Supporting information for

Synthesis and Characterization of Phosphorescent Two-Coordinate Copper(I) Complexes Bearing Diamidocarbene Ligands

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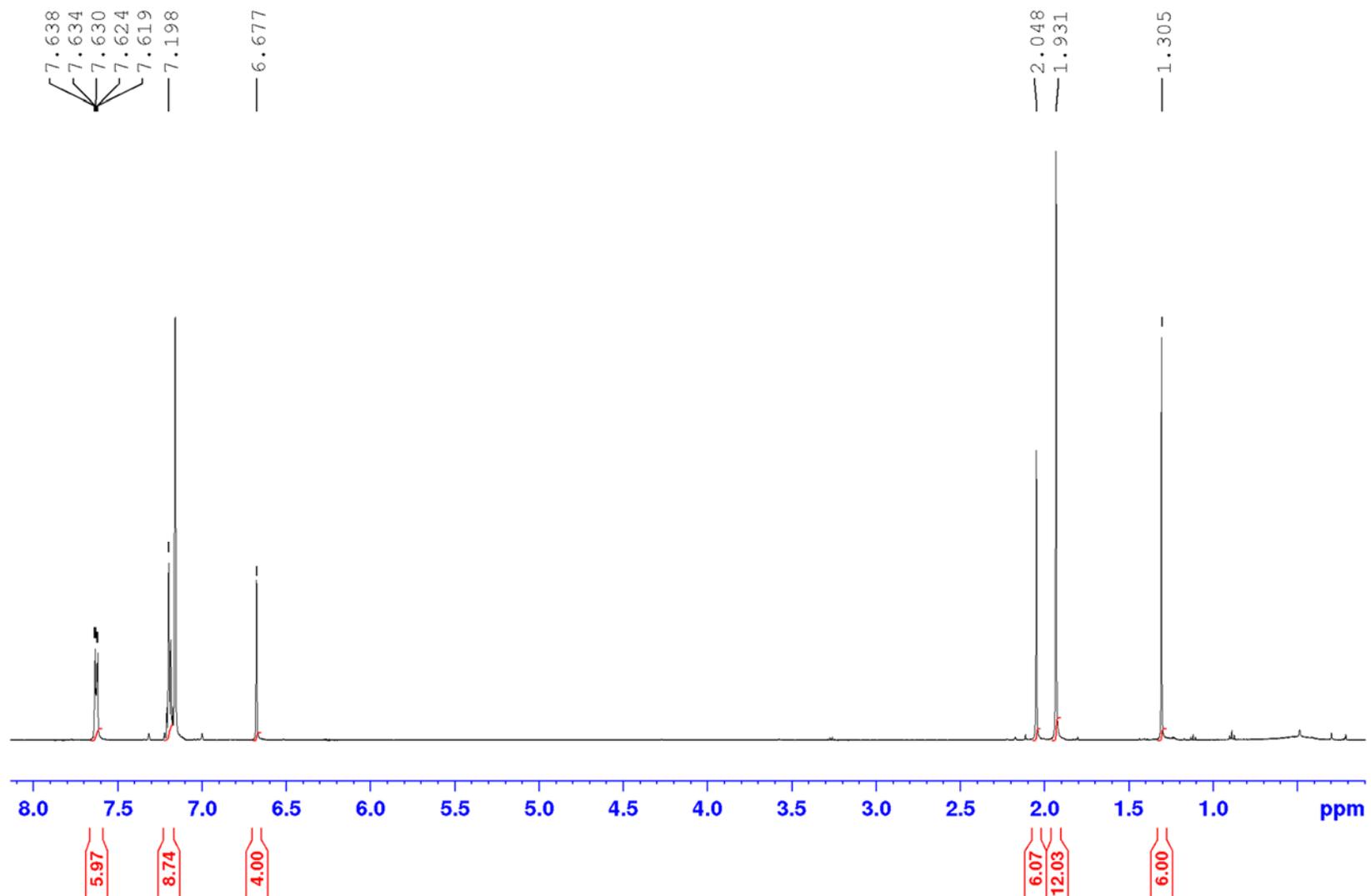
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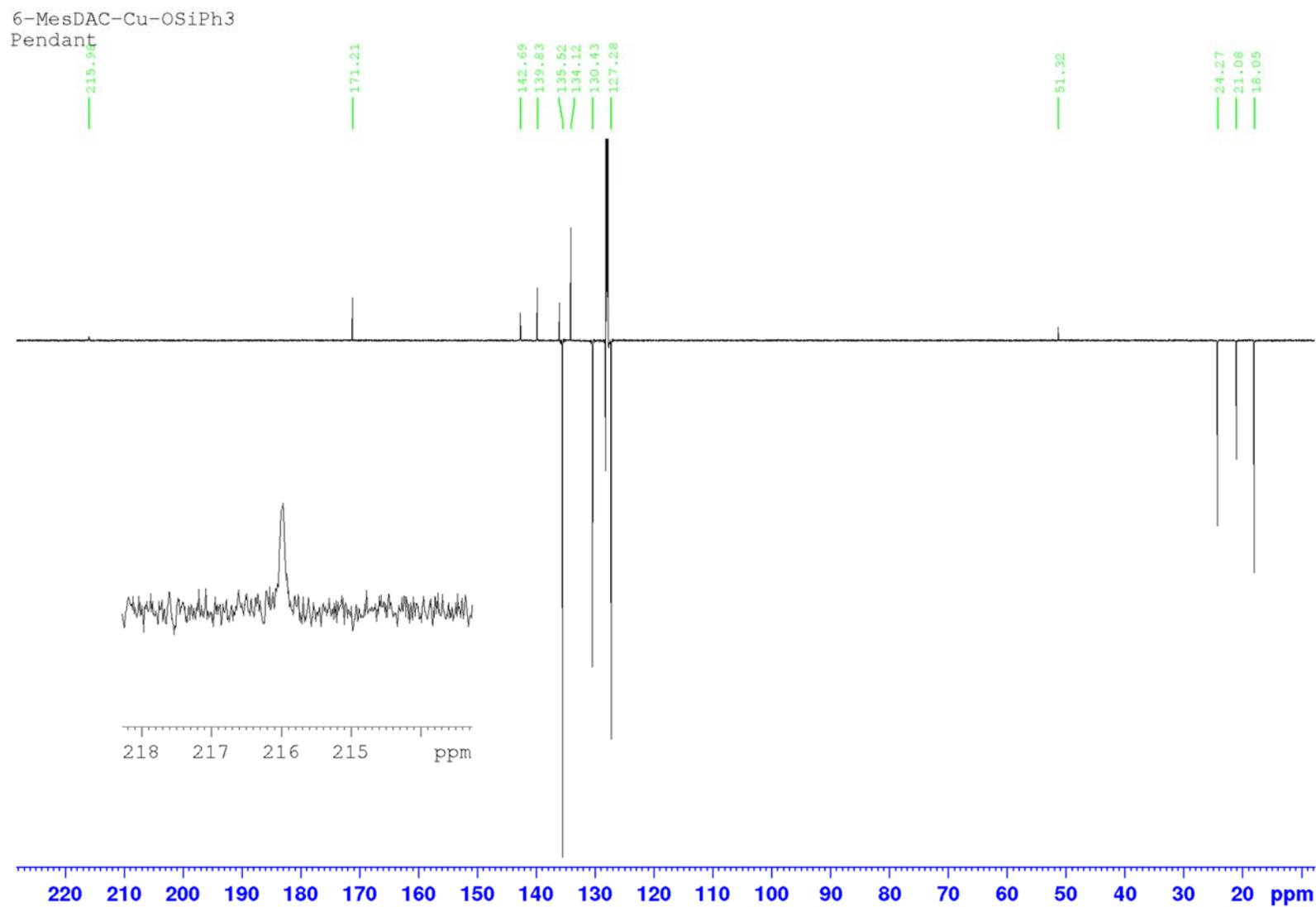
Figure S1. ^{1}H NMR spectrum (500 MHz, C$_6$D$_6$, 298 K) of (DAC)CuOSiPh$_3$ (**2**).

