The H positions calculated for $MnSO_4.4H_2O$ deviate on the average by as much as 0·2 Å from the corresponding neutron-diffraction values given by Bauer (1964) for $MgSO_4.4H_2O$, which is isostructural with $MnSO_4.4H_2O$. The n.m.r. vectors given for $MgS_2O_3.6H_2O$ appear to disagree with the hydrogen-bonding scheme suggested by the X-ray investigators (Nardelli, Fava & Giraldi, 1962). Both these compounds have been reexamined in this laboratory. The resonance component lines for $MnSO_4.4H_2O$ appear to be rather wide providing no room for improvement over the measurements made by Rao. However, the n.m.r. results for $MgS_2O_3.6H_2O$ appear to be in excellent agreement with the predictions of Nardelli *et al.* (1962).

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Refinement of the structure of diaquobisglycinatonickel(II), $Ni(NH_2CH_2COO)_2(OH_2)_2$.

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The structure of diaquobisglycinatonickel(II), determined by Stosick (*J. Amer. Chem. Soc.* (1945) **67**, 365) from three projections, has been refined with use of three-dimensional data. The metal–donor bond-lengths are Ni–N(amino) 2·08 Å, Ni–O(carboxyl) 2·06 Å, Ni–O(water) 2·10 Å, and the angle N(amino)–Ni–O(carboxyl) is 81·1°.

The structure of diaquobisglycinatonickel(II) was determined by Stosick (1945) from three incompletely resolved projections. In order to obtain accurate values of bond lengths and angles for subsequent comparison with the dimensions of nickel–peptide complexes, the structure has been reinvestigated with three-dimensional data.

The cell data are shown in Table 1. The unit-cell dimensions were determined from 104 values of θ between 58° and 81°, measured on $h0l$ and $hk0$ Weissenberg photographs calibrated with aluminum powder lines. The cell parameters were refined in ten cycles of non-linear least-squares as functions of $\sin^2\theta$. The density was determined by flotation.

Table 1. *Crystal data*

$C_4H_{12}O_6N_2Ni$ F.W. 242·7

Monoclinic. $a=7{\cdot}625(5)$, $b=6{\cdot}596(5)$, $c=9{\cdot}670(5)$ Å, $\beta=116{\cdot}57(1)°$, $U=435{\cdot}0$ Å^3. $D_m=1{\cdot}86$, $D_x=1{\cdot}85$ g.cm^{-3}, $Z=2$. λ(Cu $K\alpha_1$) = 1·5405 Å, λ(Cu $K\alpha_2$) = 1·5443 Å, a(Al) = 4·04925 Å, $\mu=34$ cm^{-1}. Space group $P2_1/c$ from systematic absences ($0k0$ absent for $k=2n+1$, $h0l$ absent for $l=2n+1$).

Two overlapping sets of data, *h0l* through *h5l* and *hk0* through *hk8*, were recorded with the same crystal specimen. Cu *Kα* radiation was used. The intensities were measured visually on Weissenberg photographs, by comparison with a series of calibrated spots. The number of independent reflexions was 967, of which 74 were unobservably weak. The data were correlated by the least-squares method of Rae (1965). Lorentz, polarization and Tunell factors, but not absorption corrections, were applied.

A modified version of the program *ORFLS* (Busing, Martin & Levy, 1962) was used for the full-matrix least-squares refinement. The function minimized was $\Sigma w||F_o|-|F_c||^2$. The weights w were given by the function $w=0{\cdot}632/[1+((F_o-15)/12)^2]$, derived from a plot of $||F_o|-|F_c||$ *versus* $|F_o|$. The atomic scattering factors of Cromer & Waber (1965) for C, N, O and Ni^{2+} were used. The values for Ni^{2+} were corrected for the real part of the anomalous scattering by subtracting 3·1 electrons over the entire sin θ range (*International Tables for X-ray Crystallography*, 1962). In the fifth cycle of refinement with anisotropic temperature factors for all atoms, no parameter shifted by more than 0·02 e.s.d. The final residual was $R=0{\cdot}095$. The positions of the hydrogen atoms could not be inferred with certainty from a difference Fourier synthesis computed after the refinement converged.

