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The Crystal Structure of 5-Acetoxy-6-methoxy-8-nitroquinoline

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The structure of 5-acetoxy-6-methoxy-8-nitroquinoline was determined from three-dimensional equiinclination Weissenberg data by a direct method. The compound crystallizes in the monoclinic system with space group $P2_1/c$. The cell data are: $a = 7.923 \pm 0.003$, $b = 9.056 \pm 0.003$, $c = 16.694 \pm 0.006$ Å, $\beta = 97.40 \pm 0.02^{\circ}$, $D_x = 1.466$ g.cm⁻³. The bond lengths are in agreement with those calculated by the valence bond theory. A comparison of the observed with the calculated exocyclic bond lengths indicates that only a small amount of resonance interaction occurs between the quinoline ring and the substituent groups. However, the bond lengths of the ring are unaffected by the resonance interaction with the substituent groups in that the observed values agree with theoretical bond distances of the unsubstituted molecule obtained in a recent self-consistent-field molecular-orbital type calculation. The exocyclic COC bond angles average 117° instead of the normal tetrahedral value owing to steric repulsions between some atoms in the methoxy and acetoxy groups and some of those in the ring. Packing and intramolecular steric requirements force the nitro and acetoxy groups to rotate out of the plane of the ring by 59° and 79° respectively. The resonance energy of the acetoxy group is sufficient to maintain its planarity in the overcrowded environment. On the contrary the quinoline ring deviates slightly but significantly from planarity.

Introduction

5-Acetoxy-6-methoxy-8-nitroquinoline (Fig. 1) is a synthetic intermediate in the preparation of 5-hydroxy-6methoxyquinoline, a reference compound for use in a study of 6-methoxyquinoline metabolites (Sax & Lynch, 1966). Its spectral and chemical properties and those of 5-hydroxy-6-methoxy-8-nitroquinoline have been determined (Griffin, Byrne, Sax & Lynch, 1966). The differences in the properties of these compounds suggest a greater diversity in their molecular structures than is implied by the mere replacement of an acetoxy by a hydroxy group. In order to ascertain the structural dissimilarities in these two molecules, both were selected for crystal structure analysis, but only the structure of the acetoxy compound is considered in this paper.

Crystal data

5-Acetoxy-6-methoxy-8-nitroquinoline, $C_{12}H_{10}O_5N_2$, M.W. 262-23 Monoclinic, space group $P2_1/c$

 $a = 7.923 \pm 0.003, b = 9.056 \pm 0.003, c = 16.694 \pm 0.006 \text{ Å}$ $\beta = 97.40 \pm 0.02^{\circ}$

$$D_x = 1.466 \text{ g.cm}^{-3}, D_m = 1.472 \text{ g.cm}^{-3}$$

Z=4

Experimental

Crystals of the acetoxy compound were provided by Dr S. M. Sax of the Department of Pathology, Western Pennsylvania Hospital, Pittsburgh, Pa. The unit-cell dimensions were measured on a Picker full circle diffractometer with Cu K α radiation (1.5418 Å). The X-ray intensity data were collected on multifilm equiinclination Weissenberg photographs with nickel-filtered Cu Ka radiation from crystals rotated about the a and b axes. Both crystals were cut to approximate a

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rectangular parallelopiped in shape. The dimensions of the one that was mounted about the *b* axis were 0.45, 0.55 and 1.15 mm in the \mathbf{a}^* , \mathbf{c} , and \mathbf{b} directions respectively. The dimensions of the crystal rotated about the *a* axis were 0.3 mm in the **b** and \mathbf{c}^* directions and 0.75 mm along **a**. Seven layers were measured on the former and six on the latter crystal. The intensity data were estimated visually by comparison with a standard scale. Interfilm and interlayer scaling of the data were performed on the IBM 1620 computer using a series of programs (University of Pittsburgh Technical Reports, 1963). The Lorentz, polarization, and spot shape corrections were applied but none were made for absorption or extinction. The 1930 observed *F*'s were scaled by a Wilson plot and the signs of 420

normalized structure factors were uniquely determined by a direct method procedure programmed for the IBM 1620 computer (Beurskens, 1963). An *E*-map synthesis gave well-resolved peaks indicating the atomic positions of the molecule. Structure factors calculated with these coordinates (assuming an overall temperature factor of $3 \cdot 0 \text{ Å}^2$) agreed reasonably well at this stage with the observed data, giving a reliability index (*R*) of 0.34.

The entire observed data, except for nine strong low order reflections probably affected by extinction, were included in the full-matrix least-squares refinement using the Busing, Martin & Levy (1962) program. The atomic form factors were taken from *International Tables for X-ray Crystallography* (1962). The Hughes (1941) weighting scheme with $4F_{\min}$ equal to 6.0 was



Fig. 1. Atomic numbering in 5-acetoxy-6-methoxy-8-nitroquinoline.

J



Fig. 2. Molecular packing viewed along normal to the bc plane.



Fig. 3. Molecular packing viewed along the b axis.

Table 1. Observed and calculated structure factors for 5-acetoxy-6-methoxy-8-nitroquinoline

The running index l is listed at the left in each group of reflections having common k and h indices. The other columns are as they follow the l index from left to right, $10F_o$ and $10F_c$.