Figure S2. $^{13}C\{^{1}H\}$ PENDANT NMR spectrum (126 MHz, C_6D_6, 298 K) of (DAC)CuOSiPh$_3$ (**2**). Inset highlights DAC NCN resonance.

Figure S3. ^{1}H NMR spectrum (500 MHz, C$_6$D$_6$, 298 K) of (DAC)CuC$_6$F$_5$ (**3**).

(6-MesDAC)CuC6F5
Pendant

216.77
171.34
140.38
135.25
134.24
130.38
51.73
24.30
20.96
18.16

218   217   216 ppm

240 220 200 180 160 140 120 100 80 60 40 20 ppm
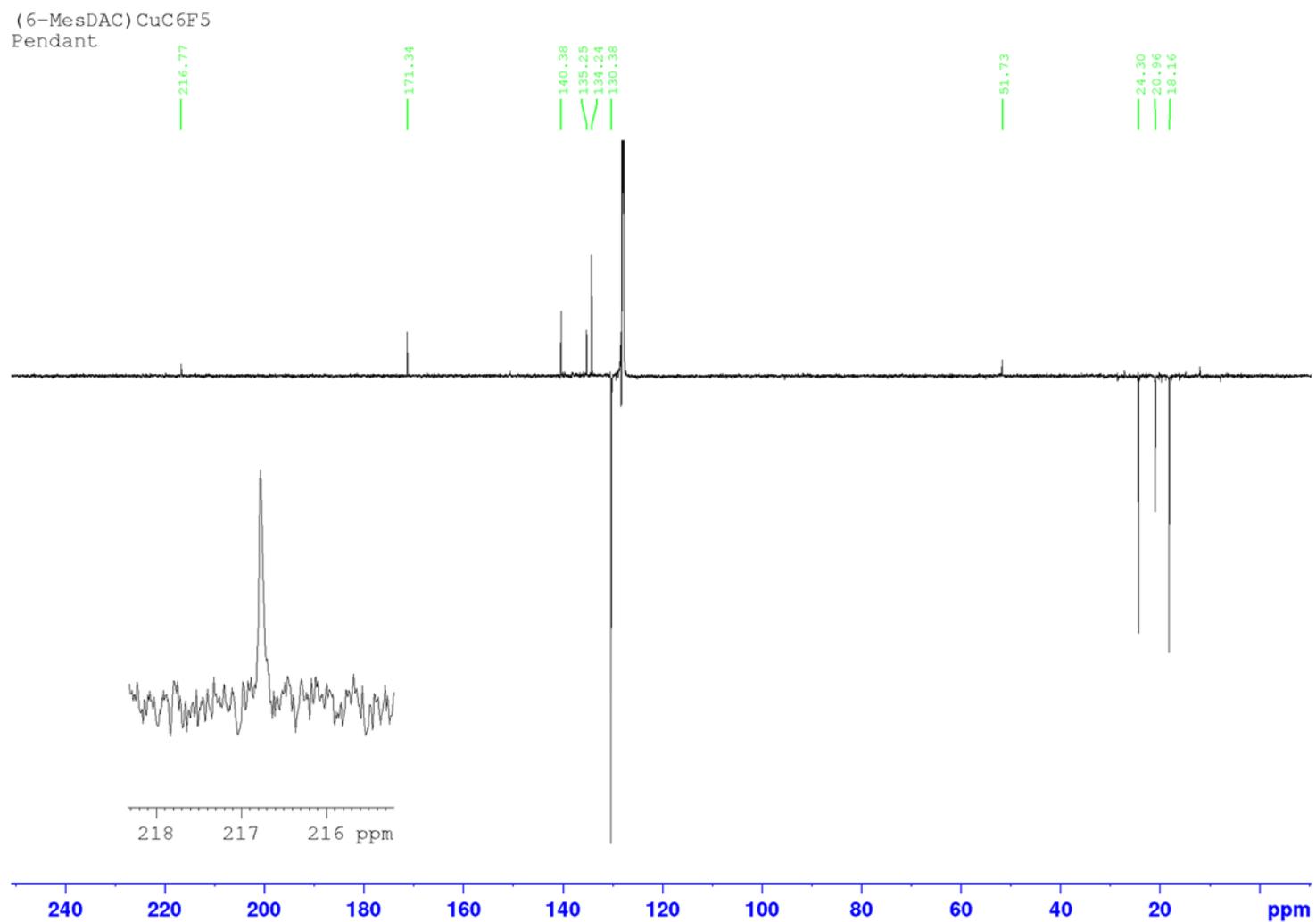
Figure S4. $^{13}C\{^{1}H\}$ PENDANT NMR spectrum (126 MHz, C_6D_6, 298 K) of (DAC)CuC$_6$F$_5$ (**3**). Inset highlights DAC N*C*N resonance.
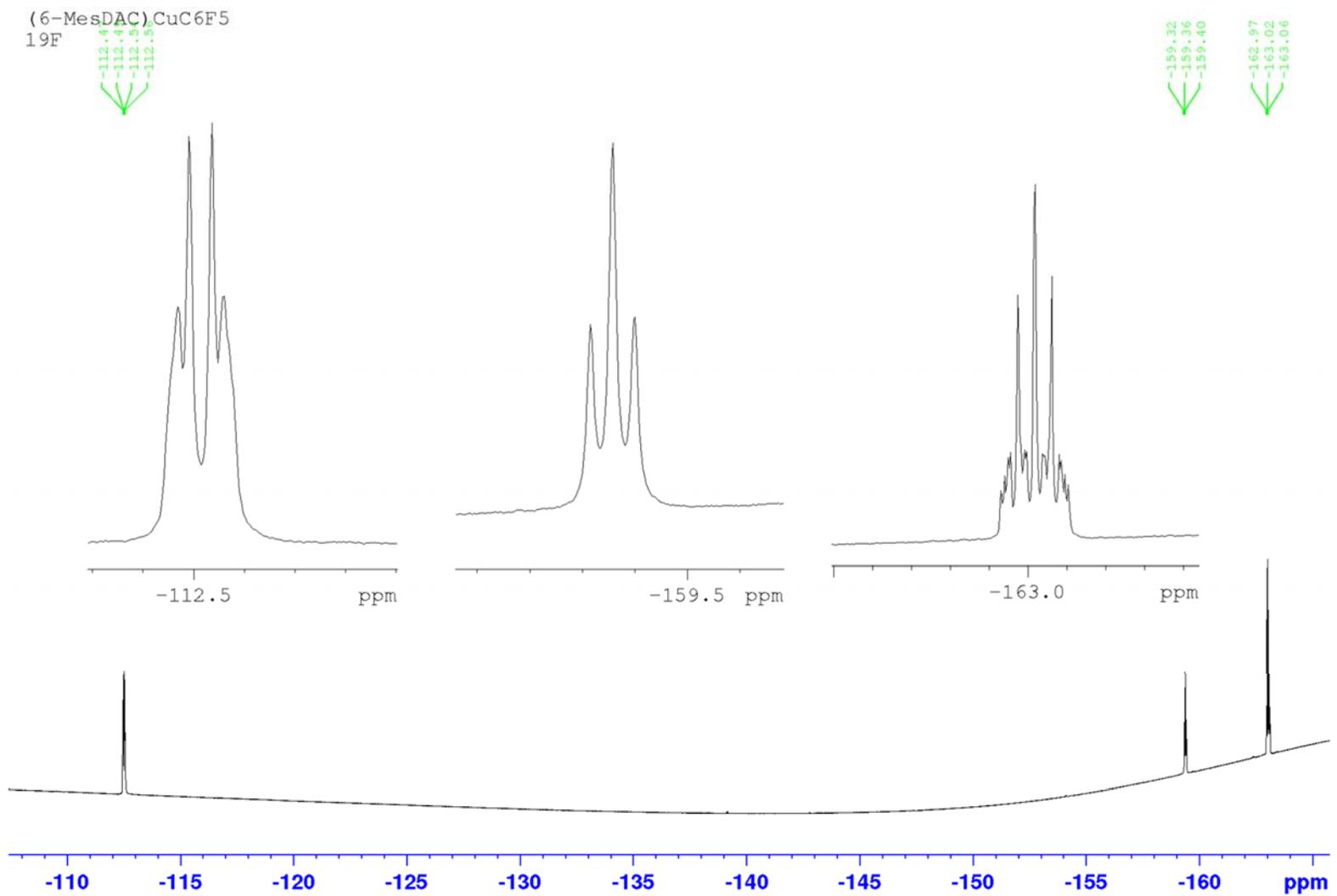
