Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular Oxygen Reduction Catalyzed by a Highly Oxidative Resistant Complex of Cobalt-hydrazone at Liquid/Liquid Interface

Mohammad-AliKamyabi[a,*], Fatemeh Soleymani-Bonoti[a], Rahman Bikas[a], Hassan Hosseini-Monfared[a], Nematollah Arshadi[a], Milosz Siczek[b] and Tadeusz Lis[b]

[a] *Department of Chemistry, Faculty of Science, University of Zanjan 45371-38791, Zanjan, Iran*

[b] *Faculty of Chemistry, University of Wroclaw, Joliot-Curie 14, Wroclaw 50-383, Poland*

Section (I):

Characterization of bis-[(E)-N'-(phenyl(pyridin-2-yl)methylene)]carbohydrazide (HL)

FT-IR (KBr, cm^{-1}): 3361 (m), 3323 (w), 3056 (w), 2868 (w), 1689 (vs, C=O), 1633 (vs), 1570 (s), 1505 (s), 1466 (s), 1429 (s), 1344 (m), 1283 (s), 1199 (m), 1132 (s), 1094 (m), 1048 (m), 992 (s), 963 (s), 908 (s), 800 (m), 763 (m), 726 (w), 698 (s), 616 (m), 524 (m), 493 (m), 493 (m), 459 (s), 404 (w). ^{1}H NMR (250 MHz, DMSO-d_6, TMS): δ = 7.26 (d, 2H, *J* =7.5 Hz), 7.31 – 7.33 (m, 2H), 7.42 (t, 1H, *J* = 3.6 Hz), 7.47 – 7.98 (tt, 1H, *J* =7.4 Hz, *J* =2.9 Hz), 7.53-7.57 (m, 4H), 7.66 – 7.69 (m, 1H), 7.85 (t, 1H, *J* = 7.2 Hz), 7.97 (dd, 1H, *J* = 7.7 Hz, *J* = 1.4 Hz), 8.00 (td, 1H, *J* = 7.80 Hz, *J* = 1.1 Hz), 8.82 (dt, 1H, *J* = 7.7 Hz, *J* = 1.7 Hz), 8.42 (d, 1H, *J* =4.3 Hz), 8.73 (m, 1H), 11.43 (s, br, 2H, N-H). ^{13}C NMR (62.90 MHz, DMSO-d_6): δ = 123.7, 124.6, 127.2, 128.7, 129.0, 129.5, 131.0, 133.4, 136.8, 138.1, 148.8, 149.0, 162.4 ppm. UV–Vis (in CH_3OH, c = 5×10^{-5}mol dm^{-3}, λ_{max} [nm] with ε [M^{-1} cm^{-1}]): 214 (24 600), 296 (21 500), 384 nm (2 300).

Two tautomeric structures of keto and enol forms were expected for HL (Scheme 1). It was found that HL is stable in keto form in solid state and in solution. In ^{1}H-NMR spectrum of HL the presence of a signal at *δ* 11.43 ppm was assigned to the common N-H group, which was consistent with the observation of a rapid loss of this signal when D_2O was added to the solution. Existence of free HL in keto form was also confirmed by a broad band at 3323 cm^{-1} due to the N-H and a very strong band at 1689 cm^{-1} due to the C=O stretching vibration in the IR spectrum of HL.

Section (II):

Characterization of the catalyst CoL

FT-IR (KBr, cm^{-1}): 3421 (s, br), 2924 (m), 2853 (m), 1675 (vs), 1618 (s), 1597 (m), 1564 (m), 1464 (s), 1442 (s), 1384 (m), 1323 (s), 1279 (s), 1264 (vs), 1239 (s), 1233 (s), 1210 (m), 1133 (vs), 1110 (m), 1018 (s), 792 (m), 779 (s), 754 (m), 744 (s), 701 (s), 646 (s), 634 (m), 586 (m), 505 (m), 444 (m). UV–Vis (in CH_3OH, c = 60 × 10^{-5}mol dm^{-3}, λ_{max} [nm] with ε [M^{-1} cm^{-1}]): 390 (1.695 × 10^4), 510 nm (1.012 × 10^4).

By comparing the IR spectrum of the complex with that of the free ligand it can be seen that, the C=O band remains in the IR spectrum of the $[Co(L)(Cl)_2]CH_3OH$,but has shifted to lower frequencies (1689 cm^{-1}in HL, 1675 cm^{-1}in $[Co(L)(Cl)_2]CH_3OH$. This finding suggests that the coordinated ligand is still in keto form. The presence of a C=O stretching vibration band, ν(C=O), at 1660 cm^{-1}suggests the absence of enolization and delocalization in the –N-C=O group in the coordinated ligand $(L)^{3-}$ [50]. The band at 1618 cm^{-1} suggests the coordination of azomethine nitrogen (C=N) to the metal core. The very broad band around 3400 cm^{-1} in IR spectra of the complex is attributed to the O−H groups of methanol molecules utilized in hydrogen bonding.

