ACTA CHEMICA SCANDINAVICA 23 (1969) 3498–3512

The Crystal Structures of Bis(ethylenediamine)nickel(II) Dibromoargentate(I), $[Ni(en)_2][AgBr_2]_2$, and Bis(ethylenediamine)nickel(II) Diiodoargentate(I), $[Ni(en)_2][AgI_2]_2$

ROLF STOMBERG

Department of Inorganic Chemistry, Chalmers Institute of Technology and University of Göteborg, P.O. Box, S-402 20 Göteborg 5, Sweden

The crystal structures of the orange compounds $[Ni(en)_2][AgBr_2]_2$ and $[Ni(en)_2][AgI_2]_2$ have been determined from Fourier calculations based on three-dimensional X-ray data, collected for $[Ni(en)_2][AgBr_2]_2$ with a Nonius integrating camera and for $[Ni(en)_2][AgI_2]_2$ with the Philips automatic single crystal diffractometer, PAILRED. Least squares refinement of the structures based on all observed reflexions yielded R values of 0.074 and 0.062, respectively.

The crystals of the two compounds are isomorphous and are composed of square planar $[Ni(en)_2]^{2+}$ ions and chains of $[AgBr_2]_n^{n-}$ or $[AgI_2]_n^{n-}$ ions. Silver is distorted tetrahedrally coordinated by four halogen atoms, the tetrahedra being linked by the sharing of edges to form $[AgX_2]_n^{n-}$ chains which extend in the direction of the shortest crystallographic axis. Two halogen atoms are sufficiently close to the nickel atom to permit weak interaction, the Ni···Br and Ni···I distances being 3.36 Å and 3.51 Å, respectively.

Average bond distances are: Ag—Br 2.72 Å, Ag—I 2.87 Å, Ni—N 1.92 Å, C—N 1.49 Å, and C—C 1.52 Å.

The determination of the crystal structures of the orange nickel(II) compounds $[Ni(en)_2][AgBr_2]_2$ and $[Ni(en)_2][AgI_2]_2$ was undertaken in order to investigate the configuration of ligands about nickel and silver. Details concerning preparation, analysis and determination of cell dimensions have already been published by Stomberg [1] and the following crystal data has also been given in the previous note.

A reduced cell, transformation matrix $\{101/010/\bar{1}00\}$, was used in all Fourier and least-squares calculations for $[Ni(en)_2][AgI_2]_2$.

$[Ni(en)_2][AgBr_2]_2$

Space group: $C2/m$

$a = 10.202 \pm 0.006$ Å
$b = 12.780 \pm 0.008$ Å
$c = 6.575 \pm 0.008$ Å
$\beta = 120.08 \pm 0.04$ Å
$V = 741.8$ Å^3
$Z = 2$

$[Ni(en)_2][AgI_2]_2$

Space group; $C2/m$

$a = 10.696 \pm 0.010$ Å
$b = 13.075 \pm 0.017$ Å
$c = 6.877 \pm 0.007$ Å
$\beta = 120.24 \pm 0.07°$
$V = 830.0$ Å^3
$Z = 2$

EXPERIMENTAL

X-Ray methods. Weissenberg photographs of the layers $h0l-h8l$ and $hk0$ for $[Ni(en)_2][AgBr_2]_2$ were recorded with a Nonius integrating camera using copper radiation. The intensities of the reflexions registered were estimated visually by comparison with an intensity scale prepared by the rotating sector method. A total of 561 independent reflexions were measured.

For $[Ni(en)_2][AgI_2]_2$ the intensities of 1576 independent $h0l-h14l$ reflexions were obtained with the Philips automatic single crystal diffractometer PAILRED using molybdenum radiation.

Computing methods. Lorentz and polarization corrections and the Patterson summation for $[Ni(en)_2][AgBr_2]_2$ were performed on a SAAB D21 computer [2,3] while the remainder of the computational work was performed on an IBM 360/50 computer using the following programmes: DATAP1,[4] DATAP2,[5] DRF,[5] LALS,[5] and DISTAN.[5] $[Ni(en)_2][AgI_2]_2$ was corrected for absorption, but extinction and dispersion effects were neglected for both crystals.

The atomic scattering factors used in the calculation of structure factors were taken from Volume III of the *International Tables for X-Ray Crystallography*, 1962.

STRUCTURE DETERMINATION

The dominant Patterson maxima for both $[Ni(en)_2][AgBr_2]_2$ and $[Ni(en)_2][AgI_2]_2$ are given in Table 1. The positions and magnitudes of the interatomic vectors indicated isomorphism, which considerably simplified

Table 1. Patterson peaks.

Peak	$[Ni(en)_2][AgBr_2]_2$				$[Ni(en)_2][AgI_2]_2$				Vector
	u	v	w	Peak height	u	v	w	Peak height	
1	0	0	0	622	0	0	0	999	origin
2	0.2635	0	−0.0178	166	0.26	0	−0.02	250	$Ag-X_2$
3	0.0071	0.1644	0.2778	160	0	0.16	0.28	230	$Ag-X_1$
4	0.2483	0	0.4272	157	0.26	0	0.42	240	$Ag-X_2$
5	0	0	1/2	141	0	0	1/2	100	Ag−Ag
6	0.2567	0.1641	0.7076	134	0.26	0.17	0.74	330	X_1-X_2
7	1/2	0.1539	1/2	106	1/2	0.16	1/2	175	$Ni-X_1$
8	0.4940	0	0.2234	100	1/2	0	0.22	160	Ag−Ni
9	0.2456	0	−0.2079	95	0.24	0	0.80	190	$Ni-X_2$
10	0	0.3133	0	64	0	0.34	0	200	X_1-X_1
11	0.5078	0	0.4201	52	0.52	0	0.42	150	X_2-X_2

the solving of the Patterson function, the only difference between the two functions being that due to the different halogen atoms. It is not possible for the eight halogen atoms to occupy the general 8-fold position of space group $C2/m$ since none of the dominant peaks with coordinates $2x$ 0 $2z$ has a corresponding peak at $2x$ $2y$ $2z$ (peaks 5 and 7 do not have correct relative peak heights, furthermore, they would lead to too short halogen-halogen distances). The halogen atoms were, therefore, assumed to occupy two 4-fold positions. The four silver atoms were assumed to occupy one 4-fold position and the two nickel atoms one of the special 2-fold positions. By taking into account the expected relative magnitudes of the interatomic vectors it was possible to identify the various peaks as is shown in Table 1, and thus to deduce the following preliminary atomic parameters, expressed in fractional coordinates, for $[Ni(en)_2][AgBr_2]_2$:

	x	y	z
Ag in 4*i*	0.007	0	0.278
Br_1 in 4*g*	0	0.160	0
Br_2 in 4*i*	0.257	0	0.709
Ni in 2*d*	$\frac{1}{2}$	0	$\frac{1}{2}$

A structure factor calculation, based on these parameters, gave an R value of 0.17. From the subsequent Fourier summations the positions of the nitrogen and carbon atoms were obtained. When these were introduced into the structure factor calculations the R value dropped to 0.14. The same atomic parameters, transformed to an I-centered cell, were then introduced into the structure factor calculation for $[Ni(en)_2][AgI_2]_2$, an R value of 0.13 being obtained.

Both structures were refined by the least-squares method. In the first three cycles isotropic temperature factors, positional parameters and an overall scale factor were refined. In the subsequent cycles the positional parameters and a scale factor for each layer were refined alternating with the refinement of positional parameters, anisotropic temperature coefficients and an overall scale factor. A total of 16 cycles of refinement was performed. Each reflexion was given the weight $w=\{a+|F_o|+c|F_o|^2+d|F_o|^3\}^{-1}$, according to Cruickshank,[6] with $a=10.0$, $c=0.012$, and $d=0.0001$ for $[Ni(en)_2][AgBr_2]_2$, and $a=80.0$, $c=0.005$, and $d=0.0001$ for $[Ni(en)_2][AgI_2]_2$. In the last cycle of refinement the maximum shift was less than 1 % of the estimated standard deviation for $[Ni(en)_2][AgBr_2]_2$ and less than 2 % for $[Ni(en)_2][AgI_2]_2$. The final R values were 0.074 and 0.062, respectively. The correctness of the proposed crystal structures was further checked by difference electron density calculations. The heights of the largest peaks in the difference maps were 30 and 15 %, respectively, of the height of a carbon atom peak.

The atomic parameters obtained in the last cycle are given in Tables 2 and 3 and observed and calculated structure factors in Tables 4 and 5. Since all computational work was based on $C2/m$ for $[Ni(en)_2][AgBr_2]_2$ and $I2/m$ for $[Ni(en)_2][AgI_2]_2$, the positional parameters for the latter compound, transformed to space group $C2/m$, are given in Table 2*a* for comparison.

Table 2a. Atomic coordinates, expressed in fractions of the cell edges, and standard deviations for $[Ni(en)_2][AgBr_2]_2$. Space group $C2/m$. $Z=2$. For comparison the values obtained for $[Ni(en)_2][AgI_2]_2$, transformed to space group $C2/m$, are given in brackets.

Atom	Position	$x \pm \sigma(x)$	$y \pm \sigma(y)$	$z \pm \sigma(z)$
Ag	4*i*	0.0061 ± 0.0002 (0.0027)	0 (0)	0.2778 ± 0.0002 (0.2775)
Br_1	4*g*	0 (0)	0.1608 ± 0.0002 (0.1675)	0 (0)
Br_2	4*i*	0.2570 ± 0.0002 (0.2597)	0 (0)	0.7050 ± 0.0003 (0.7066)
Ni	2*d*	½ (½)	0 (0)	½ (½)
N	8*j*	0.3865 ± 0.0011 (0.3874)	0.1094 ± 0.0012 (0.1069)	0.2826 ± 0.0016 (0.2939)
C	8*j*	0.4155 ± 0.0015 (0.4194)	0.2111 ± 0.0014 (0.2049)	0.4123 ± 0.0023 (0.4189)

Table 2b. Anisotropic temperature parameters β_{ij} and their standard deviations. The expression used is $\exp-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}k^2+\beta_{12}hk+\beta_{13}hl+\beta_{23}kl)$.

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ag	0.0113 2	0.0103 2	0.0207 4	0	0.0176 4	0
Br_1	0.0095 2	0.0096 3	0.0198 5	0	0.0150 5	0
Br_2	0.0082 2	0.0098 3	0.0210 5	0	0.0142 5	0
Ni	0.0083 4	0.0097 5	0.0222 9	0	0.0123 10	0
N	0.0081 12	0.0108 17	0.0186 27	0.0018 18	0.0060 29	−0.0022 25
C	0.0131 19	0.0086 18	0.0291 37	0.0080 24	0.0229 47	0.0062 36

DESCRIPTION AND DISCUSSION

The structure investigation has confirmed that the crystals of $[Ni(en)_2][AgBr_2]_2$ and $[Ni(en)_2][AgI_2]_2$ are, as expected, isomorphous and shown that they contain square planar $[Ni(en)_2]^{2+}$ ions, and chains of $[AgX_2]_n^{n-}$

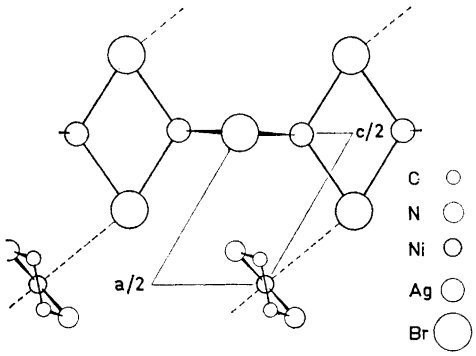

Fig. 1. Projection on (010) of part of the unit cell.

