		1·26	−0·36
10	0		1·88	2·13
	1		1·07u	0·05
	2		2·08	1·90
	3		1·32	−1·23
−10	0	1	4·89	5·06
	1		2·60	−2·56
	2		3·02	2·83
	3		2·49	−1·92
	4		1·20	−0·17
	5		1·04u	−0·48
−9	1		1·51	−0·36
	2		1·49	1·21
	3		1·45	1·49
	4		2·80	2·79
	5		1·32u	0·07
	6		1·23u	0·36
	7		1·35u	0·28
	8		1·12u	0·96
−8	0		1·65u	−0·31
	1		1·65u	−0·09
	2		2·61	2·66
	3		1·64	0·27
	4		1·62	0·94
	5		1·58u	0·84
	6		1·52u	−1·98
	7		1·76	0·91
	8		2·95	2·76
	9		1·17u	1·27
	10		2·84	2·09
−7	1		8·55	8·01
	2		10·42	−10·36
	3		12·55	12·78
	4		8·18	−7·94
	5		2·62	2·36
	6		3·09	3·22
	7		4·86	−4·88
	8		5·81	5·58
	9		1·45	0·85
	10		1·30	0·61
	11		1·34	1·27
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	1		3·11	−2·88
	2		7·72	7·65
	3		4·68	−4·28
	4		14·27	13·75
	5		5·53	−5·44
	6		1·64u	−1·18
	7		2·34	2·55
	8		9·85	−9·69
	9		3·78	3·98
	10		1·51u	−0·56
	11		1·36u	0·82
	12		2·01	1·88
	13		2·24	1·92
−5	1		7·57	−6·85
	2		2·61	−2·54
	3		17·36	−15·68
	4		7·35	6·57
	5		2·75	−2·58
	6		8·68	−9·31
	7		4·08	−3·85
	8		2·60	−1·08
	9		2·62	−2·81
	10		1·63u	−0·19
	11		2·86	2·60
	12		1·37	1·12
	13		2·14	1·43
	14		1·48	1·16
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	1		40·77	−39·51
	2		27·22	−23·21
	3		10·23	9·23
	4		18·35	−17·93
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	6		1·41	1·84
	7		2·37	−1·63
	8		1·58u	0·73
	9		4·19	3·78
	10		1·66u	−0·74
	11		2·56	−2·70
	12		1·84	1·55
	13		1·32u	−0·06
	14		1·30	0·67
−3	1		21·61	−20·57
	2		31·16	−30·73
	3		4·97	4·74
	4		17·92	18·96
	5		6·25	5·96
	6		4·84	−4·86
	7		1·72	1·38
	8		7·82	7·90
	9		8·29	−8·57
	10		8·74	9·13
	11		6·51	−6·44
	12		1·58u	0·57
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	14		1·48	−1·17
	15		1·05u	0·45
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	2		7·99	8·27
	3		25·07	27·09
	4		11·64	−11·66
	5		14·86	−14·59
	6		19·19	−18·68
	7		11·22	−12·59
	8		2·50	−2·61
	9		11·18	11·79
	10		8·23	−8·84
	11		5·99	5·98
	12		3·24	−3·66
	13		1·50u	0·50
	14		2·42	2·41
	15		2·62	−1·95
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	2		4·26	4·38
	3		6·77	−6·72
	4		23·09	−26·02
	5		25·49	−26·98
	6		22·94	−22·82
	7		8·73	−8·29
	8		4·46	−4·22
	9		1·87	2·05
	10		2·80	−2·12
	11		2·87	−2·85
	12		3·06	−3·40
	13		1·52u	−0·41
	14		1·33u	0·21
	15		1·28	0·45
0	0		42·69z	−17·95
	1		5·06	5·06
	2		4·09	−4·18
	3		4·12	−4·38
	4		24·23	27·63
	5		34·18	−36·14
	6		17·46	17·30
	7		3·87	−3·23
	8		1·73	−1·84
	9		3·05	2·89
	10		2·56	2·49
	11		4·23	−4·39
	12		2·00	1·78
	13		1·52u	−0·82
	14		1·32u	−0·47
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1	1		4·44	−4·73
	2		20·11	21·24
	3		5·69	−5·20
	4		6·67	6·56
	5		23·98	24·03
	6		20·60	−21·31
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	13		1·49u	−0·76
	14		1·28	−0·74
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	4		7·86	−8·63
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	6		2·07	−1·68
	7		1·41u	−1·20
	8		1·51u	1·14
