present model, the latter is always the ground level. Moreover, the coefficients of the free-ion orbitals in the two sets of e orbitals differ from those for the octahedral e_g and $t_{2g}\pm$ orbitals, a result which is also a feature of the D_{3d} distorted model but which has previously been neglected.[5,6]

The energy levels calculated for the explicit set of bond angles found for the $Ti(OC(NH_2)_2)_6^{3+}$ ion, *i.e.*, with the 5.6° "twist" away from an octahedron, are in terms of Dq: a_1, $-4Dq$; e(1), $-3.95Dq$; e(2), $5.95Dq$; or with $Dq = 1700$ cm^{-1}: a_1, -6800 cm^{-1}; e(1), -6720 cm^{-1}; e(2), 10,120 cm^{-1}. The ground state for this geometry is therefore $^2A_1$, a result which at first sight is at variance with the single-crystal polarization measurements.[26] There is then a small splitting ~100 cm^{-1} of the t_{2g} set, but this, together with the change in "composition" of the e(1) orbitals, is sufficient to cause a marked change in magnetic properties from those calculated for the $^2T_{2g}$ term. A more complete discussion of the influence of this type of distortion for configurations other than d^1 and on the magnetic properties of this and other trigonally distorted molecules will be discussed in detail elsewhere.[19]

(26) R. Dingle, *J. Chem. Phys.*, **50**, 545 (1969).

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The Crystal and Molecular Structure of Ethanolatotetra-μ-thiobenzoato-dinickel(II), $[Ni(C_6H_5COS)_2]_2C_2H_5OH$

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A three-dimensional crystal structure analysis using 2483 counter-diffractometric measurements has been carried out for ethanolatotetra-μ-thiobenzoato-dinickel(II), $[Ni(C_6H_5COS)_2]_2C_2H_5OH$. The cell constants were $a = 10.44$ (2) Å, $b = 11.66$ (2) Å, $c = 12.69$ (2) Å, $\alpha = 91°\ 1'$, $\beta = 92°\ 55'$, $\gamma = 93°\ 0'$ (all ±5'), $d_m = 1.54$, $d_c = 1.535$ g/cm^3, space group $P\bar{1}$, and $Z = 2$. R, after least-squares refinement with individual isotropic thermal parameters, is 0.053. The two nickel atoms in the complex are bridged by the four thiobenzoate residues so that one metal atom is surrounded by four sulfur atoms in a square-planar fashion and the other by four oxygen atoms in a similar manner. The two planes are twisted about the Ni–Ni axis by some 23° from an eclipsed configuration. The fifth coordination site of the second nickel atom is occupied by the oxygen atom of the ethanol moiety. The Ni–S distances, 2.221–2.230 (5) Å, are characteristic of square-planar, low-spin complexes while the Ni–O distances, 2.010–2.058 (7) Å, are compatible with those found in high-spin complexes. It is concluded that the observed magnetic moment of the dimer, 2.40 BM/nickel(II) ion, arises from the presence of two unpaired electron spins on the nickel ion of C_{4v} symmetry and that, despite a Ni–Ni separation of only 2.503 (4) Å, the metal–metal interaction is probably quite weak. In the crystal the molecules are held together by weak axial Ni–S interactions, 2.814 (5) Å, between the dimers so as to form centrosymmetric tetramers. These are further linked together by weak O–H···O hydrogen bonds of length 2.86 Å involving the ethanol hydroxyl group as donor to an in-plane oxygen of a neighboring molecule.

Introduction

As part of a study of reactions between sulfur donor ligands and transition metal ions[1] we have synthesized nickel(II) compounds of the general formula $Ni(RCOS)_2 \cdot 0.5C_2H_5OH$, where R is CH_3, C_2H_5, or C_6H_5. These complexes show temperature-independent magnetic moments in the range 2.3–2.4 BM/nickel(II) ion. Measurement of the molecular weights of the compounds in chloroform solution suggests the presence of binuclear species. To establish the structure of these molecules a single-crystal X-ray diffraction study of the thiobenzoate complex, R = C_6H_5, has been carried out.

Measurement of Crystal and Intensity Data

Recrystallization of the complex from anhydrous ethanol gave fragile purple-red prisms with the bounding faces (100), (010), and (001) developed. The lattice parameters, measured at room temperature, were derived from 25° precession photographs taken with Zr-filtered Mo Kα radiation (λ 0.7107 Å) and are $a = 10.44$ Å, $b = 11.66$ Å, $c = 12.69$ Å, $\alpha = 91°\ 1'$, $\beta = 92°\ 55'$, and $\gamma = 93°\ 0'$. The errors in the cell edges may be taken as the 1 part in 600 commonly associated with the precession method and imposed by uncertainty in the centering of the crystal. In the measured angles the error is ±5'. The unit cell volume is 1540 Å^3 and the calculated density on the assumption of two dimeric units of formula $Ni_2C_{26}H_{30}O_5S_4$ per unit cell is 1.535 g/cm^3, in agreement with the value of 1.54 ± 0.01 g/cm^3 measured by pycnometry of an ethyl iodide–benzene mixture. $F(000) = 732$.

The possible triclinic space groups are P1 and $P\bar{1}$. No tests were made for pyroelectric or piezoelectric effects but with $Z = 2$ the centrosymmetric space group was chosen as the more likely, a choice justified by the outcome of the analysis. This space group requires no symmetry within the dimeric units but the association of these dimers into tetramers in the

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(1) G. A. Melson, N. P. Crawford, and B. J. Geddes, *Inorg. Chem.*, **9**, 1123 (1970).

crystal by virtue of the weak Ni–S interactions found leads to a crystallographic center of symmetry being imposed on the larger unit.