Figure S5. ^{19}F NMR spectrum (470 MHz, C$_6$D$_6$, 298 K) of (DAC)CuC$_6$F$_5$ (**3**), with expansions of each signal.
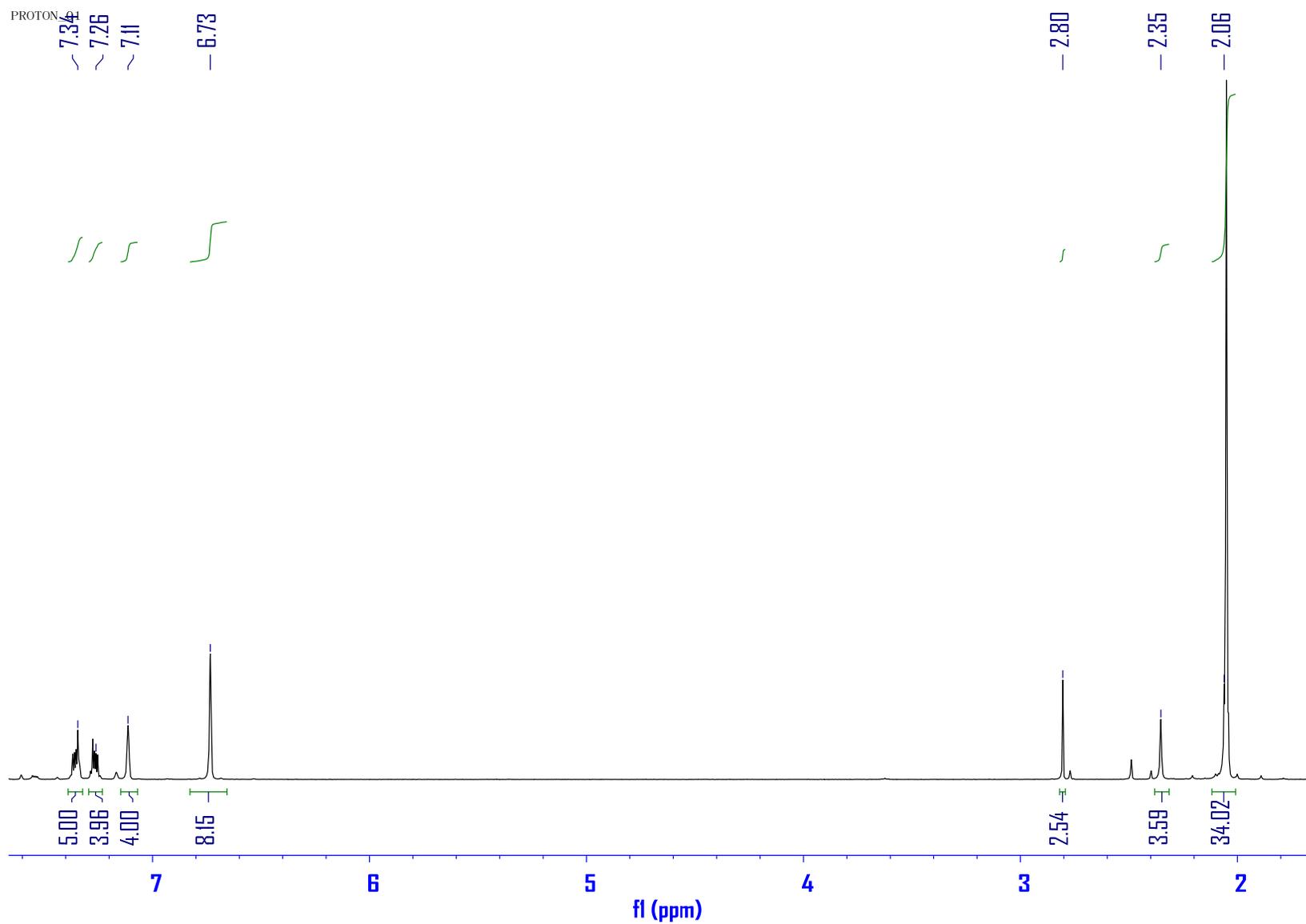
Figure S6. 1H NMR of [(IBz-3,5-Me2)2Cu][PF6] (5) in [D6]acetone
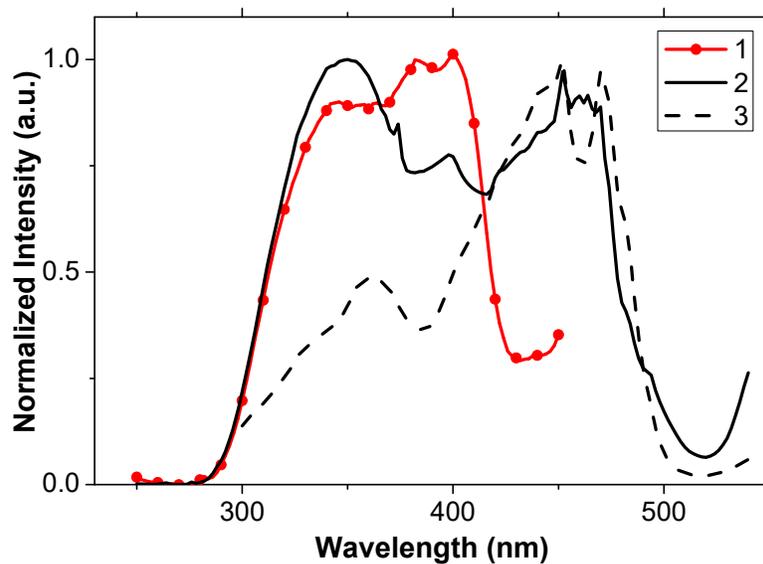
Figure S7. Excitation spectra of compounds **1**–**3** in the solid state at RT.
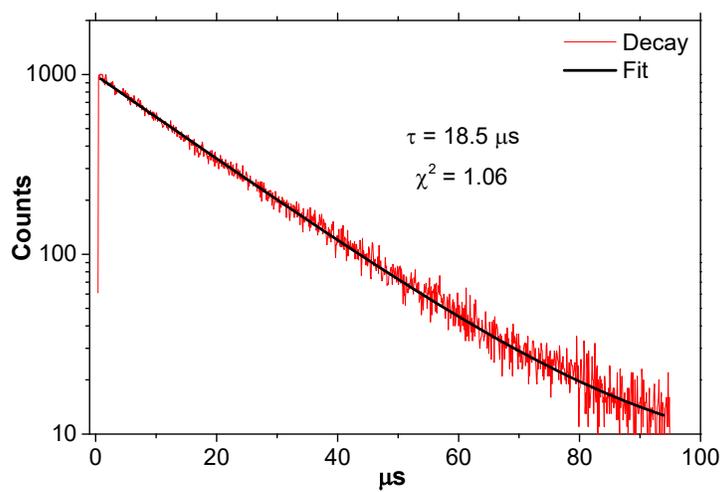
Figure S8. Emission decay transient of **1** in the solid state at RT.
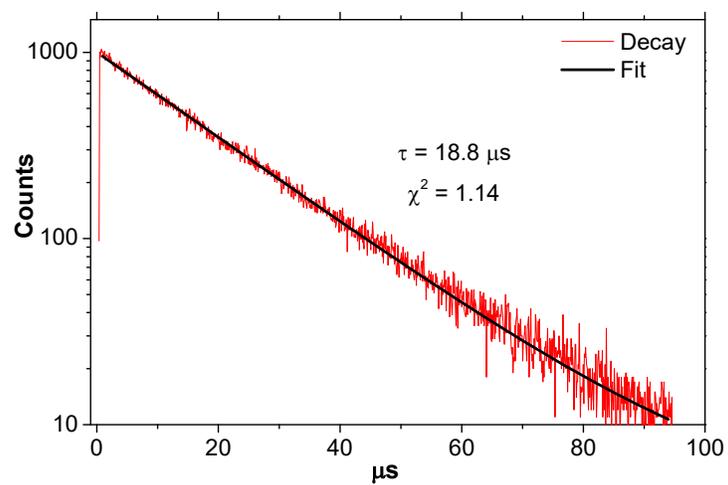
Figure S9. Emission decay transient of **1** in the solid state at 77 K.
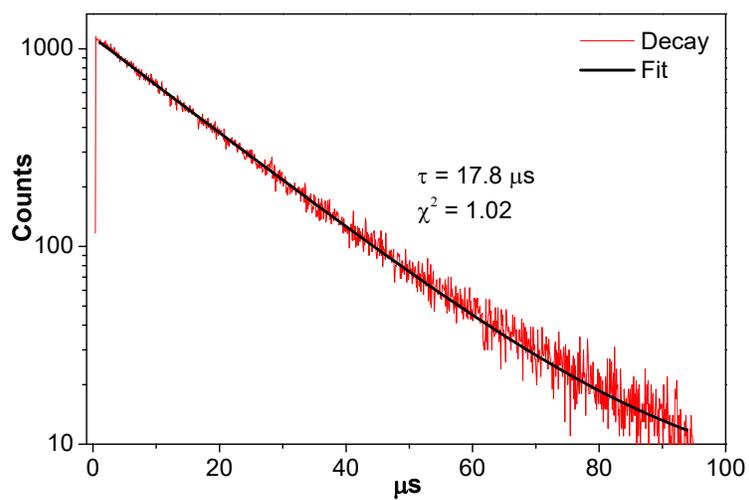
Figure S10. Emission decay transient of **1** in CH_2Cl_2 at RT.
