Table S1 Crystallographic data and refinement details for compounds $[Cu(flen)_2]BF_4.2CHCl_3$ and $[Cu(flen)_2][CuI_2]$.

Compound reference	comp1	comp2
Chemical formula	$C_{56}H_{40}CuN_4$•2($CHCl_3$)•BF_4	$C_{56}H_{40}CuN_4$•CuI_2
Formula Mass	1158.01	1149.80
Crystal system	Monoclinic	Orthorhombic
a/Å	25.2240(14)	13.848(4)
b/Å	15.1903(4)	17.564(5)
c/Å	20.1965(11)	19.573(2)
α/°	90.00	90.00
β/°	137.614(11)	90.00
γ/°	90.00	90.00
Unit cell volume/Å^3	5216.7(12)	4761(2)
Temperature/K	293(2)	293(2)
Space group	*C2/c*	*Pnna*
No. of formula units per unit cell, *Z*	4	4
No. of reflections measured	25397	34157
No. of independent reflections	4587	4209
R_{int}	0.0262	0.0270
Final R_1 values ($I > 2\sigma(I)$)	0.0612	0.0628
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1631	0.1397
Final R_1 values (all data)	0.0697	0.0812
Final $wR(F^2)$ values (all data)	0.1709	0.1531

Table S2 Cartesian coordinates used in the DFT calculation.

Atom	x	y	z
C	-1.44440	13.15328	-7.03618
H	-2.30775	12.90872	-6.79384
Cu	3.72939	13.79477	-3.40373
N	5.32341	14.55595	-4.47917
C	5.31639	13.86267	-5.76863
H	5.69709	12.97707	-5.66925
H	5.85278	14.35483	-6.40990
C	8.42617	13.95837	-5.36291
H	7.90431	13.59532	-6.04229
N	3.06798	13.13399	-5.22077
C	7.85241	14.67383	-4.32818
C	6.48511	15.74171	-2.70664
C	6.42817	14.94422	-3.95377
C	0.99633	12.10667	-4.49836
C	1.84078	12.83732	-5.46774
C	3.89249	13.75937	-6.26013
H	3.54897	14.64345	-6.46436
H	3.86218	13.22619	-7.07022
C	8.66746	15.20549	-3.29481
C	0.93964	13.21404	-6.60051
C	1.35461	11.42766	-3.35199
H	2.24041	11.40488	-3.07152
C	-0.32258	12.11426	-4.95446
C	7.82144	15.87386	-2.31317
C	9.81612	13.79735	-5.35610
H	10.22033	13.32189	-6.04502
C	5.47818	16.34628	-1.99322
H	4.59296	16.27641	-2.26960
C	10.03484	15.02017	-3.31114
H	10.56736	15.35891	-2.62768
C	10.59073	14.32293	-4.35949
H	11.51292	14.20749	-4.39081
C	0.36425	10.78056	-2.62768
H	0.58746	10.31725	-1.85299
C	-1.30494	11.47779	-4.20292