Diffraction data were collected from a single-crystal plate measuring 0.1 × 0.2 × 0.5 mm parallel to *a*, *b*, and *c*, respectively. Because of their fragility the crystals could not be cut to a more uniform shape. The crystal was mounted so as to have the reciprocal c^* axis horizontal at $\chi = 90°$ on a Picker four-circle diffractometer operated during the measurement of intensity data under the control of an SDS Sigma 2 computer. For the complex the absorption coefficient for Mo Kα radiation is 13 cm^{-1}. No absorption corrections were made though these could have been substantial for some orientations of the crystal. A study of the final agreement between the observed structure amplitudes and calculated structure factors, however, shows no indication of any serious systematic error arising from this source despite the fact that only isotropic thermal parameters have been used. Neglect of the corrections is not expected to have introduced any significant error in the positional parameters found.

Intensity data were collected using Mo Kα radiation made monochromatic by Bragg reflection from the (002) plane of a highly oriented graphite crystal mounted in the Picker incident-beam monochromator assembly. At 46 kV and 16 mA the scattered intensity at a reciprocal lattice point using this device was about 40% of that derived from the same direct beam filtered through 0.003 in. of Zr foil.

A takeoff angle of 3° was used on the direct beam. Detection of scattered radiation was by scintillation counting with pulse height discrimination. Receiving apertures on the counter were 4 mm^2 and to reduce background the counter was placed 30 cm from the crystal. The crystal was shown to be of suitable mosaicity by ω scanning. Intensity measurements were made using the θ–2θ scanning technique with scan rate 1°/min and symmetrical 2° scans for all reflections. Background measurements were made for 10 sec at both the beginning and the end of the scan range by the stationary crystal–stationary counter method. True background was assumed to be linear between these limits. Linearity of counter response was confirmed up to the higest count rates observed during the experiment.

The overall stability of the system was checked by monitoring the intensity of the (200) and (0,10,0) reflections after every 99 measurement cycles. The average deviation from the mean intensity in each case was less than 1% and random individual deviations enabled a single scale factor to be used throughout.

Over 5600 independent reciprocal lattice points were surveyed up to $2\theta = 50°$, of which 4720 yielded intensities significantly above background as defined by the background-corrected peak count exceeding three times the square root of the total number of counts involved in the measurement.

The reflection data were weighted as follows: $\sigma(F_o^2) = Lp[TC + (P(CT))^2]^{1/2}$ where $F_o^2 = (CT)(Lp)$, $TC = C_p + 0.5(t_s/t_b)(C_{b1} + C_{b2})$, $CT = C_p - 0.5 \cdot (t_s/t_b)(C_{b1} + C_{b2})$, and C_p and C_{bi} are the counts accumulated during scan and background measurements occupying times t_s and t_b, respectively. Lp is the Lorentz–polarization factor, in this case given by $(\sin 2\theta)(1 + \cos^2 2\theta_m)/(\cos^2 2\theta + \cos^2 2\theta_m)$, $2\theta_m$ being the Bragg angle for the monochromator crystal, here 12°. P is an uncertainty factor[2] to allow for effects of a nonstatistical nature and to avoid too high a weight being given to strong reflections. A value of 0.04 was used.

This function was applied to all reflections with $|F_o|$ greater than 30 on the experimental scale (18 on the absolute scale or $\simeq$2.5% of $F(000)$). To yield an adequate yet manageable set of observations, reflections having less than this amplitude were given zero weight. The final ratio of observations to parameters was better than 18:1 with 2483 reflections having nonzero weight.

Solution and Refinement of the Structure

All calculations described were carried out using programs written in this laboratory for the 16K SDS Sigma 2 computer.

From an unsharpened three-dimensional Patterson function the coordinates of the two nickel atoms were found. Approximate positions for the remaining nonhydrogen atoms were found from two successive approximations to the three-dimensional electron-density function calculated using the heavy-atom method of phase determination. These positions when included in a structure factor calculation with an overall thermal parameter $B = 3.5$ Å^2 gave a conventional R factor of 0.13.

Refinement of the parameters was by least-squares methods using the block-diagonal approximation. Matrices of dimensions 3 × 3 were used for the positional parameters of each atom, 1 × 1 matrices were used for the isotropic thermal parameters, and a 2 × 2 matrix was used for the single scale factor and overall thermal parameter.

Atomic scattering functions for the neutral atoms were used,[3] with a correction of 0.37 e$^-$ being made to the form factor for nickel to take account of the real part of the correction for anomalous dispersion.[4]

The function minimized was $\Sigma w(|F_o| - |F_c|)^2$, w being taken as $4F_o^2/\sigma^2(F_o^2)$. Damping factors of 0.5 were applied to all parameter shifts calculated to ensure steady convergence. A total of 165 parameters were varied, three positional and one isotropic thermal parameter for each atom and a single scale factor. Convergence was complete after ten cycles with the final shifts calculated in no case exceeding 0.3σ. The discrepancy factors $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $R_2 = [\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2]^{1/2}$ were 0.058 and 0.066, respectively.

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(2) W. R. Busing and H. A. Levy, *J. Chem. Phys.*, **26**, 563 (1957).

(3) H. P. Hanson, F. Herman, J. D. Lea, and S. Skillman, *Acta Cryst.*, **17**, 1040 (1964).

(4) D. T. Cromer, *ibid.*, **18**, 17 (1965).

