SUPPORTING INFORMATION

A windmill-shaped hexacopper(II) molecule built up by template self-assembly of diaqua-tetra(μ_2-N3,N9-adeninato)dicopper(II) and aqua(oxydiacetato)copper(II).

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S1A. Thermogravimetric analysis, with FT-IR spectral identification of evolved gasses.

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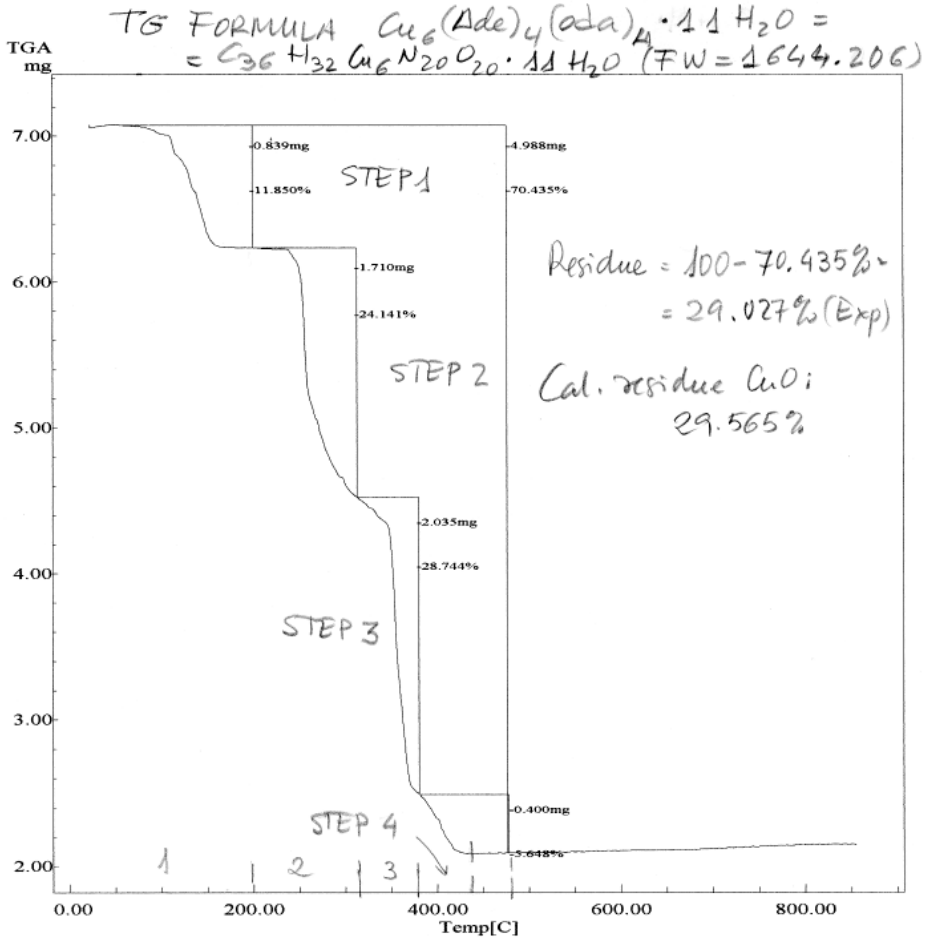
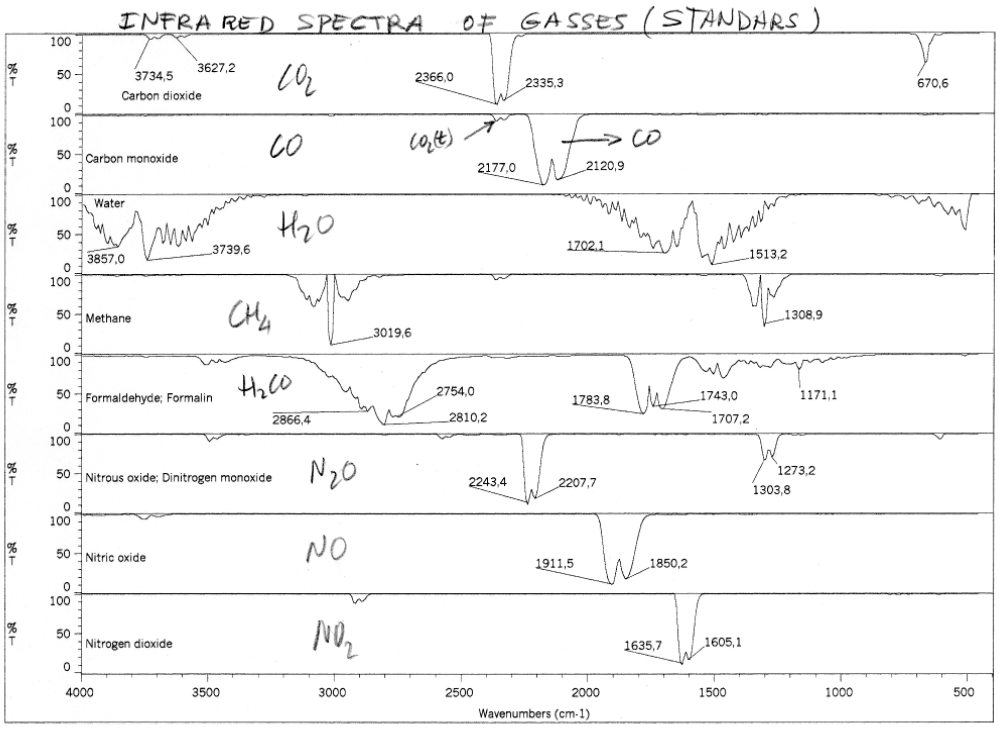
File Name:	T2100156.D20	C-286
Detector Type:	Shimadzu TGA-50H	
Acquisition Date:	10/05/04	
Acquisition Time:	09:51:44	
Sample Name:	C-286	
Weight:	7.081[mg]	
Cell:	Alumina	
Atmosphere:	Air	
Rate Flow:	100.0[ml/min]	
Operator:	MASP	

