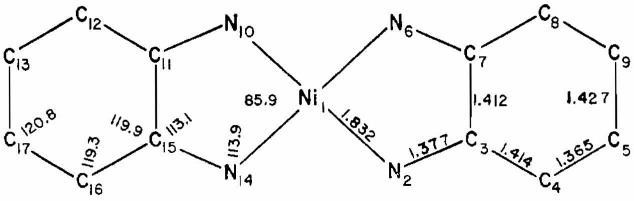

Figure 2.—The planar $Ni[C_6H_4(NH)_2]_2$ molecule showing the numbering scheme and average lengths and angles for bonds assumed to be chemically equivalent.

and 1.84 Å in bis(salicylaldiminato)nickel(II).[19] The average N–N chelate "bite" distance is 2.49 Å, and the average interligand N–N distance is 2.68 Å. The average C–N bond length of 1.38 Å is significantly longer than the 1.30 Å bond found in bis(dimethylglyoximato)nickel(II)[18] and the average length of 1.29 Å determined from various salicylaldimine complexes.[20] It is, however, much shorter than the sum (1.47 Å) of the single-bond covalent radii.[21] We note that the C–S distances in a number of sulfur-donor complexes characterized by similar electron-transfer reactions fall in the range 1.69–1.75 Å,[22] intermediate between the single- and double-bond lengths[21] of 1.81 and 1.61 Å, respectively. Thus it appears that the π bonding is delocalized throughout the ligand system. Although the differences in bond lengths within the benzene rings are of only marginal significance, the slightly shorter C_4–C_5, C_8–C_9, C_{12}–C_{13}, and C_{16}–C_{17} bonds suggest a bit of α-diimine character.

The bond lengths in the chelate rings, especially the 1.38-Å C–N distance, seem inconsistent with the early formulation[2] based on nickel(IV), but the electronic delocalization of which both they and the fact of planarity itself are indicative is consistent with the convincing evidence of Balch and Holm[7] that this is the neutral central member of a family of complexes interrelated by electron-transfer reactions. The similarity of the molecular structures of $Ni[C_6H_4(NH)_2]_2$ and $Ni[S_2C_2(C_6H_5)_2]_2$[22] should be noted because the latter compound plays the same role in a family of sulfur-bonded complexes. Others[6,7,22] have recognized that the electronic structures of highly delocalized complexes such as these cannot be adequately described by simply assigning oxidation states to the metal ions but must instead be approached through rather complete molecular orbital treatments.

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The Crystal and Molecular Structure of Tetra-n-butylammonium Tribromo(quinoline)nickelate(II), $[(n\text{-}C_4H_9)_4N][Ni(C_9H_7N)Br_3]$[1a]

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Received May 8, 1968

The structure of tetra-n-butylammonium tribromo(quinoline)nickelate(II), $[(n\text{-}C_4H_9)_4N][Ni(C_9H_7N)Br_3]$, has been determined by single-crystal X-ray diffraction methods. The crystals are triclinic, space group $P\bar{1}$, with $a = 12.282$ Å, $b = 10.291$ Å, $c = 12.726$ Å, all ± 0.002 Å; $\alpha = 101.02°$, $\beta = 99.51°$, $\gamma = 106.55°$, all $\pm 0.01°$. For $Z = 2$ the measured and calculated densities are 1.51 ± 0.01 and 1.512 g/cm^3, respectively. Counter data were collected for 5830 independent reflections by the θ–2θ scan technique. The structure was refined, including hydrogens, by least-squares methods to a conventional R value of 0.061. The anion has roughly tetrahedral coordination about the nickel by three bromine atoms and the quinoline nitrogen, with an average Ni–Br distance of 2.375 Å and an Ni–N distance of 2.029 Å. The average N–Ni–Br angle is 105.1° while the Br–Ni–Br angles average 113.3°. The coordinated quinoline is accurately planar; however, the Ni–N–Q bond makes an angle of 4.5° with the quinoline plane. The bond distances internal to the quinoline correlate well with variations predicted by π-MO theory. The cations approach the anions such that there are four distances between ion centers (Ni–N-CAT) in the range 5.98–6.89 Å. Three of the four cation butyl chains adopt the *trans* conformation while the fourth has the *gauche* conformation with a dihedral angle of 66.5°.

Introduction

Reliable evidence concerning the existence of nickel(II) complexes with tetrahedral or pseudo-tetrahedral coordination has been available only within the past decade.[2] These complexes fall into several stoichiometric classes: NiX_4^{2-}, $NiLX_3^-$, NiL_2X_2, and $Ni(L\text{–}L)_2$, where X is a halogen, L a neutral ligand such as an amine, phosphine, or phosphine oxide, and L–L repre-

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[2] For a discussion see F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry," 2nd ed, Interscience Publishers, New York, N. Y., 1966, p 883 ff.

