Supplementary Material for

The copper(II)-thiodiacetate (tda) chelate as efficient receptor of N9-(2-hydroxyethyl)adenine (9heade). Synthesis, molecular and crystal structures, physical properties and DFT calculations of $[Cu(tda)(9heade)(H_2O)]\cdot 2H_2O$.

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SM.1. Crystal data and structure refinement for $[Cu(tda)(9heade)(H_2O)]\cdot 2H_2O$.

Empirical formula	$C_{11}H_{19}CuN_5O_8S$
Formula weight	444.91
Temperature	298(2) K
Wavelength	1.54178 Å
Crystal system, space group	Triclinic, $P\bar{1}$
Unit cell dimensions	a = 5.3908(3) Å α = 62.939(3)°
	b = 12.9325(7) Å β = 86.260(3)°
	c = 13.4804(7) Å γ = 81.195(4)°
Volume	827.05(8) Å^3
Z, Calculated density	2, 1.787 Mg/m^3
Absorption coefficient	3.564 mm^{-1}
F(000)	458
Crystal size	0.140 × 0.120 × 0.120 mm
Theta range for data collection	3.682 to 66.725°
Limiting indices	$-6\leq h\leq 6$, $-14\leq k\leq 15$, $-15\leq l\leq 15$
Reflections collected/unique	10657/2881 [$R_{(int)}$=0.0486]
Completeness to θ = 67.679	95.9%
Absorption correction	Semi-empirical from equivalents
Max. / min. transmission	1.000 / 0.708
Refinement method	Full-matrix least-squares on F^2
Data / parameters	2881 / 238
Goodness-of-fit on F^2	1.132
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0415, wR_2 = 0.1173
R indices (all data)	R_1 = 0.0447, wR_2 = 0.1198
Largest diff. peak and hole	0.323 and -0.452 e.Å^{-3}

SM.2. Selected bond lengths [Å] and angles [°] for $[Cu(tda)(9heade)(H_2O)]\cdot 2H_2O$.

Cu(1)-O(4)	1.933(2)
Cu(1)-O(1)	1.962(2)
Cu(1)-N(21)	2.025(2)
Cu(1)-O(8)	2.262(2)
Cu(1)-S(1)	2.3625(8)
Cu(1)-O(2)[a]	3.060(4)
O(4)-Cu(1)-O(1)	175.04(10)
O(4)-Cu(1)-N(21)	96.16(9)
O(1)-Cu(1)-N(21)	87.56(9)
O(4)-Cu(1)-O(8)	86.36(10)
O(1)-Cu(1)-O(8)	96.03(9)
N(21)-Cu(1)-O(8)	102.95(9)
O(4)-Cu(1)-S(1)	87.22(7)
O(1)-Cu(1)-S(1)	88.77(7)
N(21)-Cu(1)-S(1)	173.58(7)
O(8)-Cu(1)-S(1)	82.67(5)
O(4)-Cu(1)-O(2)[a]	70.77(10)
O(1)-Cu(1)-O(2)[a]	105.90(9)
N(21)-Cu(1)-O(2)[a]	92.04(9)
O(8)-Cu(1)-O(2)[a]	153.95(8)
S(1)-Cu(1)-O(2)[a]	83.90(6)

Symmetry transformations used to generate equivalent atoms:
a = x-1,y,z.

SM 3. Hydrogen bonds for [Cu(tda)(9heade)(H_2O)]·2H_2O [Å and °].

