Analysis of crystallographic structures of Ni(II) complexes of α-amino acid Schiff bases; Elucidation of the substituents effect on stereochemical preferences

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Supporting Information

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(A) General Information

The chemicals were purchased from commercial sources and used without further purification. Analytical thin layer chromatography (TLC) was performed on 0.15−0.2 mm thickness silica gel plates. All products were characterized by NMR and MS spectra. ^{1}H and ^{13}C NMR spectra were recorded in deuterochloroform ($CDCl_3$) or methanol-d_4 (CD_3OD) on 400 or 500MHz instruments. Chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane. Proton coupling patterns were described as singlet (s), doublet (d), triplet (t), quartet (q), quintet (p), doublet of triplets (dt) and multiplet (m). High-resolution mass spectra (HRMS) was measured on Q-TOF spectrometer. The determination of de was performed via LC/MS analysis. Optical rotations were measured using a 1 mL cell with a 10 mm path length on an Auto pol V polarimeter and were reported as follows: $[\alpha]^{25}_{D}$ (c: g/100 mL, in solvent). Melting points were measured on melting point apparatus. All physicochemical data reported for the Ni(II) complexes are due to the single diastereomers after purification by chromatography or crystallization.

(B) General Procedures

General Procedure for the Synthesis of (*S*)-**1b**. To a stirring solution of (*S*)-**4b** (3.6 g, 7.3 mmol) in methanol (50 mL, 10 mL/g), glycine (2.8 g, 36.7 mmol) and nickel nitrate tetrahydrate (3.7 g, 14.7 mmol) was added followed by a solution of potassium carbonate (6.1 g, 44.0 mmol). The reaction mixture was stirred at 60 °C in an oil bath for 2.0 h. Then sodium hydride (0.35 g, 14.7 mmol) was added to accelerate the reaction. The resulting mixture was refluxed for 3 h and then terminated by ice water of 5% acetic acid. The mixture was extracted with dichloromethane (100 mL × 3). The combined organic layers were dried with Na_2SO_4, and then concentrated to give the crude product. The crude product was further purified by column chromatography on silica gel (dichloromethane/methanol = 40/1) to give (*S*)-**1b** (3.4 g, 77.5%) as a brown solid.

(C) Analytical Characterization Data of Products

Ni(II)-(*S*)-*N*-(2-benzoyl-4-chlorophenyl)-1-(3,4-dichlorobenzyl)pyrrolidine-2-carboxamide/2-aminoacetic acid Schiff Base Complex 1b:

Brown solid (3.4 g, yield 77.5%). mp 248-249 ^{o}C. $[\alpha]^{25}_{D}$ = +1347 (c 0.034, $CHCl_3$). ^{1}H NMR (400 MHz, CD_3OD) δ 8.82 (d, *J* = 2.0 Hz, 1H), 8.35 (dd, *J* = 8.2, 2.1 Hz, 1H), 8.01 (d, *J* = 9.3 Hz, 1H), 7.70 – 7.56 (m, 4H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.17 (dd, *J* = 9.3, 2.6 Hz, 1H), 7.07 (d, *J* = 6.4 Hz, 1H), 6.71 (d, *J* = 2.6 Hz, 1H), 4.26 (d, *J* = 12.5 Hz, 1H), 3.97 (d, *J* = 20.0 Hz, 1H), 3.72 – 3.65 (m, 1H), 3.58 (dd, *J* = 11.1, 5.8 Hz, 1H), 3.54 – 3.44 (m, 3H), 2.67 – 2.56 (m, 1H), 2.51 (ddd, *J* = 16.9, 8.1, 4.1 Hz, 1H), 2.27 – 2.16 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 180.74, 176.73, 171.06, 140.71, 134.49, 133.75, 133.57, 133.05, 132.16, 131.82, 130.92, 130.20, 129.97, 129.90, 129.61, 126.13, 125.64, 125.40, 124.91, 70.58, 62.69, 61.31, 58.41, 30.70, 23.58. HRMS (ESI) *m*/*z*: calcd for $C_{27}H_{22}Cl_3N_3NiO_3^-$ $[M - H]^-$: 598.0007, found: 598.0009.

(D) The Absolute Configuration of the Ni(II) Complexes.

X-ray Single Crystal Structure Analysis of (*S*)-1a

X-ray crystallographic data: Empirical formula, $C_{27}H_{25}N_3NiO_3$; Formula weight, 498.21; T = 273(2) K; Crystal system, orthorhombic; Space group, P 21 21 21; Unit cell dimensions, a = 9.0604(7) Å, b = 9.7307(8) Å, c = 26.482(2) Å, α = 90°, β = 90°, γ = 90°; Volume (V), 2334.8(3) $Å^3$; Z = 4; Calculated Density, 1.417 Mg/m^3; Absorption coefficient, 0.866 mm^{-1}; F(000), 1040; Theta range for data collection, 2.230 to 25.992°; Index ranges, -10<=h<=11, -12<=k<=11, -29<=l<=32; Goodness-of-fit on F^2, 1.045.

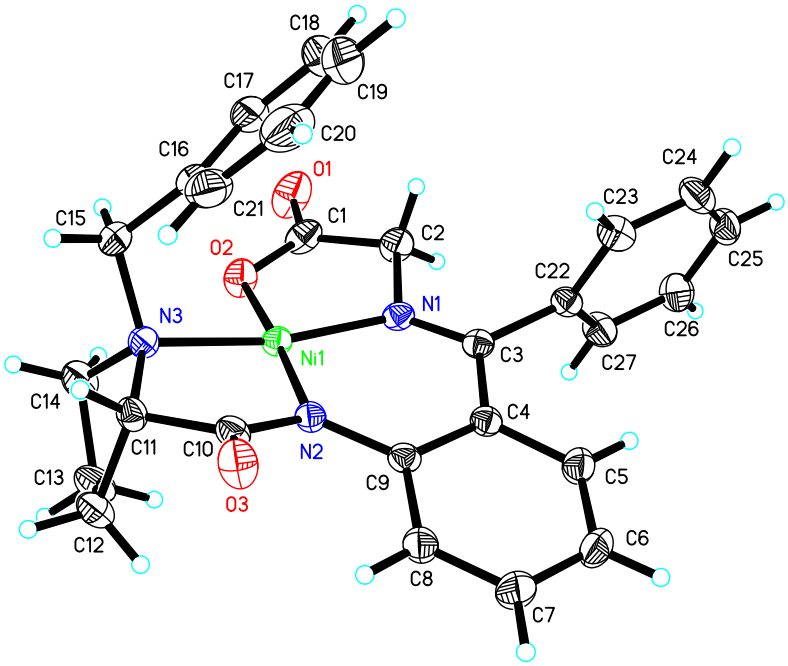

Figure S1. The crystal structure of (*S*)-**1a** by X-ray analysis. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif, the CCDC number is 1520061.

X-ray Single Crystal Structure Analysis of (*S*)-1b

X-ray crystallographic data: Empirical formula, $C_{27}H_{22}Cl_3N_3NiO_3$; Formula weight, 601.53; T = 293(2) K; Crystal system, monoclinic; Space group, P 21; Unit cell dimensions, a = 11.0422(14) Å, b = 7.6034(10) Å, c = 15.9516(19) Å, α = 90°, β = 100.367(3)°, γ = 90°; Volume (V), 1317.4(3) $Å^3$; Z = 2; Calculated Density, 1.516 Mg/m^3; Absorption coefficient, 1.076 mm^{-1}; F(000), 616; Theta range for data collection, 2.079 to 25.500°; Index ranges, -12<=h<=13, -9<=k<=7, -19<=l<=14; Goodness-of-fit on F^2, 0.994.

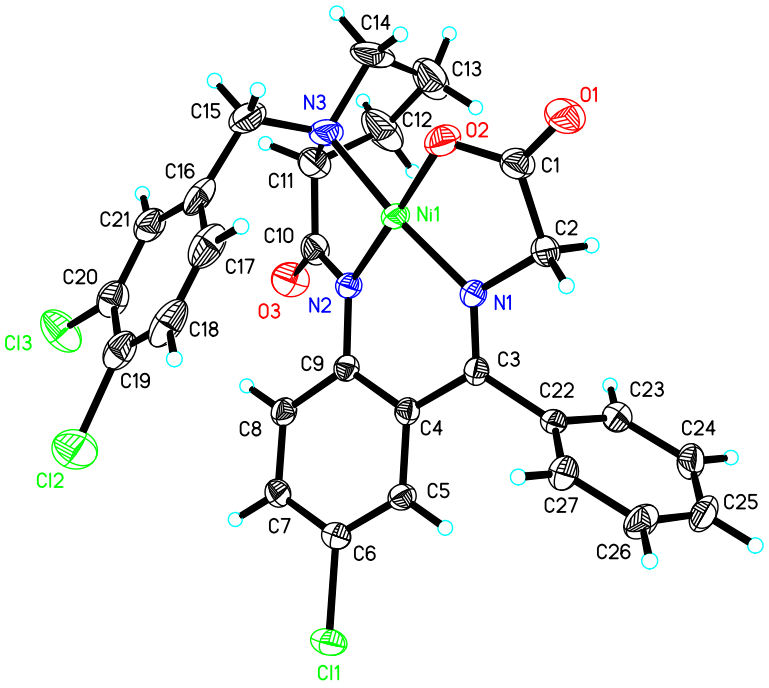

Figure S2. The crystal structure of (*S*)-**1b** by X-ray analysis. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif, the CCDC number is 1520062.

X-ray Single Crystal Structure Analysis of (*S*)(2*S*)-2a

X-ray crystallographic data: Empirical formula, $C_{28}H_{27}N_3NiO_3$; Formula weight, 512.23; T = 293(2) K; Crystal system, orthorhombic; Space group, P 21 21 21; Unit cell dimensions, = 9.7857(8) Å, b = 9.8844(8) Å, c = 25.741(2) Å, α = 90°, β = 90°, γ

= 90°; Volume (V), 2489.9(4) Å^3; Z = 4; Calculated Density, 1.366 Mg/m^3; Absorption coefficient, 0.814 mm^{-1}; F(000), 1072; Theta range for data collection, 2.207 to 25.496°; Index ranges, -11<=h<=11, -9<=k<=11, -31<=l<=30; Goodness-of-fit on F^2, 1.046.

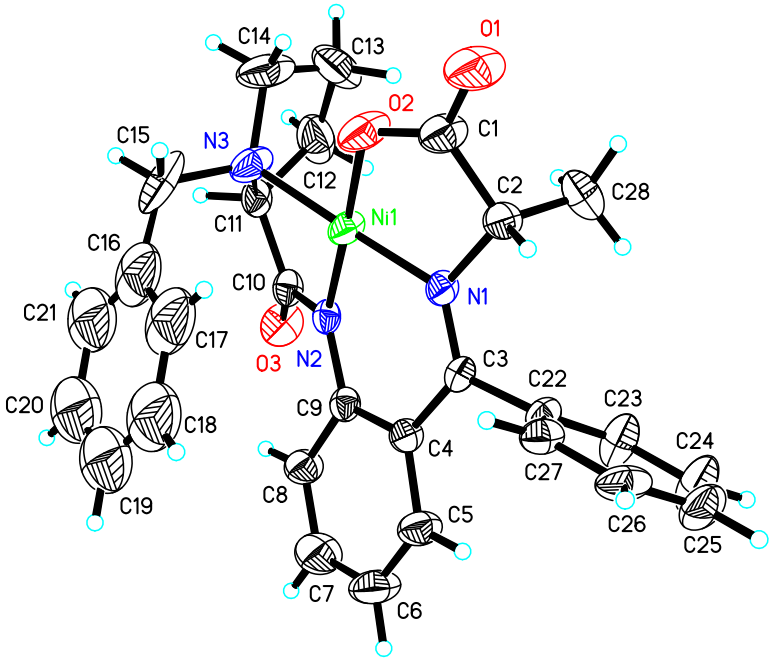

Figure S3. The crystal structure of (*S*)(2*S*)-**2a** by X-ray analysis. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif, the CCDC number is 1520063.

X-ray Single Crystal Structure Analysis of (*S*)(2*S*)-5

X-ray crystallographic data: Empirical formula, $C_{31}H_{30}Cl_3N_3NiO_3$; Formula weight, 657.64; T = 296(2) K; Crystal system, orthorhombic; Space group, P 21 21 21; Unit cell dimensions, a = 7.844(2) Å, b = 10.872(2) Å, c = 34.637(8) Å, α = 90°, β = 90°, γ = 90°; Volume (V), 2953.8(12) Å^3; Z = 4; Calculated Density, 1.479 Mg/m^3;

Absorption coefficient, 0.966 mm^{-1}; F(000), 1360; Theta range for data collection, 1.18 to 27.55°; Index ranges, -10<=h<=10, -13<=k<=13, -44<=l<=31; Goodness-of-fit on F^2, 1.025.

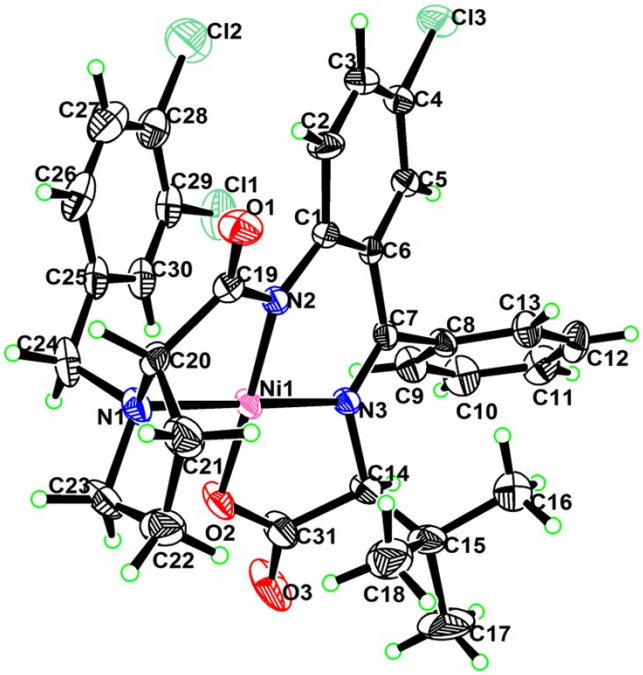

Figure S4. The crystal structure of (*S*)(2*S*)-**5** by X-ray analysis. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif, the CCDC number is 1400951.

X-ray Single Crystal Structure Analysis of (*R*)(2*R*)-6

X-ray crystallographic data: Empirical formula, $C_{37}H_{33}Cl_3N_4NiO_4$; Formula weight, 762.73; T = 293(2) K; Crystal system, monoclinic; Space group, P 21; Unit cell dimensions, a = 10.143(6) Å, b = 9.381(5) Å, c = 17.036(9) Å, α = 90°, β = 96.513(8)°, γ = 90°; Volume (V), 1610.5(16) $Å^3$; Z = 2; Calculated Density, 1.573 Mg/m^3; Absorption coefficient, 0.901 mm^{-1}; F(000), 788; Theta range for data collection, 2.021 to 25.047°; Index ranges, -11<=h<=12, -6<=k<=11, -20<=l<=19; Goodness-of-fit on F^2, 1.053.

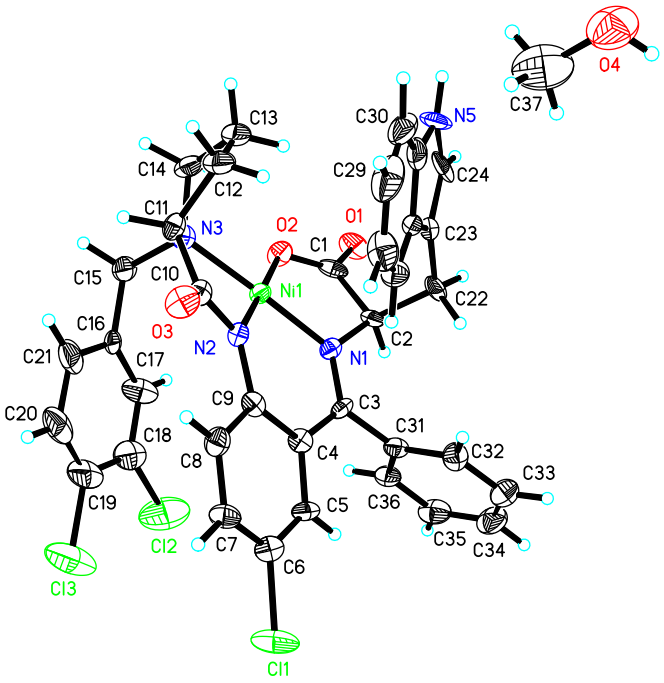

Figure S5. The crystal structure of (*R*)(2*R*)-**6** by X-ray analysis. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif, the CCDC number is 1422992.