Temp Program

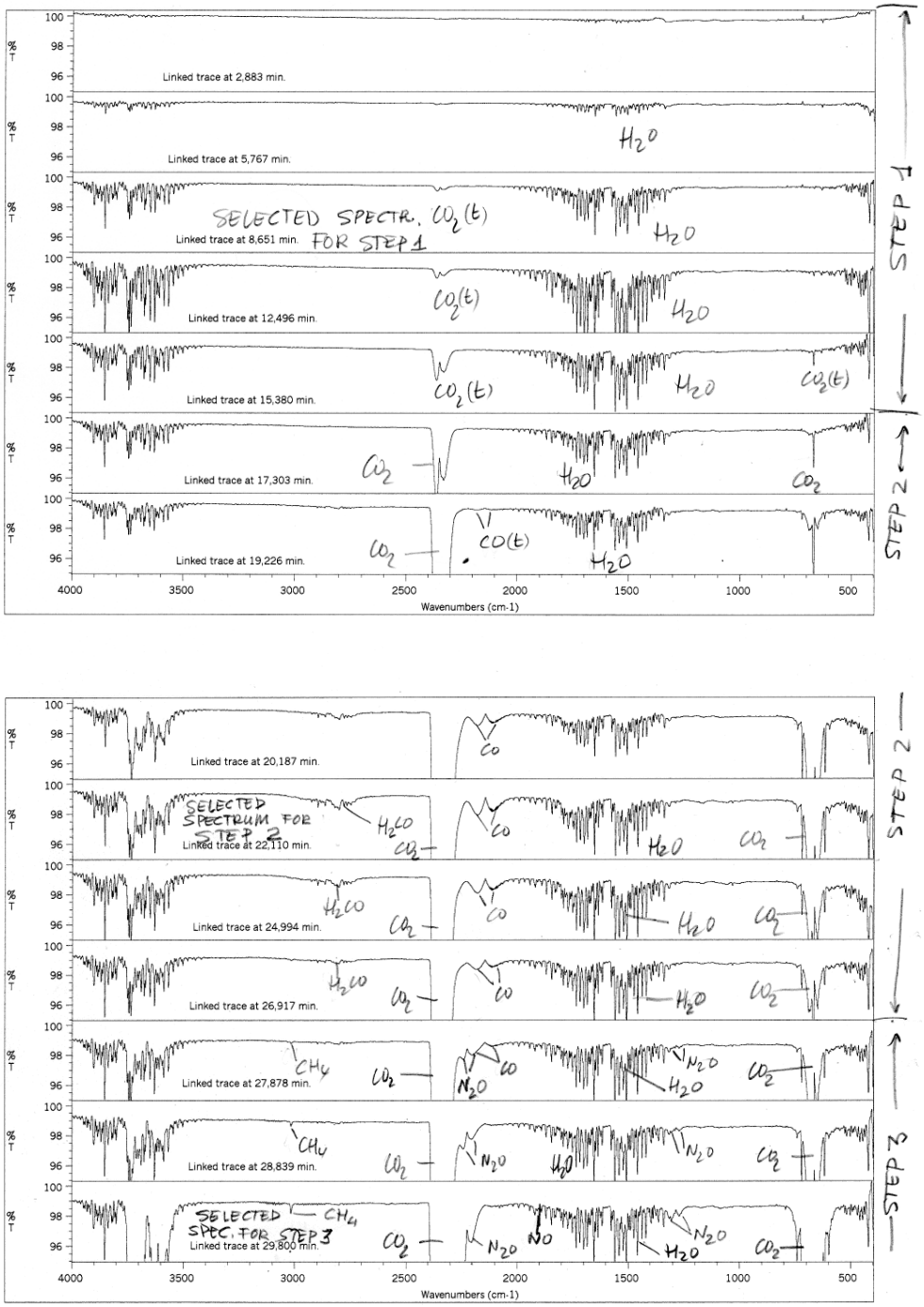
Rate [C/min]	Hold Temp [C]	Hold Time [min]
10.0	950.0	0.0