The final positional and thermal parameters are shown in Table 2, the observed and calculated structure amplitudes in Table 3, and the interatomic distances and bond angles

Table 2. *Final positional parameters* ($\times 10^4$), *and coefficients* B_{ij} ($\times 10^4$) *in the expression* $\exp -\{B_{11}h^2+B_{22}k^2+B_{33}l^2+2B_{23}kl+2B_{13}hl+2B_{12}hk\}$, (*all with their standard deviations in parentheses*)

	x/a	*y/b*	*z/c*	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ni	0	0	0	44 (2)	54 (3)	33 (2)	1 (2)	26 (2)	−3 (2)
N	2766 (7)	0413 (7)	0123 (6)	74 (10)	57 (11)	60 (6)	3 (7)	43 (7)	−10 (6)
C(1)	3249 (9)	2575 (10)	0378 (8)	64 (11)	85 (13)	76 (9)	−19 (10)	47 (8)	−26 (9)
C(2)	2278 (8)	3553 (9)	1280 (6)	65 (11)	73 (12)	33 (7)	0 (10)	21 (7)	−8 (8)
O(1)	0698 (6)	2736 (7)	1158 (5)	92 (9)	83 (9)	67 (6)	−17 (8)	55 (6)	−26 (6)
O(2)	3065 (7)	5096 (7)	2078 (6)	123 (10)	123 (11)	87 (7)	−26 (9)	37 (7)	−42 (8)
O(3)	1305 (6)	−1438 (7)	2166 (5)	83 (9)	96 (10)	54 (6)	17 (7)	38 (6)	15 (6)

Table 3. *Observed and calculated structure amplitudes* (× 10)

H	K	L	FO	FC
0	2	0	315	334
0	4	0	475	484
0	6	0	275	232
0	8	0	209	214
0	1	1	410	520
0	2	1	357	358
0	3	1	501	530
0	4	1	186	-183
0	5	1	166	161
0	6	1	76	-71
0	7	1	148	147
0	8	1	17	8
0	0	2	348	374
0	1	2	350	-387
0	2	2	260	253
0	3	2	216	199
0	4	2	417	411
0	5	2	77	-68
0	6	2	45	28
0	7	2	60	55
0	8	2	54	57
0	2	3	53	-24
0	3	3	440	487
0	4	3	73	-52
0	5	3	302	295
0	6	3	87	66
0	7	3	152	131
0	8	3	49	-45
0	0	4	414	471
0	1	4	260	-252
0	2	4	515	585
0	3	4	49	6
0	4	4	271	265
0	5	4	59	-38
0	6	4	205	185
0	7	4*	8	-4
0	1	5	358	395
0	2	5	26	-16
0	3	5	34	31
0	4	5*	9	5
0	5	5	153	144
0	6	5*	10	-17
0	7	5	96	102
0	0	6	277	281
0	1	6	199	185
0	2	6	313	317
0	3	6	42	34
0	4	6	210	210
0	5	6	124	-108
0	6	6	122	116
0	7	6*	5	10
0	1	7	239	247
0	2	7	107	-90
0	3	7	337	390
0	4	7*	10	2
0	5	7	187	180
0	6	7*	11	-30
0	0	8	280	287
0	1	8	89	-84
0	2	8	129	121
0	3	8	42	-31
0	4	8	111	116
0	5	8*	7	8
0	1	9	158	152
0	2	9	27	22
0	3	9	117	119
0	4	9	28	-20
0	0	10	190	195
0	1	10	79	-65
0	2	10	149	157
0	3	10	41	29
1	1	0	289	-335
-1	1	0	302	335
1	2	0	103	110
-1	2	0	106	110
1	3	0	135	111
-1	3	0	135	-111
1	4	0	202	198
-1	4	0	189	198
1	5	0	152	-156
-1	5	0	150	156
1	6	0	193	172
-1	6	0	181	172
1	7	0*	10	12
-1	7	0*	10	-12
1	8	0	109	118
-1	8	0	112	118
1	1	1	421	592
-1	1	1	204	209
1	2	1	272	267
-1	2	1	154	151
1	3	1	457	523
-1	3	1	175	205
1	4	1	262	-261
-1	4	1	117	106
1	5	1	260	283
-1	5	1	81	76