* - 0									
N- U	H= 0	3 122	107	4 370 364-	2 60 59-	5 144 145	7 188 182	10 117 101-	11 48 48-
4 720	850-	4 77	66	5 115 104	6 142 142	6 81 74	8 112 115-	14 153 148-	12 49 98-
8 213	170-	5 112	100	6 336 344-	8 543 535	7 49 32-	9 239 242	16 187 204-	14 41 45-
10 178	152	6 63	42	7 155 148-	10 122 134-	8 120 123-	10 72 59-	20 26 24	15 102 95-
12 158	150-	7 70	48	8 67 73-	12 343 354-	10 56 54-	11 49 48-	K= 1 H= -2	16 21 13
14 82	85	8 132	119-	9 67 64	14 99 84	11 57 52	12 27 21	1 557 758-	17 50 42-
16 159	165	9 41	33	11 70 66-	18 50 59-	12 124 129-	13 243 263-	2 477 630-	18 67 69
20 25	16-	10 77	74-	13 136 132	20 38 34	13 35 33	14 203 218	3 84 87	Ka 7 Ha -2
K= 1	на о	11 106	103	14 210 223-	Ka 1 Ha al	15 41 41	15 78 82-	4 401 483	2 117 124-
1 459	A73	14 44	41	15 115 124	1 330 400-	16 25 21-	16 74 80	6 136 162-	2 117 127-
2 409	404		24-	17 14 120	1 336 400-	10 29 21-		3 133 132-	3 10 14
2 400	110-	17 24	24-	17 34 36-	2 13 19-	10 22 10	17 31 27-	• 222 222	• /3 /8-
3 202	230-	10 21	23	10 32 32	3 228 224-	K= / H= -1	19 23 22-	7 231 216-	5 63 57
4 6UZ	087	17 110	112	19 25 20-	4 261 255-	1 257 290-	K= 4 H= 2	8 314 307-	8 98 108
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6 92	84	K= 7	н= о	0 153 156-	6 741 832	3 1 26 1 32-	1 87 96	13 41 30	11 48 48
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8 126	101	2 341	339	2 205 215-	8 3 34 321	6 46 34	3 226 228-	15 133 145-	14 36 34
9 307	262	3 144	141-	3 248 247-	9 345 303	7 85 95-	4 203 203-	16 97 100-	16 66 55-
10 211	187	6 145	146	4 261 262	11 91 78	8 40 48	5 214 216-	17 43 44-	K= 8 H= -2
11 69	56	7 59	52-	5 1 52 143-	13 72 73	9 95 117-	6 106 100-	18 53 58-	1 230 239-
12 75	73	9 84	86	6 333 320	14 79 74-	10 154 179	7 24 27	19 25 35	2 212 226
13 152	144-	11 73	78	7 103 86-	15 92 93-	12 42 40	8 62 57	20 28 25	5 156 172
14 88	80-	13 46	47-	8 54 49-	17 130 143-	13 109 88	9 166 171	K3 2 He +2	4 94 103
15 78	72	14 42	57-	9 114 107	18 69 73-	K= 8 d= ~1	10 109 100-	1 200 202-	1 10 11
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6 242	208	1 64	60-	3 154 151	11 294 281	6 47 50	6 87 83-	17 60 57-	2 49 38
7 178	146-	2 36	33-	4 18 19-	12 126 123-	7 35 39	7 53 46-	19 50 43	3 40 32
8 223	209	3 158	150	5 34 34-	13 237 231	8 75 78	8 36 39-	20 73 68-	5 83 79-
9 135	116	5 50	55	6 83 75	14 123 113-	12 45 43-	9 56 57	K= 3 H= -2	9 92 99
10 106	101-	6 55	57-	7 101 106-	16 77 79-	13 27 18	10 32 22	1 143 146	10 37 32-
11 205	181	7 96	107-	9 53 58	17 37 32-	K= 10 H= -1	11 108 113	2 285 305-	Ke 11 He -2
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K= 3	H= 0	1 56	56-	16 49 49	1 395 461	10 29 28	16 28 23	6 163 169	4 66 63-
1 375	382	2 45	40-	K= 6 H= 1	2 415 458	K= 11 H= -1	17 41 39	7 148 155	K= 0 H= 3
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3 546	611	K= 11	н= 0	1 162 185	4 565 646	2 80 80	1 86 88-	9 185 180-	2 585 672
4 419	429	2 137	125-	2 11 12	5 99 85	5 89 85	2 368 620	10 119 124	4 30 41
6 344	348-	3 112	91-	3 149 177	6 1 10 101	6 133 139-	3 89 92-	11 124 124-	A A1 52
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11 85	84	6 230	208	9 35 35-	12 321 320	12 43 33	10 57 37-	20 19 10	1 220 215-
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	142-	12 157	380- 158	11 113 124- 12 39 29-	14 233 233 15 157 165-		14 122 126-	2 294 316-	4 102 91
15 103	142-	10 386 12 157 18 62	380- 158 72-	11 113 124- 12 39 29- 14 47 59-	14 233 233 15 157 165- 16 85 80-	16 150 173- 18 48 48- 20 26 26-	14 122 126- 15 65 61	2 294 316- 3 251 244-	4 102 91 5 117 99-
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	142- 15- 142- 140- 140- 146 146 146 146 146 175- 124 68- 175- 124 68- 29 46- 29 46- 29 40- 175- 124 68- 29 40- 155 155 155 155 155 155 155 15		380- 158 72- H= 1 556 47 71- 177 104 177 104 233 243- 154- 80 1599 549 370- 72- 129- 224- 114 28	11 113 124- 12 39 229- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167- 3 151 167- 3 151 167- 3 151 167- 3 151 167- 6 56 52- 7 76 63- 9 73 894 11 94 121 16 63 75- 16 187- 1 345 394- 1 345 394- 7 55 61 9 43 52- 11 63 52- 7 5 51 61 9 43 52- 11 63 52- 7 5 51 61 9 43 52- 10 77 80- 7 55 61 9 43 52- 10 77 80- 7 55 54 125 55- 3 18 43 6 69 76	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$		$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99- 6 131 32 9 124 102 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 115 126 18 65 64- 19 48 54- K= 9 H= 3 3 38 30- 2 20- 7 163 149- 6 22 20- 7 163 149- 6 20 149- 6 20 149- 10 20 149-
	$\begin{array}{c} 142-\\ 142-\\ 51\\ 40-\\ 31-\\ 546\\ 441\\ 84-\\ 68-\\ 215\\ 37\\ 17\\ 92-\\ 29\\ 41\\ 88-\\ 41\\ 88-\\ 29\\ 41\\ 88-\\ 29\\ 41\\ 88-\\ 29\\ 41\\ 88-\\ 29\\ 41\\ 88-\\ 178\\ 38-\\ 178\\ 38-\\ 178\\ 38-\\ 178\\ 38-\\ 109\\ 109\\ 38-\\ 109\\ 100\\ 100\\ 100\\ 100\\ 100\\ 100\\ 100$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	380- 380- 158 72- 47 104 47 104 182 233- 243- 102 243- 80 64 39- 19- 42- 42- 80 159 64 39- 122- 124- 122- 124- 122- 124- 122- 124- 122- 124- 122- 124- 122- 124-	11 113 124- 12 39 29- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 4 77 83 9 73 88 10 4 65 7 46 46- 8 76 83 9 73 88 11 94 121 16 63 75- K = 8 H = 1 0 167 187- 2 220 250 3 88 87- 4 94 106 7 5 61 9 43 52- 11 63 69- K = 9 H = 1 9 43 55- 11 63 69- K = 9 H = 1 9 43 55- 11 63 69- K = 9 H = 1 8 51- 8 51-	$ \begin{array}{c} 14 & 233 & 233 \\ 15 & 157 & 165 \\ 16 & 85 & 80 \\ 17 & 27 & 77 \\ 18 & 23 & 26 \\ 18 & 23 & 26 \\ 18 & 23 & 26 \\ 18 & 23 & 26 \\ 18 & 23 & 26 \\ 18 & 23 & 26 \\ 18 & 24 & 259 \\ 18 & 24 & 259 \\ 18 & 24 & 258 \\ 18 & 24 & 258 \\ 18 & 24 & 28 \\ 18 & 24 & 28 \\ 28 & 28 & 28 \\ 18 & 24 & 28 \\ 28 & 28 & 28 \\ 28 & 28 & 28 \\ 28 & 28 &$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99 1 31 117 99 7 35 21 7 35 21 9 124 102 9 124 102 9 124 102 9 124 102 104 86 11 104 86 5 44 Ke 2 He 3 14 104 8 54- Ke 2 He 3 3 8 30- 7 163 149- 8 22 20- 7 163 149 9 44 38 6 22 20- 7 163 149- 163 20 9 44 38 107 7 72 11 162 182- 12 4 64 14 113 114- 15 218 248 16 106 104- 16 024
	142 51 400- 186 441- 546 441- 68- 37 75- 124 68- 29 17 88- 29 17 88- 17 53 109- 153 109-		380- 380- 158 72- 42- 47- 177 104 23 244- 23 244- 159 64 63 33 244- 159 64 33 244- 159 64 159 159 159 159 159 159 159 159	11 113 124 12 39 229 14 47 59 K = 7 H = 1 0 307 350 1 93 97 2 84 95 3 151 167 3 151 167 3 151 167 3 151 167 4 94 151 1 943 27 K = 8 H = 87 1 945 394 1 94 51 7 75 51 1 94 51 0 77 85 3 18 43 6 69 76 8 38 51 0 77 85 3 18 43 6 9 76 10 41 51 10 41 51 10 41 51 12 32 12 35 12 45 13 15 13 15 14 15 15 15 16	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99- 6 131 32 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 115 126 18 65 64- 19 48 54- K= 9 H= 3 3 38 30- 2 20- 7 163 169- 6 25 44 33 6 2 2 20- 7 163 169- 6 2 2 10- 1 102 182- 12 1