H	-2.19464	11.49754	-4.47522
C	5.81113	17.06326	-0.85365
H	5.14098	17.47796	-0.35943
C	1.16100	13.89305	-7.77956
H	2.01805	14.14369	-8.03688
C	8.14750	16.58021	-1.16271
H	9.02974	16.65464	-0.88361
C	-0.36453	12.82061	-6.22609
C	-1.22356	13.83836	-8.18392
H	-1.94643	14.07381	-8.71898
C	-0.93898	10.82005	-3.04974
H	-1.59183	10.39016	-2.54599
C	7.12676	17.16656	-0.44521
H	7.32979	17.64050	0.32948
C	0.05256	14.19382	-8.57739
H	0.17540	14.63889	-9.38475
C	8.90317	13.15328	0.22873
H	9.76652	12.90872	-0.01362
N	2.13536	14.55595	-2.32829
C	2.14238	13.86267	-1.03882
H	1.76168	12.97707	-1.13821
H	1.60599	14.35483	-0.39755
C	-0.96740	13.95837	-1.44454
H	-0.44554	13.59532	-0.76516
N	4.39079	13.13399	-1.58668
C	-0.39364	14.67383	-2.47927
C	0.97366	15.74171	-4.10081
C	1.03060	14.94422	-2.85368
C	6.46244	12.10667	-2.30909
C	5.61799	12.83732	-1.33971
C	3.56628	13.75937	-0.54732
H	3.90980	14.64345	-0.34310
H	3.59659	13.22619	0.26277
C	-1.20869	15.20549	-3.51265
C	6.51913	13.21404	-0.20695
C	6.10416	11.42766	-3.45546
H	5.21836	11.40488	-3.73593
C	7.78135	12.11426	-1.85299
C	-0.36267	15.87386	-4.49428
C	-2.35735	13.79735	-1.45135
H	-2.76156	13.32189	-0.76243
C	1.98059	16.34628	-4.81423
H	2.86581	16.27641	-4.53785
C	-2.57607	15.02017	-3.49631
H	-3.10859	15.35891	-4.17978
C	-3.13196	14.32293	-2.44796
H	-4.05415	14.20749	-2.41664
C	7.09452	10.78056	-4.17978
H	6.87131	10.31725	-4.95446
C	8.76371	11.47779	-2.60453
H	9.65341	11.49754	-2.33223
C	1.64764	17.06326	-5.95380
H	2.31779	17.47796	-6.44802
C	6.29777	13.89305	0.97210
H	5.44072	14.14369	1.22943
C	-0.68873	16.58021	-5.64474
H	-1.57097	16.65464	-5.92385
C	7.82330	12.82061	-0.58136
C	8.68233	13.83836	1.37647
H	9.40520	14.07381	1.91153
C	8.39775	10.82005	-3.75771
H	9.05060	10.39016	-4.26147
C	0.33201	17.16656	-6.36224
H	0.12898	17.64050	-7.13693
C	7.40621	14.19382	1.76994
H	7.28337	14.63889	2.57730

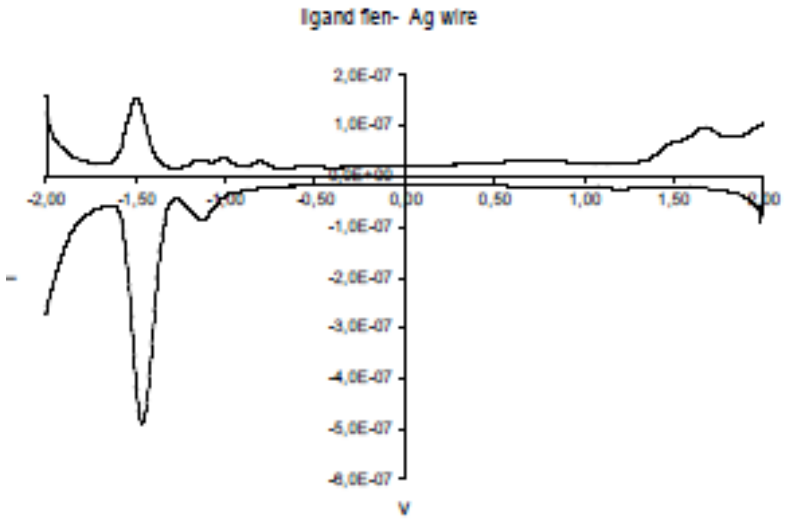

Fig S1. Differential pulse voltamogram of the **flen** ligand in CH_2Cl_2 with a Ag wire pseudoreference electrode.