	9		10·25	10·70
	10		9·36	9·59
	11		3·69	3·72
	12		1·57	1·28
2	13	1	1·42u	0·21
	14		2·53	−1·96
	15		2·82	−2·26
3	1		19·69	18·88
	2		36·48	−36·42
	3		19·68	19·37
	4		10·58	11·60
	5		7·60	7·04
	6		1·43u	−0·83
	7		3·71	−3·70
	8		2·52	2·09
	9		1·64	0·49
	10		1·66u	0·60
	11		1·61u	−0·03
	12		1·49u	−1·12
	13		1·30	−1·53
	14		1·26u	−0·16
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	3		6·66	6·99
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	7		7·39	−6·86
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7	3		3·03	−2·85
	4		1·60u	0·09
	5		1·55u	0·96
	6		1·49u	0·67
	7		1·40u	−0·23
	8		1·80	1·78
	9		2·94	−2·79
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	2		1·07u	0·61
	3		1·84	−2·00
−10	0		1·63	−2·00
	1		1·62	−1·80
	2		1·58	−1·12
	3		2·64	−2·74
	4		1·76	−0·76
	5		1·62u	0·13
	6		1·42u	0·47
	7		1·08u	−0·32
−9	1		1·96	1·83
	2		3·07	3·84
	3		1·91u	−0·72
	4		1·86	−0·90
	5		3·08	−3·05
	6		1·67	−1·58
	7		1·88	2·43
	8		2·69	−2·44
	9		1·70	1·30
−8	0		2·05	−1·89
	1		12·16	12·56
	2		5·81	5·52
	3		14·73	14·55
	4		2·04u	−0·14
	5		2·01	2·20
	6		2·40	−2·21
	7		1·88u	−0·32
	8		1·74u	1·16
	9		1·57u	−0·76
	10		1·64	−1·09
	11		1·20u	−0·71
−7	1		3·09	3·17
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	3		13·01	12·05
−7	4	2	5·72	5·98
	5		2·05u	−0·15
	6		3·25	2·76
	7		4·07	4·28
	8		4·19	4·55
	9		1·87u	1·37
	10		1·69	1·49
	11		1·80	−1·38
	12		1·39u	−1·32
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	1		1·75	−1·97
	2		8·17	7·71
	3		1·83u	0·80
	4		2·30	−1·28
	5		6·73	−6·44
	6		4·69	4·68
	7		8·91	−8·57
	8		16·50	15·31
	9		2·47	2·34
	10		3·31	3·77
	11		1·74u	1·00
	12		1·84u	−0·42
	13		1·41u	−0·71
−5	1		13·35	−13·54
	2		12·10	11·49
	3		5·25	−5·53
	4		11·24	11·59
	5		7·96	7·73
	6		17·33	−17·91
	7		14·54	13·61
	8		18·13	−17·82
	9		5·24	5·58
	10		2·02u	0·61
	11		1·92u	0·33
	12		1·72	1·16
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	14		1·27u	0·27
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	5		18·76	18·73
	6		16·93	17·25
	7		6·54	−6·23
	8		4·98	−4·50
	9		11·57	−11·94
	10		8·95	−9·20
	11		2·01u	−0·45
	12		1·87u	−0·09
	13		1·64u	0·67
	14		1·60u	0·22
−3	1		29·76	29·85
	2		1·82	1·58
	3		12·14	12·71
	4		1·66	0·81
	5		3·31	−3·47
	6		15·47	16·12
	7		2·14	2·81
	8		2·97	−3·19
	9		9·31	−9·41
	10		5·02	−4·60
	11		4·33	−4·83
	12		2·39	2·69
	13		1·75	−1·63
	14		1·79u	−0·65
	15		1·23	−1·53
−2	1		33·64	30·86
	2		5·16	−5·00
	3		3·43	3·44
	4		1·25u	1·50
	5		13·28	−13·00
	6		3·26	−3·27
	7		2·92	−2·15
	8		3·16	3·14
	9		3·08	−3·20
	10		4·07	−4·24
	11		5·23	5·41
	12		1·98u	−0·07
	13		1·80	2·08
	14		2·17	−2·74
	15		3·01	−2·54
−1	2		19·33	19·30
	3		22·48	21·13
	4		3·56	−3·84
	5		5·12	5·51
	6		3·03	2·92
	7		7·35	7·07
	8		1·80u	0·12
	9		3·06	−2·76
	10		2·03u	0·06
	11		2·05	−1·83
	12		1·99u	0·39
	13		1·83u	0·42
	14		1·56u	−0·00
	15		2·34	−1·62
0	0		93·23	−91·84
	1		4·60	4·64
	2		5·35	5·44