TABLE I

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $[(n\text{-}C_4H_9)_4N][Ni(C_9H_7N)Br_3]$[a]

```
FCA(0,0,0) =  2674

H,K=  0,  0
  L FOB FCA
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  2 308-313
  3 145-139
  4 215-205
  5  84  79
  6  17  19
  7 289-282
  8  68 -64
  9  52 -50
 10  64 -60
 11  39  36
 12   7  -4
 13  32  33
 14  56  57
 15   4  -9

H,K=  0,  1
  L FOB FCA
-15  33  37
-14  18 -16
-13  28 -22
-12  18 -19
-11  75 -70
-10   4  -1
 -9  89 -88
 -8  13 -21
 -7  89  96
 -6  77  76
 -5  28 -28
 -4 270 277
 -3  23  16
 -2 365 365
 -1 175 171
  0 461-538
  1 381-417
  2 108 109
  3  33 -37
  4  28  28
  5 214-217
  6 249-247
  7 163 162
  8  60  57
  9  71  67
 10 124 121
 11  10  20
 12  18  11
 13   8   2
 14  31 -35

H,K=  0,  2
  L FOB FCA
-15  34 -36
-14  46 -46
-13  22 -19
-12   6   5
-11  70  70
-10  18 -21
 -9  93  98
 -8 113 114
 -7 117-115
 -6 214 218
 -5 121 113
 -4  22  15
 -3  56  58
 -2 688-799
 -1 366-379
  0  42 -39
  1 118 119
  2 230 227
  3  98  96
  4 256-253
  5 198 201
  6 203 206
  7  63  59
  8  97  87
  9  50 -48
 10   9  -7
 11   8  11
 12  67 -65
 13  29 -29
 14   0   4

H,K=  0,  3
  L FOB FCA
-15   9   7
-14  16  11
-13  90  91
-12  19  12
-11  38 -35
-10  74  80
 -9  41  40
 -8  57 -56
 -7   0   7
 -6 214-214
 -5 109-105
 -4 172-176
 -3 256-259
 -2 321 335
 -1 372 396
  0  81  86
  1 153 156
  2  93 -92
  3  52 -50
  4 451 458
  5  58  55
  6 119-107
  7 148-141
  8 268-252
  9  25  18
 10  41  41
 11  74 -71
 12  19  19
 13  19  18

H,K=  0,  4
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-14  31  35
-13  53 -51
-12  17 -13
-11  46  49
-10  41 -39
 -9  44 -43
 -8 109-112
 -7 158-161
 -6  62  64
 -5  62 -59
 -4  82 -71
 -3 378 396
 -2 186 187
 -1  70 -67
  0  34 -38
  1 109-112
  2 229 234
  3  14 -10
  4 232-237
  5 114-108
  6  68 -65
  7  11  12
  8 145 140
  9  23 -24
 10  27 -31
 11  58  57
 12  21  23

H,K=  0,  5
  L FOB FCA
-15  41 -48
-14  45 -49

-13   0  17
-12  23  21
-11   0  -9
-10  69 -69
 -9  67 -69
 -8 114 116
 -7 190 196
 -6  29  31
 -5  68  70
 -4  28  29
 -3 106-111
 -2  37 -40
 -1  99 -98
  0  58 -56
  1 151 150
  2 226-216
  3 200-192
  4  81  78
  5  61  59
  6 165 156
  8  31 -33
  9  30  27
 10  11  19
 11  26 -24
 12   9   2

H,K=  0,  6
  L FOB FCA
-15  19  20
-14  25  27
-13  16 -18
-12  40 -37
-11  28  26
-10  53  51
 -9 191 195
 -8   9   2
 -7  83 -86
 -6  11   3
 -5 125-126
 -4  90 -94
 -3  36  30
 -2 119-118
 -1  31  35
  0  40  41
  1 151-142
  2 106 108
  3 153 146
  4  69  63
  5  24  20
  6 120-114
  7  44 -40
  8  61  60
  9  23 -27
 10  26 -21
 11   5   1

H,K=  0,  7
  L FOB FCA
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-12  47  51
-11  72  73
-10  42 -41
 -9 127-125
 -8  37 -35
 -7  26  29
 -6 116-115
 -5  20  19
 -4  14  -8
 -3  48 -49
 -2 111 110
 -1  16  19
  0   9 -10
  1 101  96
  2  60  55
  3  13   9
  4  41 -40
  5  73 -70
  6  13  17
  7  36  38
  8  46 -41
  9   6  -2
 10   8  -8

H,K=  0,  8
  L FOB FCA
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-11  77 -76
-10  77 -76
 -9  61  56
 -8  60  56
 -7  38  37
 -6  57  59
 -5  29 -31
 -4   0   4
 -3  61  59
 -2  20 -20
 -1  64  57
  0  42 -41
  1  76 -73
  2  14  -5
  3  38 -33
  4  33 -31
  5  53  54
  6  18 -15
  7   0  -8
  8  15  16

H,K=  0,  9
  L FOB FCA
-13  15 -16
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-10  69  67
 -9  26  20
 -8  24 -20
 -7  23 -21
 -6  17  10
 -5  66  61
 -4   8   1
 -3  72 -67
 -2  33 -36
 -1  32 -28
  0  30 -27
  1   0  11
  2  18 -21
  3  39  35
  4  26  28
  5  30 -31
  6   0  12
  7   6   8

H,K=  0, 10
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-10  31 -34
 -9  36 -35
 -8  11  -8
 -7  48  47
 -6   6  -3
 -5  64 -64
 -4  22 -26
 -3   7  10
 -2  11  12
 -1  23  18
  0  23 -19
  1   8  11
  2  80  76
  3  19 -13
  4   9 -15
  5   0   5

H,K=  0, 11
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 -9  23  25
 -8   0   5
 -7  27 -27
 -6  29 -32
 -5  25  24
 -4  32  33
 -3  26  23
 -2   3   1
 -1  12 -16
  0  15  13
  1  11  -6
  2  36 -41

H,K=  0, 12
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 -6  25  29
 -5   4  -2
 -4  11  -7
 -3  14 -15
 -2  13 -14

H,K=  1,-12
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  0  13  14
  1   0   1
  2  21 -24
  3   6   8
  4   7   8
  5  12   7
  6   0   3
  7  19 -26

H,K=  1,-11
  L FOB FCA
 -3  11  -9
 -2  10 -11
 -1   0   9
  0   2  -5
  1  16 -12
  2  19  15
  3  16  11
  4  17  17
  5   0  -9
  6  18 -15
  7  19  29
  8   5  -1
  9  24 -25
 10  20 -22

H,K=  1,-10
  L FOB FCA
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 -5   0  -5
 -4  13 -19
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 -2  43  41
 -1  10  11
  0  21  24
  1   7  -9
  2  23 -17
  3  12  19
  4  36 -36
  5  25 -25
  6  31  30
  7  32 -31
  8  32 -26
  9  18 -14
 10  17  19
 11  40  42

H,K=  1, -9
  L FOB FCA
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 -5  16  10
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 -2  23 -24
 -1  27 -25
  0  32 -30
  1  59  60
  2   7  -3
  3 104-102
  4   9  -5
  5  16 -16
  6  15 -11
  7  20  16
  8  34  32
  9  43  39
 10  31  28
 11  41 -43
 12  19 -23
 13  24  26

H,K=  1, -8
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 -8  25  19
 -7   0  -1
 -6  35  36
 -5   0   3
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 -2  14  15
 -1  63 -67
  0  81  83
  1  66 -67
  2  25 -24
  3 134 131
  4   9  -4
  5  19 -17
  6  82  81
  7  47  41
  8  14   2
  9  42 -40
 10  73 -71
 11  21  27
 13   5 -12

H,K=  1, -7
  L FOB FCA
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 -9   7  -2
 -8   0   2
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 -4  65  65
 -3  60  58
 -2  57  58
 -1  26 -30
  0  85 -87
  1 141 141
  2 172 177
  3   0   1
  4  15   8
  5  13 -15
  6 144-137
  7  94 -86
  8  62 -57
  9   0   7
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 11   5  12
 12   8 -13
 13   7  -5
 14  17  19

H,K=  1, -6
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-11   0   7
-10  32 -36
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 -8   3   1
 -7  83 -81
 -6 100 103
 -5 113 115
 -4  18  19
 -3  94  96
 -2 121-124
 -1   0  -2
  0 238 249
  1  26 -21
  2 154-150
  3 122-119
  4 231-217
  5  12  11
  6  36  35
  7  37 -38
  8 118 107
  9  55 -54
 10  26  27
 11  56  60
 12  29  28
 13  31  25
 14  16  13

H,K=  1, -5
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-11   9  -9
-10  33  33
 -9  17 -11
 -8  10   5
 -7  90  92
 -6  16  -6
 -5  67 -68
 -4  36 -36
 -3 131-136
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 -1  33  36
  0 367-396
  1 195-194
  2  85  73
  3  76  72
  4 383 379
  5   0   6
  6  27  24
  7 132 129
  8   5 -10
  9  44 -42
 10  45  43
 11  47 -51
 12  14   7
 13  38 -33
 14  57 -61
 15  13  -6

H,K=  1, -4
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-11  45  43
-10   7   7
 -9  49  49
 -8  40  37
 -7 115-116
 -6  52 -51
 -5  58 -62
 -4  42 -43
 -3 100 102
 -2 215-222
 -1 234-247
  0 247 262
  1 244 252
  2 495 514
  3  22 -15
  4 222-223
  5  48  42
  6  54  56
  7  93 -88
  8  30 -30
  9 103 -99
 10  89 -88
 11  12  -8
 12  48 -43
 13  14  11
 14  55  59
 15  33  35

H,K=  1, -3
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-11  39 -39
-10  32  29
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 -8  87 -91
 -7   0  13
 -6  71 -74
 -5 149 153
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 -3 226-225
 -2 320 329
 -1 490 520
  0 156 157
  1  77  76
  2 576-626
  3 251-250
  4 204 205
  5  66 -90
  6  90 -92
  7 127-127
  8 122-117
  9  94  94
 10  76  77
 11  20  15
 12 102 101
 13  49  45
 14   8 -21
 15  10  -2

H,K=  1, -2
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-13  62 -59
-12  35 -36
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 -8  30  31
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 -6 203 214
 -5 123-122
 -4 105-108
 -3 371 398
 -2 125-126
 -1 208-220
  0 260-266
  1 318-325
  2 372 384
  3 351 356
  4 251-254
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  6   7  -9
  7 105 104
  8 316 312
  9   6   6
 10  23 -22

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 14  19 -21
 15  20 -20

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-11  53  55
-10 100 104
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 -6 187-192
 -5 246 235
 -4  19 -20
 -3 701-862
 -2 406-442
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  0 308 319
  1 248 252
  2   6  -7
  3 158-152
  4 191 190
  5 245 243
  6 243 246
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 11  69 -59
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 13  18 -18
 14   6  12
 15  18  20

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-10  34 -31
 -9  55  54
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 -5 242-239
 -4 188-178
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  0 184 160
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  3 276 279
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  6 441-443
  7 243-237
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 11  14  14
 12  12  -8
 13  51  47
 14  26  26

H,K=  1,  1
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-13  30 -31
-12  55 -55
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-10   0   3
 -9 175-181
 -8  52 -49
 -7  64  55
 -6  48  50
 -5 327 340
 -4 202 193
 -3 156 147
 -2 228 230
 -1  96 -93
  0 335-344
  1 170 160
  2 122-116
  3  12 -14
  4 250-247
  5 273-276
  6 242 240
  7 195 185
  8   5   7
  9   0   7
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 11  13 -21
 12  52  50
 13  25 -25
 14  17 -19

H,K=  1,  2
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-13  34  31
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-11  49 -53
-10  21 -22
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 -7 150 146
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 -5 206-216
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 -3 140-139
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  5 514 519
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  7  96 -86
  8  22 -17
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 10  37  40
 11  33 -34
 12  75 -71
 13   0   2

H,K=  1,  3
  L FOB FCA
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-12  37 -35
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  5 287-263
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  8  69 -63
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 10  87 -66
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 13  12   7

H,K=  1,  4
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 -3  63  70
 -2  66 -62
 -1 250 246
  0  50  48
  1  48  41
  2  21 -19
  3 250-251
  4 166-164
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  6  49 -45
  7   0   6
  8   8   7
  9  49 -48
 10  49  48
 11  30  28
 12  17  16

H,K=  1,  5
  L FOB FCA
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-13   9 -20
-12 100-101
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-10  40  35
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 -8 184 189
 -7  45 -44
 -6  82 -83
 -5  40  43
 -4  82  76
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 -2  25 -23
 -1 242-246
  0  75 -74
  1 120-116
  2 209-198
  3 129 130
  4 125 119
  5  14   8
  6 111 104
  7  16 -19
  8  27  28
  9  66  65
 10   0  -4
 11  15 -15

H,K=  1,  6
  L FOB FCA
-15   0   5
-14  20 -28
-13  32 -30
-12 110 104
-11  17  18
-10  46  45
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 -6 122 123
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 -4  69 -72
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  0  63 -61
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  2 191 184
  3  26  11
  4  16  12
  5  10 -16
  6  45 -46
  7  59  55
  8   0  -5
  9  52 -51
 10  18 -18

H,K=  1,  7
  L FOB FCA
-14  21  22
-13  39  43
-12  22  21
-11  68 -66
-10  75 -72
 -9  46 -47
 -8  74  73
 -7  63  65
 -6  80 -79
 -5  91 -91
 -4  49 -47
 -3 148 142
 -2 141 142
 -1  12 -15
  0   0  -5
  1  61  58
  2  45 -45
  3  20 -10
  4  87 -80
  5   0  -8
  6  22  21
  7  39 -39
  8  25 -25
  9   0  11

H,K=  1,  8
  L FOB FCA
-13  18 -20
-12  37 -40
-11  26 -24
-10  55  51
 -9  41  36
 -8  72 -71
 -7  42 -40
 -6  22  16
 -5 116 117
 -4 130 127
 -3  61 -62
 -2  55 -56
 -1  19 -18
  0  69 -67
  1  24  16
  2   5   1

  3  24 -23
  4  24  24
  5  11  12
  6  22 -21
  7  19  19
  8  19  21

H,K=  1,  9
  L FOB FCA
-12  23  25
-11  36  34
-10   8 -15
 -9  41 -40
 -8  47  48
 -7  52  55
 -6  41  37
 -5  29 -29
 -4 101 -98
 -3  20  20
 -2  40  41
 -1  62 -64
  0   9   4
  1  12  -3
  2   0  -1
  3  19  19
  4  11  -1
  5   0  -7
  6  14  20

H,K=  1, 10
  L FOB FCA
-11  15 -14
-10   0  11
 -9   2  10
 -8  23  21
 -7  23 -21
 -6  70 -70
 -5  24 -26
 -4  59  58
 -3  23  23
 -2   6  -5
 -1   4   8
  0  12 -14
  1   0  -4
  2  11  25
  3  10  -2
  4   0   2

H,K=  1, 11
  L FOB FCA
 -9   4  -2
 -8  12 -11
 -7  18 -17
 -6  27  25
 -5  26  29
 -4   7   1
 -3  22 -22
 -2   3  -4
 -1  23  22
  0  29  31
  1  11 -10
  2  17 -23

H,K=  2,-12
  L FOB FCA
 -1   0   5
  0  16  21
  1  20 -21
  2   0  -1
  3   0   6
  4   7  -5
  5   4  12
  6   0   2
  7   0   3

H,K=  2,-11
  L FOB FCA
 -4  19 -23
 -3  19 -25
 -2  43  46
 -1  30  32
  0  32 -33
  1  11  10
  2  18  14
  3  17  14
  4  27  25
  5  17 -16
  6  10  10
  7   0   7
  8  40 -43
  9  30 -30
 10  13  -1

H,K=  2,-10
  L FOB FCA
 -6   0   3
 -5   0  -6
 -4  22  23
 -3  30  31
 -2  51 -51
 -1  46 -43
  0  61  59
  1  37  34
  2  30  30
  3  16 -16
  4  88 -85
  5   5   1
  6   0  -2
  7  54 -51
  8  32  34
  9  28  25
 10   2  15
 11   0 -10

H,K=  2, -9
  L FOB FCA
 -8   0  -7
 -7  17  18
 -6  10   3
 -5  33  37
 -4  23  23
 -3  47 -47
 -2  26  19
 -1   4   4
  0  11 -13
  1  14 -11
  2  66 -64
  3  34 -34
  4  43  36
  5  16  13
  6  37  36
  7  23  22
  8   0  -1
  9  17  16
 10   0  -8
 11  14  -8
 12  29  27

H,K=  2, -8
  L FOB FCA
 -9  22  26
 -8  17   7
 -7   0  -6
 -6  18  23
 -5  61 -59
 -4  40 -40
 -3 110 109
 -2  72 -74
 -1  59 -56
  0  33 -34
  1  66 -70

  2 129 125
  3 141 141
  4  55  50
  5  32  31
  6  99 -94
  7  15 -11
  8  36  37
  9  69 -66
 10   0  -1
 11   0   6
 12  43 -43
 13  25 -24

H,K=  2, -7
  L FOB FCA
-10   8  12
 -9  14 -13
 -8   4  10
 -7  20 -21
 -6 150-145
 -5  27  32
 -4  62  63
 -3  62 -63
 -2  43 -46
 -1  12   3
  0 134 137
  1 242 241
  2  79 -77
  3 105-103
  4  39 -35
  5   0  -6
  6 117 111
  7  21 -16
  8 151-146
  9  51 -49
 10  30  33
 11  23 -19
 12  42  44
 13  29  30
 14  21  21

H,K=  2, -6
  L FOB FCA
-11  22 -18
-10  40 -37
 -9  31  33
 -8  38 -39
 -7   8   1
 -6 151 157
 -5  18 -11
 -4   4 -11
 -3  81  83
 -2  19  20
 -1 205 212
  0  39 -40
  1 350-362
  2  54 -49
  3  20 -15
  4  23  16
  5  48  42
  6 136-129
  7  20  14
  8  96  94
  9  17  15
 10  66  58
 11  50  46
 12   0   1
 13   0  -0
 14  36 -37

H,K=  2, -5
  L FOB FCA
-12  14  -4
-11  25  20
-10  36  38
 -9  24 -25
 -8  95  97
 -7  40  41
 -6  59 -61
 -5  95  98
 -4  40 -39
 -3  17 -20
 -2  23 -23
 -1 384-411
  0 187-197
  1 249 249
  2 121 118
  3  17  16
  4  38 -36
  5 116-115
  6 243 236
  7 229 228
  8  51 -50
  9  28  21
 10  83 -79
 11  68 -69
 12  39 -37
 13  33 -28
 14  19  19

H,K=  2, -4
  L FOB FCA
-13  15  12
-12  33  32
-11  14 -14
-10   0  -8
 -9  71  72
 -8  98-102
 -7  82 -87
 -6  56  56
 -5 186-189
 -4  70 -68
 -3 148-155
 -2 250-257
 -1 313 335
  0 216 224
  1 132 125
  2 199 194
  3 134-132
  4 122 124
  5 379 387
  6 112-111
  7 210-204
  8 144-141
  9  93 -92
 10  39  37
 11   0  -2
 12  14  -2
 13   0   4
 14   8   6
 15  14  11

H,K=  2, -3
  L FOB FCA
-14   8   1
-13  14 -15
-12  58 -58
-11  42  42
-10  16  -4
 -9  87 -83
 -8  28  23
 -7  24 -23
 -6  11 -16
 -5  53  61
 -4  47  47
 -3 215 216
 -2 530 558
 -1 138-140
  0 281-287
  1  22  23
  2 362-372

  3 246 245
  4  45 -47
  5 410-444
  6 205-197
  7  21  19
  8 129 119
  9 167 162
 10  31 -27
 11  10  16
 12  69  70
 13   0   0
 14   4  11
 15   0  -4

H,K=  2, -2
  L FOB FCA
-14  31 -32
-13  48 -47
-12  72  75
-11  32 -28
-10  71 -74
 -9  23  22
 -8  28 -25
 -7 188 199
 -6 279 291
 -5  25  24
 -4  62  57
 -3  94 -86
 -2 459-488
 -1  28 -17
  0 336-348
  1 125 117
  2  53 -48
  3 437-460
  4 112-122
  5 335 349
  6 163 169
  7 283 275
  8  15  14
  9 102-100
 10  29  28
 11  59  65
 12  48 -49
 13  21 -24
 14  32 -35

H,K=  2, -1
  L FOB FCA
-15  17 -18
-14  28  29
-13  27  23
-12  24 -25
-11  12   4
-10  75  74
 -9  62  62
 -8 141 147
 -7  67 -73
 -6 291-300
 -5  35  27
 -4 312-326
 -3 143-130
 -2 162-167
 -1 153 159
  0 261 251
  1  50 -51
  2 221-229
  3 574 605
  4 439 460
  5  65  70
  6  14 -11
  7 268-265
  8  57 -54
  9  78  76
 10  95 -91
 11  83 -85
 12  47 -46
 13  18 -21
 14  33  36

H,K=  2,  0
  L FOB FCA
-15  39  41
-14  29 -34
-13  28 -27
-12  90  93
-11  48  51
-10  17  18
 -9  78 -81
 -8 318-334
 -7   0  12
 -6 106 107
 -5  20 -23
 -4 294 294
 -3 201-186
 -2 265 267
 -1 161 166
  0 441-468
  1  45 -49
  2 548 564
  3 155-149
  4 262-274
  5 332-324
  6 235-230
  7 144 134
  8  56  52
  9 116-108
 10  64  59
 11   0   9
 12  61  60
 13  58  61
 14  12  -6

H,K=  2,  1
  L FOB FCA
-15  39 -41
-14  11  12
-13  11  17
-12  74 -73
-11  76 -75
-10 120-125
 -9  78 -77
 -8 254 264
 -7  83  83
 -6  74  74
 -5 127 127
 -4  47 -48
 -3  35  38
 -2 475 482
 -1 172-170
  0 127 121
  1 420-412
  2 603-635
  3 143-143
  4   8   6
  5 174 171
  6 220 215
  7  65 -85
  8  18 -19
  9 146 142
 10  28  28
 11  55  57
 12  15 -18
 13  36 -40

H,K=  2,  2
  L FOB FCA
-15   6   9
-14   9  -9
-13  38 -38
-12  27 -36
-11   2 -17

-10 207 209
 -9 125 128
 -8   7  -8
 -7  11   7
 -6  72 -69
 -5  23 -23
 -4 179 172
 -3 163-163
 -2 315-325
 -1  62  67
  0 318-316
  1  63 -61
  2 221 213
  3 190 178
  4 242 232
  5  86  78
  6  94 -92
  7  56  54
  8  20 -18
  9  32  32
 10  57 -58
 11 100 -96
 12  28 -27
 13  20  25

H,K=  2,  3
  L FOB FCA
-15   0  -1
-14  19  15
-13  24  25
-12  74  75
-11 127 131
-10  95 -94
 -9 164-163
 -8  31 -31
 -7   9 -11
 -6 176 171
 -5  94 -99
 -4 497-513
 -3  71 -65
 -2 123 124
 -1  77  78
  0 328 326
  1  89  92
  2  67 -58
  3 104  97
  4 220-215
  5  43 -46
  6  47  45
  7  18  -7
  8  18  14
  9  70 -70
 10  69 -68
 11  50  50
 12  38  41

H,K=  2,  4
  L FOB FCA
-15  16  21
-14  10  10
-13   0   9
-12  35 -35
-11 164-167
-10  67 -62
 -9  54  56
 -8  31  33
 -7  23  21
 -6 155-163
 -5  57 -57
 -4 531 557
 -3 174 176
 -2  15  21
 -1  12  11
  0 141-144
  1   0 -14
  2  42 -43
  3 172-171
  4  39  36
  5  29 -26
  6  92 -87
  7  22 -15
  8   9  -7
  9  63  64
 10  84  85
 11  16 -18
 12  12 -14

H,K=  2,  5
  L FOB FCA
-15  14 -16
-14  14 -13
-13  42 -44
-12  16 -25
-11  24  15
-10 114 111
 -9   2   5
 -8  52 -52
 -7  23 -26
 -6 214 221
 -5 187 187
 -4   2 -16
 -3  99-100
 -2 191-192
 -1 103-105
  0  51  49
  1  96 -92
  2  27 -23
  3  76  74
  4  11 -12
  5  38 -34
  6  70  67
  7  13  13
  8  55  55
  9   0  -0
 10  35 -41
 11   0   3

H,K=  2,  6
  L FOB FCA
-15   0  -3
-14   0  -3
-13  61  61
-12  62  64
-11  20 -20
-10  29 -29
 -9  50 -49
 -8  75  80
 -7 111 114
 -6 155-168
 -5 172-181
 -4  85 -86
 -3  29 -27
 -2 154 153
 -1   0   8
  0 112-104
  1  76  76
  2  48  50
  3  20  23
  4 103  94
  5   0  -2
  6   9  16
  7   0   7
  8  59 -58
  9  22 -23
 10   3  13

H,K=  2,  7
  L FOB FCA
-14  15  16
-13   4   2
-12  58 -55

-11   8 -12
-10   0   5
 -9  48  48
 -8  57 -56
 -7 140-145
 -6  19 -21
 -5  87  89
 -4 110 111
 -3 109 111
 -2  26 -24
 -1  79 -80
  0 133 128
  1  32  26
  2  18 -18
  3  31 -26
  4  97 -99
  5   0  13
  6   0  -5
  7  38 -37
  8   7  12

H,K=  2,  8
  L FOB FCA
-13   0   5
-12   7  -3
-11   0   1
-10   0  -5
 -9  47 -49
 -8   8  -9
 -7  75  74
 -6  65  61
 -5  35  33
 -4  15 -10
 -3  42 -44
 -2  25  19
 -1  17  14
  0   4 -16
  1  33 -34
  2  65 -60
  3  13  -8
  4  15  18
  5  12 -13
  6   0   8
  7  28  30

H,K=  2,  9
  L FOB FCA
-12   0   5
-11   6  -4
-10  11 -12
 -9  37  38
 -8  62  64
 -7  24 -27
 -6  42 -43
 -5  58 -55
 -4  32 -31
 -3  61  63
 -2  11  -2
 -1  45 -44
  0  33 -31
  1  12  16
  2  70  70
  3   0  10
  4   7 -17
  5  15  14

H,K=  2, 10
  L FOB FCA
-11   0  -4
-10  13  13
 -9   9  -5
 -8  30 -33
 -7  33 -31
 -6   9  -1
 -5  43  43
 -4  12  20
 -3  35 -35
 -2  10  -9
 -1  15  16
  0  45  43
  1  15  11
  2  26 -26
  3  14 -16

H,K=  2, 11
  L FOB FCA
 -8   0   9
 -7  15  19
 -6  22  20
 -5  14 -15
 -4  19 -21
 -3  14  12
 -2  22  23
 -1   0   4
  0  16 -15

H,K=  3,-12
  L FOB FCA
 -1   9 -16
  0   5 -17
  1  34 -36
  2   5  11
  3  10  10
  4   2  10
  5  21  23
  6   0 -10
  7  10   3
  8   9  12

H,K=  3,-11
  L FOB FCA
 -4   0  -2
 -3   0  -9
 -2  16  17
 -1  35 -34
  0   0  -5
  1  64  60
  2  19  18
  3  19  20
  4  13 -13
  5  24 -20
  6  10   7
  7  13  14
  8   0 -12
  9   9  -6
 10  10 -13

H,K=  3,-10
  L FOB FCA
 -6  16  15
 -5   4  -6
 -4  47  48
 -3  13   8
 -2  47 -48
 -1  49  45
  0  32  30
  1   8   2
  2   9  -4
  3  73 -75
  4   8  -3
  5  54  56
  6  34 -37
  7  32 -33
  8  10 -12
  9   0   3
 10  18  17
 11  14  14

H,K=  3, -9
  L FOB FCA
 -8  17  20

 -7   0  11
 -6   9  -1
 -5  25  23
 -4  40 -43
 -3   0   2
 -2  45  45
 -1  34 -31
  0  71 -73
  1 105-104
  2  57 -56
  3 129 120
  4  54  51
  5  78 -73
  6  43  38
  7  36  34
  8  41  44
  9  54  56
 10  14 -18
 11  14  -3
 12  10  -6

H,K=  3, -8
  L FOB FCA
 -9  39  38
 -8   0 -10
 -7   8   6
 -6  21 -15
 -5  35 -34
 -4  84  88
 -3  52 -52
 -2 129-131
 -1  12   8
  0  11   6
  1 107 103
  2 126 127
  3 134-136
  4  29 -28
  5 166 157
  6  53  51
  7  36  34
  8  72 -71
  9  90 -91
 10  11 -12
 11  14 -11
 12  16 -21
 13   0  10

H,K=  3, -7
  L FOB FCA
-11  11  12
-10   9   8
 -9  24 -22
 -8  11   4
 -7  43 -43
 -6  30 -26
 -5  52  54
 -4  66 -67
 -3  31 -28
 -2 127 129
 -1  69  69
  0 162 166
  1  35 -35
  2 198-198
  3  89  89
  4  14  13
  5  37 -36
  6  56 -54
  7 108-105
  8  87 -64
  9  78  80
 10   0   7
 11  27  25
 12  12  11
 13   0   9
 14  16  17

H,K=  3, -6
  L FOB FCA
-12   7  12
-11  21 -20
-10  20  20
 -9   6  -9
 -8  84 -83
 -7  47  44
 -6  50  49
 -5  10  -6
 -4 133 134
 -3  40  45
 -2  56 -55
 -1  44  23
  0 271-278
  1  29 -24
  2 120 123
  3  92 -94
  4 101-107
  5 118-119
  6  22 -22
  7 232 222
  8 111 107
  9  65  62
 10   0   5
 11  31 -31
 12  14  11
 13  13  17
 14  29 -32

H,K=  3, -5
  L FOB FCA
-12  31 -31
-11  27  22
-10  11 -13
 -9  10  12
 -8 163 163
 -7   0   6
 -6  38  38
 -5  34  38
 -4 159-165
 -3  23  19
 -2 102-108
 -1 264-281
  0 224 226
  1 122 121
  2 240-248
  3  62 -65
  4  54  53
  5 259 260
  6 287 292
  7 135-134
  8  92 -91
  9  20 -15
 10  16 -11
 11  23  21
 12  49 -47
 13  85 -86
 14  13  16

H,K=  3, -4
  L FOB FCA
-13   7   5
-12  25  25
-11  20 -21
-10  59  54
 -9  33  29
 -8 123-123
 -7  24 -26
 -6  70 -75
 -5 195-200
 -4 186 167
 -3 132-129
 -2  42  38
 -1 218 224

  0  20 -18
  1 116-115
  2 187 196
  3 226 226
  4 260 259
  5 206-203
  6 362-368
  7  55 -55
  8  16  13
  9  15   6
 10   0  -4
 11  71 -70
 12  24  23
 13  50  58
 14   9  13

H,K=  3, -3
  L FOB FCA
-14  14  -2
-13  22 -25
-12  31  30
-11  32  32
-10 122-129
 -9 147-152
 -8  29 -25
 -7  15  11
 -6 169 192
 -5  29  38
 -4  80 -73
 -3 227 238
 -2  30  34
 -1  45 -43
  0 259 269
  1  25  32
  2 111-112
  3 167-166
  4 410-434
  5 149-149
  6 211 204
  7  90  89
  8  55  50
  9  38 -33
 10  18 -16
 11 141 144
 12  24  21
 13   0  -5
 14   7 -10

H,K=  3, -2
  L FOB FCA
-14  37 -39
-13  14  22
-12  13   5
-11 100-100
-10  47  49
 -9 120 124
 -8  91  92
 -7 172 179
 -6 151-156
 -5 163 154
 -4 318 336
 -3 180-182
 -2  31  31
 -1  24  21
  0 678-726
  1 230-229
  2 223-227
  3 190-197
  4 467 466
  5 120 123
  6  24  20
  7  31  33
  8  48 -43
  9 102  97
 10 111 106
 11  53 -46
 12  75 -79
 13  20 -26
 14  17 -17

H,K=  3, -1
  L FOB FCA
-15   0   1
-14   0  -9
-13   4 -10
-12   7   2
-11 114 115
-10  59  60
 -9  46  50
 -8 106-107
 -7 152-159
 -6  38  43
 -5  32 -28
 -4 323-336
 -3  97-100
 -2 262 266
 -1 390-400
  0 325 339
  1  51  51
  2 298 301
  3 449 463
  4 157-146
  5 115-112
  6   6   6
  7  43 -43
  8  62  76
  9  69 -65
 10 178-167
 11  46 -48
 12  13  13
 13  31  32
 14  26  29

H,K=  3,  0
  L FOB FCA
-15   4  11
-14   9  -5
-13  46  47
-12  26  32
-11  69 -68
-10  73 -71
 -9 201-204
 -8  20 -23
 -7 165 164
 -6  54 -58
 -5 224-229
 -4  72 -72
 -3  15  17
 -2 784 981
 -1 282 287
  0  42  39
  1  68  64
  2 201-189
  3 226-226
  4  31 -32
  5  63 -63
  6  12 -15
  7  35 -34
  8 166-161
  9  35 -35
 10  80  80
 11  55  56
 12  52  50
 13   0  -1

H,K=  3,  1
  L FOB FCA
-15   3   2
-14  31  33
-13  36 -41
-12  81 -78

-11  62 -65
-10  21 -20
 -9 126 127
 -8 190 190
 -7 170-175
 -6 130 137
 -5 222 222
 -4 131 135
 -3 347 347
 -2 355-365
 -1 350-351
  0  44 -39
  1 229-218
  2  93 -93
  3 201-189
  4 162-151
  5 109 111
  6  21 -16
  7  72 -70
  8 301 289
  9 109 104
 10   0   1
 11  16  -7
 12  45 -43
 13   4  -2

H,K=  3,  2
  L FOB FCA
-15   0  -3
-14  53 -54
-13   8   5
-12  51  46
-11 109 106
-10  87  84
 -9 175-177
 -8  96 -91
 -7 251 254
 -6 137 136
 -5   4   7
 -4 250-259
 -3 366-376
 -2  75 -69
 -1  86  86
  0  55  48
  1  79  79
  2  73  69
  3 150 143
  4 197 193
  5  83 -80
  6  60  61
  7 154 149
  8  60 -59
  9  92 -96
 10  58 -56
 11  38 -39
 12  26  26

H,K=  3,  3
  L FOB FCA
-15  15  15
-14  43  40
-13  33  32
-12  34  37
-11  24 -21
-10 141-138
 -9  81  84
 -8  71  70
 -7 146-148
 -6 262-289
 -5 126-135
 -4 110 105
 -3 280 301
 -2  87  86
 -1  78  78
  0  91  91
  1  61 -58
  2 254 243
  3 105 100
  4  95-100
  5  10  12
  6 172-165
  7 114-109
  8  26 -24
  9  22 -13
 10  23  21
 11  27  28
 12  16 -15

H,K=  3,  4
  L FOB FCA
-15   0   3
-14   6  -7
-13   7  -4
-12  75 -71
-11  11  12
-10  63  60
 -9  53 -54
 -8 112-117
 -7 102-103
 -6  37 -35
 -5 347 358
 -4 201 210
 -3  71 -76
 -2  40 -40
 -1   5  -3
  0  32 -33
  1  27  24
  2 182-180
  3 126-117
  4  16  -8
  5  66 -64
  6  69  67
  7  40  39
  8  13   4
  9  59  56
 10  17  22
 11   3  -3

H,K=  3,  5
  L FOB FCA
-15   6  -5
-14   6 -15
-13   0  14
-12   5  -3
-11   0 -15
-10  48 -52
 -9  48  44
 -8  75  74
 -7 124 127
 -6 172 174
 -5 147-147
 -4 193-202
 -3  13  14
 -2  50  50
 -1 104 109
  0  96 -89
  1 212-204
  2  59  60
  3  64  62
  4  22  25
  5  45  39
  6  39  39
  7   0   5
  8  21  23
  9  33 -33
 10   8 -13

H,K=  3,  6
  L FOB FCA
-14   7  11
-13  17  21

-12  22 -22
-11  36  43
-10  74  75
 -9  17  24
 -8   0   1
 -7 103-100
 -6 152-157
 -5  14 -14
 -4  89  89
 -3  21  20
 -2  15 -12
 -1 158-146
  0  66  65
  1 193 189
  2  53  50
  3  23 -26
  4  24 -16
  5   9  -3
  6  19  13
  7  28 -28
  8  35 -38
  9  10   7

H,K=  3,  7
  L FOB FCA
-14  26  34
-13   0   7
-12   8  -4
-11  11  -6
-10  32 -35
 -9  46 -42
 -8  82 -80
 -7   0 -11
 -6  77  80
 -5  45  47
 -4  13 -15
 -3  39 -33
 -2  47 -49
 -1 126 120
  0  97  94
  1  30 -31
  2  45 -43
  3  34 -23
  4  17 -24
  5  17  22
  6  32 -31
  7  10  -2
  8  18  21

H,K=  3,  8
  L FOB FCA
-13  15 -16
-12  23 -26
-11   0  -3
-10  12   4
 -9  26  22
 -8  56  54
 -7  30  34
 -6   5 -19
 -5  37 -29
 -4   6  -5
 -3 122 119
 -2  18  17
 -1  67 -69
  0  59 -61
  1   0  -7
  2  26 -26
  3  23  26
  4   0   1
  5  15 -21
  6  13  14

H,K=  3,  9
  L FOB FCA
-12  23  21
-11   7  16
-10   0  -1
 -9   8  17
 -8  16 -18
 -7  18 -19
 -6  10  -7
 -5   7  12
 -4  27  25
 -3  56 -55
 -2  90 -88
 -1  26  20
  0  39  40
  1  15  14
  2  25  29
  3  14 -20
  4   0   1

H,K=  3, 10
  L FOB FCA
-10  10  -7
 -9  14   7
 -8   3  -8
 -7   0  -9
 -6  11  -6
 -5  18  -7
 -4  24 -23
 -3   0  -2
 -2  31  35
 -1  19  16
  0  20  18
  1   0  -4
  2   7 -10

H,K=  3, 11
  L FOB FCA
 -7   7   5
 -6  15  17
 -5   0   1
 -4   9  11
 -3  12  16
 -2   7  -2

H,K=  4,-12
  L FOB FCA
 -2   0   4
 -1   3  -8
  0  38 -40
  1   0   1
  2  34  35
  3   8   7
  4   3  -3
  5  11  -9
  6   0   6
  7  26  31

H,K=  4,-11
  L FOB FCA
 -5   0  10
 -4   2 -14
 -3   5  10
 -2  24 -23
 -1  36 -36
  0  57  56
  1  32  34
  2  28 -26
  3  20 -20
  4  13 -15
  5  33  37
  6  18  21
  7  37 -37
  8   5 -10
  9   3  -2
 10  13 -15
```