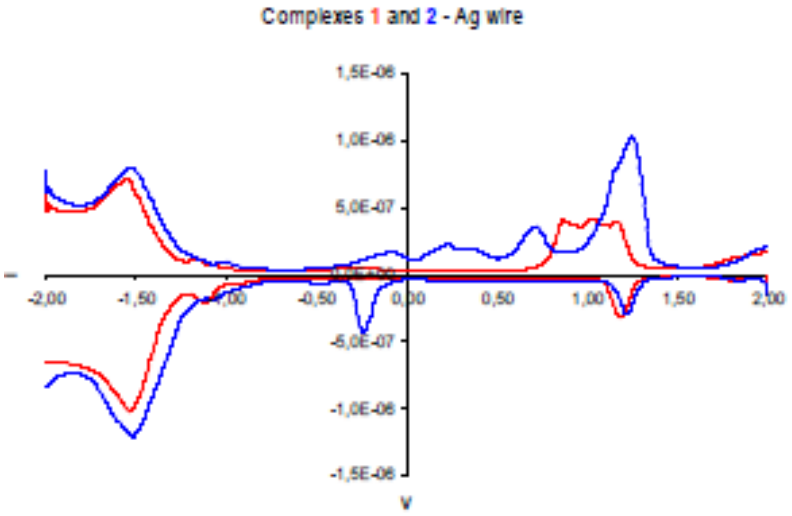

Fig S2. Differential pulse voltamogram of the two complexes in CH_2Cl_2 with a Ag wire pseudoreference electrode.

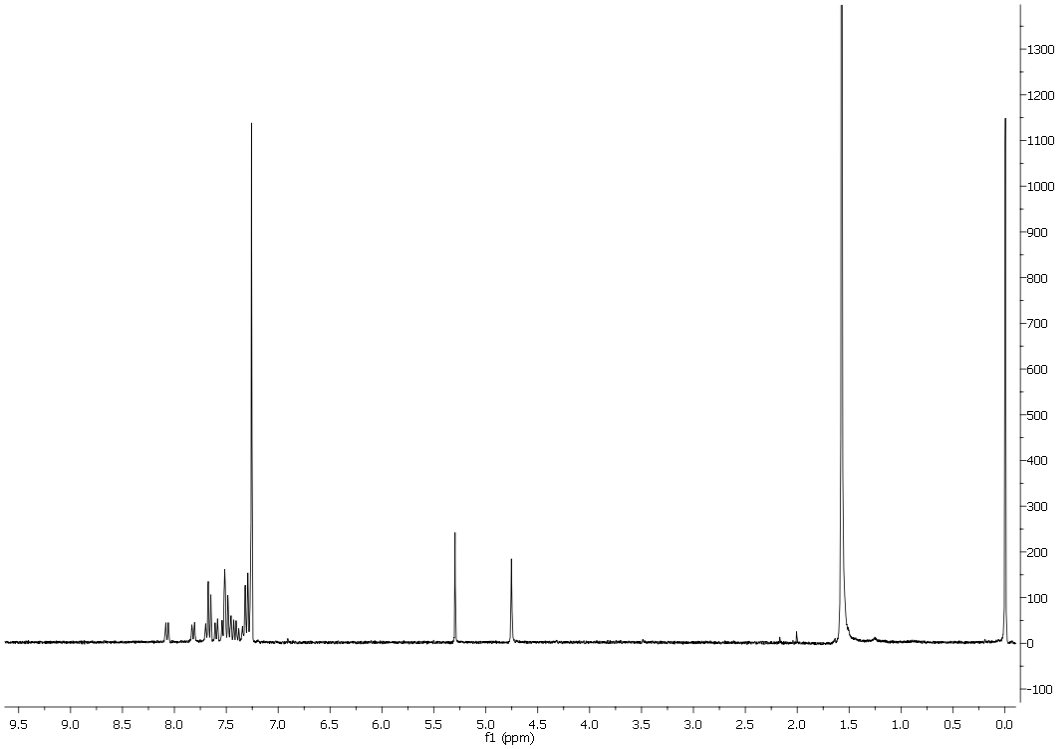

Fig S3. ^{1}H NMR spectrum of compound **1** in $CDCl_3$. The peak at ~ δ 1.5 corresponds to the protons of cyclohexane molecule used for the precipitation of the solid portion used for the measurement while that at ~ 5.3 corresponds to a dichloromethane solvent molecule.

