Supporting Information

Synthesis and Structure of an Asymmetric Copper(I) dimer with Two-coordinate and Four-coordinate Copper(I) Sites

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Synthesis of $Cu_2(pip)_2$

All manipulations were carried under anaerobic and anhydrous conditions. All the solvents were distilled under nitrogen.

To a mixture of 0.25g (1.35 mmol) of (2-Picolyliminomethyl)pyrrole and 0.15g (2.78 mmol) of NaOMe was added 20 mL of 1:1 CH_2Cl_2/MeCN. The mixture was stirred for 5 hr and added to a suspension of 0.135 g (1.35 mmol) of CuCl in 15 mL of MeCN. The resultant mixture was stirred overnight. The insoluble solid was filtered off. The filtrate was concentrated to some sticky oil under reduced pressure. Adding 2 mL of MeCN induced the crystallization of the product. The product was collected as reddish orange crystals by filtration and washed by a little MeCN and diethyl ether, giving a yield of 0.185 g. The crystals suitable for X-ray diffraction study were obtained by slowly evaporating a CH_2Cl_2 solution under MeCN atmosphere at 5 ^oC. This was achieved by sealing a vial of CH_2Cl_2 solution in a jar filled with some MeCN.

NMR Spectra for **2**.

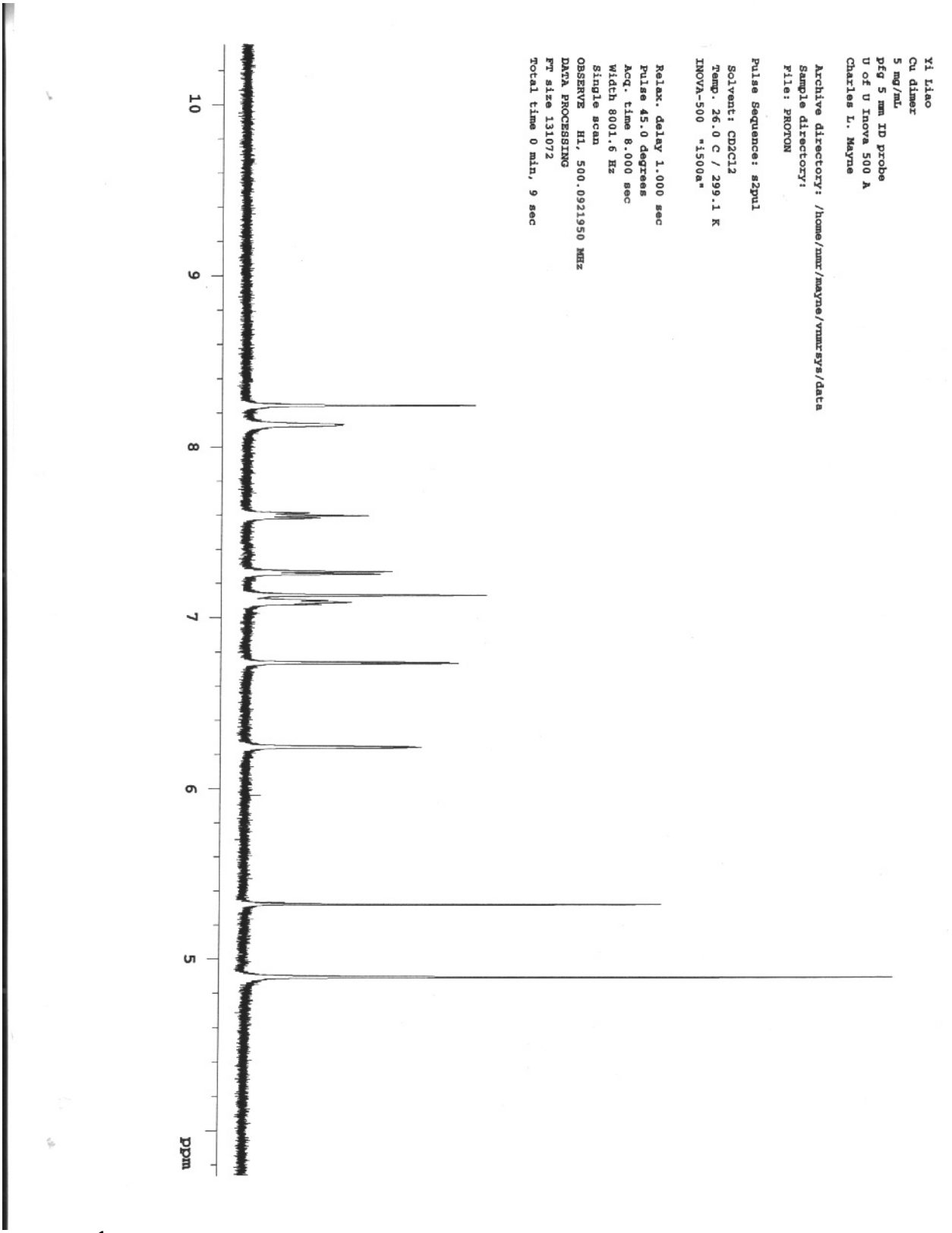

Figure 1 ^{1}H NMR of $Cu_2(pip)_2$ in CD_2Cl_2 (5 mg/mL) at 26°C.

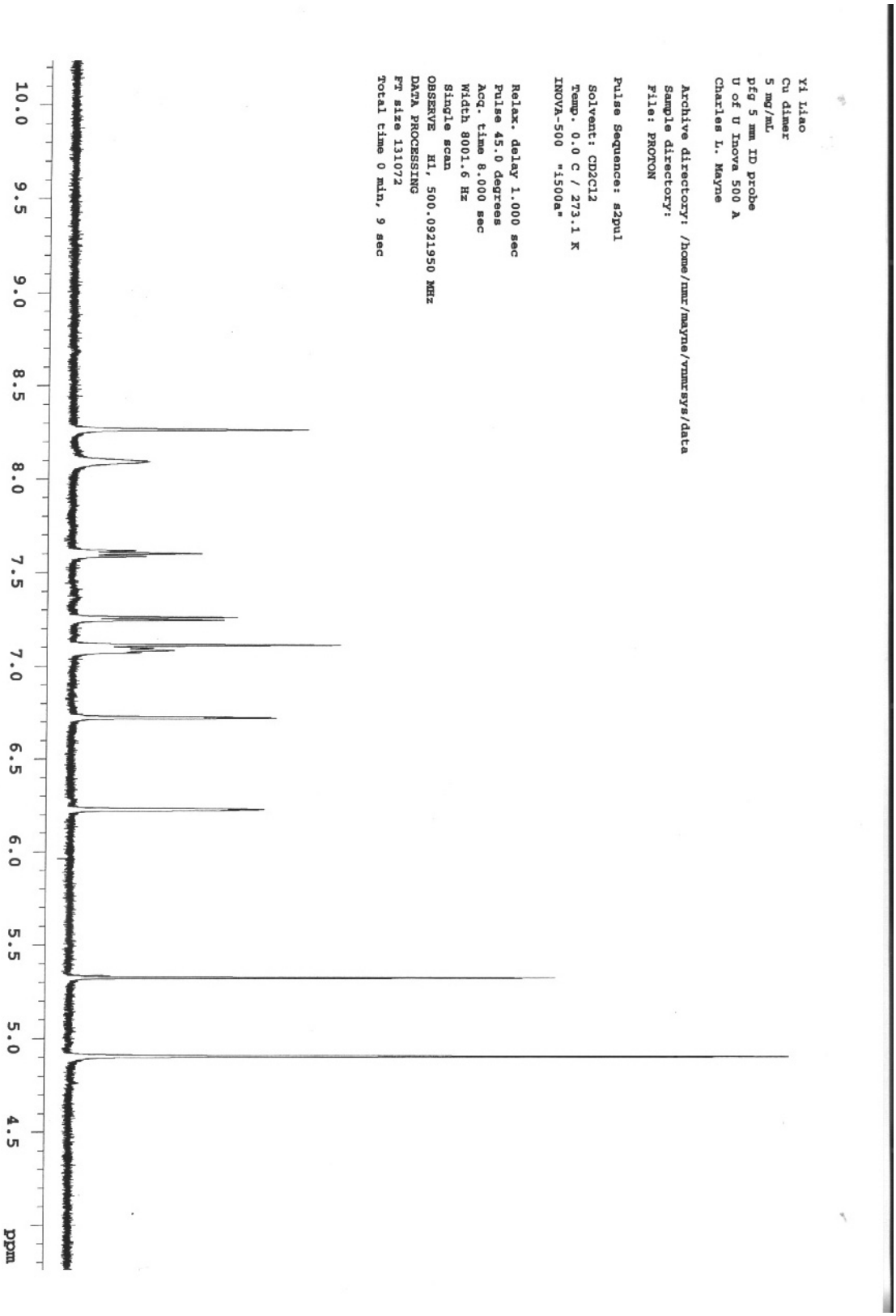

Figure 2 ^{1}H NMR of $Cu_2(pip)_2$ in CD_2Cl_2 (5 mg/mL) at 0°C.