Table 3a. Atomic coordinates and standard deviations for $[Ni(en)_2][AgI_2]_2$. Space group $I2/m$. $Z=2$. In Table 2*a* these coordinates have been transformed to space group $C2/m$.

Atom	Position	$x \pm \sigma(x)$	$y \pm \sigma(y)$	$z \pm \sigma(z)$
Ag	4*i*	0.2748 ± 0.0002	0	−0.0027 ± 0.0001
I_1	4*g*	0	0.1675 ± 0.0001	0
I_2	4*i*	0.5531 ± 0.0001	0	0.2597 ± 0.0001
Ni	2*d*	0	0	½
N	8*j*	0.0936 ± 0.0010	0.1069 ± 0.0006	0.3875 ± 0.0008
C	8*j*	0.0005 ± 0.0014	0.2049 ± 0.0006	0.4194 ± 0.0011

Table 3b. Anisotropic temperature parameters β_{ij} and their standard deviations.

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ag	0.0143 2	0.0058 1	0.0084 1	0	0.0036 2	0
I_1	0.0111 1	0.0039 0	0.0066 1	0	0.0030 1	0
I_2	0.0106 1	0.0042 0	0.0056 1	0	0.0020 1	0
Ni	0.0089 3	0.0021 1	0.0027 1	0	0.0030 3	0
N	0.0131 12	0.0032 4	0.0059 7	0.0004 11	0.0055 15	0.0020 8
C	0.0150 15	0.0026 4	0.0086 9	−0.0006 13	−0.0028 20	0.0019 10

Table 4. Observed and calculated structure factors for $[Ni(en)_2][AgBr_2]_2$. The columns are successively l, $|F_o|$ and F_c.

0 0 L			3 1 L			-4 82 80			0 - 1			-2 23 -23			3 32 30			-4 27 27		
1 25 -33			6 17 17			-5 146 -142			-1 33 33			-3 59 -61			2 68 61			-5 6 4		
2 100 -98			5 19 -18			-6 36 -31			-2 202 -206			-4 25 24			1 24 21			-6 14 15		
3 170 186			4 - 6			-7 42 38			-3 44 -42			-5 - -9			0 116 112			-7 26 30		
4 183 185			3 153 147			-8 9 -8			-4 53 47			-6 48 -51			-1 74 69					
5 68 -64			2 41 -43						-5 80 -73			-7 16 -17			-2 49 54			7 7 L		
6 25 21			1 70 -64			6 2 L			-6 128 -121						-3 14 16			3 35 39		
7 92 73			0 190 183			4 6 -4			-7 29 28			12 4 L			-4 100 99			2 4 -6		
			-1 212 223			3 19 -17						-2 32 -35			-5 32 29			1 5 -9		
2 0 L			-2 195 -221			2 16 3			9 3 L			-3 - 4			-6 - 7			0 50 47		
6 19 12			-3 76 80			1 74 -74			2 46 -45			-4 16 17			-7 16 20			-1 86 73		
5 28 30			-4 191 177			0 19 18			1 - -3			-5 50 -48						-2 70 -64		
4 90 92			-5 - 1			-1 22 -22			0 19 -18			-6 14 -17			4 6 L			-3 40 37		
3 43 41			-6 77 -72			-2 43 -39			-1 45 -45									-4 88 83		
2 59 69			-7 87 81			-3 95 -97			-2 72 -72			1 5 L			5 24 -25			-5 5 1		
1 85 85			-8 24 31			-4 54 53			-3 - 4			6 32 -36			4 62 66			-6 29 -30		
0 177 238						-5 22 -21			-4 56 -53			5 11 -10			3 67 65			-7 45 50		
-1 32 23			5 1 L			-6 72 -67			-5 42 -39			4 89 91			2 33 -29					
-2 101 141			5 - 2			-7 12 -9			-6 44 -46			3 33 32			1 16 1			9 7 L		
-3 47 45			4 51 55			-8 26 28			-7 9 -11			2 135 -135			0 202 208					
-4 128 151			3 38 35						-8 18 -20			1 136 132			-1 10 8			1 27 24		
-5 34 33			2 77 -73			8 2 L						0 114 107			-2 53 -48			0 16 18		
-6 22 20			1 96 98			3 11 13			11 3 L			-1 34 -33			-3 105 109			-1 - 11		
-7 35 38			0 126 107			2 49 -53			0 - 5			-2 84 -80			-4 132 131			-2 - -1		
			-1 9 -9			1 45 -43			-1 8 7			-3 137 145			-5 46 -48			-3 51 46		
4 0 L			-2 49 -51			0 91 88			-2 82 -85			-4 8 6			-6 19 22			-4 6 7		
5 32 -26			-3 164 164			-1 68 -66			-3 14 -18			-5 27 -26			-7 53 62			-5 18 17		
4 96 92			-4 30 25			-2 93 -92			-4 19 21			-6 15 14						-6 8 8		
3 97 94			-5 - 0			-3 20 17			-5 37 -40			-7 29 30			6 6 L			-7 16 20		
2 40 -38			-6 15 12			-4 64 63			-6 74 -79						3 13 15					
1 32 30			-7 58 53			-5 115 -111			-7 24 23			3 5 L			2 42 37			11 7 L		
0 265 300			-8 - 3			-6 28 -27						5 11 -10			1 9 8			-2 29 -26		
-1 16 9						-7 38 36			0 4 L			4 - 4			0 72 65			-3 19 16		
-2 28 -22			7 1 L			-8 11 -12			1 140 -153			-1 55 49			-1 55 49			-4 45 42		
-3 129 147			3 59 51						2 151 -165			-2 45 39			-2 45 39			-5 7 6		
-4 186 206			2 12 -19			10 2 L			3 20 17			-3 9 9			-3 9 9			-6 20 -25		
-5 71 -71			1 20 -20			1 24 -27			4 52 50			1 35 -32			-4 90 93					
-6 44 44			0 89 82			0 9 -2			5 108 -105			0 94 89			-5 32 30			0 8 L		
-7 97 86			-1 111 102			-1 - 3			6 24 -24			-1 110 113			-6 - 3			1 51 -53		
-8 23 21			-2 112 -111			-2 18 -18			7 20 20			-2 134 -143			-7 21 25			2 89 -89		
			-3 52 56			-3 62 -53						-3 62 63						3 29 30		
6 0 L			-4 143 130			-4 43 42			2 4 L			-4 89 90			8 6 L			4 50 49		
4 31 27			-5 - -1			-5 17 -15			6 12 -15			-5 8 -5			2 5 -7			5 52 -60		
3 31 31			-6 71 -65			-6 47 -49			5 30 -31			-6 53 -49			1 7 4					
2 71 65			-7 90 86			-7 9 -13			4 - -6			-7 47 51			0 95 94			2 8 L		
1 - 4			-8 28 31						3 38 -40						-1 - 1			5 6 -9		
0 84 84						12 2 L			2 35 -29			5 5 L			-2 13 -12			4 15 16		
-1 116 118			9 1 L			-2 30 -35			1 116 -119			4 25 27			-3 64 65			3 28 -24		
-2 49 55			2 12 -15			-3 10 9			0 22 14			3 18 17			-4 86 83			2 - -4		
-3 - -12			1 40 40			-4 21 23			-1 53 -58			2 43 -41			-5 30 -28			1 22 -26		
-4 171 167			0 21 19			-5 54 -55			-2 60 -58			1 56 53			-6 21 22			0 22 21		
-5 56 50			-1 - 12			-6 7 -7			-3 107 -115			0 56 49			-7 51 51			-1 24 -23		
-6 - 4			-2 - 1						-4 44 39			-1 6 -7						-2 18 -15		
-7 35 30			-3 60 59			1 3 L			-5 40 -37			-2 32 -27			10 6 L			-3 28 -26		
-8 88 71			-4 13 10			6 81 -80			-6 52 -50			-3 86 89			1 - -3			-4 25 24		
			-5 23 24			5 55 -53			-7 15 -13			-4 8 -4			0 23 23			-5 14 -16		
8 0 L			-6 - 6			4 24 24						-5 15 11			-1 32 33			-6 10 -13		
3 47 42			-7 30 30			3 37 -37			4 4 L			-6 13 -2			-2 23 20					
2 21 -17			-8 7 11			2 272 -278			5 75 -66			-7 28 29			-3 9 -10			4 8 L		
1 - -1						1 5 10			4 33 34			-8 - 2			-4 58 62			4 19 23		
0 168 155			11 1 L			0 40 24			3 27 26						-5 26 28			3 10 15		
-1 18 17			0 29 32			-1 192 -227			2 128 -130			7 5 L			-6 6 -7			2 49 -48		
-2 48 -46			-1 49 52			-2 174 -197			1 105 -99			3 52 53						1 40 -38		
-3 105 111			-2 55 -55			-3 50 56			0 169 165			2 17 -18			12 6 L			0 96 90		
-4 139 142			-3 18 18			-4 74 -78			-1 110 -117			1 40 -36			-3 27 27			-1 53 -48		
-5 59 -52			-4 79 78			-5 88 -83			-2 186 -190			0 64 62			-4 43 41			-2 80 -70		
-6 35 32			-5 - 0			-6 36 -39			-3 31 20			-1 81 77						-3 31 28		
-7 89 79			-6 42 -47			-7 7 7			-4 91 85			-2 98 -96			1 7 L			-4 46 42		
-8 33 32			-7 62 58						-5 153 -148			-3 18 18			6 18 -20			-5 66 -62		
						3 3 L			-6 36 -35			-4 102 101			5 10 10			-6 9 -8		
10 0 L			0 2 L			6 15 -16			-7 37 33			-5 - -3			4 61 63					
1 - -2			1 109 -134			5 53 -50			-8 - -12			-6 71 -67			3 46 47			6 8 L		
0 43 42			2 209 -230			4 58 -54						-7 59 64			2 64 -66			3 4 -3		
-1 45 43			3 63 48			3 47 45			6 4 L			-8 18 23			1 96 95			2 9 5		
-2 24 24			4 91 89			2 148 -145			4 - 1						0 84 105			1 29 -29		
-3 - 2			5 135 -132			1 142 -139			3 24 -23			9 5 L			-1 14 -14			0 10 8		
-4 85 87			6 18 -17			0 10 -4			2 12 -16			1 26 27			-2 9 -8			-1 - 2		
-5 42 39			7 29 29			-1 - 5			1 57 -52			0 20 19			-3 104 103			-2 9 -9		
-6 - -7						-2 263 -286			0 - -3			-1 - -2			-4 18 16			-3 51 -44		
-7 32 29			2 2 L			-3 60 -59			-1 33 -32			-2 12 -11			-5 - 3			-4 33 32		
			6 14 -17			-4 49 45			-2 55 -51			-3 45 41			-6 8 11			-5 - -4		
12 0 L			5 35 -32			-5 84 -84			-3 81 -81			-4 13 10						-6 26 -28		
-1 - -3			4 28 24			-6 127 -119			-4 43 38			-5 - 2			3 7 L			-7 4 -3		
-2 - 0			3 56 -61			-7 29 29			-5 45 -45			-6 6 -2			5 - -4					
-3 52 44			2 28 -22			-8 - -9			-6 53 -52			-7 26 25			4 - 5			8 8 L		
-4 54 52			1 90 -91						-7 16 -16						3 85 87			2 11 -24		
-5 20 -17			0 19 21			5 3 L			-8 18 18			11 5 L			2 19 -20			1 16 -18		
-6 28 21			-1 44 -51			4 - 3						-1 30 30			1 16 -9			0 48 46		
			-2 82 -81			3 23 -25			8 4 L			-2 38 -43			0 96 90			-1 27 -24		
1 1 L			-3 61 -72			2 133 -127			2 39 -44			-3 12 14			1 116 102			-2 42 -43		
6 32 -33			-4 41 40			1 - -5			1 37 -36			-4 43 51			-1 85 -74			-3 15 14		
5 - 4			-5 45 -42			0 41 -42			0 58 57			-5 11 -10			-2 42 39			-4 38 37		
4 105 104			-6 40 -38			-1 105 -99			-1 60 -60			-6 31 -32			-3 42 39			-5 50 -51		
3 75 59			-7 16 -13			-2 148 -144			-2 85 -88						-4 111 103			-6 9 -10		
2 132 -129						-3 8 10			-3 19 15			0 6 L			-5 6 5			-7 17 21		
1 160 176			4 2 L			-4 69 -72			-4 38 33			1 11 9			-6 32 -34					
0 - 150			5 65 -65			-5 82 -76			-5 103 -101			2 37 -37			-7 42 50			10 8 L		
-1 - 14			4 49 45			-6 55 -49			-6 20 -21			3 105 100						-1 - 5		
-2 48 -58			3 34 20			-7 8 -8			-7 19 18			4 113 109			5 7 L			-2 17 -9		
-3 162 175			2 119 -113			-8 34 -31			-8 10 -11			5 36 -37			4 29 32			-3 23 -24		
-4 26 21			1 113 -110									6 17 19			3 23 24			-4 20 23		
-5 - -2			0 189 199			7 3 L			10 4 L						2 33 -35			-5 - -5		
-6 19 17			-1 115 -122			3 26 27			1 29 -33			2 6 L			1 71 66			-6 17 -21		
-7 40 39			-2 194 -199			2 60 -61			0 8 -8			6 14 15			0 56 47					
			-3 57 56			1 95 -88			-1 - 5			5 13 12			-1 16 14					
												4 52 53			-2 10 -10					
															-3 92 81					