(E) Copies of ^{1}H NMR and ^{13}C NMR Spectra for the Products

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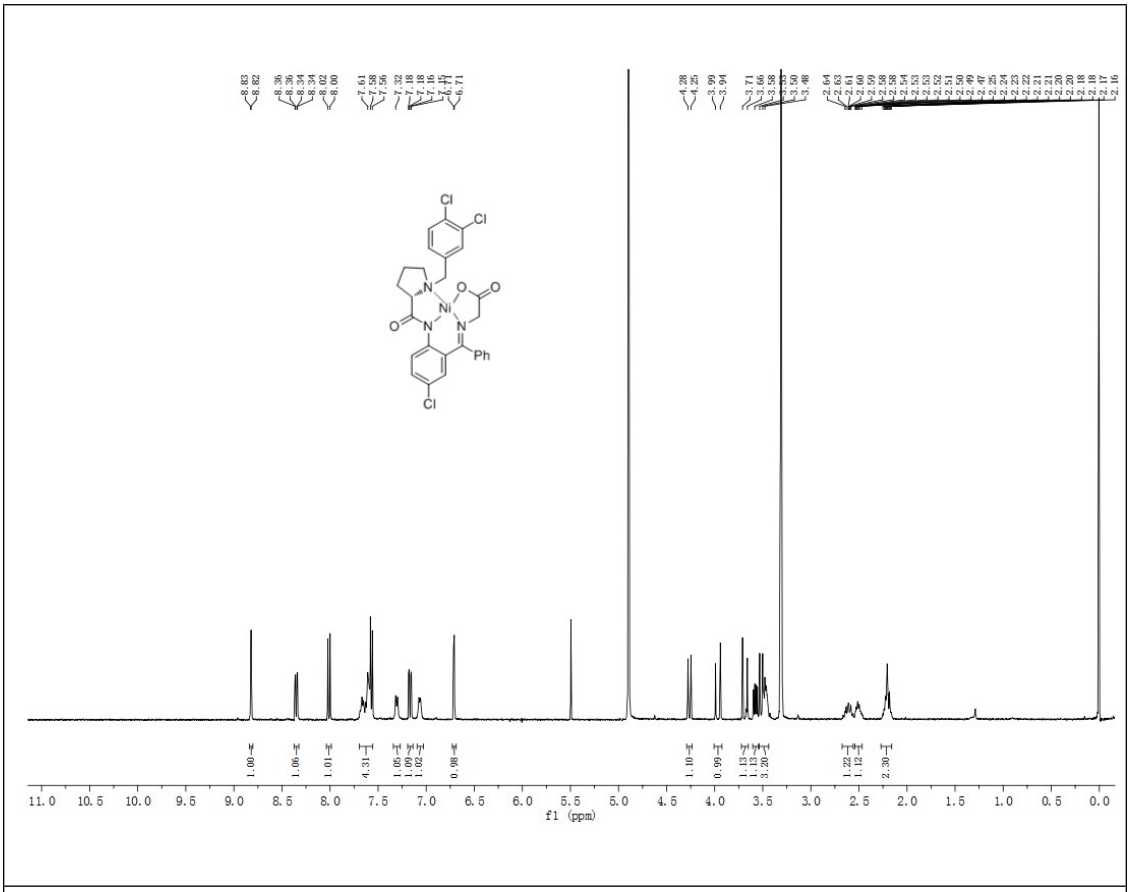
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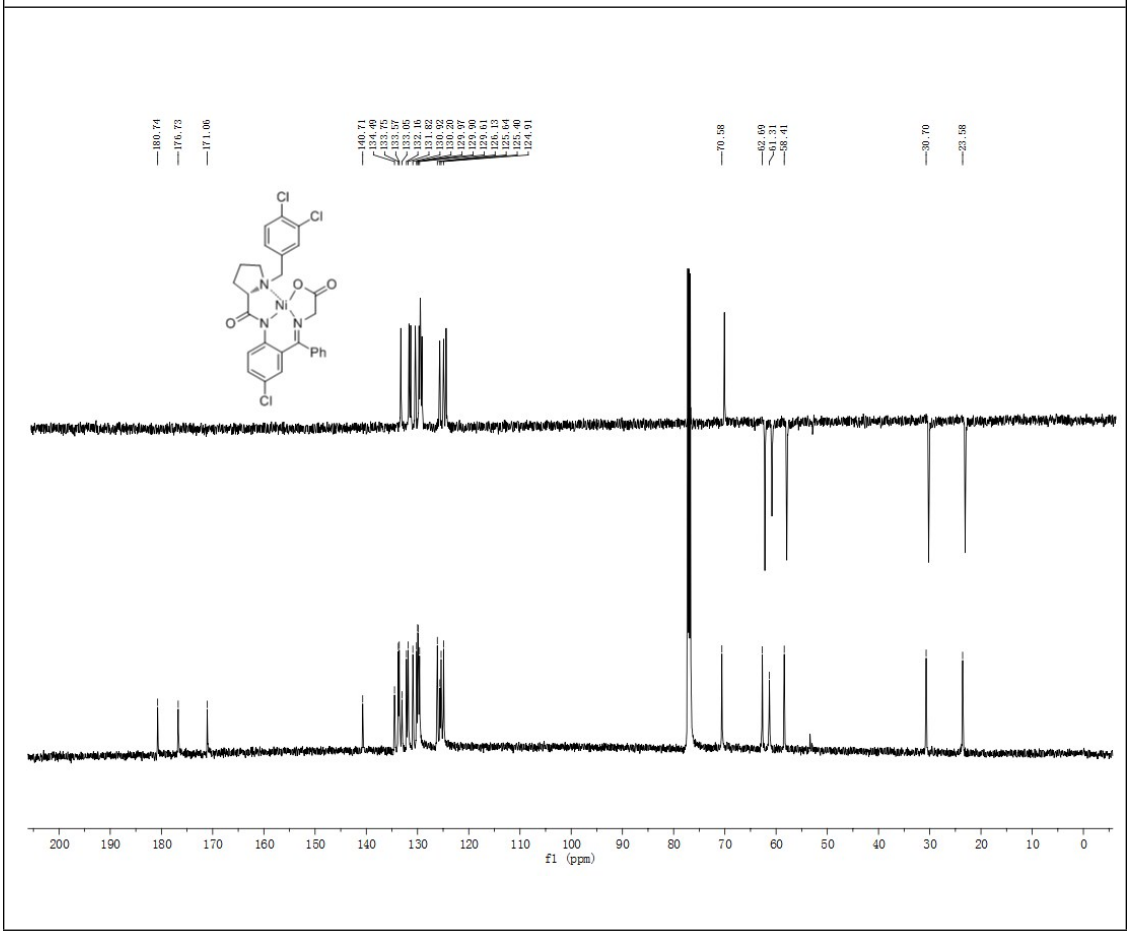
f1 (ppm)

(F) The Data for the Estimation of Parallelity in the Ni(II) Complexes

A. The data for the Ni(II) Complex (*S*)(2*S*)-2a was generated from PDB files using the software Pymol.

C5, C7, C9 (as shown in red) and C16, C18, C20 (as shown in red) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*S*)(2*S*)-**2a** (see **Figure S3** for details） as shown below.

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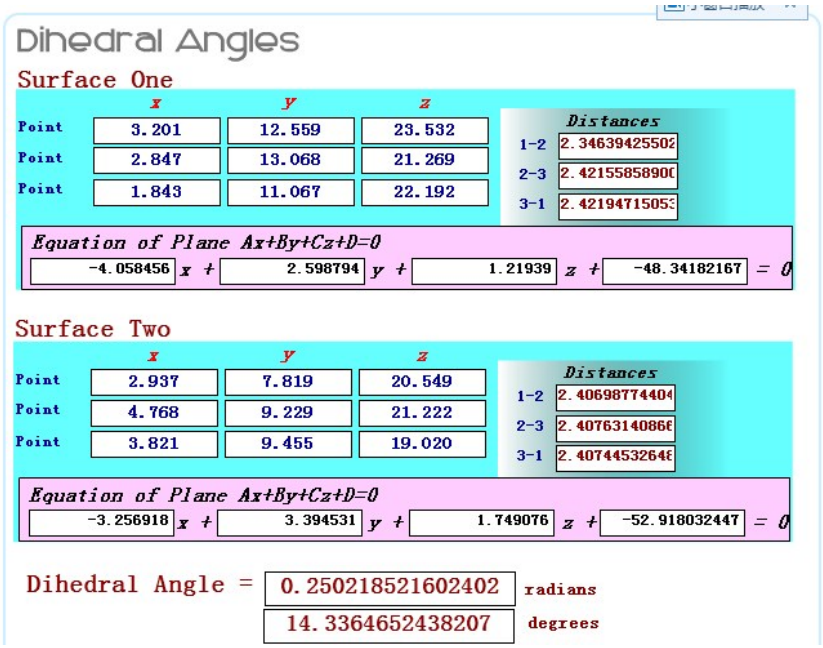

B. The data for the Ni(II) Complex (*S*)(2*S*)-2b was generated from PDB files using the software Pymol.

C6, C8, C10 (as shown in red) and C17, C19, C21 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(Ⅱ) complex (*S*)(2*S*)-**2b** as shown below.

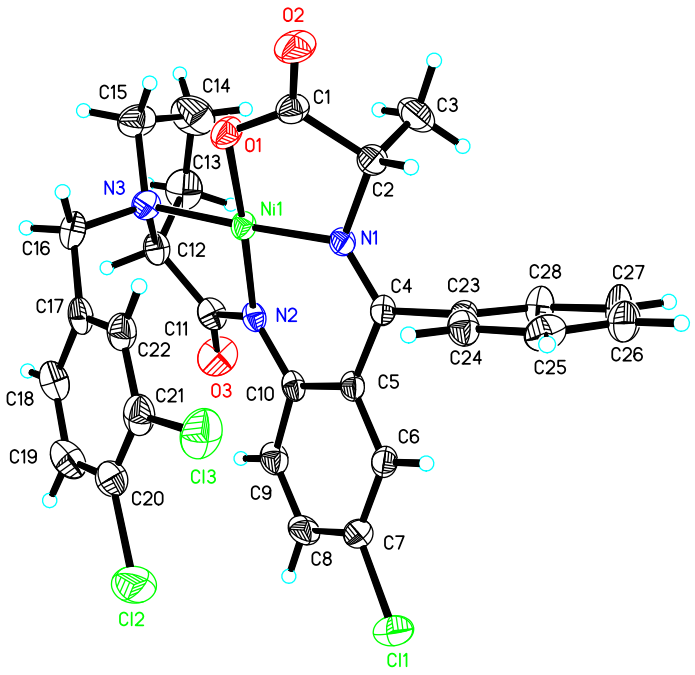

Figure S6. The crystal structure of (*S*)(2*S*)-**2b** by X-ray analysis.

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CCDC number: 1026566

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ATOM 4 CL3 0 1.308 -2.861 3.731 1.000 6.26

ATOM 5 N1 0 1.896 1.103 5.532 1.000 2.77

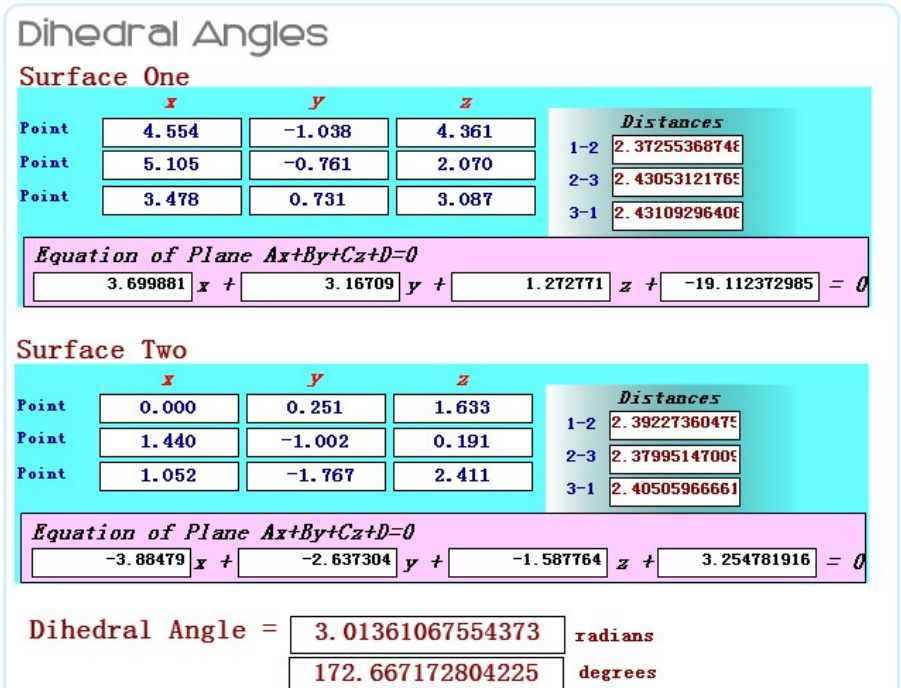
ATOM 6 N2 0 2.469 1.686 2.954 1.000 2.72

ATOM 7 N3 0 0.026 2.554 2.585 1.000 3.16

ATOM 8 O1 0 -0.526 1.750 5.132 1.000 3.70

ATOM	9	O2	0	-1.164	1.407	7.238	1.000	4.76
ATOM	10	O3	0	3.302	2.791	1.093	1.000	5.48
ATOM	11	C1	0	-0.311	1.522	6.390	1.000	3.42
ATOM	12	C2	0	1.165	1.482	6.763	1.000	3.55
ATOM	13	H2	0	1.328	0.835	7.480	1.000	4.26
ATOM	14	C3	0	1.588	2.882	7.187	1.000	5.63
ATOM	15	H3A	0	2.525	2.885	7.393	1.000	8.44
ATOM	16	H3B	0	1.089	3.146	7.964	1.000	8.44
ATOM	17	H3C	0	1.415	3.499	6.472	1.000	8.44
ATOM	18	C4	0	2.960	0.378	5.554	1.000	2.73
ATOM	19	C5	0	3.672	0.043	4.315	1.000	2.85
ATOM	20	C6	0	4.554	-1.038	4.361	1.000	3.22
ATOM	21	H6	0	4.682	-1.488	5.165	1.000	3.86
ATOM	22	C7	0	5.236	-1.450	3.247	1.000	3.75
ATOM	23	C8	0	5.105	-0.761	2.070	1.000	3.99
ATOM	24	H8	0	5.592	-1.021	1.321	1.000	4.79
ATOM	25	C9	0	4.250	0.317	1.999	1.000	3.67
ATOM	26	H9	0	4.184	0.785	1.198	1.000	4.40
ATOM	27	C10	0	3.478	0.731	3.087	1.000	2.81
ATOM	28	C11	0	2.394	2.510	1.876	1.000	3.53
ATOM	29	C12	0	1.051	3.152	1.688	1.000	3.42
ATOM	30	H12	0	0.768	3.035	0.757	1.000	4.11
ATOM	31	C13	0	1.065	4.659	2.024	1.000	5.74
ATOM	32	H13	0	1.952	4.942	2.293	1.000	6.89
ATOM	33	H13	0	0.789	5.184	1.256	1.000	6.89
ATOM	34	C14	0	0.085	4.823	3.162	1.000	6.96
ATOM	35	H14	0	0.535	4.763	4.019	1.000	8.35
ATOM	36	H14	0	-0.374	5.675	3.105	1.000	8.35
ATOM	37	C15	0	-0.866	3.690	2.978	1.000	4.90
ATOM	38	H15	0	-1.511	3.885	2.280	1.000	5.88

ATOM	39	H15	0	-1.339	3.494	3.802	1.000	5.88
ATOM	40	C16	0	-0.800	1.479	1.936	1.000	3.77
ATOM	41	H16	0	-1.533	1.243	2.525	1.000	4.52
ATOM	42	H16	0	-1.179	1.823	1.112	1.000	4.52
ATOM	43	C17	0	0.000	0.251	1.633	1.000	3.53
ATOM	44	C18	0	0.624	0.064	0.410	1.000	4.54
ATOM	45	H18	0	0.482	0.678	-0.274	1.000	5.44
ATOM	46	C19	0	1.440	-1.002	0.191	1.000	5.21
ATOM	47	H19	0	1.842	-1.118	-0.640	1.000	6.26
ATOM	48	C20	0	1.675	-1.916	1.206	1.000	4.83
ATOM	49	C21	0	1.052	-1.767	2.411	1.000	4.47
ATOM	50	C22	0	0.201	-0.704	2.619	1.000	3.86
ATOM	51	H22	0	-0.244	-0.625	3.432	1.000	4.63
ATOM	52	C23	0	3.476	-0.190	6.843	1.000	2.75
ATOM	53	C24	0	2.974	-1.387	7.321	1.000	3.51
ATOM	54	H24	0	2.315	-1.839	6.845	1.000	4.22
ATOM	55	C25	0	3.451	-1.912	8.508	1.000	4.15
ATOM	56	H25	0	3.124	-2.725	8.821	1.000	4.98
ATOM	57	C26	0	4.403	-1.238	9.224	1.000	4.84
ATOM	58	H26	0	4.705	-1.583	10.033	1.000	5.81
ATOM	59	C27	0	4.907	-0.066	8.755	1.000	5.20
ATOM	60	H27	0	5.554	0.388	9.246	1.000	6.24
ATOM	61	C28	0	4.460	0.462	7.543	1.000	4.05
ATOM	62	H28	0	4.826	1.250	7.213	1.000	4.86



C. The data for the Ni(II) Complex (*S*)(2*S*)-2c was generated from PDB files using the software Pymol.

C5, C7, C9 (as shown in red) and C16, C18, C20 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*S*)(2*S*)-**2c** as shown below.

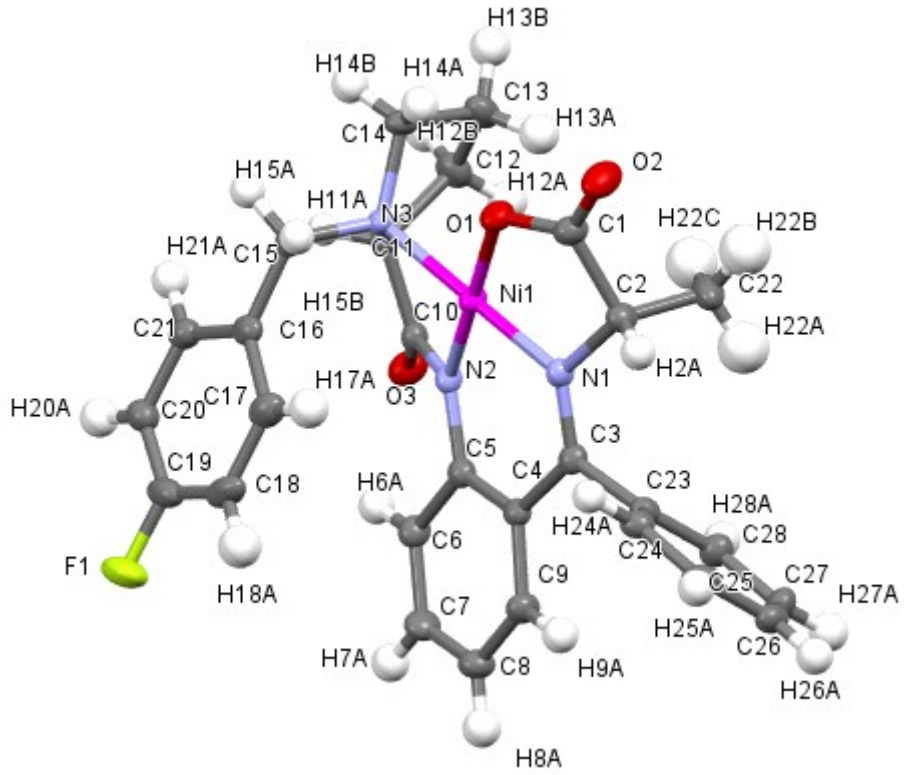


Figure S7. The crystal structure of (*S*)(2*S*)-**2c** by X-ray analysis.

HEADER CSD ENTRY VM-2 CCDC number: 769564

CRYST1 9.1541 10.2051 25.6532 90.00 90.00 90.00 P212121

SCALE1 0.109241 0.000000 0.000000 0.000000

SCALE2 0.000000 0.097990 0.000000 0.000000

SCALE3 0.000000 0.000000 0.038981 0.000000

HETATM 1 Ni1 UNK 1 3.693 6.661 10.347 1.00 1.45 Ni

ANISOU 1 Ni1 UNK 1 239 152 161 4 12 -1

Ni

HETATM 2 F1 UNK 1 -0.111 4.435 5.337 1.00 3.85 F

ANISOU 2 F1 UNK 1 420 334 709 -137 -178 -38

F

HETATM 3 O1 UNK 1 3.625 8.097 11.519 1.00 1.96

O

ANISOU 3 O1 UNK 1 365 173 208 4 23 -25
O
HETATM 4 O2 UNK 1 3.716 8.602 13.687 1.00 2.78
O
ANISOU 4 O2 UNK 1 613 235 209 -3 38 -48
O
HETATM 5 O3 UNK 1 5.084 4.735 7.252 1.00 2.28
O
ANISOU 5 O3 UNK 1 347 251 270 29 100 -12
O
HETATM 6 N1 UNK 1 3.312 5.584 11.796 1.00 1.54
N
ANISOU 6 N1 UNK 1 235 211 141 -15 4 5
N
HETATM 7 N2 UNK 1 3.827 5.253 9.150 1.00 1.45
N
ANISOU 7 N2 UNK 1 233 176 143 18 3 -16
N
HETATM 8 N3 UNK 1 4.078 7.812 8.848 1.00 1.57
N
ANISOU 8 N3 UNK 1 242 153 200 -26 -30 14
N
HETATM 9 C1 UNK 1 3.652 7.795 12.772 1.00 1.98
C
ANISOU 9 C1 UNK 1 304 216 233 -37 28 -5
C
HETATM 10 C2 UNK 1 3.652 6.295 13.060 1.00 1.81
C
ANISOU 10 C2 UNK 1 296 215 177 -33 1 -18
C

HETATM 11 H2A UNK 1 2.968 6.085 13.760 1.00 2.21
H
HETATM 12 C3 UNK 1 2.862 4.380 11.807 1.00 1.50
C
ANISOU 12 C3 UNK 1 201 193 175 34 26 -7
C
HETATM 13 C4 UNK 1 2.647 3.633 10.552 1.00 1.46
C
ANISOU 13 C4 UNK 1 197 168 191 12 -1 -8
C
HETATM 14 C5 UNK 1 3.171 4.032 9.302 1.00 1.56
C
ANISOU 14 C5 UNK 1 209 195 188 17 -5 -8
C
HETATM 15 C6 UNK 1 2.937 3.199 8.181 1.00 1.94
C
ANISOU 15 C6 UNK 1 324 229 186 -1 10 -21
C
HETATM 16 H6A UNK 1 3.276 3.455 7.332 1.00 2.37
H
HETATM 17 C7 UNK 1 2.225 2.020 8.295 1.00 2.17
C
ANISOU 17 C7 UNK 1 376 218 232 -30 -9 -68
C
HETATM 18 H7A UNK 1 2.090 1.475 7.529 1.00 2.61
H
HETATM 19 C8 UNK 1 1.706 1.626 9.517 1.00 2.23
C
ANISOU 19 C8 UNK 1 337 231 279 -64 2 -24
C