TABLE 2 (*Continued*)

h	*k*	*l*	*F*o	*F*c
0	3	2	2·14	1·77
	4		5·49	5·53
	5		8·54	−8·22
	6		6·60	−6·75
	7		3·79	−3·92
	8		3·90	3·94
	9		1·96u	−1·21
	10		4·99	−5·45
	11		3·24	3·34
	12		1·98u	−1·60
	13		1·80	2·52
	14		1·52	−1·87
	15		3·43	−2·93
1	1		22·48	20·70
	2		1·91	1·77
	3		16·89	17·19
	4		4·31	4·41
	5		3·71	−4·12
	6		14·30	14·33
	7		2·80	2·96
	8		1·90	1·71
	9		7·86	−7·78
	10		5·62	−5·19
	11		5·39	−6·02
	12		1·93	1·91
	13		1·72	−0·90
	14		1·74u	−0·14
	15		1·15	−0·80
2	0		15·96	−15·71
	1		4·21	4·46
	2		7·91	−8·41
	3		9·69	9·21
	4		10·94	9·56
	5		10·52	10·20
	6		18·94	18·51
	7		3·26	−2·90
	8		1·98	−1·82
	9		7·77	−8·14
	10		8·94	−8·92
	11		1·99	−1·98
	12		1·84u	0·03
	13		1·59u	1·15
	14		1·53u	0·60
3	1		8·51	−8·60
	2		8·46	8·69
	3		6·40	−6·88
	4		5·40	5·00
	5		10·12	10·58
	6		16·31	−16·64
	7		14·43	14·53
	8		13·32	−13·48
	9		3·24	2·49
	10		2·00u	0·30
	11		1·88u	−0·11
	12		1·67u	1·08
	13		1·69u	0·63
	14		1·11u	0·58
4	0		5·28	4·94
	1		2·88	−1·84
	2		5·68	6·01
	3		2·30	2·51
	4		1·93u	1·24
	5		3·71	−3·45
	6		5·92	6·59
	7		7·82	−8·03
	8		9·26	9·80
	9		3·14	2·90
	10		1·87	2·30
	11		1·67	1·36
	12		1·73u	0·27
	13		1·24u	−0·36
5	1		2·00	−0·52
	2		7·39	7·36
	3		10·54	9·97
	4		8·06	8·21
	5		2·06u	0·48
	6		2·05u	1·17
	7		2·46	2·41
	8		3·60	3·76
	9		1·80u	0·85
	10		2·54	2·45
	11		1·66u	−0·07
	12		1·17	−1·25
6	0		5·03	−5·09
	1		7·54	7·68
	2		4·09	4·23
	3		11·23	11·40
	4		2·01u	0·66
	5		1·97u	1·37
	6		1·90	−2·07
	7		1·80u	−1·37
	8		1·65u	1·21
	9		1·79u	0·31
	10		1·46u	−0·36
	11		0·76	−0·84
7	1		1·88	0·68
	2		1·86	2·77
	3		1·82u	0·95
	4		1·75	−0·19
	5		2·04	−2·22
	6		1·90	−2·29
	7		1·70	1·92
	8		1·86	−1·56
	9		0·95	0·89
−11	1	3	6·51	−6·60
	2		3·47	−3·53
−11	3	3	1·95u	−1·45
	4		1·64u	−1·14
−10	0		2·61u	0·12
	1		2·59u	0·57
	2		2·56u	−1·00
	3		3·50	3·46
	4		2·36u	−1·11
	5		2·20u	2·19
	6		2·42u	0·05
	7		2·03u	0·19
−9	1		3·01u	−3·01
	2		3·00u	−0·68
	3		3·62	−4·08
	4		2·89u	1·70
	5		2·78u	1·60
	6		2·64	1·63
	7		2·44u	−0·26
	8		2·17u	1·55
	9		5·43	−4·43
	10		1·39u	1·56
−8	0		10·01	−10·59
	1		8·75	−8·81
	2		16·54	−16·28
	3		13·52	−13·80
	4		11·79	−12·12