Table 5. Observed and calculated structure factors for $[Ni(en)_2][AgI_2]_2$. The columns are successively h, $|F_o|$ and F_c.

	H 21 0		0	173	160	4	66	62	-8	19	19	-3	167	-180		H 15 2		-8	93	95
1	-	-21	2	-	10	6	101	-99				-1	206	-194	7	20	-15	-6	74	78
-1	-	-21	4	46	41	8	54	-51		H 12 1		1	67	-57	5	29	-31			
			6	44	-45	10	35	-38	-9	-	2	3	68	64	3	-	-3			
	H 20 0		8	27	-23				-7	22	18	5	35	-34	1	-	4			
-4	-	7	10	-	-17		H 1 0		-5	22	-27	7	-	24	-1	-	11	-4	151	155
-2	-	6				11	43	50	-3	-	18	9	45	-45	-3	-	14	-2	29	-25
0	27	25		H 9 0		9	44	46	-1	37	31	11	-	-13	-5	-	-27	0	162	146
2	-	6	9	-	-4	7	122	133	1	80	75				-7	19	-17	2	-	-33
4	-	7	7	25	21	5	29	23	3	115	110		H 3 1					4	165	154
			5	68	-72	3	93	91	5	65	58	10	21	-24		H 14 2		6	91	86
	H 19 0		3	81	-75	1	14	-20	7	58	57	8	69	-65	-8	22	12	8	101	96
5	-	9	1	161	-153	-1	12	-20	9	-	6	6	193	-193	-6	20	-7	10	50	49
3	23	12	-1	161	-153	-3	91	91				4	176	-173	-4	-	2			
1	-	4	-3	81	-75	-5	26	23		H 11 1		2	331	-399	-2	64	-65		H 5 2	
-1	-	4	-5	70	-72	-7	135	133	8	-	2	0	50	-44	0	26	-27	9	20	-23
-3	-	12	-7	18	21	-9	46	46	6	43	-37	-2	213	-229	2	69	-69	7	40	38
-5	19	9	-9	-	-4	-11	44	50	4	-	-10	-4	41	40	4	-	3	5	-	10
									2	84	-77	-6	54	-56	6	-	2	3	176	166
	H 18 0			H 8 0			H 0 0		0	66	63	-8	19	-21	8	19	18	1	229	217
-6	-	8	-10	29	-26	-10	-	12	-2	19	15	-10	35	-37				-1	268	258
-4	38	36	-8	34	-37	-8	33	32	-4	101	104					H 13 2		-3	234	248
-2	36	39	-6	77	-70	-6	31	30	-6	34	36		H 2 1		7	-	13	-5	36	33
0	63	73	-4	38	33	-4	248	271	-8	21	25	-11	-	7	5	-	4	-7	43	44
2	37	39	-2	22	-25	-2	219	266				-9	61	-61	3	63	60	-9	31	-31
4	30	36	0	191	172	2	220	264		H 10 1		-7	52	-54	1	82	78	-11	-	9
6	-	8	2	35	-25	4	249	271	-9	42	-40	-5	203	-224	-1	93	89			
			4	37	33	6	33	30	-7	42	-41	-3	138	-153	-3	83	86		H 4 2	
	H 17 0		6	76	-70	8	33	32	-5	114	-123	-1	186	-199	-5	-	15	-10	19	22
5	-	10	8	31	-37	10	23	12	-3	95	-91	1	82	-77	-7	-	15	-8	33	34
3	-	13	10	24	-26				-1	121	-112	3	80	78	-9	21	-13	-6	27	-25
1	-	-4					H 21 1		1	69	-63	5	23	-18				-4	26	22
-1	-	-4		H 7 0		2	27	-32	3	18	16	7	40	40		H 12 2		-2	227	-241
-3	-	13	9	35	32	0	-	-15	5	-	-13	9	49	-45	-8	54	54	0	59	-55
-5	-	10	7	89	95	-2	-	-17	7	-	18	11	20	-15	-6	40	45	2	255	-255
			5	20	18				9	30	-29				-4	73	72	4	30	26
	H 16 0		3	48	45		H 20 1						H 1 1		-2	-	-9	6	-	3
-6	19	-16	1	60	-55	-3	23	-25		H 9 1		10	-	12	0	63	59	8	49	47
-4	26	15	-1	61	-55	-1	22	-26	10	22	-21	8	-	5	2	-	-5	10	29	19
-2	-	3	-3	47	45	1	20	-17	8	44	-46	6	86	-82	4	83	77			
0	48	47	-5	20	18	3	-	-4	6	135	-124	4	23	-15	6	48	48		H 3 2	
2	-	3	-7	93	95				4	133	-125	2	212	-248	8	52	52	9	84	-80
4	-	15	-9	37	32		H 19 1		2	271	-258	-2	-	-2				7	54	-53
6	26	-16				4	-	-11	0	92	-82	-4	219	245		H 11 2		5	138	-133
				H 6 0		2	27	-26	-2	138	-133	-6	63	65	9	-	-14	3	-	-10
	H 15 0		-10	-	5	0	-	3	-4	24	21	-8	48	46	7	20	16	1	10	-12
7	-	13	-8	20	24	-2	-	0	-6	41	-38	-10	18	0	5	-	15	-1	14	9
5	22	-20	-6	34	35	-4	22	21	-8	22	-24				3	102	99	-3	41	45
3	26	-28	-4	216	214				-10	35	-32		H 0 1		1	131	122	-5	115	-124
1	61	-68	-2	173	162		H 18 1					-11	32	36	-1	126	121	-7	47	-50
-1	65	-68	0	399	423	-5	-	-8		H 8 1		-9	-	-12	-3	106	111	-9	92	-93
-3	31	-28	2	177	162	-3	-	6	-9	43	-46	-7	37	34	-5	20	19	-11	30	-24
-5	22	-20	4	224	214	-1	-	8	-7	43	-44	-5	79	-82	-7	20	29			
-7	-	13	6	36	35	1	22	20	-5	140	-150	-3	54	53	-9	-	-13		H 2 2	
			8	25	24	3	31	35	-3	107	-106	1	93	110				-10	28	23
	H 14 0		10	-	5	5	-	23	-1	133	-130	3	216	254		H 10 2		-8	34	39
-8	-	-16							1	72	-63	5	115	118	-10	-	18	-6	35	-32
-6	22	-21		H 5 0			H 17 1		3	36	36	7	135	131	-8	30	30	-4	-	-5
-4	26	25	11	39	42	6	-	-12	5	-	-11	9	-	4	-6	19	-7	-2	268	-329
-2	-	-1	9	38	41	4	-	-3	7	24	26	11	-	11	-4	-	-2	0	93	-80
0	63	62	7	126	128	2	24	-22	9	33	-33				-2	141	-137	2	239	-275
2	-	-1	5	55	53	0	29	23					H 21 2		0	33	-29	4	31	29
4	28	25	3	101	96	-2	-	13		H 7 1		1	-	2	2	109	-101	6	19	-17
6	24	-21	1	51	-43	-4	40	41	10	-	11	-1	-	2	4	28	25	8	42	40
8	21	-16	-1	50	-43	-6	-	17	8	-	3				6	-	-1	10	20	17
			-3	98	96				6	68	-60		H 20 2		8	24	26			
	H 13 0		-5	53	53		H 16 1		4	-	-8	-4	-	-2					H 1 2	
7	40	50	-7	128	128	-7	-	-19	2	137	-123	-2	21	-22		H 9 2		11	-	10
5	19	18	-9	39	41	-5	49	-52	0	144	131	0	-	-9	9	58	-54	9	37	-34
3	-	23	-11	48	42	-3	40	-41	-2	15	15	2	-	-15	7	42	-40	7	31	28
1	19	-24				-1	32	-38	-4	155	165				5	80	-77	5	-	3
-1	24	-24		H 4 0		1	19	-15	-6	44	51				3	-	14	3	204	229
-3	-	23	-10	40	-35	3	-	10	-8	39	39				1	27	22	1	246	303
-5	-	18	-8	41	-41	5	-	-5	-10	-	3		H 19 2		-1	-	8	-3	215	244
-7	46	50	-6	70	-69	7	-	4				5	-	6	-3	-	11	-5	18	20
-9	-	19	-4	93	90					H 6 1		3	33	29	-5	69	-75	-7	52	58
			-2	35	-35		H 15 1		-11	30	33	1	31	36	-7	25	-26	-9	32	-32
	H 12 0		0	272	260	8	24	-28	-9	-	-1	-1	31	33	-9	52	-56	-11	-	9
-8	22	12	2	36	-35	6	70	-64	-7	27	31	-3	-	28						
-6	-	17	4	95	90	4	65	-63	-5	68	-72	-5	-	9		H 8 2			h 0 2	
-4	98	98	6	71	-69	2	103	-99	-3	16	22				-10	-	17	-10	75	72
-2	86	83	8	40	-41	0	35	-37	-1	51	46		H 18 2		-8	30	29	-8	125	128
0	189	186	10	32	-35	-2	59	-60	1	169	149	-6	21	22	-6	22	-20	-6	99	102
2	86	83				-4	-	-8	3	230	218	-4	24	26	-4	-	-12	-4	174	184
4	98	98		H 3 0		-6	23	-23	5	100	92	-2	-	1	-2	200	-195	-2	90	-87
6	-	17	11	-	13	-8	19	-12	7	102	99	0	-	24	0	55	-54	2	-	4
8	22	12	9	21	-17				9	-	6	2	-	9	2	168	-156	4	212	223
			7	29	33		H 14 1					4	35	32	4	19	16	6	104	99
	H 11 0		5	121	-116	-7	30	-29		H 5 1					6	19	-12	8	113	110
9	34	28	3	143	-138	-5	76	-83	10	-	11		H 17 2		8	30	26	10	63	58
7	58	68	1	336	-366	-3	69	-69	8	-	-4	5	-	6	10	-	13			
5	23	22	-1	328	-366	-1	65	-64	6	95	-87	3	39	38					H 18 3	
3	39	40	-3	137	-138	1	31	-27	4	40	-23	1	49	48		H 7 2		5	21	-11
1	-	-9	-5	116	-116	3	-	7	2	171	-157	-1	46	48	9	25	-25			
-1	-	-9	-7	34	33	5	20	-16	0	174	161	-3	41	42	7	-	20		H 17 3	
-3	39	40	-9	-	-17	7	-	0	-2	34	-21	-5	-	11	5	-	1	6	21	11
-5	19	22	-11	-	13				-4	156	166	-7	-	12	3	150	136	4	30	32
-7	63	68					H 13 1		-6	40	46				1	193	173	2	-	10
-9	34	28		H 2 0		8	-	-2	-8	44	44		H 16 2		-1	189	180	0	21	26
			-10	36	-38	6	38	-35	-10	-	4	-6	-	-2	-3	168	171	-2	-	-16
	H 10 0		-8	50	-51	4	-	-12				-4	-	0	-5	16	15	-4	-	-5
-10	-	-17	-6	102	-99	2	55	-49		H 4 1		-2	46	-45	-7	28	35	-6	-	-18
-8	31	-23	-4	66	62	0	50	49	-11	-	7	0	-	-17	-9	28	-27			
-6	46	-45	-2	74	-71	-2	-	7	-9	57	-55	2	34	-42					H 16 3	
-4	46	41	0	270	301	-4	63	66	-7	54	-55	4	-	5		H 6 2		-7	19	8
-2	-	10	2	77	-71	-6	20	23	-5	208	-228	6	-	2	-10	56	57	-5	-	-5

