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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 equi-inclination 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, $\beta = 97.40 \pm 0.02°$, $D_x = 1.466$ 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-6-methoxyquinoline, 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.

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Crystal data

5-Acetoxy-6-methoxy-8-nitroquinoline, $C_{12}H_{10}O_5N_2$, M.W. 262·23
Monoclinic, space group $P2_1/c$
$a = 7.923 \pm 0.003$, $b = 9.056 \pm 0.003$, $c = 16.694 \pm 0.006$ Å
$\beta = 97.40 \pm 0.02°$
$D_x = 1.466$ g.cm^{-3}, $D_m = 1.472$ 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 $K\alpha$ radiation (1·5418 Å). The X-ray intensity data were collected on multifilm equi-inclination Weissenberg photographs with nickel-filtered Cu $K\alpha$ radiation from crystals rotated about the a and b axes. Both crystals were cut to approximate a

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 a*, c, and b directions respectively. The dimensions of the crystal rotated about the *a* axis were 0·3 mm in the b and 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 3·0 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
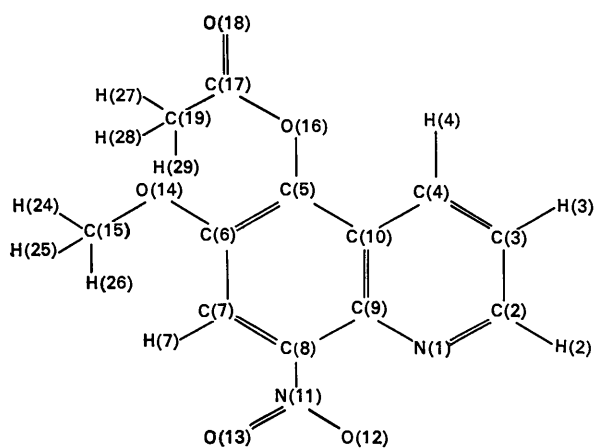

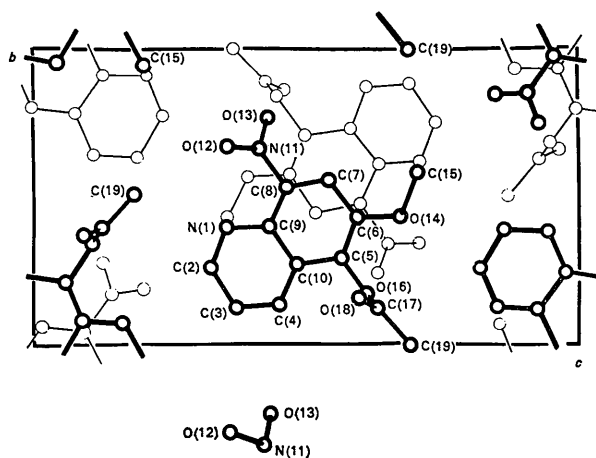Fig. 1. Atomic numbering in 5-acetoxy-6-methoxy-8-nitroquinoline.

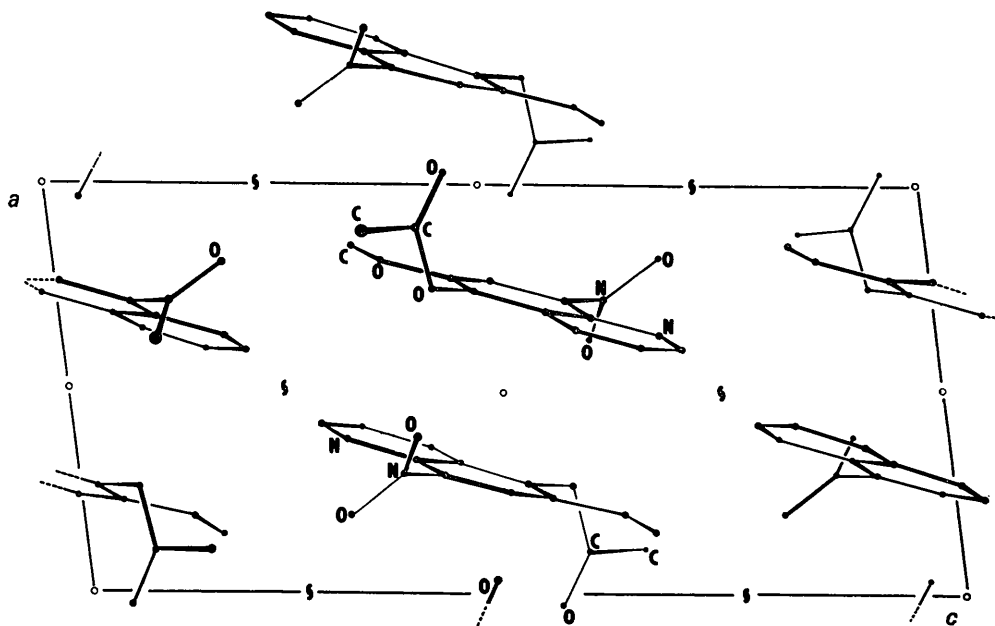Fig. 2. Molecular packing viewed along normal to the *bc* plane.