TABLE I

ATOMIC PARAMETERS AND THEIR STANDARD DEVIATIONS AS OBTAINED FROM THE FINAL CYCLE OF LEAST-SQUARES REFINEMENT[a]

Atom	x/a	y/b	z/c	10^2B, Å^2
Ni(1)	458 (1)	418 (1)	1433 (1)	222 (2)
Ni(2)	−704 (1)	462 (1)	3109 (1)	206 (2)
S(11)	213 (3)	2278 (2)	1199 (2)	299 (5)
S(12)	−1421 (2)	22 (2)	557 (2)	246 (4)
S(13)	653 (2)	−1459 (2)	1653 (2)	262 (4)
S(14)	2292 (2)	864 (2)	2361 (2)	266 (5)
O(21)	−1549 (6)	1895 (6)	2564 (5)	292 (13)
O(22)	−2149 (6)	−538 (5)	2421 (5)	254 (12)
O(23)	209 (6)	−963 (5)	3619 (5)	261 (12)
O(24)	738 (6)	1473 (5)	3796 (5)	260 (12)
O(1)	−1713 (6)	506 (5)	4459 (5)	255 (12)
C(1)	−1075 (9)	2559 (8)	1914 (8)	252 (17)
C(2)	−2413 (9)	−581 (8)	1460 (7)	213 (16)
C(3)	559 (9)	−1702 (8)	2970 (8)	268 (18)
C(4)	1844 (9)	1522 (8)	3488 (7)	227 (16)
C(5)	−2977 (11)	961 (10)	4425 (9)	373 (22)
C(6)	−3600 (11)	883 (10)	5456 (9)	386 (22)
C(11)	−1726 (10)	3667 (9)	1739 (9)	323 (20)
C(12)	−2894 (12)	3812 (11)	2155 (10)	441 (25)
C(13)	−3581 (15)	4780 (13)	1949 (12)	604 (33)
C(14)	−3086 (16)	5645 (15)	1339 (14)	721 (39)
C(15)	−1841 (18)	5556 (16)	979 (15)	810 (44)
C(16)	−1151 (15)	4520 (13)	1141 (13)	620 (34)
C(21)	−3689 (9)	−1105 (8)	1069 (8)	247 (17)
C(22)	−3939 (13)	−1432 (12)	33 (11)	528 (29)
C(23)	−5174 (15)	−1920 (13)	−290 (12)	613 (33)
C(24)	−6099 (13)	−2055 (12)	421 (11)	510 (28)
C(25)	−5809 (13)	−1772 (12)	1485 (11)	509 (28)
C(26)	−4633 (11)	−1270 (10)	1799 (9)	375 (22)
C(31)	938 (9)	−2840 (8)	3365 (8)	264 (18)
C(32)	1476 (12)	−3636 (11)	2678 (10)	446 (25)
C(33)	1881 (14)	−4657 (13)	3096 (12)	575 (31)
C(34)	1781 (13)	−4899 (12)	4170 (11)	505 (31)
C(35)	1236 (11)	−4083 (10)	4835 (9)	397 (23)
C(36)	806 (11)	−3082 (9)	4427 (9)	355 (21)
C(41)	2843 (9)	2168 (8)	4166 (8)	250 (17)
C(42)	3931 (10)	2707 (9)	3737 (8)	250 (17)
C(43)	4818 (11)	3380 (10)	4414 (9)	389 (22)
C(44)	4609 (12)	3463 (11)	5499 (10)	450 (25)
C(45)	3529 (11)	2913 (10)	5903 (9)	366 (22)
C(46)	2660 (10)	2267 (9)	5249 (8)	283 (18)

Coordinates of the Atoms of the Phenyl Rings Idealized to Regular Hexagons of Side 1.395 ± 0.01 Å in Their Least-Squares Mean Planes. Derivations from above in Parentheses

Atom	x/a	y/b	z/c
C(11)	−1724 (2)	3671 (4)	1764 (25)
C(12)	−2926 (32)	3801 (11)	2174 (19)
C(13)	−3588 (7)	4781 (1)	1959 (10)
C(14)	−3044 (42)	5630 (15)	1333 (6)
C(15)	−1835 (6)	5487 (69)	927 (52)
C(16)	−1160 (9)	4508 (12)	1137 (4)
C(21)	−3681 (8)	−1111 (6)	1074 (5)
C(22)	−3959 (20)	−1438 (6)	13 (20)
C(23)	−5163 (11)	−1921 (1)	−317 (27)
C(24)	−6113 (14)	−2086 (31)	414 (7)
C(25)	−5836 (27)	−1761 (11)	1465 (20)
C(26)	−4622 (11)	−1272 (2)	1809 (10)
C(31)	931 (7)	−2844 (4)	3377 (12)
C(32)	1459 (17)	−3621 (15)	2691 (13)
C(33)	1883 (2)	−4649 (8)	3082 (14)
C(34)	1780 (1)	−4898 (1)	4153 (17)
C(35)	1248 (12)	−4103 (20)	4819 (16)
C(36)	818 (12)	−3071 (11)	4444 (17)
C(41)	2854 (11)	2169 (1)	4162 (4)
C(42)	3914 (17)	2706 (1)	3722 (15)
C(43)	4813 (5)	3363 (17)	4363 (51)
C(44)	4636 (27)	3473 (10)	5442 (57)
C(45)	3567 (38)	2929 (16)	5876 (27)
C(46)	2675 (15)	2276 (9)	5234 (15)

Coordinates of the Hydrogen Atoms[b]

Atom	x/a	y/b	z/c
H(12)	−3348	3132	2664
H(13)	−4512	4894	2267
H(14)	−3543	6407	1152
H(15)	−1396	6163	426
H(16)	−223	4397	823
H(22)	−3208	−1309	−566
H(23)	−5373	−2175	−1147
H(24)	−7046	−2460	161
H(25)	−6574	−1889	2035
H(26)	−4400	−1020	2615
H(32)	1545	−3434	1850
H(33)	2302	−5275	2560
H(34)	2113	−5704	4456
H(35)	1161	−4289	5665
H(36)	408	−2457	4956
H(42)	4060	2623	2868
H(43)	5654	3789	4012
H(44)	5356	3998	5950
H(45)	3434	3020	6732
H(46)	1843	1854	5576
$\mathrm{H}(^5/_1)$	−2889	1873	4192
$\mathrm{H}(^5/_2)$	−3589	477	3812
$\mathrm{H}(^6/_1)$	−4558	1248	5364
$\mathrm{H}(^6/_2)$	−3005	1380	6055
$\mathrm{H}(^6/_3)$	−3704	−16	5676
H(1)	−1344	185	5119

[a] Coordinates are given as fractions of the cell edges × 10^4; the standard errors are given in parentheses and apply to the units column of the appropriate parameter. [b] The number denotes the carbon atom to which the hydrogen atom is attached.