	5		3·06u	−0·85
	6		5·20	5·10
	7		7·62	7·80
	8		2·70	3·19
	9		3·47	4·13
	10		2·11	−2·67
	11		1·98u	0·58
−7	1		4·12	−4·73
	2		7·21	−7·95
	3		15·23	−15·52
	4		7·43	−7·48
	5		8·43	−8·46
	6		3·11u	−1·04
	7		13·60	12·47
	8		5·20	5·79
	9		5·68	5·80
	10		2·59u	2·16
	11		2·25	−2·13
	12		3·28	2·52
−6	0		2·59	2·61
	1		7·15	−6·94
	2		17·94	16·99
	3		2·73	2·90
	4		11·46	10·59
	5		3·58	−3·71
	6		3·70	3·87
	7		8·45	−6·63
	8		7·26	7·07
	9		1·81u	−0·46
	10		2·89	−1·83
	11		2·62u	−0·92
	12		2·25	−2·67
	13		3·19	2·76
−5	1		13·77	15·50
	2		33·81	−34·30
	3		34·39	31·38
	4		8·29	8·08
	5		3·83	4·56
	6		2·84u	−0·37
	7		2·98u	−0·95
	8		4·34	3·81
	9		3·11u	1·66
	10		3·03u	−0·44
	11		2·86u	−0·96
	12		2·54u	−2·42
	13		2·12u	−1·95
	14		1·75	0·13
−4	0		25·16	20·27
	1		28·75	−30·17
	2		18·41	15·73
	3		2·16u	−0·11
	4		2·31	−3·36
	5		6·81	6·58
	6		5·32	−5·63
	7		2·84	−1·01
	8		7·90	7·40
	9		14·62	16·50
	10		11·15	11·23
	11		4·22	4·59
	12		2·73u	1·11
	13		2·36u	−1·10
	14		3·65	−3·24
−3	1		6·21	−6·26
	2		9·79	9·68
	3		2·72	2·78
	4		6·85	6·96
	5		21·07	18·96
	6		23·83	−23·37
	7		12·35	12·47
	8		3·56	3·98
	9		8·89	8·59
	10		14·38	13·81
	11		9·12	9·51
	12		2·84u	1·85
	13		2·50u	−1·34
	14		2·01u	−1·47
−2	0		17·30	−17·83
	1		4·65	4·37
	2		13·29	−9·98
	3		8·96	−8·44
−2	4	3	12·35	11·79
	5		29·54	−31·08
	6		20·94	22·14
	7		10·70	−10·55
	8		2·87	3·36
	9		3·03	2·96
	10		3·09u	0·74
	11		4·33	−4·28
	12		2·89	2·65
	13		2·56u	−1·94
	14		2·09u	−0·88
−1	1		18·82	17·25
	2		9·79	10·80
	3		15·60	−17·24
	4		27·00	−26·46
	5		27·44	−26·98
	6		22·99	−22·33
	7		2·69	−1·42
	8		2·87	3·21
	9		3·03	−2·98
	10		3·09u	−0·88
	11		4·33	−4·53
	12		2·87	−3·18
	13		2·54u	−0·06
	14		2·08u	0·00
0	0		5·81	4·85
	1		12·46	−10·66
	2		9·96	11·27
	3		12·91	−14·54
	4		16·05	−15·53
	5		16·08	16·19
	6		17·41	−16·23
	7		6·50	6·36
	8		2·94	−2·87
	9		12·80	−12·08
	10		12·01	−12·16
	11		7·09	−6·90
	12		3·97	−3·94
	13		2·45u	−1·53
	14		2·39	1·52
1	1		29·25	−24·42
	2		21·22	20·86
	3		7·39	7·07
	4		10·26	−8·70
	5		2·58u	0·01
	6		2·75	1·57
	7		2·91	3·37
	8		7·42	−7·68
	9		6·57	−7·02
	10		8·70	−8·86
	11		7·18	−7·49
	12		2·67	−2·73