sents a mononegative bidentate chelating agent such as N-alkylsalicylaldimato with a bulky N substituent. Detailed crystal structure studies of complexes belonging to the first,[3] third,[4] and fourth[5] of the above classes have been reported. The present work describes the structure of $[(C_4H_9)_4N^+][Ni(quinoline)Br_3^-]$, a compound belonging to the second class.

Complexes of this type are of interest for several reasons. First, they represent examples of axially distorted ligand fields of approximate C_{3v} symmetry. A thorough understanding of the spectral and magnetic properties of complexes in this class is clearly important. The present structural determination is a prelude to a series of detailed oriented single-crystal magnetic resonance, bulk magnetic anisotropy, and polarized-light studies of molecules in the isomorphous[6] series $[(C_4H_9)_4N^+][M(quinoline)Br_3^-]$, where M = Fe(II), Co(II), Ni(II), and Zn(II).

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(3) P. Pauling, *Inorg. Chem.*, **5**, 1948 (1966).

(4) G. Garton, D. E. Henn, H. M. Powell, and L. M. Venanzi, *J. Chem. Soc.*, 3625 (1963).

(5) M. R. Fox, E. C. Lingafelter, P. L. Orioli, and L. Sacconi, *Nature*, **197**, 1104 (1963); *Acta Cryst.*, **17**, 1159 (1964).

(6) D. Forster, unpublished results.

TABLE I (*Continued*)

L	FOB	FCA
H,K= 4,-10		
-7	5	14
-6	4	0
-5	11	-8
-4	45	41
-3	20	-15
-2	51	50
-1	87	86
0	80	-77
1	47	-45
2	0	-5
3	12	-19
4	69	71
5	46	-44
6	78	-78
7	0	-2
8	34	32
9	22	24
10	19	21
11	0	1
H,K= 4,-9		
-8	26	24
-7	8	-13
-6	38	37
-5	19	17
-4	20	-27
-3	13	17
-2	21	-17
-1	89	-90
0	48	49
1	7	-11
2	28	-29
3	18	-18
5	11	-3
6	106	105
7	67	65
8	31	29
9	28	-27
10	23	-26
11	14	14
12	0	-2
H,K= 4,-8		
-10	23	26
-9	7	6
-8	0	1
-7	31	30
-6	90	-88
-5	10	-13
-4	41	37
-3	153	-158
-2	18	19
-1	56	60
0	11	-13
1	60	62
2	41	-39
3	43	-43
4	145	136
5	104	95
6	10	7
7	60	-56
8	108	-107
9	25	25
10	29	34
11	33	-31
12	17	-16
13	14	-14
H,K= 4,-7		
-11	14	21
-10	18	-15
-9	7	-17
-8	43	-39
-7	76	-73
-6	87	86
-5	73	73
-4	86	-87
-3	93	93
-2	34	38
-1	51	51
0	101	99
1	54	-52
2	70	73
3	152	147
4	215	-205
5	206	-196
6	109	-107
7	73	-70
8	174	166
9	16	17
10	59	-62
11	11	14
12	25	28
13	31	32
H,K= 4,-6		
-12	0	-0
-11	17	-21
-10	10	3
-9	52	-51
-8	15	17
-7	108	108
-6	41	-41
-5	42	40
-4	93	95
-3	18	-15
-2	24	18
-1	50	-49
0	86	-87
1	53	53
2	172	-169
3	260	-259
4	29	21
5	61	53
6	191	184
7	34	29
8	79	-75
9	12	13
10	114	118
11	34	35
12	0	-4
13	26	-27
14	31	-34
H,K= 4,-5		
-13	10	-17
-12	12	-6
-11	18	18
-10	0	-6
-9	103	97
-8	30	35
-7	95	-99
-6	21	16
-5	27	-36
-4	51	-57
-3	18	17
-2	187	-189
-1	107	-111
0	42	45
1	208	-291
2	244	238
3	238	237
4	141	140
5	220	209
6	120	-112
7	142	-134
8	125	120
9	36	36
10	49	-47
11	55	-54
12	75	-78
13	17	-20
14	0	12
H,K= 4,-4		
-13	17	16
-12	20	20
-11	40	38
-10	58	57
-9	126	-126
-8	86	-85
-7	66	65
-6	97	-98
-5	24	25
-4	4	8
-3	150	-157
-2	238	245
-1	192	201
0	168	172
1	223	235
2	117	-106
3	97	-96
4	11	10
5	282	-272
6	21	-11
7	85	82
8	136	-135
9	113	-110
10	63	-59
11	7	4
12	108	107
13	47	55
14	14	8
H,K= 4,-3		
-14	6	7
-13	0	11
-12	4	4
-11	67	-65
-10	140	-144
-9	55	52
-8	56	59
-7	54	-52
-6	64	65
-5	172	-173
-4	65	67
-3	412	445
-2	27	29
-1	111	102
0	3	9
1	231	-223
2	90	-89
3	173	-170
4	205	-213
5	88	84
6	24	20
7	113	-112
8	42	42
9	60	60
10	170	165
11	83	83
12	50	-51
13	21	-23
14	0	3
H,K= 4,-2		
-14	20	-21
-13	10	11
-12	72	-77
-11	17	10
-10	140	141
-9	22	22
-8	31	28
-7	7	13
-6	117	-113
-5	250	254
-4	106	97
-3	280	-302
-2	137	-146
-1	284	-285
0	118	-113
1	213	215
2	110	-113
3	178	168
4	108	109
5	39	-41
6	107	105
7	189	182
8	84	83
9	86	85
10	128	-123
11	119	-122
12	15	-10
13	0	-10
14	5	-1
H,K= 4,-1		
-15	0	2
-14	13	15
-13	0	3
-12	106	106
-11	51	51
-10	73	-71
-9	0	-3
-8	37	-41
-7	184	187
-6	131	130
-5	362	-379
-4	470	-504
-3	138	136
-2	2	15
-1	277	284
0	81	79
1	44	-46
2	231	235
3	174	173
4	130	-110
5	112	111
6	94	-88
7	74	-76
8	100	-93
9	161	-154
10	0	7
11	49	48
12	0	6
13	14	15
H,K= 4,0		
-15	1	-1
-14	22	28
-13	48	50
-12	70	-71
-11	75	-74
-10	24	-26
-9	30	-31
-8	38	35
-7	202	-205
-6	360	-380
-5	133	139
-4	217	235
-3	507	520
-2	196	199
-1	243	-243
0	61	64
1	348	353
2	169	-165
3	17	-12
4	30	-34
5	276	-266
6	38	-35
7	105	-101
8	37	36
9	73	65
10	57	56
11	7	12
12	24	21
13	10	2
H,K= 4,1		
-15	7	-0
-14	26	-27
-13	51	-46
-12	31	30
-11	34	30
-10	52	-53
-9	32	-36
-8	69	-73
-7	116	113
-6	359	383
-5	144	146
-4	20	15
-3	203	-210
-2	285	-285
-1	177	181
0	27	29
1	352	-357
2	85	82
3	160	-157
4	49	-47
5	163	157
6	44	42
7	101	103
8	122	117
9	45	-47
10	11	-6
11	0	-7
12	0	-8
H,K= 4,2		
-15	10	-13
-14	0	-7
-13	19	21
-12	29	23
-11	41	36
-10	45	49
-9	86	86
-8	167	168
-7	16	17
-6	183	-187
-5	195	-203
-4	376	-375
-3	114	110
-2	255	260
-1	258	-259
0	217	-208
1	81	-71
2	120	121
3	286	285
4	114	112
5	31	-26
6	0	4
7	66	65
8	78	-72
9	16	-15
10	46	-44
11	0	1
12	0	-1
H,K= 4,3		
-15	13	9
-14	0	5
-13	16	18
-12	29	31
-11	16	-7
-10	14	-13
-9	30	35
-8	183	-184
-7	205	-214
-6	120	-116
-5	84	84
-4	255	296
-3	46	44
-2	252	-246
-1	190	188
0	143	146
1	323	315
2	150	147
3	188	-182
4	116	-115
5	31	29
6	112	-110
7	36	-29
8	46	-43
9	14	-14
10	40	39
11	9	-8
H,K= 4,4		
-15	5	-1
-14	7	21
-13	0	5
-12	91	-88
-11	4	3
-10	29	-29
-9	76	-79
-8	71	71
-7	82	87
-6	169	170
-5	25	25
-4	213	-213
-3	11	-16
-2	282	282
-1	141	136
0	116	-114
1	179	-175
2	213	-207
3	38	34
4	20	17
5	38	-37
6	44	44
7	7	-8
8	37	37
9	33	34
10	0	-16
H,K= 4,5		
-15	7	-5
-14	0	-10
-13	47	-52
-12	32	28
-11	31	31
-10	52	48
-9	73	74
-8	43	48
-7	30	-24
-6	40	-40
-5	79	-82
-4	92	90
-3	18	21
-2	173	-176
-1	194	-191
0	107	-99
1	62	60
2	126	131
3	9	-9
4	43	46
5	29	30
6	28	16
7	46	47
8	9	-4
9	13	-9
H,K= 4,6		
-14	39	42
-13	0	-4
-12	32	32
-11	18	18
-10	19	-12
-9	24	-21
-8	18	-18
-7	48	-47
-6	17	12
-5	44	43
-4	70	-66
-3	94	-95
-2	57	-54
-1	97	98
0	204	199
1	49	50
2	49	-48
3	20	-25
4	19	-13
5	29	27
6	0	3
7	51	-52
8	21	-18
H,K= 4,7		
-13	24	-24
-12	22	-19
-11	18	-19
-10	0	6
-9	0	5
-8	30	-29
-7	19	17
-6	24	-27
-5	38	-40
-4	87	86
-3	21	23
-2	40	35
-1	78	75
0	88	-88
1	55	-60
2	0	6
3	26	28
4	0	7
5	43	-40
6	29	-33
7	12	15
H,K= 4,8		
-12	17	20
-11	0	12
-10	0	-6
-9	0	6
-8	11	12
-7	0	-2
-6	30	29
-5	44	45
-4	6	-1
-3	36	-39
-2	40	-38
-1	48	-51
0	0	4
1	32	33
2	0	-2
3	17	-19
4	17	-18
5	25	24
H,K= 4,9		
-11	23	-26
-10	25	29
-9	22	18
-8	8	1
-7	8	8
-6	15	-18
-5	0	-4
-4	9	-5
-3	38	-36
-2	8	-4
-1	29	27
0	0	15
1	7	-13
2	15	-13
3	0	1
H,K= 4,10		
-9	11	-18
-8	18	-19
-7	0	-12
-6	12	10
-5	10	-12
-4	9	-6
-3	24	24
-2	7	13
-1	13	-14
0	0	-1
1	0	5
H,K= 5,-12		
-2	12	2
-1	11	-15
0	2	-3
1	33	35
2	14	-11
3	21	-22
4	15	15
5	12	5
6	24	30
7	26	31
H,K= 5,-11		
-5	9	-13
-4	20	-12
-3	21	21
-2	5	-17
-1	27	29
0	35	34
1	29	-29
2	8	-4
3	37	33
4	13	14
5	0	3
6	55	-55
7	54	-58
8	20	21
9	12	11
H,K= 5,-10		
-7	23	26
-6	7	-9
-5	19	17
-4	13	-5
-3	42	-40
-2	64	62
-1	17	18
0	22	-31
1	17	20
2	40	-40
3	4	-13
4	43	-40
5	51	-54
6	43	38
7	70	68
8	0	7
9	0	-7
10	12	-4
11	18	13
H,K= 5,-9		
-8	13	10
-7	0	-8
-6	45	43
-5	6	-4
-4	8	-12
-3	42	38
-2	62	-63
-1	26	-25
0	32	33
1	40	-35
2	21	19
3	46	-44
4	0	-8
5	126	125
6	22	20
7	49	-46
8	18	-10
9	10	-5
10	48	47
11	0	11
12	43	-46
H,K= 5,-8		
-10	48	51
-9	25	-29
-8	20	-24
-7	9	-11
-6	38	-38
-5	66	61
-4	62	-64
-3	94	-92
-2	67	67
-1	35	-35
0	8	-11
1	96	93
2	21	20
3	133	134
4	72	74
5	128	-122
6	60	-58
7	29	-26
8	37	34
9	12	13
10	66	-64
11	57	-64
12	0	9
H,K= 5,-7		
-11	0	8
-10	27	-35
-9	9	-3
-8	55	-53
-7	13	-13
-6	68	71
-5	86	-81
-4	13	-5
-3	90	91
-2	0	-9
-1	139	140
0	37	36
1	68	-67
2	52	55
3	53	-88
4	118	-119
5	81	76
6	61	-59
7	45	-49
8	6	-6
9	56	-53
10	45	43
11	86	87
12	34	34
13	16	21
H,K= 5,-6		
-12	37	-41
-11	18	-18
-10	0	6
-9	0	-1
-8	103	106
-7	14	18
-6	99	-98
-5	109	107
-4	46	34
-3	124	124
-2	106	106
-1	205	-211
0	69	-70
1	10	6
2	234	-233
3	0	-6
4	78	78
5	27	25
6	20	-14
7	14	14
8	6	9
9	126	127
10	20	32
11	11	-14
12	49	-51
13	37	-39
H,K= 5,-5		
-13	19	-16
-12	34	38
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11	0	3
12	20	22
H,K= 7,-6		
-12	0	2
-11	15	15
-10	33	-30
-9	31	30
-8	8	7
-7	22	25
-6	135	137
-5	0	6
-4	121	-127
-3	32	-37
-2	50	-54
-1	22	26
0	54	-53
1	316	-322
2	12	-10
3	162	158
4	41	38
5	103	99
6	16	7
7	22	19
8	96	99
9	21	24
10	0	-12
11	0	9
12	30	-31
H,K= 7,-5		
-12	0	1
-11	12	12
-10	42	43
-9	16	-7
-8	18	9
-7	18	15
-6	162	-168
-5	7	-10
-4	58	58
-3	2	-7
-2	30	32
-1	294	-288
0	100	-102
1	329	333
2	205	201
3	74	74
4	28	-29
5	72	-69
6	51	49
7	32	33
8	86	-82
9	34	-39
10	39	-39
11	45	-46
12	6	-3
H,K= 7,-4		
-13	10	-6
-12	11	7
-11	21	-21
-10	44	-43
-9	24	18
-8	86	-88
-7	92	-95
-6	131	135
-5	4	8
-4	12	-9
-3	84	89
-2	28	-27
-1	284	292
0	249	253
1	155	-152
2	142	-141
3	146	-142
4	20	-15
5	27	25
6	107	-104
7	141	-140
8	0	-11
9	28	-25
10	66	63
11	50	54
12	31	30
H,K= 7,-3		
-14	20	-17
-13	18	-22
-12	50	-50
-11	3	-10
-10	56	55
-9	48	-51
-8	57	57
-7	30	30
-6	55	-55
-5	70	69
-4	34	35
-3	69	68
-2	225	238
-1	135	-140
0	338	-355
1	118	-126
2	119	-117
3	56	58
4	80	75
5	61	-80
6	40	41
7	93	89
8	110	112
9	89	68
10	18	-15
11	19	-17
12	2	10
H,K= 7,-2		
-14	7	-10
-13	0	-9
-12	56	55
-11	15	12
-10	18	-18
-9	79	79
-8	11	-9
-7	57	58
-6	53	55
-5	13	-21
-4	15	2
-3	136	-139
-2	379	-389
-1	62	-59
0	123	123
1	207	205
2	104	104
3	90	-94
4	93	-92
5	212	210
6	124	122
7	78	78
8	70	-70
9	120	-117
10	21	-23
11	0	-6
12	27	-29
H,K= 7,-1		
-14	24	21
-13	41	40
-12	40	-40
-11	15	-15
-10	12	16
-9	18	24
-8	3	-2
-7	94	-91
-6	205	-206
-5	114	110
-4	169	-169
-3	24	-24
-2	249	252
-1	198	204
0	114	115
1	54	51
2	204	-199
3	110	110
4	141	134
5	124	-119
6	132	-127
7	161	-155
8	36	-32
9	56	54
10	0	-5
11	9	-4
H,K= 7,0		
-14	9	-13
-13	50	-49
-12	31	-29
-11	21	25
-10	8	-11
-9	91	-95
-8	134	-137
-7	20	-16
-6	101	102
-5	133	134
-4	185	188
-3	121	122
-2	55	-57
-1	45	-47
0	118	-123
1	18	-13
2	167	165
3	102	-90
4	208	-198
5	101	-97
6	27	25
7	70	67
8	82	81
9	0	1
10	22	24
11	31	34
H,K= 7,1		
-14	9	9
-13	40	40
-12	0	-4
-11	36	-40
-10	39	-44
-9	43	45
-8	216	213
-7	71	75
-6	9	10
-5	35	35
-4	109	-109
-3	106	-104
-2	51	-30
-1	151	-152
0	104	100
1	72	-70
2	205	-198
3	27	-24
4	63	63
5	205	200
6	122	116
7	37	-35
8	45	-44
9	19	19
10	0	4
H,K= 7,2		
-14	24	24
-13	26	-28
-12	0	7
-11	40	41
-10	88	88
-9	35	39
-8	128	-121
-7	95	-99
-6	69	-65
-5	81	-85
-4	38	33
-3	20	17
-2	69	-65
-1	49	51
0	4	-3
1	23	17
2	156	148
4	47	43
5	0	-15
6	131	-135
7	5	-11
8	0	12
9	29	-30
10	0	-8
H,K= 7,3		
-14	25	-23
-13	11	14
-12	19	21
-11	35	31
-10	75	-70
-9	169	-171
-8	8	-20
-7	27	23
-6	45	40
-5	75	73
-4	7	-7
-3	21	19
-2	31	34
-1	143	151
0	88	88
1	43	40
2	38	-38
3	71	-71
4	111	-114
5	34	-38
6	37	39
7	0	-1
8	13	-9
9	11	-7
H,K= 7,4		
-14	0	-1
-13	18	22
-12	27	-28
-11	75	-75
-10	12	8
-9	91	86
-8	103	101
-7	15	16
-6	59	-59
-5	27	-30
-4	80	82
-3	85	87
-2	48	-35
-1	84	-83
0	119	-128
1	50	-51
2	43	-41
3	24	-22
4	56	63
5	36	37
6	12	-11
7	20	20
8	0	-2
H,K= 7,5		
-13	29	-31
-12	0	-2
-11	82	77
-10	53	52
-9	17	-16
-8	61	-54
-7	43	-43
-6	50	50
-5	45	46
-4	100	-103
-3	83	-87
-2	13	-11
0	42	43
1	0	-10
2	36	40
3	65	68
4	5	-2
5	11	-15
6	5	5
7	10	11
H,K= 7,6		
-13	34	40
-12	22	24
-11	33	-30
-10	67	-64
-9	33	-34
-8	25	25
-7	51	51
-6	11	-8
-5	107	-110
-4	13	-13
-3	65	67
-2	64	64
-1	40	43
0	3	11
1	11	12
2	0	7
3	27	-31
4	0	-6
5	5	-1
H,K= 7,7		
-11	0	-4
-10	16	18
-9	28	26
-8	5	-9
-7	49	-47
-6	26	21
-5	15	17
-4	42	41
-3	23	24
-2	37	-36
-1	30	-33
0	7	-3
1	0	-1
2	0	-11
3	0	-6
4	7	-6
H,K= 7,8		
-10	0	-6
-9	26	-28
-8	14	-16
-7	42	43
-6	28	35
-5	14	-7
-4	28	-30
-3	32	-32
-2	0	6
-1	12	14
0	11	-12
1	13	-10
H,K= 7,9		
-6	36	-41
-5	22	-24
-4	8	12
-3	26	25
H,K= 8,-12		
-1	8	15
0	7	5
1	17	-24
2	20	26
3	13	17
4	0	-2
H,K= 8,-11		
-4	15	16
-3	13	9
-2	29	32
-1	19	-22
0	27	-32
1	58	56
2	2	-5
3	23	-23
4	25	-21
5	36	-39
6	6	6
7	0	-3
H,K= 8,-10		
-6	29	32
-5	0	-2
-4	18	17
-3	2	12
-2	57	-55
-1	36	35
0	34	29
1	56	-51
2	42	-40
3	45	-45
4	0	-5
5	50	51
6	0	-14
7	9	10
8	35	37
9	3	9
H,K= 8,-9		
-8	30	34
-7	28	31
-6	45	-48
-5	17	13
-4	37	-39
-3	34	-33
-2	91	89
-1	45	-43
0	64	-60
1	18	11
2	8	2
3	52	90
4	50	50
5	54	-52
6	28	28
7	14	14
8	0	-6
9	0	-2
10	31	-28