Table S_1. Crystallographic data of complex $[Co(L)Cl_2]\cdot CH_3OH$

	complex $[Co(L)Cl_2]\cdot CH_3OH$
Formula	$C_{25}H_{19}Cl_2CoN_6O\cdot CH_4O$
Formula weight	581.33
Crystal system	Triclinic
Space group	$P\bar{1}$
a(Å)	8.924 (3)
b(Å)	10.108(3)
c(Å)	14.354 (5)
α(°)	91.53 (3)
β(°)	103.39(3)
γ(°)	100.48 (3)
V(Å^3)	1235.4(7)
Z	2
D_x(g cm^{-3})	1.563
F(000)	596
μ(mm^{-1})	0.95
Crystal shape (color)	Block (Brown)
Crystal size (mm)	0.28 × 0.19 × 0.13
Θ range (^{0})	2.9–35.1
hkl range	-14 → 10
	-16 → 16
	-18 → 23

Reflections	
Collected	19511
Unique (R_{int})	8790 (0.037)
with $I>2\sigma(I)$	5594
$R(F)$ $[I>2\sigma(I)]$	0.050
$wR(F^2)$ [all data]	0.114
Goodness of fit	1.00
Parameters, Restraints	336, 0
$\Delta\rho_{max}/\Delta\rho_{min}$ (e $Å^{-3}$)	1.31/-0.69

Table S_2. Selected bond lengths (Å) and angles (degree) in $[Co(L)Cl_2]\cdot CH_3OH$

Co—N3	1.8652 (18)	N3—Co—N5	83.36 (8)
Co—N5	1.868 (2)	N3—Co—N2	172.10 (8)
Co—N2	1.9381 (18)	N5—Co—N2	90.60 (8)
Co—N1	2.011 (2)	N3—Co—N1	81.56 (8)
Co—Cl2	2.2450 (9)	N5—Co—N1	164.40 (7)
Co—Cl1	2.2495 (9)	N2—Co—N1	104.76 (8)
C2—O1	1.219 (3)	N3—Co—Cl2	93.57 (6)
C2—N5	1.390 (3)	N5—Co—Cl2	89.66 (6)
C2—N4	1.387 (3)	N2—Co—Cl2	91.47 (6)
N5—N6	1.347 (2)	N1—Co—Cl2	87.32 (6)
		N3—Co—Cl1	85.87 (6)
		N5—Co—Cl1	91.74 (6)
		N2—Co—Cl1	89.25 (6)
		N1—Co—Cl1	91.14 (6)
		Cl2—Co—Cl1	178.43 (2)

Section (III):

Calculation of the Galvani potential difference across theliquid|liquid interface

The Galvani potential difference across the liquid|liquid interface was controlled by the distribution of all the ions between the two phases. In order to calculate this potential, we first considered the Nernst-Donnan equation [1,2], for the different ionic species "i" present in the system:

$$\Delta^{W}_{O}\Phi = \Delta^{W}_{O}\Phi_i^{\Phi'w\rightarrow O} + (RT/Fz_i)\ln(c_i^{O}/c_i^{W}) \quad \text{(S 1)}$$

The mass balance for the species *i* is

$$(V^{O}/V^{W})\, c_{i,\,initial}{}^{O} + c_{i,\,initial}{}^{W} = (V^{O}/V^{W})\, c_i^{O} + c_i^{W} \quad \text{(S 2)}$$

$c_{i,\,initial}{}^{O}w$ and $c_{i,\,initial}{}^{W}$ → initial concentrations of the species i in the organic and aqueous phases, respectively.

c_i^{O} and c_i^{W} → The concentrations at the equilibrium.

$V^{O}/V^{W}\approx 1$

Additionally, electro neutrality condition of the both phases must be fulfilled:

For electro neutrality condition → $\sum z_i c_i^{o} = \sum z_i c_i^{w} = 0$ (S 3)

After being combined eq (S 3) with eqs. (S 1) and (S 2)

$$\sum z_i[C_i^{total}/(1+\exp(F/RT(\Delta^{W}_{O}\Phi - \Delta^{W}_{O}\Phi_i^{\Phi'w\rightarrow O})))] = 0 \qquad \text{(S 4)}$$

After solving the eq (S4), by iteration gives the Galvani potential difference of the system in equilibrium. This potential was calculated and found to be 0.536V

Section (IV):