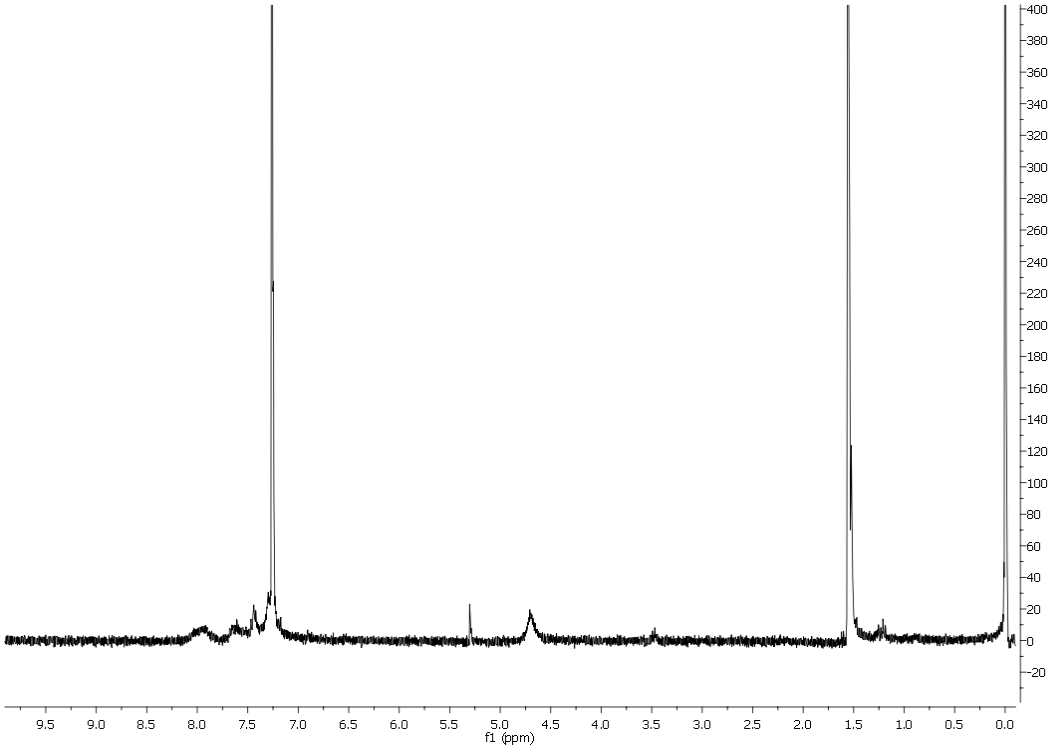

Fig S4. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