H	K	L	FO	FC
1	6	1	80	-78
-1	6	1	79	83
1	7	1	181	191
-1	7	1	157	161
1	8	1	35	-36
-1	8	1	47	52
1	0	2	317	-291
1	1	2	381	-438
-1	1	2	259	195
1	2	2	448	513
-1	2	2	397	421
1	3	2	66	44
-1	3	2	189	212
1	4	2	298	291
-1	4	2	397	393
1	5	2	153	-152
-1	5	2	24	15
1	6	2	139	134
-1	6	2	224	219
1	7	2*	10	-15
-1	7	2	51	52
1	8	2	34	27
-1	8	2	137	149
1	1	3	224	231
-1	1	3	294	308
1	2	3	262	-235
-1	2	3	182	187
1	3	3	35	-11
-1	3	3	517	574
1	4	3	36	-22
-1	4	3	21	-21
1	5	3	173	193
-1	5	3	273	280
1	6	3	77	73
-1	6	3	75	63
1	7	3	84	82
-1	7	3	82	67
-1	8	3	18	20
1	0	4	297	259
-1	0	4	55	46
1	1	4	100	68
-1	1	4	229	-222
1	2	4	442	492
-1	2	4	285	282
1	3	4	55	-30
-1	3	4	41	-3
1	4	4	62	28
-1	4	4	149	127
1	5	4	112	-87
-1	5	4	242	234
1	6	4	266	276
-1	6	4	113	107
1	7	4	45	-41
-1	7	4	34	31
-1	8	4	52	66
1	1	5	281	272
-1	1	5	455	530
1	2	5	40	-18
-1	2	5	104	74
1	3	5	249	213
-1	3	5	79	64
1	4	5	55	-58
-1	4	5	101	100
1	5	5	218	225
-1	5	5	248	214
1	6	5	112	-95
-1	6	5	53	54
1	7	5	74	72
-1	7	5	156	154
1	0	6	40	19
-1	0	6	359	369
1	1	6	153	133
-1	1	6	251	259
1	2	6	152	133
-1	2	6	343	392
1	3	6	115	-100
-1	3	6	23	-15
1	4	6	68	64
-1	4	6	301	283
1	5	6*	9	-2
-1	5	6	49	34
1	6	6	107	99
-1	6	6	166	151
-1	7	6*	7	-6
1	1	7	99	78
-1	1	7	182	177
1	2	7	67	-48
-1	2	7*	12	7
1	3	7	190	201
-1	3	7	187	194
1	4	7*	9	6
-1	4	7	104	93
1	5	7	98	99
-1	5	7	137	131
1	6	7	33	-29
-1	6	7*	12	-0
1	0	8	256	240

H	K	L	FO	FC
-1	0	8	224	228
1	1	8	71	-64
-1	1	8	113	98
1	2	8	137	127
-1	2	8	96	83
1	3	8	97	-88
-1	3	8*	12	3
1	4	8	123	120
-1	4	8	201	225
1	5	8	53	50
-1	5	8	88	73
-1	6	8*	8	18
1	1	9	116	119
-1	1	9	215	208
1	2	9	56	43
-1	2	9	69	-69
1	3	9*	8	18
-1	3	9	227	239
1	4	9	42	-43
-1	4	9	84	76
-1	5	9	97	101
1	0	10	21	-4
1	1	10	35	21
-1	1	10	33	-33
1	2	10	52	64
-1	2	10	64	60
-1	3	10	67	56
-1	4	10	102	100
-1	1	11	80	81
-1	2	11	106	106
2	0	0	142	-97
2	1	0	163	110
2	2	0	30	58
2	3	0	116	107
2	4	0	230	222
-2	4	0	206	222
2	5	0	84	-69
-2	5	0	89	69
2	6	0	92	87
2	7	0*	10	-0
2	8	0	57	68
2	1	1	60	72
-2	1	1	449	589
2	2	1	80	65
-2	2	1	162	-186
2	3	1	207	208
-2	3	1	214	225
2	4	1*	7	13
-2	4	1	44	44
2	5	1	167	161
-2	5	1	188	184
2	6	1	98	104
-2	6	1	65	48
2	7	1	97	97
-2	7	1	255	292
2	8	1	16	-7
-2	8	1	42	-37
2	0	2	163	152
-2	0	2	421	529
2	1	2	111	-47
-2	1	2	48	62
2	2	2	469	512
-2	2	2	189	203
2	3	2	29	13
-2	3	2	222	188
2	4	2	283	257
-2	4	2	207	192
2	5	2	68	58
-2	5	2	238	-251
2	6	2	214	214
-2	6	2	228	226
2	7	2*	9	1
-2	7	2	18	14
2	8	2	66	111
-2	8	2	124	136
2	1	3	267	263
-2	1	3	260	-200
2	2	3	141	-129
-2	2	3	157	125
2	3	3	91	79
-2	3	3	274	270
2	4	3	95	70
-2	4	3	117	-97
2	5	3	197	198
-2	5	3	129	123
2	6	3	56	59
-2	6	3	58	42
2	7	3	100	94
-2	7	3*	9	24
-2	8	3	34	-33
2	0	4	188	171
-2	0	4	75	-85
2	1	4	261	249
-2	1	4	325	-298
2	2	4	108	100
-2	2	4	425	426
2	3	4	37	-20