A three-dimensional difference electron-density function calculated at this time showed no evidence of significant anisotropy of thermal vibration of the atoms but indicated that the structurally most important features remaining were the hydrogen atoms. These atoms were more clearly identified by the calculation of general plane difference syntheses in the planes of the four phenyl groups and in the planes appropriate to the ethanol residue. All atoms were clearly recognizable except for the hydroxyl hydrogen.

To obtain the best positions for the hydrogen atoms the phenyl rings were adjusted in their least-squares mean planes to regular hexagons 1.395 ± 0.01 Å on a side and sites were chosen on the extension of the appropriate diagonals to give C–H distances of 1.1 Å. The five identifiable hydrogen atoms of the ethanol residue were placed in positions giving a reasonable fit between the observed locations and idealized tetrahedral geometry. The sixth was placed in the plane of the heavy atoms to give a C–O–H angle of 120°. No attempt was made to refine the parameters of the hydrogen atoms.

A final structure factor calculation was performed using these hydrogen positions (thermal parameters corresponding to those of the atoms to which the hydrogens were attached), the idealized positions of the atoms of the phenyl rings, and the positions of the remaining atoms as given in the final cycle of least-squares refinement. The values of R_1 and R_2 were 0.057 and 0.078 for the 2483 reflections involved in the refinement. R_1 was 0.087 for the complete set of observed reflections. The standard deviation of an observation of unit weight was 3.4. Inspection of the agreement between observed structure amplitudes and calculated structure factors showed no signs of significant error due to extinction.

Except in the immediate vicinity of the nickel and sulfur atoms, a final difference electron-density synthesis showed no peaks higher than one-third of the maxima associated with hydrogen atoms. Around the heavier atoms the largest positive peak, 1.1 $e^-/\text{Å}^3$, occurred between the two nickel atoms. The other peaks could be interpreted as indicating a very slight anisotropy of thermal vibration of the sulfur atoms with the major principal axis of the thermal ellipsoid more or less perpendicular to the plane of the nickel and sulfur atoms in each case.

The positional and thermal parameters of the atoms as given in the final least-squares cycle are given, together with their corresponding standard errors as derived from the inverse matrices, in Table I. Also listed are the idealized positional parameters for the phenyl ring carbon atoms. The average difference in coordinate between these two sets of values is about 1.3 times the average standard deviation in coordinate or 0.017 Å. In Table II are listed the values of $10|F_o|$ and $10F_c$ as given by the final structure factor calculation.

Description of the Structure and Discussion

An overall view of the structure showing the numbering scheme adopted is shown in Figure 1. It is seen that the thiobenzoate groups act as chelating ligands to bridge the two nickel atoms one of which is surrounded, in a square-planar manner, by the four sulfur atoms, the other being surrounded by the four oxygen atoms of the acid residues. These two planes are twisted about the Ni–Ni axis by about 23° from a fully eclipsed configuration presumably to accommodate the bite of the ligand to the metal–metal separation. The oxygen-coordinated metal atom has the vacant coordination site occupied by the oxygen atom of an ethanol molecule while the other nickel atom takes part in a weak interaction with a sulfur atom of a neighboring dimeric unit so that the structural unit in the crystal is a centrosymmetric tetramer.

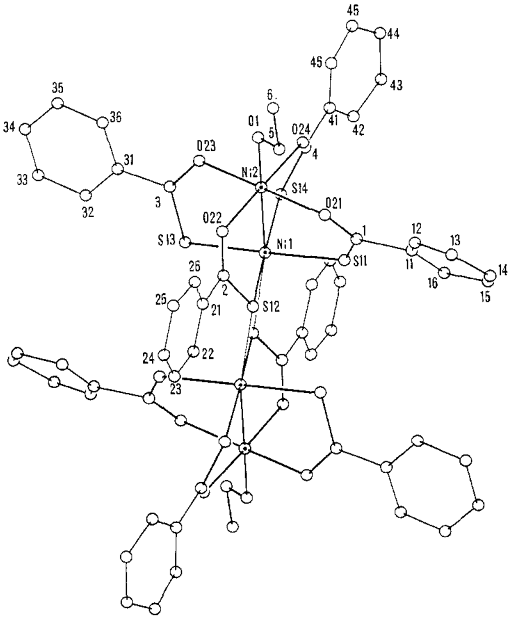

Figure 1.—View of the crystal structure showing two dimeric units of the complex. Unprefixed atoms are carbon. The weak Ni–S interactions linking the dimers together are indicated by the broken lines.

Selected intramolecular distances, angles, and torsion angles are given in Table III, together with their esd's, as derived from the data of Table I. Correlation between the parameters of different atoms has not been taken into account in deriving these error estimates though the standard errors of the cell parameters have been.

In the discussion, and in deriving intermolecular contact distances, the phenyl rings have been treated in terms of their idealized representations. The equations of their least-squares mean planes are given in Table IV together with similar equations for planes involving other groups of atoms. There are varied degrees of twist of the phenyl rings about the C–C axes linking them to the thiocarboxylate groups, most probably to achieve an efficient packing of molecules in the crystal.