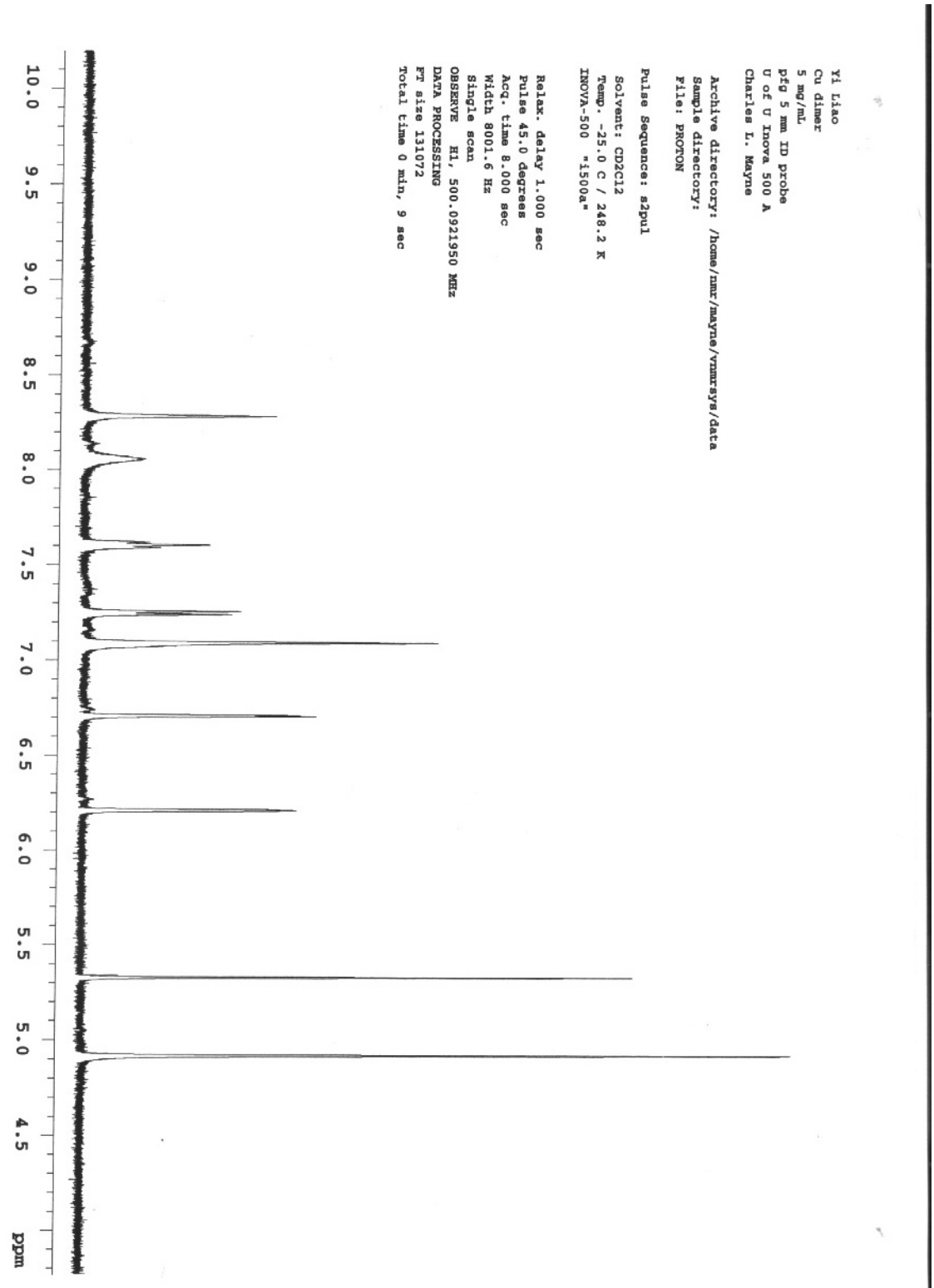

Figure 3 ^{1}H NMR of $Cu_2(pip)_2$ in CD_2Cl_2 (5 mg/mL) at -25^{o}C.

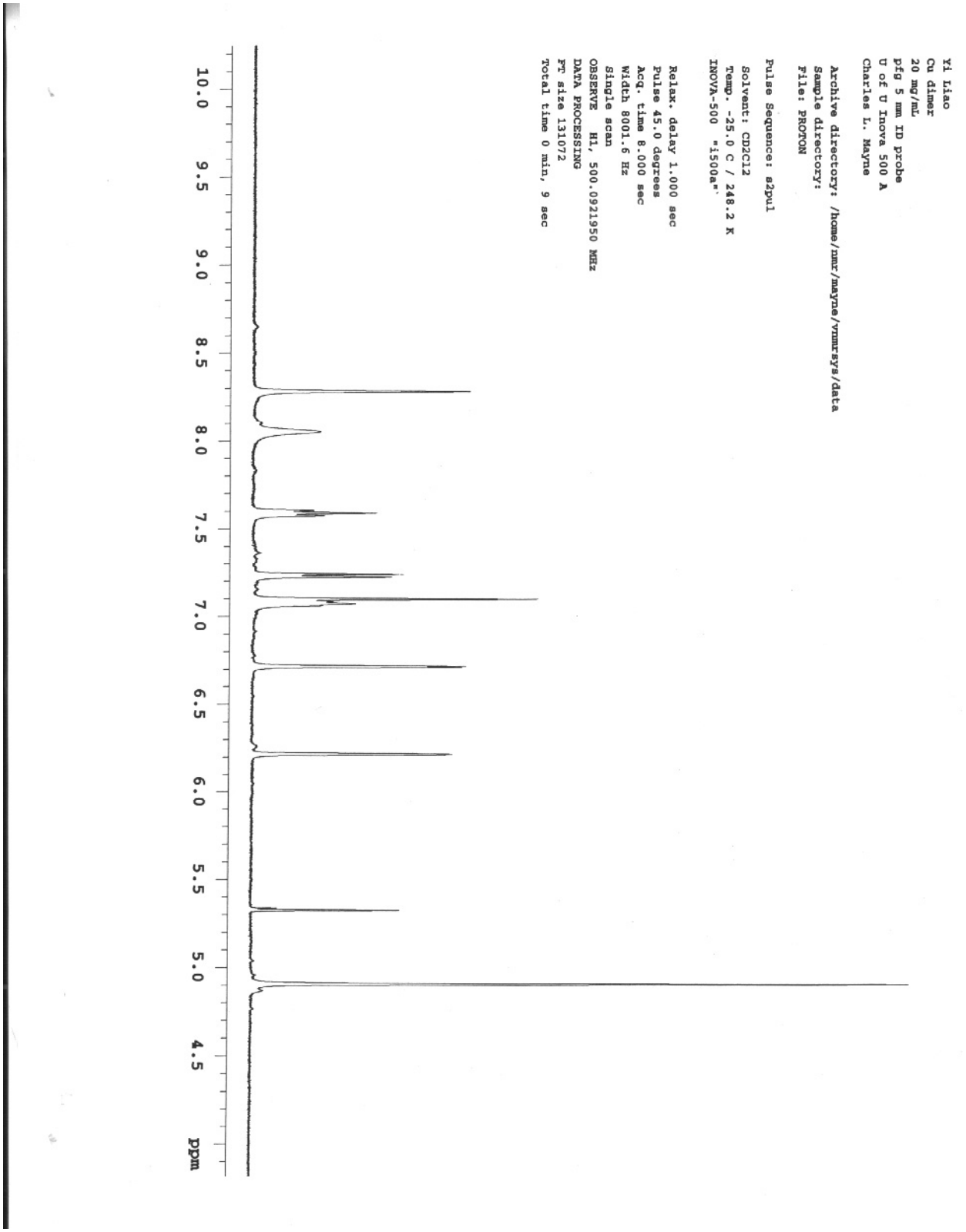

Figure 4 ^{1}H NMR of $Cu_2(pip)_2$ in CD_2Cl_2 (20 mg/mL) at -25^{o}C.