	$\begin{array}{c} 142-\\ 142-\\ 51\\ 40-\\ 31-\\ 546\\ 441\\ 86-\\ 215\\ 37\\ 175-\\ 129\\ 68-\\ 29\\ 41\\ 08-\\ 29\\ 41\\ 08-\\ 178\\ 30-\\ 178\\ 10-\\ 178\\ 109\\ 101-\\ \end{array}$		380- 380- 158 72- 42- 42- 158 47 71- 177 177 177 122 233 244- 243- 154- 86 66 64 39- 272- 129- 42- 224- 129- 42- 224- 129- 42- 224- 129- 42- 224- 129- 42- 224- 129- 42- 224- 129- 42- 224- 129- 139- 139- 139- 129- 139	11 113 124- 12 39 29- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 4 77 83 6 56 52- 7 46 46- 8 76 83 9 73 88 11 94 121 16 63 75- 8 H = 1 0 167 187- 2 220 250 3 88 87- 4 94 106 7 55 61 9 43 52- 11 63 69- K = 8 69 76 8 36 76 5 38 51- 10 41 51- K = 10 H = 1 10 41 51- 10 51- 10 41 51- 10 51-	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99 7 35 21 7 35 21 7 35 21 9 124 102 9 124 102 9 124 102 9 124 102 11 104 86 11 104 86 5 64- 19 46 54- Ke 2 He 3 3 8 30- 7 163 149- 7 163 149- 8 22 20- 7 163 149- 8 25 30- 9 44 38 10 7 7 22 11 162 182- 12 46 13 114- 13 248 16 64 17 30 24 18 248 16 106 104- 17 30 24 19 16 24- 19 16 24- 10 48- 10 44- 10 48- 10
	142- 51 42- 51 42- 51 400- 186 441 84 68- 37 75 129 68- 29 17- 53 88 29 17- 186 88 29 17- 180- 18- 17- 12- 17- 12- 17- 12- 12- 17- 12- 12- 17- 12- 12- 17- 12- 12- 17- 17- 12- 17- 17- 12- 17- 17- 17- 17- 12- 17- 17- 12- 17- 17- 17- 17- 17- 17- 17- 17- 17- 17- 17- 17- 17- 17- 10- 1		380- 380- 158 72- 42- 158 71- 177 104 123 244 159 64 63 370- 722- 42- 144 28 149 64 800 64 80 159 64 80 159 64 80 159 64 80 159 6133-370- 722 114 28 149 13- 29 143 320- 144 159 13- 20	11 113 124 12 39 229- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 3 151 167 3 151 167 3 151 167 4 94 95 11 94 121 16 63 75- 6 8 H = 1 1 345 334- 7 55 61 187- 1 345 334 7 4 94 106 7 55 61 84 87- 1 63 88 87- 1 63 89 7 7 80- 7 7 80- 7 80 55- 3 18 43 6 69 76 8 38 51- 1 6 3 55- 1 6 3 85 1 7 7 80- 7 7 80- 7 3 84 43 6 69 76 8 38 51- 1 6 4 51- K = 10 H = 1 K = 10 H = 1 H = 1 K = 10 H	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99 7 35 21- 7 35 21- 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 115 126 18 65 64- 19 48 54- Ka 2 He 3 16 22 20- 7 163 169- 6 21 102 182- 12 163 169- 6 21 102 182- 11 102 182- 12 163 169- 6 24- 11 102 182- 11 102 182- 12 163 114- 15 218 248 51- 19 30 24- 11 102 182- 11 102 182- 10 100 100 100- 10 100 100- 10 100 100 100-
	142 105- 51 46 186 186 186 186 481 481 481 481 481 481 481 481	$ \begin{array}{c} 10 & 386 \\ 12 & 157 \\ 18 & 62 \\ 20 & 36 \\ K = 1 \\ 20 & 36 \\ K = 1 \\ 1 & 47 \\ 3 & 80 \\ 4 & 188 \\ 6 & 204 \\ 4 & 188 \\ 6 & 204 \\ 8 & 284 \\ 9 & 287 \\ 10 & 177 \\ 17 & 135 \\ 18 & 54 \\ 9 & 287 \\ 10 & 177 \\ 17 & 135 \\ 18 & 54 \\ 13 & 20 \\ 42 \\ K = 2 \\ 6 \\ 2 & 595 \\ 3 & 148 \\ 5 & 231 \\ 1 & 316 \\ 5 & 231 \\ 1 & 316 \\ 5 & 231 \\ 1 & 316 \\ 5 & 231 \\ 1 & 316 \\ 5 & 231 \\ 1 & 316 \\ 1$	380- 158 72- 42- 158 456 47- 71- 177 177 107 102 23 244- 244- 244- 154- 86 60 60 60 60 64 370- 722- 244- 245- 2	11 113 124 12 39 29- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 4 77 83 9 73 88 9 73 88 11 94 121 16 63 75- 8 H = 1 0 167 187 2 220 250 3 88 487- 4 94 106 7 55 61 9 43 52- 11 63 69- 6 53 55- 16 63 75- 16 63 75- 18 80- 7 5 61 9 43 52- 11 63 69- 7 5 51 8 36 51- 10 41 51- K = 10 H = 1 1 27 35 2 38 40- 1 2 35 4 40- 1 2 7 35 2 3 84 40- 1 2 35 1 3 35	$ \begin{array}{c} 14 & 233 & 233 \\ 15 & 157 & 165 \\ 16 & 85 & 80 \\ 17 & 27 & 77 \\ 18 & 23 & 26 \\ 18 & 23 & 26 \\ 18 & 21 & 59 & 15C \\ 3 & 422 & 459 \\ 4 & 560 & 607 \\ 5 & 254 & 256 \\ 7 & 104 & 113 \\ 4 & 540 & 152 \\ 7 & 104 & 113 \\ 12 & 47 & 277 \\ 12 & 243 & 243 \\ 13 & 240 & 238 \\ 14 & 64 & 57 \\ 15 & 131 & 137 \\ 17 & 65 & 68 \\ 19 & 55 & 48 \\ 20 & 28 & 33 \\ 8 & x & 5 \\ 18 & 27 & 277 \\ 2 & 65 & 51 \\ 18 & 21 & 227 \\ 2 & 65 & 51 \\ 18 & 21 & 227 \\ 2 & 65 & 51 \\ 18 & 21 & 227 \\ 2 & 65 & 51 \\ 18 & 21 & 227 \\ 2 & 65 & 51 \\ 18 & 21 & 227 \\ 2 & 65 & 51 \\ 18 & 21 & 227 \\ 2 & 65 & 51 \\ 18 & 21 & 227 \\ 2 & 65 & 51 \\ 18 & 108 \\ 18 & 108 \\ 18 & 108 \\ 11 & 148 \\ 11 & 148 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 108 \\ 11 & 113 \\ 11 & 108 \\ 11 & 113 \\ 11 & 108 \\ 11 & 1108 \\ 11 $	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 90 1 31 132 9 124 102 9 124 102 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 105 86 14 104 86 14 105 104 14 104 104 104 14 104 104 104 104 104 104 104 104 104 1
	$\begin{array}{r} 142-\\ 105-\\ 51\\ 46\\ 400-\\ 31-\\ 546\\ 186\\ 186\\ 186\\ 186\\ 186\\ 215\\ 175-\\ 92-\\ 175-\\ 92-\\ 175-\\ 92-\\ 175-\\ 92-\\ 175-\\ 105-\\ 105-\\ 101-\\ 20\end{array}$		380- 380- 158 72- 455 71- 177 104 23 244- 159 64 800 63 370- 722- 42- 144 28 149 510- 20-	11 113 124 12 39 29- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 3 151 167 3 151 167 3 151 167 4 94 95 1 94 121 16 63 75- 6 8 H = 1 1 345 334- 7 55 61 187- 1 345 334 7 4 94 106 7 55 61 8 H = 1 9 43 52- 11 63 82 7 7 80- K = 9 H = 1 0 77 80- K = 9 H = 1 0 77 85- 3 18 43 6 69 76 8 38 51- 10 41 51- K = 10 H = 1 K = 10 H = 1 5 2 38 40- 1 5 2 40- 1 5 2 38 40- 1 5 3 38 36- 1 5 3 36- 1 5 3 36- 1 5 3 36 30- 1 5 3 30- 1	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99- 6 131 32 9 124 102 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 115 126 18 65 64- 19 48 54- K= 2 H= 3 3 38 30- 7 163 169- 6 22 20- 7 163 169- 6 22 20- 7 163 169- 8 4 33 6 22 20- 7 163 169- 8 4 22 5 44 33 6 22 20- 7 163 169- 1 102 182- 12 163 169- 1 102 182- 12 163 169- 1 102 182- 12 16 248 10 248 10- 10 248 307 1 348 387
	142 105- 51 46 186 186 186 186 481 481 481 481 481 481 481 481	$ \begin{array}{c} 10 & 380 \\ 12 & 150 \\ 12 $	380- 380- 158 72- 42- 42- 158 47- 71- 177 177 107 102 23 244- 244- 154- 80 150 150 150 150 150 150 150 15	11 113 124 12 39 29- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 4 77 83 9 73 84 9 73 84 9 73 84 11 66 52- 7 46 46- 8 76 83 9 73 88 11 94 121 16 63 75- K = 8 H = 1 0 167 187- 2 220 250 3 86 87- 4 94 106 7 55 61 9 43 52- 11 63 69- 7 6 45 5 61 9 43 51- 10 63 51- 10 63 51- 10 63 51- 10 64 51- K = 10 H = 1 1 27 35 8 36 40- 3 88 36- 4 42- 1 1 42- 1 2 35 1 2 38 40- 3 8 36- 4 42- 1 1 42- 1 3 45 1 2 38 40- 3 8 36- 4 42- 1 4 42- 1 1 42- 1 35 1 2 38 40- 3 8 36- 4 42- 1 4	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99 1 31 117 99 7 35 21 7 35 21 9 124 102 9 124 102 9 124 102 9 124 102 104 86 11 104 86 5 44 14 105 126 18 65 64- Ke 2 He 3 38 30- 7 163 149- 8 22 20- 7 163 149- 8 22 20- 7 163 149- 8 25 30- 9 46 38 107 7 72 11 162 182- 162 51 162 51 17 64 16 64 17 30 24 18 248 16 106 104- 17 30 24 18 64 17 10 24 18 64 18 10 18
	$\begin{array}{r} 142-\\ 105-\\ 51\\ 46\\ 400-\\ 31-\\ 546\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 168\\ 168$		380- 380- 158 72- H= 1 556 47- 177 104 23 244- 23 244- 159 64 370- 722- 42- 243- 159 64 370- 722- 42- 158 149 556 64 370- 72- 42- 158 149 556 64 370- 72- 42- 159 64 370- 72- 42- 159 64 370- 72- 42- 159 64 370- 72- 42- 159 64 159 64 159 64 159 64 159 64 159 64 159 64 159 64 159 64 159 64 159 64 159 64 159 64 159 159 159 64 159 159 159 159 159 159 159 159	11 113 124- 12 39 229- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 3 151 167 4 56 52- 7 46 60- 8 77 63 9 73 99 11 63 75- 6 18 H= 17- 1 345 334- 7 55 61 88 87- 1 345 334- 7 55 61 87- 1 345 334- 7 4 94 106 7 55 61 87- 1 345 334- 7 4 94 106 7 55 61 87- 1 63 89 7 7 80- 7 80- 7 80- 7 80- 7 80- 7 80- 7 80- 8 43 85 1 0 41 51- K= 10 H= 15- K= 10 H= 15- K= 10 H= 15- K= 10 H= 15- K= 10 H= 15- K= 10 H= 15- K= 10 H= 15- K= 10 H= 15- K= 10 H= 15- K= 10	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99- 6 217 99- 8 131 132 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 115 126 18 65 64- 19 48 54- K= 2 H= 3 3 38 30- 7 163 169- 6 22 20- 7 163 169- 6 22 20- 7 163 169- 6 22 20- 7 163 169- 6 22 20- 7 163 169- 8 20 20- 1 102 182- 12 16 248 10 248