Information of the DFT-B3LYP/ 6-31 G** optimized geometries

$[Co(L)Cl_2]\cdot$

HEADER

REMARK Spartan '08 exported M0001

HETATM	1	Co	UNK	0001	-0.082	-0.121	0.505
HETATM	2	N	UNK	0001	1.355	0.328	1.894
HETATM	3	C	UNK	0001	3.255	1.393	3.638
HETATM	4	C	UNK	0001	1.439	1.673	2.088
HETATM	5	C	UNK	0001	2.245	-0.461	2.505
HETATM	6	C	UNK	0001	3.206	0.023	3.390
HETATM	7	C	UNK	0001	2.368	2.231	2.970
HETATM	8	H	UNK	0001	2.191	-1.516	2.269
HETATM	9	H	UNK	0001	3.896	-0.666	3.863
HETATM	10	H	UNK	0001	2.391	3.305	3.107
HETATM	11	H	UNK	0001	3.984	1.807	4.328
HETATM	12	N	UNK	0001	-0.265	-2.060	0.551
HETATM	13	C	UNK	0001	-0.503	-4.825	0.783
HETATM	14	C	UNK	0001	-0.081	-2.682	1.733
HETATM	15	C	UNK	0001	-0.641	-2.786	-0.535
HETATM	16	C	UNK	0001	-0.760	-4.187	-0.418
HETATM	17	C	UNK	0001	-0.164	-4.054	1.895
HETATM	18	H	UNK	0001	0.103	-2.036	2.580

HETATM 19 H UNK 0001 -1.082 -4.753 -1.281

HETATM 20 H UNK 0001 0.007 -4.493 2.871

HETATM 21 H UNK 0001 -0.599 -5.904 0.860

HETATM 22 C UNK 0001 0.535 2.481 1.267

HETATM 23 C UNK 0001 0.423 3.962 1.353

HETATM 24 C UNK 0001 0.175 6.745 1.479

HETATM 25 C UNK 0001 1.256 4.780 0.574

HETATM 26 C UNK 0001 -0.539 4.546 2.193

HETATM 27 C UNK 0001 -0.659 5.935 2.253

HETATM 28 C UNK 0001 1.131 6.168 0.641

HETATM 29 H UNK 0001 1.992 4.325 -0.082

HETATM 30 H UNK 0001 -1.186 3.910 2.789

HETATM 31 H UNK 0001 -1.405 6.383 2.903

HETATM 32 H UNK 0001 1.776 6.797 0.035

HETATM 33 H UNK 0001 0.077 7.825 1.527

HETATM 34 N UNK 0001 -0.158 1.765 0.437

HETATM 35 N UNK 0001 -1.066 2.218 -0.422

HETATM 36 C UNK 0001 -1.713 1.276 -1.263

HETATM 37 O UNK 0001 -2.484 1.647 -2.119

HETATM 38 N UNK 0001 -1.303 -0.011 -0.925

HETATM 39 N UNK 0001 -1.480 -0.896 -1.887

HETATM 40 C UNK 0001 -1.084 -2.131 -1.783

HETATM 41 H UNK 0001 -1.600 -4.861 -6.403

HETATM 42 C UNK 0001 -1.498 -4.323 -5.465

HETATM 43 C UNK 0001 -1.237 -2.931 -3.033

```
HETATM   44  C   UNK  0001      -0.343  -4.468  -4.695
HETATM   45  C   UNK  0001      -2.517  -3.475  -5.025
HETATM   46  C   UNK  0001      -2.388  -2.784  -3.822
HETATM   47  C   UNK  0001      -0.212  -3.776  -3.491
HETATM   48  H   UNK  0001       0.465  -5.109  -5.036
HETATM   49  H   UNK  0001      -3.416  -3.351  -5.621
HETATM   50  H   UNK  0001      -3.170  -2.112  -3.486
HETATM   51  H   UNK  0001       0.704  -3.871  -2.913
HETATM   52 Cl   UNK  0001      -1.711   0.040   2.125
HETATM   53  H   UNK  0001      -1.287   3.203  -0.488
HETATM   54 Cl   UNK  0001       1.659  -0.232  -0.974
CONECT    1   12    2   38   34
CONECT    1   52   54
CONECT    2    5    4    1
CONECT    3    6    7   11
CONECT    4    7    2   22
CONECT    5    2    6    8
CONECT    6    5    3    9
CONECT    7    3    4   10
CONECT    8    5
CONECT    9    6
CONECT   10    7
CONECT   11    3
CONECT   12   15   14    1
CONECT   13   16   17   21
```