HETATM 20 H8A UNK 1 1.211 0.819 9.594 1.00 2.68
H
HETATM 21 C9 UNK 1 1.921 2.424 10.616 1.00 1.96
C
ANISOU 21 C9 UNK 1 293 254 198 -48 29 15
C
HETATM 22 H9A UNK 1 1.565 2.150 11.454 1.00 2.37
H
HETATM 23 C10 UNK 1 4.613 5.528 8.070 1.00 1.58
C
ANISOU 23 C10 UNK 1 216 225 159 4 -7 17
C
HETATM 24 C11 UNK 1 4.949 6.995 7.938 1.00 1.60
C
ANISOU 24 C11 UNK 1 222 223 162 2 33 11
C
HETATM 25 H11A UNK 1 4.813 7.287 6.990 1.00 1.89
H
HETATM 26 C12 UNK 1 6.406 7.302 8.374 1.00 2.37
C
ANISOU 26 C12 UNK 1 211 364 327 -27 -5 -15
C
HETATM 27 H12A UNK 1 6.849 6.485 8.717 1.00 2.84
H
HETATM 28 H12B UNK 1 6.932 7.658 7.616 1.00 2.84
H
HETATM 29 C13 UNK 1 6.271 8.356 9.488 1.00 2.47
C
ANISOU 29 C13 UNK 1 285 392 260 -117 -18 27
C

HETATM 30 H13A UNK 1 6.280 7.932 10.382 1.00 2.92
H
HETATM 31 H13B UNK 1 7.000 9.023 9.438 1.00 2.92
H
HETATM 32 C14 UNK 1 4.929 8.993 9.199 1.00 2.11
C
ANISOU 32 C14 UNK 1 375 196 231 -99 0 -6
C
HETATM 33 H14A UNK 1 4.578 9.464 9.994 1.00 2.53
H
HETATM 34 H14B UNK 1 4.990 9.629 8.442 1.00 2.53
H
HETATM 35 C15 UNK 1 2.802 8.290 8.217 1.00 1.82
C
ANISOU 35 C15 UNK 1 250 226 217 53 -9 10
C
HETATM 36 H15A UNK 1 3.018 9.023 7.588 1.00 2.21
H
HETATM 37 H15B UNK 1 2.224 8.667 8.927 1.00 2.21
H
HETATM 38 C16 UNK 1 2.022 7.239 7.476 1.00 1.85
C
ANISOU 38 C16 UNK 1 188 197 317 31 -27 21
C
HETATM 39 C17 UNK 1 1.093 6.405 8.125 1.00 2.35
C
ANISOU 39 C17 UNK 1 242 291 360 14 43 54
C
HETATM 40 H17A UNK 1 0.950 6.490 9.061 1.00 2.84
H

HETATM 41 C18 UNK 1 0.384 5.454 7.398 1.00 2.83
C
ANISOU 41 C18 UNK 1 197 280 597 -24 -5 142
C
HETATM 42 H18A UNK 1 -0.233 4.879 7.834 1.00 3.40
H
HETATM 43 C19 UNK 1 0.589 5.356 6.056 1.00 2.65
C
ANISOU 43 C19 UNK 1 269 215 524 -19 -116 -6
C
HETATM 44 C20 UNK 1 1.460 6.173 5.376 1.00 2.28
C
ANISOU 44 C20 UNK 1 298 263 306 -18 -60 -7
C
HETATM 45 H20A UNK 1 1.568 6.098 4.435 1.00 2.76
H
HETATM 46 C21 UNK 1 2.181 7.116 6.104 1.00 2.04
C
ANISOU 46 C21 UNK 1 236 234 306 -16 -11 41
C
HETATM 47 H21A UNK 1 2.793 7.685 5.654 1.00 2.45
H
HETATM 48 C22 UNK 1 5.038 5.868 13.547 1.00 3.26
C
ANISOU 48 C22 UNK 1 522 277 440 -33 -252 -1
C
HETATM 49 H22A UNK 1 5.017 4.923 13.807 1.00 4.90
H
HETATM 50 H22B UNK 1 5.296 6.414 14.320 1.00 4.90
H

HETATM 51 H22C UNK 1 5.691 5.993 12.827 1.00 4.90
H
HETATM 52 C23 UNK 1 2.532 3.656 13.084 1.00 1.56
C
ANISOU 52 C23 UNK 1 229 203 162 -44 6 -21
C
HETATM 53 C24 UNK 1 1.455 4.050 13.879 1.00 1.72
C
ANISOU 53 C24 UNK 1 231 193 229 -18 37 -34
C
HETATM 54 H24A UNK 1 0.960 4.832 13.660 1.00 2.05
H
HETATM 55 C25 UNK 1 1.108 3.293 14.995 1.00 2.03
C
ANISOU 55 C25 UNK 1 294 228 249 -69 59 -44
C
HETATM 56 H25A UNK 1 0.374 3.557 15.538 1.00 2.45
H
HETATM 57 C26 UNK 1 1.834 2.150 15.317 1.00 2.04
C
ANISOU 57 C26 UNK 1 320 257 198 -88 6 30
C
HETATM 58 H26A UNK 1 1.588 1.634 16.077 1.00 2.45
H
HETATM 59 C27 UNK 1 2.912 1.758 14.542 1.00 2.27
C
ANISOU 59 C27 UNK 1 327 260 277 8 -11 80
C
HETATM 60 H27A UNK 1 3.410 0.981 14.766 1.00 2.76
H

HETATM 61 C28 UNK 1 3.254 2.523 13.428 1.00 2.01
C
ANISOU 61 C28 UNK 1 248 262 253 3 38 27
C
HETATM 62 H28A UNK 1 3.996 2.263 12.893 1.00 2.45
H
CONECT 1 3 6 7 8
CONECT 2 43
CONECT 3 1 9
CONECT 4 9
CONECT 5 23
CONECT 6 1 10 12
CONECT 7 1 14 23
CONECT 8 1 24 32 35
CONECT 9 3 4 10
CONECT 10 6 9 11 48
CONECT 11 10
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CONECT 25 24

CONECT 26 24 27 28 29

CONECT 27 26

CONECT 28 26

CONECT 29 26 30 31 32

CONECT 30 29

CONECT 31 29

CONECT 32 8 29 33 34

CONECT 33 32

CONECT 34 32

CONECT 35 8 36 37 38

CONECT 36 35

CONECT 37 35

CONECT 38 35 39 46

CONECT 39 38 40 41

CONECT 40 39

CONECT 41 39 42 43

CONECT 42 41

CONECT 43 2 41 44

CONECT 44 43 45 46

CONECT 45 44

CONECT 46 38 44 47

CONECT 47 46

CONECT 48 10 49 50 51

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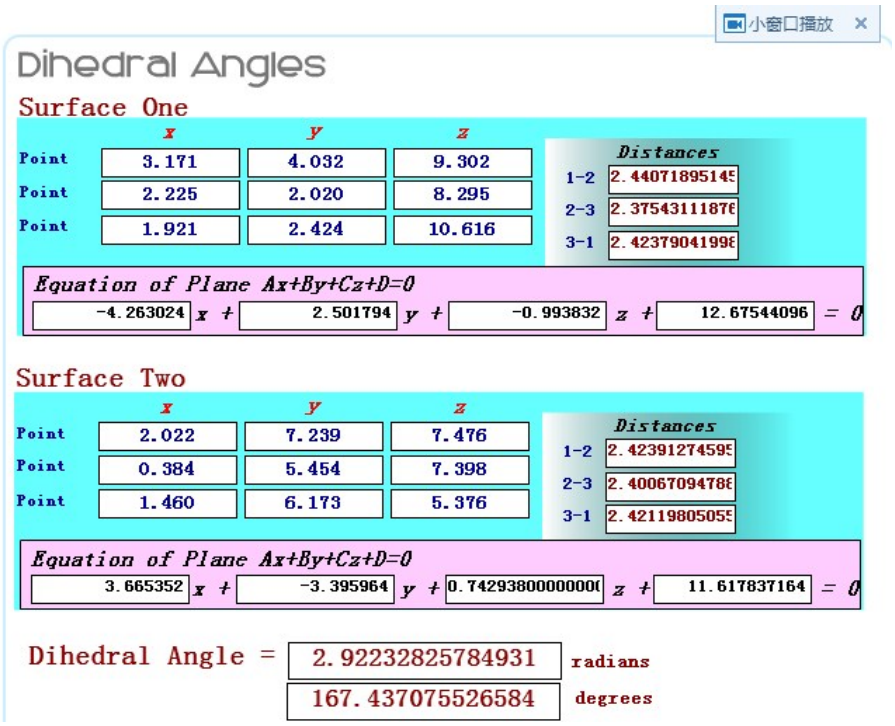

D. The data for the Ni(II) Complex (*S*)(2*S*)-2d was generated from PDB files using the software Pymol.

C6, C8, C10 (as shown in red) and C23, C25, C27 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-

angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*S*)(2*S*)-**2d** as shown below.

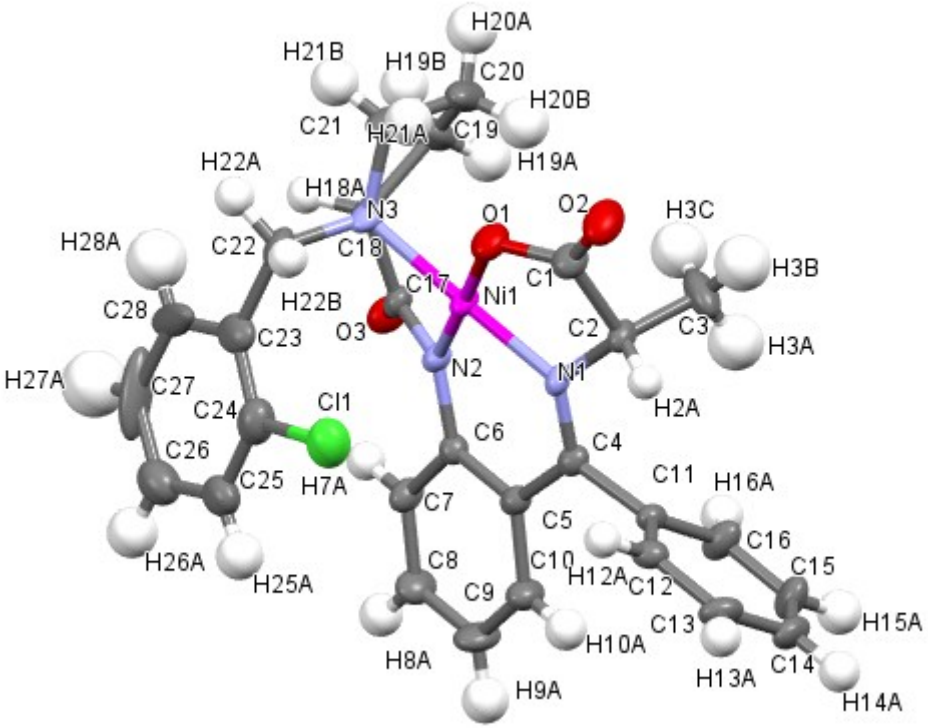

Figure S8. The crystal structure of (*S*)(2*S*)-**2d** by X-ray analysis.

HEADER CSD ENTRY 2-Cl_Ni CCDC number: 285986

CRYST1 9.3354 10.0330 25.9190 90.00 90.00 90.00 P212121

SCALE1 0.107119 0.000000 0.000000 0.000000

SCALE2 0.000000 0.099671 0.000000 0.000000

SCALE3 0.000000 0.000000 0.038582 0.000000

HETATM 1 Ni1 UNK 1 5.879 1.467 2.631 1.00 1.70 Ni

ANISOU 1 Ni1 UNK 1 342 143 162 21 5 -10

Ni

HETATM 2 Cl1 UNK 1 8.936 1.426 3.384 1.00 3.96 Cl

ANISOU 2 Cl1 UNK 1 457 629 417 -43 30 -17

Cl

HETATM 3 O1 UNK 1 6.002 2.959 1.526 1.00 2.60

O

ANISOU 3 O1 UNK 1 530 184 275 10 10 19

O

HETATM 4 O2 UNK 1 5.881 3.526 -0.634 1.00 3.40

O

ANISOU 4 O2 UNK 1 750 251 292 0 -20 73

O

HETATM 5 O3 UNK 1 4.398 -0.597 5.589 1.00 2.58

O

ANISOU 5 O3 UNK 1 430 290 259 -5 119 23

O

HETATM 6 N1 UNK 1 6.286 0.454 1.154 1.00 1.55

N

ANISOU 6 N1 UNK 1 270 169 151 -25 -2 -15

N

HETATM 7 N2 UNK 1 5.711 0.017 3.769 1.00 1.62

N

ANISOU 7 N2 UNK 1 250 175 191 8 18 -22

N

HETATM 8 N3 UNK 1 5.419 2.558 4.168 1.00 2.27

N

ANISOU 8 N3 UNK 1 460 153 250 70 10 2

N

HETATM 9 C1 UNK 1 5.952 2.689 0.249 1.00 2.32

C

ANISOU 9 C1 UNK 1 390 210 280 -10 20 30

C

HETATM 10 C2 UNK 1 5.956 1.201 -0.094 1.00 1.84

```
C
ANISOU   10  C2  UNK     1     370    180    150     10    -10     11
C
HETATM   11  H2A UNK     1       6.643   1.013  -0.796  1.00  2.21
H
HETATM   12  C3  UNK     1       4.576   0.794  -0.596  1.00  3.84
C
ANISOU   12  C3  UNK     1     560    360    540    -50   -320    100
C
HETATM   13  H3A UNK     1       4.578  -0.161  -0.822  1.00  5.76
H
HETATM   14  H3B UNK     1       4.352   1.316  -1.394  1.00  5.76
H
HETATM   15  H3C UNK     1       3.910   0.963   0.101  1.00  5.76
H
HETATM   16  C4  UNK     1       6.739  -0.751   1.107  1.00  1.71
C
ANISOU   16  C4  UNK     1     250    190    210    -20     35     -3
C
HETATM   17  C5  UNK     1       6.933  -1.540   2.324  1.00  1.71
C
ANISOU   17  C5  UNK     1     240    190    220      0     21     -7
C
HETATM   18  C6  UNK     1       6.375  -1.196   3.587  1.00  1.58
C
ANISOU   18  C6  UNK     1     250    180    170    -10      3     25
C
HETATM   19  C7  UNK     1       6.579  -2.076   4.655  1.00  2.21
C
ANISOU   19  C7  UNK     1     430    230    180     40     30     20
```

C

HETATM 20 H7A UNK 1 6.194 -1.862 5.497 1.00 2.68

H

HETATM 21 C8 UNK 1 7.309 -3.233 4.546 1.00 2.84

C

ANISOU 21 C8 UNK 1 520 280 280 100 -10 80

C

HETATM 22 H8A UNK 1 7.441 -3.789 5.306 1.00 3.40

H

HETATM 23 C9 UNK 1 7.855 -3.582 3.307 1.00 3.32

C

ANISOU 23 C9 UNK 1 590 280 390 220 30 50

C

HETATM 24 H9A UNK 1 8.347 -4.387 3.209 1.00 3.95

H

HETATM 25 C10 UNK 1 7.671 -2.746 2.232 1.00 2.61 C

ANISOU 25 C10 UNK 1 450 270 270 120 0 20

C

HETATM 26 H10A UNK 1 8.053 -2.985 1.397 1.00 3.16

H

HETATM 27 C11 UNK 1 7.087 -1.413 -0.204 1.00 1.62 C

ANISOU 27 C11 UNK 1 250 210 157 50 25 10

C

HETATM 28 C12 UNK 1 8.201 -0.992 -0.951 1.00 2.00 C

ANISOU 28 C12 UNK 1 270 210 280 40 30 36

C

HETATM 29 H12A UNK 1 8.714 -0.242 -0.676 1.00 2.37 H

HETATM 30 C13 UNK 1 8.537 -1.696 -2.102 1.00 2.53 C

ANISOU 30 C13 UNK 1 360 290 310 110 140 40

C

HETATM 31 H13A UNK 1 9.288 -1.422 -2.615 1.00 3.00 H

HETATM 32 C14 UNK 1 7.791 -2.793 -2.512 1.00 2.55 C

ANISOU 32 C14 UNK 1 470 310 190 120 60 -30

C

HETATM 33 H14A UNK 1 8.027 -3.258 -3.305 1.00 3.08 H

HETATM 34 C15 UNK 1 6.711 -3.208 -1.768 1.00 3.05 C

ANISOU 34 C15 UNK 1 420 400 340 -60 10 -160

C

HETATM 35 H15A UNK 1 6.205 -3.963 -2.045 1.00 3.63 H

HETATM 36 C16 UNK 1 6.363 -2.521 -0.617 1.00 2.66 C

ANISOU 36 C16 UNK 1 340 310 360 -70 100 -100

C

HETATM 37 H16A UNK 1 5.619 -2.812 -0.104 1.00 3.24 H

HETATM 38 C17 UNK 1 4.882 0.229 4.824 1.00 1.87

C

ANISOU 38 C17 UNK 1 290 230 190 10 0 -42

C

HETATM 39 C18 UNK 1 4.498 1.693 4.997 1.00 2.00

C

ANISOU 39 C18 UNK 1 340 230 190 60 30 -46

C

HETATM 40 H18A UNK 1 4.561 1.951 5.961 1.00 2.45

H

HETATM 41 C19 UNK 1 3.087 1.977 4.468 1.00 3.47

C

ANISOU 41 C19 UNK 1 320 500 500 160 -70 -40

C

HETATM 42 H19A UNK 1 2.692 1.161 4.072 1.00 4.18

H

HETATM 43 H19B UNK 1 2.497 2.292 5.199 1.00 4.18

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H
HETATM   44  C20 UNK     1       3.258   3.060   3.414  1.00  4.00
C
ANISOU   44  C20 UNK     1       640     550     330     360    -130    -90
C
HETATM   45 H20A UNK     1       2.509   3.706   3.442  1.00  4.74
H
HETATM   46 H20B UNK     1       3.310   2.667   2.506  1.00  4.74
H
HETATM   47  C21 UNK     1       4.573   3.729   3.797  1.00  3.50
C
ANISOU   47  C21 UNK     1       700     310     320     250    -20      20
C
HETATM   48 H21A UNK     1       4.961   4.227   3.033  1.00  4.18
H
HETATM   49 H21B UNK     1       4.455   4.345   4.562  1.00  4.18
H
HETATM   50  C22 UNK     1       6.637   3.029   4.883  1.00  2.40
C
ANISOU   50  C22 UNK     1       480     210     220     -40    -10     -50
C
HETATM   51 H22A UNK     1       6.366   3.717   5.541  1.00  2.84
H
HETATM   52 H22B UNK     1       7.236   3.464   4.227  1.00  2.84
H
HETATM   53  C23 UNK     1       7.435   1.935   5.622  1.00  3.13
C
ANISOU   53  C23 UNK     1       370     270     550     -60    -120    -70
C
HETATM   54  C24 UNK     1       8.435   1.170   5.033  1.00  3.21
```

C

ANISOU 54 C24 UNK 1 440 470 310 -70 20 -20

C

HETATM 55 C25 UNK 1 9.026 0.120 5.741 1.00 3.40

C

ANISOU 55 C25 UNK 1 380 400 510 0 -130 -60

C

HETATM 56 H25A UNK 1 9.643 -0.459 5.308 1.00 4.11

H

HETATM 57 C26 UNK 1 8.712 -0.076 7.084 1.00 3.90 C

ANISOU 57 C26 UNK 1 500 440 540 -10 -130 50

C

HETATM 58 H26A UNK 1 9.151 -0.754 7.584 1.00 4.66

H

HETATM 59 C27 UNK 1 7.745 0.728 7.698 1.00 6.76

C

ANISOU 59 C27 UNK 1 1360 1040 170 -840 10 40

C

HETATM 60 H27A UNK 1 7.515 0.583 8.610 1.00 8.13

H

HETATM 61 C28 UNK 1 7.127 1.732 6.983 1.00 5.61

C

ANISOU 61 C28 UNK 1 280 640 1210 160 -320 -620

C

HETATM 62 H28A UNK 1 6.488 2.291 7.410 1.00 6.71

H

CONECT 1 3 6 7 8

CONECT 2 54

CONECT 3 1 9

CONECT 4 9

CONECT 5 38

CONECT 6 1 10 16

CONECT 7 1 18 38

CONECT 8 1 39 47 50

CONECT 9 3 4 10

CONECT 10 6 9 11 12

CONECT 11 10

CONECT 12 10 13 14 15

CONECT 13 12

CONECT 14 12

CONECT 15 12

CONECT 16 6 17 27

CONECT 17 16 18 25

CONECT 18 7 17 19

CONECT 19 18 20 21

CONECT 20 19

CONECT 21 19 22 23

CONECT 22 21

CONECT 23 21 24 25

CONECT 24 23

CONECT 25 17 23 26

CONECT 26 25

CONECT 27 16 28 36

CONECT 28 27 29 30

CONECT 29 28

CONECT 30 28 31 32

CONECT 31 30

CONECT 32 30 33 34

CONECT 33 32

CONECT 34 32 35 36