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 $10F_c$.

```
K= 0 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  99  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     14 203 210      3  84  87    K= 7 H= -2
K= 1 H= 0       11 106 103     14 210 223-     K= 1 H= -1      15  41  41     15  78  82-     4 401 453      2 117 124-
1 459 473       14  44  41     15 115 126       1 338 400-     16  25  21-    16  74  80      5 135 152-     3  70  74
2 408 404       15  24  24-    17  34  36-      2  73  74-     18  22  16     17  31  27-     6 222 222      4  73  78-
3 262 238-      16  21  23     18  52  55       3 228 224-     K= 7 H= -1     19  23  22-     7 231 216-     5  63  57
4 602 687       17 110 115     19  25  26-      4 261 255-     1 257 290-     K= 4 H= 2       8 314 307-     8  98 108
5 265 228       18 102 118-    K= 4 H= 1        5  50  47-     2 121 124-     0  52  45      11 150 131     10  44  47
6  92  84       K= 7 H= 0      0 153 156-       6 741 832      3 126 132-     1  87  96      13  41  30     11  48  48
7 263 239       1 365 368-     1  61  69        7 122 110      5 103  99      2 153 144-     14  64  55     13  51  55
8 126 101       2 341 339      2 205 215-       8 334 321      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      4 261 262      4 261 262       11  91  78       8  40  48     5 214 216-     17  43  44-    K= 8 H= -2
11  69  56      5 121 125-     5 152 143-      13  72  73       9  95 117-     6 106 100-    18  53  58-     1 230 239-
12  75  73      6  99  99-     6 333 320       14  79  74-     10 154 179      7  24  27     20  28  25      2 212 226
13 152 144-     7 134 143-     7 103  86-      15  92  93-     12  42  40      8  62  57     K= 2 H= -2      5 156 172
14  88  80-     8  78  80-     8  54  49-      17 130 143-     13 109  88      9 166 171      1 200 202-     6  94 103
15  78  72      9 129 137-     9 114 107       18  69  73-     K= 8 H= -1     10 109 100-     2 115 116      7  70  77
16  77  74     10  59  65     10 118 122-      19  46  46      1 244 272      11 159 162      3 323 302-     8  53  57-
17  73  81      K= 9 H= 0     11  53  56-      20  36  34.     2 131 145-     12  28  39-     4 194 190-    10  57  60-
18  72  80      1  64  60-    12 112 114-      K= 2 H= -1      3  86  90-     14  46  41      5 177 166     12  34  38
19  35  26      2  36  33-    13 219 237-       1 212 243      5  79  78-     15  45  47      6  36  25-    14  54  43
20  36  36-     3 158 150     14  44  46-       2 384 447      7  56  55-     17  36  30      7 259 265-    K= 9 H= -2
21  24  24      5  50  55     15  27   5        3 434 510-     8  55  49      18  40  43      8 121 121      3 150 157-
K= 2 H= 0       6  55  57-    16  25  18        4 473 527-    10  42  49-     K= 5 H= 2       9 209 201-     4  70  76
0 202 191-      7  96 107-    17  48  57        5 137 145-    13  45  36-     0 214 229      10  67  58-     5  76  88
1 108 106       9  48  59-    19  34  28-       6 278 280-    14  77  66      1 140 152      11  97  97-     7 121 131
2  57  35-      K= 10 H= 0     K= 5 H= 1        7 284 273-    15  95 107      2  67  64      14  40  25     10  73  70
3 164 140-      0 118 110-    0  42  36-        8 204 172      K= 9 H= -1     3 103  91-     15  87  82     13  46  49-
4 344 319-      1  56  56-    1 109 109         9 294 277-     2 101 103      4 274 272-     16  90  92     K= 10 H= -2
5 397 392-      2  45  40-    2 362 403-       10 205 186      3  50  59      5 292 315-     17  60  57-     1 102  96
6 242 208       4  44  38-    3 154 151        11 294 281      6  47  50      6  87  83-     19  50  43      2  49  38
7 178 146-      K= 11 H= 0    4  18  19-       12 126 123-     7  35  39      7  53  46-     20  73  68-     3  48  32
8 223 209       2 137 125-    5  34  34-       13 237 231      8  75  78      8  36  39-     K= 3 H= -2      5  83  79-
9 135 116       3 112  91-    6  83  75        14 123 113-    12  45  43-     9  56  57      1 143 146      9  92  99
10 106 101-     5  73  60-    7 101 106-       16  77  79-    13  27  18     10  32  22      2 285 305-    10  37  32-
11 205 181      K= 0 H= 1     9  53  58        17  37  32-    K= 10 H= -1    11 108 113      3 102  91-    K= 11 H= -2
12  99  89      0 168 163-   12 286 339-       18  24  22-     5  55  41-     12  85  87-     4 439 477-     1  82  78
14  49  38      2 642 802    13 140 156-       21  46  33      7  29  25-     14 160 187-     5 296 303      2  63  52
19  36  28-     4 298 285-   14  75  85-       K= 3 H= -1      9  24  23      15  86  92-     6 163 169      3  98  96
K= 3 H= 0       6 230 208    16  49  49         1 395 461     10  29  23     16  28  23      7 148 155      4  66  63-
1 375 382       8 370 341-   K= 6 H= 1          2 415 458     K= 11 H= -1    17  41  39      8  22  20     K= 0 H= 3
2 234 213-     10 386 380-   0 203 222          3 313 318      1  75  69-    K= 6 H= 2       9 185 180-     0 399 456
3 546 611      12 157 158    1 162 185          4 565 646      2  80  80      1  86  88-    10 119 124      2 585 672