CONECT 14 17 12 18

CONECT 15 12 16 40

CONECT 16 15 13 19

CONECT 17 13 14 20

CONECT 18 14

CONECT 19 16

CONECT 20 17

CONECT 21 13

CONECT 22 4 23 34

CONECT 23 26 25 22

CONECT 24 27 28 33

CONECT 25 28 23 29

CONECT 26 23 27 30

CONECT 27 26 24 31

CONECT 28 24 25 32

CONECT 29 25

CONECT 30 26

CONECT 31 27

CONECT 32 28

CONECT 33 24

CONECT 34 22 35 1

CONECT 35 34 36 53

CONECT 36 35 37 38

CONECT 37 36

CONECT 38 36 39 1

CONECT 39 38 40

CONECT 40 39 43 15

CONECT 41 42

CONECT 42 41 45 44

CONECT 43 46 47 40

CONECT 44 47 42 48

CONECT 45 42 46 49

CONECT 46 45 43 50

CONECT 47 43 44 51

CONECT 48 44

CONECT 49 45

CONECT 50 46

CONECT 51 47

CONECT 52 1

CONECT 53 35

CONECT 54 1

END

$[Co(L)Cl_2]$·-N1H

HEADER

REMARK Spartan '08 exported M0001

HETATM 1 Co UNK 0001 -0.031 -0.109 0.616

HETATM 2 N UNK 0001 1.446 0.342 1.880

HETATM 3 C UNK 0001 3.383 1.381 3.595

HETATM 4 C UNK 0001 1.523 1.686 2.104

HETATM 5 C UNK 0001 2.362 -0.455 2.440

HETATM 6 C UNK 0001 3.346 0.021 3.306

HETATM 7 C UNK 0001 2.465 2.227 2.977

HETATM 8 H UNK 0001 2.317 -1.504 2.177

HETATM 9 H UNK 0001 4.061 -0.671 3.735

HETATM 10 H UNK 0001 2.475 3.296 3.154

HETATM 11 H UNK 0001 4.125 1.783 4.278

HETATM 12 N UNK 0001 -0.204 -2.078 0.634

HETATM 13 C UNK 0001 -0.430 -4.861 0.821

HETATM 14 C UNK 0001 0.031 -2.724 1.787

HETATM 15 C UNK 0001 -0.627 -2.802 -0.442

HETATM 16 C UNK 0001 -0.739 -4.197 -0.362

HETATM 17 C UNK 0001 -0.051 -4.106 1.924

HETATM 18 H UNK 0001 0.259 -2.100 2.641

HETATM 19 H UNK 0001 -1.098 -4.747 -1.221

HETATM 20 H UNK 0001 0.164 -4.562 2.883

HETATM 21 H UNK 0001 -0.517 -5.940 0.882

HETATM 22 C UNK 0001 0.580 2.502 1.324

HETATM 23 C UNK 0001 0.473 3.978 1.396

HETATM 24 C UNK 0001 0.226 6.759 1.495

HETATM 25 C UNK 0001 1.549 4.794 1.009

HETATM 26 C UNK 0001 -0.728 4.562 1.833

HETATM 27 C UNK 0001 -0.845 5.950 1.884

HETATM 28 C UNK 0001 1.419 6.181 1.059

```
HETATM   29  H   UNK  0001       2.471   4.345   0.653
HETATM   30  H   UNK  0001      -1.553   3.931   2.150
HETATM   31  H   UNK  0001      -1.770   6.399   2.230
HETATM   32  H   UNK  0001       2.249   6.810   0.751
HETATM   33  H   UNK  0001       0.129   7.839   1.534
HETATM   34  N   UNK  0001      -0.150   1.772   0.541
HETATM   35  N   UNK  0001      -1.088   2.230  -0.317
HETATM   36  C   UNK  0001      -1.643   1.288  -1.175
HETATM   37  O   UNK  0001      -2.272   1.555  -2.183
HETATM   38  N   UNK  0001      -1.359   0.000  -0.720
HETATM   39  N   UNK  0001      -1.489  -0.900  -1.700
HETATM   40  C   UNK  0001      -1.110  -2.153  -1.676
HETATM   41  H   UNK  0001      -1.707  -4.695  -6.356
HETATM   42  C   UNK  0001      -1.593  -4.194  -5.400
HETATM   43  C   UNK  0001      -1.297  -2.904  -2.937
HETATM   44  C   UNK  0001      -0.374  -4.259  -4.720
HETATM   45  C   UNK  0001      -2.664  -3.486  -4.851
HETATM   46  C   UNK  0001      -2.521  -2.841  -3.625
HETATM   47  C   UNK  0001      -0.222  -3.621  -3.492
HETATM   48  H   UNK  0001       0.463  -4.798  -5.152
HETATM   49  H   UNK  0001      -3.615  -3.443  -5.373
HETATM   50  H   UNK  0001      -3.366  -2.316  -3.188
HETATM   51  H   UNK  0001       0.734  -3.646  -2.979
HETATM   52 Cl   UNK  0001      -1.551  -0.013   2.307
HETATM   53  H   UNK  0001      -1.171   3.222  -0.509
```

```
HETATM   54 Cl   UNK  0001       1.564  -0.207  -1.008
HETATM   55  H   UNK  0001      -1.877  -0.502  -2.565
CONECT    1   12    2   38   34
CONECT    1   52   54
CONECT    2    5    4    1
CONECT    3    6    7   11
CONECT    4    7    2   22
CONECT    5    2    6    8
CONECT    6    5    3    9
CONECT    7    3    4   10
CONECT    8    5
CONECT    9    6
CONECT   10    7
CONECT   11    3
CONECT   12   15   14    1
CONECT   13   16   17   21
CONECT   14   17   12   18
CONECT   15   12   16   40
CONECT   16   15   13   19
CONECT   17   13   14   20
CONECT   18   14
CONECT   19   16
CONECT   20   17
CONECT   21   13
CONECT   22    4   23   34
```