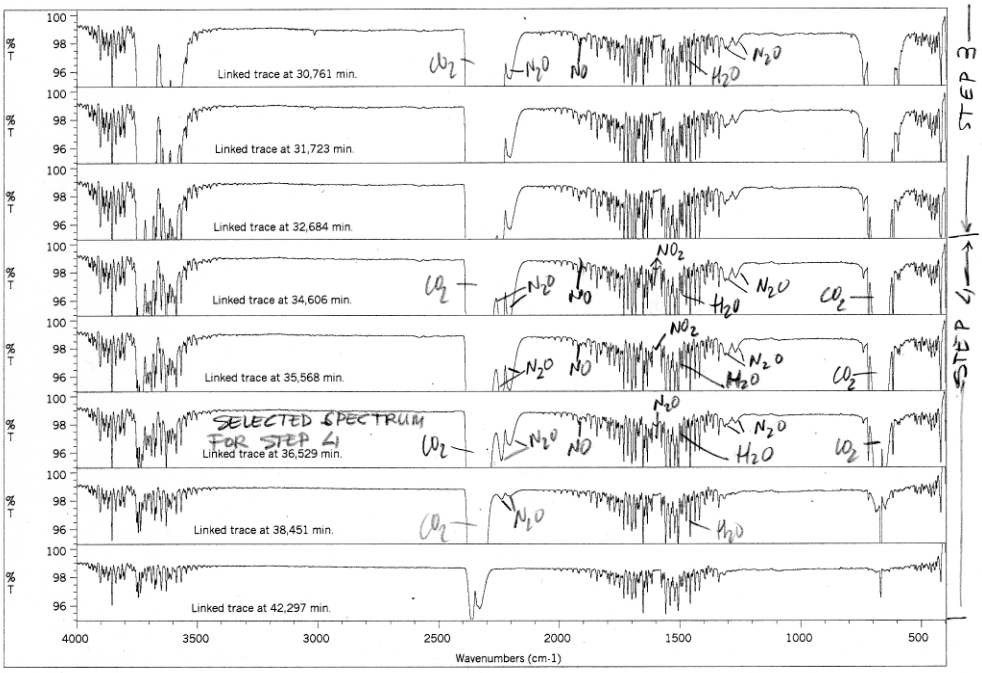
S1B. FT-IR spectra of the gasses (standards). They are used for the identification of gasses in the 22 IR spectra recorded during the experience (see S1C).



S1C. FT-IR spectra recorded during the TG analysis of compound 1-o. On the right-hand is indicated the 5 or 6 spectra corresponding to each step. Four of these spectra (one per step) were selected as is shown in S1E.



S1C (cont). FT-IR spectra recorded during the TG analysis of compound 1-o. On the right-hand is indicated the 5 or 6 spectra corresponding to each step. Four of these spectra (one per step) were selected as is shown in S1E.

