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Hexaacetonitrilenickel(II) Tetrachlorozincate. A Crystal Structure with Serious Overlap in the Patterson Function

By Inger Søtofte

Chemical Laboratory B, Technical University of Denmark, DK-2800 Lyngby, Denmark

and Rita Grønbæk Hazell and Svend Erik Rasmussen

Department of Inorganic Chemistry, Aarhus University, DK-8000 Aarhus C, Denmark

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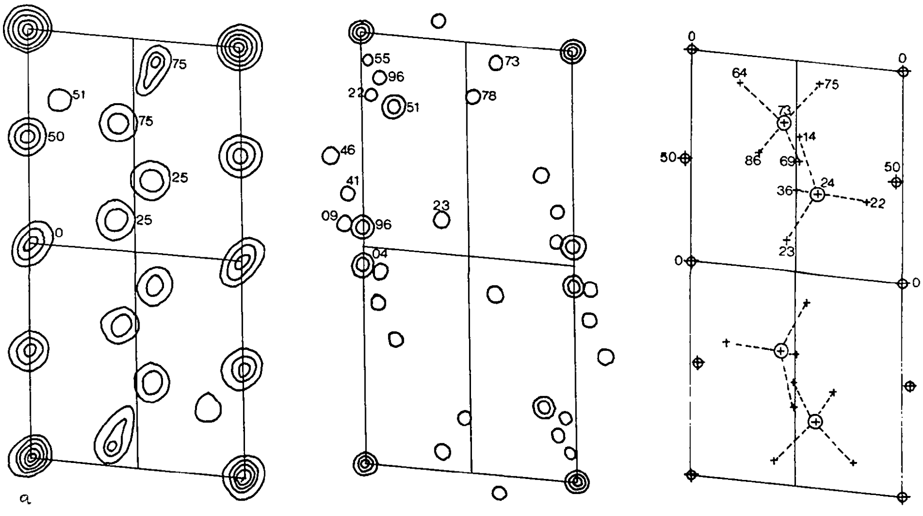
$Ni(CH_3CN)_6ZnCl_4$ crystallizes in space group $P\bar{1}$ with $a=16{\cdot}25$, $b=18{\cdot}40$, $c=8{\cdot}51$ Å, $\alpha=94{\cdot}4$, $\beta=83{\cdot}9$, $\gamma=114{\cdot}5°$, $Z=4$. Intensities were collected on a semi-automatic diffractometer. The Patterson function showed serious overlap and did not lead to the right solution; direct methods gave no new information. Reflexions with $2h+k=4n$ were systematically strong and a Patterson function calculated without these reflexions readily gave the correct positions of the metal atoms. The structure was refined by least squares with anisotropic thermal motion. The final R was 0·096 for 5580 significant reflexions. Zn is tetrahedrally coordinated by Cl atoms (average Zn–Cl 2·27 Å), Ni octahedrally by acetonitrile groups (average Ni–N 2·07 Å).

Introduction

Kern (1963) prepared a number of acrylonitrile, acetonitrile and propionitrile complexes of metal chlorides in the first transition series. He sent us samples of some of these but unfortunately, they were not well suited for X-ray work. Later, an acetonitrile–Ni compound was prepared in this laboratory as described by Kern, and well-developed blue crystals were obtained. In accordance with Kern we assumed the formula $NiCl_2(CH_3CN)_{3.5}$. This composition indicates the possibility of an unusual structure and as nitrile complexes are not well characterized in general, we decided to determine the crystal structure.

Experimental

Anhydrous materials were employed throughout. Operations were carried out in Schlenk equipment or in a glove box under dry nitrogen. A mixture of $NiCl_2$, Zn dust and white sand was extracted with dry CH_3CN and eventually a crop of royal blue crystals developed. The compound is very hygroscopic, and difficult to analyse accurately. A Ni analysis by EDTA



(*a*) (*b*) (*c*)

Fig. 1. Schematic drawings of (*a*) the Patterson function, (*b*) the 'odd' Patterson calculated without reflexions $2h+k=4n$, (*c*) the positions of the heavy atoms. The numbers indicate the y coordinates ×100.

titration and a Cl analysis were in reasonable agreement with Kern's formula.