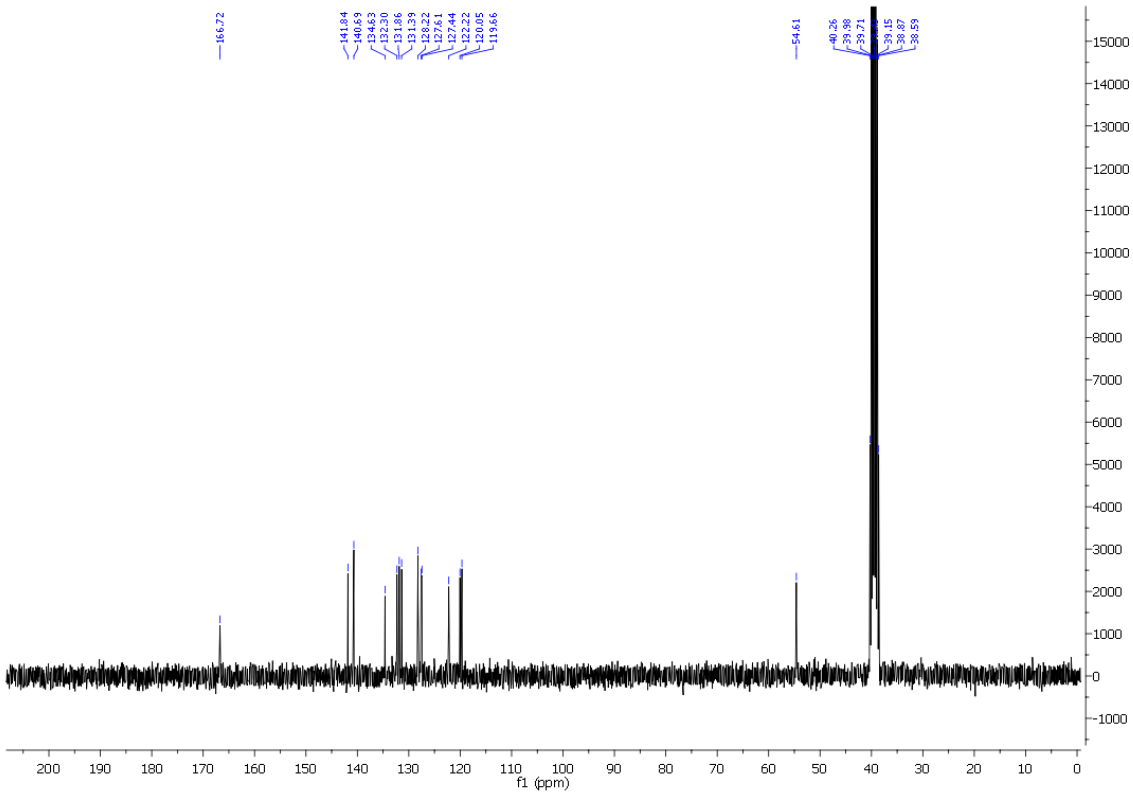

Fig S5. ^{13}C NMR for compound **1** in DMSO-d$_6$.