	142 102- 51 46 105- 105		380- 380- 158 72- 42- 47- 71- 177 177 102 233 244- 244- 244- 244- 154- 80 150 150 150 154- 80 370- 722- 244- 245- 89	11 113 124 12 39 29- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 4 77 83 9 73 88 9 73 88 11 94 121 16 63 75- 8 76 876 83 9 73 88 11 94 121 16 63 75- 8 76 81 187 2 220 250 2 250 250 1 187 4 94 106 7 55 61 9 43 52- 11 63 69- 7 5 51 10 41 51- 10 41 51- 10 41 51- 10 41 21 12 35 8 30- 6 3 76 - 5 38 40- 3 38 30- 6 41 42- 5 44	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99 1 31 117 99 7 35 21 7 35 21 9 124 102 9 124 102 9 124 102 9 124 102 18 54 14 104 86 5 44 14 104 86 5 44 4 42 5 44 3 38 30 7 163 149 8 22 20 7 163 149 8 22 20 7 163 149 8 44 8 30 9 46 38 10 77 72 11 162 182 16 64 14 103 248 16 106 10 4 17 30 24 18 248 16 106 10 4 17 30 24 18 248 16 106 10 4 17 30 24 18 58 51 17 30 24 18 58 51 17 30 24 18 58 51 19 30 24 18 58 51 19 30 24 18 58 51 19 30 24 18 58 51 19 30 24 18 248 10 248 10 248 10 248 10 248 17 30 24 18 248 10
	$\begin{array}{c} 142-\\ 142-\\ 51\\ 46\\ 40-\\ 31-\\ 546\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 18$		380- 380- 158 72- H= 1 556 471- 177 104 23 244- 243- 159 64 332 44- 159 64 349- 159 64 349- 159 64 349- 129- 42- 42- 129- 42- 14 28 149 63 349- 29- 20- 20- 20- 20- 20- 20- 20- 20	11 113 124 12 39 229 14 47 59 K = 7 H = 1 0 307 350 1 307 350 1 3 4 95 3 151 167 4 77 83 6 56 52- 7 46 60 8 77 80 1 3 4 121 1 63 75- 8 18 H = 1 1 345 334 7 55 61 9 43 52- 11 63 80 7 75 80- 7 78 80 7 78 80 7 80- 7 80- 8 4 10- 8 51- 10 4 151- K = 10 H = 15- K = 10 H = 15- K = 10 H = 15- K = 10 H = 15- K = 10 H = 15- K = 10 H = 15- K = 10 H = 15- K = 10 H = 15- K = 10 H	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99- 6 131 32 9 124 102 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 115 126 18 65 64- 19 48 54- K= 2 H= 3 3 38 30- 7 163 169- 6 22 20- 7 163 169- 6 20 264 K= 3 H= 3 0 263 303 0 263 307 189 8 51- 19 18 24 11- 10 24 11- 10 24 10- 10 24 10- 10 24 10- 10 24 10- 10 24 10- 10 4 10- 10 24 10- 10 24 10- 10 24 10- 10 24 10- 20 24 4 88 85- 20 20- 10 4 10 24 10
	$\begin{array}{c} 142-\\ 142-\\ 51\\ 46\\ 46\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 18$		380- 380- 158 72- 47- 71- 177 177 102 233 244- 244- 244- 154- 80 159 60 60 60 60 60 60 60 60 154- 29- 224- 226- 225- 255- 69 69 69 69 69 69 255- 255- 69 69 69 69 69 69 69 69 69 69	11 113 124 12 39 29- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 4 77 83 9 73 88 9 73 88 11 94 121 16 63 75- 8 76 87- 8 16 7 1 9 42 1 6 53 94- 2 220 250 3 88 87- 4 94 106 7 55 61 9 43 52- 11 63 69- K = 9 H = 1 0 167 187- 2 59 55- 5 18 40- 3 88 51- 10 51- K = 10 H = 1 1 27 35 8 36- 6 44 42- 5 44 42- 5 44 42- 5 44 42- 5 5 51	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99 1 35 117 99 7 35 21 7 35 21 9 124 102 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 105 84 14 104 86 5 44 14 52 14 7 134 K= 2 μ_m 3 3 30 30 7 163 149 7 45 14 22 20- 7 163 149 8 44 8 30 9 46 38 10 77 72 11 182 182- 12 30 9 46 38 10 24 18 248 10 2 48 30 1 30 2 49 30 2 49 30 1 49 8 25 1 102 10 2 49 30 1 49 1 2 40 40 1 102 10 1 1
	$\begin{array}{r} 142-\\ 142-\\ 51\\ 46\\ 40-\\ 31-\\ 546\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 18$		380- 380- 158 72- H= 1 556 471- 177 104- 80 244- 243- 159 64 839- 159 64 839- 159 64 839- 159 64 839- 159 64 839- 159 62- 159 639- 159 64- 122- 122- 159 64- 159 64- 122- 124- 148 135- 135- 149 149 149 149 149 149 149 149	11 113 124 12 39 229 14 47 59 K = 7 H = 1 0 307 350 1 307 350 1 3 51 167 3 151 167 3 151 167 3 151 167 4 94 95 3 151 167 4 94 121 16 63 75 6 56 52- 7 4 94 121 16 63 75- 16 187- 135 394- 7 55 61 187- 135 394 7 55 61 187- 1 35 394- 7 55 61 187- 1 63 88 87- 1 63 89 7 55 85- 3 38 43 6 69 76 8 38 51- K = 10 H = 1 K = 11 H = 1	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99- 6 131 32 9 124 102 9 124 102 9 124 102 9 124 102 104 86 11 104 86 14 105 126 18 65 64- 19 48 54- K= 2 He 3 3 38 30- 7 163 169- 7 163 169- 6 22 20- 7 163 169- 7 163 169- 1 162 122- 1 162 122- 1 162 126 1 163 169 1 161 136 1 164 166 1 166 166 1 166 166 1 166 166 1 166 166 1 166 166
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	$\begin{array}{c} 142-\\ 142-\\ 54\\ 40-\\ 31-\\ 546\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 18$		380- 380- 158 72- 4556 47- 177 104 23 244- 243- 244- 244- 244- 255 244- 159 64 64 80 84 159 64 159 64 159 244- 159 64 159 244- 159 64 159 244- 159 64 159 244- 159 64 159 244- 159 64 159 244- 159 64 159 244- 159 64 159 244- 159 64 159 244- 159 64 159 244- 129- 236-	11 113 124 12 39 229 14 47 59 K = 7 H = 1 0 307 350 1 307 350 1 3 51 167 3 151 167 3 151 167 3 151 167 4 94 95- 3 151 167 4 94 95- 3 151 167 4 94 121 16 63 75- 6 16 187- 1 345 394- 1 345 394- 1 345 394- 1 63 88 87- 1 63 89 7 55 61 187- 1 63 80 7 55 61 85- 2 38 43 6 69 76 8 38 51- 10 41 51- K = 10 H = 1 1 51 42- X = 10 H = 1 1 51 42- X = 10 H = 1 1 53 52- 3 38 35- 4 44 151- K = 10 H = 1 1 51 52 38 40- 1 0 45 15- 2 38 40- 1 0 45 15- 1 0 45 51- 1 1 H = 1 0 67 63 55 50	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99- 6 131 32 9 124 102 9 124 102 9 124 102 9 124 102 10 4 86 11 104 86 11 104 86 14 105 126 18 65 64 3 38 30- 7 163 169- 7 163 169- 7 163 169- 7 163 169- 1 162 162- 12 20- 7 163 169- 8 248- 10 48 51- 19 46 55- 10 248- 10 2
	$\begin{array}{c} 142-\\ 142-\\ 51\\ 40-\\ 31-\\ 546\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 186\\ 18$		380- 380- 158 72- 47- 71- 177 177 102 233 244- 243- 154- 80 159 60 63 64 370- 722- 244- 244- 154- 80 370- 722- 244- 245- 2	11 113 124 12 39 29- 14 47 59- K = 7 H = 1 0 307 350- 1 93 97 2 84 95- 3 151 167 4 77 83 9 73 84 9 73 84 9 73 84 9 73 84 1 94 121 16 63 75- K = 8 H = 1 0 167 187- 2 220 250 3 88 87- 4 94 106 7 55 61 9 43 52- 11 63 69- 7 40 40- 1 63 69- K = 9 H = 1 1 27 35 8 40- 3 88 51- 10 41 51- 1 27 35 8 36 7 3 51 K = 11 H = 1 1 27 65 3 15 K = 11 H = 1 1 4 22 5 44 46 6 70 68- 7 33 51 K = 11 H = 1 1 K = 10 H = 1 1 4 27 5 5 51 K = 11 H = 1 1 6 7 5 5 51 K = 11 H = 1 1 6 7 6 3 35 5 55 5 51 K = 11 H = 1 1 6 7 6 5 3 51 51 K = 11 H = 1 K = 10 H = 1 K = 11 H = 1 K = 10 H = 1 K = 10 H = 1 K = 10 H	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3 102 102 4 102 91 5 117 99 1 35 117 99 7 35 21 7 35 21 7 35 21 9 124 102 236 11 104 86 11 104 86 14 104 86 5 4-4 19 48 54- K= 2 μ 3 38 30- 7 163 149- 8 22 20- 7 163 149 8 44 42 5 44 33 6 22 20- 7 163 149- 8 25 30- 9 46 38 10 77 72 11 162 182- 12 30- 8 44 13 114- 13 124 10 248 16 106 104- 17 30 24 18 58 51- 17 30 24 18 58 51- 17 30 24 18 58 51- 17 30 24 18 58 51- 17 30 24 18 68 85- 6 213 189 7 161 133- 8 115 124 10 47 33 11 27 20
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Table 1 (cont.)