Second, proton magnetic resonance studies in one of these laboratories on salts of this stoichiometric class have revealed large dipolar isotropic shifts for the cation proton resonances in chloroform solution which are indicative of ion pairing in solution.[7-10] Several models for this ion pairing in solution have been proposed and it was hoped that the solid-state structure would illuminate the problem. In any case an accurate knowledge of the geometry of the anion is necessary for an interpretation of the isotropic proton resonance shifts of the coordinated quinoline which are both dipolar and Fermi contact in origin in the cobalt(II) and nickel(II) complexes.

Save for a very recent preliminary account[11] involving a quinoline adduct of bis(2,4-pentanedionato)copper(II), there appear to be no accurate crystal structure analyses of coordination compounds containing quinoline. This is despite the fact that quinoline is a com-

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(7) G. N. LaMar, Ph.D. Thesis, Princeton University, 1964.

(8) G. N. LaMar, *J. Chem. Phys.*, **41**, 2992 (1964); **43**, 235 (1965).

(9) R. H. Fischer, Ph.D. Thesis, Princeton University, 1967.

(10) G. N. LaMar, R. H. Fischer, and W. D. Horrocks, Jr., *Inorg. Chem.*, **6**, 1798 (1967).

(11) S. Ooi and Q. Fernando, *Chem. Commun.*, 532 (1967).

