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The Crystal and Molecular Structure of Bis(sarcosinato)nickel(II) Dihydrate

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Bis-(sarcosinato)nickel(II) dihydrate, $Ni(CH_3NHCH_2COO)_2.2H_2O$, is triclinic with $a=5{\cdot}35$ (1), $b=6{\cdot}63$ (1), $c=8{\cdot}31$ (2) Å, $\alpha=103{\cdot}6$ (3), $\beta=95{\cdot}4$ (3), $\gamma=99{\cdot}3$ (3)°, $Z=1$. Three-dimensional photographic intensities (Cu $K\alpha$ radiation) were estimated visually. The structure was solved from a Patterson synthesis and refined by the full-matrix least-squares method with anisotropic temperature factors for the atoms. Hydrogen atoms were ignored. The final R is 0·103 for 875 reflexions or 0·092 if 111 unobserved reflexions are excluded. The molecule is centrosymmetric. The chelation around nickel is octahedral. One oxygen from the carboxyl group and the nitrogen atom from each sarcosinato residue are bonded to nickel in a plane while the oxygen atoms of the two water molecules occupy the other two sites. The Ni–N(1), Ni–O(1) and Ni–O(W) distances are 1·989 (9), 1·880 (8) and 2·236 (8) Å respectively. The dimensions of the sarcosinato residue are normal.

Experimental

The nickel(II) complex of sarcosine was prepared by heating nickel carbonate with an aqueous solution of sarcosine in stoichiometric ratio. The resultant solution was evaporated slowly and blue tabular crystals of the complex obtained. The crystals were mostly twins, but single crystals could be obtained by very slow evaporation. On application of pressure the single crystals also tend to become twins.

Rotation and Weissenberg photographs about **a**, **b** and **c** (λ for Cu $K\alpha=1{\cdot}542$ Å) showed that the crystals are triclinic with $a=5{\cdot}35$ (1), $b=6{\cdot}63$ (1), $c=8{\cdot}31$ Å, $\alpha=103{\cdot}6$ (3), $\beta=95{\cdot}4$ (3), $\gamma=99{\cdot}3$ (3)°. The density measured by flotation was 1·69, while that calculated for one molecule of $Ni(C_6H_{12}N_2O_4).2H_2O$ per unit cell is also 1·69 g cm^{-3}.$\mu=27{\cdot}1$ cm^{-1}.

Since the crystals formed twins on application of pressure it was difficult to shape them to a suitable size. The crystal employed for collecting hkl data ($k=0$ to 5) was elongated along **b** and had a cross section of 0·3 × 0·4 mm. The multiple-film equi-inclination Weissenberg technique was employed with Cu $K\alpha$ radiation. Zero and higher-layer Weissenberg photographs were taken about **a** and **c** also, but the crystals used were not of suitable size, and these intensities suffered from irregular absorption. However the extra spots in the $0kl$ and $0k\bar{l}$ zones, not convered by the b-axis photographs, were included in the data.

Intensities were estimated by visual comparison with a calibrated strip and corrected for Lorentz and polarization effects. The intensities of the extended spots on the upper half of the higher-layer Weissenberg photographs as well as those of a few extended spots on the contracted side and near the central line, were multiplied by the factor $1+\Delta$, where Δ is the spot-size correction for a particular set of ϱ and ξ values (Phillips, 1954, 1956). The correction factor applied to the contracted spots on the lower half of the films was $1-0{\cdot}4\Delta$ (Singh, 1967). The intensities on each layer were separately placed on an absolute scale by Wilson's (1942) method. The space group was shown to be $P\bar{1}$ by an E-statistics test on the three-dimensional data (Hauptman & Karle, 1953) as well as an $N(z)$ test (Howells, Phillips & Rogers, 1950) on the $h0l$ reflexions.

Determination and refinement of the structure

A point-atom-sharpened Patterson synthesis revealed the structure completely. The R value at this stage was 0·28.