4 419 429      18  62  72-   2  77  72          5  99  85      5  89  85      2 368 420     11 124 124-     4  38  41
5 366 348-     20  36  42-   3 169 177          6 110 101      6 133 138-     3  89  92-    12 161 164      6  63  52
6 355 349      K= 1 H= 1     4  74  74-         7  44  57      K= 0 H= 2      4  83  77     13  61  94-    10  83  67
7 352 323-     0 432 556     5  56  60-         8  93  89-     4 148 156      5  28  20-    14  47  47-    12 121 133
8  60  58-     1  47  47     6  49  42-         9 184 170-     6 426 451      6 138 143     17  57  56-    14  67  75-
9 191 194-     3  80  71-    7  76  75-        10 106 101-     8 169 146      7  74  62-    19  36  36-    16 108 128-
10  46  37      4 188 177    8  53  45         11 118 101-    10  96  86-     9  28  20-    20  79  76     K= 1 H= 3
11  85  84      5 118 104    9  35  35-        12 321 326     12  43  33     10  57  57-    K= 4 H= -2      1 226 213-
12 234 237-     6 204 182   10  99 112         13 249 259-    14  92  95-    11  55  57-     1  58  44-     2 587 646-
13 182 186      7  24  23   11 113 124-        14 233 233     16 150 173-    13  87  90-     2 294 316-     3 102 102-
14 143 142-     8 254 244-  12  39  29-        15 157 165-    18  48  48-    14 122 126-     3 251 244-     4 102  91
15 103 105-     9 287 243-  14  47  59-        16  85  80-    20  26  26-    15  65  61      4 113 119-     5 117  99-
16  51  51     10 177 154-  K= 7 H= 1          17  72  77     K= 1 H= 2      16  62  58-     5 124 114-     6  60  51
19  42  46     12  87  80    0 307 350-        18  23  26     0 442 595-     K= 7 H= 2       6  37  22      7  35  21-
K= 4 H= 0      17 135 159    1  93  97         K= 4 H= -1     2  54  46-     0  94  96       7 165 169      8 131 132
0 388 400-     18  54  66    2  84  95-         1 130 133-     4  91  84-     1 257 272      8  23  14      9 124 102
1  38  31-     19  53  64    3 151 167          2 159 15C-     6 261 257-     2 252 273-     9  40  37     10 242 236
3 511 546      20  42  39-   4  77  83          3 422 459      7 168 158-     3 182 200     10 149 160     11 104  86
4 204 186      K= 2 H= 1     6  56  52-         4 560 607-     8 345 313      4 124 144-    11 142 143     14 115 126
5 460 441      0 445 549     7  46  46-         5 254 256      9 193 173-     5  59  50-    12 223 231-    18  65  64-
6  93  84-     1 316 370-    8  76  83          6  78  82     10  77  62-     6  45  54     13 140 143     19  46  54-
7  73  68-     2 595 722-    9  73  88          7 104 113     11  70  59-     8  71  79     14  67  65-    K= 2 H= 3
8 221 215      3 148 129-   11  94 121          8 150 152     13  68  59     10  64  76     16  52  53      0 394 472-
9  41  37       4  68  42-  16  63  75-          9 149 156     14  60  54     11  41  56-    17  34  32-     1 147 134-
10  25  17      5 231 224-  K= 8 H= 1          10  92  94     15  50  47     14  35  32     18  37  33-     2 411 450-
11  85  75-     6 140 114    0 167 187-        11 267 277     16  76  84-    K= 8 H= 2      19  17  22-     3  38  30-
13  90  92-     8 158 149    1 345 394-        12 243 243     18  71  65-     0 186 193     K= 5 H= -2      4  44  42
14 133 129      9  73  56    2 220 250         13 240 238     20  35  41-     1  86  89      1 185 190-     5  44  33
15  70  68-    10 137 133-   3  88  87-        14  64  57-    K= 2 H= 2       2 121 135-     2  31   6      6  22  20-
16  36  38-    11  41  29    4  94 106         15 131 137-    0 120 125-      3  45  53-     3  61  53-     7 163 149-
17  43  46-    13 274 286-   7  55  61         17  65  68-    1 226 256-      5  54  59-     4  34  15      8  25  30-
18  36  29     14 253 255    9  43  52-        19  55  48     2 224 222-      8  91  97      5  92  94      9  46  38
19  35  41     15 216 236-  11  63  69-        20  28  33-    3  27  18      10  77  73      6  21  20-    10  77  72
K= 5 H= 0      16  72  69    K= 9 H= 1         K= 5 H= -1     4 117 111      K= 9 H= 2       7  33  16-    11 182 182-
1  95  88-     17  84  89    0  77  80-         1 221 227-    5 298 292-      0  48  55-     8  41  14-    12  74  64
2  19  22-     18  65  69    2  59  55-         2  65  51-    6 112  90       1  65  72      9  99  99-    14 113 114-
3 204 178      19  42  39    3  38  43          3 159 162-    7  35  35       3  78  88     10 247 267-    15 218 248
4  64  53      20  24  17    6  69  76          4 118 116-    8 265 257-      4  99  99-    11 195 208-    16 106 104-
5 116 109      K= 3 H= 1     8  38  51-         5  46  46     9 126 126-      9  93  95     12 100  95-    17  30  24
6 300 319-     0 230 236    10  41  51-         6 141 148-   10  36  27-     11  69  68-    14  76  76     18  58  51-
7  97 101-     1 185 197-   K= 10 H= 1          7 159 145-   11 304 304-     12  54  47     15  63  70     19  16  24-
8 110 108-     2 262 273    1  27  35           8 115 108-   13  40  34      K= 10 H= 2     17  35  28     K= 3 H= 3
9  38  46-     3 249 247    2  38  40-         10 133 136     14  28  30      0  64  57     18  48  44      0 283 303