X-ray technique

Crystals for X-ray work were sealed in glass capillaries. Lattice type and space group were established from photographs taken with Cu and Mo radiation. A crystal 0·3 × 0·4 × 0·5 mm was used. Intensities were measured on a diffractometer of equi-inclination Weissenberg type manufactured by Supper and Pace. Mo $K\alpha$ radiation was selected by a LiF monochromator. Harmonics were excluded by a scintillation detector with a pulse height discriminator. Reflexions $hk0$ through $hk10$ ($\sin\theta/\lambda \le 0{\cdot}70$) were measured. Those having net intensities less than twice their estimated standard deviation were designated as 'unobserved' and were omitted, leaving 5580 independent, non-zero observations to be used in the determination. No absorption correction was applied. The scattering factors were those listed in *International Tables for X-ray Crystallography* (1962). Most calculations were performed with the X-RAY system (Stewart, Kundell & Baldwin, 1970).

Structure determination

The Patterson function [shown schematically in Fig. 1(*a*)] contained 7 independent peaks much larger than all others; these peaks were broad and obviously multiple and a number of solutions for 8 heavy atoms per cell seemed to fit equally well.

Direct methods were also tried. Both *SYMBAD* (Danielsen, 1969) and *MULTAN* (Main, Woolfson & Germain, 1971) gave as the more probable solutions some of those that fitted the Patterson function, but all trial structures gave R in the range 0·6–0·7; all could be refined to a somewhat lower R and all gave Fourier maps that showed some promising features as well as some unreasonable ones; none led to the solution.

Corresponding to the two big peaks in the Patterson function at $\frac{1}{2}$,0,0 and $\frac{1}{4}$,$\frac{1}{2}$,0 it was noticeable that reflexions for which $2h+k=4n$ were strong ($\langle E^2\rangle = 1{\cdot}4$) and those with $2h+k=4n+2$ were weak; reflexions with k odd were of intermediate intensity. Renormalization of the E values of these groups before use in the direct methods programs did not lead to the solution. A Patterson function calculated without the $2h+k=4n$ reflexions (Fig. 1*b*) showed better resolution than the ordinary Patterson map and was readily interpreted in terms of vectors between three pairs of heavy atoms. From the conventional Patterson map these positions were confirmed and supplemented with atoms at 0,0,0 and $\frac{1}{2}$,0,0 which would contribute to the strong reflexions only (Fig. 1*c*). This solution differed from some of those previously tried by only about 0·5 Å in some of the heavy-atom positions. Because of the serious overlap of Patterson vectors, refinement had not been able to proceed from the false minimum to the correct one even though it was quite close; since only low order data were used in the initial refinements, convergence from a greater distance had been expected.

In retrospect it is obvious that the reason the direct methods failed was that the right solution was one with the signs of all strong reflexions positive but the structure could not be recognized or refined until the weak reflexions had been given the right sign. The few reflexions that should have been negative were well down the list of E values and entered into few strong relations but were not left undetermined by the sign expansion routine. It was therefore difficult to pick out the first negative reflexions. Once the heavy atoms had been found, the full structure was obtained smoothly from Fourier maps calculated with signs from the

Table 1. *Atomic coordinates* (× 10⁴) *with standard deviations* (× 10⁴) *in parentheses*