H	K	L	FO	FC
-2	3	4	96	83
2	4	4	62	-40
-2	4	4	132	110
2	5	4	75	71
-2	5	4	49	36
2	6	4	138	150
-2	6	4	218	228
2	7	4*	6	-10
-2	7	4	34	35
-2	8	4	65	81
2	1	5	170	149
-2	1	5	362	372
2	2	5	130	108
-2	2	5	36	-35
2	3	5	288	261
-2	3	5	227	205
2	4	5	54	39
-2	4	5	50	-30
2	5	5	181	184
-2	5	5	290	277
2	6	5	59	-52
-2	6	5*	11	22
-2	7	5	121	112
2	0	6	229	197
-2	0	6	21	-11
2	1	6	45	33
-2	1	6	55	46
2	2	6	136	129
-2	2	6	263	258
2	3	6	101	-98
-2	3	6	88	-76
2	4	6	235	248
-2	4	6	60	-54
2	5	6	130	123
-2	5	6	94	82
2	6	6	67	59
-2	6	6	188	194
-2	7	6	40	-31
2	1	7	102	91
-2	1	7	161	158
2	2	7*	11	-9
-2	2	7	120	121
2	3	7	66	59
-2	3	7	48	22
2	4	7	70	63
-2	4	7	41	24
2	5	7	28	33
-2	5	7	145	139
-2	6	7	65	-54
-2	7	7	73	89
2	0	8	171	180
-2	0	8	76	45
2	1	8	34	-3
-2	1	8	179	165
2	2	8	24	24
-2	2	8	237	237
2	3	8	45	39
-2	3	8	96	-84
2	4	8	117	134
-2	4	8	233	259
-2	5	8	61	46
-2	6	8	94	87
2	1	9	138	141
-2	1	9	124	111
2	2	9	44	28
-2	2	9	133	-125
-2	3	9	135	135
-2	4	9	83	74
-2	5	9	91	87
-2	0	10	177	183
-2	1	10	62	46
-2	2	10	26	-1
-2	3	10*	10	5
-2	4	10	38	44
-2	1	11	93	88
-2	2	11	41	33
-2	3	11	98	111
3	0	0	484	577
3	1	0	75	47
3	2	0	398	411
3	3	0	245	225
3	4	0	476	531
3	5	0	131	-112
-3	5	0	142	112
3	6	0	131	102
3	7	0	62	59
3	8	0	78	114
3	1	1	184	178
-3	1	1	472	581
3	2	1	110	-97
-3	2	1	218	-225
3	3	1	309	329
-3	3	1	279	281
3	4	1	77	57
-3	4	1	42	-37
3	5	1	172	164
-3	5	1	172	144

H	K	L	FC	FC
3	6	1	145	144
-3	6	1	74	-64
3	7	1	31	30
-3	7	1	216	240
-3	8	1	39	-50
3	0	2	362	407
-3	0	2	552	655
3	1	2	135	-120
-3	1	2	58	-58
3	2	2	267	267
-3	2	2	114	-78
3	3	2	116	99
-3	3	2	42	25
3	4	2	102	77
-3	4	2	275	274
3	5	2	92	82
-3	5	2	174	-160
3	6	2	142	148
-3	6	2	36	33
3	7	2	67	64
-3	7	2*	10	-14
-3	8	2	97	107
3	1	3	422	464
-3	1	3	390	449
3	2	3	96	80
-3	2	3	77	66
3	3	3	269	270
-3	3	3	397	377
3	4	3	54	29
-3	4	3	139	-130
3	5	3	223	239
-3	5	3	177	164
3	6	3*	6	-3
-3	6	3*	11	-5
3	7	3	96	105
-3	7	3	177	178
-3	8	3	48	-58
3	0	4	278	298
-3	0	4	425	445
3	1	4	95	74
-3	1	4	226	-227
3	2	4	249	240
-3	2	4	389	440
3	3	4*	10	6
-3	3	4	162	145
3	4	4	184	182
-3	4	4	408	401
3	5	4	23	17
-3	5	4	250	-257
3	6	4	112	112
-3	6	4	179	152
-3	7	4*	8	4
3	1	5	132	126
-3	1	5	143	140
3	2	5	82	71
-3	2	5	179	-172
3	3	5	167	177
-3	3	5	260	266
3	4	5	49	40
-3	4	5	91	-82
3	5	5	88	85
-3	5	5	173	171
3	6	5	14	-13
-3	6	5	53	42
-3	7	5*	8	10
3	0	6	242	216
-3	0	6	258	285
3	1	6	76	-57
-3	1	6	215	-206
3	2	6	161	172
-3	2	6	273	291
3	3	6*	10	5
-3	3	6	41	-3
3	4	6	215	246
-3	4	6	35	-26
3	5	6	71	58
-3	5	6	41	-20
-3	6	6	192	199
-3	7	6*	7	-3
3	1	7	233	241
-3	1	7	335	380
3	2	7	44	-42
-3	2	7	95	85
3	3	7	121	118
-3	3	7	202	186
3	4	7	32	28
-3	4	7	106	-97
-3	5	7	214	219
-3	6	7	122	-117
-3	7	7	100	109
3	0	8	142	151
-3	0	8	79	46
3	1	8*	8	6
-3	1	8	47	37
3	2	8	75	77
-3	2	8	216	243
3	3	8	73	93