10  25  20                   3  38  36-        11 242 252     15  52  51-     7  57  54     19  62  63      1 348 387
11 120 128                   4  41  42-        12 182 184     17  43  47-     8  31  24-    K= 6 H= -2      2  93  84-
12 180 196                   5  44  46         13  83  83     18  45  45-     9  36  37      1  41  34-     3 260 264
13 145 154                   6  70  68-        15  25  26     19  55  54      K= 11 H= 2     2 103 103-     4  88  85-
14 100 109                   7  39  35         16  23  20-    K= 3 H= 2       0  31  35-     3  61  58-     5 213 189
16  68  74-                  9  53  51         17  29  25     0 226 233-      1  31  26      4  64  74      7 141 133-
17  41  40-                 K= 11 H= 1         18  30  32     1  22  18       2  75  72      6  28  18-     8 115 124
19  41  45-                  0  67  63         K= 6 H= -1     2  25  13-      4  57  57      7  38  32     10  47  33
K= 6 H= 0                    3  53  50          1  69  61-    3 131 131-     K= 0 H= -2      8 147 156     11  27  20
0  71  70-                   4  31  32-         2  73  65-    4 132 128       4 269 316      9  79  79-    12  44  32
1  51  41                    5  28  26-         3 132 139     5 199 174-      6 312 337-    10  66  57-    13 127 132-
2  38  18                    K= 0 H= -1         4 197 196     6 210 201-      8 275 303-                   14  81  82
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Table 1 (cont.)

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15  89  87-      2 358 415       K= 8 H= -3     14  31  30      15  36  37       4 115 105       5  82  88-      10  30  29
16  89  88       3  59  65       1 153 166-     15  45  45      17  36  33       5  62  67        6 110 102       12  37  37
17  73  71-      4 194 198       4  63  65       16  26  27      18  40  35-      7  42  44-       7  45  47-      K= 2 H= 6
18  41  39-      5  51  49-      7 115 116-      K= 6 H= 4      19  55  50       9 130 127-       8  47  41       0  47  22
K= 4 H= 3        6 271 283-     10  51  50       0 222 231      K= 4 H= -4      10  92  93-      10  60  54-       1 117 121
0  75  69-       7  96  92-     11  36  36       1  51  38       1 253 252      11  70  61-      14  74  70-       2 137 130-
1 110 102-       8 240 234      12  89  76-      2  64  67-      3 195 183       13  25  19-      15  80  83        4 125 120-
2  47  44-       9  63  43-     13  69  49-      3 169 179       5 177 183       14  39  36       16  34  29        6  43  39-
3 171 152       10  26  25      14  83  69-      4  86  81-      6  69  68-      15  92  91-      17  82  76        7  75  66-
4  40  33        12  90  78-     K= 9 H= -3      5  71  72        7  63  60       16  90  94       19  29  26        8  94  94
5 290 291        13  81  84      1  41  39       6  68  72-      8  99 104-      K= 3 H= 5       K= 3 H= -5       9 158 170-
6 158 149-       15 102 113      3  58  57-      8  54  52-      9  79  79-      0 207 202-       1 121 120       10  34  27
7 276 283        K= 2 H= -3      6  38  48-     10  30  27       10 299 347      1 117 109        2  52  49-      11 105 109-
8 204 207-       1 261 276-      7  70  66-     11  28  25       11 103 106-      2 134 136-       3  83  78       12  76  70-
10 103  98       2  67  72       8  35  29      12  22  17-      12 233 256       3  77  76-       4  92  86-      13  50  46-
11  51  49       3  88  75-      9  47  38-     13  90  91       13 102 104-      4  37  38-       5  64  49-      14  29  24-
12  59  64       4 281 303      10  26  24      14  62  62       14  39  37-      5  45  36-       6  65  56-      15  35  42
13  89  89       5 192 204-     K= 10 H= -3     15  48  46       18  75  68-      7 263 283        7  76  79       K= 3 H= 6
14  79  79       6  61  61       1  48  45       K= 7 H= 4      19  52  48-      8  91  83-       8 134 134       0 222 227
15  43  39       7  85  80-      4  28  29       0  93  99-      K= 5 H= -4      9  81  74       10 398 471        1  40  36-
16  59  55       8 231 239-      5  67  54       1 125 124-      1 117 110       11  43  39-      11 182 203-       2  40  33-
K= 5 H= 3        9  31  25-      6  38  32       3 212 215-      2 226 234-      15  30  28-      12  73  65        3 106 109
0 105 101-      10 139 137       8  18  24-      4 233 277       3  98  99-      16  39  43-      13 120 130-       4  93  91-
1  61  49-      11 221 235-      9  57  54-      5 115 123-      4  83  81-      K= 4 H= 5       14  72  69-       5  60  57
2 147 138       12 123 117       K= 11 H= -3     6  94 110       6  59  59-      0  86  79-      15  35  22-       7  71  70
3 115 120-      13  69  67       1  25  21-      8  29  33-      7 159 159       1  42  36       17  29  20        9  89  84
4  73  71        14 101 103      2  73  77-     12  47  48-      8  37  13-      2  69  69       18  37  32-      11  57  50-
5 182 190-      15  82  78       3  67  65-     13  63  69       9 152 155       3  35  28       K= 4 H= -5      13  35  37-
