Supplementary information for:

Crystallographic Structure and Quantum-Chemical Analysis of Biologically Active Co(III)-Pyridoxal-isothiosemicarbazone Complex

Fahad Abdulaziz [1], Khulood Fahad Alabbosh [2], Odeh Abdullah Odeh Alshammari [1], Wasan Mohammed Bin Tuwalah [1], Tahani Y. A. Alanazi [1], Aleksandra Rakić [3], Miljan Barić [3], Milica Marković [3], Violeta Jevtović [1,*] and Dušan Dimić [3,*]

[1] Department of Chemistry, College of Science, University of Ha'il, Ha'il 81451, Kingdom of Saudi Arabia; odeh.alshammari@uoh.edu.sa (O.A.O.A.)

[2] Department of Biology, College of Science, University of Ha'il, Ha'il 81451, Kingdom of Saudi Arabia

[3] Faculty of Physical Chemistry, University of Belgrade, Studentski Trg 12-16, 11000 Beograd, Serbia; saska@ffh.bg.ac.rs (A.R.); milica.markovic@ffh.bg.ac.rs (M.M.)

* Correspondence: v.jevtovic@uoh.edu.sa (V.J.); ddimic@ffh.bg.ac.rs (D.D.)

Table S1. Crystallographic and optimized (at B3LYP/6-31+G(H,C,N,S,O)/LanL2DZ(Co)) bond lengths (in Å) of $[Co(PLITSC\text{-}2H)(NH_3)_3]^+$

Bond	Crystallographic	Optimized
Co1-O3	1.89	1.89
Co1-N7	1.87	1.89
Co1-N11	1.97	2.05
Co1-N12	1.89	1.93
Co1-N15	1.97	1.99
Co1-N19	1.98	2.05
S2-C27	1.76	1.77
S2-C39	1.79	1.83
O3-C28	1.30	1.33
O4-H5	0.84	0.97
O4-C31	1.44	1.43

N11-N6	1.39	1.38
N6-C27	1.33	1.33
N7-H8	0.91	1.02
N7-H9	0.91	1.02
N7-H10	0.91	1.02
N11-C23	1.29	1.30
N12-H13	0.88	1.01
N12-C27	1.32	1.34
N14-C29	1.36	1.35
N14-C34	1.32	1.33
N15-H16	0.91	1.02
N15-H17	0.91	1.02
N15-H18	0.91	1.02
N19-H20	0.91	1.02
N19-H21	0.91	1.02
N19-H22	0.91	1.02
C23-H24	0.95	1.09
C23-C25	1.44	1.45
C25-C26	1.41	1.43
C25-C28	1.42	1.42
C26-C29	1.38	1.39
C31-C26	1.51	1.51
C28-C34	1.43	1.43
C29-H30	0.95	1.09
C31-H32	0.99	1.10
C31-H33	0.99	1.10
C34-C35	1.49	1.50
C35-H36	0.98	1.10
C35-H37	0.98	1.10
C35-H38	0.98	1.09
C39-H40	0.98	1.09
C39-H41	0.98	1.09
C39-H42	0.98	1.09
C34-C28	1.43	1.43

Table S2. Crystallographic and optimized (at B3LYP/6-31+G(H,C,N,S,O)/LanL2DZ(Co)) bond angles (in °) of $[Co(PLITSC\text{-}2H)(NH_3)_3]^+$

Angles optimized structure	Angles (°)	Angles (°)
A(3,1,6)	89.1	88.5

A(3,1,7)	95.7	96.1
A(3,1,10)	90.4	89.4
A(3,1,11)	87.3	84.2
A(6,1,7)	91.3	89.0
A(6,1,8)	89.1	90.7
A(6,1,11)	90.2	91.1
A(7,1,8)	82.2	82.2
A(7,1,10)	89.7	88.8
A(8,1,10)	91.8	91.3
A(8,1,11)	94.9	97.5
A(10,1,11)	88.8	91.1
A(15,2,21)	102.8	102.7
A(1,3,16)	124.4	125.5
A(18,4,22)	109.5	109.2
A(7,5,15)	108.2	110.6
A(1,6,23)	109.4	113.8
A(1,6,24)	109.5	109.4
A(1,6,25)	109.4	109.1
A(23,6,24)	109.5	106.9
A(23,6,25)	109.5	109.9
A(24,6,25)	109.5	107.6
A(1,7,5)	116.3	115.7
A(1,7,12)	126.5	125.2
A(5,7,12)	117.1	119.1
A(1,8,15)	111.0	110.2
A(1,8,26)	124.5	131.2
A(15,8,26)	124.5	118.6
A(17,9,19)	120.3	119.7
A(1,10,27)	109.4	109.3
A(1,10,28)	109.5	112.3
A(1,10,29)	109.4	111.0
A(27,10,28)	109.6	107.0
A(27,10,29)	109.5	107.1
A(28,10,29)	109.5	109.9
A(1,11,30)	109.5	102.6
A(1,11,31)	109.5	115.7
A(1,11,32)	109.5	116.0
A(30,11,31)	109.4	107.9
A(30,11,32)	109.5	107.9
A(31,11,32)	109.5	106.3
A(7,12,13)	124.0	125.6