TABLE I (*Continued*)

```
H,K=  8, -8
  L FOB FCA
 -9  18   9
 -8   0  -4
 -7  16 -11
 -6   0 -16
 -5  60 -59
 -4  60  82
 -3  16  10
 -2 132-129
 -1  13  19
  0  62  64
  1  70  73
  2 102 106
  3  62 -63
  4  97 -99
  5  17   9
  6  11  10
  7  23 -22
  8  26 -29
  9  35 -35
 10   9   4

H,K=  8, -7
  L FOB FCA
-10  11  11
 -9  36 -40
 -8   0  10
 -7  34 -30
 -6   0  15
 -5 128 128
 -4  64 -66
 -3  17 -14
 -2 171 171
 -1  31  33
  0   5   5
  1  72 -71
  2 200-208
  3  46  43
  4   0  -3
  5  38 -36
  6  20 -25
  7  23 -26
  8  16  14
  9  83  62
 10  18  19
 11  21  24

H,K=  8, -6
  L FOB FCA
-11   4  -4
-10   0   5
 -9  40  42
 -8  44 -36
 -7  54  52
 -6  17  10
 -5  41 -45
 -4  99  96
 -3 113 111
 -2 127-124
 -1 112-116
  0 179-185
  1  33 -31
  2 171 177
  4  87 -38
  5  47  46
  6   0   4
  7 103 106
  8  50  51
  9  38 -36
 10  19 -14
 11  26 -27

H,K=  8, -5
  L FOB FCA
-12  15 -12
-11  23  24
-10  15  15
 -9  18 -19
 -8  63  57
 -7  27 -30
 -6  80 -83
 -5  42 -38
 -4 165-170
 -3  46 -46
 -2   0  -9
 -1   0  -1
  0 204 213
  1 126 128
  2  70 -74
  3  13   8
  4  21  23
  5 109 112
  6  96 104
  7 119-118
  8  97 -96
  9  47 -47
 10  15 -16
 11  10   2

H,K=  8, -4
  L FOB FCA
-13   0 -14
-12   5 -11
-11  41 -38
-10  30  32
 -9  12 -15
 -8  95 -93
 -7  36 -33
 -6  35  36
 -5  53 -53
 -4 123 122
 -3 104 108
 -2 101 106
 -1 197 201
  0  63 -65
  1 105-105
  2  18 -15
  3  23 -28
  4  69  72
  5 139-148
  6 237-255
  7  11   8
  8  79  76
  9  21  19
 10  42  40
 11   0  11

H,K=  8, -3
  L FOB FCA
-13  16 -17
-12   6  -3
-11  40  39
-10  42 -43
 -9  84 -79
 -8  87  82
 -7  58  64
 -6  80  79
 -5 154 144
 -4  27 -25
 -3  21  18
 -2  79 -82
 -1 215-218
  0  75  71
  1  23  16
  2  68 -71
  3 103-105
  4 196-209
  5  20   5
  6 224 220
  7 127 130
  8   7  -7
  9  14  12
 10  16 -12
 11  18  22

H,K=  8, -2
  L FOB FCA
-14  11  10
-13  28  30
-12   0   8
-11  32 -30
-10  35  35
 -9 107 104
 -8   9  -6
 -7  14 -20
 -6  80 -80
 -5 105-106
 -4  53 -52
 -3 149-150
 -2  73 -72
 -1  84  82
  0  20 -18
  1  61 -59
  2  33  33
  3 130 132
  4 270 277
  5 129 130
  6  66 -62
  7  61 -53
  8  61 -62
  9   0  -5
 10   2  -4
 11  36 -37

H,K=  8, -1
  L FOB FCA
-14   0   5
-13  32 -34
-12   0 -14
-11  92  89
-10   2   7
 -9  35 -33
 -8  74 -75
 -7 219-219
 -6  97  95
 -5  78  78
 -4  50 -50
 -3  65  70
 -2  69  71
 -1  33  32
  0 104 113
  1  97 101
  2  72  73
  3  74  79
  4 171-175
  5 144-148
  6  70 -73
  7  33 -40
  8  31  28
  9   0  -3
 10  28 -29
 11  19  21

H,K=  8,  0
  L FOB FCA
-14  14  -2
-13  24  27
-12  23  23
-11  85 -80
-10  61 -60
 -9  47 -50
 -8   0   3
 -7 140 140
 -6 103  98
 -5  49 -51
 -4  54  54
 -3  27  25
 -2  82  89
 -1  94  99
  0  87 -94
  1  66 -63
  2 128-130
  3 198-210
  4  34 -32
  5  94  93
  6  37  39
  7  28  28
  8  26 -25
  9  21  19
 10  57  54

H,K=  8,  1
  L FOB FCA
-14  15  18
-13  33 -42
-12  23 -25
-11   8   3
-10  64  61
 -9 101 100
 -8  43  45
 -7  83 -84
 -6  48 -48
 -5  40  39
 -4  15  15
 -3  12 -16
 -2 140-142
 -1 155-157
  0  10  12
  1  34 -39
  2  60  57
  3 102 108
  4  96 103
  5  46  48
  6  16 -10
  7  17 -13
  8  50  51
  9   0  15

H,K=  8,  2
  L FOB FCA
-14  15 -20
-13   0   2
-12  66  67
-11  90  89
-10  34  37
 -9 114-104
 -8  95 -90
 -7   7   5
 -6  61  68
 -5   6 -11
 -4 105-104
 -3 165-168
 -2  64  64
 -1  96  99
  0  43  45
  1  94  99
  2  32  34
  3  15 -25
  4  25  25
  5  39 -40
  6  27 -21
  7   7  -2
  8  18 -24
  9  44 -47

H,K=  8,  3
  L FOB FCA
-14  22  27
-13  10  20
-12  39 -34
-11  69 -64
-10  68 -84
 -9  33  31
 -8 118 114
 -7  23 -26
 -6 104-111
 -5  52 -50
 -4 114 110
 -3 188 192
 -2  32  32
 -1  11  11
  0   0  14
  1  64 -70
  2  36 -41
  3   0  -6
  4  48 -46
  5  13  -2
  6   8 -13
  7  18 -25
  8   0  -5

H,K=  8,  4
  L FOB FCA
-13  34 -35
-12  16 -14
-11  37  31
-10  50  42
 -9  27  24
 -8  48 -51
 -7  17 -14
 -6  48  49
 -5 134 131
 -4  15  17
 -3  86 -88
 -2  51 -55
 -1  19 -10
  0  23 -30
  1  11 -13
  2  14   2
  3  21 -15
  4  14  19
  5  16  13
  6   7  11
  7  34  35

H,K=  8,  5
  L FOB FCA
-13  27  26
-12  27  30
-11   8   6
-10  48 -47
 -9   0  -2
 -8  48  50
 -7  70  69
 -6  19  15
 -5 116-112
 -4 108-108
 -3  43 -44
 -2  23  21
 -1  36  38
  0  14   7
  1  25 -19
  2  27  29
  3  23  19
  4  15  13
  5   0   9

H,K=  8,  6
  L FOB FCA
-12   5  -7
-11   0 -11
-10   5  13
 -9  11   9
 -8  11 -12
 -7  60 -57
 -6  57 -56
 -5   7 -15
 -4 108 109
 -3  51  51
 -2   0  -4
 -1  35 -36
  0   0  -5
  1  52  52
  2  24  23
  3  18 -15
  4  22 -24

H,K=  8,  7
  L FOB FCA
-10   0  -6
 -9  14 -22
 -8  25 -26
 -7  33  35
 -6  64  65
 -5  25  25
 -4  20 -20
 -3  26 -26
 -2   8  -3
 -1  22  21
  0   0   1
  1  24 -24
  2  14 -20

H,K=  8,  8
  L FOB FCA
 -8  25  26
 -7  14  18
 -6  51 -54
 -5  33 -36
 -4   0  -6
 -3  24  24
 -2  14  12
 -1  23 -24

H,K=  9,-11
  L FOB FCA
 -3   8   3
 -2   7   4
 -1   0  -6
  0  63  67
  1  28  28
  2  43 -45
  3  11  -9
  4  17 -22
  5  14  -3
  6   0   2

H,K=  9,-10
  L FOB FCA
 -6   5  12
 -5   0  -8
 -4  21  21
 -3   8  -4
 -2  10   6
 -1  21  18
  0  76 -74
  1  58 -57
  2   9   4
  3   7 -10
  4  41  41
  5   0  -1
  6  45 -47
  7  31  31
  8  19  23

H,K=  9, -9
  L FOB FCA
 -8  48  56
 -7  31 -37
 -6   0 -10
 -5  17  16
 -4  32 -35
 -3   8   8
 -2  13 -16
 -1  91 -91
  0  46  45
  1  61  63
  2  33  36
  3  45  43
  4  64 -63
  5  10   9
  6  77  76
  7  12   8
  8  10 -10
  9  33 -36

H,K=  9, -8
  L FOB FCA
 -9   0   6
 -8  40 -43
 -7   9 -10
 -6  14  -9
 -5  46 -45
 -4  53  53
 -3  24 -24
 -2  16  14
 -1 126 125
  0  26  30
  1  18  15
  2  14 -20
  3  43 -47
  4  50  52
  5  35  35
  6  76 -76
  7  79 -73
  8  53 -56
  9   6  -4
 10  32  34

H,K=  9, -7
  L FOB FCA
-10   7 -10
 -9   8   3
 -8  21  12
 -7  49 -46
 -6  28  26
 -5  69  67
 -4  30 -27
 -3  76  76
 -2   0   9
 -1  70 -73
  0  21 -22
  1  77 -83
  2  35  36
  3  25  24
  4 110-111
  5  81 -80
  6  10  -6
  7  50  49
  8 105 103
  9  30  35
 10   5  -6

H,K=  9, -6
  L FOB FCA
-11  16 -20
-10   0   9
 -9   0  -1
 -8  23  20
 -7 107 104
 -6  51 -50
 -5  50 -52
 -4  65  60
 -3  60 -62
 -2  42 -39
 -1  26 -28
  0  68 -64
  1  76  79
  2  11   2
  3 136-138
  4  75  77
  5 134 134
  6 104 101
  7  40  45
  8  77 -76
  9  43 -46
 10   7   9

H,K=  9, -5
  L FOB FCA
-12  26 -28
-11  28  31
-10  13   9
 -9  34  29
 -8  26  16
 -7 106-101
 -6  22 -17
 -5  45 -47
 -4  60 -62
 -3  15  16
 -2  17 -16
 -1  52  61
  0 140 142
  1  60 -59
  2  28  34
  3 197 208
  4  42  43
  5  43 -50
  6 115-113
  7 110-107
  8   7  -5
  9   6  11
 10  22 -25

H,K=  9, -4
  L FOB FCA
-12  21  21
-11  14  11
-10   1 -11
 -9  89 -89
 -8  56 -54
 -7  23  27
 -6   0  -2
 -5  53  55
 -4  61  58
 -3  56 -56
 -2  81  85
 -1  54  50
  0   7   1
  1  88  88
  2  32  22
  3 190-191
  4 110-107
  5  87 -89
  6  31  32
  7  56  50
  8  11  -3
  9  15 -11
 10  12  12

H,K=  9, -3
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-13  14 -13
-12  12  -9
-11  21 -21
-10  54 -57
 -9  53  46
 -8 114 112
 -7  41  44
 -6  95  93
 -5  47 -49
 -4  16 -10
 -3  97 100
 -2  56 -56
 -1  79 -80
  0  25 -21
  1 223-220
  2  21 -24
  3   0  -5
  4  25  22
  5  55  57
  6  62  62
  7   8 -17
  8   9  16
  9  32  34
 10  38  41

H,K=  9, -2
  L FOB FCA
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-12   0  -3
-11  39  39
-10 123 121
 -9  33  35
 -8 103 -98
 -7  92 -93
 -6   0   6
 -5  23  22
 -4  20  21
 -3 186-185
 -2 100 -96
 -1  15 -15
  2  83  80
  3 134 131
  4 108 104
  5  42 -42
  6  52 -49
  7   0   4
  8   0  -6
  9   0 -10
 10  49 -52

H,K=  9, -1
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-12  38  40
-11  21  26
-10 103 -99
 -9  81 -79
 -8  63 -61
 -6  66  67
 -5 142-154
 -4 141-142
 -3 112 108
 -2 122 120
 -1 176 178
  0  66  64
  1  24  22
  2  10   5
  3  53 -56
  4  66 -63
  5  11   9
  6  26 -24
  7  50 -47
  8  40 -40
  9  30 -34
 10  27  25

H,K=  9,  0
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-14  17 -16
-13   0  -8
-12  37 -36
-11  52 -54
-10  37  33
 -9  82  79
 -8  34  28
 -7  23  22
 -6 107-105
 -5 103 105
 -4 185 188
 -3 105 107
 -2  11   2
 -1 127-127
  0 114-108
  1  74 -74
  2  57 -96
  3  66 -60
  4  51  53
  5  47 -49
  6  11  11
  7  14  15
  8  35  37
  9  63  66

H,K=  9,  1
  L FOB FCA
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-13  19 -26
-12  40  34
-11  62  60
-10  35  32
 -9  19 -19
 -8  84 -76
 -7  50  54
 -6 164 164
 -5   0   6
 -4 117-115
 -3 216-217
 -2 116-114
 -1  26  27
  0  55  53
  1  21 -21
  2   0  -3
  3  36  36
  4  57  56
  5  40  38
  6  32  30
  7  27  29
  8  11  18

H,K=  9,  2
  L FOB FCA
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-12  10   2
-11  25 -23
-10  47 -40
 -9   0  20
 -8  97  93
 -7  29 -27
 -6 166-163
 -5 108-110
 -4  30 -29
 -3  36  34
 -2 189 187
 -1  40  35
  0  44 -40
  1  45  43
  2  48  45
  3  66  67
  4   0  -6
  5  30 -30
  6  21 -20
  7  30 -34
  8  31 -31

H,K=  9,  3
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-12  10  -5
-11  27 -19
-10   4   5
 -9  26  23
 -8  70 -67
 -7  54 -55
 -6  55  52
 -5 132 132
 -4  78  79
 -3  36  36
 -2  97 -96
 -1  39 -38
  0  35  30
  1  15  17
  2  15 -22
  3  69 -69
  4  53 -52
  5   0 -14
  6   0 -11
  7  10   4

H,K=  9,  4
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-11  10  -9
-10  15 -15
 -9  14  -8
 -8  30  28
 -7  84  84
 -6  64  63
 -5  13  -8
 -4 126-126
 -3  44 -43
 -2  55  52
 -1  37  41
  0  38 -40
  1  73 -72
  2  25 -25
  3  29  30
  4  31  35
  5  20  22

H,K=  9,  5
  L FOB FCA
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-11   2   4
-10  10  12
 -9  40  38
 -8   9   5
 -7  36 -37
 -6  81 -78
 -5  42 -42
 -4  76  76
 -3  41  43
 -2  42 -39
 -1  63 -64
  0  24 -22
  1  77  76
  2  58  64
  3   9  -3
  4  15 -11

H,K=  9,  6
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-10  14   2
 -9  36 -36
 -8  23 -28
 -7  12  12
 -6  11  10
 -5  17  21
 -4   0   1
 -3  25 -28
 -2   5  -2
 -1  32  34
  0  39  38
  1   9  -6
  2  36 -39

H,K=  9,  7
  L FOB FCA
 -8  33  36
 -7   9  11
 -6  30 -29
 -5   8   5
 -4  15  12
 -3  22  22
 -2  20  21
 -1  12 -10

H,K= 10,-11
  L FOB FCA
 -2  14 -15
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  0  46  51
  1  41 -44
  2  13 -15
  3  26  27
  4  10   7
  5   5 -10

H,K= 10,-10
  L FOB FCA
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 -4  10  14
 -3  19 -18
 -2  23  22
 -1   9 -12
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  1  23  23
  2  13  13
  3  21 -18
  4  10 -10
  5  21 -22
  6  37  40
  7  48  63

H,K= 10, -9
  L FOB FCA
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 -6  19  21
 -5  24 -25
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 -3   4  -2
 -2  79 -75
 -1   9  -1
  0  46  47
  1  25 -20
  2  16  13
  3   0  -2
  4  28  26
  5  83  85
  6  20  11
  7  54 -58
  8  18 -17

H,K= 10, -8
  L FOB FCA
 -8  45 -47
 -7  25 -26
 -6  31 -30
 -5  33  30
 -4  13  18
 -3  35 -26
 -2  82  83
 -1  30  33
  0  11  -9
  1  57  51
  2  30  25
  3   0  -6
  4  35  35
  5 116-115
  6  45 -47
  7   0   0
  8   9  -2
  9  19  18

H,K= 10, -7
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-10  35 -39
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 -8   2  13
 -7  29  29
 -6  54  54
 -5  34 -33
 -4  16  12
 -3  64  59
 -2  21 -26
 -1   9 -11
  0  10   9
  1  39 -39
  2  16 -14
  3 103-105
  4  75 -72
  5  53  53
  6  50  49
  7  32  30
  8   7   9
  9  17 -12

H,K= 10, -6
  L FOB FCA
-10  29  29
 -9  24  22
 -8  53  52
 -7  30  27
 -6  87 -85
 -5  23  17
 -4   2  -6
 -3 103-101
 -2   5  -1
 -1  74 -71
  0  87 -83
  1  42  41
  2  57 -59
  3  78  81
  4 115 113
  5  65  64
  6   4  16
  7   7  -8
  8  13  -2
  9  35  40

H,K= 10, -5
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-11  20  20
-10  20 -16
 -9  10  -1
 -8  87 -87
 -7  35 -35
 -6  77  74
 -5  17  22
 -4  40 -37
 -3  38 -35
 -2  95 -95
 -1  92 100
  0 144 140
  1  75  76
  2  83  81
  3  27  24
  4  45 -43
  5  65 -63
  6  55 -56
  7   7  -6
  8   0  -6
  9  69 -72

H,K= 10, -4
  L FOB FCA
-12   9  13
-11   0 -10
-10  44 -45
 -9  68 -66
 -8  83  80
 -7  40  41
 -6  85 -82
 -5   6   7
 -4  10  14
 -3 111 114
 -2 174 168
 -1   6  -7
  0  84 -79
  1  48 -48
  2  58 -58
  3  66 -64
  4  45 -46
  5  46 -44
  6  47  46
  7  41 -42
  8  19 -26
  9  48  46

H,K= 10, -3
  L FOB FCA
-12   9  -9
-11   0  -9
-10  54  52
 -9  82  80
 -8  54 -55
 -7  45 -47
 -6  60  59
 -5  65  63
 -4 112 111
 -3  45 -45
 -2 203-203
 -1  76 -78
  0  85 -89
  1  74 -67
  2  47  46
  3  37  33
  4  47  47
  5  72  74
  6  14  -5
  7  46  47
  8  78  80
  9  17  20

H,K= 10, -2
  L FOB FCA
-13   0   4
-12  13  16
-11  42  42
-10  13  -7
 -9  36 -33
 -8  10  16
 -7 112 108
 -6   9   1
 -5  88 -88
 -4 199-202
 -3  93 -88
 -2 107 107
 -1 100  99
  0  57  55
  1  35  33
  2  46 -45
  3  51  54
  4  57  53
  5  18  21
  6  31  31
  7  26 -26
  8  76 -78
  9  44 -48

H,K= 10, -1
  L FOB FCA
-13  12  20
-12   0   2
-11  43 -39
-10  26 -23
 -9   0  -3
 -8  22 -19
 -7   9  -5
 -6 130-129
 -5  71 -70
 -4 129 128
 -3 163 162
 -2  56  55
 -1  17  20
  0  72 -75
  1  47  46
  2  92  90
  3  43 -45
  4  55 -56
  5  74 -73
  6  66 -66
  7  19 -18
  8  12   3
  9  27  24

H,K= 10,  0
  L FOB FCA
-13  12 -12
-12  20 -23
-11  15  14
-10  17  12
 -9  62 -64
 -8  20 -13
 -7  36  32
 -6 111 111
 -5 176 173
 -4   7  -8
 -3 130-128
 -2  80 -75
 -1  15 -11
  0  85  86
  1  21 -17
  2 161-163
  3  24 -23
  4  10 -12
  5  16  11
  6  54  52
  7  41  43
  8  33  37

H,K= 10,  1
  L FOB FCA
-13   0   3
-12  20  17
-11  14  -7
-10   0   8
 -9  50  47
 -8  54  53
 -7  71  69
 -6   9   3
 -5 128-130
 -4 100 -97
 -3  21  23
 -2  62  80
 -1  53 -52
  0 130-128
  1  56 -55
  2  51  54
  3 118 120
  4  45  46
  5  20  19
  6  14 -12
  7  14  -3

H,K= 10,  2
  L FOB FCA
-13   0   8
-12   4   4
-11   0   2
-10  15  13
 -9  15 -16
 -8  32 -27
 -7 102-100
 -6  73 -72
 -5  34  32
 -4  69  65
 -3  40  39
 -2  63 -61
 -1   0 -21
  0 103 104
  1  89  87
  2  45  49
  3  21 -15
  4  51 -53
  5  23 -25
  6   0   1

H,K= 10,  3
  L FOB FCA
-12   9   1
-11  41 -43
-10   0 -12
 -9  41 -42
 -7  58  57
 -6  56  90
 -5  21  18
 -4  52 -52
 -3   9  -8
 -2  67  65
 -1  91  93
  0  17 -17
  1  76 -79
  2  64 -65
  3  30 -34
  4  21  20
  5  11  13

H,K= 10,  4
  L FOB FCA
-11  10   8
-10  30  30
 -9  45  44
 -8  35  32
 -7  10  -5
 -6  41 -36
 -5   7  -2
 -4  23  20
 -3  35  35
 -2  37 -33
 -1  99-101
  0  44 -47
  1  10  15
  2  19  19
  3  18  25
  4  14 -10

H,K= 10,  5
  L FOB FCA
-10  15 -16
 -9  26 -26
 -8   7  -9
 -7  13 -14
 -6  19 -16
 -5  16  17
 -4   7   4
 -3  42 -43
 -2  18 -20
 -1  25  25
  0  41  44
  1  30  35
  2   5   9

H,K= 10,  6
  L FOB FCA
 -9  21  20
 -8  14  17
 -7  31 -34
 -6   6   5
 -5   0  -4
 -4  13 -12
 -3  29  29
 -2  32  38
 -1  14  18
  0   0  -3

H,K= 11,-11
  L FOB FCA
  0   1 -15
  1  13 -25

H,K= 11,-10
  L FOB FCA
 -4   0 -16
 -3   0 -14
 -2  27  25
 -1  18 -22
  0   0  -5
  1   6  13
  2  44 -45
  3  12  -5
  4  11  11
  5  17  24

H,K= 11, -9
  L FOB FCA
 -6  14  16
 -5  20 -25
 -4  29  29
 -3  23 -17
 -2  74 -65
 -1  15  24
  0   7   0
  1   6   9
  2  58  56
  3  16  11
  4  34  35
  5   7  17
  6  41 -44

H,K= 11, -8
  L FOB FCA
 -8  14  14
 -7   0   7
 -6   0   2
 -5  12  16
 -4  56 -51
 -3  18 -11
 -2  65  64
 -1   1   5
  0  37  37
  1  42  38
  2  66 -65
  3   8  -3
  4  31 -36
  5  63 -62
  6  15  17
  7  13  13

H,K= 11, -7
  L FOB FCA
 -9   6  14
 -8  10  -9
 -7  25  27
 -6   6  -4
 -5  13  -6
 -4  98  88
 -3  61  53
 -2  16 -12
 -1  27 -26
  0  72 -74
  1  31 -27
  2  30 -30
  3  26 -22
  4  15  16
  5  44  41
  6  19 -23
  7   0  -2
  8  14  20

H,K= 11, -6
  L FOB FCA
-10  23  29
 -9   0   5
 -8   0  -5
 -7  24 -30
 -6  20  16
 -5 104  98
 -4  70 -68
 -3 116-111
 -2  83 -81
 -1  33 -33
  0  79  79
  1  10   8
  2  35 -31
  3  87  87
  4  10   6
  5   5  11
  6  60  62
  7  15  10
  8   3  13

H,K= 11, -5
  L FOB FCA
-11  16 -16
-10  13 -18
 -9   0  -1
 -8  16 -13
 -7  10   8
 -6  35 -35
 -5 104 -99
 -4  46 -42
 -3  56  53
 -2  90  92
 -1  66  83
  0  54 -56
  1   9   9
  2  66  62
  3   7  -4
  4  22  24
  5   9   7
  6  52 -51
  7  43 -42
  8  46 -45

H,K= 11, -4
  L FOB FCA
-11  16 -15
-10   8   2
 -9   8  -6
 -8  11  15
 -7  53 -52
 -6  16  -4
 -5 108  99
 -4  97  92
 -3  98  97
 -2  11   6
 -1  87 -84
  0  24  21
  1  13   6
  2  30 -27
  3  59 -57
  4 109-114
  5  46 -45
  6   8 -12
  7   0  12
  8  43  44

H,K= 11, -3
  L FOB FCA
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-11   8 -10
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 -8   0  -6
 -7  92  87
 -6  71  66
 -5  12  -5
 -4  55 -55
 -3 170-170
 -2  10  -9
 -1  44  43
  0  25 -22
  1  90 -87
  2  65 -66
  3  25 -26
  4 106 107
  5 104 104
  6  32  33
  7  29  31
  8   0   1

H,K= 11, -2
  L FOB FCA
-12  10   8
-11  23  22
-10  20 -20
 -9  14 -20
 -8  93  91
 -7  36 -34
 -6  89 -85
 -5 131-128
 -4  57 -55
 -3 122 119
 -2  54  51
 -1 112-109
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  1  87  86
  2 126 126
  3 111 109
  4   0  -6
  5  54 -50
  6  21 -21
  7  19 -19
  8  14 -16

H,K= 11, -1
  L FOB FCA
-12   9   9
-11   0  -4
-10   0 -10
 -9  60 -57
 -8  37 -36
 -7  41 -41
 -6  20  18
 -5 126 121
 -4 104 104
 -3  41 -41
 -2  60 -58
 -1 113 110
  0  92  95
  1  41  42
  2  84 -86
  3 101 -98
  4  69 -69
  5  26 -27
  6  16 -22
  7  11  -8

H,K= 11,  0
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-11   0 -11
-10  32 -33
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 -7  73  66
 -6  34  31
 -5  45 -41
 -4  66 -64
 -3  51  53
 -2  55  58
 -1   6 -12
  0  81 -84
  1 149-153
  2  23 -24
  3  68  65
  4  19  20
  5  12  19
  6  10  12
  7  24  20

H,K= 11,  1
  L FOB FCA
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-11  26  25
-10  23  25
 -9  22  24
 -8   0   2
 -7  49 -43
 -6  57 -50
 -5  12   2
 -4  41  39
 -3  33 -34
 -2  52 -50
 -1  32 -34
  0  22 -27
  1  86  86
  2 110 114
  3  11  11
  4   0  -3
  5   6  -7
  6  30  32

H,K= 11,  2
  L FOB FCA
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-11  25 -22
-10  11 -16
 -9  40 -36
 -8   0  -4
 -7   0   9
 -6  49  44
 -5  38 -41
 -4  44 -44
 -3  13 -12
 -2  31  32
 -1  93  94
  0  79  83
  1  15 -18
  2  43 -46
  3  27 -32
  4   0   1
  5   4   5

H,K= 11,  3
  L FOB FCA
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-10  30  33
 -9   5   1
 -8  21 -26
 -7  19 -15
 -6  14 -13
 -5  16  14
 -4  52  50
 -3  66  66
 -2  33  34
 -1  38 -39
  0  57 -60
  1  29 -30
  2   5  11
  3  16  18
  4  16 -14

H,K= 11,  4
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-10  25 -25
 -9   0   1
 -8  10  15
 -7  28  28
 -6  20  22
 -5   8   9
 -4  21 -20
 -3  31 -31
 -2  51 -54
 -1  33 -32
  0  24  28
  1  27  32
  2   5  -2

H,K= 11,  5
  L FOB FCA
 -8   7   6
 -7  26 -25
 -6  28 -28
 -5  31 -33
 -4   2  -6
 -3   6   7
 -2   1  13
 -1  31  37
  0   6   4

H,K= 12,-10
  L FOB FCA
 -2  26 -32
 -1  44 -50
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  1   7   3
  2  20 -22
  3   5  12

H,K= 12, -9
  L FOB FCA
 -5  15 -17
 -4  10  -4
 -3  34 -36
 -2   0  10
 -1  52  54
  0   0  -5
  1   0  16
  2  15  17
  3  20  20
  4  26  29
  5   6  -4

H,K= 12, -8
  L FOB FCA
 -7  12 -11
 -6   0  -2
 -5  15 -16
 -4  14 -14
 -3  76  78
 -2  36  36
 -1  28 -28
  0  32  29
  1  33 -35
  2   0  -3
  3  17  14
  4  30 -35
  5  32 -31
  6  20 -25

H,K= 12, -7
  L FOB FCA
 -8  24 -22
 -7   0   4
 -6   6  10
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 -4  60  56
 -3  75 -71
 -2  34 -33
 -1  11 -14
  0   8  -6
  1  18 -17
  2  36 -39
  3  77 -75
  4   0   8
  5  29  26
  6  29  33

H,K= 12, -6
  L FOB FCA
 -9   0   5
 -8  12   6
 -7   2   4
 -6  54  51
 -5  55 -54
 -4  90 -85
 -3  12   9
 -2   8   4
 -1  23  28
  0  14  19
  1  57 -56
  2   1  18
  3 105 101
  4  41  39
  5  24  28
  6   6  -5
  7  20 -19

H,K= 12, -5
  L FOB FCA
-10  17  14
 -9  11  -8
 -8   0  -9
 -7  29 -26
 -6  95 -90
 -5  21 -19
 -4  59  56
 -3  48  50
 -2  30  33
 -1  38 -38
  0  24 -25
  1 113 115
  2  71  68
  3  26 -25
  4  51 -49
  5  50 -54
  6  32 -35
  7  15  -8

H,K= 12, -4
  L FOB FCA
-10  15 -17
 -9   6   1
 -8  15 -16
 -7   0  -1
 -6  88  85
 -5  64  62
 -4  30 -24
 -3  26 -28
 -2   5  -7
 -1  58  58
  0  95  90
  1 100-104
  2 118-114
  3  84 -84
  4  15   6
  5  44  44
  6   0  -3
  7   0  -1

H,K= 12, -3
  L FOB FCA
-11   5   1
-10  10  11
 -9   0   3
 -8  75  75
 -7  48  41
 -6  33 -32
 -5  64 -61
 -4   0   2
 -3  40  42
 -2  29  29
 -1  90 -92
  0 113-113
  1  31 -32
  2  51  48
  3  77  80
  4  43  45
  5  20 -26
  6  21  28
  7  28  29

H,K= 12, -2
  L FOB FCA
-11  19  25
-10  32 -32
 -9  12  -4
 -8  24 -20
 -7  82 -78
 -6   0  10
 -5  12  10
 -4  23 -24
 -3  49 -48
 -2 101-100
 -1  20  23
  0  99 100
  1 128 128
  2  71  74
  3  29 -32
  4  39 -38
  5  12  10
  6   0  -2

H,K= 12, -1
  L FOB FCA
-11  22 -21
-10  27 -27
 -9  19  19
 -8  14  -2
 -7  10  -4
 -6  34 -32
 -5  22  16
 -4  16   9
 -3  52  51
 -2 101  99
 -1  83  79
  0  13  -9
  1  91 -92
  2  62 -66
  3  12  -9
  4  11  23
  5  23 -25
  6  40 -40

H,K= 12,  0
  L FOB FCA
-11  15  14
-10   8   4
 -9  27  25
 -8  18 -22
 -7  15  16
 -6  47  46
 -5  14  15
 -4  49  51
 -3  45  46
 -2  53 -52
 -1 111-113
  0  93 -96
  1   7  -1
  2  67  72
  3   0  -7
  4  46 -46
  5   0  -6

H,K= 12,  1
  L FOB FCA
-11   0  -2
-10  17 -15
 -9  15  -2
 -8  35  39
 -7  15  17
 -6  34 -34
 -5  62 -62
 -4  49 -49
 -3  77 -76
 -2   8  -2
 -1  60  56
  0  47  50
  1  42  44
  2  32 -35
  3   8  -6
  4  53  53

H,K= 12,  2
  L FOB FCA
-10  22  27
 -9   3  -2
 -8  34 -34
 -7  32 -32
 -6  29 -29
 -5   8  -2
 -4  44  43
 -3  42  44
 -2  32  32
 -1  12  10
  0  12 -13
  1   0  -1
  2  22  26
  3  14  11

H,K= 12,  3
  L FOB FCA
 -9  30 -33
 -8   0   6
 -7  44  44
 -6  29  27
 -5  30  34
 -4   7  -1
 -3   3  -7
 -2  26 -23
 -1  19 -25
  0  21  20
  1  12  -3

H,K= 12,  4
  L FOB FCA
 -7  10  -9
 -6  32 -32
 -5  15 -16
 -4   7  -3
 -3   5  -7
 -2   6  -6
 -1   9  11

H,K= 13, -9
  L FOB FCA
 -3   0   4
 -2  33  45
 -1   0   7
  0  20 -19
  1   9  -9
  2  19  20

H,K= 13, -8
  L FOB FCA
 -5   0   9
 -4  30  40
 -3  25  26
 -2  35 -36
 -1  15  13
  0  61  56
  1   6  11
  2  12  19
  3  57 -58
  4  48 -46

H,K= 13, -7
  L FOB FCA
 -7  24  24
 -6   6  11
 -5  10  12
 -4  13 -21
 -3  49 -51
 -2  35  34
 -1  24  16
  0  56 -55
  1  67 -65
  2  62 -63
  3  15  15
  4  35  34
  5  22  18

H,K= 13, -6
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 -8   6 -10
 -7   0   4
 -6   0  -8
 -5  55 -60
 -4   0   1
 -3  33  35
 -2  46 -45
 -1  41 -44
  0  48 -46
  1  51  53
  2 103 102
  3  49  49
  4  10  -5
  5   1 -10

H,K= 13, -5
  L FOB FCA
 -9  20 -25
 -8   0 -11
 -7   3   4
 -6  21 -21
 -5  26  37
 -4  31 -29
 -3  22 -20
 -2  35  34
 -1  75  73
  0 112 111
  1  52  47
  2  65 -66
  3  64 -62
  4   0  -6
  5  15 -16

H,K= 13, -4
  L FOB FCA
 -9  15  11
 -8   5  -6
 -7  15  12
 -6  11  11
 -5   0   4
 -4  36  34
 -3  51  46
 -2  12   9
 -1  20 -14
  0  89 -90
  1  93 -93
  2   1  -1
  3  26  26
  4   0   5
  5  13 -16

H,K= 13, -3
  L FOB FCA
-10   3  -4
 -9   0  -1
 -8  12   8
 -7  11  10
 -6  33  30
 -5  15  -4
 -4  20 -17
 -3  26 -24
 -2  77  78
 -1  95 -95
  0  21  24
  1  72  72
  2  22  21
  3  11  10
  4   0 -13
  5  19  17

H,K= 13, -2
  L FOB FCA
-10   0   3
 -9  44  48
 -8   5 -10
 -7  42 -43
 -6  42 -43
 -5  37 -35
 -4  11  11
 -3  12 -11
 -2  28  30
 -1 105 106
  0  29  31
  1  30 -33
  2   0   4
  3  13   9
  4  49  51
  5  11  12

H,K= 13, -1
  L FOB FCA
-10  13  20
 -9   0 -12
 -8  37 -34
 -7  13 -15
 -6   0  -5
 -5  30  27
 -4  39  38
 -3  56  54
 -2  18  15
 -1  31 -30
  0  44 -38
  1  25  25
  2  14  15
  3  22 -23
  4  62 -61

H,K= 13,  0
  L FOB FCA
-10  23 -26
 -9  13  10
 -8  33  33
 -7  67  65
 -6  30  32
 -5  12  -8
 -4  30 -29
 -3  40 -42
 -2  17 -16
 -1   0   2
  0  22 -23
  1   0   6
  2  52 -57
  3  17 -17

H,K= 13,  1
  L FOB FCA
 -9  35  37
 -8   0   9
 -7  49 -46
 -6  52 -53
 -5  12  -2
 -4   3   8
 -3   0  -6
 -2  12 -11
 -1  24 -26
  0   6   1
  1  30  30
  2  28  25

H,K= 13,  2
  L FOB FCA
 -8  36 -38
 -7   4   4
 -6  23  26
 -5  20  21
 -4  12  -2
 -3   7  -7
 -2  14  13
 -1  20  20
  0  27  29

H,K= 13,  3
  L FOB FCA
 -6  13 -15
 -5   9 -13
 -4   4   7
 -3  30  29

H,K= 14, -8
  L FOB FCA
 -2  10  16
 -1  48  45
  0   9 -17

H,K= 14, -7
  L FOB FCA
 -4   6  -1
 -3   7   8
 -2  11  13
 -1  56 -55
  0  48 -46
  1   6  -5
  2  23  27

H,K= 14, -6
  L FOB FCA
 -6  15 -15
 -5  28 -24
 -4  12  -7
 -3  33 -35
 -2  36 -33
 -1   5  -2
  0  27  27
  1  40  46
  2  11   2
  3  22 -19

H,K= 14, -5
  L FOB FCA
 -7  33 -33
 -6  23 -18
 -5  10  18
 -4   8  -2
 -3  36  38
 -2  44  42
 -1  33  34
  0  16  17
  1  27 -27
  2  24 -21
  3  33  35

H,K= 14, -4
  L FOB FCA
 -7  41  41
 -6  23  22
 -5  17  18
 -4  59  59
 -3  11  -9
 -2  21 -22
 -1  17 -23
  0  26 -28
  1   0  -8
  2   0  -1
  3  30 -29

H,K= 14, -3
  L FOB FCA
 -8  36  35
 -7  15 -13
 -6   4  -5
 -5  33 -34
 -4  50 -50
 -3  43 -42
 -2   6  -5
 -1  14 -12
  0   0   5
  1   5 -16
  2   5  -2
  3  25  24

H,K= 14, -2
  L FOB FCA
 -8  35 -34
 -7  46 -47
 -6  28 -31
 -5  19  23
 -4  36  36
 -3   5   6
 -2  10  -1
 -1  17  14
  0  14  15
  1  43  44
  2  39  37

H,K= 14, -1
  L FOB FCA
 -8  10   4
 -7  62  63
 -6  50  49
 -5  11  -6
 -4  32 -31
 -3  21  21
 -2  35  34
 -1  16  17
  0   0   5
  1  17 -20

H,K= 14,  0
  L FOB FCA
 -7  25 -29
 -6  39 -41
 -5   6  12
 -4  33  33
 -3   0  -2
 -2  34 -33
 -1  57 -55
  0  19 -14

H,K= 14,  1
  L FOB FCA
 -6  36  36
 -5  14  14
 -4  27 -28
 -3  40 -40
 -2  22 -22

H,K= 15, -5
  L FOB FCA
 -3   5  -6
 -2   0  -1
 -1  12  12

H,K= 15, -4
  L FOB FCA
 -4  10   7
 -3  32  21
 -2  26  27
 -1  12 -15

H,K= 15, -3
  L FOB FCA
 -5  21  32
 -4  10   8
 -3  21 -30
 -2  52 -52
 -1  21 -19

H,K= 15, -2
  L FOB FCA
 -4  53 -55
 -3   0  -8
 -2  48  48
```