```
CONECT   35   34
CONECT   36   27   34   37
CONECT   37   36
CONECT   38    5    7   39
CONECT   39    8   38   40   41
CONECT   40   39
CONECT   41   39   42   43   44
CONECT   42   41
CONECT   43   41
CONECT   44   41   45   46   47
CONECT   45   44
CONECT   46   44
CONECT   47    8   44   48   49
CONECT   48   47
CONECT   49   47
CONECT   50    8   51   52   53
CONECT   51   50
CONECT   52   50
CONECT   53   50   54   61
CONECT   54    2   53   55
CONECT   55   54   56   57
CONECT   56   55
CONECT   57   55   58   59
CONECT   58   57
CONECT   59   57   60   61
CONECT   60   59
CONECT   61   53   59   62
CONECT   62   61
MASTER        0    0    0    0    0    0    0    3   62    0   62    0
END
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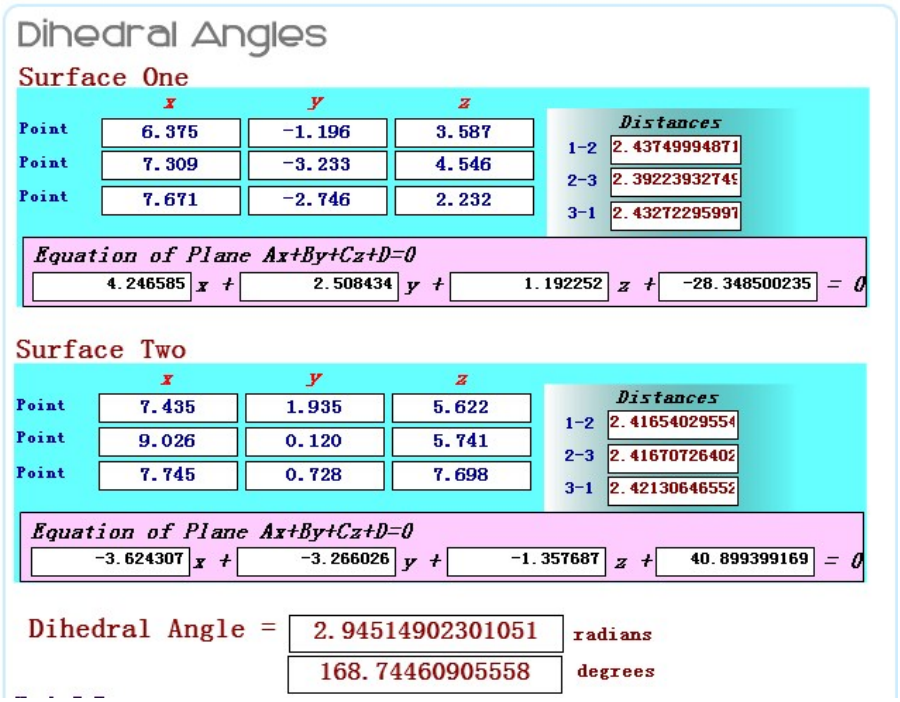

E. The data for the Ni(II) Complex (*S*)(2*S*)-2e was generated from PDB files using the software Pymol.

C7, C9, C11 (as shown in red) and C27, C29, C31 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*S*)(2*S*)-**2e** as shown below.

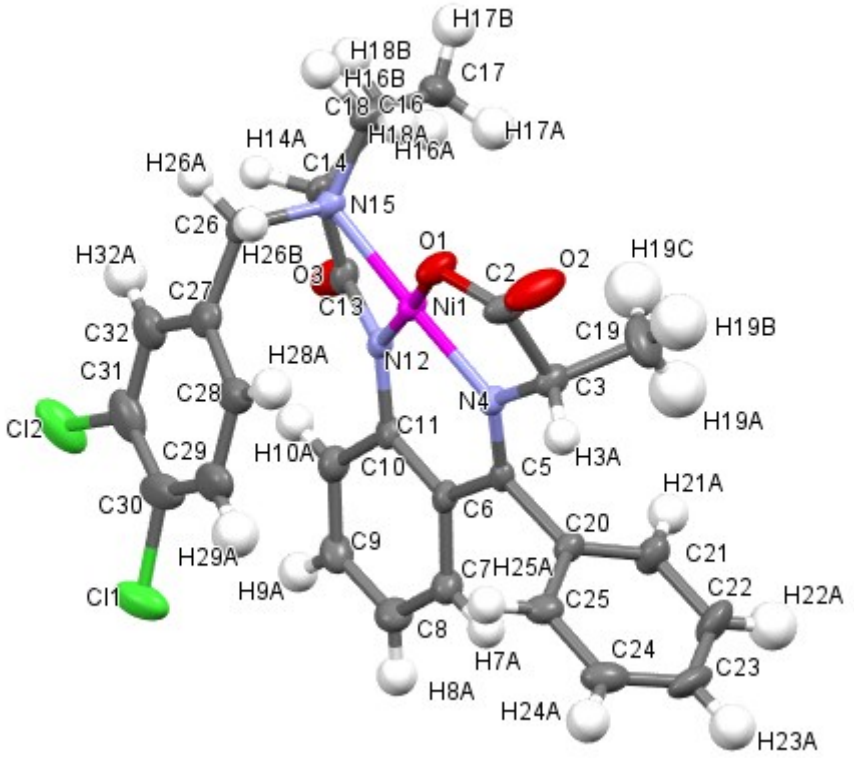

Figure S9. The crystal structure of (*S*)(2*S*)-**2e** by X-ray analysis.

HEADER CSD ENTRY Ni-CPB-(S)-Ala CCDC number: 204805

CRYST1 9.1360 10.7340 26.3380 90.00 90.00 90.00 P212121

SCALE1 0.109457 0.000000 0.000000 0.000000

SCALE2 0.000000 0.093162 0.000000 0.000000

SCALE3 0.000000 0.000000 0.037968 0.000000

HETATM 1 Ni1 UNK 1 -12.778 7.105 4.051 1.00 1.51 Ni

ANISOU 1 Ni1 UNK 1 177 244 154 5 2 37

Ni

HETATM 2 Cl1 UNK 1 -11.001 2.191 0.992 0.80 4.15 Cl

ANISOU 2 Cl1 UNK 1 391 257 930 -1 89 -29

Cl

HETATM 3 Cl2 UNK 1 -11.763 4.226 -1.300 0.80 4.23 Cl

ANISOU 3 Cl2 UNK 1 771 340 497 -140 350 -87

Cl

HETATM 4 O1 UNK 1 -14.228 7.148 5.215 1.00 2.26

O

ANISOU 4 O1 UNK 1 200 450 210 70 47 110

O

HETATM 5 O2 UNK 1 -14.740 7.005 7.391 1.00 4.21

O

ANISOU 5 O2 UNK 1 340 930 330 300 180 260

O

HETATM 6 O3 UNK 1 -10.696 8.147 0.915 1.00 2.74

O

ANISOU 6 O3 UNK 1 300 450 290 0 60 150

O

HETATM 7 C2 UNK 1 -13.951 6.936 6.471 1.00 2.42

C

ANISOU 7 C2 UNK 1 320 370 230 120 50 110

C

HETATM 8 C3 UNK 1 -12.467 6.681 6.740 1.00 1.97

C

ANISOU 8 C3 UNK 1 230 340 180 40 30 40

C

HETATM 9 H3A UNK 1 -12.365 5.888 7.340 1.00 2.37

H

HETATM 10 N4 UNK 1 -11.785 6.424 5.450 1.00 1.47

N

ANISOU 10 N4 UNK 1 170 240 150 0 0 10

N

HETATM 11 C5 UNK 1 -10.644 5.793 5.405 1.00 1.50

C

ANISOU 11 C5 UNK 1 220 180 170 -50 -20 10

C

HETATM 12 C6 UNK 1 -9.960 5.540 4.151 1.00 1.58

C

ANISOU 12 C6 UNK 1 190 250 160 -40 -10 0

C

HETATM 13 C7 UNK 1 -8.886 4.626 4.172 1.00 2.11

C

ANISOU 13 C7 UNK 1 240 330 230 20 0 -30

C

HETATM 14 H7A UNK 1 -8.632 4.238 4.999 1.00 2.53

H

HETATM 15 C8 UNK 1 -8.190 4.276 3.034 1.00 2.42

C

ANISOU 15 C8 UNK 1 230 350 340 40 20 -10

C

HETATM 16 H8A UNK 1 -7.465 3.664 3.082 1.00 2.92

H

HETATM 17 C9 UNK 1 -8.559 4.827 1.836 1.00 2.34

C

ANISOU 17 C9 UNK 1 230 390 270 -10 60 -70

C

HETATM 18 H9A UNK 1 -8.105 4.572 1.040 1.00 2.84

H

HETATM 19 C10 UNK 1 -9.585 5.747 1.767 1.00 2.13 C

ANISOU 19 C10 UNK 1 280 320 210 -20 0 0

C

HETATM 20 H10A UNK 1 -9.806 6.128 0.927 1.00 2.61

H

HETATM 21 C11 UNK 1 -10.316 6.141 2.913 1.00 1.61 C

ANISOU 21 C11 UNK 1 150 260 200 -50 -20 -40

C

HETATM 22 N12 UNK 1 -11.400 7.005 2.814 1.00 1.47

N

ANISOU 22 N12 UNK 1 210 200 150 -30 -14 10

N

HETATM 23 C13 UNK 1 -11.558 7.833 1.741 1.00 1.87 C

ANISOU 23 C13 UNK 1 250 280 180 -60 -10 20

C

HETATM 24 C14 UNK 1 -12.930 8.447 1.633 1.00 1.71 C

ANISOU 24 C14 UNK 1 270 220 160 0 -30 30

C

HETATM 25 H14A UNK 1 -13.291 8.297 0.714 1.00 2.05

H

HETATM 26 N15 UNK 1 -13.869 7.855 2.640 1.00 1.68

N

ANISOU 26 N15 UNK 1 220 220 200 10 -10 40

N

HETATM 27 C16 UNK 1 -14.702 9.010 3.105 1.00 2.32 C

ANISOU 27 C16 UNK 1 320 320 240 90 -20 60

C

HETATM 28 H16A UNK 1 -15.119 8.818 3.980 1.00 2.76

H

HETATM 29 H16B UNK 1 -15.412 9.224 2.447 1.00 2.76 H

HETATM 30 C17 UNK 1 -13.709 10.138 3.213 1.00 2.82 C

ANISOU 30 C17 UNK 1 480 250 340 80 -60 -30

C

HETATM 31 H17A UNK 1 -13.142 10.044 4.019 1.00 3.40

H

HETATM 32 H17B UNK 1 -14.163 11.018 3.234 1.00 3.40 H

HETATM 33 C18 UNK 1 -12.890 9.963 1.933 1.00 2.45 C

ANISOU 33 C18 UNK 1 410 210 310 -40 -60 10

C

HETATM 34 H18A UNK 1 -11.958 10.269 2.068 1.00 2.92
H
HETATM 35 H18B UNK 1 -13.290 10.479 1.188 1.00 2.92 H
HETATM 36 C19 UNK 1 -11.882 7.917 7.417 1.00 3.95 C
ANISOU 36 C19 UNK 1 500 570 430 20 70 -260
C
HETATM 37 H19A UNK 1 -10.956 7.737 7.683 1.00 5.92
H
HETATM 38 H19B UNK 1 -12.413 8.137 8.210 1.00 5.92 H
HETATM 39 H19C UNK 1 -11.901 8.671 6.790 1.00 5.92 H
HETATM 40 C20 UNK 1 -10.029 5.244 6.664 1.00 1.71 C
ANISOU 40 C20 UNK 1 210 270 170 20 0 30
C
HETATM 41 C21 UNK 1 -9.009 5.928 7.293 1.00 2.55 C
ANISOU 41 C21 UNK 1 350 340 280 -60 -80 70
C
HETATM 42 H21A UNK 1 -8.708 6.757 6.940 1.00 3.00
H
HETATM 43 C22 UNK 1 -8.422 5.407 8.447 1.00 3.63 C
ANISOU 43 C22 UNK 1 470 590 320 30 -200 50
C
HETATM 44 H22A UNK 1 -7.739 5.891 8.897 1.00 4.34
H
HETATM 45 C23 UNK 1 -8.838 4.189 8.923 1.00 3.18 C
ANISOU 45 C23 UNK 1 410 540 260 230 -50 100
C
HETATM 46 H23A UNK 1 -8.453 3.838 9.719 1.00 3.87
H
HETATM 47 C24 UNK 1 -9.814 3.471 8.260 1.00 2.84 C
ANISOU 47 C24 UNK 1 380 350 350 130 110 110

```
C
HETATM   48 H24A UNK     1      -10.066   2.612   8.576  1.00  3.40
H
HETATM   49  C25 UNK     1      -10.428   4.003   7.132  1.00  2.16           C
ANISOU   49  C25 UNK     1      230    280    310     60     40     40
C
HETATM   50 H25A UNK     1      -11.114   3.520   6.687  1.00  2.61
H
HETATM   51  C26 UNK     1      -14.750   6.765   2.081  1.00  1.92           C
ANISOU   51  C26 UNK     1      190    300    240    -70    -40     50
C
HETATM   52 H26A UNK     1      -15.215   7.096   1.272  1.00  2.29
H
HETATM   53 H26B UNK     1      -15.437   6.520   2.752  1.00  2.29           H
HETATM   54  C27 UNK     1      -13.935   5.543   1.728  1.00  2.29           C
ANISOU   54  C27 UNK     1      230    300    340   -100    -60      0
C
HETATM   55  C28 UNK     1      -13.667   4.583   2.708  1.00  2.58           C
ANISOU   55  C28 UNK     1      280    250    450    -60    -70    -10
C
HETATM   56 H28A UNK     1      -14.097   4.647   3.553  1.00  3.08
H
HETATM   57  C29 UNK     1      -12.787   3.542   2.473  1.00  3.34           C
ANISOU   57  C29 UNK     1      400    260    610    -80   -130    -50
C
HETATM   58 H29A UNK     1      -12.608   2.899   3.147  1.00  4.03
H
HETATM   59  C30 UNK     1      -12.179   3.456   1.251  1.00  3.29           C
ANISOU   59  C30 UNK     1      240    240    770    -70    -80    -20
C
```

HETATM 60 C31 UNK 1 -12.479 4.346 0.227 1.00 3.45 C

ANISOU 60 C31 UNK 1 410 410 490 -210 90 -150

C

HETATM 61 C32 UNK 1 -13.384 5.400 0.482 1.00 2.76 C

ANISOU 61 C32 UNK 1 350 310 390 -130 -10 -60

C

HETATM 62 H32A UNK 1 -13.610 6.011 -0.211 1.00 3.32 H

HETATM 63 Cl2' UNK 1 -12.125 2.571 3.226 0.20 6.55 Cl

ANISOU 63 Cl2' UNK 1 900 280 1310 -40 -820 -70 Cl

HETATM 64 Cl1' UNK 1 -10.900 2.516 0.345 0.20 6.40 Cl

ANISOU 64 Cl1' UNK 1 280 400 1750 -30 -320 -760 Cl

CONECT 1 4 10 22 26

CONECT 2 59

CONECT 3 60

CONECT 4 1 7

CONECT 5 7

CONECT 6 23

CONECT 7 4 5 8

CONECT 8 7 9 10 36

CONECT 9 8

CONECT 10 1 8 11

CONECT 11 10 12 40

CONECT 12 11 13 21

CONECT 13 12 14 15

CONECT 14 13

CONECT 15 13 16 17

CONECT 16 15

CONECT 17 15 18 19

CONECT 18 17

CONECT 19 17 20 21

CONECT 20 19

CONECT 21 12 19 22

CONECT 22 1 21 23

CONECT 23 6 22 24

CONECT 24 23 25 26 33

CONECT 25 24

CONECT 26 1 24 27 51

CONECT 27 26 28 29 30

CONECT 28 27

CONECT 29 27

CONECT 30 27 31 32 33

CONECT 31 30

CONECT 32 30

CONECT 33 24 30 34 35

CONECT 34 33

CONECT 35 33

CONECT 36 8 37 38 39

CONECT 37 36

CONECT 38 36

CONECT 39 36

CONECT 40 11 41 49

CONECT 41 40 42 43

CONECT 42 41

CONECT 43 41 44 45

CONECT 44 43

CONECT 45 43 46 47

CONECT 46 45

CONECT 47 45 48 49

CONECT 48 47

CONECT 49 40 47 50

CONECT 50 49

CONECT 51 26 52 53 54

CONECT 52 51

CONECT 53 51

CONECT 54 51 55 61

CONECT 55 54 56 57

CONECT 56 55

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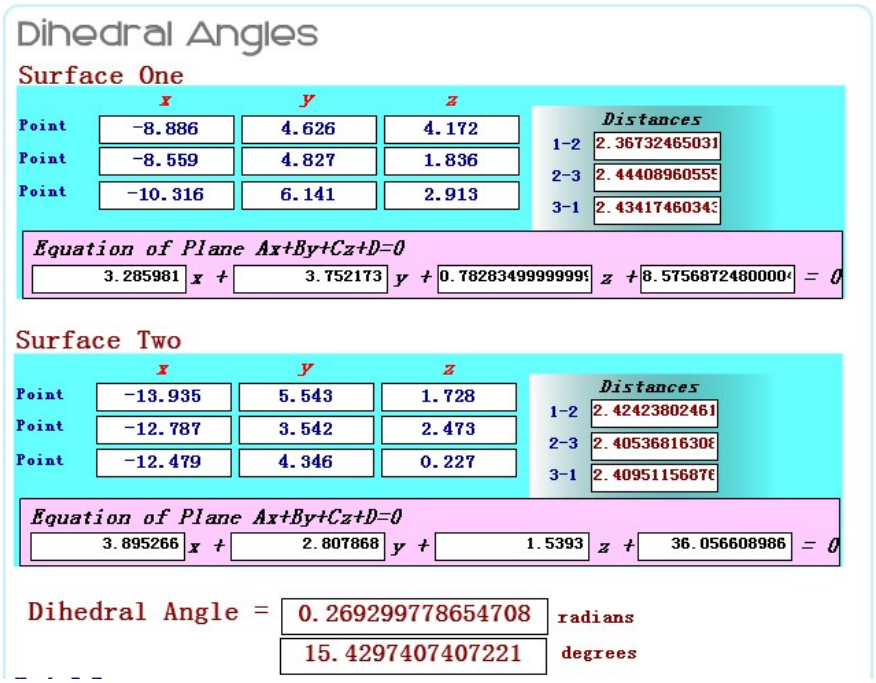
MASTER 0 0 0 0 0 0 0 3 64 0 62 0

END



F. The data for the Ni(II) Complex (*S*)(2*S*)-2f was generated from PDB files using the software Pymol.

C6, C8, C10 (as shown in red) and C23, C25, C27 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*S*)(2*S*)-**2f** as shown below.