Excluding the weak Ni–S interaction, the closest approach between molecules involves the ethanol oxygen atom and O(23) in location $\bar{x}, \bar{y}, 1 - \bar{z}$. This distance is 2.86 (1) Å and although no positive identification of the hydrogen atom of the ethanol moiety could be made, the geometry of the situation is such that a weak hydrogen bond is almost certainly formed between these atoms. Thus, the angles Ni(2)–O(1)–O(23′) and O(23′)–O(1)–C(5) are 117 and 115° with the angle O(23′)–O(1)–H(1) being 33°. O(23′) lies 1.58 Å from the plane of the ethanol residue.

Other intermolecular contacts correspond to normal van der Waals interactions. Those less than 3.8 Å which are of most interest are listed in Table V.

Before discussing the bond distances we may observe that there is a high degree of internal consistency in the values found for chemically equivalent bond types, with the exception of what appear to be significant, and not unexpected, differences among the Ni–O

TABLE II

OBSERVED STRUCTURE AMPLITUDES AND CALCULATED STRUCTURE FACTORS ON 10 TIMES THE ABSOLUTE SCALE AS DERIVED FROM THE FINAL STRUCTURE FACTOR CALCULATION. COLUMN HEADINGS ARE k, l, $10|F_o|$, AND $10F_c$

***** [illegible] = 0 *****			
0	2	506	-511
0	3	780	-725
0	4	633	-625
0	5	194	-215
0	6	322	273
0	7	701	618
0	10	432	-374
0	11	414	-370
0	13	316	243
1	13	488	431
1	11	553	-482
1	10	701	-662
1	7	753	742
1	6	274	281
1	5	216	-201
1	4	328	-319
1	3	235	214
1	2	478	-466
1	0	1909	1985
1	-1	753	770
1	-2	461	-465
1	-5	273	-274
1	-6	468	457
1	-11	301	-295
1	-13	288	248
2	-13	253	267
2	-12	262	-250
2	-11	405	-376
2	-8	323	-317
2	-6	215	-220
2	-5	191	-167
2	-4	351	342
2	-2	1151	-1113
2	-1	729	692
2	0	751	714
2	2	272	234
2	4	435	-452
2	5	732	-702
2	6	484	468
2	7	333	311
2	8	208	-206
2	10	597	-479
2	11	464	-405
2	13	436	382
3	13	199	197
3	12	250	226
3	11	241	-203
3	10	448	-448
3	8	370	-369
3	7	224	-212
3	5	429	-397
3	3	267	284
3	2	407	384
3	1	493	-488
3	-2	312	-307
3	-3	236	-211
3	-4	181	181
3	-5	247	-239
3	-6	162	-172
3	-7	527	491
3	-8	319	-278
3	-11	459	-397
3	-12	510	-443
4	-12	620	-535
4	-11	413	-367
4	-7	690	646
4	-6	576	-521
4	-5	773	-740
4	-4	180	-176
4	-2	509	479
4	-1	858	879
4	0	194	205
4	1	255	-243
4	3	321	312
4	4	340	-347
4	6	435	431
4	7	359	-348
4	8	386	-374
4	11	335	-323
4	12	230	224
5	10	196	-203
5	8	350	-318
5	7	194	-220
5	6	679	715
5	2	272	-264
5	1	294	-324
5	-1	1454	1483
5	-2	693	721
5	-5	812	-808
5	-6	586	-569
5	-7	437	428
5	-8	298	264
5	-9	347	-320
5	-10	181	182
5	-12	352	-320
6	-9	460	-446
6	-7	380	375
6	-6	533	-498
6	-5	330	-353
6	-3	470	454
6	-2	348	384
6	-1	1036	1081
6	1	723	-705
6	5	624	632
6	6	601	617
6	7	199	-206
6	8	527	-512
6	9	209	-208
6	10	345	-332
6	12	217	212
7	12	211	195
7	9	350	-327
7	8	234	-250
7	7	429	-467
7	6	470	475
7	5	464	454
7	4	406	-412
7	2	308	331
7	0	288	-293
7	-1	473	465
7	-3	276	322
7	-9	234	-254
8	-13	329	-291
8	-11	237	256
8	-4	235	235
8	-1	305	328
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-10	-3	197	-195
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-11	-4	255	284
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-12	-2	198	-211
-12	-4	224	244
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-1	6	510	-523
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-1	2	237	227
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2	-13	225	-206
2	-7	254	-306
2	-5	191	196
2	-4	222	-211
2	-3	373	397
2	-2	787	830
2	-1	292	-304
2	0	198	-175
2	3	256	-266
2	4	256	290
2	5	248	269
2	7	220	-202
2	8	604	-575
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8	6	208	-232
9	5	261	-280
9	2	192	-206
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9	-8	284	-275
10	-8	274	-254
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10	-2	258	-267
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9	0	210	219
9	3	195	185
8	6	225	-259
8	5	320	-335
8	4	189	195
8	3	254	281
8	-8	259	-279
7	-8	267	-261
7	-7	218	-213
7	-6	192	165
7	-5	230	214
7	-4	213	193
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7	3	376	397
7	4	362	403
7	5	387	-406
7	6	318	-343
6	6	414	-456
6	5	224	-245
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6	3	262	276
6	-1	234	-223
6	-4	206	235
6	-5	259	263
6	-7	501	-501
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5	-8	279	-238
5	-7	578	-553
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-1	-6	221	-244
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-1	4	278	-274
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-2	10	256	-234
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-2	8	210	-189
-2	7	196	-176
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-2	4	393	-396
-2	2	426	460
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-2	-2	212	204
-2	-7	182	-151
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-2	-13	247	-244
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-3	-7	193	-196
-3	-3	248	-223
-3	-2	312	324
-3	-1	600	624
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-3	6	203	209
-3	9	396	-379
-3	10	264	-263
-3	12	220	193
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-4	6	305	316
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-4	-1	744	793
-4	-2	406	426
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TABLE II (*Continued*)