	x	y	z
Zn(1)	8475 (1)	7698 (1)	776 (2)
Zn(2)	3162 (1)	7404 (1)	797 (2)
Ni(1)	10000 (0)	5000 (0)	5000 (0)
Ni(2)	5000 (0)	5000 (0)	5000 (0)
Ni(3)	2628 (1)	2 (1)	4696 (2)
Cl(1)	7530 (3)	8168 (3)	−195 (7)
Cl(2)	9267 (3)	8583 (3)	2554 (7)
Cl(3)	9469 (3)	7581 (3)	−1196 (6)
Cl(4)	7681 (3)	6469 (3)	1887 (6)
Cl(5)	1842 (2)	6396 (2)	176 (5)
Cl(6)	3152 (4)	8572 (2)	66 (7)
Cl(7)	3231 (6)	7328 (5)	3418 (8)
Cl(8)	4343 (3)	7238 (4)	−561 (9)
N(1)	11186 (10)	5025 (8)	3759 (16)
N(2)	9308 (9)	3861 (7)	4267 (15)
N(3)	9720 (8)	5409 (7)	2979 (15)
N(4)	3867 (8)	4019 (7)	4413 (14)
N(5)	5164 (9)	5482 (7)	2710 (16)
N(6)	5849 (9)	4465 (8)	4199 (17)
N(7)	1717 (8)	433 (6)	4116 (14)
N(8)	1808 (8)	−1087 (8)	3837 (14)
N(9)	3508 (9)	−465 (7)	5307 (14)
N(10)	3435 (9)	1120 (7)	5549 (15)
N(11)	3338 (8)	337 (7)	2525 (16)
N(12)	1962 (8)	−289 (7)	6956 (16)
C(1)	11827 (13)	5056 (10)	3025 (20)
C(2)	12678 (13)	5123 (15)	2126 (23)
C(3)	8903 (10)	3258 (9)	3679 (18)
C(4)	8420 (12)	2468 (8)	3065 (22)
C(5)	9601 (8)	5576 (7)	1806 (17)
C(6)	9431 (11)	5779 (9)	271 (18)
C(7)	3216 (11)	3475 (10)	4266 (19)
C(8)	2332 (14)	2777 (12)	4051 (27)
C(9)	5400 (9)	5773 (8)	1577 (18)
C(10)	5666 (12)	6153 (10)	−29 (20)
C(11)	6419 (10)	4316 (9)	3766 (17)
C(12)	7172 (12)	4061 (15)	3318 (23)
C(13)	1155 (9)	591 (7)	3766 (17)
C(14)	412 (11)	788 (10)	3377 (30)
C(15)	1371 (11)	−1657 (8)	3257 (18)
C(16)	826 (14)	−2388 (10)	2437 (26)
C(17)	3905 (9)	−813 (9)	5706 (20)
C(18)	4378 (11)	−1264 (11)	6195 (25)
C(19)	3798 (12)	1719 (9)	6069 (21)
C(20)	4278 (17)	2502 (11)	6716 (30)
C(21)	3673 (9)	518 (7)	1308 (16)
C(22)	4097 (13)	748 (11)	−322 (19)
C(23)	1685 (9)	−344 (8)	8227 (18)
C(24)	1345 (14)	−397 (12)	9882 (21)

Table 2. *Mean square vibration amplitudes,* $U_{ij} \times 10^4$ *with standard deviations* ($\times 10^4$) *in parentheses*