15 89 87- 16 89 88 17 73 71-	2 358 415 3 59 65	K= 8 H= -3 1 153 166-	14 31 30 15 45 45	15 36 37 17 36 33	4 115 105 5 62 67	5 82 88- 6 110 102	10 30 29 12 37 37
18 41 39- K= 4 H= 3	5 51 49-	7 115 116-	K= 6 H= 4 0 222 231	10 40 35- 19 55 50 K= 4 H= -4	9 130 127- 10 92 93-	7 45 47- 8 47 41	K= 2 H= 6 0 47 22
0 75 69-	7 96 92- 8 240 234	11 36 36 12 89 76-	1 51 38 2 64 67-	L 253 252 3 195 183	11 70 61-	14 74 70- 15 80 83	2 137 130-
2 47 44- 3 171 152	9 63 43- 10 26 25	13 69 49- 14 83 69-	3 169 1/9 4 86 81-	5 177 183 6 69 68-	14 39 36 15 92 91-	16 34 29 17 82 76	6 43 39- 7 75 66-
4 40 33 5 290 291	12 90 78- 13 81 84	K∓ 9 H≃ −3 1 41 39	5 71 72 6 68 72-	7 63 60 8 99 104-	16 90 94 K≖ 3 H= 5	19 29 26 K= 3 H= -5	8 94 94 9 158 170-
7 276 283	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3 58 57- 6 38 48-	8 54 52- 10 30 27	9 79 79- 10 299 347	0 207 202- 1 117 109	1 121 120 2 52 49-	10 34 27 11 105 109-
10 103 98	2 67 72	8 35 29	12 22 17-	11 103 106- 12 233 256	2 134 136- 3 77 76-	3 83 78 4 92 86-	12 76 70- 13 50 46-
12 59 64	4 281 303 5 192 204-	10 26 24 K= 10 H= -3	14 62 62	14 39 37-	5 45 36-	5 64 49- 6 65 56- 7 74 70	14 29 24- 15 35 42
14 79 79 15 43 39	6 61 61 7 85 80-	1 48 45 4 28 29	K= 7 H= 4 0 93 99-	L9 52 48-	8 91 83- 9 81 74	8 134 134 10 398 471	0 222 227
16 59 55 K= 5 H= 3	8 231 239- 9 31 25-	5 67 54 6 38 32	1 125 124- 3 212 215-	1 117 110 2 226 234-	11 43 39- 15 30 28-	11 182 203- 12 73 65	2 40 33-
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3 115 120-	12 123 117	K = 11 H = -3 1 25 21 = -3	6 94 110 8 29 33-	6 59 59- 7 159 159	0 86 79- 1 42 36	15 35 22- 17 29 20	7 71 70 9 89 84
5 182 190-	15 82 78 16 74 79	3 67 65-		8 37 13- 9 152 155	2 69 69 3 35 28	18 37 32- K= 4 H= -5	11 57 50- 13 35 37-
7 67 77 8 163 169-	17 36 36-	0 43 48-	0 252 271-	11 105 93	5 140 138-	2 105 90-	K= 4 H= 6
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12 121 129 13 114 124	1 83 90- 2 434 485-	K= 1 H= 4 0 66 57	4 64 66 6	16 54 48 17 46 36-	0 93 77 L 74 67-	6 147 157- 7 39 37	4 56 52-
14 134 140 15 74 70	3 174 186- 4 36 33	1 411 437 2 358 366	7 54 59- 10 66 61-	18 38 32- K= 6 H= -4	2 88 91 3 57 50-	8 186 211 9 283 326	7 56 58- 8 82 80-
17 42 48-	5 127 132 6 143 139	3 342 352 4 79 64	K≈ 9 H≠ 4 1 108 99	1 53 48 2 105 110	5 33 29 6 83 77-	10 121 134 11 167 183	10 23 20 11 74 67
0 44 40	8 177 182	5 189 194- 6 179 174 7 77 41-	2 43 43 3 26 24	3 34 23 4 93 91-	7 45 38 8 66 65	12 71 69- 13 46 48-	12 40 35 13 31 25
3 108 120-	10 262 282-	9 118 105	9 63 78- Ka 10 Ha A	7 38 35	9 38 31- 10 29 22-	14 58 59 15 26 25-	K= 5 H= 6 1 103 98-
5 142 139-	12 396 457-	12 69 61 13 43 43	0 86 85-	9 88 85 10 32 23-			2 33 29 3 26 17
8 74 75 9 39 39	15 48 44 16 25 8	16 67 69 K= 2 H= 4	2 59 51-	13 38 31 14 47 44-	K= 6 H= 5 0 87 89-	1 152 154-	5 42 41 A 59 54-
10 188 214- 11 119 130 [°]	17 58 61- 20 23 24	0 36 41- 1 115 117	4 30 26- 5 40 41	15 47 35 16 45 41-	1 82 83- 2 82 74	3 112 112-	7 51 51-
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16 33 38-	2 140 126 3 180 183-	4 71 67- 5 108 106	4 69 73 6 270 323	1 65 64- 2 203 206	5 54 58 7 78 76	9 91 93 11 25 21-	12 33 36- K= 6 H= 6
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2 201 222	8 100 87	11 99 100 12 89 87	K= 1 H= -4	5 39 34- 6 147 144- 7 52 19	12 64 64	15 26 24	4 147 164 5 156 187-
4 90 93 5 141 156-	10 158 164-	13 67 67-	2 178 185	12 81 61-	K= 7 H= 5	2 22 13	7 57 53-
6 38 38 8 109 121	13 69 53- 14 73 67	17 43 43 18 25 32	4 44 38 5 25 25	K* 8 H= -4 3 119 118-	2 57 54- 3 75 72	4 68 76 5 108 120-	9 39 38 10 41 38
11 60 68- K= 8 H= 3	15 77 7/ 16 38 40-	K= 3 H= 4 0 89 75-	6 334 378 7 203 208	5 188 198- 7 33 38-	4 142 160- 5 94 107	7 22 21 8 123 135-	11 35 33 K= 7 H= 6
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4 201 234-	2 41 44-	5 112 117	10 37 31-	12 52 39- 13 35 25	K= 8 H= 5 1 82 77-	11 72 68 15 42 39-	2 60 62 3 25 19
9 64 57-	4 379 414- 5 90 76	8 76 62	13 136 157	1 66 63	5 62 56-	K= 7 H= -5	• 28 32- 5 85 72
11 35 24- 12 58 60	6 28 15 7 93 79	10 52 51 11 28 13	15 65 68 19 60 61-	6 38 33 7 108 80-	8 28 30 10 22 29	3 33 40-	K= 8 H= 6 2 136 149
13 25 30 K= 9 H= 3	8 71 73- 9 189 194-	12 53 57 13 37 27	20 31 27- K= 2 H= -4	8 79 62- K= 10 H= -4	K= 9 H= 5 0 68 60-	5 89 96- 6 153 163	3 83 83 4 25 30
	10 148 150- 11 127 127-	15 81 68 16 104 107-	1 134 139 2 126 128-	1 34 24- 2 32 28-	1 71 63- 2 104 101-	7 55 59- 8 96 106	6 50 52- K= 9 H= 6
3 40 46 4 27 28	13 41 31	K= 4 H=	4 115 110 5 359 420-	3 40 .42 4 59 47 5 87 70	3 49 44- K= 10 H= 5	10 40 38- 11 54 45	1 38 35 K= 0 H= +6
5 80 84 6 31 27-	16 61 52 18 69 59-	2 54 52- 3 112 89	6 133 142-	7 52 49-	K= 0 H= →5 2 45 51-	13 33 40 14 53 41	2 109 200- 4 82 83- 6 158 172-
8 22 28- 9 35 36-	K= 6 H= -3 L 77 77-	4 67 55 5 127 123	8 111 113 9 72 64	0 103 107 2 302 335-	4 278 332 6 278 327	3 72 64-7 7 74 61	8 47 45 10 67 60
10 43 43 K= 10 H= 3	2 212 235 3 84 80-	6 146 144 7 198 200	10 119 116 12 56 51-	4 68 75- 6 85 79	8 158 179- 14 188 213-	8 38 39- 9 57 49-	12 159 181-
2 75 69-	4 165 176- 5 103 107	8 79 75- 10 64 60-	13 39 31 14 47 43-	8 61 63 10 142 159	16 99 96- 18 82 79	10 54 46 11 20 12	16 32 30- 18 31 28
5 41 38	7 133 136	12 82 81 15 26 26-	15 68 69. 16 35 32	12 125 139-	K= 1 H= -5 2 23 10	12 63 57 K= 0 H= 6	K= 1 H= -6 1 107 105
K= 11 H= 3 0 71 79	9 35 34- 10 35 39	16 27 33 K= 5 H= 4	18 73 64 19 83 70-	0 42 23 3 35 30	3 123 132- 3 86 89 5 83 86	2 40 41	2 40 37 3 72 70
1 23 28 K= 0 H= -3	11 76 76- 13 87 89-	0 64 45- 1 84 69-	20 22 17 K= 3 H= -4	4 166 162 5 28 30	7 114 111 8 51 49	6 49 57 8 52 46	5 42 34-
2 188 225	14 47 47- 16 28 29-	2 77 66- 3 141 144-	1 100 89 2 382 433	7 99 102- 9 52 48-	9 43 35 10 76 76	14 47 52- K= 1 H= 6	7 104 107- 8 30 28-
6 772 135- 8 194 166-	K= 7 H= -3 1 73 67 2 127 125	4 59 58- 5 76 83 6 133 135	3 167 159 4 33 28-	11 92 92- 12 51 56	11 70 64 13 41 42-	0 93 91- 1 76 69-	10 61 60 11 50 37-
12 116 114-	3 77 72-	7 121 118	0 20 39- 7 179 185- 9 74 70-	14 38 28- 15 121 120	14 101 114- 16 57 62-	2 227 241- 3 363 386-	12 58 53
16 119 127 18 51 55	7 188 204 8 167 176-	4 76 75 10 45 97-	10 124 131-	K= 2 H= 5 0 85 A5-	19 33 38- Km 2 Hm - K	+ 248 274- 5 152 146- 6 63 60	10 91 33- 17 37 34 18 25 33-
20 /3 70- Ka- L Ha +3	9 89 91 10 61 64-	11 56 53- 12 34 14-	12 49 43 13 58 56-	1 54 59 2 227 236	1 144 151 2 60 62-	7 55 47 8 44 40	K= 2 H= -6 1 152 159-
1 31 77-	16 35 29-	13 70 70-	14 63 53-	3 179 178	4 43 33-	9 51 44-	45