CONECT 23 26 25 22

CONECT 24 27 28 33

CONECT 25 28 23 29

CONECT 26 23 27 30

CONECT 27 26 24 31

CONECT 28 24 25 32

CONECT 29 25

CONECT 30 26

CONECT 31 27

CONECT 32 28

CONECT 33 24

CONECT 34 22 35 1

CONECT 35 34 36 53

CONECT 36 35 37 38

CONECT 37 36

CONECT 38 36 39 1

CONECT 39 38 40 55

CONECT 40 39 43 15

CONECT 41 42

CONECT 42 41 45 44

CONECT 43 46 47 40

CONECT 44 47 42 48

CONECT 45 42 46 49

CONECT 46 45 43 50

CONECT 47 43 44 51

CONECT 48 44

CONECT 49 45

CONECT 50 46

CONECT 51 47

CONECT 52 1

CONECT 53 35

CONECT 54 1

CONECT 55 39

END

$[Co(L)Cl_2]$·-N2H

HEADER

REMARK Spartan '08 exported M0001

HETATM 1 Co UNK 0001 -0.159 -0.160 0.650

HETATM 2 N UNK 0001 1.417 0.295 1.771

HETATM 3 C UNK 0001 3.517 1.338 3.275

HETATM 4 C UNK 0001 1.546 1.643 1.937

HETATM 5 C UNK 0001 2.348 -0.510 2.291

HETATM 6 C UNK 0001 3.413 -0.031 3.052

HETATM 7 C UNK 0001 2.574 2.189 2.702

HETATM 8 H UNK 0001 2.248 -1.567 2.079

HETATM 9 H UNK 0001 4.139 -0.728 3.453

HETATM 10 H UNK 0001 2.629 3.263 2.834

HETATM 11 H UNK 0001 4.327 1.742 3.873

HETATM 12 N UNK 0001 -0.315 -2.115 0.682

HETATM 13 C UNK 0001 -0.736 -4.867 0.851

HETATM 14 C UNK 0001 -0.086 -2.785 1.825

HETATM 15 C UNK 0001 -0.786 -2.793 -0.399

HETATM 16 C UNK 0001 -1.009 -4.173 -0.325

HETATM 17 C UNK 0001 -0.263 -4.158 1.948

HETATM 18 H UNK 0001 0.210 -2.187 2.676

HETATM 19 H UNK 0001 -1.410 -4.686 -1.189

HETATM 20 H UNK 0001 -0.054 -4.642 2.895

HETATM 21 H UNK 0001 -0.908 -5.937 0.907

HETATM 22 C UNK 0001 0.547 2.454 1.219

HETATM 23 C UNK 0001 0.475 3.932 1.258

HETATM 24 C UNK 0001 0.291 6.719 1.302

HETATM 25 C UNK 0001 1.521 4.713 0.740

HETATM 26 C UNK 0001 -0.664 4.554 1.799

HETATM 27 C UNK 0001 -0.749 5.946 1.821

HETATM 28 C UNK 0001 1.422 6.103 0.762

HETATM 29 H UNK 0001 2.394 4.235 0.305

HETATM 30 H UNK 0001 -1.462 3.951 2.225

HETATM 31 H UNK 0001 -1.624 6.424 2.249

HETATM 32 H UNK 0001 2.228 6.705 0.353

HETATM 33 H UNK 0001 0.220 7.802 1.319

HETATM 34 N UNK 0001 -0.269 1.709 0.543

HETATM 35 N UNK 0001 -1.279 2.164 -0.230

HETATM 36 C UNK 0001 -2.130 1.260 -0.819

```
HETATM   37  O   UNK  0001      -3.074   1.536  -1.500
HETATM   38  N   UNK  0001      -1.741  -0.154  -0.473
HETATM   39  N   UNK  0001      -1.703  -0.887  -1.708
HETATM   40  C   UNK  0001      -1.201  -2.072  -1.652
HETATM   41  H   UNK  0001      -0.912  -4.528  -6.413
HETATM   42  C   UNK  0001      -0.974  -4.041  -5.445
HETATM   43  C   UNK  0001      -1.140  -2.795  -2.946
HETATM   44  C   UNK  0001       0.040  -4.229  -4.504
HETATM   45  C   UNK  0001      -2.068  -3.226  -5.142
HETATM   46  C   UNK  0001      -2.149  -2.598  -3.903
HETATM   47  C   UNK  0001      -0.041  -3.615  -3.256
HETATM   48  H   UNK  0001       0.899  -4.849  -4.743
HETATM   49  H   UNK  0001      -2.857  -3.080  -5.872
HETATM   50  H   UNK  0001      -2.989  -1.955  -3.662
HETATM   51  H   UNK  0001       0.762  -3.744  -2.538
HETATM   52 Cl   UNK  0001      -1.584  -0.034   2.433
HETATM   53  H   UNK  0001      -1.441   3.161  -0.336
HETATM   54 Cl   UNK  0001       1.305  -0.202  -1.072
HETATM   55  H   UNK  0001      -2.513  -0.498   0.117
CONECT    1   12    2   38   34
CONECT    1   52   54
CONECT    2    5    4    1
CONECT    3    6    7   11
CONECT    4    7    2   22
CONECT    5    2    6    8
```