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	361 (9)	366 (8)	574 (11)	112 (7)	52 (8)	67 (7)
Zn(2)	478 (10)	394 (9)	654 (12)	78 (8)	−111 (9)	−43 (8)
Ni(1)	368 (13)	299 (12)	419 (14)	65 (10)	−29 (11)	30 (10)
Ni(2)	283 (11)	259 (11)	506 (15)	39 (9)	74 (10)	−4 (10)
Ni(3)	316 (8)	299 (8)	429 (10)	115 (7)	−33 (7)	−12 (7)
Cl(1)	506 (23)	558 (24)	1199 (43)	267 (20)	−29 (25)	183 (26)
Cl(2)	660 (29)	734 (30)	874 (35)	91 (24)	−33 (25)	−262 (26)
Cl(3)	755 (28)	646 (26)	676 (27)	455 (23)	263 (23)	310 (21)
Cl(4)	596 (26)	519 (23)	851 (32)	143 (20)	174 (23)	269 (22)
Cl(5)	398 (18)	379 (17)	686 (25)	66 (15)	3 (17)	−15 (17)
Cl(6)	827 (32)	372 (20)	1021 (38)	177 (21)	81 (28)	20 (22)
Cl(7)	1437 (64)	1200 (53)	788 (41)	204 (46)	−402 (42)	−60 (36)
Cl(8)	457 (25)	892 (37)	1600 (59)	339 (25)	−131 (31)	−314 (38)
N(1)	530 (81)	506 (72)	552 (82)	207 (63)	−116 (68)	−27 (60)
N(2)	550 (77)	435 (70)	484 (74)	73 (60)	−168 (61)	11 (57)
N(3)	423 (65)	451 (65)	449 (73)	44 (52)	−51 (55)	109 (55)
N(4)	462 (69)	473 (70)	334 (65)	97 (59)	−21 (53)	−6 (52)
N(5)	608 (80)	360 (58)	480 (75)	210 (56)	−5 (63)	−110 (54)
N(6)	462 (74)	516 (74)	679 (88)	152 (62)	262 (67)	65 (63)
N(7)	493 (67)	364 (58)	427 (69)	132 (52)	−126 (56)	12 (49)
N(8)	542 (72)	491 (69)	360 (64)	197 (59)	−34 (54)	63 (52)
N(9)	508 (69)	415 (60)	432 (69)	175 (54)	−51 (56)	−22 (51)
N(10)	586 (74)	403 (62)	480 (74)	238 (57)	−71 (60)	22 (53)
N(11)	460 (69)	333 (58)	723 (82)	108 (52)	71 (61)	14 (54)
N(12)	407 (65)	411 (61)	666 (83)	174 (53)	42 (60)	40 (56)
C(1)	606 (112)	616 (99)	507 (92)	286 (88)	−255 (86)	−59 (74)
C(2)	745 (116)	1480 (188)	638 (116)	736 (129)	90 (94)	78 (116)
C(3)	470 (81)	474 (84)	460 (87)	166 (69)	−65 (69)	86 (68)
C(4)	633 (106)	316 (67)	890 (122)	112 (68)	−226 (92)	−123 (71)
C(5)	360 (65)	236 (54)	434 (78)	77 (48)	54 (57)	−9 (51)
C(6)	681 (99)	497 (82)	433 (82)	274 (75)	−173 (73)	41 (64)
C(7)	524 (91)	505 (93)	435 (87)	−21 (77)	4 (71)	43 (70)
C(8)	694 (124)	714 (116)	1072 (160)	−343 (98)	11 (112)	−187 (110)
C(9)	453 (74)	349 (66)	438 (82)	72 (57)	35 (63)	−51 (59)
C(10)	733 (110)	587 (99)	524 (97)	75 (84)	−62 (84)	82 (77)
C(11)	372 (74)	578 (89)	400 (79)	80 (67)	−3 (62)	−148 (65)
C(12)	572 (104)	1406 (191)	725 (118)	584 (121)	−66 (88)	−337 (118)
C(13)	402 (74)	344 (61)	443 (79)	117 (55)	−51 (61)	94 (54)
C(14)	423 (84)	623 (101)	1543 (208)	225 (77)	−291 (107)	352 (115)
C(15)	588 (94)	324 (72)	488 (86)	154 (68)	−171 (73)	−89 (62)
C(16)	869 (135)	411 (85)	1008 (144)	157 (88)	−469 (115)	−201 (88)
C(17)	324 (70)	399 (76)	726 (103)	103 (60)	116 (68)	83 (70)
C(18)	501 (92)	727 (115)	1036 (145)	342 (87)	−51 (92)	196 (102)
C(19)	610 (102)	350 (82)	683 (105)	151 (76)	−25 (83)	−132 (74)
C(20)	1202 (175)	466 (98)	1265 (186)	152 (106)	−274 (146)	−419 (111)
C(21)	422 (72)	332 (62)	415 (74)	−49 (53)	−245 (60)	−71 (52)
C(22)	729 (115)	706 (111)	404 (88)	44 (92)	177 (83)	135 (78)
C(23)	422 (73)	441 (70)	497 (83)	89 (58)	−103 (63)	14 (60)
C(24)	856 (138)	917 (133)	411 (96)	−72 (108)	153 (93)	−115 (89)