H	K	L	FO	FC
-3	3	8	77	-72
-3	4	8	176	175
-3	5	8	66	-54
-3	6	8	50	92
-3	1	9	111	99
-3	2	9	62	-48
-3	3	9	114	114
-3	4	9*	9	-1
-3	5	9	78	68
-3	0	10	156	154
-3	1	10	57	-40
-3	2	10	145	137
-3	3	10	46	-33
-3	4	10	155	156
-3	1	11	172	162
-3	2	11	71	-63
-3	3	11	88	88
-3	0	12	83	94
4	0	0	319	290
4	1	0	225	-215
4	2	0	382	421
4	3	0	168	146
4	4	0	248	240
4	5	0	158	-139
-4	5	0	150	139
4	6	0	171	156
4	7	0	52	46
4	1	1	371	409
-4	1	1	201	204
4	2	1	113	-106
-4	2	1	77	-55
4	3	1	384	380
-4	3	1	275	284
4	4	1	78	-69
-4	4	1	116	108
4	5	1	252	258
-4	5	1	124	110
4	6	1	39	25
-4	6	1	25	-14
4	7	1	64	56
-4	7	1	68	71
4	0	2	255	229
-4	0	2	630	762
4	1	2	155	-136
-4	1	2	55	44
4	2	2	303	319
-4	2	2	265	267
4	3	2	48	-36
-4	3	2	126	-110
4	4	2	47	-28
-4	4	2	327	337
4	5	2*	9	-7
-4	5	2	197	209
4	6	2	184	195
-4	6	2	141	136
4	7	2	22	-28
-4	7	2*	8	-7
4	1	3	263	250
-4	1	3	552	665
4	2	3	117	108
-4	2	3	154	144
4	3	3	107	83
-4	3	3	321	316
4	4	3	69	-54
-4	4	3	41	-28
4	5	3	137	140
-4	5	3	189	173
4	6	3	89	-85
-4	6	3	18	-15
-4	7	3	247	250
4	0	4	143	118
-4	0	4	268	282
4	1	4	70	59
-4	1	4	118	92
4	2	4	349	323
-4	2	4	221	210
4	3	4	78	-72
-4	3	4	133	118
4	4	4	225	228
-4	4	4	341	353
4	5	4	33	-26
-4	5	4	95	-86
4	6	4	93	107
-4	6	4	24	24
-4	7	4*	7	11
4	1	5	186	179
-4	1	5	274	277
4	2	5	99	-89
-4	2	5	79	-60
4	3	5	161	155
-4	3	5	321	342
4	4	5*	8	-7
-4	4	5	42	43
4	5	5	102	100
-4	5	5	182	177
-4	6	5	123	118
-4	7	5	51	47

H	K	L	FO	FC
4	0	6	124	116
-4	0	6	454	510
4	1	6*	9	3
-4	1	6	86	-72
4	2	6	96	88
-4	2	6	409	433
4	3	6	37	-24
-4	3	6	39	10
4	4	6	65	72
-4	4	6	244	228
-4	5	6	42	33
-4	6	6	185	188
-4	7	6*	6	0
4	1	7	135	146
-4	1	7	314	344
4	2	7	39	-36
-4	2	7	31	-14
4	3	7	67	100
-4	3	7	196	186
-4	4	7	18	12
-4	5	7	184	186
-4	6	7*	12	-7
-4	0	8	296	294
-4	1	8	120	116
-4	2	8	169	174
-4	3	8	22	-19
-4	4	8	111	106
-4	5	8	42	31
-4	6	8	86	89
-4	1	9	237	225
-4	2	9	72	64
-4	3	9	265	274
-4	4	9*	9	5
-4	5	9	155	151
-4	0	10	240	242
-4	1	10	57	-47
-4	2	10	149	154
-4	3	10	68	-56
-4	4	10	246	270
-4	5	10	57	50
-4	1	11	189	181
-4	2	11	46	-38
-4	3	11	75	77
-4	0	12	183	205
-4	2	12	64	82
5	0	0	96	-60
5	1	0	183	-162
5	2	0	192	188
5	3	0	75	-62
5	4	0	36	19
5	5	0	52	48
5	6	0	122	126
5	7	0	27	-35
5	1	1	224	221
-5	1	1	137	122
5	2	1*	11	-10
-5	2	1	60	-31
5	3	1	76	96
-5	3	1	311	344
5	4	1	41	-23
-5	4	1	136	119
5	5	1	147	155
-5	5	1	192	192
5	6	1	25	-15
-5	6	1	30	30
-5	7	1	43	44
5	0	2	157	146
-5	0	2	359	396
5	1	2	92	80
-5	1	2	62	-63
5	2	2	273	267
-5	2	2	250	240
5	3	2	120	-104
-5	3	2	75	-62
5	4	2	118	104
-5	4	2	174	163
5	5	2	36	23
-5	5	2	144	153
5	6	2	135	164
-5	6	2	202	204
-5	7	2	25	19
5	1	3	125	107
-5	1	3	168	180
5	2	3	23	18
-5	2	3	118	103
5	3	3	46	37
-5	3	3	89	83
5	4	3*	9	-11
-5	4	3	26	15
5	5	3	99	102
-5	5	3	64	42
-5	6	3*	9	7
-5	7	3	133	157
5	0	4*	10	3
-5	0	4	200	176
5	1	4	126	116
-5	1	4*	8	11