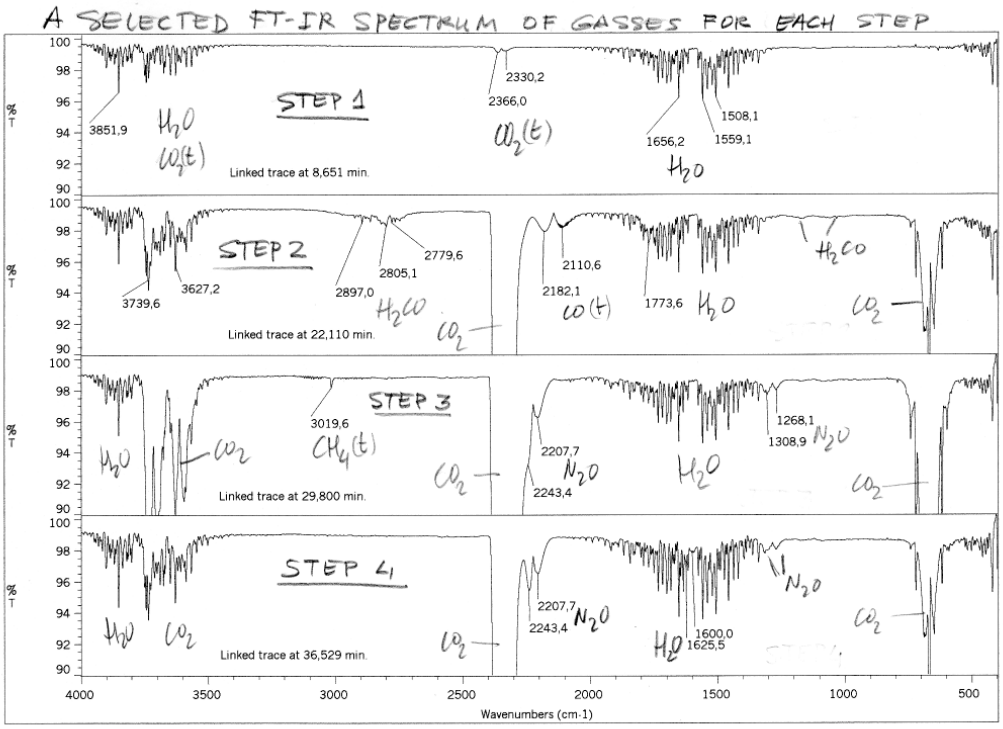


S1D. Summary of the Thermogravimetric experience for compound **1-o**.

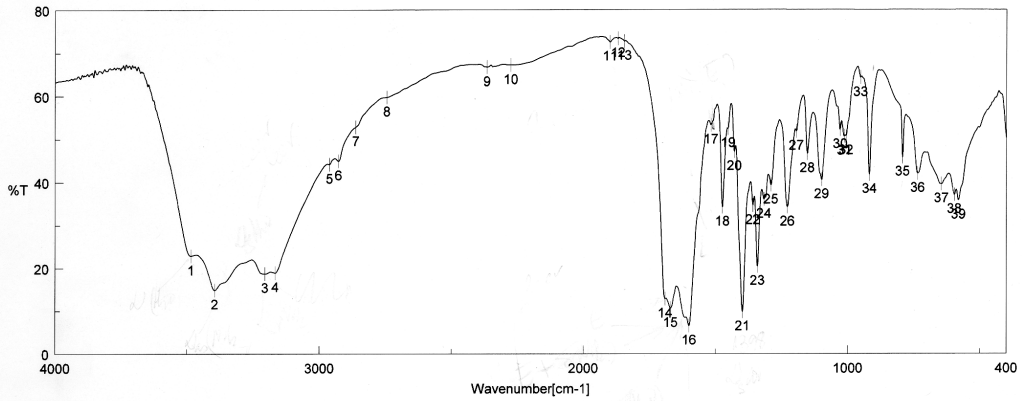
Step	temp (ºC)	time (min)	IR Nº	Weight loss % Exp.	Calcd*.	Gasses or residue
1	r.t. – 200	2 - 15	5	11.850	12.053	(11)H_2O, CO_2(t)**
2	200 - 315	15 - 27	6	24.141	-	***, H_2CO, CO
3	315 - 380	27 - 33	6	28.744	-	***, CO, N_2O, NO
4	380 - 435	33 - 44	5	5.648	-	***, N_2O, NO, NO_2(t)
Residue	480	-	-	29.565	29.027	CuO

* Calculated values for $C_{36}H_{32}Cu_6N_{20}O_{20}\cdot 11H_2O$ (FW 1644.206)
** t = trace amounts
*** In additon to H_2O and CO_2

S1E. Selected FT-IR spectra of gasses for each step.



S2. FT-IR spectrum of compound **1-o** in solid state (KBr disc).