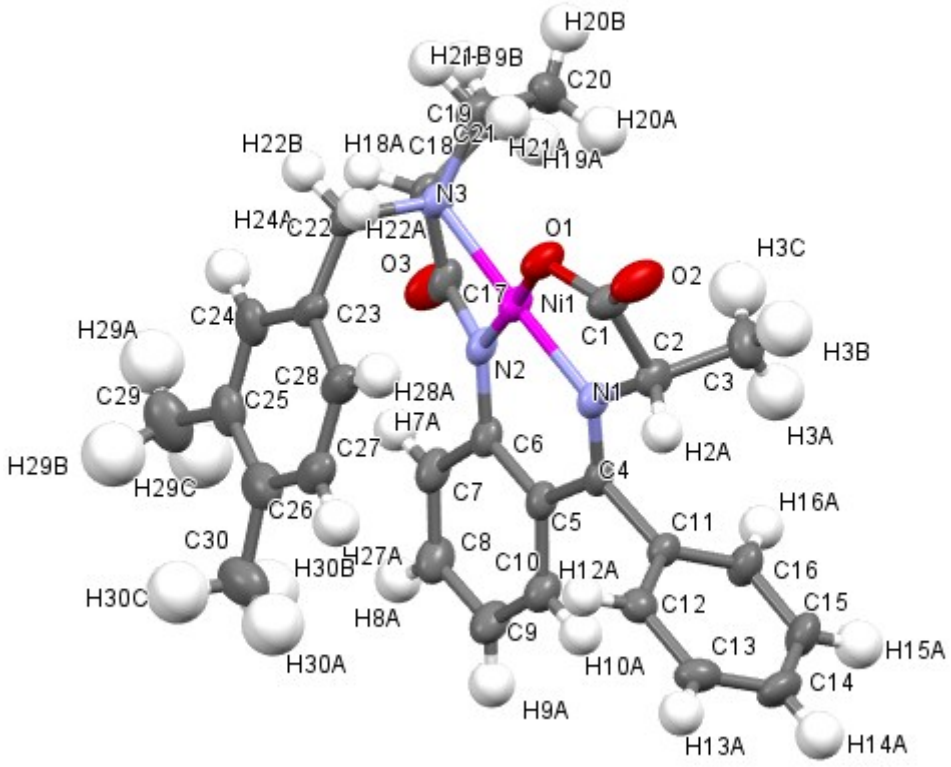


Figure S10. The crystal structure of (*S*)(2*S*)-**2f** by X-ray analysis.

HEADER CSD ENTRY Mal-4 CCDC number: 285985

CRYST1 9.3420 10.5929 26.2970 90.00 90.00 90.00 P212121

SCALE1 0.107043 0.000000 0.000000 0.000000

SCALE2 0.000000 0.094403 0.000000 0.000000

SCALE3 0.000000 0.000000 0.038027 0.000000

HETATM 1 Ni1 UNK 1 3.702 3.629 17.170 1.00 2.14 Ni

ANISOU 1 Ni1 UNK 1 270 370 175 -3 4 -51

Ni

HETATM 2 O1 UNK 1 5.176 3.619 18.306 1.00 2.84

O

ANISOU 2 O1 UNK 1 291 554 234 68 -29 -112

O

HETATM 3 O2 UNK 1 5.757 3.840 20.447 1.00 3.86

O

ANISOU 3 O2 UNK 1 389 793 284 167 -100 -168

O

HETATM 4 O3 UNK 1 1.611 2.574 14.046 1.00 3.92

O

ANISOU 4 O3 UNK 1 399 752 340 1 -81 -245

O

HETATM 5 N1 UNK 1 2.732 4.299 18.595 1.00 2.09

N

ANISOU 5 N1 UNK 1 295 323 176 -21 0 -24

N

HETATM 6 N2 UNK 1 2.294 3.694 15.964 1.00 2.09

N

ANISOU 6 N2 UNK 1 271 351 173 -40 11 -24

N

HETATM 7 N3 UNK 1 4.780 2.902 15.738 1.00 2.33

N

ANISOU 7 N3 UNK 1 319 357 211 16 10 -39

N

HETATM 8 C1 UNK 1 4.926 3.844 19.557 1.00 2.82

C

ANISOU 8 C1 UNK 1 358 469 243 92 -37 -91

C

HETATM 9 C2 UNK 1 3.446 4.053 19.877 1.00 2.57

C

ANISOU 9 C2 UNK 1 354 434 188 47 -40 -40

C

HETATM 10 H2A UNK 1 3.340 4.844 20.480 1.00 3.08

H

HETATM 11 C3 UNK 1 2.918 2.807 20.569 1.00 3.90

C

ANISOU 11 C3 UNK 1 520 601 359 32 -12 160

C

HETATM 12 H3A UNK 1 1.968 2.928 20.777 1.00 5.84

H

HETATM 13 H3B UNK 1 3.419 2.658 21.398 1.00 5.84

H

HETATM 14 H3C UNK 1 3.027 2.034 19.978 1.00 5.84

H

HETATM 15 C4 UNK 1 1.591 4.896 18.574 1.00 2.05

C

ANISOU 15 C4 UNK 1 299 279 201 -66 26 -17

C

HETATM 16 C5 UNK 1 0.844 5.118 17.332 1.00 2.20

C

ANISOU 16 C5 UNK 1 269 352 214 -52 -2 -1

C

HETATM 17 C6 UNK 1 1.182 4.522 16.088 1.00 2.23

C

ANISOU 17 C6 UNK 1 242 374 231 -75 2 1

C

HETATM 18 C7 UNK 1 0.384 4.867 14.972 1.00 2.78

C

ANISOU 18 C7 UNK 1 304 529 223 -50 -10 -3

C

HETATM 19 H7A UNK 1 0.594 4.495 14.124 1.00 3.32

H

HETATM 20 C8 UNK 1 -0.678 5.721 15.074 1.00 3.25

C

ANISOU 20 C8 UNK 1 339 619 275 -4 -42 39

C

HETATM 21 H8A UNK 1 -1.185 5.930 14.300 1.00 3.87

H

HETATM 22 C9 UNK 1 -1.028 6.286 16.292 1.00 3.22

C

ANISOU 22 C9 UNK 1 294 616 312 51 1 12

C

HETATM 23 H9A UNK 1 -1.772 6.873 16.362 1.00 3.87

H

HETATM 24 C10 UNK 1 -0.270 5.974 17.393 1.00 2.77 C

ANISOU 24 C10 UNK 1 310 483 260 4 8 -19

C

HETATM 25 H10A UNK 1 -0.506 6.355 18.232 1.00 3.32

H

HETATM 26 C11 UNK 1 0.973 5.435 19.845 1.00 2.18

C

ANISOU 26 C11 UNK 1 283 353 193 35 8 -14

C

HETATM 27 C12 UNK 1 1.381 6.663 20.333 1.00 2.47

C

ANISOU 27 C12 UNK 1 310 329 298 43 -21 14

C

HETATM 28 H12A UNK 1 2.072 7.147 19.896 1.00 3.00

H

HETATM 29 C13 UNK 1 0.764 7.186 21.473 1.00 3.03
C
ANISOU 29 C13 UNK 1 401 386 366 109 -51 -96
C
HETATM 30 H13A UNK 1 1.041 8.028 21.816 1.00 3.63
H
HETATM 31 C14 UNK 1 -0.243 6.485 22.104 1.00 3.48 C
ANISOU 31 C14 UNK 1 466 555 303 152 74 -84
C
HETATM 32 H14A UNK 1 -0.646 6.836 22.889 1.00 4.18
H
HETATM 33 C15 UNK 1 -0.663 5.272 21.594 1.00 3.54 C
ANISOU 33 C15 UNK 1 466 531 347 -19 159 24
C
HETATM 34 H15A UNK 1 -1.368 4.799 22.021 1.00 4.26
H
HETATM 35 C16 UNK 1 -0.059 4.741 20.459 1.00 2.99 C
ANISOU 35 C16 UNK 1 413 396 327 -76 97 -38
C
HETATM 36 H16A UNK 1 -0.352 3.910 20.107 1.00 3.55
H
HETATM 37 C17 UNK 1 2.463 2.892 14.869 1.00 2.68
C
ANISOU 37 C17 UNK 1 364 451 203 -80 25 -46
C
HETATM 38 C18 UNK 1 3.839 2.300 14.752 1.00 2.30
C
ANISOU 38 C18 UNK 1 365 341 168 -23 24 -48
C
HETATM 39 H18A UNK 1 4.187 2.446 13.827 1.00 2.76

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H
HETATM   40  C19 UNK     1       3.818    0.782   15.065  1.00  3.33
C
ANISOU   40  C19 UNK     1       560      354     352     -53     91     -43
C
HETATM   41 H19A UNK     1       2.894    0.475   15.244  1.00  4.03
H
HETATM   42 H19B UNK     1       4.187    0.263   14.308  1.00  4.03
H
HETATM   43  C20 UNK     1       4.686    0.622   16.300  1.00  3.70
C
ANISOU   43  C20 UNK     1       715      390     301      95     60      16
C
HETATM   44 H20A UNK     1       4.150    0.696   17.130  1.00  4.42
H
HETATM   45 H20B UNK     1       5.160   -0.248   16.296  1.00  4.42           H
HETATM   46  C21 UNK     1       5.651    1.770   16.169  1.00  3.13
C
ANISOU   46  C21 UNK     1       440      477     272     113    -24     -98
C
HETATM   47 H21A UNK     1       6.090    1.967   17.035  1.00  3.79
H
HETATM   48 H21B UNK     1       6.345    1.576   15.492  1.00  3.79
H
HETATM   49  C22 UNK     1       5.616    4.023   15.167  1.00  2.78
C
ANISOU   49  C22 UNK     1       276      451     331     -38     57     -96
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HETATM   50 H22A UNK     1       6.335    4.252   15.807  0.70  3.32
H
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HETATM 51 H22B UNK 1 6.044 3.715 14.329 0.70 3.32
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ANISOU 52 C23 UNK 1 340 250 390 -40 150 -62
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HETATM 53 C24 UNK 1 4.219 5.392 13.629 0.70 3.08
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ANISOU 53 C24 UNK 1 470 340 360 -154 30 42
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HETATM 54 H24A UNK 1 4.457 4.806 12.920 0.70 3.71
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HETATM 55 C25 UNK 1 3.282 6.407 13.423 0.70 3.37
C
ANISOU 55 C25 UNK 1 500 410 370 -190 -10 57
C
HETATM 56 C26 UNK 1 2.945 7.287 14.452 0.70 3.50
C
ANISOU 56 C26 UNK 1 350 430 550 -100 0 70
C
HETATM 57 C27 UNK 1 3.610 7.190 15.679 0.70 3.32
C
ANISOU 57 C27 UNK 1 422 380 461 -105 141 -59
C
HETATM 58 H27A UNK 1 3.434 7.823 16.367 0.70 4.03
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HETATM 59 C28 UNK 1 4.528 6.169 15.890 0.70 3.05
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ANISOU 59 C28 UNK 1 430 340 390 -85 113 -84
C

HETATM 60 H28A UNK 1 4.973 6.098 16.728 0.70 3.71
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HETATM 61 C29 UNK 1 2.638 6.505 12.095 0.70 5.00
C
ANISOU 61 C29 UNK 1 840 520 540 -200 -200 50
C
HETATM 62 H29A UNK 1 2.993 5.807 11.508 0.70 7.50
H
HETATM 63 H29B UNK 1 2.824 7.385 11.707 0.70 7.50
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HETATM 64 H29C UNK 1 1.669 6.390 12.191 0.70 7.50
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HETATM 65 C30 UNK 1 1.882 8.333 14.292 0.70 4.74
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ANISOU 65 C30 UNK 1 520 450 830 -50 -20 100
C
HETATM 66 H30A UNK 1 1.803 8.847 15.126 0.70 7.11
H
HETATM 67 H30B UNK 1 1.026 7.902 14.093 0.70 7.11
H
HETATM 68 H30C UNK 1 2.123 8.936 13.559 0.70 7.11
H
HETATM 69 H22C UNK 1 6.255 3.664 14.545 0.30 3.32
H
HETATM 70 H22D UNK 1 6.098 4.461 15.873 0.30 3.32
H
HETATM 71 C23' UNK 1 4.714 5.017 14.466 0.30 3.79 C
ANISOU 71 C23' UNK 1 490 260 690 -200 520 -320
C
HETATM 72 C24' UNK 1 4.134 6.041 15.234 0.30 3.26 C

ANISOU 72 C24' UNK 1 540 390 310 -290 120 -190
C
HETATM 73 H24B UNK 1 4.417 6.098 16.138 0.30 3.95
H
HETATM 74 C25' UNK 1 3.187 6.986 14.821 0.30 2.76 C
ANISOU 74 C25' UNK 1 300 230 520 10 170 -190
C
HETATM 75 C26' UNK 1 2.755 6.886 13.493 0.30 3.84 C
ANISOU 75 C26' UNK 1 300 240 920 40 330 70
C
HETATM 76 C27' UNK 1 3.383 5.939 12.670 0.30 2.66 C
ANISOU 76 C27' UNK 1 340 350 320 30 50 170
C
HETATM 77 H27B UNK 1 3.154 5.931 11.747 0.30 3.16
H
HETATM 78 C28' UNK 1 4.324 5.004 13.120 0.30 2.40 C
ANISOU 78 C28' UNK 1 280 270 360 10 90 -50
C
HETATM 79 H28B UNK 1 4.694 4.367 12.517 0.30 2.84
H
HETATM 80 C29' UNK 1 2.565 7.933 15.807 0.30 6.37 C
ANISOU 80 C29' UNK 1 740 130 1550 -10 810 -150
C
HETATM 81 H29D UNK 1 1.898 8.488 15.350 0.30 9.55
H
HETATM 82 H29E UNK 1 3.260 8.507 16.191 0.30 9.55
H
HETATM 83 H29F UNK 1 2.131 7.421 16.520 0.30 9.55
H
HETATM 84 C30' UNK 1 1.650 7.747 12.896 0.30 5.55 C

ANISOU 84 C30' UNK 1 450 310 1350 150 330 390

C

HETATM 85 H30D UNK 1 1.327 8.378 13.572 0.30 8.29

H

HETATM 86 H30E UNK 1 0.910 7.172 12.604 0.30 8.29

H

HETATM 87 H30F UNK 1 2.000 8.242 12.128 0.30 8.29

H

CONECT 1 2 5 6 7

CONECT 2 1 8

CONECT 3 8

CONECT 4 37

CONECT 5 1 9 15

CONECT 6 1 17 37

CONECT 7 1 38 46 49

CONECT 8 2 3 9

CONECT 9 5 8 10 11

CONECT 10 9

CONECT 11 9 12 13 14

CONECT 12 11

CONECT 13 11

CONECT 14 11

CONECT 15 5 16 26

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CONECT 28 27

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CONECT 32 31

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CONECT 34 33

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CONECT 36 35

CONECT 37 4 6 38

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CONECT 39 38

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CONECT 46 7 43 47 48

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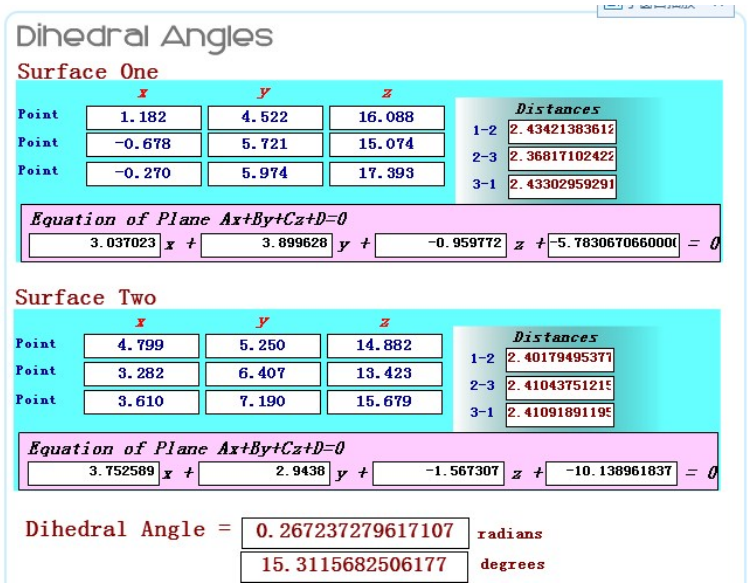

G. The data for the Ni(II) Complex (*S*)(2*S*)-2g was generated from PDB files using the software Pymol.

C5, C7, C9 (as shown in red) and C16, C18, C20 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*S*)(2*S*)-**2g** as shown below.

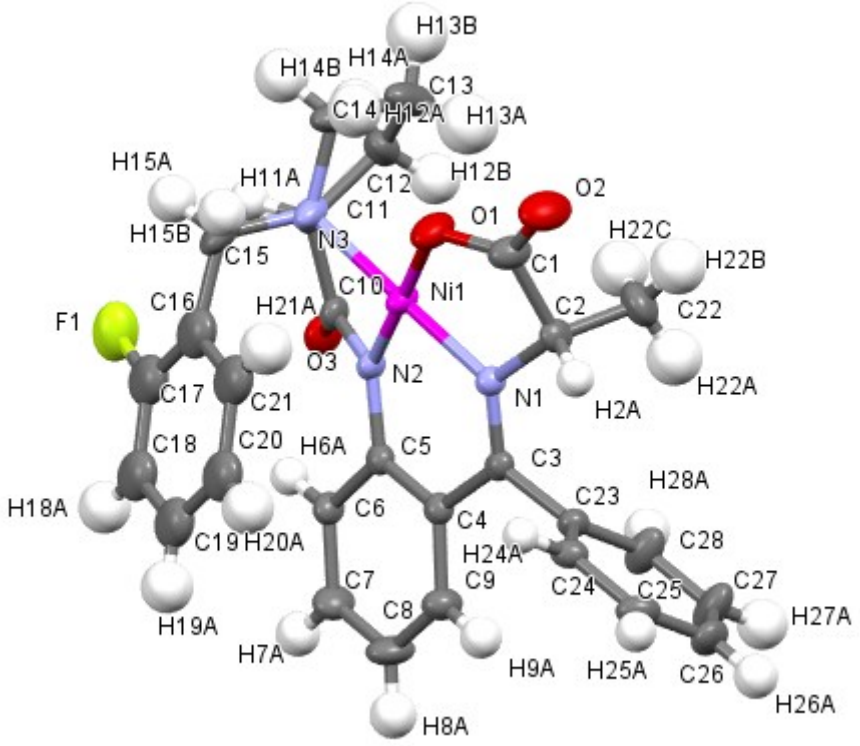

Figure S11. The crystal structure of (*S*)(2*S*)-**2g** by X-ray analysis.