A(7,12,33)	118.0	115.4
A(13,12,33)	118.0	119.0
A(12,13,14)	119.0	119.0
A(12,13,16)	122.2	122.8
A(14,13,16)	118.8	118.2
A(13,14,17)	119.0	118.0
A(13,14,18)	121.6	122.6
A(17,14,18)	119.2	119.4
A(2,15,5)	112.4	113.3
A(2,15,8)	125.5	125.5
A(5,15,8)	122.1	121.2
A(3,16,13)	126.2	124.5
A(3,16,19)	116.3	117.1
A(13,16,19)	117.5	118.5
A(9,17,14)	122.4	123.9
A(9,17,34)	118.8	115.8
A(14,17,34)	118.8	120.3
A(4,18,14)	108.5	109.0
A(4,18,35)	110.0	110.1
A(4,18,36)	110.0	110.9
A(14,18,35)	110.0	110.6
A(14,18,36)	110.0	108.7
A(35,18,36)	108.4	107.5
A(9,19,16)	121.8	121.8
A(9,19,20)	118.7	118.1
A(16,19,20)	119.5	120.1
A(19,20,37)	109.5	111.4
A(19,20,38)	109.5	111.4
A(19,20,39)	109.5	109.1
A(37,20,38)	109.5	107.0
A(37,20,39)	109.5	108.9
A(38,20,39)	109.4	109.0
A(2,21,40)	109.5	112.1
A(2,21,41)	109.5	104.9
A(2,21,42)	109.5	112.1
A(40,21,41)	109.4	108.1
A(40,21,42)	109.5	111.2
A(41,21,42)	109.5	108.1

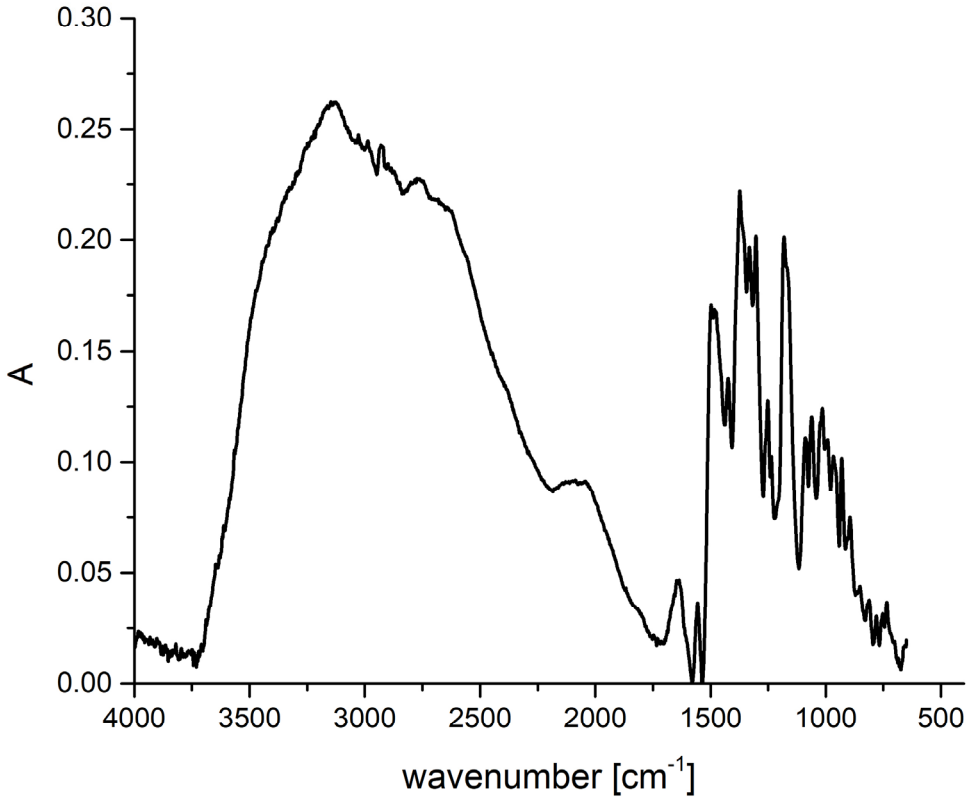

Figure S1. IR spectrum of **1**.