Refinement was carried out by the method of least squares using a modified version of the *ORFLS* program of Busing, Martin & Levy (1962) adapted to a 32K core memory CDC 3600 computer at the Tata Institute of Fundamental Research, Bombay. The function minimized in the program was $\sum w(F_o-F_c)^2$, where $w=1/\sigma^2$ and σ is the standard deviation of an intensity: for $F_o<1{\cdot}5$, $\sigma=0{\cdot}30\ F_o$, for $1{\cdot}5 \langle F_o \rangle 3{\cdot}5$ and $F_o>30{\cdot}0$, $\sigma=0{\cdot}15\ F_o$, for the rest $\sigma=0{\cdot}075\ F_o$. This estimate does not include absorption effects, for which no correction was applied. The scattering factors for C, N, O and Ni were taken from *International Tables for X-ray Crystallography* (1962). The scattering factor of Ni was corrected for anomalous dispersion.

Four cycles of full-matrix refinement with isotropic temperature factors and three with anisotropic reduced R to 0·100. A difference Fourier synthesis calculated at this stage showed no special features, indicating that the structure is correct. The hydrogen atoms, however, could not be located. After two more cycles of anisotropic refinement the final R was 0·092 for 764 observed reflexions or 0·103 if 111 unobserved reflex-

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ions were included, the unobserved reflexions being assigned half the minimum observable intensity.

The final positional and thermal parameters with their standard deviations are given in Table 1. The observed and calculated structure factors are given in Table 2. A drawing of the molecule is shown in Fig. 1.

Discussion

(*a*) *Molecular characteristics*

The bond lengths and angles are given in Table 3 and in Fig. 2. The main features of the structure of the nickel complex of sarcosine are similar to those of the transition-metal complexes of other amino acids. The Ni atom is octahedrally coordinated. The nitrogen atom and one oxygen atom from the carboxyl group of each of the centrosymmetrically related ligands are bonded to nickel and form almost a square planar configuration, the O(1)–Ni–N(1) angle being 90·5 (3)°. The Ni–O(1) and Ni–N(1) distances are 1·880 (6) and 2·046 (7) Å respectively. The Ni–O(1) distance is the shortest so far reported for transition-metal amino-acid chelates.

The oxygen of the two water molecules completes the coordination with Ni–O(*W*) = 2·263 (6) Å. The Ni–O(*W*) bond makes an angle of 86° 15′ with the plane of the coordination square, while the O(*W*)–Ni–O(1) and O(*W*)–Ni–N(1) angles are 91·5 (2) and 86·5 (3)° respectively.

The carboxyl group is substantially planar. The equation of the least-squares plane passing through the atoms C(2), C(1), O(1) and O(2) is

$$0{\cdot}6189X' + 0{\cdot}7222Y' - 0{\cdot}3088Z' = 0{\cdot}1995$$

where X', Y', Z' are coordinates in Å referred to a set of orthogonal axes given by

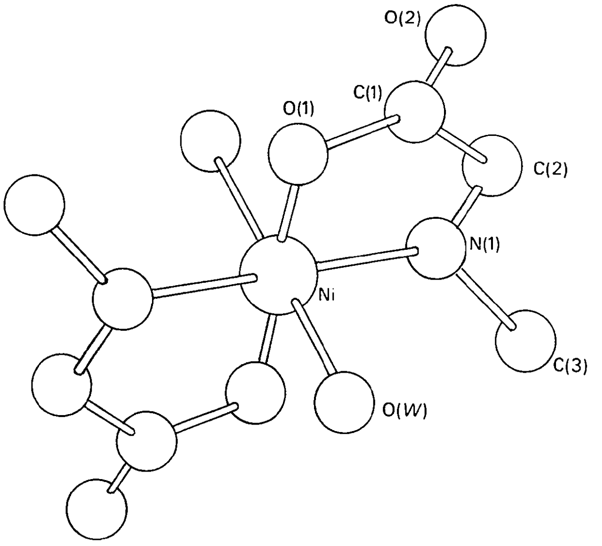

Fig. 1. A drawing of bis(sarcosinato)nickel(II) dihydrate.