CONECT 6 5 3 9

CONECT 7 3 4 10

CONECT 8 5

CONECT 9 6

CONECT 10 7

CONECT 11 3

CONECT 12 15 14 1

CONECT 13 16 17 21

CONECT 14 17 12 18

CONECT 15 12 16 40

CONECT 16 15 13 19

CONECT 17 13 14 20

CONECT 18 14

CONECT 19 16

CONECT 20 17

CONECT 21 13

CONECT 22 4 23 34

CONECT 23 26 25 22

CONECT 24 27 28 33

CONECT 25 28 23 29

CONECT 26 23 27 30

CONECT 27 26 24 31

CONECT 28 24 25 32

CONECT 29 25

CONECT 30 26

CONECT 31 27

CONECT 32 28

CONECT 33 24

CONECT 34 22 35 1

CONECT 35 34 36 53

CONECT 36 35 37 38

CONECT 37 36

CONECT 38 36 39 1 55

CONECT 39 38 40

CONECT 40 39 43 15

CONECT 41 42

CONECT 42 41 45 44

CONECT 43 46 47 40

CONECT 44 47 42 48

CONECT 45 42 46 49

CONECT 46 45 43 50

CONECT 47 43 44 51

CONECT 48 44

CONECT 49 45

CONECT 50 46

CONECT 51 47

CONECT 52 1

CONECT 53 35

CONECT 54 1

CONECT 55 38

END

$[Co(L)Cl_2]^{\cdot}$-N3H

HEADER

REMARK Spartan '08 exported M0001

HETATM 1 Co UNK 0001 -0.116 -0.128 0.481

HETATM 2 N UNK 0001 1.332 0.287 1.856

HETATM 3 C UNK 0001 3.481 1.274 3.351

HETATM 4 C UNK 0001 1.540 1.630 1.985

HETATM 5 C UNK 0001 2.204 -0.543 2.431

HETATM 6 C UNK 0001 3.282 -0.092 3.198

HETATM 7 C UNK 0001 2.600 2.154 2.721

HETATM 8 H UNK 0001 2.051 -1.602 2.263

HETATM 9 H UNK 0001 3.953 -0.814 3.650

HETATM 10 H UNK 0001 2.737 3.226 2.781

HETATM 11 H UNK 0001 4.316 1.654 3.931

HETATM 12 N UNK 0001 -0.378 -2.048 0.561

HETATM 13 C UNK 0001 -0.891 -4.769 0.861

HETATM 14 C UNK 0001 -0.310 -2.643 1.769

HETATM 15 C UNK 0001 -0.740 -2.779 -0.523

HETATM 16 C UNK 0001 -1.004 -4.152 -0.378

HETATM 17 C UNK 0001 -0.539 -3.996 1.964

HETATM 18 H UNK 0001 -0.103 -1.994 2.609

```
HETATM   19  H   UNK  0001     -1.319  -4.714  -1.245
HETATM   20  H   UNK  0001     -0.464  -4.415   2.960
HETATM   21  H   UNK  0001     -1.098  -5.829   0.964
HETATM   22  C   UNK  0001      0.583   2.471   1.243
HETATM   23  C   UNK  0001      0.452   3.929   1.388
HETATM   24  C   UNK  0001      0.112   6.691   1.622
HETATM   25  C   UNK  0001      0.503   4.746   0.242
HETATM   26  C   UNK  0001      0.242   4.506   2.653
HETATM   27  C   UNK  0001      0.063   5.883   2.761
HETATM   28  C   UNK  0001      0.340   6.123   0.365
HETATM   29  H   UNK  0001      0.729   4.310  -0.729
HETATM   30  H   UNK  0001      0.186   3.877   3.536
HETATM   31  H   UNK  0001     -0.117   6.327   3.735
HETATM   32  H   UNK  0001      0.400   6.753  -0.516
HETATM   33  H   UNK  0001     -0.021   7.764   1.714
HETATM   34  N   UNK  0001     -0.139   1.746   0.444
HETATM   35  N   UNK  0001     -1.352   2.195  -0.143
HETATM   36  C   UNK  0001     -1.741   1.197  -1.373
HETATM   37  O   UNK  0001     -2.336   1.711  -2.270
HETATM   38  N   UNK  0001     -1.297  -0.013  -1.009
HETATM   39  N   UNK  0001     -1.375  -0.912  -2.024
HETATM   40  C   UNK  0001     -1.024  -2.142  -1.842
HETATM   41  H   UNK  0001     -0.958  -5.036  -6.371
HETATM   42  C   UNK  0001     -0.977  -4.462  -5.450
HETATM   43  C   UNK  0001     -1.033  -2.986  -3.069
```

```
HETATM   44  C   UNK  0001      0.053  -4.602  -4.518
HETATM   45  C   UNK  0001     -2.030  -3.580  -5.196
HETATM   46  C   UNK  0001     -2.057  -2.841  -4.017
HETATM   47  C   UNK  0001      0.026  -3.871  -3.332
HETATM   48  H   UNK  0001      0.882  -5.273  -4.718
HETATM   49  H   UNK  0001     -2.832  -3.468  -5.920
HETATM   50  H   UNK  0001     -2.865  -2.145  -3.819
HETATM   51  H   UNK  0001      0.844  -3.965  -2.623
HETATM   52 Cl   UNK  0001     -1.845   0.171   2.020
HETATM   53  H   UNK  0001     -1.339   3.162  -0.484
HETATM   54 Cl   UNK  0001      1.636  -0.311  -0.940
HETATM   55  H   UNK  0001     -2.075   2.043   0.592
CONECT    1   12    2   38   34
CONECT    1   52   54
CONECT    2    5    4    1
CONECT    3    6    7   11
CONECT    4    7    2   22
CONECT    5    2    6    8
CONECT    6    5    3    9
CONECT    7    3    4   10
CONECT    8    5
CONECT    9    6
CONECT   10    7
CONECT   11    3
CONECT   12   15   14    1
```