HEADER CSD ENTRY VM3 CCDC number: 769563

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SCALE2 0.000000 0.100366 0.000000 0.000000

SCALE3 0.000000 0.000000 0.039244 0.000000

HETATM 1 Ni1 UNK 1 1.364 8.478 22.861 1.00 2.07 Ni

ANISOU 1 Ni1 UNK 1 418 198 169 -63 -17 -7

Ni

HETATM 2 F1 UNK 1 2.328 8.822 18.324 0.50 4.73
F
ANISOU 2 F1 UNK 1 561 802 433 131 -50 -20
F
HETATM 3 O1 UNK 1 1.529 6.975 23.938 1.00 3.16
O
ANISOU 3 O1 UNK 1 701 220 281 -62 -73 32
O
HETATM 4 O2 UNK 1 1.549 6.364 26.083 1.00 3.94
O
ANISOU 4 O2 UNK 1 790 344 363 -141 -134 155
O
HETATM 5 O3 UNK 1 -0.207 10.599 19.988 1.00 2.72
O
ANISOU 5 O3 UNK 1 431 392 212 -20 -81 11
O
HETATM 6 N1 UNK 1 1.830 9.469 24.354 1.00 1.68
N
ANISOU 6 N1 UNK 1 263 203 172 -14 -25 16
N
HETATM 7 N2 UNK 1 1.161 9.955 21.765 1.00 1.77
N
ANISOU 7 N2 UNK 1 291 230 152 -43 -11 -15
N
HETATM 8 N3 UNK 1 0.862 7.421 21.316 1.00 2.87
N
ANISOU 8 N3 UNK 1 625 233 234 -111 44 -33
N
HETATM 9 C1 UNK 1 1.558 7.217 25.217 1.00 2.76
C

ANISOU 9 C1 UNK 1 482 272 293 -80 -91 50
C
HETATM 10 C2 UNK 1 1.574 8.696 25.584 1.00 2.15
C
ANISOU 10 C2 UNK 1 361 301 154 -56 -33 43
C
HETATM 11 H2A UNK 1 2.295 8.873 26.254 1.00 2.53
H
HETATM 12 C3 UNK 1 2.291 10.676 24.389 1.00 1.67
C
ANISOU 12 C3 UNK 1 200 222 212 13 -11 -21
C
HETATM 13 C4 UNK 1 2.442 11.484 23.176 1.00 1.81
C
ANISOU 13 C4 UNK 1 272 213 204 7 6 15
C
HETATM 14 C5 UNK 1 1.844 11.156 21.930 1.00 1.75
C
ANISOU 14 C5 UNK 1 251 212 201 14 21 2
C
HETATM 15 C6 UNK 1 2.016 12.048 20.857 1.00 2.19
C
ANISOU 15 C6 UNK 1 404 255 173 -55 23 22
C
HETATM 16 H6A UNK 1 1.617 11.849 20.018 1.00 2.61
H
HETATM 17 C7 UNK 1 2.757 13.214 20.995 1.00 2.96
C
ANISOU 17 C7 UNK 1 541 272 311 -93 -12 71
C

HETATM 18 H7A UNK 1 2.858 13.799 20.253 1.00 3.55
H
HETATM 19 C8 UNK 1 3.350 13.524 22.208 1.00 3.31
C
ANISOU 19 C8 UNK 1 572 282 403 -190 -91 52
C
HETATM 20 H8A UNK 1 3.863 14.319 22.299 1.00 3.95
H
HETATM 21 C9 UNK 1 3.189 12.678 23.276 1.00 2.65
C
ANISOU 21 C9 UNK 1 420 294 293 -102 -53 24
C
HETATM 22 H9A UNK 1 3.593 12.900 24.103 1.00 3.16
H
HETATM 23 C10 UNK 1 0.305 9.749 20.717 1.00 2.19
C
ANISOU 23 C10 UNK 1 355 315 163 -44 11 -44
C
HETATM 24 C11 UNK 1 -0.073 8.293 20.538 1.00 2.50 C
ANISOU 24 C11 UNK 1 454 343 151 -151 55 -66
C
HETATM 25 H11A UNK 1 -0.041 8.048 19.570 1.00 2.92
H
HETATM 26 C12 UNK 1 -1.464 7.991 21.109 1.00 3.96 C
ANISOU 26 C12 UNK 1 530 611 363 -282 155 -121
C
HETATM 27 H12A UNK 1 -2.092 7.736 20.388 1.00 4.74
H
HETATM 28 H12B UNK 1 -1.826 8.777 21.588 1.00 4.74 H
HETATM 29 C13 UNK 1 -1.229 6.812 22.078 1.00 5.66 C

ANISOU 29 C13 UNK 1 973 884 294 -671 35 -13
C
HETATM 30 H13A UNK 1 -1.182 7.132 23.012 1.00 6.79
H
HETATM 31 H13B UNK 1 -1.960 6.147 22.003 1.00 6.79 H
HETATM 32 C14 UNK 1 0.069 6.217 21.657 1.00 4.36
C
ANISOU 32 C14 UNK 1 932 415 311 -393 12 -11
C
HETATM 33 H14A UNK 1 0.488 5.707 22.396 1.00 5.21
H
HETATM 34 H14B UNK 1 -0.043 5.623 20.872 1.00 5.21 H
HETATM 35 C15 UNK 1 2.072 6.976 20.564 1.00 3.49
C
ANISOU 35 C15 UNK 1 721 260 344 31 -50 -111
C
HETATM 36 H15A UNK 1 1.792 6.644 19.674 0.50 4.18
H
HETATM 37 H15B UNK 1 2.492 6.223 21.048 0.50 4.18
H
HETATM 38 C16 UNK 1 3.089 8.063 20.378 0.50 4.18
C
ANISOU 38 C16 UNK 1 431 573 584 110 101 -162
C
HETATM 39 C17 UNK 1 3.180 8.979 19.314 0.50 4.18
C
ANISOU 39 C17 UNK 1 431 573 584 110 101 -162
C
HETATM 40 C18 UNK 1 4.151 9.999 19.341 0.50 4.18
C

ANISOU 40 C18 UNK 1 431 573 584 110 101 -162
C
HETATM 41 H18A UNK 1 4.214 10.617 18.619 0.50 4.97
H
HETATM 42 C19 UNK 1 5.029 10.101 20.436 0.50 4.18
C
ANISOU 42 C19 UNK 1 431 573 584 110 101 -162
C
HETATM 43 H19A UNK 1 5.683 10.789 20.457 0.50 4.97
H
HETATM 44 C20 UNK 1 4.939 9.188 21.499 0.50 4.18
C
ANISOU 44 C20 UNK 1 431 573 584 110 101 -162
C
HETATM 45 H20A UNK 1 5.532 9.259 22.238 0.50 4.97
H
HETATM 46 C21 UNK 1 3.969 8.165 21.468 0.50 4.18
C
ANISOU 46 C21 UNK 1 431 573 584 110 101 -162
C
HETATM 47 H21A UNK 1 3.909 7.545 22.187 0.50 4.97
H
HETATM 48 C22 UNK 1 0.220 9.068 26.167 1.00 3.89
C
ANISOU 48 C22 UNK 1 512 533 434 -71 202 45
C
HETATM 49 H22A UNK 1 0.251 9.986 26.509 1.00 5.76
H
HETATM 50 H22B UNK 1 0.002 8.455 26.901 1.00 5.76
H