H	K	L	FO	FC
5	2	4	70	60
-5	2	4	168	175
5	3	4	77	-68
-5	3	4	149	137
5	4	4	135	148
-5	4	4	181	167
5	5	4	19	25
-5	5	4*	9	14
-5	6	4	118	121
-5	7	4	60	64
5	1	5	113	111
-5	1	5	298	294
5	2	5	108	-109
-5	2	5	129	115
5	3	5	135	135
-5	3	5	296	284
5	4	5	36	40
-5	4	5	25	-3
-5	5	5	202	204
-5	6	5	66	68
-5	7	5	128	132
5	0	6	178	203
-5	0	6	63	-52
5	1	6	30	16
-5	1	6	84	-60
5	2	6	22	11
-5	2	6	307	316
-5	3	6	84	58
-5	4	6	164	147
-5	5	6	50	45
-5	6	6	139	134
-5	1	7	190	186
-5	2	7	90	-73
-5	3	7	61	37
-5	4	7	100	102
-5	5	7	136	139
-5	6	7	126	121
-5	0	8	256	246
-5	1	8	161	173
-5	2	8	269	275
-5	3	8*	12	0
-5	4	8	40	30
-5	5	8	59	59
-5	6	8	206	208
-5	1	9	165	152
-5	2	9	93	69
-5	3	9	222	208
-5	4	9	53	40
-5	5	9	163	168
-5	0	10	103	103
-5	1	10	107	83
-5	2	10	103	90
-5	3	10	75	-59
-5	4	10	124	129
-5	1	11	132	123
-5	2	11*	9	6
-5	3	11	123	129
-5	0	12	180	209
6	0	0	173	157
6	1	0	111	-107
6	2	0	203	-280
6	3	0*	11	-6
6	4	0	172	167
6	5	0	100	99
6	6	0	82	94
6	1	1	174	169
-6	1	1	167	162
6	2	1	29	25
-6	2	1	93	-73
6	3	1	56	-38
-6	3	1	249	249
6	4	1	59	51
-6	4	1*	10	-3
6	5	1	75	78
-6	5	1	154	156
-6	6	1	52	-53
6	0	2	129	120
-6	0	2	187	171
6	1	2	139	131
-6	1	2*	11	-8
6	2	2	121	112
-6	2	2	32	15
6	3	2	55	43
-6	3	2	87	-79
6	4	2	142	141
-6	4	2	146	150
6	5	2*	5	-1
-6	5	2	32	-21
-6	6	2	50	50
6	1	3	131	129
-6	1	3	155	133
6	2	3	23	-23
-6	2	3	102	-84
6	3	3	164	186
-6	3	3	195	175
6	4	3	63	53
-6	4	3*	11	0