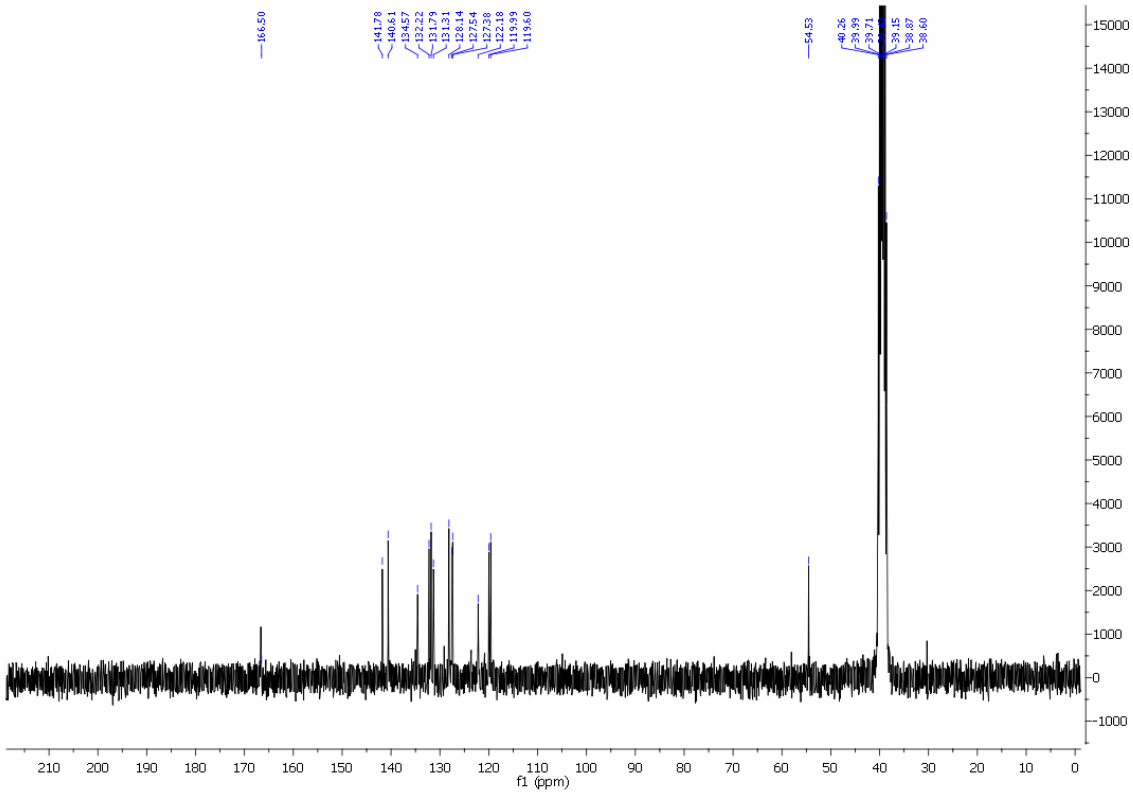

Fig S6. ^{13}C NMR for compound **2** in DMSO-d$_6$.

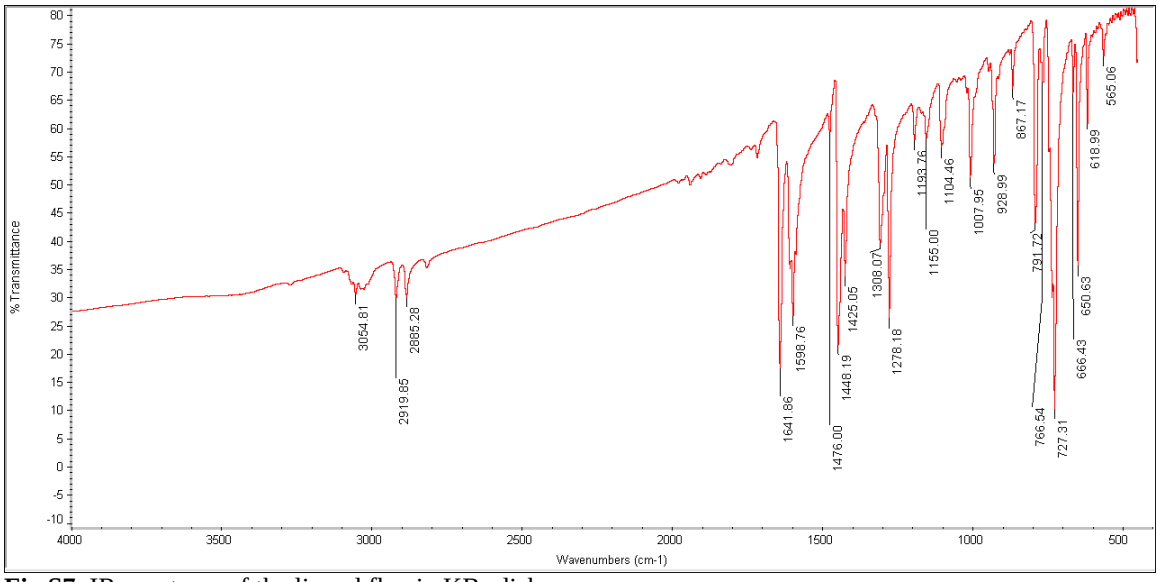

Fig S7. IR spectrum of the ligand flen in KBr disk.