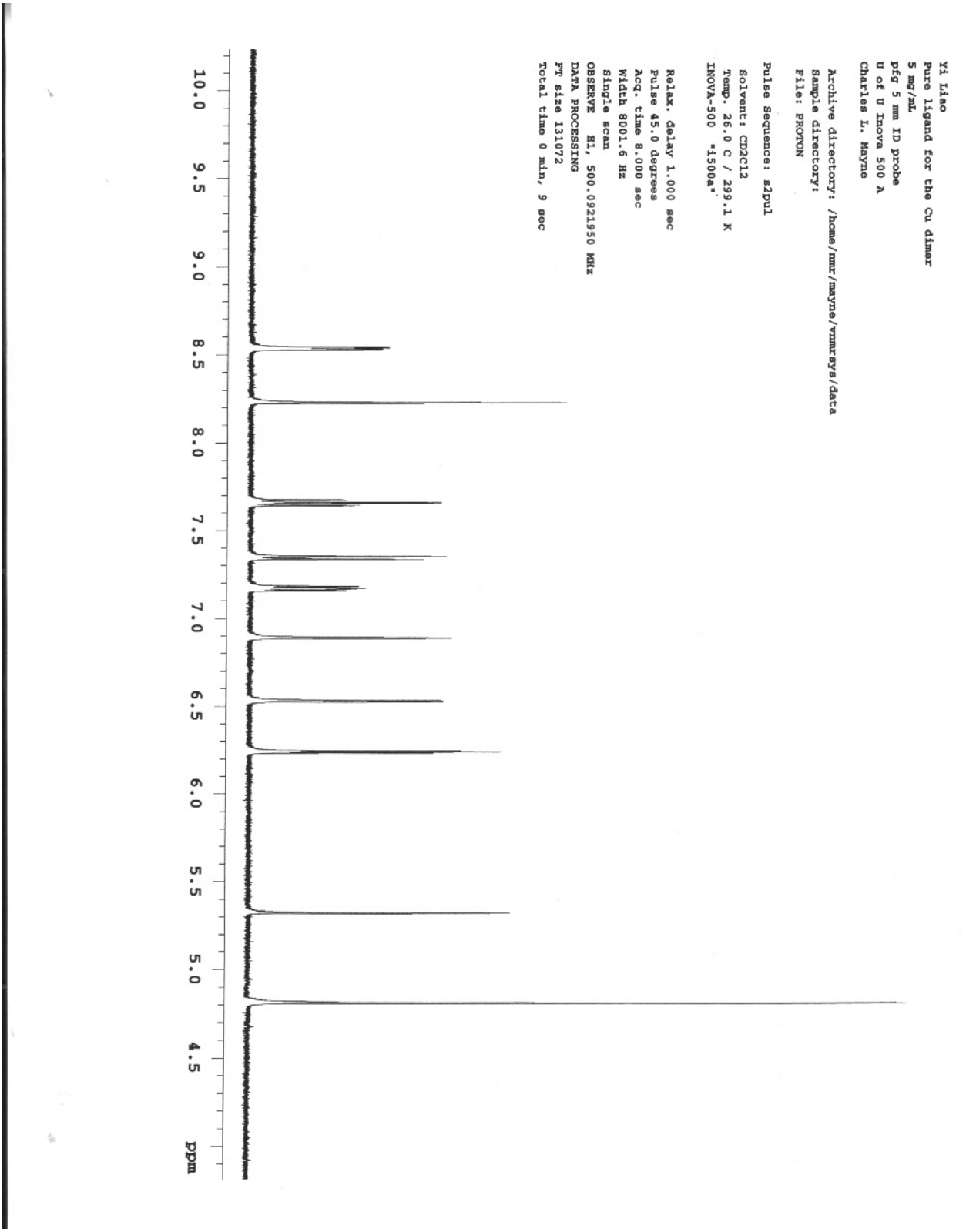

Figure 5 ^{1}H NMR of (2-picolyliminomethyl)pyrrole in CD_2Cl_2 (25 mg/mL) at -25^{o}C.

Computational Results for $Cu^{I}_{2}(pip)_{2}$ [pip = (2-picolyliminomethyl)pyrrole dianion]

exptl (cry -1571.10689518 (0.00)
twisted optimized: -1571.07955175 (17.16 kcal/mol)

exptl.:
========

# b3lyp/lanl2dz guess=read freq
Charge = 0 Multiplicity = 1

6	-3.52657	-1.0313	-1.91182
6	-3.96295	-2.37408	-2.04734
6	-3.19571	-3.13209	-1.13703
6	-2.30022	-2.22794	-0.49408
6	-1.32713	-2.58861	0.48847
6	0.50151	-2.38493	2.02637
6	1.1362	-1.2484	2.81065
6	1.33849	-1.29958	4.20128
6	1.94546	-0.20557	4.84662
6	2.32457	0.91421	4.08272
6	2.08709	0.89245	2.69794
6	-2.35012	3.22074	1.11321
6	-1.83224	4.53256	1.26459
6	-0.57091	4.53427	0.63148
6	-0.35256	3.21534	0.13576
6	0.81838	2.77745	-0.55663
6	2.37674	1.31453	-1.64232
6	2.30058	-0.03104	-2.34452
6	2.81446	-0.24824	-3.63539
6	2.71294	-1.53052	-4.20721
6	2.09042	-2.55839	-3.47425
6	1.59892	-2.26364	-2.19134
29	-1.86909	0.69671	-0.25581
29	0.64496	-0.24134	0.08433
7	-2.52489	-0.93233	-0.97992
7	-0.3327	-1.84035	0.92745
7	1.51313	-0.16669	2.0767
7	-1.46671	2.41932	0.43583
7	1.16024	1.53055	-0.82146
7	1.70827	-1.03119	-1.63771
1	-3.90065	-0.15376	-2.42372
1	-4.73709	-2.73197	-2.71294
1	-3.25191	-4.19968	-0.96005
1	-1.45705	-3.60191	0.89559
1	1.31433	-3.00136	1.60178
1	-0.07486	-3.02828	2.70749
1	1.01805	-2.17122	4.76502
1	2.10516	-0.22124	5.92147
1	2.78075	1.7851	4.54287
1	2.34254	1.73797	2.06641
1	-3.30902	2.84059	1.44195
1	-2.32058	5.36074	1.76058

1	0.11886	5.36539	0.54382
1	1.47448	3.596	-0.88673
1	2.52363	2.11158	-2.38599
1	3.2675	1.30783	-0.98844
1	3.27301	0.57085	-4.18226
1	3.09738	-1.71865	-5.20614
1	1.97693	-3.55707	-3.8842
1	1.09315	-3.01514	-1.59256

Full point group C1 NOp 1
116 alpha electrons 116 beta electrons

SCF Done: E(RB+HF-LYP) = -1571.10689518 A.U. after 3 cycles
Convg = 0.4783D-08 -V/T = 2.1013
S**2 = 0.0000

Total atomic charges:

		1
1	C	-0.202442
2	C	-0.305498
3	C	-0.385429
4	C	0.326884
5	C	-0.255873
6	C	-0.436670
7	C	0.301128
8	C	-0.331327
9	C	-0.173445
10	C	-0.178533
11	C	-0.243865
12	C	-0.202612
13	C	-0.305492
14	C	-0.385563
15	C	0.326900
16	C	-0.255160
17	C	-0.436847
18	C	0.300577
19	C	-0.330608
20	C	-0.173599
21	C	-0.178642
22	C	-0.243116
23	Cu	0.332806
24	Cu	0.371982
25	N	-0.376652
26	N	-0.206381
27	N	-0.159436
28	N	-0.376654
29	N	-0.205995
30	N	-0.160666
31	H	0.222203
32	H	0.231445
33	H	0.230966
34	H	0.205294