H	K	L	FO	FC
-6	5	3	88	79
-6	6	3*	7	0
6	0	4	143	148
-6	0	4	436	506
6	1	4*	7	9
-6	1	4	129	-111
6	2	4	31	29
-6	2	4	121	97
6	3	4	23	16
-6	3	4	55	43
-6	4	4	180	183
-6	5	4	83	-82
6	1	5	43	55
-6	1	5	132	109
-6	2	5	159	141
-6	3	5	164	143
-6	4	5	124	-136
-6	5	5	98	91
-6	6	5	53	-54
-6	0	6	96	-87
-6	1	6	198	-200
-6	2	6	144	146
-6	3	6	93	93
-6	4	6	165	142
-6	5	6	75	-69
-6	6	6	48	47
-6	1	7	210	220
-6	2	7	104	-76
-6	3	7	127	100
-6	4	7	34	-18
-6	5	7	169	158
-6	6	7	41	37
-6	0	8	101	75
-6	1	8	52	-32
-6	2	8	227	235
-6	3	8	34	16
-6	4	8	36	27
-6	5	8	81	-68
-6	1	9	101	89
-6	2	9*	11	-5
-6	3	9	29	27
-6	4	9*	8	2
-6	5	9	85	96
-6	0	10	64	50
-6	1	10	99	92
-6	2	10	132	134
-6	3	10	23	-11
-6	4	10	62	61
-6	1	11	71	96
-6	2	11	51	-36
-6	3	11	151	178
-6	0	12	82	108
-6	1	12	52	-52
7	0	0	190	181
7	1	0	58	-90
7	2	0	236	271
7	3	0	74	41
7	4	0	109	105
7	5	0	18	-14
7	1	1	218	-240
-7	1	1	181	185
7	2	1	25	-5
-7	2	1	20	13
7	3	1	123	117
-7	3	1	98	97
7	4	1	20	10
-7	4	1*	8	-11
-7	5	1	90	93
7	0	2	94	91
-7	0	2	166	137
7	1	2	80	74
-7	1	2	153	150
7	2	2	136	141
-7	2	2	206	211
7	3	2	29	28
-7	3	2	107	-98
-7	4	2	192	228
-7	5	2	36	33
7	1	3	85	87
-7	1	3	261	273
7	2	3	18	-19
-7	2	3	161	-155
-7	3	3	260	278
-7	4	3	55	52
-7	5	3	138	136
-7	0	4	436	473
-7	1	4	62	44
-7	2	4	69	55
-7	3	4	85	-79
-7	4	4	142	144
-7	5	4*	7	-8
-7	1	5	177	146
-7	2	5	75	70
-7	3	5	197	197
-7	4	5	76	-67
-7	5	5	66	66
-7	6	5*	2	-41

H	K	L	FC	FC
-7	0	6	321	320
-7	1	6	90	-68
-7	2	6	192	183
-7	3	6	26	21
-7	4	6	238	257
-7	5	6	57	-49
-7	1	7	213	202
-7	2	7	20	-2
-7	3	7	218	213
-7	4	7	80	-73
-7	5	7	141	140
-7	0	8	125	119
-7	1	8	130	-110
-7	2	8	162	154
-7	3	8	39	-28
-7	4	8	115	115
-7	1	9	235	249
-7	2	9	25	-22
-7	3	9	54	47
-7	0	10	185	171
-7	1	10	106	87
-7	2	10	167	164
-7	3	10*	7	-15
-7	1	11	77	75
-7	2	11	62	-58
8	0	0	76	83
8	1	0	74	69
8	2	0	129	143
8	3	0	41	-37
8	1	1	94	110
-8	1	1	179	176
8	2	1*	4	1
-8	2	1	102	99
-8	3	1	76	69
-8	0	2	58	43
-8	1	2	89	69
-8	2	2	256	279
-8	3	2*	9	9
-8	4	2	133	150
-8	1	3	150	146
-8	2	3	50	-48
-8	3	3	120	129
-8	4	3	88	79
-8	0	4	167	185
-8	1	4	77	58
-8	2	4	137	134
-8	3	4*	10	-12
-8	4	4	96	98
-8	1	5	230	244
-8	2	5*	10	8
-8	3	5	181	176
-8	4	5	54	50
-8	0	6	244	255
-8	1	6	72	59
-8	2	6	167	174
-8	3	6	75	59
-8	4	6	101	111
-8	1	7	93	86
-8	2	7	84	66
-8	3	7	188	201
-8	4	7*	6	8
-8	0	8	144	128
-8	1	8	79	-62
-8	2	8	226	230
-8	3	8*	8	-9
-8	4	8	89	100
-8	1	9	236	247
-8	2	9	25	21
-8	3	9	86	90
-8	0	10	101	105
-8	1	10	95	97
-8	2	10	151	165
-9	0	2	44	51
-9	1	2*	7	-1
-9	2	2	53	64
-9	1	3	35	38
-9	2	3	43	38
-9	0	4	100	87
-9	1	4	45	-48
-9	2	4	87	91
-9	1	5	120	131
-9	2	5	46	-39
-9	3	5	43	44
-9	0	6	104	117
-9	1	6*	8	8
-9	2	6*	7	19
-9	3	6	96	100
-9	1	7	76	64
-9	2	7	48	41
-9	3	7	142	141
-9	0	8	63	54
-9	1	8	90	-83
-9	2	8	142	153
-9	1	9	49	58