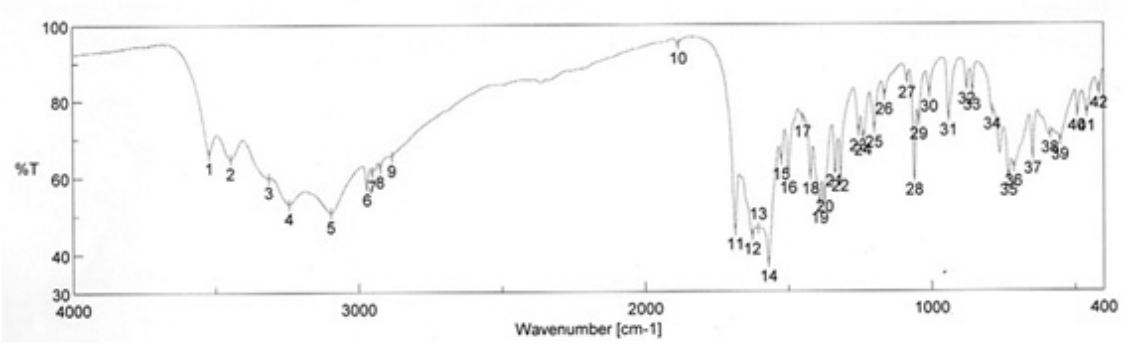
D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
O(1)-H(1B)...O(8)[a]	0.85	1.86	2.699(3)	168.2
O(1)-H(1A)...O(9)[b]	0.85	1.79	2.622(3)	163.7
O(2)-H(2C)...O(4)	0.85	2.50	3.108(4)	129.7
O(2)-H(2C)...O(5)	0.85	1.86	2.691(4)	164.7
O(2)-H(2D)...O(5)[c]	0.85	1.98	2.816(3)	167.8
O(3)-H(3A)...O(9)[b]	0.85	1.98	2.819(3)	169.9
O(3)-H(3B)...N(23)[a]	0.85	2.11	2.918(4)	157.7
O(32)-H(32)...O(3)	0.82	1.93	2.744(3)	170.8
N(26)-H(26A)...O(2)[a]	0.86	1.96	2.757(4)	154.0
N(26)-H(26B)...N(27)[d]	0.86	2.18	2.980(4)	154.1
C(2)-H(2A)...O(32)[e]	0.97	2.35	3.297(4)	165.2
C(6)-H(6B)...O(32)[e]	0.97	2.53	3.443(4)	156.4
C(22)-H(22)...O(1)[f]	0.93	2.52	3.412(4)	161.2
C(22)-H(22)...O(8)	0.93	2.61	3.282(4)	129.6

Symmetry transformations used to generate equivalent atoms:

a = x-1,y,z; b = -x+1,-y+1,-z+1; c = -x+2,-y+1,-z+2; d = -x,-y,-z+2; e = x,y+1,z; f = x+1,y,z

SM 4. FT-IR spectra

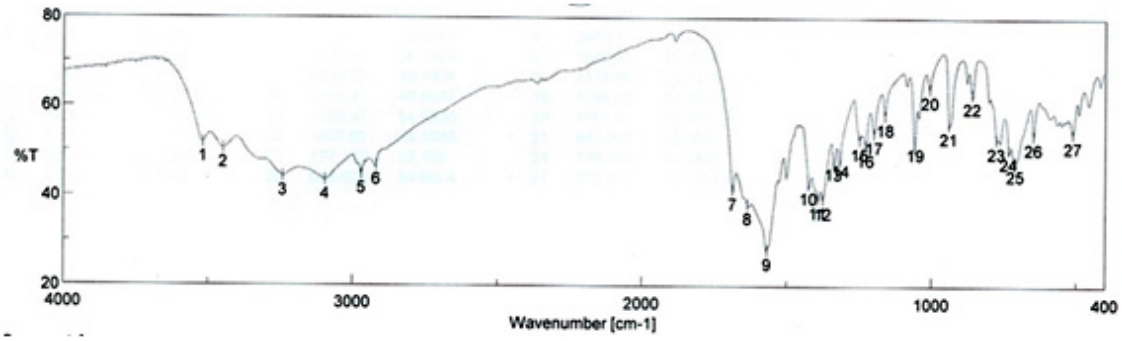
SM.4-a. Minimally ground sample of compound 1.