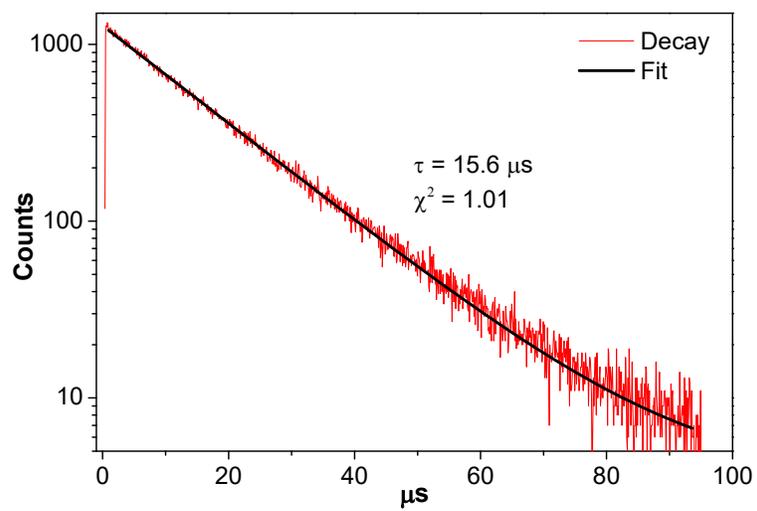
Figure S11. Emission decay transient of **2** in the solid state at RT.
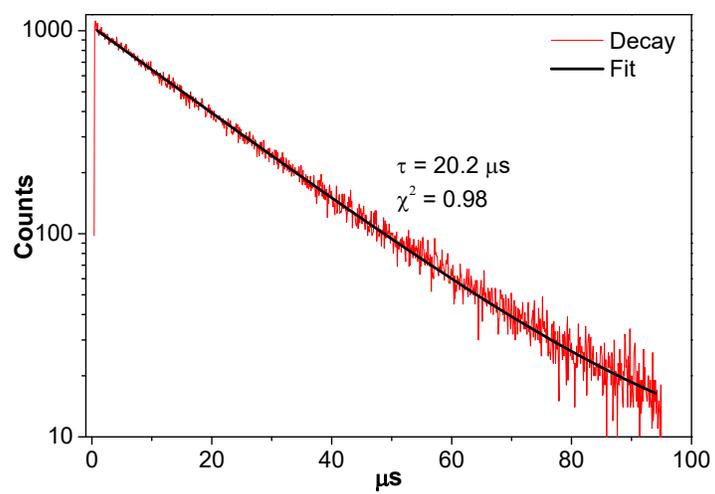
Figure S12. Emission decay transient of **2** in the solid state at 77 K
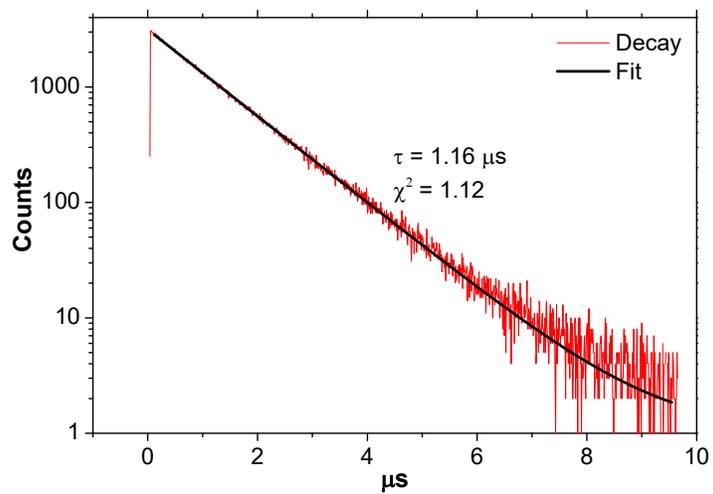
Figure S13. Emission decay transient of **2** in CH$_2$Cl$_2$ at RT.
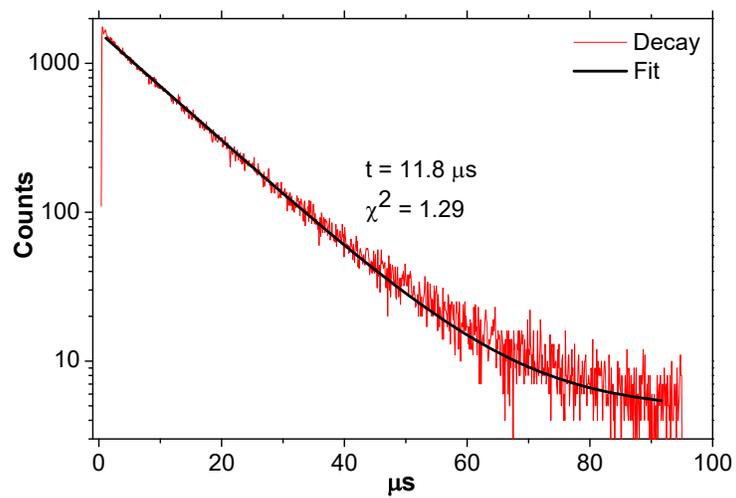
Figure S14. Emission decay transient of **3** in the solid state at RT.
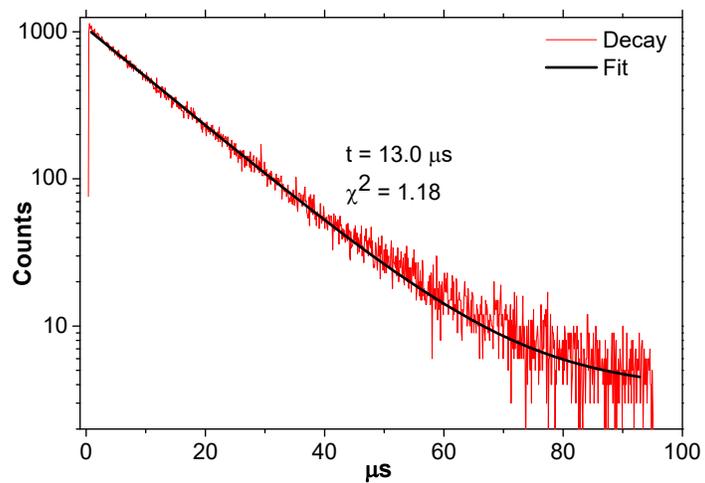
Figure S15. Emission decay transient of **3** in the solid state at 77K.
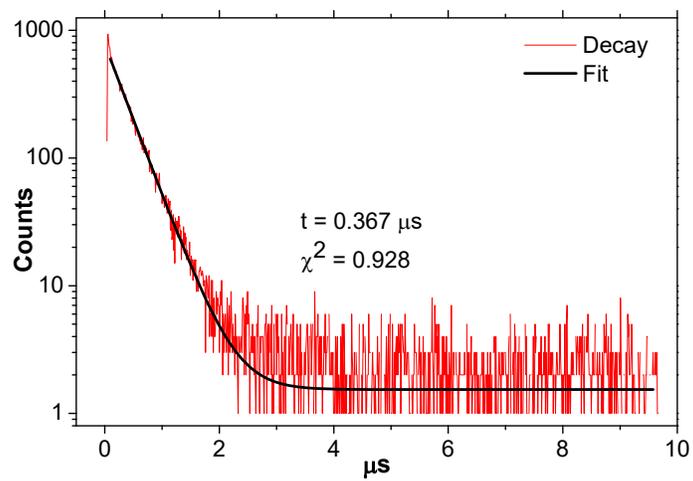