CONECT 13 16 17 21

CONECT 14 17 12 18

CONECT 15 12 16 40

CONECT 16 15 13 19

CONECT 17 13 14 20

CONECT 18 14

CONECT 19 16

CONECT 20 17

CONECT 21 13

CONECT 22 4 23 34

CONECT 23 26 25 22

CONECT 24 27 28 33

CONECT 25 28 23 29

CONECT 26 23 27 30

CONECT 27 26 24 31

CONECT 28 24 25 32

CONECT 29 25

CONECT 30 26

CONECT 31 27

CONECT 32 28

CONECT 33 24

CONECT 34 22 35 1

CONECT 35 34 36 53 55

CONECT 36 35 37 38

CONECT 37 36

CONECT 38 36 39 1

CONECT 39 38 40

CONECT 40 39 43 15

CONECT 41 42

CONECT 42 41 45 44

CONECT 43 46 47 40

CONECT 44 47 42 48

CONECT 45 42 46 49

CONECT 46 45 43 50

CONECT 47 43 44 51

CONECT 48 44

CONECT 49 45

CONECT 50 46

CONECT 51 47

CONECT 52 1

CONECT 53 35

CONECT 54 1

CONECT 55 35

END

$[Co(L)Cl_2]$·-OH

HEADER

REMARK Spartan '08 exported M0001

HETATM 1 Co UNK 0001 0.105 -0.130 0.460

HETATM 2 N UNK 0001 1.559 0.304 1.783

HETATM 3 C UNK 0001 3.488 1.332 3.518

HETATM 4 C UNK 0001 1.643 1.646 2.014

HETATM 5 C UNK 0001 2.465 -0.498 2.348

HETATM 6 C UNK 0001 3.443 -0.027 3.226

HETATM 7 C UNK 0001 2.579 2.185 2.893

HETATM 8 H UNK 0001 2.416 -1.546 2.082

HETATM 9 H UNK 0001 4.149 -0.724 3.662

HETATM 10 H UNK 0001 2.595 3.254 3.067

HETATM 11 H UNK 0001 4.228 1.729 4.205

HETATM 12 N UNK 0001 -0.167 -2.056 0.561

HETATM 13 C UNK 0001 -0.689 -4.774 0.904

HETATM 14 C UNK 0001 0.017 -2.659 1.750

HETATM 15 C UNK 0001 -0.659 -2.778 -0.479

HETATM 16 C UNK 0001 -0.929 -4.145 -0.312

HETATM 17 C UNK 0001 -0.208 -4.012 1.963

HETATM 18 H UNK 0001 0.316 -2.018 2.567

HETATM 19 H UNK 0001 -1.349 -4.700 -1.139

HETATM 20 H UNK 0001 -0.032 -4.437 2.944

HETATM 21 H UNK 0001 -0.899 -5.831 1.024

HETATM 22 C UNK 0001 0.712 2.469 1.224

HETATM 23 C UNK 0001 0.501 3.925 1.398

HETATM 24 C UNK 0001 0.035 6.659 1.710

HETATM 25 C UNK 0001 1.459 4.852 0.958

HETATM 26 C UNK 0001 -0.692 4.369 1.994

HETATM 27 C UNK 0001 -0.918 5.738 2.148

HETATM 28 C UNK 0001 1.220 6.217 1.116

HETATM 29 H UNK 0001 2.373 4.507 0.485

HETATM 30 H UNK 0001 -1.416 3.644 2.359

HETATM 31 H UNK 0001 -1.834 6.081 2.619

HETATM 32 H UNK 0001 1.958 6.935 0.773

HETATM 33 H UNK 0001 -0.144 7.722 1.832

HETATM 34 N UNK 0001 0.060 1.751 0.370

HETATM 35 N UNK 0001 -0.883 2.231 -0.494