35 H 0.228088
36 H 0.208191
37 H 0.236255
38 H 0.236753
39 H 0.232832
40 H 0.242840
41 H 0.222276
42 H 0.231464
43 H 0.231013
44 H 0.205162
45 H 0.208942
46 H 0.228162
47 H 0.236215
48 H 0.236775
49 H 0.232841
50 H 0.242512
Sum of Mulliken charges= 0.00000

freqs:
Low frequencies --- -3.6571 -2.7924 -0.0007 0.0005 0.0009 2.9829
Low frequencies --- 14.6734 15.6397 19.7287
Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	14.5176	15.6161	19.6326
Red. masses --	5.5759	5.9108	4.9830
Frc consts --	0.0007	0.0008	0.0011
IR Inten --	0.2423	1.1444	1.0596

	4	5	6
	?A	?A	?A
Frequencies --	34.1889	48.4966	59.4479
Red. masses --	4.8600	6.5435	4.5844
Frc consts --	0.0033	0.0091	0.0095
IR Inten --	0.2862	0.2663	0.3597

	7	8	9
	?A	?A	?A
Frequencies --	72.5546	75.1845	80.1475
Red. masses --	5.0049	6.5648	5.5372
Frc consts --	0.0155	0.0219	0.0210
IR Inten --	0.1448	0.3484	0.3587

	10	11	12
	?A	?A	?A
Frequencies --	85.7522	101.4359	112.0140
Red. masses --	4.8421	5.2616	12.2600
Frc consts --	0.0210	0.0319	0.0906
IR Inten --	0.0083	1.7157	0.3496

	13	14	15
	?A	?A	?A
Frequencies --	123.4557	143.2977	143.6728
Red. masses --	6.2837	10.5832	7.6925

Frc consts --	0.0564	0.1280	0.0936
IR Inten --	0.1451	0.3903	0.0386
	16	17	18
	?A	?A	?A
Frequencies --	170.0133	179.1708	194.3377
Red. masses --	6.3711	5.9019	5.1767
Frc consts --	0.1085	0.1116	0.1152
IR Inten --	3.9605	9.6641	6.4373
	19	20	21
	?A	?A	?A
Frequencies --	205.5619	207.4953	224.1166
Red. masses --	5.3237	5.1410	6.0623
Frc consts --	0.1325	0.1304	0.1794
IR Inten --	1.3720	0.2106	0.0096
	22	23	24
	?A	?A	?A
Frequencies --	269.3379	271.0257	289.8458
Red. masses --	5.4513	5.6780	4.0177
Frc consts --	0.2330	0.2457	0.1989
IR Inten --	1.1605	1.1258	23.0964
	25	26	27
	?A	?A	?A
Frequencies --	291.7155	295.1439	308.4973
Red. masses --	4.8255	4.9514	3.5712
Frc consts --	0.2419	0.2541	0.2002
IR Inten --	4.1931	3.5229	4.3138
	28	29	30
	?A	?A	?A
Frequencies --	358.8135	364.1774	386.5865
Red. masses --	3.6864	3.1696	6.8027
Frc consts --	0.2796	0.2477	0.5990
IR Inten --	24.1005	0.2923	17.8753
	31	32	33
	?A	?A	?A
Frequencies --	410.9346	421.3298	427.2403
Red. masses --	4.4162	3.3203	3.1499
Frc consts --	0.4394	0.3473	0.3388
IR Inten --	2.0701	0.1199	9.9174
	34	35	36
	?A	?A	?A
Frequencies --	436.4524	485.8345	487.6510
Red. masses --	4.6205	3.1871	3.2031
Frc consts --	0.5186	0.4432	0.4488
IR Inten --	2.8068	4.1802	0.9373
	37	38	39
	?A	?A	?A
Frequencies --	543.2905	547.8221	626.4028
Red. masses --	5.3925	5.6147	2.7374
Frc consts --	0.9378	0.9928	0.6328
IR Inten --	4.2179	5.4210	8.2120
	40	41	42
	?A	?A	?A

Frequencies --	627.2395	641.2868	642.5343
Red. masses --	2.7526	5.9653	6.0339
Frc consts --	0.6381	1.4454	1.4677
IR Inten --	11.5391	0.0145	6.3286
	43	44	45
	?A	?A	?A
Frequencies --	654.9589	656.6877	695.3594
Red. masses --	5.5751	5.5212	4.4409
Frc consts --	1.4091	1.4028	1.2651
IR Inten --	0.2423	8.5948	0.2290
	46	47	48
	?A	?A	?A
Frequencies --	697.1500	765.8056	766.7458
Red. masses --	4.4596	3.7043	3.8273
Frc consts --	1.2770	1.2800	1.3257
IR Inten --	14.1171	3.7154	0.5922
	49	50	51
	?A	?A	?A
Frequencies --	776.1151	776.5752	783.9695
Red. masses --	1.2942	1.2944	1.3703
Frc consts --	0.4593	0.4599	0.4962
IR Inten --	91.4658	76.8794	49.6174
	52	53	54
	?A	?A	?A
Frequencies --	784.2960	799.8515	803.0451
Red. masses --	1.3754	3.6069	3.5522
Frc consts --	0.4985	1.3596	1.3497
IR Inten --	42.5075	0.9193	90.7101
	55	56	57
	?A	?A	?A
Frequencies --	847.4617	848.1611	870.7272
Red. masses --	1.3588	1.3561	4.0150
Frc consts --	0.5750	0.5748	1.7935
IR Inten --	0.7219	0.2553	2.0206
	58	59	60
	?A	?A	?A
Frequencies --	871.1150	908.0963	908.8264
Red. masses --	3.9872	5.1748	5.0471
Frc consts --	1.7827	2.5142	2.4562
IR Inten --	1.0576	0.2872	0.3912
	61	62	63
	?A	?A	?A
Frequencies --	913.8316	914.1721	923.7304
Red. masses --	1.3986	1.3916	1.3248
Frc consts --	0.6881	0.6852	0.6660
IR Inten --	0.6146	0.8927	0.7847
	64	65	66
	?A	?A	?A
Frequencies --	924.3119	958.5565	958.7115
Red. masses --	1.3255	1.6302	1.6308
Frc consts --	0.6672	0.8825	0.8831
IR Inten --	0.7218	15.3939	9.7937

	67	68	69
	?A	?A	?A
Frequencies --	990.3677	991.2297	1009.3168
Red. masses --	1.5049	1.4994	4.1386
Frc consts --	0.8696	0.8680	2.4840
IR Inten --	4.9901	0.2399	5.2380
	70	71	72
	?A	?A	?A
Frequencies --	1009.4321	1011.7286	1013.3119
Red. masses --	5.2407	2.7537	2.8576
Frc consts --	3.1463	1.6607	1.7288
IR Inten --	5.6061	5.7156	28.6303
	73	74	75
	?A	?A	?A
Frequencies --	1014.6060	1016.5855	1034.8425
Red. masses --	3.5608	2.4134	2.6145
Frc consts --	2.1597	1.4695	1.6496
IR Inten --	26.6214	20.5423	5.7673
	76	77	78
	?A	?A	?A
Frequencies --	1035.3250	1040.0696	1040.2896
Red. masses --	2.6040	1.3629	1.3626
Frc consts --	1.6445	0.8687	0.8688
IR Inten --	10.9823	0.2217	0.2344
	79	80	81
	?A	?A	?A
Frequencies --	1067.3736	1068.2582	1081.2346
Red. masses --	2.3005	2.2991	1.3115
Frc consts --	1.5442	1.5458	0.9033
IR Inten --	2.8657	3.8439	75.8614
	82	83	84
	?A	?A	?A
Frequencies --	1082.1596	1119.0863	1121.5688
Red. masses --	1.3331	2.3980	2.5191
Frc consts --	0.9198	1.7694	1.8670
IR Inten --	114.2743	0.2184	4.0613
	85	86	87
	?A	?A	?A
Frequencies --	1128.1317	1128.2052	1198.3578
Red. masses --	1.6419	1.6419	1.0967
Frc consts --	1.2312	1.2313	0.9279
IR Inten --	0.6216	5.2319	0.6893
	88	89	90
	?A	?A	?A
Frequencies --	1198.4157	1222.2754	1223.4602
Red. masses --	1.0965	1.6762	1.6694
Frc consts --	0.9278	1.4754	1.4723
IR Inten --	6.6086	10.6384	15.2017
	91	92	93
	?A	?A	?A
Frequencies --	1229.2462	1229.7038	1267.4330
Red. masses --	1.2128	1.2105	2.2080