	13		2·26	1·51
	14		2·06u	1·40
2	0		27·17	−28·17
	1		31·31	28·74
	2		18·18	−19·24
	3		6·29	5·77
	4		12·71	−12·16
	5		8·85	−8·54
	6		2·92u	−0·73
	7		3·03	1·96
	8		3·79	3·11
	9		4·37	−3·36
	10		2·98u	−1·97
	11		2·76u	0·01
	12		2·44u	1·51
	13		1·97u	−0·20
3	1		10·12	−8·78
	2		6·56	5·96
	3		8·32	−7·37
	4		7·74	−7·67
	5		4·25	−4·15
	6		7·20	7·26
	7		3·79	−3·87
	8		3·08	1·04
	9		3·64	−3·93
	10		2·78	−2·03
	11		2·47u	2·18
	12		2·06u	−1·52
	13		2·20	2·20
4	0		3·68	3·75
	1		5·22	5·63
	2		8·85	9·60
	3		5·73	5·23
	4		12·35	11·94
	5		5·81	6·43
	6		3·09u	−0·82
	7		3·01u	−0·19
	8		8·43	−8·73
	9		5·03	−5·14
	10		2·41u	−1·85
	11		2·47u	−1·55
	12		2·19	2·56
5	1		7·89	6·34
	2		7·25	8·03
	3		11·49	11·43
	4		7·74	8·33
	5		3·64	4·13
	6		2·87u	0·46
	7		2·72	−2·61
	8		5·00	−5·97
	9		2·20u	−0·48
	10		2·22u	−1·65
	11		1·17u	1·39
6	0	3	2·89	−1·61
	1		2·87u	−0·43
	2		2·84	2·36
	3		2·78u	−0·22
	4		2·69	2·20
	5		2·56u	0·22
	6		2·39u	−0·57
	7		2·16u	−2·55
	8		2·89	2·05
	9		1·58	−2·33
−11	1	4	4·09u	3·54
	2		3·95	3·95
	3		3·71u	2·07
	4		3·26	2·16
	5		2·43	0·97
−10	0		4·59u	−2·48
	1		4·56	−5·48
	2		4·51u	−1·29
	3		4·37	−3·70
	4		5·11	4·10
	5		3·90u	1·07
	6		3·54u	0·51
	7		3·68	3·10
	8		2·05u	−3·36
−9	1		5·20	−6·67
	2		23·95	−25·71
	3		5·09	−6·32
	4		11·70	−12·69
	5		4·81	3·87
	6		4·56	−2·26
	7		4·23u	−0·54
	8		3·76u	1·29
	9		3·84	0·39
	10		3·59	1·65
−8	0		7·49	−7·81
	1		12·44	−11·60
	2		16·37	−15·89
	3		12·47	−13·13
	4		6·50	−6·21
	5		5·25	−4·53
	6		5·14	−3·04
	7		6·03	−5·16
	8		7·30	−7·88
	9		4·18	−3·71
	10		4·37u	1·26
	11		3·23u	0·57
−7	1		6·14	−6·74
	2		5·06	−3·83
	3		5·14u	−3·44
	4		6·42	4·24
	5		5·31u	−0·03
	6		13·02	13·17
	7		23·83	−21·41
	8		5·09	5·14
	9		15·15	−16·52
	10		4·34u	−2·83
	11		3·71	−0·74
	12		3·37u	0·52
−6	0		20·10	19·08
	1		9·04	−9·86
	2		10·81	11·48
	3		21·48	−19·69
	4		4·92	−1·96
	5		6·22	3·29
	6		14·77	−15·98
	7		30·28	29·42
	8		19·47	−17·72
	9		11·50	12·83
	10		4·81	−3·47
	11		4·31	−2·03
	12		3·62u	−0·36
	13		3·04u	−0·45
−5	1		3·95	5·13
	2		10·42	−10·31
	3		12·83	−8·13
	4		25·71	−25·62
	5		20·46	−18·90
	6		7·08	−7·21
	7		5·20	−5·91