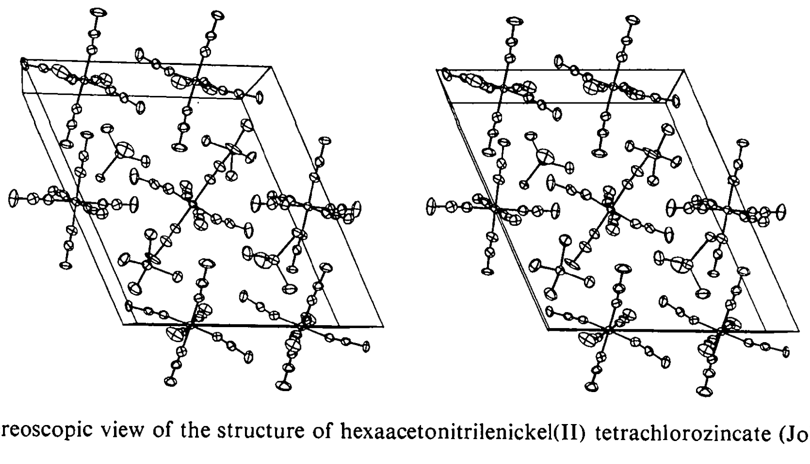


Fig. 2. Stereoscopic view of the structure of hexaacetonitrilenickel(II) tetrachlorozincate (Johnson, 1965).

heavy-atom contributions and it became clear that the unit cell contained 2×2 Zn atoms each with a tetrahedron of Cl atoms around them and 2+1+1 Ni atoms each octahedrally surrounded by acetonitrile groups.

The structure was refined by least squares, first with isotropic and later anisotropic temperature factors. The weights were $w=xy$, where if $0{\cdot}33F_o>|F_c|$, then $w=10^{-9}$, else if $\sin\theta>0{\cdot}22$, then $x=1$, else $x=\sin\theta/0{\cdot}22$, and if $62>F_o$, then $y=1$, else $y=62/F_o$. The refinement terminated with $R=0{\cdot}096$ for 5580 reflexions.

Crystal data

$Ni(CH_3CN)_6ZnCl_4$. Crystal system: triclinic. $a=16{\cdot}25$ (5), $b=18{\cdot}40$ (5), $c=8{\cdot}51$ (5) Å, $\alpha=94{\cdot}4$ (5), $\beta=83{\cdot}9$ (5), $\gamma=114{\cdot}5$ (5)°. $V=2302$ Å^3, $Z=4$, $d_c=1{\cdot}48$ g cm^{-3}. Space group: $P\bar{1}$.

Coordinates and anisotropic temperature factor parameters are given in Tables 1 and 2, bond lengths and angles in Tables 3 and 4.*

Discussion

The compound was analysed for Ni by precipitating dimethylglyoximenickel as well as by EDTA titration. The percentages found differed by a factor of about two. Dimethylglyoxime is a rather specific reagent for Ni whereas EDTA will titrate the sum of Ni and Zn. We did not, however, realize the presence of Zn until the structure was solved. We consider it possible that the compound '$NiCl_2(CH_3CN)_{3.5}$' reported by Kern (1963) is identical with that reported here as the preparative methods employed were the same in both cases.