Table 5. Continued.

-3	-	4	-1	75	75		H 16 4		-8	25	27	2	28	-26	-6	39	41	2	17	7
-1	23	-26	1	16	17	-6	-	-11	-6	40	39	0	-	8	-8	36	35	4	25	27
1	39	-42	3	19	18	-4	18	19	-4	193	198	-2	18	-1	-10	-	6			
3	40	-40	5	41	-46	-2	-	9	-2	175	167	-4	25	24					H 17 6	
5	39	-43	7	29	30	0	38	44	0	349	355	-6	-	11		H 6 5		5	-	7
7	-	-14	9	-	3	2	-	1	2	123	117				-11	-	25	3	22	27
						4	-	8	4	139	135		H 16 5		-9	-	-12	1	41	38
	H 15 3			H 5 3		6	22	-17	6	-	5	-7	18	-20	-7	24	22	-1	43	44
6	-	-18	10	-	-6				8	20	15	-5	42	-45	-5	47	-49	-3	39	46
4	-	5	8	24	26		H 15 4		10	-	6	-3	28	-30	-3	50	48	-5	25	19
2	37	-40	6	42	41	7	-	8				-1	27	-28	-1	50	47	-7	-	15
0	26	-27	4	180	180	5	25	-20		H 5 4		1	17	-9	1	121	114			
-2	88	-92	2	42	39	3	29	-27	9	38	34	3	-	6	3	154	155		H 16 6	
-4	54	-58	0	163	154	1	51	-53	7	96	93	5	-	-4	5	75	75	-6	-	-3
-6	52	-59	-2	168	-147	-1	60	-62	5	33	34				7	67	68	-4	-	-5
-8	30	-28	-4	14	-11	-3	39	-38	3	74	60		H 15 5		9	-	-1	-2	36	-37
			-6	73	-70	-5	31	-37	1	13	-8	6	41	-38				0	-	-11
	H 14 3		-8	-	-3	-7	-	2	-1	32	-32	4	43	-43		H 5 5		2	22	-23
-7	-	12	-10	-	7				-3	47	47	2	83	-81	10	-	12	4	-	11
-5	-	-10					H 14 4		-5	-	-5	0	35	-37	8	-	14	6	-	6
-3	-	-2		H 4 3		-8	-	-16	-7	96	97	-2	46	-46	6	17	-37			
-1	43	-47	-11	-	-13	-6	23	-23	-9	39	38	-4	-	2	4	-	-2		H 15 6	
1	62	-64	-9	36	-37	-4	17	19	-11	49	47	-6	18	-11	2	134	-128	7	24	-18
3	57	-55	-7	55	50	-2	19	7				-8	-	-9	0	78	71	5	26	-29
5	54	-61	-5	23	-24	0	61	60		H 4 4					-2	-	-2	3	-	-7
7	26	-22	-3	31	30	2	-	-8	-10	30	-30		H 14 5		-4	158	163	1	-	1
			-1	153	-139	4	-	2	-8	42	-39	-9	28	-27	-6	63	66	-1	-	1
	H 13 3		1	197	-187	6	29	-30	-6	65	-65	-7	30	-26	-8	46	46	-3	-	4
8	-	9	3	148	-138	8	-	-15	-4	78	76	-5	54	-60	-10	-	8	-5	-	-22
6	19	17	5	168	-167				-2	-	7	-3	39	-39				-7	-	-10
4	61	66	7	35	-40		H 13 4		0	237	228	-1	42	-43		H 4 5				
2	21	17	9	38	-41	7	39	44	2	49	-41	1	-	-17	-11	-	-2		H 14 6	
0	40	45				5	17	20	4	28	24	3	-	10	-9	69	-64	-8	18	11
-2	51	-52		H 3 3		3	28	27	6	79	-82	5	-	-3	-7	52	-53	-6	18	-12
-4	-	-14	10	37	-39	1	-	1	8	37	-35	7	-	3	-5	163	-159	-4	18	-18
-6	35	-33	8	27	-30	-1	-	-8	10	21	-23				-3	90	-93	-2	66	-65
-8	-	-5	6	51	-55	-3	19	20					H 13 5		-1	131	-122	0	18	-21
			4	52	46	-5	-	5		H 3 4		8	-	1	1	44	-35	2	37	-39
	H 12 3		2	174	-167	-7	42	43	9	-	-5	6	19	-22	3	49	48	4	-	8
-9	-	9	0	56	-44	-9	-	21	7	40	36	4	-	-14	5	-	-6	6	-	0
-7	57	62	-2	349	-378				5	66	-64	2	60	-58	7	23	18			
-5	51	53	-4	173	-178		H 12 4		3	81	-78	0	-	10	9	40	-36		H 13 6	
-3	90	93	-6	199	-200	-8	-	18	1	206	-205	-2	-	-7				7	-	4
-1	38	43	-8	81	-80	-6	23	30	-1	249	-248	-4	54	54		H 3 5		5	-	1
1	20	10	-10	35	-35	-4	101	107	-3	117	-119	-6	20	24	10	-	-17	3	39	45
3	-	4				-2	93	95	-5	139	-130	-8	-	16	8	42	-41	1	70	67
5	20	-24		H 2 3		0	173	171	-7	26	23				6	132	-134	-1	71	70
7	-	15	-9	45	-43	2	73	71	-9	-	-14		H 12 5		4	136	-137	-3	67	70
			-7	44	44	4	76	75	-11	20	19	-9	-	-6	2	288	-319	-5	20	19
	H 11 3		-5	35	-34	6	17	11				-7	-	7	0	125	-116	-7	28	23
8	-	18	-3	52	53	8	-	11		H 2 4		-5	27	-30	-2	202	-206	-9	-	-5
6	25	24	-1	136	-122				-10	35	-35	-3	18	14	-4	-	15			
4	86	87	1	204	-210		H 11 4		-8	38	-39	-1	19	20	-6	43	-45		H 12 6	
2	21	22	3	165	-172	9	24	22	-6	56	-57	1	58	55	-8	25	-21	-8	43	47
0	79	81	5	180	-190	7	56	59	-4	91	96	3	73	75	-10	23	-33	-6	33	37
-2	56	-50	7	44	-40	5	34	34	-2	9	-8	5	39	37				-4	52	52
-4	-	-7	9	38	-41	3	44	42	0	244	233	7	29	32		H 2 5		-2	-	-2
-6	45	-44				1	-	-5	2	45	-44				-11	-	0	0	55	56
-8	-	-7		H 1 3		-1	21	-22	4	42	43		H 11 5		-9	72	-68	2	17	17
			8	33	36	-3	27	28	6	82	-80	8	-	4	-7	61	-64	4	68	69
	H 10 3		6	42	42	-5	19	14	8	41	-38	6	24	-28	-5	190	-207	6	40	42
-9	26	-25	4	180	187	-7	59	63	10	30	-27	4	-	-11	-3	117	-127	8	39	41
-7	-	19	2	11	12	-9	31	25				2	64	-61	-1	152	-139			
-5	22	-16	-2	134	-136					H 1 4		0	40	39	1	37	-34		H 11 6	
-3	24	28	-4	-	-4		H 10 4		9	34	33	-2	-	-1	3	45	42	7	-	9
-1	47	-50	-6	101	-100	-10	25	-22	7	111	110	-4	72	74	5	26	-24	5	-	1
1	109	-102	-8	-	-14	-8	19	-22	5	55	55	-6	25	32	7	-	9	3	54	53
3	104	-100	-10	-	8	-6	26	-26	3	85	87	-8	32	27	9	47	-41	1	84	80
5	107	-107				-4	48	48	1	39	38	-10	-	7				-1	95	94
7	19	-25		H 0 3		-2	-	-2	-3	56	54					H 1 5		-3	101	103
9	-	-22	-11	27	23	0	99	96	-5	-	13		H 10 5		10	-	15	-5	34	29
			-9	-	14	2	-	-18	-7	122	124	-9	34	-35	8	-	10	-7	29	29
	H 9 3		-7	137	137	4	21	22	-9	37	39	-7	38	-36	6	58	-60	-9	-	-10
8	-	-19	-5	113	111	6	37	-42	-11	50	48	-5	105	-110	4	-	-16			
6	38	-38	-3	251	280	8	24	-24				-3	67	-64	2	142	-144		H 10 6	
4	17	9	1	25	20					H 0 4		-1	53	-53	-2	19	-18	-10	-	12
2	114	-107	3	-	-7		H 9 4		-10	-	5	1	-	2	-4	151	160	-8	-	12
0	38	-30	5	77	-73	7	22	22	-8	33	34	3	29	32	-6	55	57	-6	-	-18
-2	211	-196	7	38	42	5	35	-34	-6	61	61	5	-	-7	-8	-	54	-4	-	-10
-4	118	-115	9	-	8	3	49	-49	-4	245	265	7	-	6	-10	19	14	-2	102	-101
-6	138	-139				1	144	-139	-2	163	174	9	26	-21				0	40	-37
-8	60	-62		H 21 4		-1	175	-170	2	125	132					H 0 5		2	84	-83
-10	23	-25	1	-	-16	-3	83	-83	4	172	186		H 9 5		-11	32	35	4	-	14
			-1	-	-18	-5	67	-72	6	-	11	8	28	-28	-9	-	-7	6	18	5
	H 8 3					-7	-	18	8	-	14	6	92	-92	-7	32	30	8	23	21
-9	30	-32		H 20 4		-9	-	-10	10	-	1	4	94	-92	-5	77	-79			
-7	20	23	-4	-	7							2	185	-178	-3	54	56		H 9 6	
-5	21	-25	-2	-	2		H 8 4			H 21 5		0	59	-55	1	173	194	9	37	-35
-3	27	29	0	-	14	-10	25	-26	0	-	-17	-2	117	-113	3	191	211	7	32	-29
-1	72	-75	2	-	-1	-8	27	-28	-2	-	-19	-4	-	-3	5	84	85	5	62	-62
1	150	-137				-6	38	-36				-6	34	-33	7	81	80	3	19	-23
3	134	-125		H 19 4		-4	60	60		H 20 5		-8	-	-12	9	-	1	1	-	-10
5	131	-134	3	-	11	-2	-	-4	-1	-	-14	-10	20	-19				-1	-	6
7	32	-32	1	-	-2	0	144	131	1	-	-4					H 21 6		-3	33	34
9	30	-29	-1	-	-7	2	21	-23	3	18	2		H 8 5		-1	-	5	-5	43	-44
			-3	-	6	4	32	28				-9	51	-49				-7	-	-22
	H 7 3		-5	-	8	6	54	-54		H 19 5		-7	50	-51		H 20 6		-9	53	-53
10	-	-5				8	26	-29	4	-	-7	-5	141	-147	-4	-	-4			
8	24	24		H 18 4					2	20	-15	-3	94	-93	-2	-	-18		H 8 6	
6	36	33	-6	-	18		H 7 4		0	-	7	-1	95	-88	0	-	-10	-10	-	15
4	144	139	-4	38	43	9	27	29	-2	-	0	1	22	-21	2	-	-15	-8	-	17
2	24	22	-2	37	38	7	85	84	-4	-	14	3	28	23				-6	20	-20
0	136	128	0	58	59	5	44	40				5	22	-20		H 19 6		-4	-	-9
-2	115	-104	2	29	32	3	63	62		H 18 5		7	-	2	3	-	12	-2	126	-125
-4	-	-12	4	31	33	1	13	-9	-5	-	-14	9	26	-30	1	-	19	0	34	-35
-6	72	-69				-1	40	-37	-3	-	2				-1	-	25	2	98	-94
-8	-	-9		H 17 4		-3	39	41	-1	-	10		H 7 5		-3	24	28	4	28	27
			5	23	19	-5	-	9	1	26	24	8	-	4	-5	-	10	6	-	9
	H 6 3		3	25	22	-7	89	90	3	25	27	6	51	-48				8	27	27
-11	-	16	1	-	5	-9	32	33	5	-	13	4	26	-23		H 18 6				
-9	-	15	-1	-	-2	-11	39	40				2	124	-120	-6	-	18		H 7 6	
-7	118	121	-3	-	14					H 17 5		0	56	48	-4	-	24	9	-	-14
-5	99	97	-5	-	12		H 6 4		6	-	-14	-2	23	-19	-2	-	6	7	-	12
-3	191	187	-7	27	28	-10	-	9	4	-	-10	-4	109	112	0	-	19	5	-	0