	8		23·14	22·48
	9		11·83	11·17
	10		7·22	8·32
	11		5·75	6·50
	12		4·12u	−1·43
	13		3·98u	0·04
−4	0		16·34z	−21·84
	1		5·83	−6·25
	2		18·39	−19·22
	3		3·84u	0·89
	4		7·74	−5·44
	5		16·06	−15·13
	6		4·76u	−1·74
	7		5·03u	−2·91
	8		7·41	7·73
	9		12·47	11·45
	10		11·70	11·71
	11		4·92	−2·88
	12		4·40	3·73
	13		3·65u	−1·31
	14		2·99	3·36
−3	1		63·24	67·24
	2		31·33	−31·33
	3		3·51u	−1·85
	4		11·36	9·21
	5		4·26u	0·67
−3	6	4	4·62u	2·38
	7		4·92u	−3·01
	8		7·33	6·37
	9		5·31u	3·45
	10		5·28	−3·46
	11		5·03u	1·98
	12		6·44	−6·88
	13		3·84u	2·48
	14		3·40	1·73
−2	1		26·13	−28·49
	2		46·29	57·47
	3		11·72	−11·61
	4		18·06	−17·61
	5		4·23u	0·56
	6		34·59	−5·53
	7		4·92	−4·26
	8		5·17	−3·63
	9		5·31u	0·88
	10		5·28	4·79
	11		5·03u	−1·89
	12		4·59	0·13
	13		3·87u	0·22
	14		3·46u	2·52
−1	1		54·64	54·23
	2		9·57	−7·40
	3		18·64	−17·92
	4		4·01	1·48
	5		4·37	3·07
	6		4·70	−3·78
	7		4·98	−1·73
	8		5·23u	−1·60
	9		5·31	4·54
	10		5·25u	1·00
	11		7·88	7·15
	12		4·48	4·67
	13		3·76u	2·07
	14		3·21u	−1·28
0	0		3·68u	−2·62
	1		3·73u	2·31
	2		20·88	−19·89
	3		4·09	−4·28
	4		10·20	−8·37
	5		16·04	−15·01
	6		4·89	−1·32
	7		9·59	−9·68
	8		5·28u	2·92
	9		5·31	4·14
	10		13·66	13·20
	11		4·81u	1·74
	12		4·26	4·22
	13		3·46u	−2·15
1	1		12·55	11·97
	2		10·34	−8·58
	3		6·44	−3·05
	4		12·11	−10·97
	5		18·86	−18·32
	6		5·14u	−0·17
	7		12·91	−13·33
	8		8·41	8·67
	9		9·04	8·60
	10		6·06	7·24
	11		5·50	6·55
	12		3·84u	−0·24
	13		3·51u	−1·07
2	0		10·76	10·37
	1		4·84	−5·14
	2		9·79	8·88
	3		10·01	−9·28
	4		5·11	−5·03
	5		11·09	10·79
	6		21·87	−22·28
	7		21·24	21·02
	8		12·22	−12·09
	9		4·98	6·00
	10		4·56	1·14
	11		3·98u	−0·68
	12		3·90u	−0·38
3	1		5·23	−3·33
	2		5·25u	−3·30
	3		6·47	−5·04
	4		5·31u	−2·76
	5		9·21	−7·78
	6		11·14	10·66
	7		13·02	−13·62
	8		4·84u	1·75
	9		4·45	−6·08
	10		3·93	−4·21
	11		3·87u	−1·23
4	1		5·31	−5·10
	2		8·35	−7·33
	3		14·35	−14·02
	4		7·33	−6·48
	5		5·03	−5·33
	6		4·84u	−1·75
	7		4·56	−1·12
	8		4·15u	−2·66
	9		3·62	−5·52
	10		3·48u	−0·57
5	2		11·34	−12·94
	3		4·73	−5·62
	4		7·91	−9·39
	5		4·34	1·65
	6		4·01u	1·79
	7		3·59u	−0·16
	8		3·65	0·32