6 103  86-      16  74  79       K= 0 H= 4      K= 8 H= 4       10 142 140       4  72  60-       1  64  58       14  20  19-
7  67  77       17  36  36-      0  43  48-      0 252 271-      11 105  93       5 140 138-       2 105  90-      K= 4 H= 6
8 163 169-      18  39  37-      6 157 167-      1 122 128-      12  77  82-      6  93  88-       3 180 194       0  53  48-
9 115 113       20  42  39       8  52  46       2 118 132-      13  31  20-      7 112 113-       4  30  24-       2  28  20-
10  99  92-      K= 3 H= -3     12  77  81-      3  88  89-      14  64  59       K= 5 H= 5        5  76  73        3  25  20-
12 121 129       1  83  90-      K= 1 H= 4       4  64  66       16  54  48       0  93  77        6 147 157-       4  56  52-
13 114 124       2 434 485-      0  66  57       6  56  41       17  46  36-      1  74  67-       7  39  37        6 148 154-
14 134 140       3 174 186-      1 411 437       7  54  59-      18  38  32-      2  88  91        8 186 211        7  56  58-
15  74  70        4  36  33      2 358 366      10  66  61-      K= 6 H= -4      3  57  50-       9 283 326        8  82  80-
16  29  24        5 127 132      3 342 352       K= 9 H= 4       1  53  44       5  33  29       10 121 134       10  23  20
17  42  48-       6 143 139      4  79  64       1 108  99       2 105 110       6  83  77-      11 167 183       11  74  67
K= 6 H= 3         7 147 159-     5 189 194-      2  43  43       3  34  23       7  45  38       12  71  69-      12  40  35
0  44  40         8 177 182      6 179 174       3  26  24       4  93  91-      8  66  65       13  46  48-      13  31  25
1  73  76         9 143 135-     7  77  61-      8  30  35-      6  94  96-      9  38  31-      14  58  59       K= 5 H= 6
3 108 120-       10 262 282-     9 118 105       9  63  78-      7  38  35       10  29  22-      15  26  25-      1 103  98-
4 138 135        11  95  86     10  88  84       K= 10 H= 4      8  54  51-      12  88  90-      16  21  18-       2  33  29
5 142 139-       12 396 457-    12  69  61       0  86  85-      9  88  85       13  31  23-      18  39  37        3  26  17
6  98  97        13 124 123     13  43  43       1  56  44       10  32  23-      14  85  94-      K= 5 H= -5       4  56  57
8  74  75        15  48  44     16  67  69       2  59  51-      13  38  31       K= 6 H= 5        1 152 154-       5  42  41
9  39  39        16  25   8     K= 2 H= 4        3  41  34       14  47  44-      0  87  89-       2 171 177        6  59  56-
10 188 214-      17  58  61-     0  36  41-      4  30  26-      15  47  35       1  82  83-       3 112 112-       7  51  51-
11 119 130-      20  23  24      1 115 117       5  40  41       16  45  41-      2  82  74        4 131 130        8 140 142-
12  44  56-      K= 4 H= -3      2 118 121       K= 0 H= -4      17  34  34-      3 106 119-       6 144 155-       9  54  50-
13 115 119        1 221 238      3  82  71-      2 212 255       K= 7 H= -4      4 124 137        7 115 120       10  45  39-
14  52  53         2 140 126      4  71  67-      4  69  73       1  65  64-      5  54  58        9  91  93       12  33  36-
16  33  38-        3 180 183-     5 108 106       6 270 323       2 203 206       7  78  76       11  25  21-      K= 6 H= 6
K= 7 H= 3          4  91  72      6 113 108-     10 268 320-      3 129 126-      8  46  51-      12  54  44       0  32  29-
0  44  47-         5  38  33-     8  84  78-     14 139 153       4  97  84       10  73  68       13  31  29        2  39  98-
1  54  43-         7 103  94     10 131 131      16 137 150       5  59  54-      11  24  24-      15  26  24        4 147 164
2 201 222          8 100  87     11  99 100       K= 1 H= -4      6 147 144-      12  64  64       16  44  38        5 156 187-
3 190 203-         9 237 243-    12  89  87       1  15  10-      7  52  39       13  72  82-      K= 6 H= -5       6 117 119
4  90  93         10 158 164-    13  67  67-      2 178 185      12  81  61-      K= 7 H= 5        2  22  13        7  57  53-
5 141 156-        11 306 322-    15  46  44-      3 198 206-     15  58  46-      0  41  40        3  38  43-       8  28  24
6  38  38         13  69  53-    17  43  43       4  44  38       K= 8 H= -4      2  57  54-       4  68  76        9  39  38
8 109 121         14  73  67     18  25  32       5  25  25       3 119 118-      3  75  72        5 108 120-      10  41  38
11  60  68-       15  77  77     K= 3 H= 4        6 334 378       5 188 198-      4 142 160-       7  22  21       11  35  33
K= 8 H= 3         16  38  40-     0  89  75-      7 203 208       7  33  38-      5  94 107        8 123 135-      K= 7 H= 6
0 158 173         19  48  44-     1 202 201       8 265 303       8  57  50       6  43  45        9  96 100       0  34  26
1 234 261         K= 5 H= -3      2 153 149       9  42  37      11  43  36-      8  33  33-      10  61  62-       1  34  34
3 179 195          1 135 126      3 100  82      10  37  31-     12  52  39-      9  96 100       11  72  68        2  60  62
4 201 234-         2  41  44-     5 112 117      11  64  69      13  35  25       10  61  62-      15  42  39-       3  25  19