Table 3. *Bond lengths* (Å)
with standard deviations in parentheses

Zn(1)–Cl(1)	2·284 (11)	N(3)—C(5)	1·116 (21)
Zn(1)–Cl(2)	2·251 (17)	N(4)—C(7)	1·130 (20)
Zn(1)–Cl(3)	2·270 (14)	N(5)—C(9)	1·076 (21)
Zn(1)–Cl(4)	2·275 (17)	N(6)—C(11)	1·094 (25)
Zn(2)–Cl(5)	2·276 (18)	N(7)—C(13)	1·137 (23)
Zn(2)–Cl(6)	2·269 (10)	N(8)—C(15)	1·123 (19)
Zn(2)–Cl(7)	2·258 (15)	N(9)—C(17)	1·161 (25)
Zn(2)–Cl(8)	2·257 (13)	N(10)–C(19)	1·110 (20)
Ni(1)–N(1)	2·081 (19)	N(11)–C(21)	1·113 (20)
Ni(1)–N(2)	2·032 (18)	N(12)–C(23)	1·118 (21)
Ni(1)–N(3)	2·071 (18)	C(1)—C(2)	1·466 (30)
Ni(2)–N(4)	2·064 (19)	C(3)—C(4)	1·442 (22)
Ni(2)–N(5)	2·119 (19)	C(5)—C(6)	1·458 (24)
Ni(2)–N(6)	2·052 (19)	C(7)—C(9)	1·501 (25)
Ni(3)–N(7)	2·056 (17)	C(9)—C(10)	1·500 (25)
Ni(3)–N(8)	2·048 (18)	C(11)–C(12)	1·492 (32)
Ni(3)–N(9)	2·066 (17)	C(13)–C(14)	1·467 (28)
Ni(3)–N(10)	2·078 (18)	C(15)–C(16)	1·465 (24)
Ni(3)–N(11)	2·043 (19)	C(17)–C(18)	1·443 (31)
Ni(3)–N(12)	2·079 (19)	C(19)–C(20)	1·443 (26)
N(1)—C(1)	1·140 (26)	C(21)–C(22)	1·478 (23)
N(2)—C(3)	1·155 (20)	C(23)–C(24)	1·449 (25)

Zn–Cl	2·268 (5)
Ni–N	2·066 (5)
N—C	1·123 (6)
C—C	1·467 (8)

Table 4. *Angles* (°)
with standard deviations in parentheses

Cl(1) –Zn(1)–Cl(2)	108·1 (0·3)
Cl(1) –Zn(1)–Cl(3)	110·4 (0·4)
Cl(1) –Zn(1)–Cl(4)	111·3 (0·3)
Cl(2) –Zn(1)–Cl(3)	108·6 (0·4)
Cl(2) –Zn(1)–Cl(4)	111·0 (0·4)
Cl(3) –Zn(1)–Cl(4)	107·4 (0·3)
Cl(5) –Zn(2)–Cl(6)	107·8 (0·3)
Cl(5) –Zn(2)–Cl(7)	107·5 (0·2)
Cl(5) –Zn(2)–Cl(8)	109·1 (0·3)
Cl(6) –Zn(2)–Cl(7)	113·0 (0·3)
Cl(6) –Zn(2)–Cl(8)	109·5 (0·3)
Cl(7) –Zn(2)–Cl(8)	109·9 (0·4)
N(1)—Ni(1)–N(2)	90·0 (0·6)
N(1)—Ni(1)–N(3)	88·4 (0·6)
N(2)—Ni(1)–N(3)	89·1 (0·6)
N(4)—Ni(2)–N(5)	90·0 (0·5)
N(4)—Ni(2)–N(6)	92·1 (0·6)
N(5)—Ni(2)–N(6)	89·1 (0·6)
N(7)—Ni(3)–N(8)	88·4 (0·6)
N(7)—Ni(3)–N(10)	90·0 (0·6)
N(7)—Ni(3)–N(11)	90·1 (0·6)
N(7)—Ni(3)–N(12)	90·8 (0·6)
N(8)—Ni(3)–N(9)	90·2 (0·6)
N(8)—Ni(3)–N(11)	91·2 (0·5)
N(8)—Ni(3)–N(12)	91·7 (0·5)
N(9)—Ni(3)–N(10)	91·4 (0·6)
N(9)—Ni(3)–N(11)	91·3 (0·6)
N(9)—Ni(3)–N(12)	87·9 (0·6)
N(10)–Ni(3)–N(11)	88·7 (0·5)
N(10)–Ni(3)–N(12)	88·3 (0·5)
Ni(1)–N(1)—C(1)	177·0 (1·6)
Ni(1)–N(2)—C(3)	171·3 (1·4)
Ni(1)–N(3)—C(5)	172·7 (1·4)
Ni(2)–N(4)—C(7)	172·4 (1·2)
Ni(2)–N(5)—C(9)	167·8 (1·4)
Ni(2)–N(6)—C(11)	167·2 (1·1)
Ni(3)–N(7)—C(13)	172·8 (1·0)
Ni(3)–N(8)—C(15)	174·8 (1·2)
Ni(3)–N(9)—C(17)	171·4 (1·0)
Ni(3)–N(10)–C(19)	173·8 (1·4)
Ni(3)–N(11)–C(21)	175·3 (1·4)
Ni(3)–N(12)–C(23)	170·5 (1·0)
N(1)—C(1)—C(2)	177·5 (1·7)
N(2)—C(3)—C(4)	174·5 (2·0)
N(3)—C(5)—C(6)	178·9 (1·1)
N(4)—C(7)—C(8)	177·3 (2·2)
N(5)—C(9)—C(10)	176·3 (1·6)
N(6)—C(11)–C(12)	174·3 (1·8)
N(7)—C(13)–C(14)	177·7 (1·6)
N(8)—C(15)–C(16)	177·5 (1·6)
N(9)—C(17)–C(18)	178·5 (1·4)
N(10)–C(19)–C(20)	179·0 (1·8)
N(11)–C(21)–C(22)	178·7 (1·7)
N(12)–C(23)–C(24)	178·6 (1·3)