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-5	-1	808	821
-5	0	534	577
-5	2	196	-176
-5	4	200	-203
-5	6	202	195
-5	10	192	-177
-6	10	213	-197
-6	7	221	-221
-6	0	193	200
-6	-1	499	550
-6	-2	224	-216
-6	-5	211	-215
-6	-6	309	-302
-6	-7	303	327
-6	-8	231	225
-6	-11	297	-267
-7	-1	292	308
-7	7	225	-219
-7	10	247	-239
-8	6	251	237
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-8	-2	293	-290
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-8	-4	190	189
-9	-2	407	-437
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-9	4	275	-287
-9	5	214	-189
-10	4	194	-223
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-6	-7	359	366
-6	-6	214	-218
-6	-5	249	-254
-6	-4	218	-240
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-6	1	196	-172
-6	3	213	242
-6	6	266	251
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-5	6	561	546
-5	1	215	-212
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-5	-1	370	399
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-5	-7	374	357
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-4	-6	223	-196
-4	-5	352	-375
-4	-4	274	-269
-4	-2	190	184
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-4	1	379	-403
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-3	6	473	445
-3	5	353	367
-3	2	188	192
-3	1	272	-283
-3	0	212	-230
-3	-1	421	441
-3	-5	259	-269
-3	-6	237	-282
-3	-9	220	-202
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-2	-5	205	-217
-2	-1	311	319
-2	0	284	-297
-2	2	456	457
-2	5	388	386
-2	6	283	285
-1	7	244	-230
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-1	2	365	390
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-1	-2	259	256
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2	6	243	-257
2	7	368	-379
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6	4	340	361
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7	6	227	-257
7	5	194	-244
7	4	270	293
7	3	218	226
7	2	229	229
7	1	182	186
7	-1	324	-344
7	-8	241	-236
8	-4	165	-168
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8	1	193	202
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6	0	361	-373
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2	3	350	349
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-5	2	208	-234
-5	1	283	-287
-5	-5	307	-310
-5	-6	239	-243
-5	-7	202	212
-4	-6	210	-205
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6	2	209	218
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7	-5	193	177
****** H = 11 *****			
5	-5	336	335
3	-7	195	178
3	2	217	213
2	2	301	310
2	0	331	-346
2	-4	221	214
1	-4	309	318
1	0	393	-398
1	1	249	-291
1	2	228	240
0	4	211	-222
0	2	198	213
0	1	355	-355
0	-4	224	218
-1	1	286	-286
-1	4	181	-169
-2	3	190	193
-2	1	231	-221
-2	-7	212	199
-3	1	360	-358
-3	2	214	-232
-3	4	188	181
-4	4	193	202
-4	2	197	-207
-4	1	508	-517
-4	-3	274	277
-5	-3	233	233
-5	1	291	-304
-5	2	255	-282
-6	2	296	-301
-7	-1	214	-223
-7	2	257	-274
****** H = 12 *****			
-4	-3	238	252
-4	1	244	-254
-3	3	188	183
-3	-3	214	216
-2	-3	219	194
-1	-3	215	179
0	-4	303	307
0	-3	227	214
1	1	193	-196
1	-4	336	346
2	-4	300	293
2	-2	195	-183

TABLE III

INTRAMOLECULAR INTERATOMIC DISTANCES (Å), ANGLES (DEG), AND TORSION ANGLES (DEG) WITH THEIR ASSOCIATED STANDARD ERRORS AS CALCULATED FROM THE PARAMETERS OF TABLE I

Distances

Ni(1)–Ni(2)	2.503 (4)	S(11)–C(1)	1.702 (10)
Ni(1)–S(11)	2.221 (5)	S(12)–C(2)	1.718 (10)
Ni(1)–S(12)	2.227 (5)	S(13)–C(3)	1.707 (11)
Ni(1)–S(13)	2.230 (5)	S(14)–C(4)	1.709 (10)
Ni(1)–S(14)	2.228 (5)	O(21)–C(1)	1.244 (12)
Ni(1)–S(12′)	2.814 (5)	O(22)–C(2)	1.236 (11)
Ni(2)–O(21)	2.044 (7)	O(23)–C(3)	1.262 (12)
Ni(2)–O(22)	2.010 (7)	C(1)–C(11)	1.506 (14)
Ni(2)–O(23)	2.056 (7)	C(2)–C(21)	1.493 (13)
Ni(2)–O(24)	2.015 (7)	C(3)–C(31)	1.492 (14)
Ni(2)–O(1)	2.058 (7)	C(4)–C(41)	1.484 (13)
C(5)–C(6)	1.493 (17)	C(5)–O(1)	1.446 (13)
S(11)···O(21)	2.617 (8)	O(21)···O(22)	2.873 (10)
S(12)···O(22)	2.605 (8)	O(22)···O(23)	2.895 (10)
S(13)···O(23)	2.621 (8)	O(23)···O(24)	2.867 (10)
S(14)···O(24)	2.613 (8)	O(24)···O(21)	2.855 (10)