Table 1. *Positional coordinates and anisotropic temperature factors with estimated standard deviations*

Anisotropic temperature factors are in the form $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+\beta_{12}hk+\beta_{13}hl+\beta_{23}kl)]$ and are multiplied by 10^4.

	x/a	y/b	z/c	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ni	0·0000	0·0000	0·0000	479 (10)	269 (10)	124 (3)	186 (8)	20 (4)	2 (4)
O(1)	−0·1857 (10)	0·2229 (8)	0·0329 (7)	253 (21)	168 (23)	210 (10)	146 (18)	0 (11)	60 (11)
C(1)	−0·1213 (13)	0·3488 (11)	0·1786 (8)	380 (29)	118 (27)	134 (10)	148 (22)	−28 (14)	45 (12)
O(2)	−0·2291 (12)	0·4908 (9)	0·2382 (7)	327 (24)	466 (30)	124 (9)	192 (23)	29 (11)	38 (13)
C(2)	0·0811 (14)	0·3015 (12)	0·2988 (10)	519 (30)	599 (33)	196 (12)	336 (24)	−18 (13)	79 (14)
N(1)	0·2157 (14)	0·1311 (12)	0·2275 (9)	437 (28)	351 (26)	135 (10)	243 (21)	67 (12)	60 (12)
C(3)	0·2739 (16)	0·0169 (13)	0·3548 (10)	640 (32)	293 (32)	251 (12)	182 (24)	−13 (14)	18 (14)
O(*W*)	0·3025 (11)	0·1842 (9)	−0·1074 (7)	484 (24)	244 (23)	127 (9)	247 (18)	31 (11)	55 (10)

Table 2. *Observed and calculated structure factors*

Within each group the columns, reading from left to right, contain the values *l*, 10F_o and 10F_c. Unobserved reflexions are omitted.