HETATM 36 C UNK 0001 -1.494 1.239 -1.226

HETATM 37 O UNK 0001 -2.344 1.572 -2.181

HETATM 38 N UNK 0001 -1.160 0.002 -0.956

HETATM 39 N UNK 0001 -1.406 -0.901 -1.945

HETATM 40 C UNK 0001 -1.072 -2.139 -1.768

HETATM 41 H UNK 0001 -1.617 -5.067 -6.240

HETATM 42 C UNK 0001 -1.511 -4.486 -5.329

HETATM 43 C UNK 0001 -1.241 -2.994 -2.974

HETATM 44 C UNK 0001 -0.377 -4.642 -4.530

HETATM 45 C UNK 0001 -2.506 -3.579 -4.957

HETATM 46 C UNK 0001 -2.370 -2.830 -3.792

HETATM 47 C UNK 0001 -0.242 -3.905 -3.355

HETATM 48 H UNK 0001 0.407 -5.333 -4.824

HETATM 49 H UNK 0001 -3.389 -3.456 -5.576

HETATM 50 H UNK 0001 -3.134 -2.117 -3.502

HETATM 51 H UNK 0001 0.653 -4.015 -2.750

```
HETATM   52 Cl   UNK  0001      -1.520   0.113   2.059
HETATM   53  H   UNK  0001      -1.353   3.100  -0.257
HETATM   54 Cl   UNK  0001       1.764  -0.340  -1.068
HETATM   55  H   UNK  0001      -2.174   2.464  -2.521
CONECT    1   12    2   38   34
CONECT    1   52   54
CONECT    2    5    4    1
CONECT    3    6    7   11
CONECT    4    7    2   22
CONECT    5    2    6    8
CONECT    6    5    3    9
CONECT    7    3    4   10
CONECT    8    5
CONECT    9    6
CONECT   10    7
CONECT   11    3
CONECT   12   15   14    1
CONECT   13   16   17   21
CONECT   14   17   12   18
CONECT   15   12   16   40
CONECT   16   15   13   19
CONECT   17   13   14   20
CONECT   18   14
CONECT   19   16
CONECT   20   17
```

CONECT 21 13

CONECT 22 4 23 34

CONECT 23 26 25 22

CONECT 24 27 28 33

CONECT 25 28 23 29

CONECT 26 23 27 30

CONECT 27 26 24 31

CONECT 28 24 25 32

CONECT 29 25

CONECT 30 26

CONECT 31 27

CONECT 32 28

CONECT 33 24

CONECT 34 22 35 1

CONECT 35 34 36 53

CONECT 36 35 37 38

CONECT 37 36 55

CONECT 38 36 39 1

CONECT 39 38 40

CONECT 40 39 43 15

CONECT 41 42

CONECT 42 41 45 44

CONECT 43 46 47 40

CONECT 44 47 42 48

CONECT 45 42 46 49

CONECT 46 45 43 50

CONECT 47 43 44 51

CONECT 48 44

CONECT 49 45

CONECT 50 46

CONECT 51 47

CONECT 52   1

CONECT 53 35

CONECT 54   1

CONECT 55 37

END

References:

[1] H. Hosseini-Monfared, H. Falakian, R. Bikas, P. Mayer, Intramolecular hydrogen bond effect on keto-enolization of aroylhydrazone in copper(II) complexes,Inorg. Chim. Acta349 (2013) 526.