Figure S16. Emission decay transient of **3** in CH_2Cl_2 at RT.
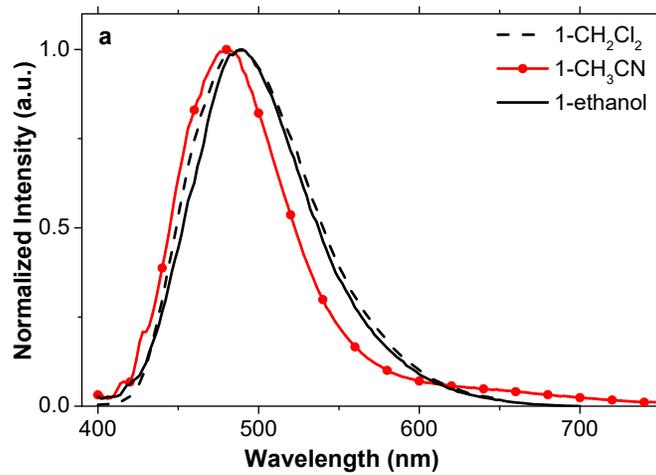
Figure S17. Emission spectra of **1** in different solvents at RT.
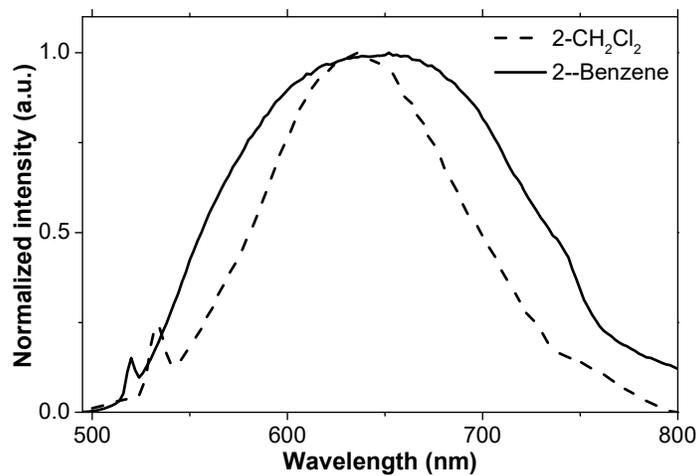
Figure S18. Emission spectra of **2** in CH$_2$Cl$_2$ and benzene at RT.
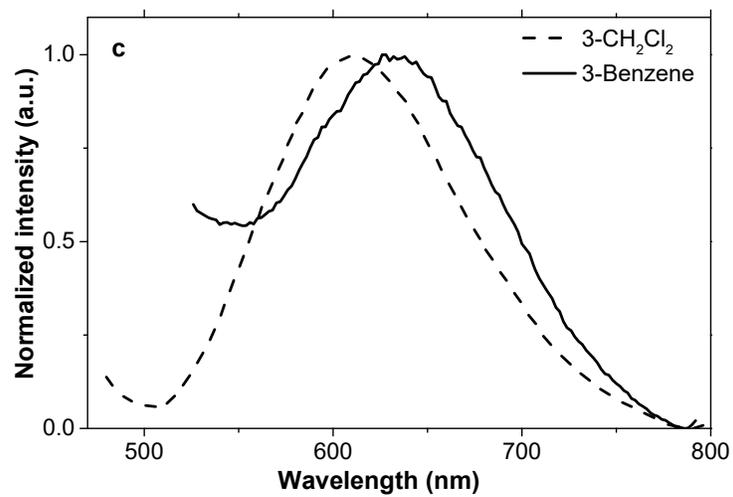
Figure S19. Emission spectra of **3** in CH$_2$Cl$_2$ and benzene at RT.
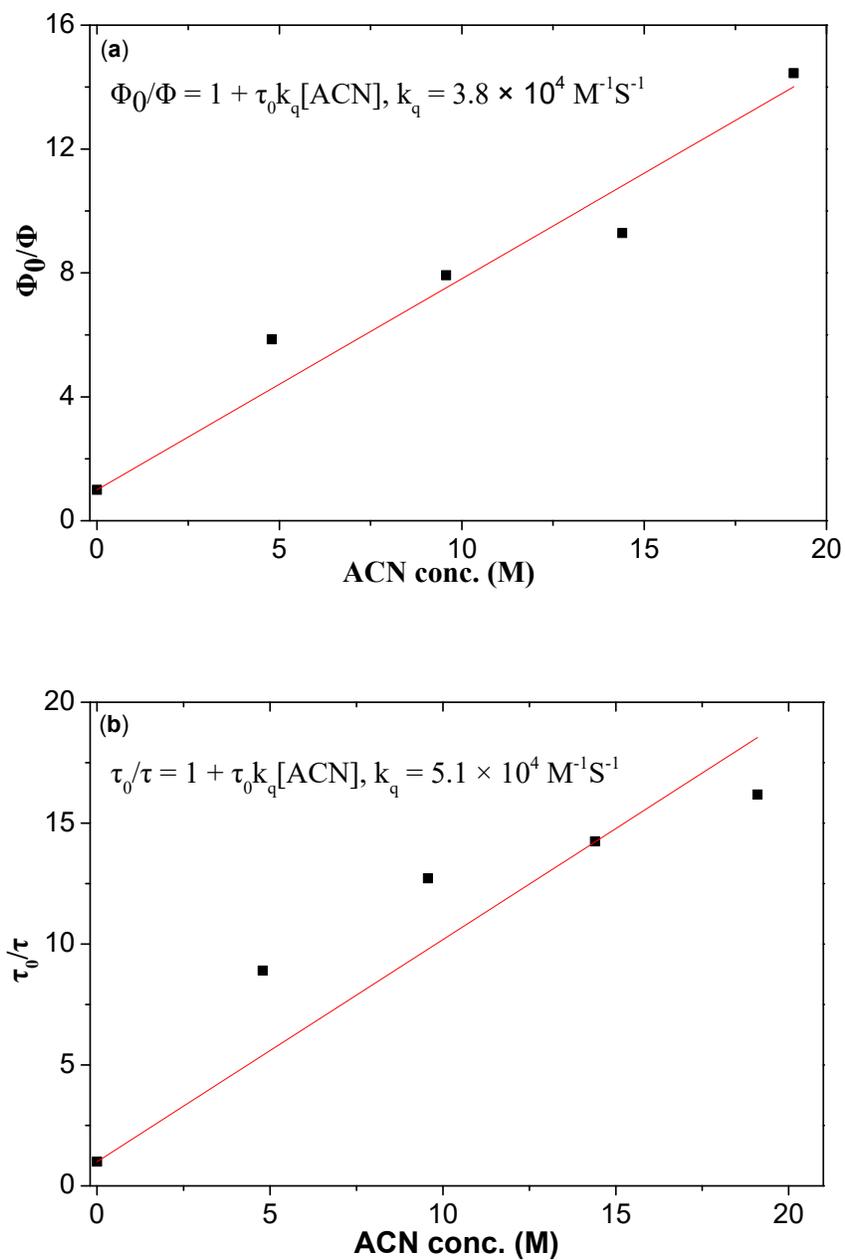
Figure S20. Stern-Volmer plot of [(DAC)$_2$Cu][BF4] (**1**) quenching by acetonitrile in CH$_2$Cl$_2$. Equation used: (a) $\Phi_0/\Phi = 1 + \tau_0 k_q$ [ACN]; (b) $\tau_0/\tau = 1 + \tau_0 k_q$ [ACN].