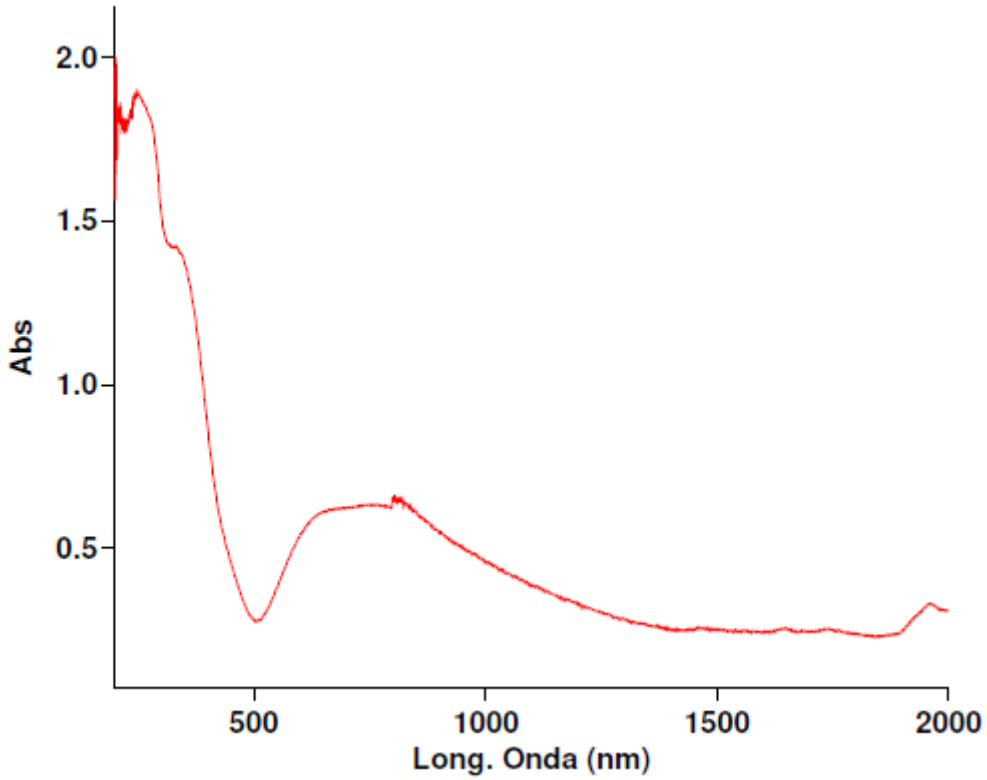
[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3521.38	66.0202	2	3446.17	64.6513	3	3313.11	59.7551
4	3242.72	52.928	5	3097.12	50.7111	6	2969.84	57.806
7	2951.52	61.3051	8	2924.52	62.3599	9	2884.02	65.2647
10	1883.15	94.5863	11	1686.44	45.9874	12	1627.63	44.7063
13	1606.41	46.3469	14	1570.74	37.5623	15	1525.42	64.0976
16	1500.35	60.5881	17	1450.21	75.1749	18	1423.21	60.349
19	1391.39	52.7427	20	1373.07	55.6248	21	1339.32	62.3386
22	1319.07	61.0095	23	1255.43	71.5281	24	1239.04	70.3587
25	1200.47	72.415	26	1164.79	81.0214	27	1084.76	85.3574
28	1059.69	59.9967	29	1044.26	74.4588	30	1007.62	81.7111
31	940.128	75.4933	32	876.488	83.6893	33	858.168	82.1281
34	787.779	77.0193	35	730.889	59.7875	36	713.533	62.1769
37	647.001	65.4159	38	586.254	70.798	39	551.542	69.0303
40	492.723	76.5139	41	458.975	76.4116	42	415.585	82.4419

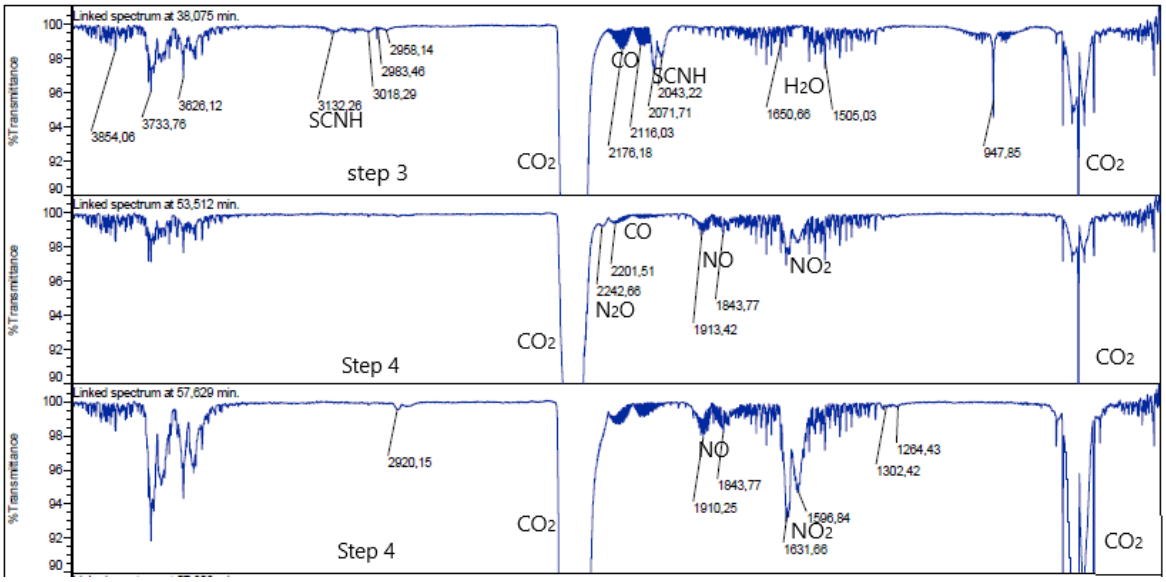
SM 4-b.Ground sample of compound 1.



SM 5. Electronic spetrun (diffuse reflectance)



SM.6. TGA analysis. Three FT-IR spectra of the evolved gases during the TGA of compound 1.



SM.7. ESR spectra.