7 100 112-         3 179 168      6  70  60-     12 119 117-     K= 9 H= -4      11  72  68       16  36  32        4  28  32-
9  64  57-         4 379 414-     8  76  62      13 138 157       1  66  63       15  42  39-      K= 7 H= -5       5  85  72
10  55  48         5  90  76      9 128 136-     14  47  34-      5 120 102-      16  36  32        1  28  29        6  91  94-
11  35  24-        6  28  15     10  52  51      15  65  68       6  38  33       K= 8 H= 5        3  33  40-      K= 8 H= 6
12  58  60         7  93  79     11  28  13      19  60  61-      7 108  80-      1  82  77-       4  52  54-       2 136 149
13  25  30         8  71  73-    12  53  57      20  31  27-      8  79  62-      2 123 123-       5  89  96-       3  83  83
K= 9 H= 3          9 189 194-    13  37  27      K= 2 H= -4      K= 10 H= -4     5  62  56-       6 153 163        4  25  30
0 130 130         10 148 150-    15  81  68       1 134 139      1  34  24-      6  89  89        7  55  59-       6  50  52-
1 160 171         11 127 127-    16 104 107-      2 126 128-     2  32  28-      8  28  30        8  96 106       K= 9 H= 6
2  41  38         12  42  39     17  35  35       3  29  22-      3  46  42      10  22  29       10  40  38-       1  38  35
3  40  46         13  41  31     K= 4 H= 4        4 115 110      4  59  47       K= 9 H= 5       11  54  45       K= 0 H= -6
4  27  28         15  48  44-     1  73  59-      5 359 420-      5  87  79       0  68  60-      13  53  48        2 169 200-
5  80  84         16  61  52      2  54  52-      6 133 142-      7  52  49-      1  71  63-      K= 8 H= -5       4  82  83-
6  31  27-        18  69  59-     3 112  89       7  29  23-      K= 0 H= 5       2 104 101-       3  72  64-       6 158 172-
8  22  28-        K= 6 H= -3      4  67  55       8 111 113      0 103 107       3  49  44-       7  74  61        8  47  45
9  35  36-         1  77  77-     5 127 123       9  72  64      2 302 335-      K= 10 H= 5       8  38  39-      10  67  60
10  43  43         2 212 235      6 146 144      10 119 116      4  68  75-      0  50  56-       9  57  49-      12 159 181-
K= 10 H= 3         3  84  80-     7 198 200      12  56  51-     6  85  79       K= 0 H= -5      10  54  46       14 182 198-
1  51  51-         4 165 176-     8  79  75-     13  39  31      8  61  63       2  45  51-      11  20  12       16  32  30-
2  75  69-         5 103 107     10  64  60-     14  47  43-     10 142 159       4 278 332       12  63  57       18  31  28
4  41  33-         7 133 136     11  97  99-     15  68  69      12 125 139-      5 278 327       K= 0 H= 6       K= 1 H= -6
5  41  38          8  46  49     12  82  81      16  35  32-     14  84  90-      8 158 179-       0 103 109-      1 107 105
6  29  34          9  35  34-    15  26  26-     17  73  72      K= 1 H= 5       14 188 213-       2  40  41        2  40  37
K= 11 H= 3        10  35  39     16  27  33      18  73  64      2  23  10       16  99  96-       4 173 176-       3  72  70
0  71  79         11  76  76-    K= 5 H= 4       19  83  70-     3 123 132-      18  82  79        6  49  57        4 137 150-
1  23  28         13  87  89-    0  64  45-      20  22  17      4  86  89       K= 1 H= -5       8  52  46        5  42  34-
K= 0 H= -3        14  47  47-    1  84  69-      K= 3 H= -4      5  83  86       2  23  10       14  47  52-       6  65  48-
2 188 225         16  28  29-    2  77  66-      1 100  89      7 114 111       3  38  43-      K= 1 H= 6        7 104 107-
4 154 146-        K= 7 H= -3     3 141 144-      2 582 433      8  51  49       4  68  76        0  93  91-       8  30  28-
6 592 735-         1  75  67     4  59  58-      3 167 159      9  43  35       5 108 120-       1  76  69-      10  61  60
8 194 166-         2 127 125     5  96  83       4  33  28-    11  92  92-       7  22  21        2 227 241-      11  50  37-
10  40  29          3  77  72-    6 133 125       6  56  59-    12  51  56       8 123 135-       3 363 386-      12  58  53
12 116 114-        4 154 155     7 121 118       7 179 185-    13  41  42-       9  96 100        4 248 274-      13  47  49-
14  62  64-         7 188 204     8  65  65       9  74  70-    14 101 114-      10  61  62-       5 152 146-      16  41  33-
16 119 127         8 167 176-    9  76  75      10 124 131-    16  57  62-      11  72  68        6  63  60       17  37  34
18  51  55          9  89  91    10  95  97-     11 113 122-    18  39  43-      15  42  39-       7  55  47       18  25  23-
20  73  70-        10  61  64-   11  56  53-     12  49  43     19  33  38-      16  36  32        8  44  40       K= 2 H= -6
K= 1 H= -3        16  35  29-    12  34  14-     13  58  56-    K= 2 H= -5                          9  51  46-      1 152 159-
1  81  77-                       13  70  70-     14  63  53-    1 144 151                                            ·1     45
                                                               2  60  62-
                                                               4  43  33-
```