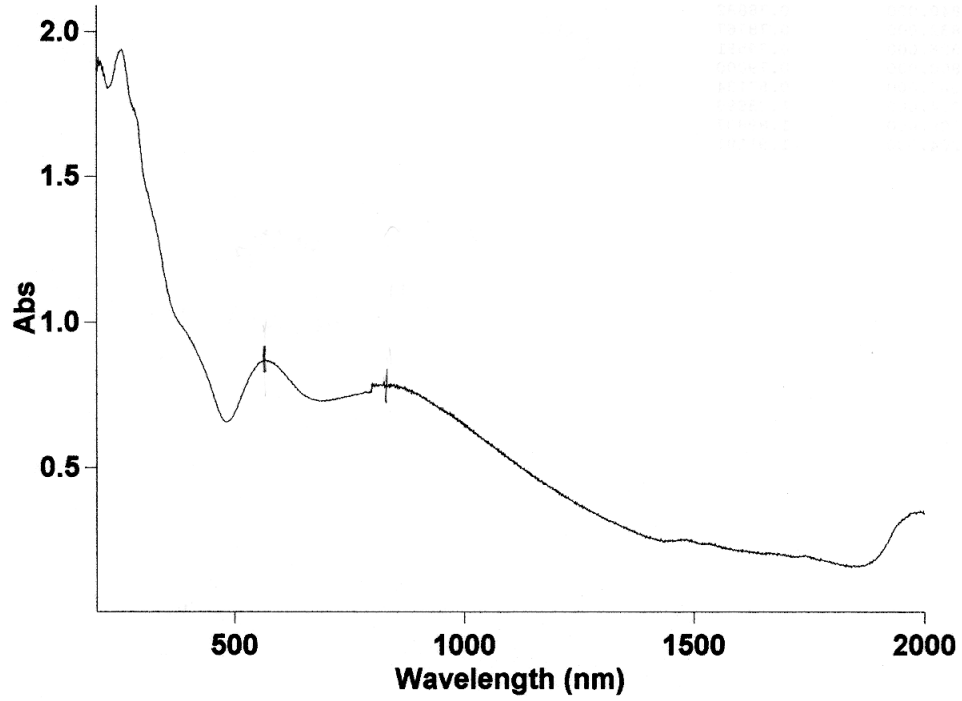
Accumulation	180	Resolution	4 cm-1
Zero Filling	ON	Apodization	Cosine
Gain	2	Scanning Speed	2 mm/sec
Date/Time	07/10/2003 17:02		
Operator	Tiziana-12		
File Name	Tz-12		
Sample Name	Cu(ODA)(Adeh)		
Comment	muestra 1		

1: 3484.74, 22.8832	2: 3394.10, 14.9205	3: 3206.08, 18.7656	4: 3167.51, 18.9750
5: 2962.13, 44.1621	6: 2927.41, 44.9489	7: 2861.84, 52.8762	8: 2744.21, 59.7541
9: 2366.23, 66.7470	10: 2275.59, 67.2269	11: 1900.50, 72.5879	12: 1869.65, 73.3987
13: 1845.54, 72.7636	14: 1691.27, 12.8600	15: 1671.02, 10.6349	16: 1600.63, 6.5882
17: 1517.70, 53.3272	18: 1474.31, 34.2741	19: 1453.10, 52.5079	20: 1428.99, 47.1366
21: 1398.14, 9.8723	22: 1358.60, 34.6141	23: 1341.25, 20.4892	24: 1317.14, 36.0421
25: 1291.11, 39.3534	26: 1228.43, 34.2759	27: 1194.69, 51.8475	28: 1153.22, 46.6370
29: 1099.23, 40.5898	30: 1029.80, 52.2327	31: 1014.37, 50.6727	32: 1007.62, 50.7930
33: 952.66, 64.2769	34: 918.91, 41.8268	35: 793.56, 45.8353	36: 735.71, 42.0274
37: 646.04, 39.5822	38: 596.86, 37.0814	39: 581.43, 35.8234	

Wavenumbers in cm^{-1} (the number of the band is indicated in brackets).

H_2O	ν_{as} 3485 [1]	ν_s ~ 3280	δ 1625
Ade	$\nu_{as}(NH_2)$ 3390 [2], 3350 π(C-H) 794 [35]	$\nu_s(NH_2)$ 3206 [3], 3168 [4]	$\delta(NH_2)$ 1671 [15]
oda	ν_{as}(COO) 1601 [16]	ν_s(COO) 1398 [21]	

S3. Electronic (reflectance) spectrum of compound **1-o**.



Maxima	840 nm	11900 cm^{-1}
	567 nm	17640 cm^{-1}

S4. X-band ESR spectrum of compound **1-o** at room temperature. Apparent gi_{so} = 2.137.