The compound is built from $[Ni(CH_3CN)_6]^{2+}$ and $ZnCl_4^{2-}$ ions. Each of the three independent Ni atoms is octahedrally coordinated to six N atoms and the two independent Zn atoms are each coordinated to

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31369 (24 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

four Cl atoms forming nearly regular tetrahedra (Fig. 2). Table 3 includes some mean values of bond lengths and angles for the acetonitrile groups and the tetrachlorozincate ions. The Ni–N distances show no significant differences and the mean differences of the angles from 90° are only two standard deviations.

The dimensions of the acetonitrile groups agree with the results of other studies (Einstein, Enwall, Morris & Sutton, 1971; Marstokk & Strømme, 1968; Swanson, Shriver & Ibers, 1969) in which no significant differences from those of acetonitrile itself (Costain, 1958; Danford & Livingston, 1955) were found.

The coordination of the acetonitrile groups is not quite linear, the mean of the Ni–N–C angles is 172°. The distribution shows a spread corresponding to twice the estimated standard deviations, but since these are usually underestimated (Hamilton & Abrahams, 1970), it would seem to indicate that these angles are hardly influenced by packing forces. The N–C–C angles on the other hand are probably 180°. For a normal distribution around 180° the expected mean is $180° - 0{\cdot}8\sigma$, taking all angles ≤ 180 and integrating this one-sided distribution. In this case $\sigma = 2°$ (from least squares, probably underestimated), expected mean therefore 178·4° which is not significantly different from the mean value found, 177·4°. The sample standard deviation of the distribution around 177·4° is only 1·2° and the distribution is clearly skew, showing that the real mean is much closer to 180°.

The tetrachlorozincate ions are regular tetrahedra, the distances differing by an average of only one standard deviation from the mean and the angles by 1·5° (4 e.s.d.'s). The bond lengths and angles are in good agreement with the results of other recent studies of Zn complexes (Freeman, Marzilli & Maxwell, 1970; Gainsford, House & Robinson, 1971; Irland, House & Robinson, 1970; Wiesner, Srivastava, Kennard, Di Vaira & Lingafelter, 1967).

Table 5. *Shortest intermolecular contacts*

Cl(4) –C(9)	3·420 (23)	x	y	z
Cl(4) –C(7)	3·455 (27)	$1-x$	$1-y$	$1-z$
Cl(3) –C(14)	3·521 (29)	$1-x$	$1-y$	$-z$
Cl(5) –C(12)	3·465 (30)	$1-x$	$1-y$	$-z$
Cl(5) –C(5)	3·465 (26)	$-1+x$	y	z
Cl(6) –C(21)	3·466 (21)	x	$1+y$	z
Cl(7) –C(18)	3·491 (32)	x	$1+y$	z
C(20)–C(9)	3·295 (30)	$1-x$	$1-y$	$1-z$

All short intermolecular distances correspond to those expected for van der Waals forces; the shortest are collected in Table 5. Fig. 2 shows how the acetonitrile groups radiating from different Ni atoms weave together to leave room for the anions.

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