Table S1. Lowest vertical energy transitions for complexes **1–4** determined from TD-DFT calculations.

complex	states	λ (nm)	f	Major contribution[a]
1	S_1	396	0.0058	HOMO → LUMO (84%) HOMO → LUMO+1 (6%)
	T_1	430	0	HOMO → LUMO (72%) HOMO-8 → LUMO (10%) HOMO-9 → LUMO+1 (7%)
2	S_1	510	0.0032	HOMO-1 → LUMO (31%) HOMO → LUMO (28%) HOMO-6 → LUMO (16%) HOMO-2 → LUMO (14%)
	T_1	561	0	HOMO → LUMO (41%) HOMO-6 → LUMO (23%) HOMO-2 → LUMO (13%) HOMO-1 → LUMO (12%)
3	S_1	494	0.0021	HOMO-2 → LUMO (76%) HOMO-1 → LUMO (21%)
	T_1	540	0	HOMO-2 → LUMO (74%) HOMO-1 → LUMO (18%)
4	S_1	645	0.0049	HOMO-2 → LUMO (78%) HOMO-1 → LUMO (15%)
	T_1	703	0	HOMO → LUMO (83%) HOMO-2 → LUMO (12%)

[a] transitions with >5% contribution

Table S2. Selected frontier orbitals for complexes **1**–**4**.