Table 1 (cont.)

[Structure factor listing — multi-column numeric table]

used throughout the refinement. The quantity minimized was $\Sigma w(F_o - KF_c)^2$, 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

	x	y	z
N(1)	0·3753 (3)	0·6143 (3)	0·3123 (2)
C(2)	0·4125 (5)	0·7464 (4)	0·2872 (2)
C(3)	0·4061 (5)	0·8770 (4)	0·3324 (3)
C(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)
C(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·C06 (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 R index 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 $B = 3\cdot5$ 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):
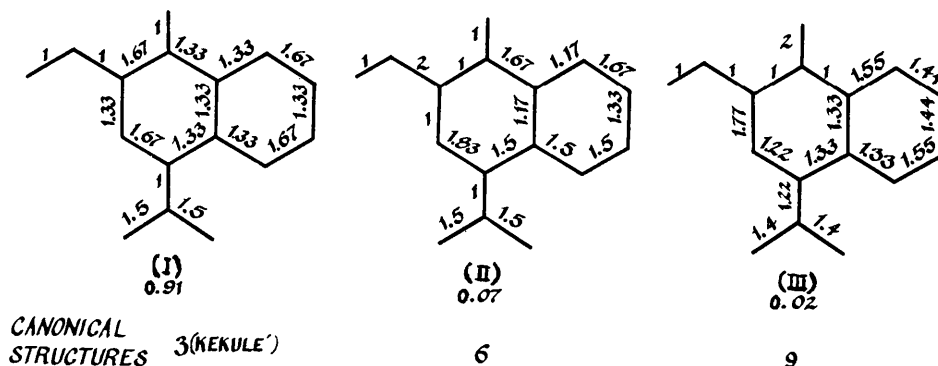
by Dewar & Gleicher (1966) (Table 4). Moreover, the C(8)–N(11) and C(5)–O(16) bond numbers show that there is no major degree of resonance between the nitro or acetoxy group and the quinoline ring. Only a small amount of resonance occurs between the methoxy group and the ring system, as indicated by 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 $\exp[-2\pi^2(h^2a^{*2}U_{11}\cdots\cdots+2klb^*c^*U_{23})]$.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
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)	−0·0090 (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 (0·0012)
C(7)	0·0497 (0·0014)	0·0225 (0·0014)	0·0335 (0·0014)	−0·0026 (0·0011)	0·0060 (0·0011)	0·0003 (0·0011)
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)	−0·0009 (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 (0·0011)
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 (0·0010)
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)	0·0108 (0·0009)
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)	0·0051 (0·0011)	0·0016 (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)	0·0503	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)	0·0503	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)	0·0503	0·0523	0·0507	0·0000	0·0000	0·0000
H(28)	0·0503	0·0523	0·0507	0·0000	0·0000	0·00C0
H(29)	0·0503	0·0523	0·0507	0·0000	0·0000	0·0000