h = 0, k = 0		
1	47	50
3	251	218
4	240	240
5	146	154
6	66	71
7	47	50
8	70	78
9	75	64
h = 1, k = 0		
0	451	437
1	320	337
2	386	388
3	272	284
4	251	224
5	173	196
6	120	114
7	71	66
8	41	41
9	32	34
h = −1, k = 0		
1	153	−154
2	144	−147
3	127	120
4	238	214
5	120	108
6	150	130
7	110	100
8	39	36
9	29	26
h = 2, k = 0		
0	170	−153
1	55	61
2	362	241
3	162	149
4	51	44
5	77	71
6	157	162
7	113	119
8	30	27
9	15	16
h = −2, k = 0		
1	72	71
2	240	218
3	164	154
4	131	117
5	82	71
6	92	89
7	82	71
h = 3, k = 0		
0	51	45
1	49	42
2	110	105
3	97	92
4	27	−35
5	32	−25
6	58	65
7	55	60
8	31	35
h = −3, k = 0		
1	96	107
2	136	157
3	82	93
4	54	55
5	47	52
6	26	28
7	45	41
8	42	46
h = 4, k = 0		
0	117	111
1	36	35
2	63	70
3	85	75
4	46	38
5	28	21
h = −4, k = 0		
1	73	80
3	64	64
4	109	116
5	82	78
h = 5, k = 0		
0	53	52
1	50	44
2	47	41
3	39	36
4	62	55
5	41	46
h = −5, k = 0		
1	63	65
2	45	40
3	61	65
4	89	86
h = 6, k = 0		
1	32	29
2	39	32
h = −6, k = 0		
1	35	42
h = 0, k = 1		
0	269	281
1	32	29
2	382	353
3	395	363
4	79	76
5	57	52
6	52	45
8	40	35
9	47	45
−1	425	434
−2	512	505
−3	129	133
−4	68	71
−5	182	179
−6	212	192
−7	238	194
−8	89	87
−9	70	60
−10	42	38
h = 1, k = 1		
0	79	87
1	86	−96
2	336	319
3	369	337
4	226	216
5	146	138
6	67	70
7	61	65
8	44	42
−1	619	634
−2	475	503
−3	118	104
−4	201	187
−5	203	238
−6	216	206
−7	79	82
−9	45	28
−10	79	26
h = −1, k = 1		
0	231	218
1	295	252
5	85	89
6	89	100
7	30	32
8	53	51
9	90	85
−1	82	86
−2	261	236
−3	282	282
−4	230	212
−5	39	24
−7	99	97
−8	119	111
−9	50	48
h = 2, k = 1		
0	232	210
1	202	218
2	110	109
3	54	62
4	160	166
5	130	142
6	95	86
7	62	62
8	40	44
−1	313	338
−2	312	277
−3	99	101
−4	128	133
−5	81	90
−7	39	41
−8	38	42
h = −2, k = 1		
1	108	111
2	102	101
3	77	79
4	181	164
5	172	161
6	117	105
7	70	76
8	56	50
9	67	45
−1	30	−26
−3	295	214
−4	300	283
−5	38	42
−6	26	−20
−7	60	59
−8	52	54
h = 3, k = 1		
0	179	157
1	215	234
2	80	81
4	36	47
5	93	91
6	51	60
8	26	21
−3	48	52
−4	36	34
−7	52	53
−8	66	64
h = −3, k = 1		
0	135	147
1	102	99
2	278	263
3	308	289
4	120	125
5	42	43
6	85	86
7	82	87
8	52	48
−1	122	124
−3	62	59
−4	76	86
−5	54	62
−6	60	65
−7	36	33
h = 4, k = 1		
1	99	91
2	53	50
5	41	43
−1	25	−22
−3	39	41
−4	38	41
−5	56	59
−6	65	56
h = −4, k = 1		
0	196	179
1	123	117
2	138	131
3	167	153
4	35	39
6	60	59
7	82	76
8	37	39
−1	170	160
−2	122	126
−3	67	72
−4	28	26
−5	52	57
−6	63	60
h = −5, k = 1		
0	79	77
1	76	81
4	43	40
5	50	47
6	45	41
−1	52	49
−2	60	65
−3	72	76
−4	63	59
−5	50	46
h = −6, k = 1		
0	31	32
1	51	38
4	32	28
h = 0, k = 2		
0	99	113
1	65	71
2	130	118
3	179	166
4	143	146
5	78	87
7	43	38
8	58	66
9	26	25
−1	54	−57
−2	54	−49
−3	97	92
−4	156	175
−5	278	245
−6	146	137
−7	43	40
−8	69	73
−9	62	70
h = 1, k = 2		
0	39	−38
1	160	145