Table 5. Continued.

3	87	85		H 17 7		6	-	11	-1	-	2	6	-	1	-7	23	-17	-6	34	33
1	135	127	-6	-	-15	8	-	7	1	-	7	4	70	73				-4	67	69
-1	146	140	-4	-	-8				3	18	16	2	64	61		H 15 9		-2	16	-14
-3	155	154	-2	-	-14		H 6 7		5	-	15	0	195	187	-6	20	-13	0	31	28
-5	34	36	0	21	17	9	-	9				-2	112	108	-4	-	-10	2	74	-72
-7	45	44	2	-	8	7	26	24		H 16 8		-4	139	144	-2	34	-36	4	-	-13
-9	-	-17	4	-	19	5	29	-28	4	-	3	-6	50	51	0	28	-27	6	28	-26
-11	-	6				3	16	-11	2	-	-1	-8	25	28	2	45	-51	8	-	9
				H 16 7		1	-	-4	0	26	27	-10	-	7	4	33	-30			
	H 6 6		5	23	-30	-1	41	39	-2	-	11				6	28	-25		H 4 9	
-10	59	54	3	25	-33	-3	126	125	-4	20	20		H 5 8					9	-	-23
-8	80	80	1	34	-35	-5	63	65	-6	-	-1	-11	39	34		H 14 9		7	18	-1
-6	52	55	-1	24	-25	-7	88	89				-9	23	27	5	-	-7	5	-	-12
-4	81	85	-3	-	-1	-9	-	15		H 15 8		-7	71	71	3	-	5	3	26	25
-2	41	-37	-5	-	-7	-11	21	18	-7	-	3	-5	-	-2	1	-	0	1	-	10
0	107	97	-7	-	5				-5	27	-25	-3	18	14	-1	23	-18	-1	47	-42
2	12	10		H 5 7					-3	30	-29	-1	48	-44	-3	25	-26	-3	52	-53
4	122	120		H 15 7		-10	-	1	-1	43	-47	1	-	-2	-5	48	-48	-5	116	-119
6	61	62	-8	25	-29	-8	18	-19	1	32	-33	3	58	53	-7	25	-24	-7	45	-46
8	60	64	-6	48	-49	-6	57	-60	3	-	-10	5	41	42				-9	45	-47
			-4	38	-39	-4	-	7	5	-	-4	7	62	58		H 13 9		-11	-	-3
	H 5 6		-2	50	-50	-2	40	-36				9	24	18	-8	-	13			
9	22	-21	0	-	-8	0	129	125		H 14 8					-6	-	13		H 3 9	
7	-	4	2	19	-24	2	33	33	6	-	-18		H 4 8		-4	28	26	-10	21	-17
5	-	-14	4	-	1	4	102	103	4	-	2	8	24	-24	-2	-	-7	-8	18	-11
3	97	93	6	22	-12	6	27	24	2	-	-8	6	47	-50	0	-	6	-6	27	-29
1	149	143				8	-	17	0	29	28	4	-	11	2	34	-34	-4	17	-8
-1	155	146		H 14 7					-2	-	3	2	31	-28	4	22	-11	-2	120	-118
-3	155	156	7	-	-10		H 4 7		-4	21	20	0	106	99	6	-	-13	0	77	-73
-5	25	25	5	42	-40	9	-	-16	-6	-	-4	-2	-	4				2	165	-168
-7	56	49	3	47	-46	7	-	-16	-8	-	-8	-4	61	65		H 12 9		4	75	-77
-9	19	-19	1	46	-48	5	99	-101				-6	21	-16	7	-	15	6	70	-71
-11	-	6	-1	34	-31	3	110	-111		H 13 8		-8	22	-19	5	20	20	8	18	-17
			-3	-	4	1	134	-126	-9	-	16	-10	29	-24	3	41	44			
	H 4 6		-5	-	-9	-1	93	-83	-7	28	33				1	61	62		H 2 9	
-10	27	23	-7	-	6	-3	30	28	-5	-	3		H 3 8		-1	25	22	9	29	-26
-8	24	28				-5	19	-21	-3	-	7	-11	-	14	-3	-	15	7	-	-1
-6	30	-32		H 13 7		-7	31	32	-1	-	-14	-9	-	-12	-5	-	-20	5	-	-10
-4	30	-32	-8	-	-13	-9	28	-27	1	-	3	-7	-	12	-7	-	1	3	28	25
-2	204	-199	-6	28	-31	-11	-	-5	3	30	26	-5	89	-93	-4	-	-7	1	-	-2
0	39	-38	-4	-	-8				5	32	23	-3	81	-87				-1	33	-36
2	128	-121	-2	23	-22		H 3 7		7	25	27	-1	166	-155		H 11 9		-3	53	-56
4	36	35	0	39	37	-10	35	-36				1	106	-103	-10	-	5	-5	114	-121
6	-	-1	2	-	9	-8	81	-80		H 12 8		3	25	-27	-8	-	19	-7	45	-47
8	25	28	4	38	36	-6	150	-157	6	-	4	5	15	-16	-6	21	24	-9	54	-54
10	-	11	6	-	7	-4	118	-122	4	43	43	7	23	26	-4	44	43	-11	-	-6
						-2	203	-201	2	47	43	9	-	-2	-2	-	-8			
	H 3 6			H 12 7		0	19	-16	0	106	106				0	-	5		H 1 9	
9	52	-51	7	-	9	2	93	-94	-2	67	68		H 2 8		2	44	-45	-10	-	10
7	43	-42	5	21	-18	4	14	16	-4	78	80	8	22	-22	4	-	-8	-8	35	37
5	91	-90	3	-	-11	6	52	-44	-6	30	32	6	57	-54	6	-	-13	-6	47	47
3	15	-9	1	-	-9	8	33	-25	-8	24	18	4	-	8				-4	85	91
1	20	19	-1	-	13	10	24	-30				2	30	-29		H 10 9		-2	23	-25
-1	24	21	-3	58	57					H 11 8		0	126	123	7	-	0	0	14	15
-3	52	51	-5	35	35		H 2 7		-9	21	20	-2	20	19	5	-	-3	2	89	-92
-5	72	-74	-7	44	47	-11	-	-8	-7	41	40	-4	66	71	3	-	15	4	14	-9
-7	19	-21	-9	-	9	9	23	-22	-5	-	1	-6	21	-25	1	-	-4	6	-	-25
-9	72	-70				7	27	-26	-3	21	15	-8	24	-23	-1	37	35	8	18	10
-11	-	-21		H 11 7		5	110	-114	-1	-	-8	-10	27	-23	-3	38	-32			
			-10	-	0	3	116	-119	1	-	10				-5	61	-65		H 0 9	
	H 2 6		-8	-	-9	1	144	-146	3	33	32		H 1 8		-7	30	-29	9	-	-5
-10	26	23	-6	33	-32	-1	122	-117	5	25	26	-11	41	43	-9	34	-34	7	38	38
-8	25	27	-4	-	-6	-3	9	6	7	39	38	-9	33	29				5	47	50
-6	31	-30	-2	33	-31	-5	31	-31				-7	69	71		H 9 9		3	102	106
-4	16	-11	0	59	57	-7	36	37		H 10 8		-5	15	-15	-10	20	-16	1	86	91
-2	183	-193	2	23	24	-9	28	-29	8	-	-14	-3	27	26	-8	-	-9	-3	41	45
2	134	-137	4	60	59				6	32	-33	1	-	6	-6	16	-14	-5	36	-35
4	45	44	6	-	12		H 1 7		4	-	-2	3	49	51	-4	-	-2	-7	17	14
6	18	10	8	-	6	-10	-	1	2	18	-16	5	17	39	-2	80	-80	-9	21	-18
8	35	37				-8	19	-14	0	70	67	7	67	67	0	64	-61	-11	22	16
10	-	13		H 10 7		-6	61	-64	-2	19	17	9	21	24	2	112	-113			
			7	-	-14	-4	16	-8	-4	41	37				4	49	-51		H 19 10	
	H 1 6		5	59	-57	-2	75	-80	-6	17	-16		H 0 8		6	46	-45	-1	-	17
9	27	-21	3	56	-56	2	44	44	-8	-	-15	8	-	8	8	19	-13			
7	-	14	1	71	-69	4	120	125	-10	-	-13	6	-	-8					H 18 10	
5	-	-10	-1	59	-57	6	21	21				4	73	76		H 8 9		-4	-	9
3	94	96	-3	-	4	8	-	12		H 9 8		2	61	64	7	-	-2	-2	-	1
1	143	148	-5	-	-9	10	-	-9	-9	-	-8	0	198	247	5	-	-7	0	-	13
-3	195	216	-7	27	26				-7	-	-1	-2	134	142	3	-	16	2	-	9
-5	40	42	-9	-	-13		H 0 7		-5	64	-67	-4	160	172	1	-	-5			
-7	50	52				9	20	9	-3	58	-57	-6	48	45	-1	46	-45		H 17 10	
-9	29	-30		H 9 7		7	34	29	-1	98	-92	-8	25	26	-3	46	43	3	21	11
-11	-	6	-10	25	-24	5	26	-26	1	74	-68	-10	-	10	-5	83	-84	1	-	21
			-8	45	-48	3	-	10	3	26	-29				-7	34	-36	-1	26	26
	F 0 6		-6	94	-97	1	11	10	5	18	-17		H 20 9		-9	43	-41	-3	23	28
-10	61	58	-4	82	-85	-3	140	146	7	-	15	-1	-	-11				-5	-	12
-8	88	84	-2	135	-132	-5	80	85				1				H 7 9				
-6	60	62	0	-	-12	-7	121	125		H 8 8			H 19 9		-10	-	8		H 16 10	
-4	117	122	2	45	-44	-9	26	25	8	-	-16	-2	-	-4	-8	32	28	-6	-	-3
-2	46	-45	4	-	19	-11	22	21	6	39	-39	0	-	-4	-6	32	31	-4	-	-4
2	26	-27	6	27	-27				4	-	1	2	-	-14	-4	56	60	-2	23	-19
4	132	137	8	-	-19		H 20 8		2	18	-21				-2	21	-19	0	-	-4
6	76	76				0	-	13	0	88	82		H 18 9		0	16	11	2	-	-10
8	78	79		H 8 7		-2	-	6	-2	18	18	3	-	17	2	69	-68	4	-	9
10	-	35	9	-	-17				-4	48	47	1	-	14	4	-	-13			
			7	-	-22		H 19 8		-6	18	-19	-1	-	6	6	-	-22		H 15 10	
	F 20 7		5	79	-82	-5	-	1	-8	23	-19	-3	-	5	8	-	6	5	-	-14
1	-	-18	3	83	-84	-3	-	4	-10	-	-17	-5	-	-5				3	-	-7
-1	-	-15	1	105	-100	-1	-	0								H 6 9		1	-	0
-3	-	-4	-1	85	-83	1	-	3		H 7 8			H 17 9		9	-	-4	-1	-	6
			-3	-	-5	3	22	7	-11	33	32	-6	-	10	7	26	27	-3	-	15
	H 19 7		-5	23	-23				-9	24	25	-4	22	15	5	30	35	-5	-	-4
-4	-	-6	-7	22	25		H 18 8		-7	55	58	-2	-	-4	3	86	84	-7	-	-3
-2	-	-10	-9	24	-20	4	-	15	-5	-	-2	0	20	-1	1	87	83			
0	-	12				2	19	18	-3	32	30	2	20	-17	-1	44	43		H 14 10	
2	-	9		H 7 7		0	41	43	-1	23	-23	4	-	-5	-3	34	30	-8	-	4
			-10	-	-1	-2	32	32	1	-	6				-5	38	-39	1	-	-6
	H 18 7		-8	-	-18	-4	33	32	3	46	46		H 16 9		-7	-	7	-4	-	-6
3	-	-2	-6	57	-57	-6	-	13	5	38	38	5	-	-4	-9	18	-11	-2	30	-31
1	-	-2	-4	-	-14				7	55	54	3	-	4	-11	-	16	0	18	-12
-1	-	3	-2	59	-56		H 17 8		9	21	20	1	-	-1				2	-	-19
-3	-	17	0	93	85	-7	26	18				-1	-	-15		F 5 9		4	-	10
-5	-	14	2	25	21	-5	-	6		H 6 8		-3	22	-20	-10	23	13	6	-	7
			4	81	80	-3	-	11	8	-	7	-5	35	-33	-8	30	34			