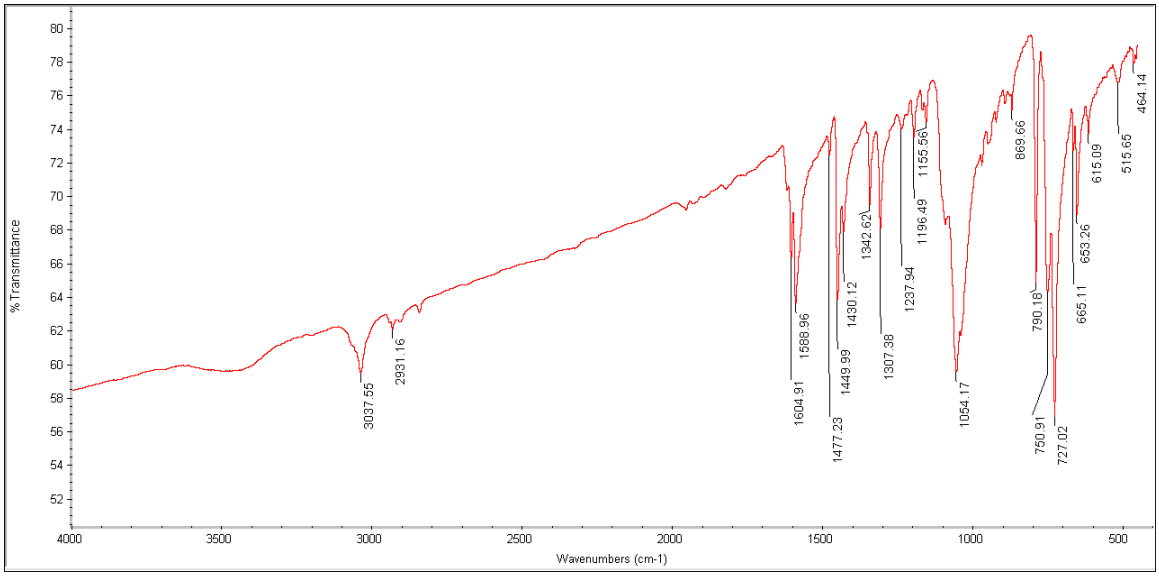

Fig S8. IR spectrum of compound **1** in KBr disk.

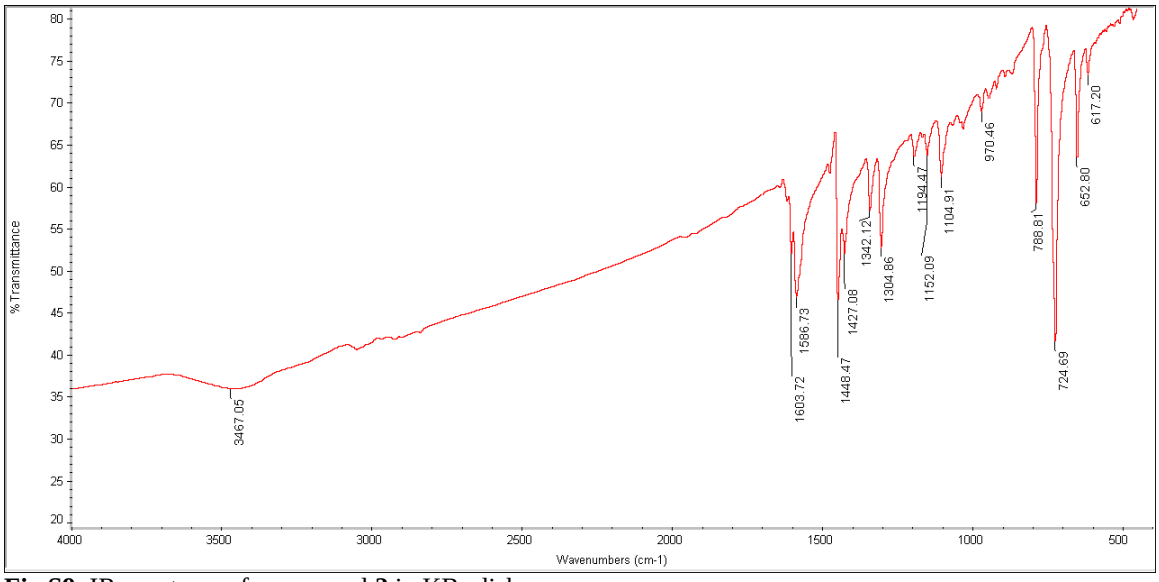

Fig S9. IR spectrum of compound **2** in KBr disk.