2	182	184
4	46	47
5	80	87
6	50	54
7	52	55
8	44	41
−1	92	88
−2	347	375
−3	461	474
−4	260	225
−5	81	75
−6	91	106
−7	85	92
−8	54	50
−9	26	34
−10	37	30
h = −1, k = 2		
0	358	324
1	313	294
2	108	116
3	162	159
4	151	160
5	42	48
6	43	47
7	79	74
8	82	78
9	50	45
−1	220	214
−2	43	47
−3	180	−170
−4	41	46
−5	230	205
−6	31	40
−8	58	64
−9	80	82
−10	66	68
h = 2, k = 2		
0	115	104
1	299	263
2	179	194
3	72	80
4	38	55
5	31	27
6	30	39
−1	152	160
−3	225	242
−4	60	69
−6	61	68
−7	91	97
−8	57	61
−9	33	36
−10	25	30
h = −2, k = 2		
0	145	138
1	301	276
2	210	235
3	38	32
4	80	82
5	181	164
6	171	157
7	91	96
8	37	41
−1	320	301
−2	298	279
−3	109	106
−4	151	143
−5	101	109
−6	36	39
h = 3, k = 2		
0	131	126
1	98	94
2	98	79
3	130	136
4	109	105
5	44	39
−1	105	91
−2	103	98
−3	50	58
−4	33	39
−5	69	73
−6	72	61
−7	33	36
−8	32	38
−9	25	30
h = −3, k = 2		
0	91	100
1	210	196
2	300	277
3	107	104
4	80	71
5	170	153
6	141	130
7	34	27
−1	158	161
−2	105	165
−3	200	193
−4	154	141
−5	79	89
−6	102	108
−7	87	92
−8	27	31
h = 4, k = 2		
0	60	60
3	43	47
4	60	64
−1	74	66
−3	27	23
−4	42	39
−5	39	41
h = −4, k = 2		
0	180	181
1	90	97
2	77	70
3	91	98
4	56	54
5	45	59
−1	146	140
−2	85	87
−3	70	63
−4	51	60
−5	60	69
−6	70	63
−7	70	74
h = −5, k = 2		
0	78	65
1	36	−30
2	36	−32
3	51	44
4	42	48
−1	120	113
−2	50	57
−4	48	51
−5	33	37
h = −6, k = 2		
1	26	26
3	41	36
4	37	32
5	22	19
−1	27	20
h = 0, k = 3		
0	59	68
2	120	113
3	154	170
4	79	90
5	120	102
6	151	115
7	67	72
−1	87	94
−2	170	165
−3	133	144
−5	90	98
−6	186	178
−7	63	57
−8	34	−26
−10	38	33
h = 1, k = 3		
0	132	119
1	60	53
2	52	60
6	59	56
−1	162	174
−2	79	73
−3	80	81
−4	88	90
−5	45	46
−6	61	72
−7	49	45
−9	42	40
−10	40	48
h = −1, k = 3		
0	332	295
1	345	316
2	161	154
3	230	212
4	200	211
5	106	115
6	70	64
7	29	27
−1	111	125
−2	188	177
−3	92	83
−5	104	106
−6	159	144
−7	104	106
−8	47	49
h = 2, k = 3		
0	173	151
1	159	157
2	42	30
3	29	25
4	40	41
−1	50	56
−3	99	60
−4	144	156
−5	102	95
−6	40	37
−7	61	65
−8	72	75
−9	47	49
h = −2, k = 3		
0	390	371
1	340	318
2	54	62
3	42	41
4	190	184
5	101	105
7	28	25
8	56	52
−1	331	315
−2	261	237
−3	176	186
−4	170	161
−5	70	67
−6	41	35
−7	74	70
−8	93	84
−9	59	60
h = 3, k = 3		
1	75	83
2	60	53
3	59	54
4	30	35
5	29	28
−1	27	31
−2	45	51
−3	105	112
−4	126	134
−5	81	87
−6	30	36
−7	32	33
−8	29	35
−9	21	20
h = −3, k = 3		
0	63	70
1	60	41
2	64	60
3	49	60
4	98	96
5	80	86
6	30	35
7	46	38
8	43	39
−1	155	152
−2	165	160
−3	168	181
−4	170	161
−5	101	105
−6	76	71
−7	50	40
−8	59	54
−9	49	48
h = −4, k = 3		
0	61	−63
1	23	26
2	141	133
3	108	109
4	26	21
5	13	10
6	38	37
7	32	34
−2	93	87
−3	71	70
−5	76	68
−6	72	78
−7	51	42
−8	42	40
h = −5, k = 3		
1	73	70
3	84	87
5	34	39
6	28	27
−1	19	16
−2	62	59
−5	14	11
h = −6, k = 3		