Table 5. Continued.

H 13 10			-6	20	-20	-4	-	-7	H 3 11			H 7 12			H 11 13			-3	21	21
5	-	-1	-4	19	-15	-6	23	-17	8	-	-16	5	-	21	4	-	-6	1	40	48
3	-	16	-2	93	-93	-8	-	-8	6	23	-23	3	20	24	2	-	-22	3	37	40
1	26	29	0	26	-24				4	-	11	1	-	7	0	-	-2	5	-	13
-1	37	38	2	56	-55	H 12 11			2	26	-28	-1	-	-13	-2	-	-9			
-3	47	50	4	29	29	-9	-	9	0	-	3	-3	-	3	-4	31	14	H 15 14		
-5	24	20	6	-	13	-7	31	30	-2	88	-87	-5	-	-8	-6	-	10	-1	-	5
-7	25	17	8	-	20	-5	21	19	-4	64	-65	-7	26	27				-3	-	7
-9	-	-4				-3	27	27	-6	83	-85	-9	-	15	H 10 13					
			H 3 10			-1	-	3	-8	56	-50				-7	36	-22	H 14 14		
H 12 10			1	-	-4	-10	23	-26				H 6 12			-5	48	-33	-4	-	-7
-8	-	28	3	-	-5				H 2 11			-8	19	18	-3	-	-17	-2	-	-13
-6	19	20	5	-	-6	-9	-	-14	-7	-	22	-6	36	33	-1	-	-11	0	-	0
-4	24	25				-5	14	-17	-3	-	-1	-4	82	79	1	-	3			
-2	-	-5	H 11 11			-1	66	-64	-1	66	-64	-2	72	66	3	-	3	H 12 14		
0	28	26	6	-	3	1	73	-73	1	73	-73	0	95	90	5	-	-7	2	-	9
2	-	11	4	28	25	3	60	-61	3	60	-61	2	28	26				0	-	15
4	36	40	2	-	13	5	49	-49	5	49	-49	4	26	26	H 9 13			-2	-	1
6	25	25	0	33	34	7	-	-8	7	-	-8				4	-	-29			
			-2	-	-7							H 5 12			2	54	-55	H 11 14		
H 11 10			-4	-	-3				H 1 11			5	21	27	0	29	-32	-3	36	35
7	-	2	-6	21	-22				8	-	2	3	31	31	-2	45	-42	-1	28	25
5	-	-1	-8	-	-12				6	-	5	1	-	15	-4	-	-13	1	22	18
3	30	26				H 10 11			4	48	51	-1	-	-4	-6	-	-15			
1	45	46	H 2 10			-9	-	-10	2	20	19	-3	19	14				H 10 14		
-1	52	54	-10	-	16	-7	-	8	0	38	68	-5	-	-7	H 8 13			2	-	-7
-3	62	63	-8	-	12	-5	18	-11	-4	-	0	-7	30	30	-7	-	-25	0	-	-4
-5	19	24	-6	26	-27	-3	-	-2	-6	40	-42	-9	-	16	-5	48	-45	-2	24	-21
-7	28	26	-4	28	-28	-1	40	-39	-8	26	-22				-3	-	-17	-4	-	-5
-9	-	-2	-2	103	-107	1	52	-50	-10	-	-6	H 4 12			-1	-	-12			
			0	23	-22	3	39	-43				-8	-	-9	1	-	5	H 9 14		
H 10 10			2	55	-56	5	35	-33	H 9 11			-6	-	-3	3	-	5	-3	-	18
-10	-	13	4	23	29	7	-	-7	6	-	-17	-4	42	42	5	-	-6	-1	-	4
-8	19	11	6	-	8				4	-	1	-2	22	22				1	-	-2
-6	-	-12	8	-	19	H 1 10			2	29	-27	0	51	51	H 7 13					
-4	20	-17				9	-	-9	0	-	-3				6	-	-7	H 8 14		
-2	53	-56	H 1 10			7	-	1	-2	56	-56	H 0 11			4	-	-6	2	-	-11
0	-	-8	9	-	-9	5	-	-11	-4	42	-43	-11	-	15	2	27	-33	0	-	-7
2	25	-23	7	-	1	3	41	44	-6	60	-62	-9	-	12	0	-	-3	-2	32	-30
4	20	23	5	-	-11	1	61	117	-8	44	-41	4	-	-4	-2	-	-12	-4	-	-10
6	-	8	3	41	44	-1	79	84	-10	-	-6	6	23	-25	-6	28	16			
			1	79	84	-3	33	33	H 8 11									H 7 14		
H 9 10			-1	61	117	-5	47	44				H 3 12			H 6 13			-5	20	21
7	-	-20	-3	33	33	-7	-	-12	-9	-	15	7	-	13	-7	-	-11	-3	45	45
5	42	-36	-7	47	44	-9	-	-8	-11	73	-70	5	18	-3	-1	45	-46	-1	38	32
3	-	-12	-9	-	-8	-11	-	6	-1	45	-46	3	-	-11	-5	59	-57	1	27	24
1	-	5	-11	-	6				-5	59	-57	1	37	-41	-7	-	-3	-5	-	-14
-1	-	9				H 7 11			-7	-	-3	-1	73	-70	-9	-	-8	-3	25	18
-3	22	20	H 0 10			-9	-	-12	-9	-	-8	-3	45	-46				-1	-	20
-5	19	-22	-10	53	46	-7	-	13				-5	59	-57	H 2 12			1	38	37
-7	-	-5	-8	59	58	-5	-	-12	H 15 12			-7	-	-3				3	31	36
-9	29	-26	-6	33	33	-3	-	-2	-3	-	-12	-9	-	-8	-8	-	-9	5	-	15
			-4	44	45	-1	21	-17	-1	21	-17				-6	-	-2			
H 8 10			0	66	70							H 14 12			-4	34	40	H 5 13		
-10	-	13	2	22	23	H 7 11			-4	19	16	-8	-	-9	-2	14	12	4	-	-7
-8	-	9	4	83	87	1	59	-57	-2	18	12	-6	-	-2	0	43	45	2	38	-40
-6	18	-20	6	49	46	3	48	-48	0	28	20	-4	34	40	2	17	-20	0	-	-10
-4	27	-24	8	25	43	5	38	-36	2	20	-4	-2	14	12	4	-	-5	-2	-	-20
-2	73	-75	7	-	-6							0	43	45	6	-	-29	-4	26	28
0	16	-16				H 13 12			H 1 12			2	17	-20				-6	28	21
2	36	-37	H 19 11			3	-	13	7	-	34	4	-	-5	H 1 12			-8	-	17
4	24	19	0	-	5	1	-	5	5	23	31	6	-	-29	7	-	34			
6	-	6	-2	-	-3	-1	-	-3	3	37	37				5	23	31	H 4 14		
8	-	14				-3	-	5	1	-	12	H 12 12			3	37	37	-9	45	-32
			H 18 11			-5	-	-2	-3	-	5	-6	-	22	1	-	12	-7	-	-25
H 7 10			-5	-	8				-5	22	-7	-4	48	46	-3	-	5	-5	58	-52
7	-	1	-3	-	11	H 7 11			-7	41	40	-5	22	-7	-5	22	-7	-3	-	-22
5	-	-8	-1	-	1	8	-	1	-9	-	19	-2	41	38	-7	41	40	-1	25	-22
3	31	30	1	-	-4	6	-	5				0	52	48	-9	-	19	1	-	2
1	60	58				4	41	42	H 6 11			2	-	15				3	-	9
-1	73	72	H 17 11			2	23	20				4	-	14	H 0 12			5	-	-5
-3	95	91	2	-	6	0	53	51	-11	26	12				-10	-	8			
-5	27	29	0	-	12	-2	14	-14	-9	-	15	H 11 12			-8	20	26	H 3 13		
-7	35	32	-2	-	-2	-4	-	-3	-7	58	56	3	26	21	-6	51	47	6	-	-27
-9	-	-8	-4	-	-1	-6	-	-9	-5	30	32	1	-	8	-4	95	97	4	29	-33
-11	-	4	-6	-	-9				-3	47	47	-1	-	-6	0	95	106	2	65	-76
						H 6 10			-1	-	-1	-3	-	6	2	32	- 35	0	42	-46
H 16 11			H 5 11			1	17	-9	-5	-	1	2	32	- 35						
-7	-	4	8	-	-1	3	-	-8	-7	-	22	4	30	38	H 15 13			H 2 14		
-5	-	-5	6	-	2	5	-	-11				6	-	-1	0	-	-22	-2	-	-16
-3	-	-5	4	48	47	7	-	11	H 10 12						-2	-	-23	-4	-	-10
-1	22	-20	2	22	24				-6	-	5	H 15 13			-4	-	-7	-6	-	-12
1	24	-22	0	60	57	H 5 11			-4	28	28	0	-	-22				-8	-	-5
3	-	-17	-2	27	-25	8	-	-1	-2	-	12	-2	-	-23	H 2 13					
			-4	-	-9	6	-	2	0	31	30	-4	-	-7	-9	41	-33	H 1 14		
H 15 11			-6	32	-34	4	48	47	2	-	-4				-7	32	-29	-7	25	27
4	-	-1	-8	-	-13	2	22	24	4	-	3	H 14 13			-5	61	-59	-5	25	29
2	-	-12	-10	-	-3	0	60	57				-5	-	-22	-3	-	-21	-3	116	62
0	-	-8				-2	27	-25	H 9 12			-3	-	-13	-1	16	-16	1	27	29
-2	26	-33	H 4 11			-4	-	-9	5	-	3	-1	-	-13	1	-	9	3	-	12
-4	27	-28	-11	-	-4	-6	32	-34	3	-	-1	1	-	-3	3	-	11			
-6	23	-30	-9	-	-10	-8	-	-13	1	26	-24				5	-	-6	H 0 14		
			-7	25	23	-10	-	-3	-1	51	-48	H 13 13						2	-	15
H 14 11			-5	25	-19				-3	38	-33	2	-	-18	H 1 13			0	44	27
-9	-	-10	-3	-	-11	H 8 12			-5	40	-33	0	-	-7	6	-	-12	-4	21	24
-7	25	23	-1	72	-66	-8	19	-5	-7	-	3	-2	-	-10	4	-	-10	-6	16	18
1	71	-68	-2	-	8	-6	-	0				-4	-	10	2	35	-43			
3	55	-55	0	33	31	-4	26	27	H 12 13			-6	-	9	0	-	-1			
5	45	-47	2	-	-12	-2	-	8	-7	-	0				-4	25	28			
7	-	-11	4	22	-3	1	33	23	-5	-	-9	H 8 12			-6	-	17			
			6	-	-21	3	30	22	-3	-	9	-7	-	0	-8	35	19			
									-1	-	13	-5	-	-9						
									4	22	-3	-3	-	9	H 0 13					
									6	-	-21	-1	-	13	-9	-	-12			
												1	33	23	-7	-	-3			
												3	30	22	-5	-	-26			