1	HOMO-9: -10.0 eV	HOMO-8: -9.68 eV	HOMO: -8.85 eV	LUMO: -4.97 eV	LUMO+1: -4.88 eV
2	HOMO-6: -6.27 eV	HOMO-2: -5.98 eV	HOMO-1: -5.91 eV	HOMO: -5.90 eV	LUMO: -2.60 eV
3	HOMO-2: -6.08 eV	HOMO-1: -5.91 eV	HOMO: -5.85 eV	LUMO: -2.66 eV	
4	HOMO-2: -5.17 eV	HOMO-1: -5.15 eV	HOMO: -4.86 eV	LUMO: -2.49 eV	
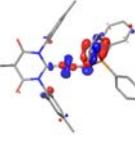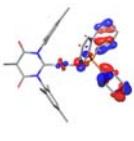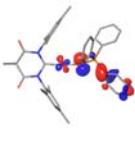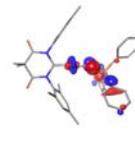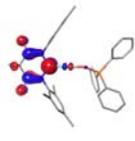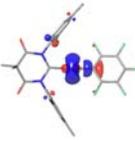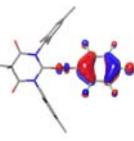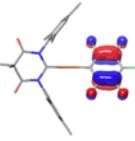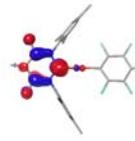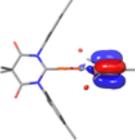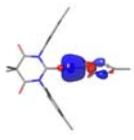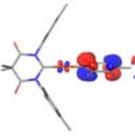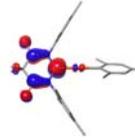
Table S3. Atom positions for the geometry optimized ground and triplet excited states of complexes **1**–**4**.

Complex **1**:
Optimized ground state

		angstroms	
atom	x	y	z
Cu1	8.4767946503	4.7273451835	3.6606234862
N2	8.5018963448	4.9218186620	0.7293719452
O3	5.5972346053	2.8521498384	7.5591411561
O4	8.3092578182	5.3735362831	-1.5091554232
O5	12.3259510781	3.7280800977	0.3154239526
O6	7.6585298341	7.0092272122	8.2711294318
N7	10.5083291990	4.1816939918	1.6338344642
N8	6.9515017527	3.7982437505	5.9714067039
N9	8.0179294588	5.8265754405	6.3406342410
C10	8.9824306916	4.8995670742	-0.6258208746
C11	6.6706243414	7.9896364286	4.9444560378
H12	6.3802304312	7.1573765151	4.2928565094
H13	6.3525029083	8.9153019511	4.4585733209
H14	6.1033443945	7.8956946666	5.8777560392
C15	8.8081608836	6.9533230754	5.8604467010
C16	7.1362812463	5.4089178231	0.8800713920
C17	7.7464788936	4.7945170337	5.5041748081
C18	9.2303990255	4.5995440087	1.8276279097
C19	12.1919868105	4.8750056917	3.2905855262
C20	7.3507589987	1.5484382028	5.0611535791
C21	4.9685247585	1.7241561194	3.5940306245
H22	4.0302526382	1.7818195576	3.0465987608
C23	6.0832007064	4.5043288224	0.6842015647
C24	11.3481606880	3.8757797231	2.7856193716
C25	5.3590036453	2.8164079967	4.3715913381
C26	7.5114182619	5.9672316683	7.6794371467
C27	11.1574191888	4.0305303800	0.3619790483
C28	8.9274082465	9.1226530393	4.8480810812
H29	8.4384271892	9.9586958362	4.3531689490
C30	8.1573481605	8.0129241270	5.2103078692
C31	5.7292876570	0.5509437792	3.5258486161
C32	6.9154301204	0.4850028698	4.2631174853
H33	7.5061830753	-0.4279667211	4.2404969811
C34	12.2011890460	6.2721946394	2.7196813356
H35	12.8934015702	6.9101838536	3.2738371894
H36	11.2118124887	6.7405982032	2.7639681251
H37	12.5252921398	6.2654996765	1.6729620318
C38	6.3849971030	3.7268283556	7.2889817133
C39	9.9699554231	2.7684726754	-1.4026556044

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H40          10.9034304918          2.2435581433         -1.6204864125
H41           9.3808413133          2.8509519296         -2.3196008040
H42           9.4015896274          2.1857886530         -0.6704259795
C43          10.1725024783          6.9982463429          6.1875141004
C44           6.8758991194          4.7396196469          8.3076380790
C45           7.9895226798          4.0304915574          9.1433135409
H46           8.8342990464          3.7150088011          8.5229687521
H47           7.5610717720          3.1496699506          9.6284635842
H48           8.3539315801          4.7196400190          9.9095386549
C49           5.2741927017         -0.6106192852          2.6750884875
H50           4.1961686346         -0.7752424203          2.7709825679
H51           5.7844291569         -1.5368622676          2.9526957280
H52           5.4792155667         -0.4253101794          1.6134202354
C53           8.6010412913          1.4168256134          5.8989533253
H54           8.3715009135          1.4857162783          6.9690127906
H55           9.3387925059          2.1938548518          5.6674288625
H56           9.0756895287          0.4470191232          5.7301173965
C57           5.5963049261          7.2334125858          1.1000648514
H58           5.4080261514          8.2964016707          1.2345814645
C59          10.3053681163          4.2022237199         -0.8824132687
C60          10.8361483100          5.8919594973          6.9718020090
H61          10.4331586548          5.8347781695          7.9901545706
H62          11.9104939428          6.0698001991          7.0555259947
H63          10.6990886880          4.9132298830          6.5000972193
C64           6.5679919727          2.7116912415          5.0796305347
C65           4.4843129309          4.0442515749          4.4714701042
H66           4.1464560530          4.2057129482          5.5018757548
H67           3.5953382031          3.9362547372          3.8457820174
H68           5.0084947244          4.9493830560          4.1447585885
C69          10.8954378892          8.1302420613          5.8032535989
H70          11.9516795767          8.1868984203          6.0568034781
C71           4.5131282477          6.3638061970          0.9219544019
C72          11.3832079435          2.5537580126          3.2594591078
C73           8.0653656337          7.7603784087          1.1851146824
H74           8.6892376837          7.7453772248          0.2837170392
H75           8.7118737186          7.5384677276          2.0417486489
H76           7.6916743217          8.7795745695          1.3090252127
C77           4.7787854228          5.0068900949          0.7201671650
H78           3.9504813586          4.3209930042          0.5581158371
C79          13.0654781778          4.5241264908          4.3251622964
H80          13.7368939330          5.2832352489          4.7196536076
C81          10.2939189711          9.2025628013          5.1354361164
C82           3.0970161649          6.8883341191          0.9360620535
H83           2.3871442230          6.1390861594          0.5754432222
H84           2.9986004852          7.7780144381          0.3049883801
H85           2.7913730014          7.1769329021          1.9488592071
C86          10.5315800670          1.4698072222          2.6421109741
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atom	x	y	z
H87	10.6998655809	0.5145855103	3.1451524477
H88	10.7782920612	1.3296836029	1.5831210789
H89	9.4609608162	1.6960368592	2.7052543790
C90	13.1227430532	3.2268516797	4.8411515911
C91	6.9188957671	6.7843717625	1.0689413703
C92	12.2682032227	2.2584923456	4.2992450800
H93	12.3146645451	1.2376999316	4.6727310813
C94	6.3339214266	3.0439552121	0.3942033059
H95	5.3900538039	2.4978202616	0.3276908030
H96	6.9389458437	2.5672861915	1.1731632067
H97	6.8531572837	2.9150710660	-0.5627279297
C98	5.7153786538	5.1600675245	9.2318115058
H99	6.0844244636	5.8501044526	9.9920124118
H100	5.2901380879	4.2759727358	9.7092621546
H101	4.9221227375	5.6619222970	8.6694599593
C102	14.0877256376	2.8657695809	5.9457381835
H103	13.5580725154	2.6460873671	6.8808132375
H104	14.7931508282	3.6770096100	6.1447546086
H105	14.6664566585	1.9721391418	5.6877299541
C106	11.1021193794	10.4139669558	4.7353938835
H107	10.4768676327	11.3090921827	4.6704042438
H108	11.5692789829	10.2690523437	3.7532041509
H109	11.9057871134	10.6115945982	5.4511806690
C110	11.1020724782	4.9735056125	-1.9567549704
H111	11.3512801563	5.9838702861	-1.6179258126
H112	10.5036839126	5.0553980607	-2.8654310743
H113	12.0315074767	4.4439990670	-2.1715795255