Angles

Ni(1)–Ni(2)–O(21)	87.6 (2)	Ni(2)–Ni(1)–S(11)	91.46 (13)
Ni(1)–Ni(2)–O(22)	90.0 (2)	Ni(2)–Ni(1)–S(12)	88.67 (16)
Ni(1)–Ni(2)–O(23)	90.3 (2)	Ni(2)–Ni(1)–S(13)	88.25 (13)
Ni(1)–Ni(2)–O(24)	90.1 (2)	Ni(2)–Ni(1)–S(14)	89.15 (16)
O(21)–Ni(2)–O(22)	90.3 (3)	S(11)–Ni(1)–S(12)	89.50 (15)
O(22)–Ni(2)–O(23)	90.8 (3)	S(12)–Ni(1)–S(13)	89.11 (14)
O(23)–Ni(2)–O(24)	89.6 (3)	S(13)–Ni(1)–S(14)	92.33 (15)
O(24)–Ni(2)–O(21)	89.4 (3)	S(14)–Ni(1)–S(11)	89.06 (15)
O(21)–Ni(2)–O(23)	177.6 (3)	S(11)–Ni(1)–S(13)	178.58 (26)
O(22)–Ni(2)–O(24)	179.7 (12)	S(12)–Ni(1)–S(14)	177.35 (19)
O(21)–Ni(2)–O(1)	91.2 (3)	Ni(1)–S(12)–Ni(1′)	97.50 (16)
O(22)–Ni(2)–O(1)	88.7 (3)	C(6)–C(5)–O(1)	112.9 (9)
O(23)–Ni(2)–O(1)	91.0 (3)	C(5)–O(1)–Ni(2)	119.6 (6)
O(24)–Ni(2)–O(1)	91.2 (3)	Ni(1)–Ni(2)–O(1)	178.2 (2)
Ni(2)–O(21)–C(1)	124.3 (6)	Ni(1)–S(11)–C(1)	103.8 (4)
Ni(2)–O(22)–C(2)	123.9 (6)	Ni(1)–S(12)–C(2)	105.7 (3)
Ni(2)–O(23)–C(3)	121.0 (6)	Ni(1)–S(13)–C(3)	106.9 (4)
Ni(2)–O(24)–C(4)	123.5 (6)	Ni(1)–S(14)–C(4)	105.0 (3)
S(11)–C(1)–O(21)	124.5 (7)	S(13)–C(3)–O(23)	123.2 (7)
S(12)–C(2)–O(22)	122.9 (7)	S(14)–C(4) O(24)	124.3 (7)
O(21)–C(1)–C(11)	116.6 (8)	S(11)–C(1)–C(11)	118.8 (7)
O(22)–C(2)–C(21)	118.7 (8)	S(12)–C(2)–C(21)	118.2 (7)
O(23)–C(3)–C(31)	119.1 (9)	S(13)–C(3)–C(31)	117.7 (7)
O(24)–C(4)–C(41)	117.1 (8)	S(14)–C(4)–C(41)	118.6 (7)

Torsion Angles

O(21)–Ni(2)–Ni(1)–S(11)	22.7	O(23)–Ni(2)–Ni(1)–S(13)	25.1
O(21)–Ni(2)–Ni(1)–S(12)	66.8	O(23)–Ni(2)–Ni(1)–S(14)	67.3
O(21)–Ni(2)–Ni(1)–S(13)	155.9	O(23)–Ni(2)–Ni(1)–S(11)	156.3
O(21)–Ni(2)–Ni(1)–S(14)	111.7	O(23)–Ni(2)–Ni(1)–S(12)	114.2
O(22)–Ni(2)–Ni(1)–S(12)	23.5	O(24)–Ni(2)–Ni(1)–S(14)	22.3
O(22)–Ni(2)–Ni(1)–S(13)	65.7	O(24)–Ni(2)–Ni(1)–S(11)	66.7
O(22)–Ni(2)–Ni(1)–S(14)	158.0	O(24)–Ni(2)–Ni(1)–S(12)	156.2
O(22)–Ni(2)–Ni(1)–S(11)	112.9	O(24)–Ni(2)–Ni(1)–S(13)	114.6

distances. This suggests that the error estimates given are realistic.

The geometry of the structure shows some interesting features which allow a plausible interpretation of the bonding and magnetic properties of the complex.

TABLE IV

DIRECTION COSINES FOR LEAST-SQUARES MEAN PLANES THROUGH CERTAIN GROUPS OF ATOMS. THE COEFFICIENTS ARE APPLIED TO CARTESIAN COORDINATES FOR THE ATOMS OBTAINED FROM THE FRACTIONAL COORDINATES OF TABLE I BY APPLICATION OF THE MATRIX

$$\begin{matrix} 10.43600 & -0.61221 & -0.64686 \\ 0.00000 & 11.64292 & -0.25870 \\ 0.00000 & 0.00000 & 12.67185 \end{matrix}$$

	Plane			
	a	b	c	d
Sulfur atoms[a]	−0.5304	0.0314	0.8471	1.3858
Oxygen atoms[b]	−0.5409	0.0218	0.8408	3.8252
Ethanol residue[c]	0.3463	0.8986	0.2695	1.2184
Phenyl 1	0.3765	0.4366	0.8171	2.8680
Phenyl 2	0.3559	−0.9156	0.1872	0.0971
Phenyl 3	0.8772	0.4336	0.2061	0.2223
Phenyl 4	0.5551	−0.8152	0.1656	0.3328
Thiocarboxyl 1[d]	0.5552	0.4078	0.7248	2.1739
Thiocarboxyl 2[d]	−0.5119	0.8561	0.0708	0.8383
Thiocarboxyl 3[d]	0.9259	0.3427	0.1585	0.3498
Thiocarboxyl 4[d]	0.2183	−0.8280	0.5165	1.2399

[a] Deviations (Å): S(11), 0.019; S(12), −0.019; S(13), 0.018; S(14), −0.018; Ni(1), −0.024. [b] Deviations (Å): O(21), 0.020; O(22), −0.019; O(23), 0.019; O(24), −0.020; Ni(2), 0.019. [c] Deviation: O(23′), 1.58 Å. [d] The angles of tilt of the four thiocarboxyl groups with respect to the planes of the phenyl rings to which they are attached are 168, 162, 173, and 152°, respectively.