Table 6. Bond distances and angles in $[Ni(en)_2][AgBr_2]_2$ and $[Ni(en)_2][AgI_2]_2$.

The number in parenthesis after the atom symbol denotes:

(1)	x	y	z	(5)	$\bar{x}$	$\bar{y}$	$\bar{z}$	(9)	x	y	$1+z$
(2)	$\bar{x}$	y	$1-z$	(6)	$-\frac{1}{2}+x$	$\frac{1}{2}-y$	z	(10)	$1-x$	$\bar{y}$	$1-z$
(3)	$1-x$	y	$1-z$	(7)	$\frac{1}{2}-x$	$\frac{1}{2}-y$	$1-z$				
(4)	x	$\bar{y}$	z	(8)	$\frac{1}{2}-x$	$\frac{1}{2}-y$	$\bar{z}$				

	Distance (Å) X=Br	Distance (Å) X=I
$Ag(1)-X_1(1)$	2.730 ± 0.002	2.895 ± 0.001
$Ag(1)-X_2(1)$	2.689 ± 0.002	2.845 ± 0.002
$Ag(1)-X_2(2)$	2.742 ± 0.002	2.863 ± 0.002
$Ni(1)-N(1)$	1.919 ± 0.013	1.922 ± 0.007
$N(1)-C(1)$	1.500 ± 0.022	1.484 ± 0.011
$C(1)-C(3)$	1.520 ± 0.027	1.510 ± 0.020
	Angle (°) X=Br	**Angle (°) X=I**
$X_1(1)-Ag(1)-X_1(4)$	97.71 ± 0.08	98.29 ± 0.05
$X_1(1)-Ag(1)-X_2(1)$	112.92 ± 0.05	111.56 ± 0.03
$X_1(1)-Ag(1)-X_2(2)$	109.45 ± 0.04	109.91 ± 0.04
$X_2(1)-Ag(1)-X_2(2)$	113.30 ± 0.06	114.46 ± 0.05
$X_2(1)\cdots Ni(1)-N(1)$	90.4 ± 0.3	90.9 ± 0.2
$N(1)-Ni(1)-N(3)$	86.4 ± 0.7	86.7 ± 0.4
$Ni(1)-N(1)-C(1)$	109.5 ± 0.8	109.0 ± 0.5
$N(1)-C(1)-C(3)$	104.9 ± 0.8	105.8 ± 0.6

Table 7. Interatomic distances other than bond distances. Distances less than 4.5 Å are included. Symbols are explained in Table 6.

$Ag(1)-Ag(2)$	2.99	3.09
$Ag(1)-Ag(5)$	3.59	3.79
$Ni(1)-Ag(1)$	4.49	>4.50
$Ag(1)-N(1)$	4.11	4.28
$Ag(1)-N(5)$	4.10	4.29
$Ag(1)-C(6)$	4.01	4.18
$Ag(1)-C(7)$	4.10	4.26
$X_1(1)-X_1(4)$	4.11	4.38
$X_1(1)-X_2(2)$	4.47	>4.50
$X_1(1)-N(1)$	3.48	3.67
$X_1(1)-N(8)$	3.95	4.08
$X_1(1)-C(1)$	3.77	3.96
$X_1(1)-C(7)$	3.88	4.00
$X_1(1)-C(8)$	3.62	3.78
$X_2(1)-Ni(1)$	3.36	3.51
$X_2(1)-N(1)$	3.88	3.97
$X_2(1)-N(9)$	3.62	3.82
$X_2(1)-N(10)$	3.86	4.02
$X_2(1)-C(1)$	4.09	4.17
$X_2(1)-C(7)$	4.00	4.20
$Ni(1)-C(1)$	2.80	2.78
$N(1)-N(4)$	2.80	2.80
$N(1)-N(10)$	3.84	3.84
$N(1)-N(3)$	2.63	2.64
$N(1)-C(4)$	4.16	4.14
$C(1)-C(7)$	4.20	4.45

ions extending parallel to the shortest crystallographic axis. Bond distances and angles are given in Table 6 and interatomic distances less than 4.5 Å other than bond distances in Table 7. Fig. 1 shows the projection on (010) of part of the unit cell.

There is good agreement between corresponding bond distances and angles in the two compounds, the differences in the lengths of the Ni—N, N—C, and C—C bonds being only $\frac{1}{2}\sigma$, σ, and $\frac{1}{2}\sigma$, respectively. The N—C and C—C bond distances do not differ significantly from the normal single bond values.

Distorted AgX_4 tetrahedra are linked by the sharing of edges to form $[AgX_2]_n^{n-}$ ions. Corresponding angles in the $[AgBr_2]_n^{n-}$ and $[AgI_2]_n^{n-}$ ions, though significantly different, do not differ by more than 1.4°. Only one angle in the AgX_4 unit has the tetrahedral value, while one, being approximately 98°, differs by as much as 12°.

The Ag—Br and Ag—I bond distances have normal values. The average Ag—I distance in $[Ni(en)_2][AgI_2]_2$ is 2.87 Å (2.845—2.895 Å), while, *e.g.*, 2.81 Å has been found in AgI,[7] 2.85 Å in the $Ag_4I_6^{2-}$ and AgI_2^- ions,[8] and 2.78 Å in the $[AgI_3]_n^{2n-}$ ion, the latter being built up from linked tetrahedra.[9]

The configuration about the nickel atom can be described as being square planar, though there are two halogen atoms, *trans* to each other, in octahedral positions, the Ni···X direction being almost perpendicular to the NiN_4 plane. It is possible that there is weak interaction between these halogen atoms and the nickel atom, since the Ni···Br and Ni···I distances, 3.36 Å and 3.51 Å, respectively, although about 0.7 Å longer than the normal single bond values, found in octahedral nickel complexes,[10,11] are considerably shorter than the closest contact distances of about 4 Å found in typical square planar nickel complexes.[12,13] The ligand field exerted by the halogen atoms is, of course, not strong enough to raise the energy of the d_{z^2} orbital sufficiently to make the promotion of one d_{z^2} electron to the empty $d_{x^2-y^2}$ orbital energetically more favourable than spin pairing. $[Ni(en)_2][AgX_2]_2$ is, therefore, diamagnetic in contrast to the true octahedral nickel complexes, which are paramagnetic.