0	51	44
1	54	48
2	29	26
−1	38	35
−2	15	11
−3	17	18
h = 0, k = 4		
0	160	166
1	52	60
2	120	109
3	135	130
4	85	81
5	87	78
6	65	57
7	31	38
−1	187	196
−2	192	206
−3	260	260
−4	132	124
−5	29	23
−6	24	21
−7	50	46
−8	42	44
−9	22	17
h = 1, k = 4		
0	96	102
1	129	114
2	125	111
3	37	41
4	50	55
5	75	69
6	35	32
−1	30	27
−2	61	60
−3	65	71
−4	27	30
−5	44	47
−7	70	80
−8	53	57
−9	16	18
h = −1, k = 4		
0	102	115
1	53	58
2	151	131
3	262	241
4	140	129
5	28	23
6	42	38
−1	151	174
−2	191	205
−3	153	141
−4	192	180
−5	199	190
−6	130	113
−7	73	68
−8	53	50
−9	42	37
h = 2, k = 4		
1	29	37
2	25	20
3	33	28
4	52	46
5	30	38
−1	30	32
−2	32	29
−4	23	24
−5	56	59
−6	65	56
−7	46	53
−8	27	32
−9	15	12
h = −2, k = 4		
1	138	144
2	160	147
3	136	117
4	37	55
7	50	40
−1	162	157
−2	107	100
−3	72	75
−4	116	131
−5	121	107
−6	83	88
−7	83	80
−8	70	61
−9	78	71
h = 3, k = 4		
0	42	39
3	18	15
4	18	14
−1	75	71
−2	62	57
−3	44	36
−4	46	41
−5	69	76
−6	44	49
h = −3, k = 4		
0	98	107
1	98	106
2	52	49
3	37	31
5	49	36
6	67	59
7	46	40
−1	30	28
−2	33	30
−3	152	165
−4	138	120
−6	28	21
−7	38	30
−8	21	25
h = −4, k = 4		
0	48	46
1	98	88
2	39	35
3	28	32
4	52	55
5	80	85
6	79	72
7	27	31
−1	58	−59
−2	15	−14
−3	99	97
−4	73	70
−5	35	39
−6	35	36
−7	17	17
h = −5, k = 4		
0	97	88
1	90	91
2	56	62
3	77	81
4	76	70
5	25	26
−1	46	53
−2	27	31
−5	50	44
−6	52	49
h = −6, k = 4		
0	72	66
1	40	37
2	29	32
3	35	38
−1	109	101
−2	81	78
−3	15	17
h = 0, k = 5		
0	114	117
1	135	125
2	121	126
3	42	44
4	18	−14
5	25	22
6	39	40
−1	121	112
−2	142	147
−3	141	158
−4	98	88
−5	66	61
−6	62	56
−7	38	32
−8	43	40
−9	45	42
h = 1, k = 5		
0	79	74
1	111	106
2	110	113
3	74	68
4	55	49
−1	67	73
−2	49	44
−3	56	59
−4	80	88
−5	55	59
−6	35	29
−7	27	26
−8	42	41
−9	36	40
h = −1, k = 5		
0	41	36
1	68	78
2	58	50
3	34	26
5	48	40
6	50	65
−1	46	42
−2	151	143
−3	145	156
−4	130	121
−5	123	137
−6	99	90
−7	43	47
−8	27	20
−9	14	10
h = 2, k = 5		
0	22	18
1	36	32
2	30	25
3	51	45
−1	29	21
−2	47	41
−3	45	60
−4	63	58
−5	137	123
h = −2, k = 5		
0	69	60
1	70	70
2	49	45
3	37	44
4	68	64
5	59	53
−1	55	61
−2	30	−20
−3	49	−55
−4	34	31
−5	93	89
−6	85	81
−7	61	62
−9	17	18
h = −3, k = 5		
0	150	163
1	40	40
2	34	29
3	37	34
4	54	50
5	40	41
6	22	21
−1	[illegible]	168
−3	45	44
−4	22	21
−5	29	27
−6	17	19
−7	25	23
−8	26	31
h = −4, k = 5		
0	91	94
1	29	33
2	52	46
3	66	67
4	51	51
5	59	65
−1	[illegible]	[illegible]
−2	115	105
−3	85	91
−4	50	44
−5	17	19
−6	21	22
−7	29	24
h = −5, k = 5		
0	25	23
1	49	55
2	88	81
3	71	76
4	47	42
−1	47	42
−2	85	96
−3	81	97
−4	51	49
−5	27	23
h = −6, k = 5		
0	35	32
−1	35	37
−2	42	39
h = 0, k = 6		
0	89	97
1	48	52
2	18	15
4	16	16
5	54	49
−1	47	52
−2	12	14
−3	52	57
−4	26	29
−5	41	37
−6	66	60
−7	58	59
h = 0, k = 7		
2	30	31
3	32	38
−3	23	25