Table 4. *Bond lengths and estimated standard deviations*

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. *Some least-squares planes of atoms and some dihedral angles*

Coefficients in $AX + BY + CZ - D = 0$ referred to the crystallographic axes (X, Y, Z in Å)

Plane	A	B	C	D
Quinoline ring	0·9163	−0·1243	0·2595	3·3862
Pyridine moiety	0·9109	−0·1327	0·2702	2·3769
Benzenoid moiety	0·9226	−0·1138	0·2466	3·3508
Nitro group	0·7952	0·3723	−0·5771	−0·6339
Acetoxy group	0·1612	0·6890	−0·7214	−1·2715

Deviations from the plane (Å)

	Quinoline	Pyridine	Benzene	Acetoxy	Nitro
N(1)	−0·000	0·002	0·045		
C(2)	0·013	−0·002	0·078		
C(3)	0·015	−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	0·016	−0·016		
C(9)	−0·018	−0·000	0·008		
C(10)	−0·020	−0·002	0·006		
O(16)				0·001	
C(17)				0·002	
O(18)				−0·004	
C(19)				0·001	

Dihedral angles

Intersecting planes	Angle
Acetoxy and benzenoid	79·1°
Nitro and benzenoid	59·2
Pyridine and benzenoid	1·8

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

(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)H₃ 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)···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(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.

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*

Atoms	Distance
C(15)···C(6)	2·392 Å
C(15)···C(7)	2·835
C(15)···H(7)	2·68
H(24)···C(6)	2·71
H(24)···C(7)	2·78
H(24)···H(7)	2·40
H(25)···H(7)	2·40
H(26)···C(6)	2·57
H(26)···C(7)	2·70
O(16)···C(6)	2·39
C(17)···C(5)	2·339
C(17)···O(14)	3·013
C(17)···C(6)	3·068
O(18)···C(5)	2·639
O(18)···C(6)	3·139

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