Table 4. *Distances and angles in diaquobisglycinatonickel*(II)

Code for superscripts:

	Atom at				Atom at		
(none)	x,	y,	z	v	$1-x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$
′	$-x$,	$-y$,	$-z$	vi	$-x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$
″	x,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$	vii	x,	$-1+y$,	z
‴	$-x$,	$-\frac{1}{2}+y$,	$\frac{1}{2}-z$	viii	$1-x$,	$-\frac{1}{2}+y$,	$\frac{1}{2}-z$
iv	x,	$1+y$,	z	ix	x,	$\frac{1}{2}-y$,	$-\frac{1}{2}+z$

(*a*) Bond-lengths
(E.s.d.'s = 0·01 Å)

Ni —N	2·08 Å
Ni —O(1)	2·06
Ni —O(3)	2·10
N—C(1)	1·47
C(1)–C(2)	1·52
C(2)–O(1)	1·28
C(2)–O(2)	1·26

(*b*) Bond angles
(E.s.d.'s in parentheses)

N—Ni —O(1)	81·1 (5)°
N—Ni —O(3)	89·2 (5)
O(1)–Ni —O(3)	87·8 (5)
Ni —N—C(1)	108·1 (5)
N—C(1)–C(2)	111·1 (6)
C(1)–C(2)–O(1)	116·8 (7)
C(1)–C(2)–O(2)	118·4 (7)
O(1)–C(2)–O(2)	124·8 (9)
C(2)–O(1)–Ni	115·0 (6)

(*c*) Hydrogen-bonds and closest non-bonded contact
(E.s.d.'s = 0·01 Å)

O(1)$\cdots$H–O(3$^{\mathrm{vi}}$)	O(3)–H$\cdots$O(1‴)	2·73 Å
O(2)$\cdots$H–O(3$^{\mathrm{iv}}$)	O(3)–H$\cdots$O(2$^{\mathrm{vii}}$)	2·67
O(2)$\cdots$H–N″	N—H$\cdots$O(2$^{\mathrm{ix}}$)	3·07
O(2)$\cdots\cdots$N$^{\mathrm{v}}$	N $\cdots\cdots$O(2$^{\mathrm{viii}}$)	3·31

(*d*) Bond angles at hydrogen-bonded atoms

Ni —N$\cdots\cdots$O(2$^{\mathrm{ix}}$)	116·1°	C(2) —O(2)$\cdots$O(3$^{\mathrm{iv}}$)	127·2°
C(1)–N$\cdots\cdots$O(2$^{\mathrm{ix}}$)	98·4	N″ $\cdots\cdots$O(2)$\cdots$O(3$^{\mathrm{iv}}$)	79·0
Ni —O(1)$\cdots$O(3$^{\mathrm{vi}}$)	114·8	Ni—O(3)$\cdots$O(1$^{\mathrm{iii}}$)	122·7
C(2)–O(1)$\cdots$O(3$^{\mathrm{vi}}$)	128·0	Ni—O(3)$\cdots$O(2$^{\mathrm{vii}}$)	112·0
C(2)–O(2)$\cdots$N″	106·3	O(1‴)$\cdots$O(3)$\cdots$O(2$^{\mathrm{vii}}$)	105·7

in Table 4. The oxygen atom of the water molecule is represented by O(3). Both single and stereoscopic views of the structure have already been published elsewhere (Freeman, Guss & Sinclair, 1968; Freeman, 1967*b*).

Discussion

Comparisons of this structure with those of glycine (Marsh, 1958) and bisglycinatocopper(II) hydrate (Freeman, Snow, Nitta & Tomita, 1964) show that the dimensions of the amino acid are not significantly changed by chelation. Because the metal–ligand bond-lengths in the Ni(II) complex are 0·08 Å longer, the N(amino)–metal–O(carboxyl) angles in the chelate rings are 4° smaller than in the Cu(II) complex. The degree of 'puckering' of the glycinatonickel(II) chelate rings is among the highest recorded for α-amino acid complexes (Freeman, 1967*a*). The Ni and N(amino) atoms lie at 0·26 and 0·61 Å from the plane of the carboxyl group, respectively [compared with deviations of 0·006, −0·103 Å and 0·126, 0·162 Å in the crystallographically independent chelate rings in bisglycinatocopper(II) hydrate]. The only respect in which our description of the structure differs from Stosick's is that we do not identify the vector from the N(amino) atom to O(2$^{\mathrm{viii}}$) as a potential hydrogen bond. The atoms are 3·13 Å apart and the interatomic vector makes unacceptable angles with the bonds at the N(amino) atom.

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