•

Table 1 (cont.)

				14 97 94-	0 80 43	PA 84 6	3 41 36
4 64 65	13 32 29-	11 52 55	2 90 96	14 21 24-	7 20 72	3 35 34-	
5 86 82	14 45 45-	K= 2 H= 7	3 61 59	K= 4 H= -7	10 51 50-	2 23 20-	3 44 44
4 47 31	15 24 17	0 49 41-	4 63 58-	2 40 41	K= 3 H= 8	5 95 106-	K= 4 H= 9
		1 167 168	5 66 66	4 102 105	0 105 112-	6 53 55-	0 17 19-
/ 04 01-	10 43 40	1 107 100	7 46 40-	5 48 43	1 67 69	7 91 110-	1 16 14-
8 27 24-	K= 6 H= -0	2 49 30-			2 44 97-	10 30 26	2 58 57-
9 70 66-	1 22 9-	4 128 125-	8 17 17	0 4/ 4/-		12 26 23-	X . 5 Ma 9
10 63 62	3 22 20-	5 150 159-	K= 0 H= -7	7 93 95-	3 96 90	12 23 23-	0 50 54-
12 52 48	4 54 54	6 109 107-	2 83 85-	8 123 141-	5 22 20	13 20 20-	0 90 94-
14 37 35	6 40 36-	7 37 33-	4 208 234-	9 182 214-	6 29 26	K= 4 H= -8	1 32 31-
16 24 27-	8 60 60m	8 50 48-	6 67 82-	10 84 104	7 26 7-	1 55 52	K= 0 H= -9
19 20 21-	10 11 14	10 48 41	8 18 42-	11 82 95-	8 16 16	3 60 62	2 59 59
10 01 4/-	10 33 34		10 60 68-	12 10 10	10 13 4	5 48 48	10 34 38-
17 60 52	13 29 21-	12 40 40	10 39 88-			A A3 AA	12 67 86-
K= 3 H= -6	14 26 21	13 25 30	12 11 13	K= 3 H= -/		e 184 200	Ka I Ha -9
1 76 68-	15 16 2	K= 3 H= 7	14 99 126	1 51 50	0 34 29-	0 104 207	
2 104 91-	K= 7 H= -6	U 48 44-	16 33 45-	2 1/3 181-	1 41 31-	9 20 28-	2 44 40-
3 106 106-	1 62 57	1 39 27-	K= 1 H= -7	6 42 38	4 38 26-	12 26 24-	3 /3 80
1 01 70	3 79 75	2 39 25	1 56 47	8 33 28	8 34 32	K= 5 H= -8	4 44 47-
4 61 76	3 14 13			9 43 44	Ka SHA d	1 67 55-	5 44 46
5 37 27-	4 140 147	3 40 40		10 41 41-	0 29 27	A 29 23-	6 35 36
7 131 136	5 59 50	4 47 31	4 121 101	10 83 03-		1 20 13	10 59 56-
8 97 89	6 76 60	5 1 19 1 24	5 86 80-	13 99 50-	1 20 11		11 29 20-
11 50 46-	8 99 78-	6 45 43	6 56 47	14 34 37	2 34 23	0 17 17	11 27 20-
12 26 24	9 46 38	7 35 24-	8 79 95-	K= 6 H= -7	3 46 41	/ 8/ 83	Ka 2 ma - 4
13 25 23-	12 40 39	8 40 39	12 41 49	1 26 33	4 25 17	8 70 66-	1 37 31-
14 11 25	13 34 29	9 85 76-	13 47 49	3 45 54	5 46 43-	9 90 91	3 44 41-
14 31 23		10 51 55	Ka 2 Ha +7	6 30 27-	6 38 32	10 40 38-	5 30 36-
15 44 40-	K= 8 H= -0	10 33 44	1 1 2 1 2 1 2 1 2 1 2 1 2	7 50 55-	Ka A Ha A	11 60 64	7 53 46
16 29 27-	4 41 41	11 30 20-	1 121 127-	0 16 18-	0 24 24	Ka 6 He -R	8 66 60
17 21 21-	5 42 36	K= 4 H= /	2 28 22-	4 10 10-		1 1 1 75	0 25 22
K= 4 H= -6	8 46 42	0, 74 73	3 57 59-	10 38 41-	1 25 20-		7 E 7 Ma - 0
1 61 53-	9 29 27	1 27 27-	4 28 15-	12 30 34-	2 31 32	3 15 15-	K* 3 H= -7
2 74 74	K. 4 H6	2 27 31-	5 28 28	K= 0 H= 8	3 22 23-	4 15 15-	2 38 35
1 14 14	1 51 50	3 38 36-	6 40 36	0 99 112	4 26 23-	5 30 29-	6 114 107
4 36 36		4 59 42-	8 48 47	2 121 131	5 60 81	8 36 46-	7 48 45
2 22 23-	3 21 17		10 18 21-	4 49 51	K= 0 H= -8	9 16 16-	8 104 108
6 1 26 131	• 22 27-	3 66 66			A AA 27	K . 0 H . 9	10 32 31-
8 145 156-	5 20 20-	0 20 9/-	11 42 32		a 35 34-	0 31 27-	K= 4 H= -9
9 83 86	6 47 55	7 79 75	12 00 04	N= 1 //= 0	0 39 30-		1 1 24
10 252 286-	K= 0 H= 7	9 40 35	13 32 28-	C 62 50-	10 32 20	0 47 33-	1 31 60
12 63 61	0 73 72	10 25 26	15 32 30-	L 62 53-	12 82 107	K# T H# A	2 17 10-
14 40 36	2 108 113	11 38 30	K= 3 H= -7	3 59 51	K= 1 H= -8	0 25 30-	3 17 0-
	4 104 221	K. 5 H. 7	1 28 13	4 150 173	2 113 115	1 35 30-	4 44 38
10 67 00	4 194 201	0 145 154	3 62 47	5 116 125	4 54 57	2 48 48-	5 35 29
17 53 41	0 122 139	0 145 154	1 10 14-	4 45 76	5 49 76	4 30 36-	6 103 108
K= 5 H= -6	8 43 39	1 43 42	3 37 34-		7 40 40	7 24 12	7 107 114
2 41 30-	10 70 72-	3 29 19-	a 28 19-	A= 2 m= 8		· · · · · · · · · · · · · · · · · · ·	AA AA-
3 56 44	12 39 37-	4 33 23-	5 65 63-	U 26 6	11 30 32	A- 4 II- 7	0
4 51 40-	K= 1 H= 7	5 45 41	6 48 37-	1 46 40-	12 47 52-	U 47 41	N= 3 H= -9
5 34 27-	0 115 104-	7 40 32	7 94 108-	2 25 4-	13 30 28	1 50 50-	• 38 39-
4 17 11-	3 73 64-	A 5A 58-	8 233 284-	3 86 85	K= 2 H= -8	2 19 23	K= 0 H=-10
	3 13 30-	0 17 10-	0 44 49-	à A3 A1	1 74 35-	3 42 41-	4 58 68-
1 13 61-			10 112 122-	5 21 23	2 38 22-	5 58 58	6 43 54-
8 58 56-	2 41 41-	10 34 30-	10 112 122-		4 41 44-	6 46 50	K= 1 H=+10
9 83 79-	6 54 50-	K= 6 H= 7	11 02 81	0 77 3/	· · · · · · · · · · · · · · · · · · ·		A 37 AL
10 76 73	8 83 103	0 71 70	12 57 68	7 63 61-	K= 3 H= -0	N- 3 H- 9	

used throughout the refinement. The quantity minimized was $\sum w(F_o - KF_c)^2$, K being a single scale factor. After four isotropic cycles the R index was reduced to