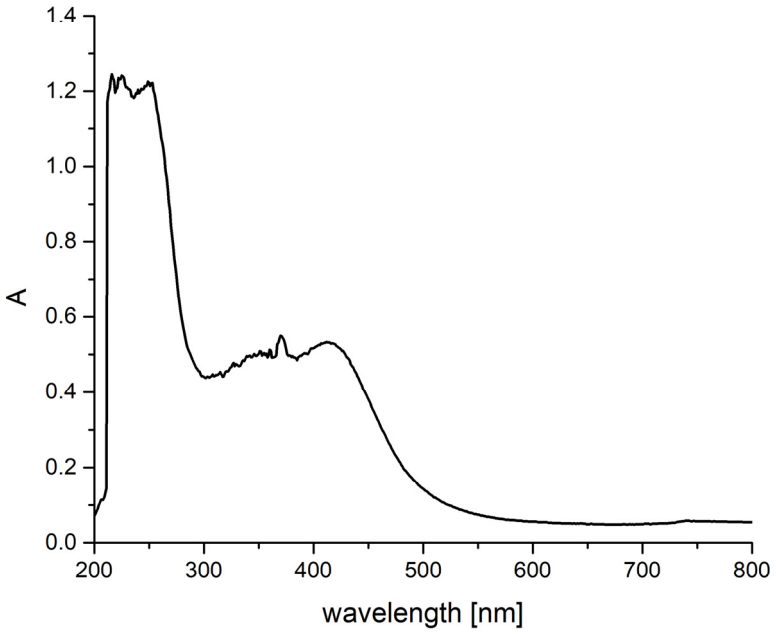

Figure S2. UV-VIS spectrum of **1**.

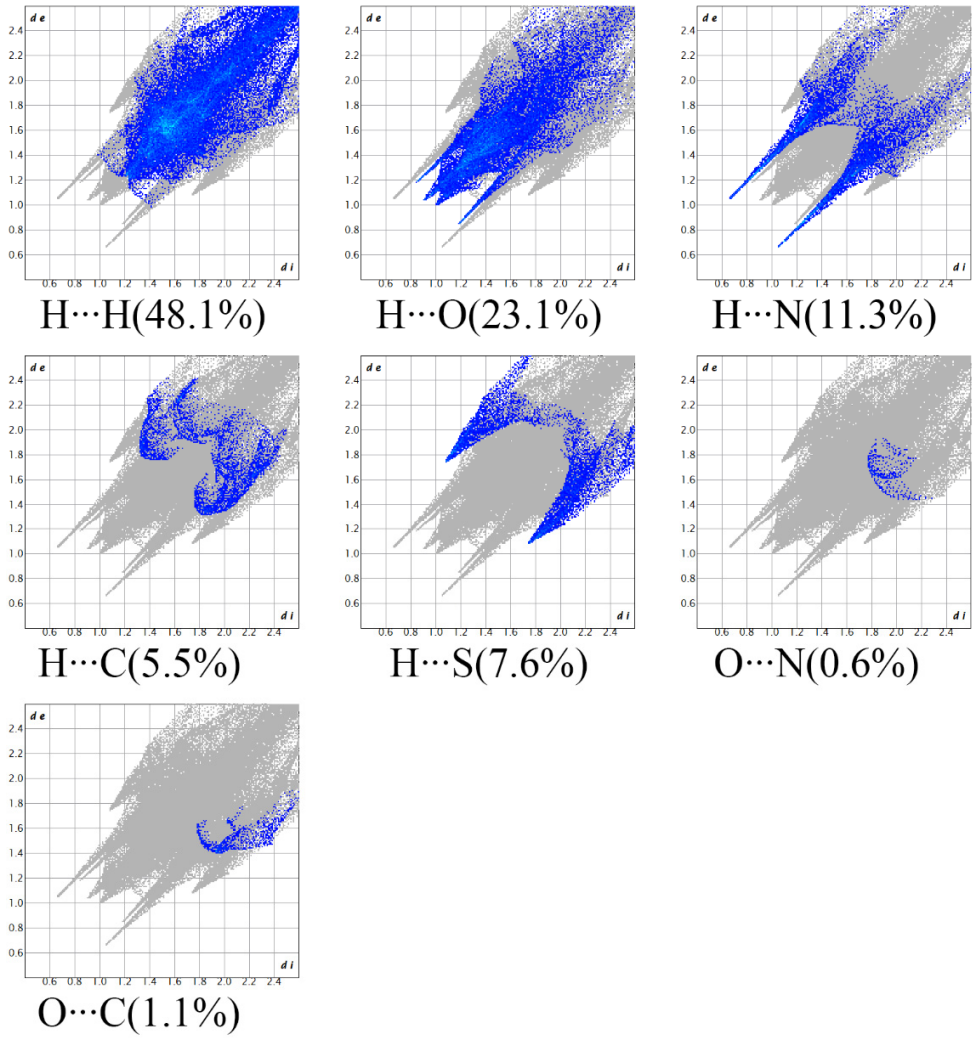

Figure S3. The fingerprint plots for the most important interactions within crystal structure of **1**.