TABLE 3

Atomic co-ordinates and standard deviations (in Å) referred to axes *a*,*b*,*c*, and L,M,N

Atom	x σ	y σ	z σ	L	M	N
O(1) *	−1·467 (4)	−2·190 (3)	1·416 (4)	2·608	−0·523	0·064
C(2)	−0·502 (4)	−1·347 (4)	1·717 (5)	1·401	−0·494	0·009
C(3)	−0·877 (4)	0·079 (4)	1·458 (5)	0·659	0·771	−0·002
C(4)	−2·548 (5)	0·398 (9)	0·692 (9)	1·512	2·016	−0·041
C(5)	0·206 (4)	0·991 (3)	1·845 (4)	−0·665	0·779	0·002
C(6)	−0·035 (7)	2·470 (6)	1·672 (9)	−1·529	2·000	0·002
C(7)	1·803 (4)	0·545 (4)	2·573 (5)	−1·387	−0·514	0·005
O(8)	2·815 (3)	1·369 (3)	2·987 (4)	−2·603	−0·528	0·042
C(9)	2·157 (4)	−0·862 (4)	2·760 (5)	−0·649	−1·751	−0·044
C(10)	1·093 (5)	−1·757 (4)	2·372 (6)	0·653	−1·758	−0·037
H(11)	−2·96 (6)	−0·49 (5)	0·56 (7)	2·38	1·62	−0·06
H(12)	−2·68 (12)	0·88 (11)	1·13 (13)	1·31	2·45	0·49
H(13)	−2·72 (7)	1·24 (7)	0·33 (8)	1·02	2·74	−0·28
H(14)	0·90 (9)	2·94 (7)	1·91 (8)	−2·47	1·78	−0·13
H(15)	−0·13 (6)	2·84 (6)	2·36 (9)	−1·67	2·32	0·75
H(16)	−0·91 (7)	2·58 (5)	0·81 (7)	−1·08	2·62	−0·48
H(17)	3·31 (5)	−1·13 (4)	3·22 (6)	−1·21	−2·65	−0·09
H(18)	1·22 (3)	−2·67 (3)	2·43 (4)	1·20	−2·50	−0·10

* Refer to diagram for numbering of atoms.

Components of unit vectors L,M,N, referred to the *a**,*b**,*c** axes

Axis	a^*	b^*	c^*
L	−6·1068	−8·4650	0·5887
M	−5·4238	8·9963	−0·0680
N	−3·8042	0·7623	7·3400

can be obtained from the components of the unit vector N: $-3{\cdot}804x + 0{\cdot}762y + 7{\cdot}340z + 1{\cdot}831 = 0$ where x, y, and z are fractional co-ordinates referred to *a*,*b*,*c*; the atomic N co-ordinates give the deviations from the "best plane." No attempt has been made to analyse the thermal parameters of the heavy atoms in terms of rigid-body vibrations because of the indefiniteness in u_{33}.

Bond Lengths and Angles.—Table 4 gives the experimental bond lengths; the averaged e.s.d. of the bond lengths are 0·006 (C–C, C=O) and 0·07 Å (C–H); the e.s.d. of the bond angles are 0·4° (CCC, CCO) and 4° (CCH). Assuming *mm* symmetry in the isolated molecule we have averaged chemically equivalent bond lengths and angles (Figure). We note that the bond scatter in the present structure is greater than the e.s.d. would lead us to expect, and further that the averaged bond lengths here do not compare satisfactorily with those of the 2,6-isomer [4] and of duroquinone.[1] Also, we have not been able to locate the hydrogen atoms of the two methyl groups in reasonable positions, and we must therefore conclude that the accuracy of this structure