Table	2	Atomic	coordinates	and	e.s.d	.'s
raute	<i></i>	111011110	coorainaico	ann	C.D	

	x	у	Z
N(1)	0.3753(3)	0.6143 (3)	0.3123(2)
C(2)	0.4125(5)	0.7464 (4)	0.2872(2)
Č(3)	0.4061 (5)	0.8770 (4)	0.3324(3)
Č(4)	0.3583(4)	0.8709 (3)	0.4080(2)
C(5)	0.2661(4)	0.7118(3)	0.5167 (2)
C(6)	0.2324 (4)	0.5739 (3)	0.5459 (2)
C(7)	0·2436 (4)	0.4490 (3)	0.4964 (2)
C(8)	0·2856 (4)	0.4681 (3)	0.4200 (2)
Č(9)	0.3264 (3)	0.6065 (3)	0.3879 (2)
C(10)	0.3154(3)	0.7317(3)	0.4385 (2)
N(11)	0.2837(3)	0.3360 (3)	0.3689 (2)
O(12)	0.1880 (4)	0.3348 (3)	0.3059 (2)
O(13)	0.3769 (3)	0.2330 (3)	0.3938 (2)
O(14)	0.1868 (4)	0.5700 (3)	0.6215 (1)
C(15)	0.1485 (5)	0.4296 (4)	0.6541 (2)
O(16)	0.2591 (3)	0.8349 (2)	0.5655 (1)
C(17)	0.1013 (4)	0.8854 (3)	0.5754 (2)
O(18)	-0.0251(3)	0.8387 (3)	0.5373 (2)
C(19)	0.1132 (5)	1.0043 (4)	0.6378 (2)
H(2)	0.447 (7)	0.756 (6)	0.233 (4)
H(3)	0.440 (6)	0·976 (6)	0.308 (4)
H(4)	0.352 (6)	0·964 (6)	0.441 (3)
H(7)	0.216 (6)	0.346 (6)	0.507 (3)
H(24)	0.065 (7)	0.366 (7)	0.622 (4)
H(25)	0.131 (7)	0.448 (7)	0.711 (3)
H(26)	0.240 (7)	0.367 (6)	0.652 (4)
H(27)	0∙C 0 6 (7)	0.070 (7)	0.641 (4)
H(28)	0 ·145 (7)	- 0 ·048 (7)	0.703 (4)
H(29)	0.201 (7)	0 ∙069 (6)	0.622 (4)

0.156. Anisotropic thermal parameters were then introduced, and after three cycles of refinement, the Rindex reduced to 0.101. At this point, an $(F_{obs} - F_{calc})$ difference synthesis yielded the hydrogen atomic coordinates. These were refined in three cycles while all other parameters were fixed including the hydrogen temperature factors, which were assumed to be isotropic with B = 3.5 Å². Following this, the thermal and positional parameters of the other atoms were refined with the hydrogen parameters fixed. After four cycles the resulting final R value was 0.088. The observed and calculated structure factors are listed in Table 1. The atomic coordinates and their thermal parameters together with their e.s.d.'s are given in Tables 2 and 3, respectively. The projection of the unit cell along a* is shown in Fig. 2, and along the **b** axis in Fig. 3.

Discussion

The observed bond distances, their estimated standard deviations, and the estimated bond lengths after an adjustment for thermal motion by a procedure of Busing & Levy (1964) are listed in Table 4. In calculating the corrections to the ring bonds, in-phase thermal motion was assumed for the ring atoms. A 'riding' motion was assumed for all the other atoms. In Table 4 the adjusted distances are compared with the calculated bond lengths that one might expect from simple valence bond theory. The latter were obtained by the method of Pauling (1960) from the tabulated bond numbers which were derived on the assumption that canonical structures involving independent resonance of the quinoline ring and the substituents contribute 91% to the hybrid structure, while structures with double bonding between the ring and either the acetoxy or methoxy group contribute 2 and 7% respectively. The three classes of resonance structures are represented summarily by the composite structures (I), (II) and (III):

by Dewar & Gleicher (1966) (Table 4). Moreover, the C(8)-N(11) and C(5)-O(16) bond numbers show that there is no major degree of resonance between the nitro or acetoxy group and the quinoline ring. Only a small amount of resonance occurs between the methoxy group and the ring system, as indicated by the C(6)-O(14) bond distance.

The dihedral angles which are listed in Table 5 and the valency angles in Table 6 show the effects of intra-



The bond numbers are the average of those in the equally weighted canonical structures that contribute to the composite structure. The bond lengths of the ring are virtually unaffected by resonance with the substituent groups in that the observed values agree within the uncertainty limits with theoretical distances in the unsubstituted molecule as obtained recently in a self-consistent-field molecular-orbital type calculation

molecular steric repulsions. The exocyclic COC angles in the methoxy and acetoxy groups are significantly larger than tetrahedral due mainly to steric repulsions. In the case of the methoxy group this repulsion is between the methyl group and atoms C(6), C(7) and H(7); in the acetoxy group C(17) and O(18) interact sterically with C(5) of the ring. Similarly, the deviation of the exocyclic angles at C(6) from 120° is due to the steric

 Table 3. Thermal parameters and e.s.d.'s

Thermal parameters are in the form $\exp\left[-2\pi^2(h^2a^{*2}U_{11}\cdots+2klb^*c^*U_{23})\right]$.						
	U_{11}	U_{22}	U_{33}	U_{12}	1/12	Um
N(1)	0.0465 (0.0019)	0.0360 (0.0020)	0.0359 (0.0018)	-0.0007(0.0016)	0.0128 (0.0015)	0.0008 (0.0015)
C(2)	0.0549 (0.0019)	0.0475 (0.0017)	0.0438 (0.0022)	-0.0067(0.0015)	0.0174 (0.0015)	0.0066 (0.0015)
C(3)	0.0562 (0.0016)	0.0329 (0.0015)	0.0585 (0.0018)	-0.0090(0.0013)	0.0146 (0.0013)	0.0112(0.0013)
C(4)	0.0439 (0.0013)	0.0260(0.0014)	0.0501(0.0015)	-0.0048(0.0011)	0.0065 (0.0011)	-0.0004(0.0011)
C(5)	0.0358 (0.0016)	0.0243 (0.0015)	0.0371(0.0014)	-0.0026(0.0012)	0.0041 (0.0012)	-0.0000(0.0011)
C(6)	0.0449 (0.0016)	0.0294 (0.0014)	0.0300 (0.0015)	-0.0007 (0.0012)	0.0044 (0.0012)	-0.0040(0.0017)
C(7)	0.0497 (0.0014)	0.0225 (0.0014)	0.0335(0.0014)	-0.0026 (0.0011)	0.0060 (0.0012)	-0.0040(0.0012)
C (8)	0.0382 (0.0013)	0.0242 (0.0014)	0.0333 (0.0014)	-0.0000(0.0010)	0.0050 (0.0010)	-0.0052(0.0011)
C(9)	0.0320 (0.0013)	0.0252(0.0013)	0.0324 (0.0015)	0.0006 (0.0011)	0.0032 (0.0011)	-0.00092(0.0011)
C (10)	0.0324 (0.0014)	0.0241(0.0012)	0.0379 (0.0013)	-0.0026(0.0010)	0.0037 (0.0010)	-0.0017(0.0010)
N(11)	0.0471 (0.0022)	0.0236 (0.0015)	0.0355 (0.0013)	-0.0011(0.0014)	0.0100 (0.0013)	-0.0064 (0.0010)
O(12)	0.0968 (0.0015)	0.0434 (0.0013)	0.0374(0.0019)	-0.0008(0.0011)	-0.0083 (0.0013)	-0.0105(0.0012)
O(13)	0.0564 (0.0018)	0.0312(0.0013)	0.0723(0.0012)	0.0134(0.0012)	0.0072 (0.0011)	-0.0090(0.0012)
O(14)	0.0797 (0.0022)	0.0359 (0.0019)	0.0323 (0.0018)	-0.0032(0.0016)	0.0173 (0.0016)	-0.0033(0.0015)
C(15)	0.0650 (0.0011)	0.0446 (0.0011)	0.0423(0.0012)	-0.0008(0.0008)	0.0149 (0.0009)	-0.00033(0.0013)
O(16)	0.0379 (0.0015)	0.0263 (0.0014)	0.0416 (0.0014)	0.0002(0.0011)	0.0025 (0.0011)	-0.0134(0.0011)
C(17)	0.0403 (0.0012)	0.0274 (0.0014)	0.0315 (0.0016)	0.0031 (0.0010)	$0.0023 (0.0011) \\ 0.0051 (0.0011)$	-0.0154(0.0011)
O(18)	0.0400 (0.0022)	0.0414 (0.0023)	0.0587(0.0019)	-0.0040(0.0017)	0.0013 (0.0016)	-0.0060(0.0016)
C(19)	0.0672 (0.0014)	0.0503 (0.0015)	0.0431(0.0014)	0.0178(0.0011)	0.0002 (0.0010)	-0.0157(0.0011)
H(2)	0.0503	0.0523	0.0507	0.0000	0.0000	0.0000
H(3)	0.0203	0.0523	0.0507	0.0000	0.0000	0.0000
H(4)	0.0503	0·0523	0.0507	0.0000	0.0000	0.0000
H(7)	0.0503	0.0523	0.0507	0.0000	0.0000	0.0000
H(24)	0.0503	0.0523	0.0507	0.0000	0.0000	0.0000
H(25)	0.0203	0.0523	0.0507	0.0000	0.0000	0.0000
H(26)	0.0503	0.0523	0.0507	0.0000	0.0000	0.0000
H(27)	0.0203	0.0523	0.0507	0.0000	0.0000	0.0000
H(28)	0.0503	0.0523	0.0507	0.0000	0.0000	0.0000
H(29)	0.0503	0.0523	0.0507	0.0000	0.0000	0.0000

D(obs) is the experimental bond length. D(adj) is the experimental bond length after applying an estimated adjustment for thermal motion. D(calc) is the bond length that is predicted by the valence bond theory for the corresponding tabulated bond number, B.N.