[a] The signs of FCA apply to the real part of the structure factor.

mon ligand which participates in a wide variety of transition metal complexes. Only very recently has an accurate determination of any quinoline derivative appeared.[12] Since quinoline occupies a fundamental position in heterocyclic chemistry reliable structural information on this molecule is desirable.

Experimental Section

Crystals of tetra-*n*-butylammonium tribromo(quinoline)-nickelate(II), $[(n\text{-}C_4H_9)_4N][Ni(C_9H_7N)Br_3]$, were prepared according to the method of Forster[6] by mixing stoichiometric quantities of *anhydrous* nickel bromide dissolved in a minimum of *n*-butyl alcohol with tetra-*n*-butylammonium bromide and quinoline dissolved in a minimum quantity of ethanol. A crystal of approximate dimensions 0.23 × 0.20 × 0.18 mm was chosen for intensity measurements and was mounted on a quartz fiber with the c^* axis of the triclinic cell parallel to the spindle axis of the instrument. A primitive unit cell was chosen and the cell dimensions were determined at room temperature by a least-squares treatment of 51 carefully centered reflections using a General Electric XRD-5 unit equipped with manual goniostat, scintillation counter, and pulse height discriminator using unfiltered molybdenum radiation (λ 0.70926 Å for $K\alpha_1$). These are: $a = 12.282 \pm 0.002$ Å, $b = 10.291 \pm 0.002$ Å, $c = 12.726 \pm 0.002$ Å, $\alpha = 101.02 \pm 0.01°$, $\beta = 99.51 \pm 0.01°$, $\gamma = 106.55 \pm 0.01°$. The standard deviations were estimated from the least-squares analysis. The density measured by flotation in a carbon tetrachloride–methylcyclohexane mixture is 1.51 ± 0.01 g/cm^3 which compares favorably with the calculated density of 1.512

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[12] M. Sax and R. Desiderato, *Acta Cryst.*, **23**, 319 (1967).

g/cm^3 calculated for $Z = 2$. With two formula units per unit cell, space group P$\bar{1}$ was suggested; furthermore the top 15 non-origin peaks in the Patterson function were interpretable on this basis. The choice of P$\bar{1}$ was confirmed by the subsequent refinement of the structure. All atoms occupy general positions and no molecular symmetry conditions are imposed by space group symmetry.

The intensity data were recorded on an automated GE XRD-5 diffractometer. Nickel-filtered (at the receiving slit) copper radiation (λ 1.54051 Å for $K\alpha_1$) with a 20-mA source current, a 2° takeoff angle, and a θ–2θ scan technique was employed. Scans commenced at 2θ values 0.8° below the calculated $K\alpha_1$ position proceeded through the $K\alpha_1 - K\alpha_2$ separation and on to 0.8° beyond the $K\alpha_2$ peak position at a rate of 1°/min. A 10-sec background count was taken 0.4° from each end of the peak scan. The background correction for each reflection was obtained from the average of the two background counts prorated to the duration of the peak scan. In order to avoid errors due to counter saturation, reflections with $2\theta \leq 45°$ were remeasured with a source current of 6 mA. All 6-mA data were less than 500,000 total counts and in the final audit of the raw data reflections with total count values greater than this were deleted. Six standard reflections were recorded every 100 measurements. These showed evidence of crystal deterioration such that by the end of the 2-week period of data collection they had decreased from 7 to 31% at a steady rate depending on the particular reflection. The data were taken in batches: 2θ = 0–90, 90–120, and 120–147°. On the basis of an average decay of 30% over the period of the measurements of a representative sample of several hundred 0–90° data remeasured at the end, these batches were assigned scale factors of 1.00, 1.11, and 1.25, respectively. The 6-mA data were averaged in with the 20-mA data using a scale factor of 4.53 obtained from a comparison of 37 reflections of intermediate intensity. Of the 5830 independent reflections measured, 5388 were observed to be nonzero. The corrected intensities, I, were assigned standard deviations according to the formula

$$\sigma(I) = [\mathrm{TC} + 0.25(t_c/t_b)^2(B_1 + B_2) + (0.05I)^2]^{1/2}$$

where TC is the total integrated peak count obtained in a scan time, t_c, B_1 and B_2 are the two background counts each obtained in time, t_b, and $I = \mathrm{TC} - 0.5(t_c/t_b)(B_1 + B_2)$. The linear absorption coefficient of the crystal is $\mu = 63.6$ cm^{-1}. The intensity of the 003 reflection showed no greater than a 5% diminution from its maximum value as a function of ϕ, suggesting that absorption effects are not of great importance. No absorption corrections were applied to the data.

