Synthetic Analogue Approach for the Functional Domains of Copper(II)- Bleomycins and Its DNA Cleavage Activity

Shanta Dhar, Munirathinam Nethaji and Akhil R. Chakravarty*

Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India, E-mail: <u>arc@ipc.iisc.ernet.in</u>

Supplementary Material

<i>T</i> (K)	$\chi_{\rm M}T({\rm cm}^3{\rm M}^{-1}{\rm K})$	Т	$\chi_{\rm M} T$
304.9372	0.5076	262.3832	0.48157
304.5652	0.50831	261.0794	0.47837
304.1172	0.50404	259.7579	0.4797
303.6163	0.50465	258.4077	0.47925
303.0258	0.50204	257.0608	0.47779
302.3688	0.50095	255.7137	0.47686
301.6748	0.49927	254.3484	0.47664
300.9801	0.49647	252.9791	0.47398
300.2648	0.49908	251.6022	0.4753
299.4325	0.4977	250.2649	0.47415
298.5959	0.49796	248.8763	0.4715
297.7283	0.49824	247.4945	0.47188
296.8395	0.49485	246.1232	0.46995
295.9128	0.4923	244.7147	0.4682
294.9246	0.49342	243.3239	0.46845
293.9548	0.4916	241.9178	0.4694
292.9802	0.49402	240.5147	0.46748
291.9806	0.49044	239.1073	0.46958
290.9355	0.49196	237.673	0.46705
289.9257	0.48923	236.2566	0.46979
288.9715	0.48513	234.8206	0.46863
288.0023	0.48761	233.3875	0.4686
287.0179	0.48463	231.927	0.4684
285.9096	0.48432	230.5073	0.46716
284.7789	0.48359	229.0621	0.46727
283.6016	0.48393	227.5719	0.46456
282.3979	0.48576	226.1495	0.46572
281.1985	0.48447	224.6821	0.4649
279.9725	0.48626	223.2096	0.46515
278.7368	0.48387	221.738	0.46343
277.5258	0.48264	220.277	0.4644
276.3156	0.48492	218.7973	0.46408
275.0783	0.48601	217.3479	0.46257
273.8624	0.48431	215.8581	0.46266
272.6194	0.48287	214.3809	0.46209
271.3629	0.48519	212.9204	0.46101
270.1137	0.48293	211.4291	0.46115
268.8406	0.48268	209.9405	0.46024
267.5888	0.48284	208.4488	0.46116
266.3092	0.48183	206.9538	0.45999
264.9875	0.4812	205.4636	0.45924
263.68	0.48041	203.9043	0.46038

Table S1 Magnetic susceptibilities (per copper) at various temperatures for 1

202.4112	0.45865	135.4148	0.4408
200.9052	0.45763	133.9763	0.44001
199.406	0.45738	132.5309	0.44098
197.929	0.45659	131.0301	0.43756
196.4057	0.45552	129.5777	0.43841
194.9135	0.45727	128.0958	0.43798
193.4003	0.45687	126.6658	0.43763
191.8986	0.4545	125.2059	0.4378
190.3894	0.45569	123.7124	0.43796
188.8572	0.45404	122.2292	0.4382
187.3462	0.45427	120.7536	0.43694
185.8372	0.45403	119.2427	0.43559
184.3085	0.45332	117.7615	0.43546
182.7662	0.45326	116.2353	0.43481
181.2121	0.45339	114.6919	0.43459
179.714	0.45194	113.169	0.43363
178.1781	0.44997	111.6372	0.43307
176.648	0.45163	110.0628	0.43276
175.1418	0.45087	108.4748	0.43272
173.6197	0.44963	106.8788	0.43313
172.0903	0.44878	105.268	0.43307
170.565	0.45073	103.6039	0.43188
169.0372	0.44988	101.9164	0.43046
167.5001	0.45097	100.2077	0.43047
165.9813	0.45589	98.44734	0.42962
164.4907	0.44506	96.75623	0.42996
163.0007	0.4443	94.99219	0.429
161.5327	0.44577	93.15894	0.42839
160.1015	0.44734	91.24302	0.42793
158.7243	0.44252	89.33935	0.42698
157.371	0.44579	87.39486	0.42687
156.0443	0.44694	85.36035	0.42545
154.7641	0.44402	83.26105	0.42517
153.4459	0.44495	81.07485	0.42435
152.0989	0.44454	78.80109	0.42298
150.7694	0.44534	76.52352	0.42357
149.4032	0.44333	73.97924	0.42248
148.052	0.44411	71.42128	0.42234
146.6835	0.44379	68.66427	0.42172
145.3176	0.44272	65.60815	0.42047
143.9112	0.44058	62.23225	0.41786
142.5399	0.44015	58.34161	0.4095
141.1352	0.44096	54.13036	0.41045
139.6964	0.44135	49.44511	0.41703
138.2928	0.44076	44.04317	0.41537
136.8336	0.44146	42.20851	0.42999

41.00587	0.42967
39.77706	0.43031
38.61408	0.43008
37.41167	0.42988
37.32558	0.40798
36.01581	0.42946
34.55149	0.42969
32.85503	0.42918
31.02279	0.4306
29.37218	0.4095
28.87441	0.43344
25.95456	0.4343
22.14638	0.46202
22.07177	0.43594
18.81545	0.47207
17.64652	0.47123
17.23671	0.60383
17.16497	0.47259
17.10732	0.47859
17.09288	0.48977
17.00594	0.48466
16.99141	0.48088
16.87462	0.48545
16.84528	0.48617



Fig. S3 Temperature dependence of magnetic susceptibility (o, per copper) and the magnetic moment (Δ , per copper) for [Cu₂(R'SSR)₂(SO₄)₂] (1). Theoretical fitting of the experimental data is shown by solid line.



Fig. S2 Unit cell packing diagram of $[Cu_2(R'SSR)_2(SO_4)_2]$ (1)