D(D-G) are theoretical bond lengths in quinoline calculated by an SCF-MO method (Dewar & Gleicher, 1966). The distances and their e.s.d.'s are in Å.

Bond	D(obs)	e.s.d.	D(adj)	B.N.	D(calc)	D(D-G)
N(1) - C(2)	1.314	0.005	1.314	1.653	1.298	1.314
C(2) - C(3)	1.408	0.005	1.408	1.335	1.422	1.424
C(3) - C(4)	1.365	0.006	1.365	1.663	1.372	1.374
C(4) - C(10)	1.416	0.004	1.416	1.326	1.424	1.424
C(10) - C(5)	1.422	0.005	1.422	1.350	1.419	1.429
C(5) - C(6)	1.379	0.004	1.379	1.607	1.379	1.373
C(6) - C(7)	1.410	0.004	1.410	1.319	1.425	1.426
C(7) - C(8)	1.371	0.005	1.371	1.670	1.371	1.370
C(8) - C(9)	1.416	0.004	1.416	1.321	1.425	1.436
C(9) - C(10)	1.423	0.004	1.423	1.320	1.425	1.409
C(9) - N(1)	1.370	0.004	1.371	1.345	1.354	1.352
C(8) - N(11)	1.469	0.004	1.472	1.004	1.449	
N(11)-O(12)	1.214	0.004	1.245	1.498	1.260	
N(11)-O(13)	1.229	0.004	1.252	1.498	1.260	
C(6)—O(14)	1.358	0.004	1.373	1.07	1.381	
O(14)–C(15)	1.430	0.005	1.431	1.003	1.432	
C(5)—O(16)	1.386	0.004	1.389	1.02	1.395	
O(16)–C(17)	1.362	0.004	1.365	1.12	1.369	
C(17)-O(18)	1.193	0.004	1.211	1.88	1.219	
C(17) - C(19)	1.492	0.006	1.513	1.00	1.504	
C(15)-H(24)	0.98					
C(15)-H(25)	0.98					
C(15)-H(26)	0.93					
C(19)-H(27)	1.04					
C(19)–H(28)	1.17					
C(19)-H(29)	0.97					
C(2) - H(2)	0.99					
C(3) - H(3)	1.04					
C(4) - H(4)	1.01					
C(7) - H(7)	0.99					

Table 5. S	Some least-	squares plan	es of atom	s and some	dihedral	angles

		Coefficie	nts in $AX + BY$	+CZ-D=0 re	eferred to
		the	crystallographic	e axes (X, Y, Z i	n A)
Plar	ne	A	В	С	D
Quinoline	ring	0.9163	-0.1243	0.2595	3.3862
Pyridine 1	noiety	0.9109	-0.1327	0.2202	2.3769
Benzenoio	1 moiety	0.9226	-0.1138	0.2466	3.3508
Nitro gro	up	0.7952	0.3723	-0.5771	-0.6339
Acetoxy g	group	0.1612	0.6890	-0.7214	-1.2715
		Deviations fr	om the plane (Å)	
	Quinoline	Pyridine	Benzene	Acetoxy	Nitro
N(1)	-0.000	0.002	0.045		
C(2)	0.013	-0.005	0.078		
C(3)	0.012	-0.000	0.082		
C(4)	0.002	0.002	0.051		
C(5)	-0.017	0.019	-0.012	-0.170	
C(6)	0.020	0.072	0.004		
C(7)	0.027	0.080	0.011		-0.035
C(8)	-0.020	0.000	-0.016		
C(9)	-0.020	-0.002	0.008		
O(16)	0 020	0 002	0 000	0.001	
C(17)				0.002	
O(18)				-0.004	
C(19)				0.001	
		Dihec	iral angles		
		Intersecting p Acetoxy and be Nitro and benz	planes , enzenoid enoid	Angle 79·1° 59·2	
		i ynume anu be	.uzenoid	10	

repulsion between the methoxy group and the ring. The intramolecular contacts involved in these steric interactions are included in Table 7. Certain of the angles in the ring differ significantly from their mean value of 120° . However, the angles C(10)–C(9)–N(1), C(9)-N(1)-C(2) and N(1)-C(2)-C(3) are normal for this heterocyclic system (Pauling, 1960). Repulsion between O(12) and the unshared electron pair on N(1)prevents the nitro group from lying in the plane of the quinoline ring (Fig. 2). The 59° rotation out of the plane produces a normal van der Waals contact of 2.929 Å between N(1) and O(12). While this angle corresponds to an estimated resonance energy of 1.7 kcal.mole⁻¹ between the nitro group and the ring, the C(8)-N(11) distance indicates negligible resonance

Table 6. Valency angles and their standard deviations

	Angle	e.s.d.	
C(9) - N(1) - C(2)	116·2°	0·3°	
N(1) - C(2) - C(3)	124.6	0.4	
C(2) - C(3) - C(4)	119.7	0.4	
C(3) - C(4) - C(10)	118.5	0.4	
C(4) - C(10) - C(9)	117.4	0.3	
C(4) - C(10) - C(5)	123.3	0.3	
C(9) - C(10) - C(5)	119.2	0.3	
C(10) - C(5) - C(6)	121.9	0.3	
C(5) - C(6) - C(7)	119.3	0.3	
C(6) - C(7) - C(8)	119-1	0.3	
C(7) - C(8) - C(9)	123.9	0.3	
C(8) - C(9) - C(10)	116.5	0.3	
C(8) - C(9) - N(1)	119.9	0.3	
C(10) - C(9) - N(1)	123.4	0.3	
C(9) - C(8) - N(11)	119.1	0.3	
C(7) - C(8) - N(11)	116.9	0.3	
C(8) - N(11) - O(13)	117.4	0.3	
C(8) - N(11) - O(12)	117.9	0.3	
O(12) - N(11) - O(13)	124.6	0.3	
C(7) - C(6) - O(14)	124.6	0.3	
C(5) - C(6) - O(14)	116.1	0.3	
C(6) - O(14) - C(15)	118.1	0.3	
C(10) - C(5) - O(16)	118.3	0.3	
C(6) - C(5) - O(16)	119.7	0.3	
C(5) - O(16) - C(17)	116.7	0.3	
O(16) - C(17) - O(18)	122.4	0.4	
O(16)-C(17)-C(19)	110.5	0.3	
O(18) - C(17) - C(19)	127.0	0.4	

Table 7. Some intramolecular distances between non-bonded atoms

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Atoms	Distance
$C(15) \cdots C(6)$	2∙392 Å
$C(15) \cdots C(7)$	2.835
$C(15) \cdots H(7)$	2.68
$H(24) \cdots C(6)$	2.71
$H(24) \cdots C(7)$	2.78
$H(24) \cdots H(7)$	2.40
$H(25) \cdots H(7)$	2.40
$H(26) \cdots C(6)$	2.57
$H(26) \cdots C(7)$	2.70
$O(16) \cdots C(6)$	2.39
$C(17) \cdots C(5)$	2.339
$C(17) \cdots O(14)$	3.013
$C(17) \cdots C(6)$	3.068
$O(18) \cdots C(5)$	2.639
$O(18) \cdots C(6)$	3.139

(Trotter, 1960). Presumably packing forces and intramolecular steric requirements govern the magnitude of the out-of-plane rotation, while resonance plays an insignificant role. Repulsions between either O(18) or the $C(19)H_3$ methyl group and O(14) or H(4) prevent the acetoxy group from lying in the plane of the ring. The rotation of this group by 79° out of the plane decreases the O(18) \cdots C(5) contact to 2.639 Å, about 0.3 Å less than a normal van der Waals distance. Evidently, resonance energy maintains the planarity of the acetoxy group to the extent of forcing this somewhat close intramolecular contact. These resonance effects are evident also in the C(17)-O(18) and C(17)-O(18)O(16) bond lengths and numbers.

Equations of some least-squares planes of atoms and the displacements of atoms out of the plane are listed in Table 5. The method of Schomaker, Waser, Marsh & Bergman (1959) was used for computing the equations. The quinoline ring is significantly non-planar although the largest atomic out of plane displacement is only 0.027 Å. While the pyridine moiety is planar to within 0.002 Å, the six membered ring of carbon atoms bearing the three bulky substituent groups is significantly non-planar. Very likely the steric interactions of the substituents induce the deviations from planarity. The intermolecular contacts are at the normal van der Waals distances except for the somewhat close 2.31 Å contact between O(18) of one molecule and H(7) in another molecule related to it by a symmetry center and unit translations in the **b** and **c** directions. The molecular packing is shown in Figs.2 and 3.

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