Frc consts --	1.0797	1.0785	2.0897
IR Inten --	3.6613	0.5568	18.5339
	94	95	96
	?A	?A	?A
Frequencies --	1267.5361	1289.4425	1289.7207
Red. masses --	2.1778	3.5453	3.5075
Frc consts --	2.0616	3.4730	3.4375
IR Inten --	10.6496	14.4645	5.9745
	97	98	99
	?A	?A	?A
Frequencies --	1308.0636	1308.2618	1322.7488
Red. masses --	4.5870	4.4846	1.6225
Frc consts --	4.6242	4.5224	1.6726
IR Inten --	1.2603	2.7289	5.5195
	100	101	102
	?A	?A	?A
Frequencies --	1323.4946	1367.8137	1368.8656
Red. masses --	1.6188	1.9694	2.0161
Frc consts --	1.6707	2.1709	2.2258
IR Inten --	10.8834	18.6070	2.7868
	103	104	105
	?A	?A	?A
Frequencies --	1394.1432	1396.1451	1401.2832
Red. masses --	1.7163	1.6902	2.6892
Frc consts --	1.9654	1.9412	3.1112
IR Inten --	103.9653	198.7367	37.0137
	106	107	108
	?A	?A	?A
Frequencies --	1402.1704	1436.3754	1437.2582
Red. masses --	2.7275	2.9961	3.0597
Frc consts --	3.1595	3.6420	3.7238
IR Inten --	41.8627	21.6823	63.1620
	109	110	111
	?A	?A	?A
Frequencies --	1457.9828	1458.4395	1467.0592
Red. masses --	2.7332	2.7513	2.0652
Frc consts --	3.4231	3.4479	2.6189
IR Inten --	9.1301	72.2934	18.6413
	112	113	114
	?A	?A	?A
Frequencies --	1467.1738	1493.7202	1494.0116
Red. masses --	2.0482	1.2964	1.3010
Frc consts --	2.5977	1.7043	1.7109
IR Inten --	25.4432	29.2201	51.3118
	115	116	117
	?A	?A	?A
Frequencies --	1506.5278	1506.6559	1524.5074
Red. masses --	1.6906	1.6973	4.2901
Frc consts --	2.2607	2.2700	5.8746
IR Inten --	7.4567	13.8979	4.4853
	118	119	120
	?A	?A	?A

Frequencies --	1524.8109	1609.6409	1610.0333
Red. masses --	4.2974	5.9999	5.9856
Frc consts --	5.8869	9.1591	9.1417
IR Inten --	0.1860	8.2599	33.5161
	121	122	123
	?A	?A	?A
Frequencies --	1632.4465	1632.4797	1653.1466
Red. masses --	5.5458	5.5564	5.8053
Frc consts --	8.7075	8.7244	9.3475
IR Inten --	21.1183	10.4438	443.8060
	124	125	126
	?A	?A	?A
Frequencies --	1654.1455	2980.9464	2981.4822
Red. masses --	5.8087	1.0647	1.0646
Frc consts --	9.3643	5.5745	5.5757
IR Inten --	670.8341	40.3729	105.3515
	127	128	129
	?A	?A	?A
Frequencies --	3050.9800	3051.2286	3060.7861
Red. masses --	1.0890	1.0892	1.0929
Frc consts --	5.9725	5.9745	6.0324
IR Inten --	43.6619	14.3156	108.6602
	130	131	132
	?A	?A	?A
Frequencies --	3061.1384	3204.8117	3204.9329
Red. masses --	1.0927	1.0878	1.0878
Frc consts --	6.0330	6.5826	6.5830
IR Inten --	13.1490	3.9036	2.9861
	133	134	135
	?A	?A	?A
Frequencies --	3216.6721	3216.8732	3225.2292
Red. masses --	1.0901	1.0901	1.0961
Frc consts --	6.6458	6.6466	6.7175
IR Inten --	0.0770	0.1204	13.3166
	136	137	138
	?A	?A	?A
Frequencies --	3225.3954	3242.1572	3242.3851
Red. masses --	1.0961	1.0912	1.0912
Frc consts --	6.7182	6.7581	6.7592
IR Inten --	33.5296	2.7285	4.5287
	139	140	141
	?A	?A	?A
Frequencies --	3244.0611	3244.1478	3255.6688
Red. masses --	1.1011	1.1011	1.0945
Frc consts --	6.8276	6.8277	6.8354
IR Inten --	14.8183	31.7233	19.5491
	142	143	144
	?A	?A	?A
Frequencies --	3255.7713	3282.3994	3282.5293
Red. masses --	1.0945	1.1074	1.1073
Frc consts --	6.8356	7.0294	7.0298
IR Inten --	6.2802	23.2757	24.1321

Zero-point correction= 0.385829 (Hartree/Particle)
Thermal correction to Energy= 0.412794
Thermal correction to Enthalpy= 0.413738
Thermal correction to Gibbs Free Energy= 0.324621
Sum of electronic and zero-point Energies= -1570.721066
Sum of electronic and thermal Energies= -1570.694101
Sum of electronic and thermal Enthalpies= -1570.693157
Sum of electronic and thermal Free Energies= -1570.782274

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	259.032	101.298	187.562
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	44.480
ROTATIONAL	0.889	2.981	36.220
VIBRATIONAL	257.255	95.336	106.862
VIBRATION 1	0.593	1.986	7.271
VIBRATION 2	0.593	1.986	7.126
VIBRATION 3	0.593	1.986	6.671
VIBRATION 4	0.594	1.983	5.570
VIBRATION 5	0.595	1.978	4.878
VIBRATION 6	0.597	1.974	4.475
VIBRATION 7	0.599	1.967	4.083
VIBRATION 8	0.599	1.966	4.013
VIBRATION 9	0.600	1.963	3.887
VIBRATION 10	0.601	1.959	3.755
VIBRATION 11	0.604	1.948	3.427
VIBRATION 12	0.607	1.940	3.234
VIBRATION 13	0.610	1.929	3.046
VIBRATION 14	0.616	1.910	2.759
VIBRATION 15	0.616	1.909	2.754
VIBRATION 16	0.625	1.879	2.435
VIBRATION 17	0.629	1.868	2.337
VIBRATION 18	0.635	1.848	2.186
VIBRATION 19	0.640	1.832	2.083
VIBRATION 20	0.641	1.829	2.066
VIBRATION 21	0.649	1.804	1.926
VIBRATION 22	0.674	1.730	1.600
VIBRATION 23	0.675	1.727	1.590
VIBRATION 24	0.686	1.693	1.475
VIBRATION 25	0.687	1.689	1.464
VIBRATION 26	0.689	1.683	1.444
VIBRATION 27	0.698	1.658	1.370
VIBRATION 28	0.734	1.557	1.127
VIBRATION 29	0.738	1.546	1.104
VIBRATION 30	0.755	1.499	1.013
VIBRATION 31	0.775	1.447	0.923
VIBRATION 32	0.784	1.424	0.887
VIBRATION 33	0.789	1.411	0.868
VIBRATION 34	0.797	1.391	0.838
VIBRATION 35	0.842	1.281	0.695