Solution and Refinement of the Structure

On the basis of the space group P$\bar{1}$ a Patterson[13] synthesis located the three bromine atoms and the nickel atom. Four cycles of least-squares[13] refinement of these four atoms yielded a conventional R value[14] of 0.385. A Fourier synthesis[13] based on these positions disclosed the remaining 27 nonhydrogen atoms. Several cycles of least-squares refinement with all of the atoms treated isotropically yielded $R = 0.157$. At this point the nickel atom and three bromine atoms were refined anisotropically and R dropped to 0.083. Owing to a programming error, the above refinements were obtained using only *hkl* data with $h \leq 9$. When all 5830 data were included in the full-matrix least-squares refinement R became 0.089. All 31 heavy atoms were then refined anisotropically yielding $R = 0.077$. A difference Fourier map computed at this point disclosed all 41 hydrogen atoms. These were first refined keeping the heavy atoms fixed, and then the heavy atoms were refined holding the hydrogens fixed by the full-matrix least-squares method. A final $R = 0.061$ was obtained. The error in an observation of unit weight is 1.45. Atomic scattering factors and dispersion corrections were taken from the "International Tables."[15] The final refined hydrogen atom positions correspond quite closely to those predicted on the basis of the heavy-atom structure. Table I gives the final observed and calculated structure factors. The final heavy-atom positional and anisotropic thermal parameters are given in Table II, while the hydrogen positional and isotropic thermal parameters are set out in Table III. The hydrogen parameters are of course of lower accuracy, and, since they are of no particular chemical interest in the present structure, they will not be considered further.

Description and Discussion of the Structure

Over-all Structure.—The crystal consists of a lattice of discrete tetra-*n*-butylammonium cations and tribromo(quinoline)nickelate(II) anions. A stereo pair showing an anion and cation as they are juxtaposed in the unit cell (which is comprised of two such units related by a center of symmetry) is provided in Figure 1. Each cation is surrounded by four nearest neighbor anions such that nickel–tetrabutylammonium nitrogen distances (Ni–N-CAT) of 5.982, 6.133, 6.723, and 6.855 Å occur. Owing to the highly unsymmetrical nature of the anion when taken as a unit and the large van der Waals contribution to the lattice forces in a crystal as organic in nature as the present, the crystal lattice does not approximate any of the well-known simple ionic structures for 1:1 salts. It is perhaps significant that each of the anion bromines is approximately equidistant from two cation nitrogens at distances ranging from 4.5 to 5.4 Å. The cation butyl chains are for the most part fully extended (Figure 1) which produces a structure with heavy interleaving of anion and cation features. In view of the solution work on the systems [cation$^+$][M(($C_6H_5)_3$P)I_3^-] (cation = $(C_4H_9)_4N^+$ or $(C_6H_5)_4As^+$; M = Co or Ni), wherein ion pairing is required to explain the cation proton isotropic magnetic resonance shifts, the mode of nearest neighbor anion–cation approach in the solid is of interest. For the $(C_6H_5)_3$P complexes it was assumed that the cation–anion approach was along the C_3 axis of the anion on the side opposite the bulky $(C_6H_5)_3$P ligand. In the present solid-state structure none of the nearest neighbor cations approaches the anion along what would correspond to the C_3 axis, *i.e.*, along the nickel–quinoline nitrogen (Ni–N-Q) bond axis on the side opposite

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[13] Computations were performed on the CDC 6600 computer at Lawrence Radiation Laboratory. The following computer programs were used for the operations indicated: Instrumental setting: Zalkin's GONIO (a modification of a program written by Larsen) and EULERA; refinement of cell dimensions: Hope's CELDIM; reduction of new data: Zalkin's AUDIT and INCOR; Patterson and Fourier syntheses: Zalkin's FORDAP; least-squares refinement: Zalkin's LS 300 (a modification of the Gantzel–Sparks–Trueblood full-matrix) program which minimizes $\Sigma w|\Delta F|^2/\Sigma w|F_o|^2$, $w = 1/\sigma^2(F)$; interatomic distance and angle computation: Zalkin's DISTAN; calculation of least-squares planes: Chu's LSPLAN; graphical representation of atomic positions and molecular stereochemistry: Zalkin's ATMPLT and Johnson's ORTEP; preparation of Table I: Zalkin's LIST.

[14] $R = \Sigma||F_o| - |F_o||/\Sigma|F_o|$.

[15] "International Tables for Crystallography," Vol. III, The Kynoch Press, Birmingham, England, 1962, p 201 ff.

TABLE II

FINAL NONHYDROGEN FRACTIONAL COORDINATES AND ANISOTROPIC THERMAL PARAMETERS[a] FOR $[(n\text{-}C_4H_9)_4N][Ni(C_9H_7N)Br_3]$[b,c]

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ni	0.2134 (1)	0.3607 (1)	0.2190 (1)	3.51 (2)	4.50 (3)	4.18 (3)	1.58 (2)	0.78 (2)	1.31 (2)
Br(1)	0.0435 (0)	0.2958 (1)	0.0743 (0)	4.17 (2)	8.27 (3)	5.20 (2)	2.38 (2)	0.04 (1)	1.76 (2)
Br(2)	0.3959 (0)	0.4142 (1)	0.1692 (0)	3.46 (2)	8.03 (3)	7.24 (3)	1.66 (2)	1.53 (2)	3.66 (2)
Br(3)	0.1852 (1)	0.5274 (1)	0.3593 (0)	9.21 (3)	6.90 (3)	5.79 (2)	4.96 (2)	1.16 (2)	0.33 (2)
N-Q	0.2100 (2)	0.1820 (3)	0.2656 (2)	3.6 (1)	4.3 (1)	3.5 (1)	1.1 (1)	1.0 (1)	0.8 (1)
C(2)-Q	0.1412 (3)	0.0605 (4)	0.1946 (3)	4.5 (2)	4.6 (2)	4.3 (2)	1.0 (1)	1.4 (1)	0.6 (1)
C(3)-Q	0.1374 (4)	−0.0706 (4)	0.2125 (4)	5.7 (2)	4.3 (2)	5.9 (2)	1.0 (1)	2.7 (1)	0.6 (1)
C(4)-Q	0.2051 (4)	−0.0788 (4)	0.3040 (4)	6.0 (2)	4.5 (2)	6.8 (2)	2.0 (2)	3.5 (2)	2.2 (2)
C(5)-Q	0.3537 (4)	0.0461 (5)	0.4788 (4)	6.3 (2)	8.5 (3)	6.6 (2)	3.9 (2)	2.6 (2)	4.4 (2)
C(6)-Q	0.4244 (4)	0.1675 (6)	0.5494 (4)	6.2 (2)	11.2 (4)	4.9 (2)	4.1 (3)	1.4 (2)	3.7 (2)
C(7)-Q	0.4240 (4)	0.2966 (5)	0.5279 (3)	4.9 (2)	7.7 (2)	4.4 (2)	2.2 (2)	0.3 (1)	1.2 (2)
C(8)-Q	0.3545 (3)	0.3024 (4)	0.4349 (3)	4.1 (1)	5.7 (2)	4.2 (2)	1.5 (1)	0.8 (1)	1.2 (1)
C(9)-Q	0.2804 (3)	0.1766 (4)	0.3595 (3)	3.3 (1)	5.0 (2)	3.6 (1)	1.7 (1)	1.4 (1)	1.6 (1)
C(10)-Q	0.2795 (3)	0.0471 (4)	0.3816 (3)	4.6 (2)	5.3 (2)	5.2 (2)	2.2 (1)	2.5 (1)	2.6 (1)
N-CAT	0.7879 (2)	0.5569 (2)	0.2339 (2)	2.7 (1)	3.5 (1)	3.6 (1)	1.0 (1)	0.9 (1)	0.9 (1)
$C(1)\text{-}C_4H_9(1)$	0.7205 (3)	0.6552 (3)	0.2096 (3)	3.3 (1)	3.5 (1)	4.3 (1)	1.5 (1)	1.1 (1)	1.1 (1)
$C(2)\text{-}C_4H_9(1)$	0.7784 (3)	0.7690 (3)	0.1579 (3)	4.3 (1)	4.1 (1)	4.7 (2)	1.7 (1)	1.7 (1)	1.4 (1)
$C(3)\text{-}C_4H_9(1)$	0.6989 (4)	0.8531 (4)	0.1328 (3)	5.9 (2)	5.1 (2)	6.3 (2)	3.0 (2)	2.5 (2)	2.4 (2)
$C(4)\text{-}C_4H_9(1)$	0.7497 (5)	0.9660 (5)	0.0777 (4)	10.2 (3)	6.6 (2)	8.5 (3)	4.5 (2)	4.3 (3)	4.7 (2)
$C(1)\text{-}C_4H_9(2)$	0.9066 (3)	0.6371 (4)	0.3117 (3)	2.8 (1)	4.5 (1)	4.0 (1)	1.1 (1)	0.7 (1)	0.7 (1)
$C(2)\text{-}C_4H_9(2)$	0.9050 (3)	0.7176 (4)	0.4236 (3)	3.6 (1)	5.0 (2)	4.1 (1)	0.8 (1)	0.6 (1)	0.2 (1)
$C(3)\text{-}C_4H_9(2)$	1.0283 (3)	0.7918 (4)	0.4922 (3)	3.8 (1)	6.2 (2)	4.4 (2)	1.2 (1)	0.6 (1)	−0.0 (1)
$C(4)\text{-}C_4H_9(2)$	1.0348 (4)	0.8675 (5)	0.6080 (5)	5.4 (2)	7.2 (2)	4.9 (2)	1.7 (2)	0.3 (2)	−1.0 (2)
$C(1)\text{-}C_4H_9(3)$	0.7136 (3)	0.4546 (3)	0.2850 (3)	3.7 (1)	3.7 (1)	4.4 (1)	0.9 (1)	1.0 (1)	1.2 (1)
$C(2)\text{-}C_4H_9(3)$	0.7611 (3)	0.3415 (4)	0.3120 (4)	4.4 (2)	5.0 (2)	6.7 (2)	1.6 (1)	1.1 (1)	2.9 (2)
$C(3)\text{-}C_4H_9(3)$	0.6738 (4)	0.2392 (5)	0.3553 (4)	6.3 (2)	6.0 (2)	6.7 (2)	0.9 (2)	1.4 (2)	3.1 (2)
$C(4)\text{-}C_4H_9(3)$	0.5642 (4)	0.1514 (5)	0.2738 (4)	6.0 (2)	5.0 (2)	9.1 (3)	0.8 (2)	2.5 (2)	2.3 (2)
$C(1)\text{-}C_4H_9(4)$	0.8100 (3)	0.4813 (3)	0.1291 (3)	3.3 (1)	4.1 (1)	3.9 (1)	1.5 (1)	1.0 (1)	0.8 (1)
$C(2)\text{-}C_4H_9(4)$	0.7006 (3)	0.3863 (4)	0.0444 (3)	4.0 (1)	5.0 (2)	4.0 (1)	1.8 (1)	0.7 (1)	0.2 (1)
$C(3)\text{-}C_4H_9(4)$	0.7323 (3)	0.3117 (4)	−0.0550 (3)	4.2 (2)	6.2 (2)	5.1 (2)	2.0 (1)	0.4 (1)	−0.4 (2)
$C(4)\text{-}C_4H_9(4)$	0.6230 (4)	0.2148 (6)	−0.1398 (4)	5.3 (2)	8.7 (3)	6.5 (2)	1.9 (2)	−0.1 (2)	−2.4 (2)

[a] Anisotropic thermal parameters are of the form $\exp[-0.25(B_{11}b_1{}^2h^2 + B_{22}b_2{}^2k^2 + B_{33}b_3{}^2l^2 + 2B_{12}b_1b_2hk + 2B_{13}b_1b_3hl + B_{23}b_2b_3kl)]$, when b_i is the ith reciprocal axis. [b] In this and subsequent tables the standard deviations of the least significant figure(s) are given in parentheses. [c] The atom labeling conforms to that indicated in the figures. Q denotes a quinoline molecule, and N-CAT is the tetra-n-butylammonium nitrogen.

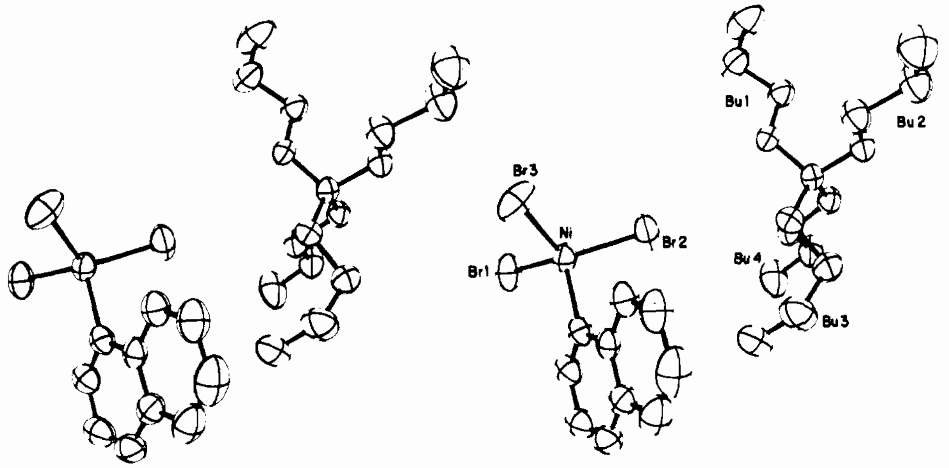

Figure 1.—Stereoscopic pair showing anion and cation as they are juxtaposed in the unit cell.

the quinoline. In fact, the nearest neighbor cation nitrogen to nickel vectors make angles of 69.0, 94.3, 117.5, and 126° with the Ni–N-Q bond axis. Of course solution and solid-state structures need not be identical or even closely related. The solid-state structure is determined by the conditions of minimization of the free energy of the entire crystal lattice while ion-pair formation in solution involves but a single cation–anion interaction plus solvation energy considerations. Even in solution the model proposed for the $(C_6H_5)_3P$ complexes is considerably less probable for the present system since quinoline has far less bulk and stereochemical influence than $(C_6H_5)_3P$.

Anion Geometry.—The bond angles and distances internal to the $[Ni(quinoline)Br_3^-]$ anion are set out in Table IV. A projection of the anion viewed down

TABLE III

FINAL HYDROGEN ATOM FRACTIONAL COORDINATES AND ISOTROPIC THERMAL PARAMETERS[a,b] FOR $[(n\text{-}C_4H_9)_4N][Ni(C_9H_7N)Br_3]$

Atom	x	y	z	B
H(2)-Q	0.087 (3)	0.075 (4)	0.127 (3)	3.1 (8)
H(3)-Q	0.088 (3)	−0.161 (4)	0.161 (3)	3.2 (8)
H(4)-Q	0.201 (4)	−0.180 (5)	0.306 (4)	5.9 (12)
H(5)-Q	0.335 (4)	−0.068 (5)	0.494 (4)	5.2 (11)
H(6)-Q	0.475 (5)	0.167 (6)	0.611 (5)	7.2 (14)
H(7)-Q	0.469 (4)	0.382 (4)	0.566 (4)	4.5 (10)
H(8)-Q	0.363 (3)	0.388 (4)	0.420 (3)	2.7 (8)
H(1)C(1)C_4H_9(1)	0.640 (3)	0.597 (3)	0.163 (2)	0.9 (6)
H(2)C(1)C_4H_9(1)	0.698 (3)	0.697 (3)	0.275 (3)	1.9 (7)
H(1)C(2)C_4H_9(1)	0.797 (3)	0.728 (4)	0.093 (3)	3.4 (9)
H(2)C(2)C_4H_9(1)	0.848 (5)	0.851 (6)	0.229 (5)	8.3 (16)
H(1)C(3)C_4H_9(1)	0.624 (3)	0.793 (4)	0.089 (3)	2.3 (7)
H(2)C(3)C_4H_9(1)	0.677 (4)	0.891 (4)	0.200 (3)	3.6 (9)
H(1)C(4)C_4H_9(1)	0.696 (4)	1.004 (5)	0.047 (4)	4.7 (10)
H(2)C(4)C_4H_9(1)	0.811 (6)	1.035 (6)	0.109 (5)	8.6 (17)
H(3)C(4)C_4H_9(1)	0.762 (4)	0.940 (4)	0.003 (3)	3.6 (9)
H(1)C(1)C_4H_9(2)	0.949 (3)	0.577 (3)	0.309 (2)	1.1 (6)
H(2)C(1)C_4H_9(2)	0.954 (3)	0.700 (4)	0.265 (3)	2.2 (7)
H(1)C(2)C_4H_9(2)	0.859 (3)	0.793 (4)	0.413 (3)	3.5 (9)
H(2)C(2)C_4H_9(2)	0.875 (5)	0.657 (5)	0.472 (5)	7.0 (14)
H(1)C(3)C_4H_9(2)	1.078 (4)	0.722 (5)	0.500 (4)	4.7 (10)
H(2)C(3)C_4H_9(2)	1.064 (4)	0.854 (5)	0.458 (4)	5.9 (12)
H(1)C(4)C_4H_9(2)	0.990 (5)	0.929 (5)	0.613 (4)	6.3 (13)
H(2)C(4)C_4H_9(2)	1.113 (4)	0.919 (4)	0.651 (4)	4.2 (10)
H(3)C(4)C_4H_9(2)	0.996 (6)	0.797 (7)	0.641 (6)	9.6 (19)
H(1)C(1)C_4H_9(3)	0.637 (3)	0.407 (3)	0.227 (2)	1.4 (6)
H(2)C(1)C_4H_9(3)	0.701 (3)	0.499 (3)	0.348 (3)	1.7 (6)
H(1)C(2)C_4H_9(3)	0.770 (3)	0.298 (4)	0.242 (3)	2.9 (8)
H(2)C(2)C_4H_9(3)	0.826 (4)	0.378 (5)	0.374 (4)	4.9 (11)
H(1)C(3)C_4H_9(3)	0.717 (6)	0.183 (6)	0.392 (5)	8.2 (16)
H(2)C(3)C_4H_9(3)	0.653 (5)	0.275 (5)	0.408 (4)	6.0 (13)
H(1)C(4)C_4H_9(3)	0.521 (4)	0.087 (4)	0.316 (4)	4.2 (10)
H(2)C(4)C_4H_9(3)	0.509 (4)	0.196 (5)	0.248 (4)	4.6 (10)
H(3)C(4)C_4H_9(3)	0.581 (5)	0.114 (5)	0.197 (5)	6.4 (13)
H(1)C(1)C_4H_9(4)	0.861 (3)	0.432 (3)	0.156 (3)	1.3 (6)
H(2)C(1)C_4H_9(4)	0.854 (3)	0.558 (3)	0.104 (3)	1.6 (6)
H(1)C(2)C_4H_9(4)	0.647 (3)	0.305 (4)	0.080 (3)	2.7 (8)
H(2)C(2)C_4H_9(4)	0.657 (3)	0.433 (4)	0.026 (3)	2.4 (7)
H(1)C(3)C_4H_9(4)	0.777 (5)	0.389 (5)	−0.088 (4)	6.6 (13)
H(2)C(3)C_4H_9(4)	0.779 (5)	0.260 (5)	−0.028 (4)	6.1 (13)
H(1)C(4)C_4H_9(4)	0.563 (5)	0.298 (7)	−0.177 (5)	9.0 (18)
H(2)C(4)C_4H_9(4)	0.645 (5)	0.165 (6)	−0.219 (5)	8.1 (16)
H(3)C(4)C_4H_9(4)	0.593 (6)	0.154 (6)	−0.114 (5)	8.5 (17)