The Ni···X interaction seems to be responsible for the opening of the $X_2—Ag—X_2$ angle, which is 4—5° greater than the tetrahedral value.

The Ni—N bond distances, 1.92 Å in both $[Ni(en)_2][AgBr_2]_2$ and $[Ni(en)_2][AgI_2]_2$, are significantly shorter than the distances found in octahedral nickel complexes (see Table 8). They are, however, slightly longer than the values observed in true square planar nickel complexes (see Table 8), and this bond weakening may be a consequence of the nickel-halogen interaction.

The nickel atom and the four nitrogen atoms all lie exactly in a plane and the carbon atoms are displaced 0.38 Å from this plane in $[Ni(en)_2][AgBr_2]_2$ and 0.36 Å in $[Ni(en)_2][AgI_2]_2$. The corresponding distance is 0.29 Å in $[Ni(en)_3](NO_3)_2$,[20] 0.34 Å in $[Co(en)_2Cl_2]Cl(HCl)(H_2O)$,[32] 0.34 Å in $[Ni(NCS)_2(en)_2]$,[17] 0.33 Å in both *trans*-$[CrCl_2(H_2O)_2en]Cl$[33] and $[Cr(O_2)_2(H_2O)en](H_2O)$,[34] and 0.37 Å in $[(en)_2Ni(NCS)_2Ni(en)_2]I_2$ and $[(en)_2Ni(NCS)_2Ni(en)_2](ClO_4)_2$.[19]

Table 8. Ni—N distances in some Ni(II) complexes,

Octahedral complexes:		Distance (Å)	Ref.
Diaquobis(glycinato)nickel(II)	$[Ni(H_2O)_2(C_2H_4NO_2)_2]$	2.09	14
Dichlorotetrakis(pyrazole)-nickel(II)	$[NiCl_2(C_3H_4N_2)_4]$	2.087—2.097	15
Bis(isoselenocyanato)tetrakis-(dimethylformamide)nickel(II)	$[Ni(NCSe)_2(HCON(CH_3)_2)_4]$	2.05	16
trans-Bis(isothiocyanato)bis-(ethylenediamine)nickel(II)	$[Ni(NCS)_2(en)_2]$	2.09—2.15	17
Chloroisothiocyanatobis-(ethylenediamine)nickel(II)	$[NiCl(NCS)(en)_2]$	2.06—2.13	18
Bromoisothiocyanatobis-(ethylenediamine)nickel(II)	$[NiBr(NCS)(en)_2]$		
Di-μ-isothiocyanato-bis{bis-(ethylenediamine)nickel(II)}iodide	$[(en)_2Ni(NCS)_2Ni(en)_2]I_2$	2.04—2.13	19
Di-μ-isothiocyanato-bis{bis-(ethylenediamine)nickel(II)} perchlorate	$[(en)_2Ni(NCS)_2Ni(en)_2](ClO_4)_2$		
Tris(ethylenediamine)nickel(II) nitrate	$[Ni(en)_3](NO_3)_2$	2.12	20
trans-Bis(2,4-pentanedionato)-dipyridinenickel(II)	$[Ni(C_5H_7O_2)_2(py)_2]$	2.112	21
Square planar complexes:			
Bis(salicylaldiminato)nickel(II)	$[Ni(C_7H_6NO)_2]$	1.84	13
Bis(salicylaldoximato)nickel(II)	$[Ni(C_6H_5NO_2)_2]$	1.83	22
Etioporphyrinatonickel(II)	$[Ni(C_{32}H_{36}N_4)]$	1.84	23
Bis(dimethylglyoximato)nickel(II)	$[Ni(C_4H_7N_2O_2)_2]$	1.85 *	24
Bis(*N*-methylsalicylaldiminato)-nickel(II)	$[Ni(C_8H_8NO)_2]$	1.90	26
Bis(glyoximato)nickel(II)	$[Ni(C_2H_3N_2O_2)_2]$	1.866—1.880	27, 28
Bis(dehydroaceticacidmonoimido)-nickel(II)	$[Ni(C_8H_8NO_3)_2]$	1.825—1.839	29
Bis(*o*-phenylenediamino)nickel(II)	$[Ni(C_6H_6N_2)_2]$	1.823—1.841	30
Bis(pyridine-2-carboxamido)-nickel(II) dihydrate	$[Ni(C_6H_5N_2O)_2](H_2O)_2$	1.87—1.92	31

A comparatively large number of nickel complexes with the empirical formula $Ni(en)_2XY$ have been the subject of structural investigations during the last ten years.[11,17,35–43] According to Porai-Koshits, who, together with his co-workers, has performed the most extensive investigations of these compounds, they can be divided into four groups according to their structure and the nature of the ligands X and Y.[44] It is obvious that $[Ni(en)_2][AgBr_2]_2$ and $[Ni(en)_2][AgI_2]_2$ belong to the first group, $[Ni(en)_2]X_2$, since they are diamagnetic and contain square planar $[Ni(en)_2]^{2+}$ ions.

After completing the structure determinations the author received a letter from Lingafelter,[43] in connection with the author's note on $[Ni(en)_2][AgX_2]_2$,[1] to the effect that he was performing structure analyses of the isomorphous

* This value has been obtained by a least-squares refinement [25] of the data given by Godycki *et al*,. who reported the values 1.90 and 1.87 Å.

$[Ni(en)_2][AgBr_2]_2$, $[Cu(en)_2][AgBr_2]_2$ and $[Ni(en)_2][AgBrI]_2$. The preliminary parameters given by Lingafelter for $[Ni(en)_2][AgBr_2]_2$ are in good agreement with those obtained in the present investigation.

Acknowledgements. I wish to thank Professor G. Lundgren for reading the manuscript and Dr. Susan Jagner for revising the English text. A grant from the *Swedish Natural Science Research Council* is gratefully acknowledged.

REFERENCES

1. Stomberg, R. *Acta Chem. Scand.* **22** (1968) 2022.
2. Abrahamsson, S. and Larsson, K. *Arkiv Kemi* **24** (1965) 383.
3. Larsson, K. *Arkiv Kemi* **24** (1964) 17.
4. Lindgren, O. *Private communication.*
5. Modified by Lindqvist, O. and Lindgren, O. and in use at this Department. DATAP2 was originally written by Coppens, P., Leiserowitz, L. and Rabinowich, D., LALS by Gantzel, R., Sparks, K. and Trueblood, K., and DRF and DISTAN by Zalkin, A.
6. Cruickshank, D. W. J. *The Equations of Structure Refinements*, Glasgow 1964.
7. Wilsey, R. B. *Phil. Mag.* **46** (1923) 487.
8. Dallinga, G. and Mackor, E. L. *Rec. Trav. Chim.* **75** (1956) 796.
9. Brink, C. and MacGillavry, C. H. *Acta Cryst.* **2** (1949) 158.
10. Antsyshkina, A. S. and Porai-Koshits, M. A. *Kristallografiya* **3** (1958) 676.
11. Antsyshkina, A. S. and Porai-Koshits, M. A. *Dokl. Acad. Nauk SSSR* **143** (1962) 105.
12. Vannerberg, N. G. *Acta Chem. Scand.* **18** (1964) 2385.
13. Stewart, J. M. and Lingafelter, E. C. *Acta Cryst.* **12** (1959) 842.
14. Stosick, A. J. *J. Am. Chem. Soc.* **67** (1945) 365.
15. Reimann, C. W., Mighell, A. D. and Mauer, F. A. *Acta Cryst.* **23** (1967) 135.
16. Tsintsadze, G. V., Porai-Koshits, M. A. and Antsyshkina, A. S. *Zh. Struct. Khim.* **8** (1967) 296.
17. Brown, B. W. and Lingafelter, E. C. *Acta Cryst.* **16** (1963) 753.
18. Shvelashvili, A. E. and Porai-Koshits, M. A. *Zh. Struct. Khim.* **9** (1968) 646.
19. Shvelashvili, A. E. *Abstract 9—61 of the Communications to the 7th International Congress of Crystallography, Moscow 1966.*
20. Swink, L. N. and Atoji, M. *Acta Cryst.* **13** (1960) 639.
21. Elder, R. C. *Inorg. Chem.* **7** (1968) 2316.
22. Merritt, L. L., Jr., Guare, C. and Lessor, A. E., Jr. *Acta Cryst.* **9** (1956) 253.
23. Crute, M. B. *Acta Cryst.* **12** (1959) 24.
24. Godycki, L. E. and Rundle, R. E. *Acta Cryst.* **6** (1953) 487.
25. Williams, D. E., Wohlauer, G. and Rundle, R. E. *J. Am. Chem. Soc.* **81** (1959) 755.
26. Frasson, E., Panattoni, C. and Sacconi, L. *J. Phys. Chem.* **63** (1959) 1908.
27. Calleri, M., Ferraris, G. and Viterbo, D. *Acta Cryst.* **22** (1967) 468.
28. Murmann, R. K. and Schlemper, E. O. *Acta Cryst.* **23** (1967) 667.
29. Kiryu, S. *Acta Cryst.* **23** (1967) 392.
30. Hall, G. S. and Soderberg, R. H. *Inorg. Chem.* **7** (1968) 2300.
31. Chang, S. C., Park, D. Y. and Li, N. C. *Inorg. Chem.* **7** (1968) 2144.
32. Nakahara, A., Saito, Y. and Kuroya, H. *Bull. Chem. Soc. Japan* **25** (1952) 331.
33. Stomberg, R. and Larking, I. *Acta Chem. Scand.* **23** (1969) 343.
34. Stomberg, R. *Arkiv Kemi* **24** (1965) 47.
35. Lewellin, F. J. and Waters, F. M. *J. Chem. Soc.* **1962** 3845.
36. Shvelashvili, A. E., Porai-Koshits, M. A. and Antsyshkina, A. S. *Zh. Struckt. Khim.* **5** (1964) 147.
37. Barinskij, R. L., Shvelashvili, A. E. and Maljokov, B. A. *Zh. Strukt. Khim.* **5** (1964) 497.
38. Porai-Koshits, M. A. and Minacheva, L. Kh. *Zh. Strukt. Khim.* **5** (1964) 642.
39. Shvelashvili, A. E., Porai-Koshits, M. A. and Antsyshkina, A. S. *Zh. Strukt. Khim.* **5** (1964) 797.

40. Shvelashvili, A. E., Porai-Koshits, M. A. and Antsyshkina, A. S. *Zh. Strukt. Khim.* **6** (1965) 168.
41. Shvelashvili, A. E., Porai-Koshits, M. A. and Antsyshkina, A. S. *Zh. Strukt. Khim.* **6** (1965) 170.
42. Shvelashvili, A. E. and Porai-Koshits, M. A. *Zh. Strukt. Khim.* **9** (1968) 646.
43. Lingafelter, E. C. *Private communication* (1969).
44. Porai-Koshits, M. A. *Abstract 9—49 of the Communications to the 7th International Congress of Crystallography, Moscow 1966.*

Received April 28, 1969.