VIBRATION 36	0.844	1.277	0.690
VIBRATION 37	0.898	1.154	0.558
VIBRATION 38	0.903	1.144	0.549
	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.484808-149	-149.314430	-343.809181
TOTAL V=0	0.142331D+29	28.153300	64.825368
VIB (BOT)	0.611204-165	-165.213814	-380.418865
VIB (BOT) 1	0.142711D+02	1.154459	2.658240
VIB (BOT) 2	0.132668D+02	1.122768	2.585268
VIB (BOT) 3	0.105512D+02	1.023304	2.356244
VIB (BOT) 4	0.605432D+01	0.782066	1.800773
VIB (BOT) 5	0.426326D+01	0.629742	1.450034
VIB (BOT) 6	0.347391D+01	0.540819	1.245281
VIB (BOT) 7	0.284160D+01	0.453563	1.044367
VIB (BOT) 8	0.274117D+01	0.437936	1.008385
VIB (BOT) 9	0.256951D+01	0.409851	0.943716
VIB (BOT) 10	0.239941D+01	0.380105	0.875223
VIB (BOT) 11	0.202267D+01	0.305925	0.704418
VIB (BOT) 12	0.182767D+01	0.261897	0.603041
VIB (BOT) 13	0.165398D+01	0.218529	0.503182
VIB (BOT) 14	0.141771D+01	0.151586	0.349040
VIB (BOT) 15	0.141386D+01	0.150406	0.346322
VIB (BOT) 16	0.118536D+01	0.073849	0.170042
VIB (BOT) 17	0.112133D+01	0.049732	0.114513
VIB (BOT) 18	0.102822D+01	0.012087	0.027832
VIB (BOT) 19	0.967918D+00	-0.014161	-0.032608
VIB (BOT) 20	0.958169D+00	-0.018558	-0.042731
VIB (BOT) 21	0.881062D+00	-0.054993	-0.126627
VIB (BOT) 22	0.717789D+00	-0.144003	-0.331580
VIB (BOT) 23	0.712705D+00	-0.147090	-0.338688
VIB (BOT) 24	0.659835D+00	-0.180565	-0.415766
VIB (BOT) 25	0.654936D+00	-0.183801	-0.423217
VIB (BOT) 26	0.646106D+00	-0.189696	-0.436791
VIB (BOT) 27	0.613485D+00	-0.212196	-0.488599
VIB (BOT) 28	0.511230D+00	-0.291383	-0.670935
VIB (BOT) 29	0.501898D+00	-0.299384	-0.689358
VIB (BOT) 30	0.465535D+00	-0.332048	-0.764568
VIB (BOT) 31	0.430238D+00	-0.366292	-0.843418
VIB (BOT) 32	0.416329D+00	-0.380563	-0.876279
VIB (BOT) 33	0.408703D+00	-0.388592	-0.894767
VIB (BOT) 34	0.397201D+00	-0.400990	-0.923313
VIB (BOT) 35	0.342521D+00	-0.465312	-1.071421
VIB (BOT) 36	0.340708D+00	-0.467618	-1.076730
VIB (BOT) 37	0.290715D+00	-0.536533	-1.235413
VIB (BOT) 38	0.287067D+00	-0.542017	-1.248040
VIB (V=0)	0.179439D+13	12.253916	28.215684
VIB (V=0) 1	0.147799D+02	1.169672	2.693269
VIB (V=0) 2	0.137763D+02	1.139131	2.622947
VIB (V=0) 3	0.110631D+02	1.043876	2.403614
VIB (V=0) 4	0.657494D+01	0.817892	1.883265
VIB (V=0) 5	0.479248D+01	0.680560	1.567048
VIB (V=0) 6	0.400971D+01	0.603113	1.388719

VIB (V=0) 7	0.338525D+01	0.529591	1.219429
VIB (V=0) 8	0.328640D+01	0.516720	1.189792
VIB (V=0) 9	0.311771D+01	0.493835	1.137098
VIB (V=0) 10	0.295095D+01	0.469962	1.082128
VIB (V=0) 11	0.258355D+01	0.412217	0.949165
VIB (V=0) 12	0.239483D+01	0.379274	0.873311
VIB (V=0) 13	0.222790D+01	0.347896	0.801059
VIB (V=0) 14	0.200329D+01	0.301744	0.694792
VIB (V=0) 15	0.199966D+01	0.300957	0.692979
VIB (V=0) 16	0.178649D+01	0.252002	0.580255
VIB (V=0) 17	0.172775D+01	0.237481	0.546821
VIB (V=0) 18	0.164335D+01	0.215729	0.496735
VIB (V=0) 19	0.158943D+01	0.201242	0.463378
VIB (V=0) 20	0.158078D+01	0.198872	0.457919
VIB (V=0) 21	0.151305D+01	0.179853	0.414128
VIB (V=0) 22	0.137477D+01	0.138230	0.318286
VIB (V=0) 23	0.137060D+01	0.136911	0.315250
VIB (V=0) 24	0.132788D+01	0.123158	0.283582
VIB (V=0) 25	0.132398D+01	0.121881	0.280642
VIB (V=0) 26	0.131698D+01	0.119579	0.275340
VIB (V=0) 27	0.129143D+01	0.111071	0.255751
VIB (V=0) 28	0.121509D+01	0.084609	0.194820
VIB (V=0) 29	0.120845D+01	0.082229	0.189339
VIB (V=0) 30	0.118317D+01	0.073048	0.168198
VIB (V=0) 31	0.115962D+01	0.064317	0.148096
VIB (V=0) 32	0.115064D+01	0.060939	0.140317
VIB (V=0) 33	0.114578D+01	0.059103	0.136090
VIB (V=0) 34	0.113857D+01	0.056359	0.129771
VIB (V=0) 35	0.110607D+01	0.043783	0.100813
VIB (V=0) 36	0.110505D+01	0.043381	0.099888
VIB (V=0) 37	0.107837D+01	0.032769	0.075453
VIB (V=0) 38	0.107655D+01	0.032033	0.073759
ELECTRONIC	0.100000D+01	0.000000	0.000000
TRANSLATIONAL	0.431614D+09	8.635096	19.883043
ROTATIONAL	0.183776D+08	7.264288	16.726641

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twisted alternative (optimized):
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b3lyp/lanl2dz guess=read freq

Charge = 0 Multiplicity = 1

6	1.5277	-0.66479	3.17635
6	0.95537	-1.5733	4.12571
6	-0.03347	-2.30264	3.4384
6	-0.02831	-1.81121	2.09577
6	-0.80292	-2.14749	0.95911
6	-1.42934	-1.88932	-1.35892
6	-2.91152	-1.55634	-1.21404
6	-3.90897	-2.4671	-1.61298

6	-5.26643	-2.1283	-1.48351
6	-5.60405	-0.87121	-0.9497
6	-4.57042	-0.00589	-0.56973
6	3.75686	-1.97375	-0.3504
6	5.10216	-2.12085	-0.73561
6	4.94925	0.03411	-1.84013
6	3.60428	0.11103	-1.41723
6	2.74544	1.26703	-1.69725
6	0.68172	2.50825	-1.45157
6	0.07975	3.11067	-0.22098
6	0.49099	4.24796	0.4918
6	-0.40697	4.3921	1.5966
6	-1.32287	3.33429	1.50622
29	1.04485	-0.20838	0.03342
29	-1.94852	0.98323	-0.10273
7	0.94208	-0.80447	1.9603
7	-0.61145	-1.50269	-0.19321
7	-3.25202	-0.33575	-0.69537
7	3.01824	-0.89147	-0.69036
7	1.56166	1.33075	-1.15157
7	-1.03402	2.54658	0.39775
1	2.30951	0.06522	3.34479
1	1.23147	-1.66502	5.16833
1	-0.67696	-3.07646	3.83926
1	-1.55632	-2.93885	1.0543
1	-1.34226	-2.96534	-1.58182
1	-1.03451	-1.35164	-2.23093
1	-3.61392	-3.43133	-2.0157
1	-6.04069	-2.82752	-1.78704
1	-6.63717	-0.56361	-0.82695
1	-4.78227	0.97545	-0.15888
1	3.25235	-2.72817	0.24626
1	5.65563	-3.00892	-0.44636
1	5.3852	0.84949	-2.41157
1	3.13241	2.05735	-2.34769
1	1.24944	3.26946	-2.0082
1	-0.11272	2.12781	-2.11268
1	1.32844	4.88943	0.24409
1	-0.3909	5.16495	2.35427
1	-2.15054	3.09729	2.1627
6	5.7059	-1.09817	-1.49801
1	6.74382	-1.18141	-1.80873

Full point group C1 NOp 1

116 alpha electrons 116 beta electrons

SCF Done: E(RB+HF-LYP) = -1571.07955175 A.U. after 3 cycles
Convg = 0.7801D-08 -V/T = 2.1014
S**2 = 0.0000

Total atomic charges:

		1
1	C	-0.278106
2	C	-0.284810
3	C	-0.407882
4	C	0.373426
5	C	-0.218014
6	C	-0.463495
7	C	0.310439
8	C	-0.336738
9	C	-0.163694
10	C	-0.189422
11	C	-0.152404
12	C	-0.263834
13	C	-0.175816
14	C	-0.279779
15	C	0.279927
16	C	-0.235678
17	C	-0.487752
18	C	0.384083
19	C	-0.434293
20	C	-0.309853
21	C	-0.219836
22	Cu	0.414761
23	Cu	0.358100
24	N	-0.325535
25	N	-0.245699
26	N	-0.276738
27	N	-0.163290
28	N	-0.166041
29	N	-0.416625
30	H	0.227078
31	H	0.229175
32	H	0.231650
33	H	0.223377
34	H	0.205511
35	H	0.234499
36	H	0.245466
37	H	0.244261
38	H	0.242043
39	H	0.250552
40	H	0.251447
41	H	0.231956
42	H	0.231972
43	H	0.228528
44	H	0.192981
45	H	0.215347
46	H	0.224101
47	H	0.220714
48	H	0.200146
49	C	-0.192194
50	H	0.235989

Sum of Mulliken charges= 0.00000

Low frequencies --- -3.0824 -0.0005 -0.0002 0.0006 1.2528 6.0910 Low frequencies --- 13.3953 27.6184 31.2558

Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
Raman scattering activities (A**4/AMU), Raman depolarization ratios,
reduced masses (AMU), force constants (mDyne/A) and normal coordinates:

	1	2	3
	?A	?A	?A
Frequencies --	13.2168	27.6074	31.1600
Red. masses --	5.8971	6.1296	5.9986
Frc consts --	0.0006	0.0028	0.0034
IR Inten --	1.4690	0.7223	0.4400

	4	5	6
	?A	?A	?A
Frequencies --	34.5671	42.5312	47.8155
Red. masses --	5.4636	6.2729	5.2984
Frc consts --	0.0038	0.0067	0.0071
IR Inten --	1.1329	0.5842	0.7237

	7	8	9
	?A	?A	?A
Frequencies --	65.7354	78.9172	85.5562
Red. masses --	5.4228	6.9443	5.8566
Frc consts --	0.0138	0.0255	0.0253
IR Inten --	0.8794	0.9245	0.2776

	10	11	12
	?A	?A	?A
Frequencies --	90.9139	111.6643	115.0475
Red. masses --	5.5378	6.0691	5.6790
Frc consts --	0.0270	0.0446	0.0443
IR Inten --	0.0796	0.9263	0.8510

	13	14	15
	?A	?A	?A
Frequencies --	117.1137	144.7177	154.4844
Red. masses --	8.4142	5.6173	6.2919
Frc consts --	0.0680	0.0693	0.0885
IR Inten --	0.8430	4.2587	5.5069

	16	17	18
	?A	?A	?A
Frequencies --	162.1540	176.1516	189.3643
Red. masses --	6.0634	5.7250	7.3749
Frc consts --	0.0939	0.1047	0.1558
IR Inten --	4.0657	1.2416	3.4916

	19	20	21
	?A	?A	?A
Frequencies --	212.1883	219.8271	231.7023
Red. masses --	5.0234	5.4914	4.6422
Frc consts --	0.1333	0.1563	0.1468
IR Inten --	0.0076	2.3995	8.2500

Zero-point vibrational energy 1013759.5 (Joules/Mol)
242.29434 (kcal/Mol)

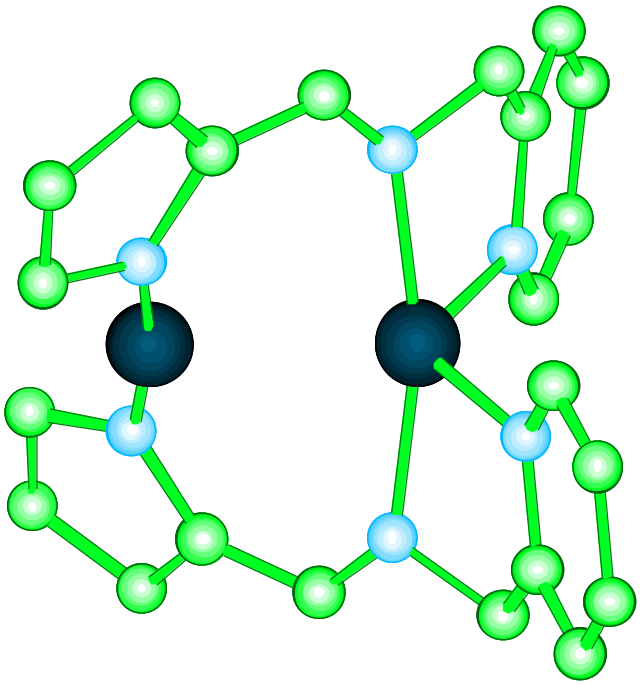
Zero-point correction= 0.386121 (Hartree/Particle)
Thermal correction to Energy= 0.412841
Thermal correction to Enthalpy= 0.413785
Thermal correction to Gibbs Free Energy= 0.325725
Sum of electronic and zero-point Energies= -1570.693431
Sum of electronic and thermal Energies= -1570.666711
Sum of electronic and thermal Enthalpies= -1570.665767
Sum of electronic and thermal Free Energies= -1570.753827

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	259.062	101.103	185.338
ELECTRONIC	0.000	0.000	0.000
TRANSLATIONAL	0.889	2.981	44.480
ROTATIONAL	0.889	2.981	36.408
VIBRATIONAL	257.284	95.141	104.450
VIBRATION 1	0.593	1.987	7.457
VIBRATION 2	0.593	1.984	5.994
VIBRATION 3	0.594	1.983	5.754
VIBRATION 4	0.594	1.983	5.548
VIBRATION 5	0.595	1.980	5.138
VIBRATION 6	0.595	1.978	4.906
VIBRATION 7	0.597	1.971	4.277
VIBRATION 8	0.600	1.963	3.918
VIBRATION 9	0.601	1.959	3.759
VIBRATION 10	0.602	1.956	3.640
VIBRATION 11	0.607	1.940	3.240
VIBRATION 12	0.608	1.937	3.182
VIBRATION 13	0.608	1.935	3.147
VIBRATION 14	0.616	1.908	2.741
VIBRATION 15	0.620	1.898	2.616
VIBRATION 16	0.622	1.889	2.525
VIBRATION 17	0.628	1.872	2.369
VIBRATION 18	0.633	1.855	2.234
VIBRATION 19	0.643	1.822	2.025
VIBRATION 20	0.647	1.811	1.961
VIBRATION 21	0.653	1.793	1.866
VIBRATION 22	0.669	1.743	1.652
VIBRATION 23	0.679	1.714	1.546
VIBRATION 24	0.696	1.664	1.389
VIBRATION 25	0.697	1.661	1.380
VIBRATION 26	0.706	1.634	1.306
VIBRATION 27	0.724	1.584	1.185
VIBRATION 28	0.732	1.562	1.137
VIBRATION 29	0.747	1.520	1.052
VIBRATION 30	0.760	1.487	0.991
VIBRATION 31	0.793	1.401	0.853
VIBRATION 32	0.800	1.384	0.828
VIBRATION 33	0.807	1.365	0.801
VIBRATION 34	0.817	1.342	0.770
VIBRATION 35	0.832	1.304	0.722
VIBRATION 36	0.865	1.228	0.634