TABLE 4

Experimental bond lengths and angles

Bond		Angles	
O(1)–C(2)	1·21 Å	O(1)–C(2)–C(3)	121·8°
O(8)–C(7)	1·22	O(1)–C(2)–C(10)	119·3
C(2)–C(3)	1·47	O(8)–C(7)–C(5)	119·8
C(7)–C(5)	1·48	O(8)–C(7)–C(9)	120·2
C(2)–C(10)	1·47	C(3)–C(2)–C(10)	119·0
C(7)–C(9)	1·44	C(5)–C(7)–C(9)	120·0
C(3)–C(4)	1·51	C(2)–C(3)–C(5)	120·7
C(5)–C(6)	1·50	C(7)–C(5)–C(3)	118·9
C(3)–C(5)	1·33	C(2)–C(10)–C(9)	120·4
C(10)–C(9)	1·30	C(7)–C(9)–C(10)	121·0
		C(2)–C(3)–C(4)	115·2
C(4)–H(11)	0·9$_6$	C(5)–C(3)–C(4)	124·1
C(4)–H(12)	0·7$_1$	C(6)–C(5)–C(3)	125·6
C(4)–H(13)	0·9$_0$	C(7)–C(5)–C(6)	115·6
C(6)–H(14)	0·9$_7$		
C(6)–H(15)	0·8$_3$	H(11)–C(4)–C(3)	100
C(6)–H(16)	0·9$_1$	H(12)–C(4)–C(3)	109
C(9)–H(17)	1·0$_6$	H(13)–C(4)–C(3)	111
C(10)–H(18)	0·9$_2$		
		H(14)–C(6)–C(5)	112
		H(15)–C(6)–C(5)	114
		H(16)–C(6)–C(5)	106
		H(17)–C(9)–C(10)	122
		H(17)–C(9)–C(7)	117
		H(18)–C(10)–C(2)	113
		H(18)–C(10)–C(9)	126

TABLE 5

Intermolecular contacts *

A_{000}	$\bar{A}_{\bar{1}00}$	Å	A_{000}	$\bar{B}_{\bar{1}00}$	Å
C(4)	C(4)	3·58	H(12)	H(14)	2·78
C(4)	H(11)	3·12			
				$B_{0\bar{1}1}$	
	$\bar{A}_{101}$		H(17)	H(15)	2·76
O(8)	H(17)	2·57			
				$\bar{B}_{000}$	
	$B_{\bar{1}\bar{1}0}$		O(8)	C(6)	3·47
O(1)	C(6)	3·49	O(8)	H(15)	2·77
O(1)	H(13)	3·20			
O(1)	H(16)	2·65		B_{001}	
			O(8)	C(10)	3·55
	$\bar{B}_{\bar{1}\bar{1}0}$		O(8)	H(18)	2·79
O(1)	C(10)	3·39			
O(1)	H(18)	2·79			

* Listed are contacts shorter than 3·6 Å for C · · · C, C · · · O, O · · · O, 3·2 Å for C · · · H, O · · · H, and 2·8 Å for H · · · H.

Co-ordinates of equivalent positions	Symbol
xyz	A
$\bar{x}\bar{y}\bar{z}$	$\bar{A}$
$\bar{x}, \frac{1}{2} + y, \frac{1}{2} - z$	B
$x, \frac{1}{2} - y, \frac{1}{2} + z$	$\bar{B}$

A_{pqr} denotes fractional co-ordinates $p + x, q + y, r + z$.

analysis is inferior to that of the 2,6-isomer in spite of the greater volume of data. This difference is partly due to the instability of the 2,3-dimethyl compound during *X*-ray photography, and is perhaps also associated with its low melting point.

Packing Arrangement.—The molecular packing arrangement seen along [001] is shown in Figure 2 of Part XV;[1] intermolecular distances $<3{\cdot}6$ Å are listed in Table 5. Contacts between double bonds and their relation to the photo-behaviour of the solid quinone are discussed in Part XV.

We thank Professor G. M. J. Schmidt for suggesting the problem, and acknowledge support of this work by The National Bureau of Standards, Washington, D.C.

[6/654 *Received, May* 31*st*, 1966]