HETATM 51 H22C UNK 1 -0.466 9.000 25.471 1.00 5.76 H

HETATM 52 C23 UNK 1 2.676 11.311 25.686 1.00 1.91 C

ANISOU 52 C23 UNK 1 263 251 212 -55 -14 -13 C

HETATM 53 C24 UNK 1 3.826 10.940 26.366 1.00 1.96 C

ANISOU 53 C24 UNK 1 260 212 271 -34 -55 41 C

HETATM 54 H24A UNK 1 4.372 10.237 26.032 1.00 2.37 H

HETATM 55 C25 UNK 1 4.180 11.603 27.546 1.00 2.55 C

ANISOU 55 C25 UNK 1 352 303 314 -102 -131 63 C

HETATM 56 H25A UNK 1 4.966 11.347 28.014 1.00 3.00 H

HETATM 57 C26 UNK 1 3.393 12.630 28.038 1.00 3.03 C

ANISOU 57 C26 UNK 1 464 436 252 -131 -33 -101 C

HETATM 58 H26A UNK 1 3.638 13.079 28.838 1.00 3.55 H

HETATM 59 C27 UNK 1 2.245 13.000 27.355 1.00 3.87 C

ANISOU 59 C27 UNK 1 450 551 470 81 -63 -275 C

HETATM 60 H27A UNK 1 1.695 13.698 27.693 1.00 4.66 H

HETATM 61 C28 UNK 1 1.895 12.354 26.178 1.00 3.16

C

ANISOU 61 C28 UNK 1 343 474 383 120 -114 -160

C

HETATM 62 H28A UNK 1 1.118 12.625 25.701 1.00 3.71

H

HETATM 63 F1' UNK 1 4.175 8.487 21.810 0.50 4.72 F

ANISOU 63 F1' UNK 1 562 802 431 131 -55 -24

F

HETATM 64 H15C UNK 1 1.778 6.410 19.848 0.50 4.18

H

HETATM 65 H15D UNK 1 2.607 6.437 21.150 0.50 4.18

H

HETATM 66 C16' UNK 1 2.953 8.027 19.972 0.50 4.18 C

ANISOU 66 C16' UNK 1 431 573 584 110 101 -162

C

HETATM 67 C17' UNK 1 3.918 8.812 20.569 0.50 4.18 C

ANISOU 67 C17' UNK 1 431 573 584 110 101 -162

C

HETATM 68 C18' UNK 1 4.564 9.868 19.904 0.50 4.18 C

ANISOU 68 C18' UNK 1 431 573 584 110 101 -162

C

HETATM 69 H18B UNK 1 5.222 10.386 20.352 0.50 4.97

H

HETATM 70 C19' UNK 1 4.224 10.149 18.564 0.50 4.18 C

ANISOU 70 C19' UNK 1 431 573 584 110 101 -162

C

HETATM 71 H19B UNK 1 4.648 10.857 18.094 0.50 4.97

H

HETATM 72 C20' UNK 1 3.242 9.356 17.932 0.50 4.18 C

ANISOU 72 C20' UNK 1 431 573 584 110 101 -162

```
C
HETATM   73 H20B UNK     1       3.000   9.526  17.029  0.50  4.97
H
HETATM   74 C21' UNK     1       2.625   8.319  18.640  0.50  4.18           C
ANISOU   74 C21' UNK     1       431     573    584     110     101    -162
C
HETATM   75 H21B UNK     1       1.964   7.794  18.202  0.50  4.97
H
CONECT    1    3    6    7    8
CONECT    2   39
CONECT    3    1    9
CONECT    4    9
CONECT    5   23
CONECT    6    1   10   12
CONECT    7    1   14   23
CONECT    8    1   24   32   35
CONECT    9    3    4   10
CONECT   10    6    9   11   48
CONECT   11   10
CONECT   12    6   13   52
CONECT   13   12   14   21
CONECT   14    7   13   15
CONECT   15   14   16   17
CONECT   16   15
CONECT   17   15   18   19
CONECT   18   17
CONECT   19   17   20   21
CONECT   20   19
CONECT   21   13   19   22
CONECT   22   21
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CONECT 23 5 7 24

CONECT 24 8 23 25 26

CONECT 25 24

CONECT 26 24 27 28 29

CONECT 27 26

CONECT 28 26

CONECT 29 26 30 31 32

CONECT 30 29

CONECT 31 29

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CONECT 37 35

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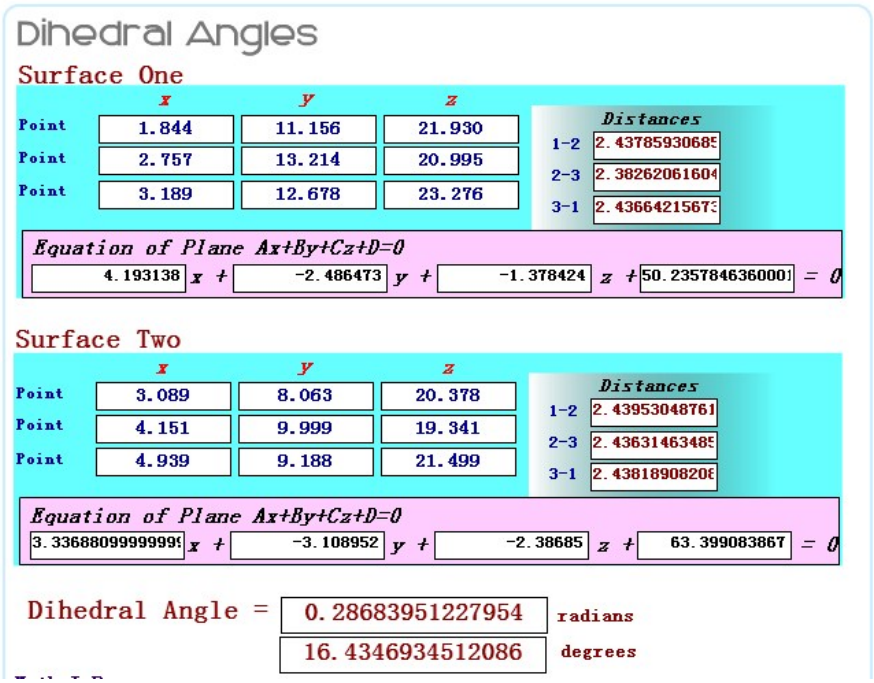

H. The data for the Ni(II) Complex (*R*)(2*R*)-2h was generated from PDB files using the software Pymol.

C5, C7, C9 (as shown in red) and C16, C18, C20 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*R*)(2*R*)-**2h** as shown below.

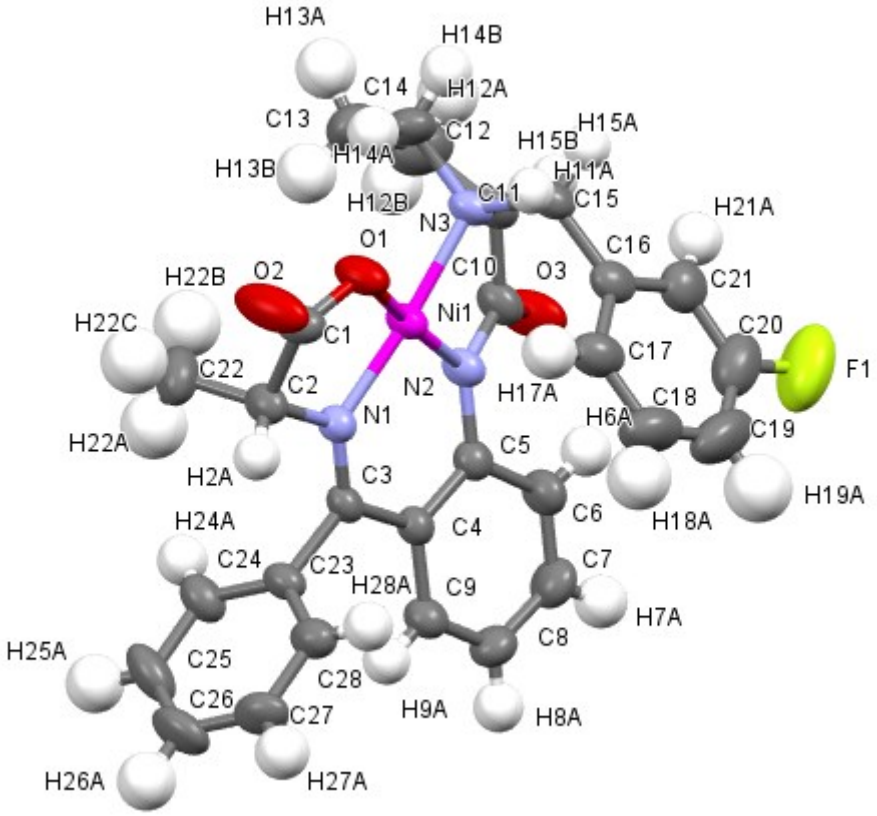

Figure S12. The crystal structure of (*R*)(2*R*)-**2h** by X-ray analysis.

HEADER CSD ENTRY VM-1 CCDC number: 769562

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SCALE2 0.000000 0.041597 0.000000 0.000000

SCALE3 0.000000 0.000000 0.080301 0.000000

HETATM 1 Ni1 UNK 1 2.019 15.990 5.813 1.00 2.74 Ni

ANISOU 1 Ni1 UNK 1 383 340 316 88 -33 -11

Ni

HETATM 2 F1 UNK 1 4.533 19.810 1.877 1.00 9.99

F

ANISOU 2 F1 UNK 1 1528 1290 978 -434 487 35

F

HETATM 3 O1 UNK 1 1.589 16.420 7.570 1.00 3.97

O

ANISOU 3 O1 UNK 1 605 549 355 259 -14 -42
O
HETATM 4 O2 UNK 1 1.949 15.823 9.662 1.00 6.40
O
ANISOU 4 O2 UNK 1 1077 1014 340 594 -43 -36
O
HETATM 5 O3 UNK 1 1.727 16.114 1.920 1.00 5.66
O
ANISOU 5 O3 UNK 1 844 954 351 390 -158 -58
O
HETATM 6 N1 UNK 1 3.053 14.617 6.510 1.00 2.65
N
ANISOU 6 N1 UNK 1 376 336 293 41 -1 2
N
HETATM 7 N2 UNK 1 2.554 15.738 4.063 1.00 2.90
N
ANISOU 7 N2 UNK 1 418 379 306 70 -51 -20
N
HETATM 8 N3 UNK 1 0.810 17.363 5.168 1.00 3.02
N
ANISOU 8 N3 UNK 1 378 370 400 97 -59 -13
N
HETATM 9 C1 UNK 1 2.041 15.607 8.463 1.00 3.45
C
ANISOU 9 C1 UNK 1 422 532 356 119 9 -41
C
HETATM 10 C2 UNK 1 2.658 14.334 7.911 1.00 3.26
C
ANISOU 10 C2 UNK 1 489 432 319 94 39 28
C

HETATM 11 H2A UNK 1 3.450 14.092 8.437 1.00 3.95
H
HETATM 12 C3 UNK 1 4.006 13.970 5.941 1.00 2.60
C
ANISOU 12 C3 UNK 1 389 267 333 29 -37 3
C
HETATM 13 C4 UNK 1 4.429 14.240 4.555 1.00 2.64
C
ANISOU 13 C4 UNK 1 383 314 307 12 -15 1
C
HETATM 14 C5 UNK 1 3.745 15.117 3.687 1.00 2.85
C
ANISOU 14 C5 UNK 1 403 317 361 5 -14 -38
C
HETATM 15 C6 UNK 1 4.348 15.399 2.446 1.00 3.87
C
ANISOU 15 C6 UNK 1 575 518 376 85 10 95
C
HETATM 16 H6A UNK 1 3.953 16.025 1.883 1.00 4.66
H
HETATM 17 C7 UNK 1 5.501 14.777 2.042 1.00 4.30
C
ANISOU 17 C7 UNK 1 569 658 409 -33 118 29
C
HETATM 18 H7A UNK 1 5.868 14.982 1.213 1.00 5.13
H
HETATM 19 C8 UNK 1 6.121 13.852 2.856 1.00 3.81
C
ANISOU 19 C8 UNK 1 437 540 472 43 104 -49
C

HETATM 20 H8A UNK 1 6.883 13.405 2.565 1.00 4.58
H
HETATM 21 C9 UNK 1 5.598 13.602 4.099 1.00 3.40
C
ANISOU 21 C9 UNK 1 475 385 432 72 5 -19
C
HETATM 22 H9A UNK 1 6.028 12.994 4.656 1.00 4.11
H
HETATM 23 C10 UNK 1 1.701 16.265 3.130 1.00 3.55
C
ANISOU 23 C10 UNK 1 545 418 385 78 -106 4
C
HETATM 24 C11 UNK 1 0.577 17.062 3.726 1.00 3.45
C
ANISOU 24 C11 UNK 1 440 435 434 62 -138 3
C
HETATM 25 H11A UNK 1 0.493 17.908 3.237 1.00 4.11
H
HETATM 26 C12 UNK 1 -0.774 16.314 3.669 1.00 5.72 C
ANISOU 26 C12 UNK 1 484 844 845 -64 -108 -245
C
HETATM 27 H12A UNK 1 -1.440 16.843 3.202 1.00 6.87
H
HETATM 28 H12B UNK 1 -0.676 15.463 3.217 1.00 6.87 H
HETATM 29 C13 UNK 1 -1.167 16.113 5.107 1.00 5.53 C
ANISOU 29 C13 UNK 1 487 691 924 -27 36 -13
C
HETATM 30 H13A UNK 1 -2.131 16.124 5.210 1.00 6.63
H
HETATM 31 H13B UNK 1 -0.819 15.275 5.450 1.00 6.63 H

HETATM 32 C14 UNK 1 -0.539 17.277 5.798 1.00 4.10 C

ANISOU 32 C14 UNK 1 365 606 587 100 -27 13

C

HETATM 33 H14A UNK 1 -0.470 17.121 6.753 1.00 4.90

H

HETATM 34 H14B UNK 1 -1.048 18.088 5.646 1.00 4.90 H

HETATM 35 C15 UNK 1 1.401 18.723 5.403 1.00 3.32

C

ANISOU 35 C15 UNK 1 454 354 455 98 -62 -65

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HETATM 36 H15A UNK 1 0.837 19.386 4.975 1.00 3.95

H

HETATM 37 H15B UNK 1 1.400 18.905 6.355 1.00 3.95

H

HETATM 38 C16 UNK 1 2.800 18.866 4.882 1.00 3.54

C

ANISOU 38 C16 UNK 1 469 312 564 10 -70 -93

C

HETATM 39 C17 UNK 1 3.885 18.538 5.692 1.00 4.58

C

ANISOU 39 C17 UNK 1 513 509 719 52 -113 -99

C

HETATM 40 H17A UNK 1 3.735 18.244 6.562 1.00 5.53

H

HETATM 41 C18 UNK 1 5.155 18.640 5.234 1.00 6.31

C

ANISOU 41 C18 UNK 1 479 757 1160 31 -44 -150

C

HETATM 42 H18A UNK 1 5.864 18.420 5.793 1.00 7.58

H

HETATM 43 C19 UNK 1 5.407 19.065 3.954 1.00 7.12
C
ANISOU 43 C19 UNK 1 552 812 1340 -161 241 -267
C
HETATM 44 H19A UNK 1 6.279 19.138 3.638 1.00 8.53
H
HETATM 45 C20 UNK 1 4.337 19.380 3.149 1.00 5.96
C
ANISOU 45 C20 UNK 1 890 606 767 -218 225 -150
C
HETATM 46 C21 UNK 1 3.030 19.297 3.604 1.00 4.43
C
ANISOU 46 C21 UNK 1 610 434 641 -70 -32 -70
C
HETATM 47 H21A UNK 1 2.321 19.530 3.049 1.00 5.29
H
HETATM 48 C22 UNK 1 1.630 13.230 7.992 1.00 5.49
C
ANISOU 48 C22 UNK 1 849 541 696 -81 275 42
C
HETATM 49 H22A UNK 1 2.010 12.414 7.656 1.00 8.21
H
HETATM 50 H22B UNK 1 0.863 13.467 7.467 1.00 8.21
H
HETATM 51 H22C UNK 1 1.366 13.107 8.908 1.00 8.21
H
HETATM 52 C23 UNK 1 4.796 12.922 6.699 1.00 2.98
C
ANISOU 52 C23 UNK 1 426 382 325 113 2 15
C

HETATM 53 C24 UNK 1 4.397 11.604 6.705 1.00 3.90
C
ANISOU 53 C24 UNK 1 674 362 447 81 -35 -2
C
HETATM 54 H24A UNK 1 3.611 11.349 6.279 1.00 4.66
H
HETATM 55 C25 UNK 1 5.182 10.658 7.355 1.00 5.17
C
ANISOU 55 C25 UNK 1 1069 381 516 161 -25 75
C
HETATM 56 H25A UNK 1 4.903 9.770 7.377 1.00 6.24
H
HETATM 57 C26 UNK 1 6.357 11.007 7.962 1.00 5.22
C
ANISOU 57 C26 UNK 1 837 631 514 331 -70 136
C
HETATM 58 H26A UNK 1 6.885 10.361 8.372 1.00 6.24
H
HETATM 59 C27 UNK 1 6.744 12.313 7.957 1.00 4.52
C
ANISOU 59 C27 UNK 1 458 793 468 140 -87 94
C
HETATM 60 H27A UNK 1 7.539 12.559 8.374 1.00 5.45
H
HETATM 61 C28 UNK 1 5.965 13.284 7.341 1.00 3.66
C
ANISOU 61 C28 UNK 1 458 529 404 105 33 41
C
HETATM 62 H28A UNK 1 6.231 14.174 7.359 1.00 4.42
H

HETATM 63 Ni2 UNK 1 8.462 19.990 12.019 1.00 2.90 Ni

ANISOU 63 Ni2 UNK 1 402 393 306 139 4 15

Ni

HETATM 64 F2 UNK 1 5.636 16.510 8.308 1.00 8.74

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ANISOU 64 F2 UNK 1 1272 996 1052 -1 -511 -303

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HETATM 65 O4 UNK 1 8.929 19.688 13.801 1.00 4.50

O

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O

HETATM 66 O5 UNK 1 8.654 20.524 15.832 1.00 6.40

O

ANISOU 66 O5 UNK 1 1077 1014 340 594 -43 -36

O

HETATM 67 O6 UNK 1 8.701 19.841 8.133 1.00 4.69

O

ANISOU 67 O6 UNK 1 631 804 346 214 106 74

O

HETATM 68 N4 UNK 1 7.519 21.467 12.627 1.00 3.16

N

ANISOU 68 N4 UNK 1 494 407 299 127 -33 -24

N

HETATM 69 N5 UNK 1 7.878 20.149 10.275 1.00 2.71

N

ANISOU 69 N5 UNK 1 374 344 311 78 17 -2

N

HETATM 70 N6 UNK 1 9.638 18.572 11.397 1.00 2.98

N

ANISOU 70 N6 UNK 1 365 368 400 85 36 62

N

HETATM 71 C29 UNK 1 8.552 20.612 14.616 1.00 5.05

C

ANISOU 71 C29 UNK 1 766 803 349 388 -71 -11

C

HETATM 72 C30 UNK 1 8.006 21.863 13.967 1.00 4.76

C

ANISOU 72 C30 UNK 1 764 692 352 333 -157 -114

C

HETATM 73 H30A UNK 1 7.268 22.225 14.502 1.00 5.68

H

HETATM 74 C31 UNK 1 6.627 22.162 12.012 1.00 2.92

C

ANISOU 74 C31 UNK 1 393 378 339 95 28 18

C

HETATM 75 C32 UNK 1 6.100 21.779 10.704 1.00 2.75

C

ANISOU 75 C32 UNK 1 380 332 333 28 -6 36

C

HETATM 76 C33 UNK 1 6.696 20.776 9.894 1.00 2.59

C

ANISOU 76 C33 UNK 1 345 314 324 12 12 35

C

HETATM 77 C34 UNK 1 6.024 20.409 8.713 1.00 3.26

C

ANISOU 77 C34 UNK 1 500 385 353 18 -38 -21

C

HETATM 78 H34A UNK 1 6.372 19.727 8.187 1.00 3.95

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HETATM 79 C35 UNK 1 4.870 21.031 8.322 1.00 3.75

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ANISOU 79 C35 UNK 1 516 485 424 -3 -142 2

C

HETATM 80 H35A UNK 1 4.439 20.756 7.545 1.00 4.50

H

HETATM 81 C36 UNK 1 4.337 22.065 9.071 1.00 3.81

C

ANISOU 81 C36 UNK 1 415 503 529 89 -105 55

C

HETATM 82 H36A UNK 1 3.578 22.516 8.778 1.00 4.58

H

HETATM 83 C37 UNK 1 4.937 22.415 10.242 1.00 3.42

C

ANISOU 83 C37 UNK 1 401 451 449 102 -38 20

C

HETATM 84 H37A UNK 1 4.564 23.095 10.753 1.00 4.11

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HETATM 85 C38 UNK 1 8.741 19.651 9.349 1.00 3.13

C

ANISOU 85 C38 UNK 1 445 346 400 53 66 -2

C

HETATM 86 C39 UNK 1 9.852 18.827 9.928 1.00 3.13

C

ANISOU 86 C39 UNK 1 425 392 371 121 116 30

C

HETATM 87 H39A UNK 1 9.902 17.970 9.454 1.00 3.71

H

HETATM 88 C40 UNK 1 11.211 19.553 9.815 1.00 4.78

C

ANISOU 88 C40 UNK 1 421 674 723 68 152 215

C

HETATM 89 H40A UNK 1 11.856 19.001 9.346 1.00 5.76

H

HETATM 90 H40B UNK 1 11.113 20.393 9.340 1.00 5.76

H

HETATM 91 C41 UNK 1 11.650 19.794 11.240 1.00 4.90

C

ANISOU 91 C41 UNK 1 400 557 905 24 14 35

C

HETATM 92 H41A UNK 1 12.616 19.763 11.319 1.00 5.92

H

HETATM 93 H41B UNK 1 11.332 20.653 11.564 1.00 5.92

H

HETATM 94 C42 UNK 1 11.010 18.661 11.988 1.00 3.92

C

ANISOU 94 C42 UNK 1 347 602 541 123 -11 -27

C

HETATM 95 H42A UNK 1 11.500 17.835 11.854 1.00 4.74

H

HETATM 96 H42B UNK 1 10.967 18.852 12.939 1.00 4.74

H

HETATM 97 C43 UNK 1 9.058 17.221 11.681 1.00 3.49

C

ANISOU 97 C43 UNK 1 427 422 478 131 68 94

C

HETATM 98 H43A UNK 1 9.578 16.547 11.217 1.00 4.18

H

HETATM 99 H43B UNK 1 9.118 17.042 12.633 1.00 4.18

H

HETATM 100 C44 UNK 1 7.629 17.119 11.251 1.00 3.67

C

ANISOU 100 C44 UNK 1 470 357 566 24 43 92

C

HETATM 101 C45 UNK 1 6.600 17.469 12.138 1.00 4.14

C

ANISOU 101 C45 UNK 1 473 540 561 38 78 113

C

HETATM 102 H45A UNK 1 6.812 17.703 13.012 1.00 4.97

H

HETATM 103 C46 UNK 1 5.287 17.474 11.745 1.00 5.26

C

ANISOU 103 C46 UNK 1 487 643 867 30 62 98

C

HETATM 104 H46A UNK 1 4.622 17.694 12.357 1.00 6.32

H

HETATM 105 C47 UNK 1 4.952 17.160 10.474 1.00 5.51

C

ANISOU 105 C47 UNK 1 515 488 1090 0 -68 18

C

HETATM 106 H47A UNK 1 4.064 17.182 10.198 1.00 6.63

H

HETATM 107 C48 UNK 1 5.948 16.812 9.604 1.00 5.30

C

ANISOU 107 C48 UNK 1 857 416 740 -97 -282 -40

C

HETATM 108 C49 UNK 1 7.287 16.776 9.959 1.00 4.36

C

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HETATM 109 H49A UNK 1 7.938 16.528 9.344 1.00 5.21

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ANISOU  110  C50 UNK     1     1048    810    898    138   -570   -204
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HETATM  111 H50A UNK     1       8.809  23.675  13.439  1.00 10.90           H
HETATM  112 H50B UNK     1       9.855  22.511  13.359  1.00 10.90           H
HETATM  113 H50C UNK     1       9.443  23.100  14.752  1.00 10.90           H
HETATM  114  C51 UNK     1       6.033  23.383  12.647  1.00  3.43
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ANISOU  114  C51 UNK     1      553    442    308    143    -42    -18
C
HETATM  115  C52 UNK     1       6.508  24.642  12.321  1.00  4.64
C
ANISOU  115  C52 UNK     1      763    421    580     39   -161    -36
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HETATM  116 H52A UNK     1       7.216  24.725  11.725  1.00  5.61
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HETATM  117  C53 UNK     1       5.947  25.765  12.865  1.00  6.47
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ANISOU  117  C53 UNK     1     1340    474    645    157   -329    -60
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HETATM  118 H53A UNK     1       6.280  26.605  12.644  1.00  7.74
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HETATM  119  C54 UNK     1       4.922  25.654  13.716  1.00  7.50
C
ANISOU  119  C54 UNK     1     1646    679    525    578   -203   -173
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HETATM  120 H54A UNK     1       4.546  26.420  14.083  1.00  9.00
H
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ANISOU 121 C55 UNK 1 1231 920 552 498 298 -15
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HETATM 122 H55A UNK 1 3.700 24.367 14.632 1.00 8.53
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HETATM 123 C56 UNK 1 4.988 23.283 13.514 1.00 5.29
C
ANISOU 123 C56 UNK 1 860 600 548 286 202 70
C
HETATM 124 H56A UNK 1 4.655 22.446 13.748 1.00 6.32
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ANISOU 125 Cl1 UNK 1 860 837 810 122 -94 -250
Cl