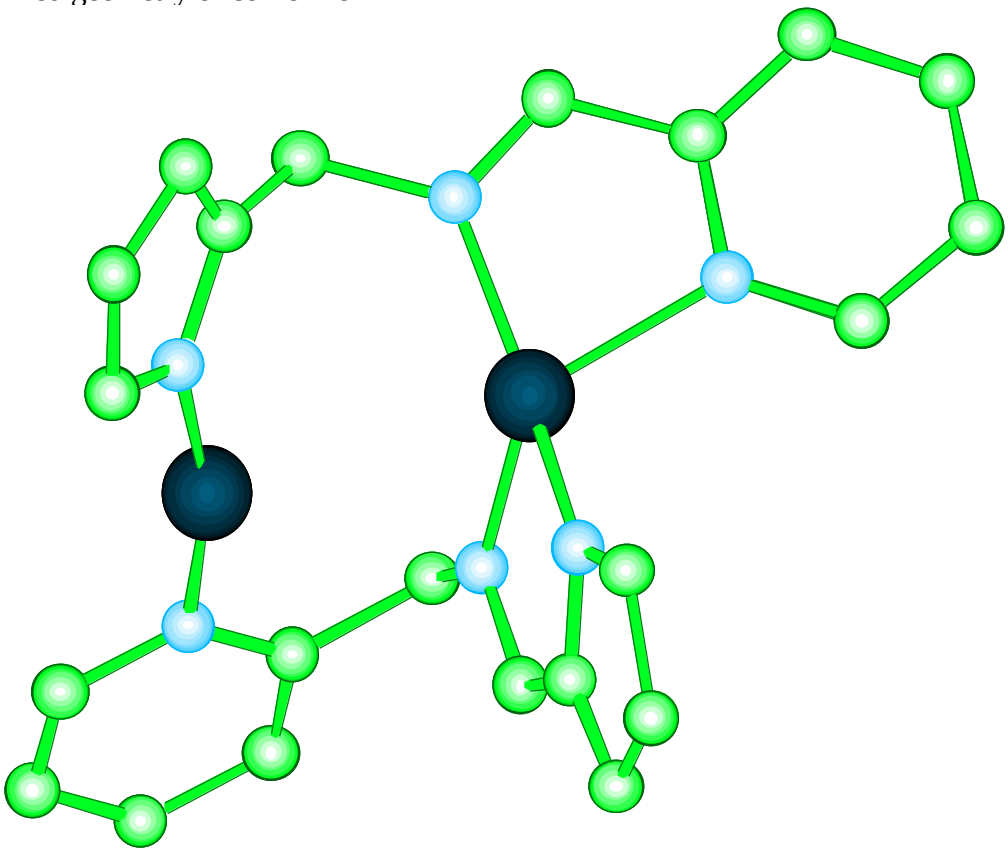
VIBRATION 37	0.890	1.172	0.575
VIBRATION 38	0.892	1.169	0.572
VIBRATION 39	0.980	0.989	0.416

	Q	LOG10(Q)	LN(Q)
TOTAL BOT	0.150626-149	-149.822099	-344.978132
TOTAL V=0	0.602348D+28	27.779847	63.965462
VIB (BOT)	0.172751-165	-165.762579	-381.682444
VIB (BOT) 1	0.156763D+02	1.195242	2.752147
VIB (BOT) 2	0.750063D+01	0.875098	2.014987
VIB (BOT) 3	0.664412D+01	0.822437	1.893732
VIB (BOT) 4	0.598794D+01	0.777278	1.789748
VIB (BOT) 5	0.486378D+01	0.686974	1.581817
VIB (BOT) 6	0.432427D+01	0.635913	1.464243
VIB (BOT) 7	0.313925D+01	0.496825	1.143983
VIB (BOT) 8	0.261006D+01	0.416651	0.959374
VIB (BOT) 9	0.240498D+01	0.381112	0.877543
VIB (BOT) 10	0.226118D+01	0.354336	0.815889
VIB (BOT) 11	0.183353D+01	0.263288	0.606243
VIB (BOT) 12	0.177829D+01	0.250003	0.575654
VIB (BOT) 13	0.174611D+01	0.242072	0.557391
VIB (BOT) 14	0.140324D+01	0.147133	0.338785
VIB (BOT) 15	0.131084D+01	0.117549	0.270666
VIB (BOT) 16	0.124593D+01	0.095492	0.219879
VIB (BOT) 17	0.114172D+01	0.057560	0.132536
VIB (BOT) 18	0.105716D+01	0.024139	0.055582
VIB (BOT) 19	0.935218D+00	-0.029087	-0.066976
VIB (BOT) 20	0.899885D+00	-0.045813	-0.105488
VIB (BOT) 21	0.849419D+00	-0.070878	-0.163203
VIB (BOT) 22	0.742271D+00	-0.129437	-0.298040
VIB (BOT) 23	0.692426D+00	-0.159627	-0.367554
VIB (BOT) 24	0.621419D+00	-0.206615	-0.475750
VIB (BOT) 25	0.617833D+00	-0.209129	-0.481537
VIB (BOT) 26	0.585487D+00	-0.232483	-0.535311
VIB (BOT) 27	0.534853D+00	-0.271766	-0.625764
VIB (BOT) 28	0.515062D+00	-0.288140	-0.663467
VIB (BOT) 29	0.481036D+00	-0.317823	-0.731814
VIB (BOT) 30	0.456790D+00	-0.340283	-0.783532
VIB (BOT) 31	0.402904D+00	-0.394798	-0.909056
VIB (BOT) 32	0.393418D+00	-0.405146	-0.932882
VIB (BOT) 33	0.383019D+00	-0.416780	-0.959672
VIB (BOT) 34	0.371227D+00	-0.430360	-0.990940
VIB (BOT) 35	0.352926D+00	-0.452317	-1.041498
VIB (BOT) 36	0.319367D+00	-0.495709	-1.141413
VIB (BOT) 37	0.297285D+00	-0.526827	-1.213063
VIB (BOT) 38	0.296045D+00	-0.528643	-1.217244
VIB (BOT) 39	0.235813D+00	-0.627432	-1.444716
VIB (V=0)	0.690823D+12	11.839367	27.261150
VIB (V=0) 1	0.161842D+02	1.209092	2.784037
VIB (V=0) 2	0.801728D+01	0.904027	2.081599
VIB (V=0) 3	0.716290D+01	0.855089	1.968916
VIB (V=0) 4	0.650878D+01	0.813500	1.873152

VIB (V=0) 5	0.538942D+01	0.731542	1.684437
VIB (V=0) 6	0.485308D+01	0.686017	1.579613
VIB (V=0) 7	0.367882D+01	0.565708	1.302591
VIB (V=0) 8	0.315752D+01	0.499346	1.149788
VIB (V=0) 9	0.295641D+01	0.470764	1.083975
VIB (V=0) 10	0.281581D+01	0.449603	1.035248
VIB (V=0) 11	0.240048D+01	0.380298	0.875669
VIB (V=0) 12	0.234725D+01	0.370559	0.853244
VIB (V=0) 13	0.231629D+01	0.364793	0.839966
VIB (V=0) 14	0.198966D+01	0.298779	0.687964
VIB (V=0) 15	0.190296D+01	0.279429	0.643410
VIB (V=0) 16	0.184251D+01	0.265410	0.611128
VIB (V=0) 17	0.174640D+01	0.242145	0.557559
VIB (V=0) 18	0.166944D+01	0.222570	0.512485
VIB (V=0) 19	0.156049D+01	0.193260	0.444998
VIB (V=0) 20	0.152946D+01	0.184539	0.424916
VIB (V=0) 21	0.148565D+01	0.171917	0.395854
VIB (V=0) 22	0.139497D+01	0.144564	0.332871
VIB (V=0) 23	0.135408D+01	0.131645	0.303123
VIB (V=0) 24	0.129760D+01	0.113140	0.260514
VIB (V=0) 25	0.129481D+01	0.112205	0.258361
VIB (V=0) 26	0.126993D+01	0.103780	0.238963
VIB (V=0) 27	0.123217D+01	0.090669	0.208774
VIB (V=0) 28	0.121784D+01	0.085589	0.197076
VIB (V=0) 29	0.119383D+01	0.076941	0.177164
VIB (V=0) 30	0.117724D+01	0.070866	0.163175
VIB (V=0) 31	0.114213D+01	0.057716	0.132896
VIB (V=0) 32	0.113622D+01	0.055463	0.127708
VIB (V=0) 33	0.112984D+01	0.053018	0.122079
VIB (V=0) 34	0.112274D+01	0.050281	0.115775
VIB (V=0) 35	0.111201D+01	0.046109	0.106169
VIB (V=0) 36	0.109329D+01	0.038736	0.089193
VIB (V=0) 37	0.108170D+01	0.034108	0.078537
VIB (V=0) 38	0.108107D+01	0.033854	0.077951
VIB (V=0) 39	0.105282D+01	0.022353	0.051470
ELECTRONIC	0.100000D+01	0.000000	0.000000
TRANSLATIONAL	0.431614D+09	8.635096	19.883043
ROTATIONAL	0.202015D+08	7.305384	16.821269



Full optimized geometry of conformer **2**



Full optimized geometry of conformer **3**

TOC

Synthesis and Structure of an Asymmetric Copper(I) dimer with Two-coordinate and Four-coordinate Copper(I) Sites

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An asymmetric copper(I) dimer with both two- and four-coordinate copper(I) sites was synthesized and studied by X-ray diffraction and DFT calculations and shown to be more stable than the symmetric form.