$$X' = X + Y\cos\gamma + Z\cos\beta$$

$$Y' = Y\sin\gamma + Z\left(\frac{\cos\alpha - \cos\beta\,.\,\cos\gamma}{\sin\gamma}\right)$$

$$Z' = Z(\sin^2\gamma - \cos^2\alpha - \cos^2\beta + 2\cos\alpha\,.\,\cos\beta\,.\,\cos\gamma)^{1/2}/\sin\gamma\,.$$

The deviations from this plane of the atoms O(1), O(2), C(1), C(2), N(1), C(3) and Ni are −0·041, 0·004, 0·041, −0·023, 0·038, 0·105 and 0·833 Å respectively.

The dimensions of the sarcosinato residue do not differ significantly from those of other metal–amino acid complexes. The only exception is the angle C(1)–C(2)–N(1), whose value [115·7 (7)°] is somewhat high. As a result, the distance N(1)–O(1) [2·790 (9) Å] differs from the average value of 2·66 (1) Å found in other metal–amino acid complexes (Freeman, 1967). No great significance, however, can be attached to this deviation due to the presence of absorption errors in the data.

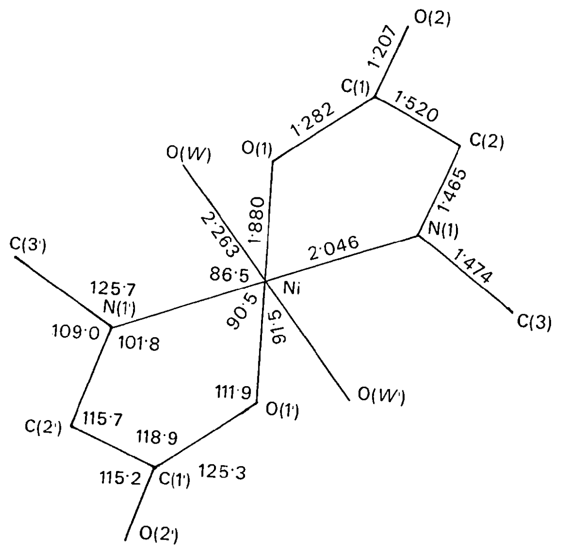

Fig. 2. Dimensions of the molecule.

(*b*) *Intermolecular characteristics*

The packing of the molecules is shown in Fig. 3. Three hydrogen atoms, two from the water molecule and one from the nitrogen atom, are available for hydrogen-bond formation. From Table 3 it can be seen that O(*W*) has five close neighbours, of which two are N(1) atoms of the two centrosymmetric parts of the molecule. The O(*W*)···acceptor–C angles are also reasonably near the tetrahedral value. Without a knowledge of the positions of the hydrogen atoms it is not possible to ascertain which three of the five sites are involved in hydrogen-bond formation.

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Table 3. *Bond distances and angles with their estimated standard deviations*

Ni—O(1)	1·880 (6) Å	N(1)—C(3)	1·474 (12) Å
Ni—N(1)	2·046 (7)	O(1)—N(1)	2·790 (9)
Ni—O(*W*)	2·263 (6)	N(1)—O(1^i)	2·767 (9)
O(1)–C(1)	1·282 (10)	O(*W*)–O(1)	2·979 (9)
O(2)–C(1)	1·207 (9)	O(W^i)–O(1)	2·904 (9)
C(1)–C(2)	1·520 (11)	O(*W*)–N(1)	2·958 (10)
C(2)–N(1)	1·465 (11)	O(W^i)–N(1)	3·141 (9)
O(1)—Ni—N(1)	90·5 (3)°	O(1)—Ni—O(*W*)	91·5 (2)°
N(1)—Ni—O(*W*)	86·5 (3)	Ni—O(1)–C(1)	111·9 (5)
Ni—N(1)–C(2)	101·8 (5)	Ni—N(1)–C(3)	125·2 (5)
O(1)—C(1)–O(2)	125·3 (7)	O(1)—C(1)–C(2)	118·9 (6)
O(2)—C(1)–C(2)	115·2 (7)	C(1)—C(2)–N(1)	115·7 (7)
O(2)—N(1)–C(3)	109·0 (7)	O(1)—N(1)–Ni	42·4 (2)
N(1)—O(1)–Ni	47·2 (2)	N(1)—O(1)–C(1)	64·9 (4)
O(1)—N(1)–C(2)	60·0 (4)	O(1)—N(1)–C(3)	142·9 (6)
N(1)—O(1^i)–Ni	47·7 (2)	N(1)—O(1^i)–C(1^i)	159·2 (5)
O(1^i)—N(1)–C(2)	143·9 (6)	O(1^i)—N(1)–C(3)	92·8 (5)
O(*W*)–O(1)–Ni	49·4 (2)	O(*W*)–O(1)–C(1)	105·0 (4)
O(W^i)–O(1)–Ni	51·2 (2)	O(W^i)–O(1)–C(1)	102·6 (4)
O(*W*)–N(1)–Ni	49·8 (2)	O(*W*)–N(1)–C(2)	105·4 (6)
O(*W*)–N(1)–C(3)	145·2 (4)	O(W^i)–N(1)–Ni	46·0 (2)
O(W^i)–N(1)–C(2)	91·0 (5)	O(W^i)–N(1)–C(3)	88·7 (5)
Intermolecular distance and angle			
O(W^{ii})–O(2)	2·692 (11) Å	O(W^{ii})–O(2)–C(1)	125·8 (5)°