HETATM 126 Cl2 UNK 1 -0.945 11.316 5.219 1.00 9.43 Cl
ANISOU 126 Cl2 UNK 1 779 1938 867 437 214 49
Cl
HETATM 127 Cl3 UNK 1 1.372 12.533 4.044 1.00 10.52 Cl
ANISOU 127 Cl3 UNK 1 1536 1263 1199 -769 -197 -132
Cl
HETATM 128 C57 UNK 1 0.269 11.218 3.984 1.00 4.87
C
ANISOU 128 C57 UNK 1 495 607 747 119 40 -96
C
HETATM 129 H57A UNK 1 0.777 10.393 4.126 1.00 5.84
H
HETATM 130 O7 UNK 1 7.531 21.384 5.839 1.00 8.96
O
ANISOU 130 O7 UNK 1 1115 1450 838 261 42 -27

O

HETATM 131 H7B UNK 1 7.932 21.136 4.994 1.00 13.42

H

HETATM 132 H7C UNK 1 7.956 20.934 6.594 1.00 13.42

H

CONECT 1 3 6 7 8

CONECT 2 45

CONECT 3 1 9

CONECT 4 9

CONECT 5 23

CONECT 6 1 10 12

CONECT 7 1 14 23

CONECT 8 1 24 32 35

CONECT 9 3 4 10

CONECT 10 6 9 11 48

CONECT 11 10

CONECT 12 6 13 52

CONECT 13 12 14 21

CONECT 14 7 13 15

CONECT 15 14 16 17

CONECT 16 15

CONECT 17 15 18 19

CONECT 18 17

CONECT 19 17 20 21

CONECT 20 19

CONECT 21 13 19 22

CONECT 22 21

CONECT 23 5 7 24

CONECT 24 8 23 25 26

CONECT 25 24

CONECT 26 24 27 28 29

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CONECT 28 26

CONECT 29 26 30 31 32

CONECT 30 29

CONECT 31 29

CONECT 32 8 29 33 34

CONECT 33 32

CONECT 34 32

CONECT 35 8 36 37 38

CONECT 36 35

CONECT 37 35

CONECT 38 35 39 46

CONECT 39 38 40 41

CONECT 40 39

CONECT 41 39 42 43

CONECT 42 41

CONECT 43 41 44 45

CONECT 44 43

CONECT 45 2 43 46

CONECT 46 38 45 47

CONECT 47 46

CONECT 48 10 49 50 51

CONECT 49 48

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CONECT 52 12 53 61

CONECT 53 52 54 55

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CONECT 56 55

CONECT 57 55 58 59

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CONECT 60 59

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CONECT 64 107

CONECT 65 63 71

CONECT 66 71

CONECT 67 85

CONECT 68 63 72 74

CONECT 69 63 76 85

CONECT 70 63 86 94 97

CONECT 71 65 66 72

CONECT 72 68 71 73 110

CONECT 73 72

CONECT 74 68 75 114

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CONECT 76 69 75 77

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CONECT 105 103 106 107

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CONECT 109 108

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CONECT 111 110

CONECT 112 110

CONECT 113 110

CONECT 114 74 115 123

CONECT 115 114 116 117

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CONECT 119 117 120 121

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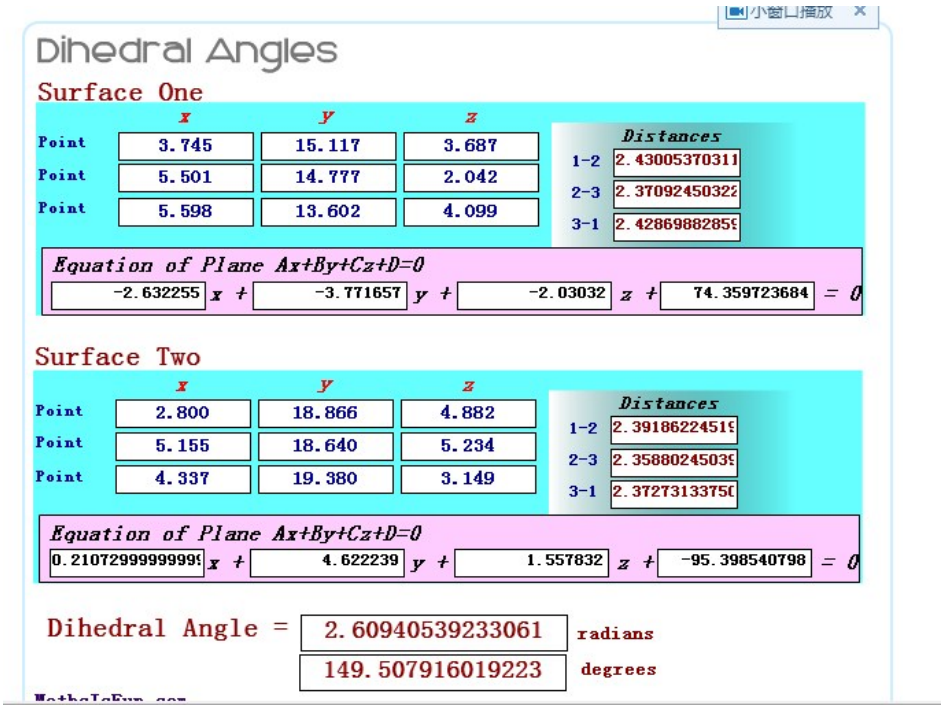

I. The data for the Ni(II) Complex (*S*)(2*S*)-5 was generated from PDB files using the software Pymol.

C1, C3, C5 (as shown in red) and C25, C27, C29 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*S*)(2*S*)-**5** (see **Figure S4** for details） as shown below.

HEADER CSD ENTRY mo_2015202_0m CCDC number: 1400951

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SCALE2 0.000000 0.091979 0.000000 0.000000

SCALE3 0.000000 0.000000 0.028871 0.000000

HETATM 1 Ni1 UNK 1 2.021 3.704 28.686 1.00 2.96 Ni

ANISOU 1 Ni1 UNK 1 583 274 269 90 79 25

Ni

HETATM 2 Cl1 UNK 1 6.073 4.880 31.141 1.00 6.25 Cl

ANISOU 2 Cl1 UNK 1 586 1101 687 44 -20 270

Cl

HETATM 3 Cl2 UNK 1 5.636 7.968 31.629 1.00 7.85 Cl

ANISOU 3 Cl2 UNK 1 759 1199 1024 -286 117 -314 Cl

HETATM 4 Cl3 UNK 1 3.384 6.965 34.811 1.00 5.23 Cl

ANISOU 4 Cl3 UNK 1 867 639 481 -128 -89 -160 Cl

HETATM 5 O1 UNK 1 0.171 7.129 28.878 1.00 4.07 O

ANISOU 5 O1 UNK 1 660 342 546 182 -80 -15 O

HETATM 6 O2 UNK 1 2.713 2.181 27.877 1.00 4.69 O

ANISOU 6 O2 UNK 1 1090 382 310 265 191 28 O

HETATM 7 O3 UNK 1 3.222 0.071 28.302 1.00 8.53 O

ANISOU 7 O3 UNK 1 2100 530 610 700 530 59 O

HETATM 8 N2 UNK 1 1.416 5.241 29.498 1.00 2.46 N

ANISOU 8 N2 UNK 1 392 255 286 42 38 14 N

HETATM 9 C7 UNK 1 2.358 3.234 31.441 1.00 2.73 C

ANISOU 9 C7 UNK 1 400 349 290 23 77 48 C

HETATM 10 N3 UNK 1 2.100 2.755 30.264 1.00 2.77 N

ANISOU 10 N3 UNK 1 510 237 307 52 50 5 N

HETATM 11 C19 UNK 1 0.804 6.130 28.620 1.00 3.06
C
ANISOU 11 C19 UNK 1 450 321 390 -25 43 2
C
HETATM 12 C20 UNK 1 0.950 5.706 27.178 1.00 3.08
C
ANISOU 12 C20 UNK 1 500 281 390 27 30 116
C
HETATM 13 H20 UNK 1 1.166 6.491 26.632 1.00 3.71
H
HETATM 14 C21 UNK 1 -0.337 5.050 26.633 1.00 5.08 C
ANISOU 14 C21 UNK 1 620 850 460 -110 -30 -90
C
HETATM 15 H21A UNK 1 -0.951 4.854 27.356 1.00 6.08
H
HETATM 16 H21B UNK 1 -0.777 5.639 26.002 1.00 6.08 H
HETATM 17 C22 UNK 1 0.096 3.779 25.953 1.00 5.68
C
ANISOU 17 C22 UNK 1 1160 530 470 -90 -210 20
C
HETATM 18 H22A UNK 1 -0.329 3.694 25.084 1.00 6.87
H
HETATM 19 H22B UNK 1 -0.138 3.006 26.490 1.00 6.87 H
HETATM 20 C23 UNK 1 1.592 3.890 25.804 1.00 4.86
C
ANISOU 20 C23 UNK 1 1070 510 268 250 0 -27
C
HETATM 21 H23A UNK 1 1.825 4.351 24.984 1.00 5.84
H
HETATM 22 H23B UNK 1 2.006 3.014 25.801 1.00 5.84

H

HETATM 23 N1 UNK 1 2.021 4.688 27.012 1.00 3.54

N

ANISOU 23 N1 UNK 1 610 435 299 120 72 61

N

HETATM 24 C24 UNK 1 3.399 5.270 26.766 1.00 4.74

C

ANISOU 24 C24 UNK 1 580 800 420 140 200 230

C

HETATM 25 H24A UNK 1 4.000 4.553 26.508 1.00 5.68

H

HETATM 26 H24B UNK 1 3.348 5.893 26.026 1.00 5.68

H

HETATM 27 C25 UNK 1 3.964 5.970 27.944 1.00 4.00

C

ANISOU 27 C25 UNK 1 450 610 460 0 190 170

C

HETATM 28 C30 UNK 1 4.672 5.240 28.897 1.00 4.16

C

ANISOU 28 C30 UNK 1 520 580 480 70 150 150

C

HETATM 29 H30 UNK 1 4.797 4.327 28.773 1.00 4.97

H

HETATM 30 C29 UNK 1 5.194 5.851 30.023 1.00 4.40

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ANISOU 30 C29 UNK 1 440 710 520 10 140 210

C

HETATM 31 C28 UNK 1 5.021 7.208 30.217 1.00 5.05

C

ANISOU 31 C28 UNK 1 460 750 710 -160 170 -10

C

HETATM 32 C27 UNK 1 4.338 7.939 29.276 1.00 5.55

C

ANISOU 32 C27 UNK 1 590 500 1020 -10 150 100

C

HETATM 33 H27 UNK 1 4.221 8.853 29.400 1.00 6.63

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HETATM 34 C26 UNK 1 3.828 7.338 28.160 1.00 5.16

C

ANISOU 34 C26 UNK 1 530 610 820 10 90 370

C

HETATM 35 H26 UNK 1 3.380 7.854 27.529 1.00 6.16

H

HETATM 36 C1 UNK 1 1.712 5.596 30.810 1.00 2.60

C

ANISOU 36 C1 UNK 1 370 282 334 -12 65 -21

C

HETATM 37 C6 UNK 1 2.298 4.665 31.705 1.00 2.48

C

ANISOU 37 C6 UNK 1 320 308 314 -27 85 4

C

HETATM 38 C14 UNK 1 1.996 1.298 29.974 1.00 3.55

C

ANISOU 38 C14 UNK 1 790 229 328 120 10 58

C

HETATM 39 H14 UNK 1 2.501 0.807 30.657 1.00 4.26

H

HETATM 40 C15 UNK 1 0.541 0.785 29.970 1.00 4.50

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ANISOU 40 C15 UNK 1 1000 269 440 -50 -80 12

C

HETATM 41 C16 UNK 1 -0.144 1.063 31.302 1.00 6.24 C

ANISOU 41 C16 UNK 1 900 830 640 -250 110 -80

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HETATM 42 H16A UNK 1 -0.158 2.009 31.464 1.00 9.40

H

HETATM 43 H16B UNK 1 0.340 0.626 32.008 1.00 9.40

H

HETATM 44 H16C UNK 1 -1.043 0.728 31.277 1.00 9.40 H

HETATM 45 C17 UNK 1 0.586 -0.727 29.750 1.00 8.32 C

ANISOU 45 C17 UNK 1 1800 280 1080 -150 -200 -110

C

HETATM 46 H17A UNK 1 -0.307 -1.062 29.642 1.00 12.48 H

HETATM 47 H17B UNK 1 0.997 -1.149 30.508 1.00 12.48 H

HETATM 48 H17C UNK 1 1.097 -0.921 28.960 1.00 12.48 H

HETATM 49 C18 UNK 1 -0.313 1.430 28.880 1.00 6.37 C

ANISOU 49 C18 UNK 1 1090 660 670 -170 -160 70

C

HETATM 50 H18A UNK 1 0.145 1.373 28.039 1.00 9.55

H

HETATM 51 H18B UNK 1 -0.468 2.353 29.099 1.00 9.55 H

HETATM 52 H18C UNK 1 -1.154 0.971 28.818 1.00 9.55 H

HETATM 53 C31 UNK 1 2.700 1.130 28.630 1.00 4.90

C

ANISOU 53 C31 UNK 1 1070 410 380 210 110 40

C

HETATM 54 C8 UNK 1 2.774 2.314 32.553 1.00 2.91

C

ANISOU 54 C8 UNK 1 510 336 259 44 3 13

C

HETATM 55 C9 UNK 1 3.983 1.632 32.459 1.00 4.11
C
ANISOU 55 C9 UNK 1 530 540 490 140 30 50
C
HETATM 56 H9 UNK 1 4.555 1.790 31.745 1.00 4.90
H
HETATM 57 C10 UNK 1 4.328 0.718 33.440 1.00 4.92
C
ANISOU 57 C10 UNK 1 570 690 610 160 -80 130
C
HETATM 58 H10 UNK 1 5.128 0.248 33.369 1.00 5.92
H
HETATM 59 C11 UNK 1 3.507 0.499 34.511 1.00 4.95
C
ANISOU 59 C11 UNK 1 760 600 520 0 -200 260
C
HETATM 60 H11 UNK 1 3.741 -0.125 35.160 1.00 5.92
H
HETATM 61 C12 UNK 1 2.338 1.204 34.623 1.00 4.53
C
ANISOU 61 C12 UNK 1 560 730 430 -90 -30 240
C
HETATM 62 H12 UNK 1 1.786 1.063 35.357 1.00 5.45
H
HETATM 63 C13 UNK 1 1.967 2.120 33.657 1.00 3.66
C
ANISOU 63 C13 UNK 1 470 530 390 60 10 96
C
HETATM 64 H13 UNK 1 1.179 2.604 33.750 1.00 4.34
H

HETATM 65 C5 UNK 1 2.788 5.119 32.948 1.00 2.96
C
ANISOU 65 C5 UNK 1 420 345 360 3 45 -13
C
HETATM 66 H5 UNK 1 3.176 4.510 33.536 1.00 3.55
H
HETATM 67 C4 UNK 1 2.701 6.436 33.306 1.00 3.55
C
ANISOU 67 C4 UNK 1 500 460 390 -100 50 -100
C
HETATM 68 C3 UNK 1 2.063 7.317 32.488 1.00 3.96
C
ANISOU 68 C3 UNK 1 700 315 490 -20 100 -80
C
HETATM 69 H3 UNK 1 1.968 8.202 32.753 1.00 4.74
H
HETATM 70 C2 UNK 1 1.559 6.920 31.278 1.00 3.46
C
ANISOU 70 C2 UNK 1 570 253 490 17 -30 -30
C
HETATM 71 H2 UNK 1 1.104 7.538 30.751 1.00 4.18
H
CONECT 1 6 8 10 23
CONECT 2 30
CONECT 3 31
CONECT 4 67
CONECT 5 11
CONECT 6 1 53
CONECT 7 53
CONECT 8 1 11 36

CONECT 9 10 37 54

CONECT 10 1 9 38

CONECT 11 5 8 12

CONECT 12 11 13 14 23

CONECT 13 12

CONECT 14 12 15 16 17

CONECT 15 14

CONECT 16 14

CONECT 17 14 18 19 20

CONECT 18 17

CONECT 19 17

CONECT 20 17 21 22 23

CONECT 21 20

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CONECT 23 1 12 20 24

CONECT 24 23 25 26 27

CONECT 25 24

CONECT 26 24

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CONECT 28 27 29 30

CONECT 29 28

CONECT 30 2 28 31

CONECT 31 3 30 32

CONECT 32 31 33 34

CONECT 33 32

CONECT 34 27 32 35

CONECT 35 34

CONECT 36 8 37 70

CONECT 37 9 36 65

CONECT 38 10 39 40 53

CONECT 39 38

CONECT 40 38 41 45 49

CONECT 41 40 42 43 44

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CONECT 54 9 55 63

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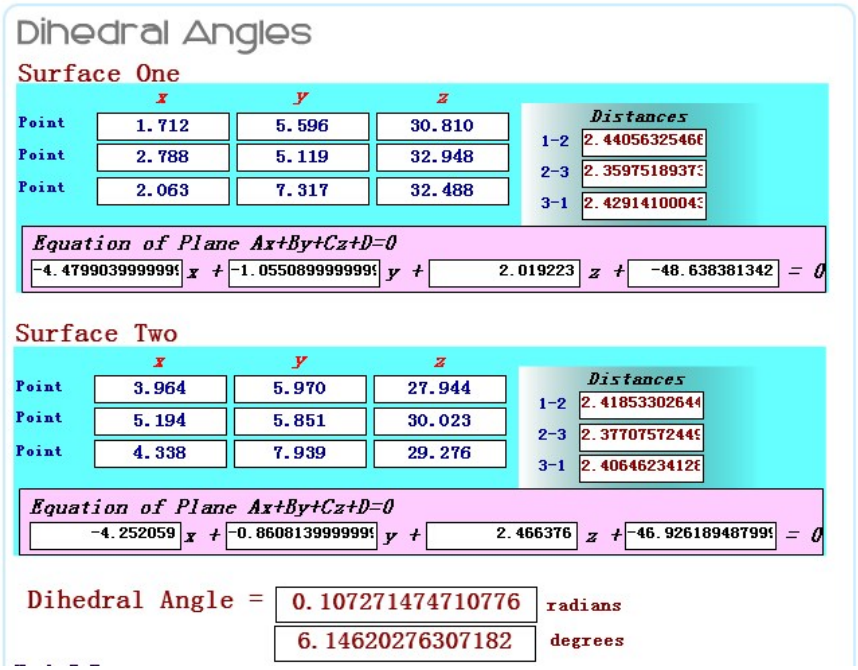
MASTER 0 0 0 0 0 0 0 3 71 0 71 0

END



J. The data for the Ni(II) Complex (*R*)(2*R*)-6 was generated from PDB files using the software Pymol.

C5, C7, C9 (as shown in red) and C16, C18, C20 (as shown in blue) were selected and calculated *via* http://www.mathsisfun.com/geometry/dihedral-angles.html to estimate the degree of parallelity of the *o*-amino-benzophenone and benzyl rings in the Ni(II) Complex (*R*)(2*R*)-**6** (see **Figure S5** for details） as shown below.

CRYST1 10.143 9.381 17.036 90.00 96.51 90.00 P 1 21 1

CCDC number: 1422992

SCALE1 0.098592 0.000000 0.011256 0.000000

SCALE2 0.000000 0.106597 0.000000 0.000000

SCALE3 0.000000 0.000000 0.059080 0.000000

ATOM 1 NI1 0 0.363 2.031 11.306 1.000 2.41

ATOM	2	CL1	0	-0.890	1.875	18.126	1.000	6.17
ATOM	3	CL2	0	-3.099	0.094	14.366	1.000	10.32
ATOM	4	CL3	0	-4.298	2.605	15.609	1.000	9.62
ATOM	5	N1	0	1.232	0.885	12.416	1.000	2.43
ATOM	6	N2	0	0.069	3.297	12.577	1.000	2.61
ATOM	7	N3	0	-0.619	3.149	10.147	1.000	3.23
ATOM	8	N5	0	4.727	2.807	9.403	1.000	4.80
ATOM	9	H5A	0	5.113	3.044	8.672	1.000	5.76
ATOM	10	O1	0	1.831	-0.976	9.531	1.000	4.17
ATOM	11	O2	0	0.638	0.787	10.008	1.000	3.38
ATOM	12	O3	0	-0.209	5.559	12.652	1.000	4.19
ATOM	13	O4	0	8.596	7.781	11.532	1.000	8.84
ATOM	14	H4	0	9.087	7.175	11.784	1.000	13.26
ATOM	15	C1	0	1.462	-0.123	10.296	1.000	3.48
ATOM	16	C2	0	2.015	-0.082	11.652	1.000	2.54
ATOM	17	H2	0	1.915	-0.966	12.062	1.000	3.04
ATOM	18	C3	0	1.166	0.831	13.677	1.000	2.41
ATOM	19	C4	0	0.435	1.805	14.441	1.000	2.33
ATOM	20	C5	0	0.140	1.507	15.734	1.000	3.12
ATOM	21	H5	0	0.394	0.679	16.072	1.000	3.75
ATOM	22	C6	0	-0.492	2.347	16.527	1.000	3.08
ATOM	23	C7	0	-0.842	3.556	16.078	1.000	3.55
ATOM	24	H7	0	-1.261	4.158	16.650	1.000	4.26
ATOM	25	C8	0	-0.590	3.913	14.786	1.000	3.46
ATOM	26	H8	0	-0.826	4.762	14.488	1.000	4.16
ATOM	27	C9	0	0.005	3.036	13.926	1.000	2.54
ATOM	28	C10	0	-0.136	4.505	12.082	1.000	3.00
ATOM	29	C11	0	-0.376	4.498	10.590	1.000	2.80
ATOM	30	H11	0	-1.132	5.077	10.359	1.000	3.36
ATOM	31	C12	0	0.881	4.943	9.861	1.000	4.38

ATOM	32	H12	0	0.760	5.820	9.464	1.000	5.25
ATOM	33	H12	0	1.640	4.972	10.464	1.000	5.25
ATOM	34	C13	0	1.069	3.918	8.827	1.000	4.84
ATOM	35	H13	0	1.281	4.331	7.975	1.000	5.80
ATOM	36	H13	0	1.792	3.320	9.070	1.000	5.80
ATOM	37	C14	0	-0.181	3.193	8.740	1.000	4.14
ATOM	38	H14	0	-0.047	2.301	8.385	1.000	4.97
ATOM	39	H14	0	-0.824	3.663	8.186	1.000	4.97
ATOM	40	C15	0	-2.039	2.765	10.198	1.000	3.66
ATOM	41	H15	0	-2.553	3.407	9.685	1.000	4.39
ATOM	42	H15	0	-2.142	1.899	9.774	1.000	4.39
ATOM	43	C16	0	-2.589	2.694	11.541	1.000	3.24
ATOM	44	C17	0	-2.590	1.500	12.252	1.000	4.56
ATOM	45	H17	0	-2.228	0.732	11.872	1.000	5.47
ATOM	46	C18	0	-3.133	1.453	13.531	1.000	5.30
ATOM	47	C19	0	-3.674	2.600	14.099	1.000	5.57
ATOM	48	C20	0	-3.673	3.795	13.388	1.000	5.51
ATOM	49	H20	0	-4.035	4.562	13.768	1.000	6.61
ATOM	50	C21	0	-3.131	3.842	12.109	1.000	5.54
ATOM	51	H21	0	-3.130	4.641	11.634	1.000	6.64
ATOM	52	C22	0	3.491	0.283	11.620	1.000	3.26
ATOM	53	H22	0	3.802	0.353	12.536	1.000	3.91
ATOM	54	H22	0	3.973	-0.452	11.208	1.000	3.91
ATOM	55	C23	0	3.864	1.526	10.914	1.000	3.22
ATOM	56	C24	0	4.438	1.548	9.734	1.000	4.33
ATOM	57	H24	0	4.616	0.801	9.210	1.000	5.20
ATOM	58	C25	0	4.326	3.670	10.382	1.000	4.71
ATOM	59	C26	0	3.759	2.859	11.371	1.000	2.56
ATOM	60	C27	0	3.317	3.462	12.498	1.000	3.89
ATOM	61	H27	0	2.932	2.965	13.183	1.000	4.67

ATOM	62	C28	0	3.447	4.824	12.610	1.000	5.33
ATOM	63	H28	0	3.152	5.249	13.383	1.000	6.40
ATOM	64	C29	0	3.985	5.543	11.640	1.000	6.49
ATOM	65	H29	0	4.072	6.460	11.764	1.000	7.79
ATOM	66	C30	0	4.397	5.028	10.523	1.000	5.72
ATOM	67	H30	0	4.730	5.565	9.841	1.000	6.86
ATOM	68	C31	0	1.793	-0.223	14.399	1.000	2.96
ATOM	69	C32	0	2.995	0.029	15.052	1.000	3.96
ATOM	70	H32	0	3.382	0.873	15.004	1.000	4.75
ATOM	71	C33	0	3.618	-0.982	15.775	1.000	5.09
ATOM	72	H33	0	4.421	-0.813	16.211	1.000	6.11
ATOM	73	C34	0	3.039	-2.244	15.846	1.000	5.50
ATOM	74	H34	0	3.456	-2.920	16.329	1.000	6.60
ATOM	75	C35	0	1.838	-2.495	15.193	1.000	4.95
ATOM	76	H35	0	1.451	-3.339	15.241	1.000	5.94
ATOM	77	C36	0	1.215	-1.485	14.470	1.000	3.46
ATOM	78	H36	0	0.411	-1.653	14.034	1.000	4.15
ATOM	79	C37	0	7.289	7.364	11.588	1.000	10.05
ATOM	80	H37	0	7.232	6.559	12.109	1.000	15.08
ATOM	81	H37	0	6.969	7.193	10.699	1.000	15.08
ATOM	82	H37	0	6.752	8.047	11.995	1.000	15.08

Dihedral Angles

Surface One

	x	y	z
Point	0.140	1.507	15.734
Point	-0.842	3.556	16.078
Point	0.005	3.036	13.926

Distances	
1-2	2.29805591750
2-3	2.37042464550
3-1	2.37169348778

Equation of Plane Ax+By+Cz+D=0

-4.230568 x + -1.821896 y + -1.224863 z + 22.609871234 = 0

Surface Two

	x	y	z
Point	-2.589	2.694	11.541
Point	-3.133	1.453	13.531
Point	-3.673	3.795	13.388

Distances	
1-2	2.40751261678
2-3	2.40769869377
3-1	2.40804194315

Equation of Plane Ax+By+Cz+D=0

-4.483117 x + -1.152392 y + -1.944188 z + 13.935627843 = 0

Dihedral Angle = 0.201130624418388 radians

11.5239359100045 degrees