TABLE V

SELECTED INTERMOLECULAR CONTACTS (Å) LESS THAN 3.8 Å

(1) Contacts between Asymmetric Units[a]

Ni(1)···S(12)	2.81	S(12)···S(12)	3.35
S(11)···S(12)	3.77	S(12)···S(13)	3.40
S(11)···S(13)	3.78	S(14)···C(22)	3.61

(2) Contacts between Neighboring Molecules in Different Cells

S(12)···C(24)	21100	3.79	O(24)···O(1)	12001	3.39
S(13)···C(25)	11100	3.72	O(24)···C(36)	12001	3.41
C(6)···C(43)	22100	3.66	C(4)···O(1)	12001	3.55
C(6)···C(44)	22100	3.62	C(5)···C(36)	12001	3.49
C(12)···C(23)	21100	3.64	O(1)···C(36)	12001	3.34
C(34)···C(41)	22010	3.66	O(1)···C(46)	12001	3.38
S(14)···C(6)	12001	3.72	C(26)···C(45)	12001	3.70
O(23)···O(24)	12001	3.53	C(6)···C(6)	12$\bar{1}$01	3.62
O(23)···C(6)	12001	3.67	C(34)···C(35)	1201$\bar{1}$	3.62
O(23)···O(1)	12001	2.86	C(35)···C(35)	1201$\bar{1}$	3.31
O(23)···C(46)	12001	3.68			

[a] The first atom is at x, y, z, as given in Table I; the second is at $\bar{x}$, $\bar{y}$, $\bar{z}$. [b] The five-digit code specifies the actual contact as follows: *e.g.*, 2110$\bar{1}$, the first atom is at symmetry position 2, $\bar{x}$, $\bar{y}$, $\bar{z}$, in the basic unit cell; the second is at symmetry position 1, x, y, z, in the cell at $x + 1$, y, $z - 1$.

The metal–metal interaction is apparently sufficiently strong to induce the observed twist of the Ni–S and Ni–O planes about the Ni–Ni axis needed to accommodate the bite of the ligand. (It is possible, but less likely, that this is simply the best solution to the packing requirements.) However, although the Ni–Ni separation is only slightly greater than that found in nickel metal,[5] 2.492 (<1) Å, we believe that it corresponds to only a weak interaction in this compound. We are led to this conclusion by the following pieces of evidence. First, the equatorial Ni–S bond distances are in the range of those found for square-planar complexes of nickel(II) containing negatively charged sulfur donor ligands,[6–11] all of which are low-spin complexes. Second, the fifth, axial, Ni–S interaction linking the dimers into tetramers in the crystal is clearly very weak being possibly no more than a dipole–dipole attraction. Thus, its length is greater than those found for similar weak Ni–S interactions in bis(dithiobenzoato)nickel(II),[6] 2.77 (1) Å, and in tetra(thiourea)nickel(II) thiosulfate,[12] 2.72(4) Å. In addition, it does not appear to survive in solution where molecular weight measurements indicate only dimers to be present.

While the Ni–S distances indicate an effectively square-planar configuration for that nickel atom, the Ni–O distances are characteristic of high-spin octahedral or square-pyramidal nickel(II) complexes.[13–17]

The complex has an observed temperature-independent magnetic moment of 2.40 BM/nickel(II) ion ($\theta = -15^\circ$) corresponding to the presence of two unpaired electron spins in the dimeric unit. It is clear from the geometry of the complex that the two nickel atoms exist in quite different environments. If we assume that the two metal atoms interact only weakly with one another, then it is possible to rationalize the magnetic behavior. We conclude that the effective coordination pattern for the nickel ion coordinated to the sulfur ligands is square planar and that the weak axial interactions are not of sufficient strength to disturb the arrangement of orbital energies expected for such a configuration of local D_{4h} symmetry. For the other metal atom which is surrounded by five oxygen donors the effective local symmetry will be C_{4v}.

For the D_{4h} nickel atom the strong ligand field results in complete pairing of the electron spins and a singlet ground state.[18–20] Ciampolini had discussed the splitting of terms for the nickel(II) ion in a field of C_{4v} symmetry.[21] With the exception of large field strengths, such as those resulting from P or As donors, the ion is expected to have a triplet ground state. Thus, for the dimer, the only significant contribution to the magnetic moment will come from this nickel ion and will be characteristic of two unpaired electrons, in agreement with observation. Finally, Ciampolini[21] and Sacconi, *et al.*,[22] have studied the reflectance spectra of some high-spin square-pyramidal nickel(II) complexes. Characteristic of these spectra is a low-energy absorption band, assigned to the transition $^3B_1 \rightarrow {}^3E$ in C_{4v} symmetry, at 7700 cm^{-1}. Such a band is also observed in the reflectance spectra of these thiocarboxylate complexes.[1]

The presence of different coordination environments within a crystal associated with apparently anomalous magnetic properties has been described previously by Kilbourn, Powell, and Darbyshire for the interallogon compound bis(benzyldiphenylphosphinato)dibromonickel(II)[23] and by Nyburg and Wood for the so-called Lifschitz complexes.[24] However, we believe this to be the first case observed where one chelating ligand with two different ligand donor types produces this effect within a single molecule giving rise to an intra-allogon compound.

While this article was in preparation, our attention was drawn to a preliminary communication by Bonamico, Dessy, and Fares[25] describing a structure analysis of this compound undertaken using photographic data. Their results appear to be in good agreement with those reported here.

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