[a] The isotropic thermal parameters have the form $\exp(-B\cdot(\sin^2\theta)/\lambda^2)$. [b] The atom labeling conforms to the code described in footnote c of Table II.

the crystal a axis indicating the atom labeling and selected bond distances is provided in Figure 2. The nickel atom is surrounded in a roughly tetrahedral fashion by the three bromine atoms and the quinoline nitrogen. The three Ni–Br distances must be considered identical to within the accuracy of the determination, with an average value of 2.375 Å. As expected for tetrahedral coordination this distance is less than that predicted (~2.50 Å) on the basis of covalent radii for Ni–Br distances in octahedral nickel complexes. A Ni–Br distance of 2.58 Å has been reported[16] for the octahedral complex $Ni(py)_4Br_2$ in a determination of marginal accuracy. The present Ni–Br distance is in good agreement with that predicted (2.39 Å) from the Ni–Cl distance (2.27 Å) in $NiCl_4^{2-}$ [3] and $Ni((C_6H_5)_3P)_2Cl_2$[4] when the difference in the Cl and Br radii is taken into account. The observed Ni–N distance of 2.029 Å is also consistent with a definite shortening of bond lengths in tetrahedral complexes as compared with their octahedral counterparts.

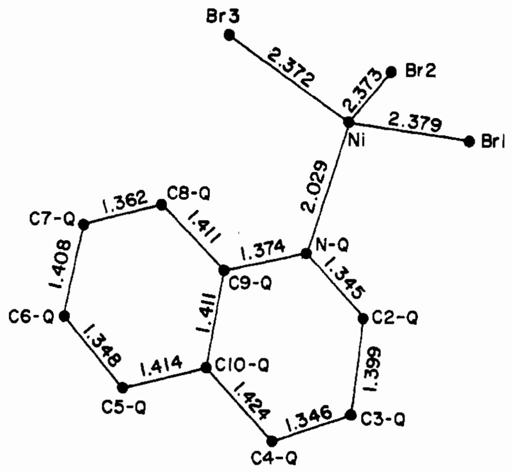

Figure 2.—Anion geometry viewed down the crystal a axis showing bond distances.

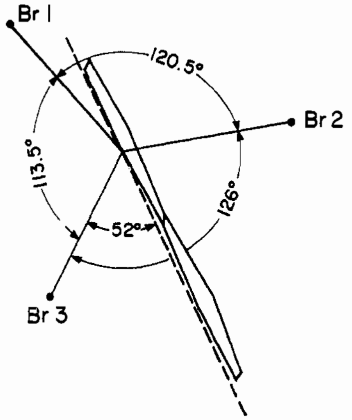

Figure 3.—Projection of the anion on the plane normal to the Ni–N bond. The angles quoted refer to the projection and not the actual bond angles.

The pseudo-tetrahedral geometry around the nickel is best described in terms of distortion from idealized C_{3v} symmetry with the N-Q–Ni bond taken as the C_3 axis. The three N-Q–Ni–Br angles are 105.1, 99.7, and 111.5° to Br(1), Br(2), and Br(3), respectively, for an average angle of 105.4°, slightly less than the tetrahedral angle. The three Br–Ni–Br angles also vary slightly among themselves (see Table IV) and average 113.3°, slightly above the tetrahedral angle. This indicates that on the average there is a slightly greater steric repulsion of the halogens among themselves than with the coordinated quinoline. The observed distortions from the average values quoted above can be understood in terms of specific interactions of the bromine atoms with the quinoline. Figure 3 shows the anion viewed down the Ni–N-Q bond. The angles between the three (N-Q, Ni, Br) planes are indicated in the figure. The quinoline benzo group provides greater steric interaction with the coordinated bromines than the hydrogen of the quinoline 2 position (H(2)-Q) and the benzo group roughly bisects the angle between the N-Q–Ni–Br(2) and –Br(3) planes, being however somewhat nearer the –Br(3) plane. The angle between these two planes (126°) is the largest of the three. The

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(16) A. S. Antsyshkina and M. A. Porai-Koshits, *Kristallografiya*, **3**, 676 (1958).

TABLE IV

BOND DISTANCES AND ANGLES OF $[(n\text{-}C_4H_9)_4N][Ni(C_7H_9N)Br_3]$

Anion Distances, Å

Ni–Br(1)	2.379 (2)	C(4)-Q–C(10)-Q	1.424 (6)
Ni–Br(2)	2.373 (1)	C(5)-Q–C(10)-Q	1.414 (6)
Ni–Br(3)	2.372 (2)	C(5)-Q–C(6)-Q	1.348 (8)
Ni–N-Q	2.029 (3)	C(6)-Q–C(7)-Q	1.408 (8)
N-Q–C(2)-Q	1.345 (5)	C(7)-Q–C(8)-Q	1.362 (5)
N-Q–C(9)-Q	1.374 (4)	C(8)-Q–C(9)-Q	1.411 (5)
C(2)-Q–C(3)-Q	1.399 (5)	C(9)-Q–C(10)-Q	1.411 (5)
C(3)-Q–C(4)-Q	1.346 (6)		

Anion Angles, deg

Br(1)–Ni–N-Q	105.1 (1)	C(3)-Q–C(4)-Q–C(10)-Q	119.1 (4)
Br(2)–Ni–N-Q	99.7 (0)	C(4)-Q–C(10)-Q–C(9)-Q	118.8 (3)
Br(3)–Ni–N-Q	111.5 (1)	C(4)-Q–C(10)-Q–C(5)-Q	122.0 (4)
Br(1)–Ni–Br(2)	116.8 (0)	C(5)-Q–C(10)-Q–C(9)-Q	119.2 (4)
Br(1)–Ni–Br(3)	104.5 (0)	C(10)-Q–C(5)-Q–C(6)-Q	120.3 (5)
Br(2)–Ni–Br(3)	118.5 (0)	C(5)-Q–C(6)-Q–C(7)-Q	120.4 (4)
Ni–N-Q–C(2)-Q	117.1 (2)	C(6)-Q–C(7)-Q–C(8)-Q	121.3 (4)
Ni–N-Q–C(9)-Q	124.5 (2)	C(7)-Q–C(8)-Q–C(9)-Q	119.3 (4)
C(2)-Q–N-Q–C(9)-Q	118.2 (3)	C(8)-Q–C(9)-Q–C(10)-Q	119.5 (3)
N-Q–C(2)-Q–C(3)-Q	123.0 (3)	C(8)-Q–C(9)-Q–N-Q	119.5 (3)
C(2)-Q–C(3)-Q–C(4)-Q	120.0 (4)	C(10)-Q–C(9)-Q–N-Q	121.0 (3)

Cation Distances, Å

N-CAT–C(1)-C_4H_9(1)	1.522 (4)	N-CAT–C(1)-C_4H_9(3)	1.508 (4)
C(1)-C_4H_9(1)–C(2)-C_4H_9(1)	1.511 (5)	C(1)-C_4H_9(3)–C(2)-C_4H_9(3)	5.513 (5)
C(2)-C_4H_9(1)–C(3)-C_4H_9(1)	1.513 (5)	C(2)-C_4H_9(3)–C(3)-C_4H_9(3)	1.528 (6)
C(3)–C_4H_9(1)–C(4)-C_4H_9(1)	1.509 (7)	C(3)-C_4H_9(3)–C(4)-C_4H_9(3)	1.480 (7)
N-CAT–C(1)-C_4H_9(2)	1.520 (4)	N-CAT–C(1)-C_4H_9(4)	1.516 (4)
C(1)-C_4H_9(2)–C(2)-C_4H_9(2)	1.510 (5)	C(1)-C_4H_9(4)–C(2)-C_4H_9(4)	1.514 (5)
C(2)-C_4H_9(2)–C(3)-C_4H_9(2)	1.512 (5)	C(2)-C_4H_9(4)–C(3)-C_4H_9(4)	1.518 (5)
C(3)-C_4H_9(2)–C(4)-C_4H_9(2)	1.507 (6)	C(3)-C_4H_9(4)–C(4)-C_4H_9(4)	1.520 (7)

Cation Angles, deg

C(1)-C_4H_9(1)–N-CAT–C(1)-C_4H_9(2)	111.1 (2)	N-CAT–C(1)-C_4H_9(2)–C(2)-C_4H_9(2)	116.0 (3)
C(1)-C_4H_9(1)–N-CAT–C(1)-C_4H_9(3)	106.2 (2)	C(1)-C_4H_9(2)–C(2)-C_4H_9(2)–C(3)-C_4H_9(2)	110.4 (3)
C(1)-C_4H_9(1)–N-CAT–C(1)-C_4H_9(4)	110.7 (2)	C(2)-C_4H_9(2)–C(3)-C_4H_9(2)–C(4)-C_4H_9(2)	113.9 (3)
C(1)-C_4H_9(2)–N-CAT–C(1)-C_4H_9(3)	110.8 (2)	N-CAT–C(1)-C_4H_9(3)–C(2)-C_4H_9(3)	115.8 (3)
C(1)-C_4H_9(2)–N-CAT–C(1)-C_4H_9(4)	107.0 (2)	C(1)-C_4H_9(3)–C(2)-C_4H_9(3)–C(3)-C_4H_9(3)	110.5 (3)
C(1)-C_4H_9(3)–N-CAT–C(1)-C_4H_9(4)	111.0 (2)	C(2)-C_4H_9(3)–C(3)-C_4H_9(3)–C(4)-C_4H_9(3)	115.4 (4)
N-CAT–C(1)-C_4H_9(1)–C(2)-C_4H_9(1)	116.2 (3)	N-CAT–C(1)-C_4H_9(4)–C(2)-C_4H_9(4)	114.6 (3)
C(1)-C_4H_9(1)–C(2)-C_4H_9(1)–C(3)-C_4H_9(1)	110.3 (3)	C(1)-C_4H_9(4)–C(2)-C_4H_9(4)–C(3)-C_4H_9(4)	110.4 (3)
C(2)-C_4H_9(1)–C(3)-C_4H_9(1)–C(4)-C_4H_9(1)	113.1 (4)	C(2)-C_4H_9(4)–C(3)-C_4H_9(4)–C(4)-C_4H_9(4)	110.7 (3)

steric repulsion between H(2)-Q and Br(1) forces Br(1) away from the quinoline and compresses the angle between the –Br(1) and –Br(3) planes to 113.5°. This is below the ideal angle of 120°, which the angle between the –Br(1) and –Br(2) planes approximates quite closely. Variations in the N-Q–Ni–Br angles may be readily understood by similar reasoning.

Quinoline.—As expected the quinoline molecule is quite accurately planar with none of the atoms deviating from the least-squares plane through all ten atoms by more than 0.011 Å. An interesting fact of the coordination is that the nickel atom lies 0.158 Å from the quinoline plane such that the Ni–N-Q bond makes an angle of 4.5° with this plane. This can be seen in Figure 3. Similar deviations have been found in the coordination of other heterocycles to metals.[17]

The bond angles internal to quinoline are normal. Of the 14 of these listed in Table IV all but one are within 2° of 120°; the exception is 123°. There are significant variations in the C–C and C–N bond lengths in quinoline which are analogous to those found in naphthalene.[18] The present bond distances compare favorably with the crystal structure results of Sax and Desiderato[12] on the quinoline nucleus of 5-acetoxy-6-methoxy-8-quinoline as indicated in Figure 4. The bond length variations correlate well with those predicted[19] by self-consistent field molecular orbital (SCFMO) theory. As shown in Figure 4 the agreement is satisfactory both for the present results and for those of Sax and Desiderato,[12] particularly with respect to trends. As predicted by the theory, the introduction of a heteroatom does not induce any marked changes in the carbon–carbon bond length pattern from those observed in naphthalene.[18] Agreement of the present results with the bond length predictions of a somewhat more elaborate MO calculation[20] is good but

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[17] E. B. Fleischer, C. K. Miller, and L. E. Webb, *J. Am. Chem. Soc.*, **86**, 2342 (1964), and references therein.

[18] D. W. J. Cruickshank and R. A. Sparks, *Proc. Roy. Soc.* (London), **A258**, 270 (1960); see also electron diffraction results of A. Almenningen, O. Bastiansen, and F. Dyvik, quoted by O. Bastiansen and P. N. Skanche, *Advan. Chem. Phys.*, **3**, 323 (1961).

[19] K. Nishimoto and L. S. Forster, *Theoret. Chim. Acta*, **4**, 155 (1966).

[20] M. J. S. Dewar and G. J. Gleicher, *J. Chem. Phys.*, **44**, 759 (1966).

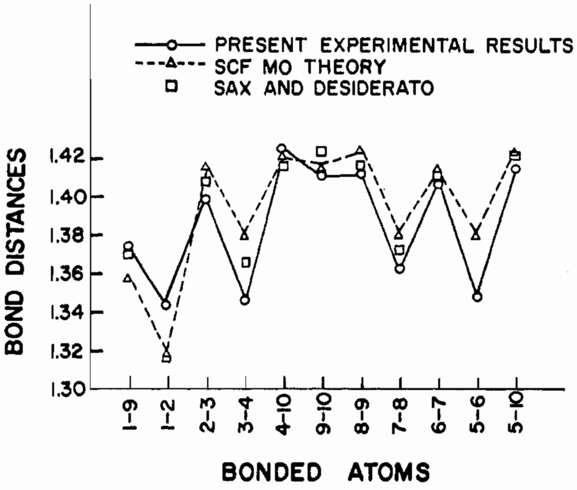

Figure 4.—Comparison of the present observed bond distances with those predicted by self-consistent field molecular orbital theory and those determined[12] for the quinoline nucleus of 5-acetoxy-6-methoxy-8-nitroquinoline. The quinoline atoms are labeled as in Figure 2.

slightly less satisfactory. It is noteworthy that coordination to the $NiBr_3^-$ moiety apparently produces a negligible perturbation on the quinoline structure.

Cation Geometry.—The configuration of the tetra-n-butylammonium ion in this structure is illustrated in Figure 1. Three of the butyl chains adopt the *trans* conformation but the fourth (Bu(3)) adopts a *gauche* conformation. A similar configuration was found[21a] for $(C_4H_9)_4N^+$ in $[(C_4H_9)_4N^+]_2[Co(MNT)_2^{2-}]$, where MNT = maleonitrile dithiolate; however, in two other structures[21b,22] containing this cation all of the butyl groups adopt the *trans* configuration. The energy differences involved are not great and packing considerations are undoubtedly decisive. In order to facilitate a comparison with other structures,[21] the dihedral angles between the planes defined by carbons 1, 2, 3 and 2, 3, 4 were computed for each of the butyl chains. The results are presented in Table V. The dihedral angle for the *gauche* chain is 66.5°, quite close to the value (71.6°) found in the $[(C_4H_9)_4N^+]_2[Co(MNT)_2^{2-}]$ structure.[21a] The *trans* chains have dihedral angles somewhat larger than those found earlier,[21] but the butyl chains are nevertheless reasonably planar. The present average N-CAT–C(1) distance of 1.517 Å is in almost perfect agreement with those found earlier, as is the average butyl chain C–C distance of 1.511 Å. The six tetrahedral angles at the nitrogen (C(1)–N-CAT–C(1)) average 109.5°. The mean value of the four N–C–C angles is 115.7° while that of the eight C–C–C angles is 111.8°, again in excellent agreement with previous determinations.[21]

TABLE V

THE DIHEDRAL ANGLES FOR THE FOUR BUTYL CHAINS IN THE TETRA-n-BUTYLAMMONIUM ION

Plane 1 defined by atoms	Plane 2 defined by atoms	Dihedral angle, deg
C(1), C(2), and C(3) of $C_4H_9(1)$	C(2), C(3), and C(4) of $C_4H_9(1)$	15.1
C(1), C(2), and C(3) of $C_4H_9(2)$	C(2), C(3), and C(4) of $C_4H_9(2)$	12.6
C(1), C(2), and C(3) of $C_4H_9(3)$	C(2), C(3), and C(4) of $C_4H_9(3)$	66.5
C(1), C(2), and C(3) of $C_4H_9(4)$	C(2), C(3), and C(4) of $C_4H_9(4)$	13.1

Orientation of the Complex in the Crystal.—Finally, since one of the major purposes of the present determination is to provide information to enable the interpretation of oriented single-crystal experiments, we present in Table VI the angles that the principal bonds in the anion make with the respective crystal axes.

TABLE VI

ANGLES MADE BY VARIOUS ANION BONDS WITH THE CRYSTAL AXES[a]

Bond	Angle (deg) with—		
	a axis	b axis	c axis
Ni–N-Q	79.1	17.0	62.0
Ni–Br(1)	48.0	83.3	54.9
Ni–Br(2)	22.7	89.2	62.1
Ni–Br(3)	61.6	51.6	50.3

[a] All angles are given as acute.

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