Symmetry code:

i	$-x,\ -y,\ -z$
ii	$-x,\ 1-y,\ -z$

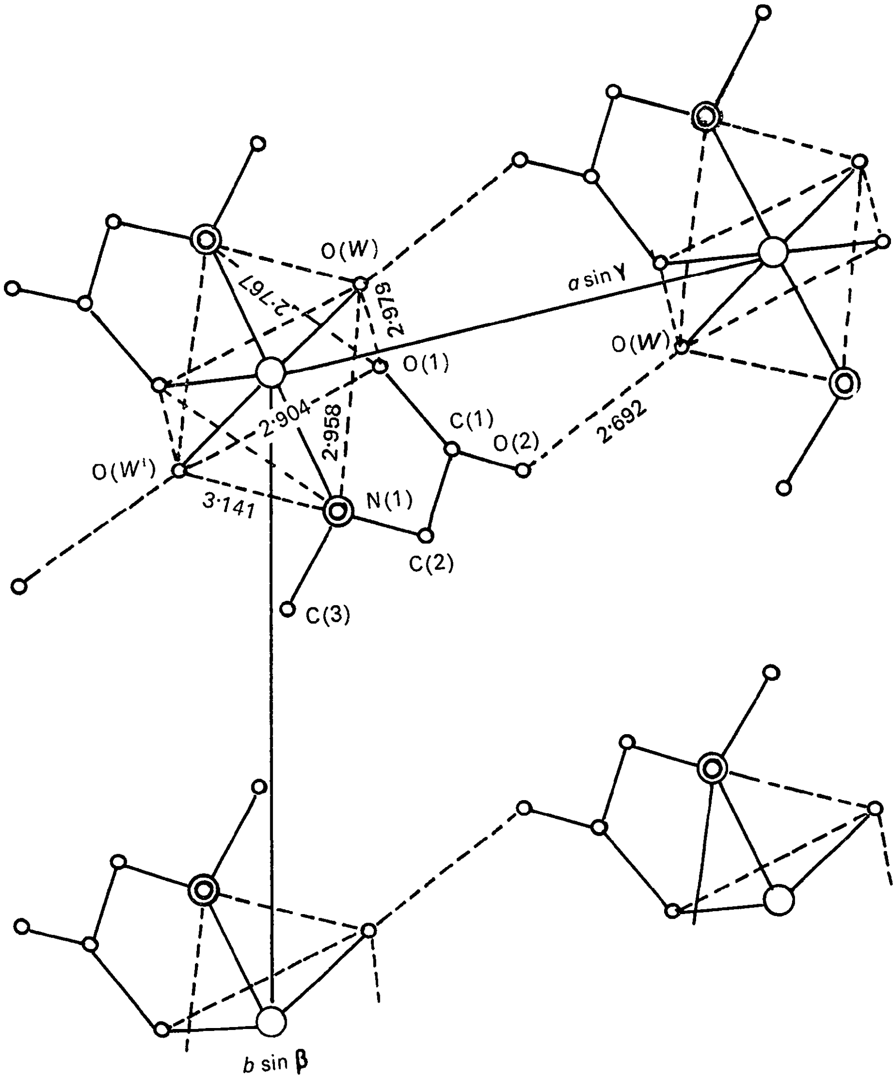

Fig. 3. Packing of the molecule in projection down **c**.

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