Optimized triplet excited state

angstroms

atom	x	y	z
Cu1	8.4527828388	4.7210010044	3.7002069874
N2	8.5115820861	5.1667916523	0.7719769728
O3	6.0433714458	2.5616138297	7.6922425888
O4	8.2719508498	5.6798432621	-1.4477497954
O5	12.1231996559	3.5045918051	0.1847689453
O6	7.4944213757	7.1078077873	8.1605064030
N7	10.3643696230	4.0154332941	1.5619127471
N8	7.1188652209	3.6832791725	6.0495682779
N9	7.8184343236	5.9038689341	6.2754493840
C10	8.9237220743	5.1114482661	-0.6048669154
C11	6.1361558915	7.9234358460	5.0702772554
H12	5.8378169268	6.9566077688	4.6546782183
H13	5.6874523411	8.7109764595	4.4611286965
H14	5.7182686787	7.9975411716	6.0809061551

C15	8.4497265420	7.0746685022	5.7006009765
C16	7.2686003473	5.8915546067	1.0079162269
C17	7.7438131076	4.7777298961	5.4730782831
C18	9.1830213195	4.6263792944	1.8174291273
C19	12.0385335652	4.3188168311	3.3429540805
C20	8.0107891795	1.4710510039	5.4238357690
C21	5.8169324164	1.0864461512	3.7085490370
H22	4.9517219822	0.9167701563	3.0722371210
C23	6.0553924372	5.1880642343	0.9355180188
C24	11.1461367035	3.4724018385	2.6654741152
C25	5.9176532871	2.2921884745	4.4013505785
C26	7.3472164089	6.0366386335	7.5730212542
C27	10.9909665249	3.9156946578	0.2701698692
C28	8.2521745052	9.2419254329	4.6766643654
H29	7.6372874128	10.0290849190	4.2474832014
C30	7.6351191722	8.0749246906	5.1225824270
C31	6.7748060762	0.0695820171	3.8461639569
C32	7.8586054014	0.2829427481	4.7102148439
H33	8.5883752582	−0.5104916213	4.8518755070
C34	12.1664878241	5.7821902560	2.9920905452
H35	12.9354942662	6.2575577667	3.6049545287
H36	11.2315345138	6.3313092721	3.1507181100
H37	12.4556461966	5.9114024522	1.9427460263
C38	6.5700501035	3.6099705437	7.3218103418
C39	9.6319662516	2.9376568043	−1.5536955856
H40	10.4890523638	2.3236816534	−1.8406155428
H41	9.0359574842	3.1625391332	−2.4413542069
H42	9.0139352175	2.3713709380	−0.8495773458
C43	9.8439403727	7.2502594395	5.8616012660
C44	6.6508588427	4.8419092756	8.2216207321
C45	7.4313987470	4.4585586458	9.5053572944
H46	8.4559502885	4.1482851371	9.2727569689
H47	6.9255152051	3.6299864885	10.0054466300
H48	7.4760681621	5.3204649255	10.1746021178
C49	6.6387470081	−1.2206056563	3.0785015040
H50	5.5894069420	−1.5094254409	2.9661493264
H51	7.1699091849	−2.0394764459	3.5710293848
H52	7.0553266170	−1.1206459135	2.0672658677
C53	9.1296078330	1.6370627094	6.4205556355
H54	8.7297853721	1.5937040132	7.4402132688
H55	9.6420697783	2.5962066788	6.3027500105
H56	9.8679193690	0.8395450542	6.3130596720
C57	6.1078884923	7.9745805989	1.2395569713
H58	6.1256231180	9.0585119211	1.3242784422
C59	10.1480191072	4.2772711492	−0.9388466678
C60	10.6775628733	6.2351566101	6.6040191982
H61	10.3718105173	6.1930669533	7.6559234410

H62	11.7353305811	6.5071665812	6.5745068832
H63	10.5703742161	5.2292417020	6.1872025064
C64	7.0388533379	2.4810381678	5.2434458907
C65	4.8141531549	3.3185353470	4.3292684883
H66	4.3327049417	3.4251694274	5.3079994006
H67	4.0488189564	3.0140036067	3.6115854188
H68	5.1876590105	4.3037883893	4.0348899606
C69	10.4095941415	8.4360845259	5.3962267268
H70	11.4763388870	8.5980691404	5.5303699671
C71	4.8749483224	7.3125643269	1.1993676862
C72	11.0934017433	2.0894585215	2.9049289027
C73	8.6298275659	8.0425223692	1.0974972668
H74	9.1189332981	7.9280408632	0.1229644778
H75	9.3290716202	7.6968481033	1.8664729354
H76	8.4634406076	9.1100020917	1.2576204965
C77	4.8715186928	5.9218052658	1.0499199177
H78	3.9218474543	5.3958437779	0.9890038726
C79	12.8541806856	3.7485854749	4.3242460854
H80	13.5596023638	4.3855005539	4.8522342212
C81	9.6343267615	9.4448260633	4.8028317021
C82	3.5814596098	8.0825541207	1.3138982039
H83	2.7591947741	7.5607002524	0.8164908807
H84	3.6694472095	9.0795201305	0.8722633799
H85	3.2963480928	8.2151192008	2.3648388254
C86	10.2156933479	1.1749182459	2.0835784099
H87	10.2475787322	0.1562234016	2.4757952287
H88	10.5586991974	1.1350709964	1.0428224970
H89	9.1691567034	1.4967822993	2.0809051980
C90	12.8169410788	2.3811459793	4.6154721076
C91	7.3205740907	7.2895897782	1.1353581332
C92	11.9311972872	1.5714722288	3.8943399278
H93	11.9141407380	0.5012228275	4.0860280610
C94	6.0156251214	3.6985668755	0.6873552670
H95	4.9831731163	3.3432956317	0.6509363750
H96	6.5335795482	3.1345735190	1.4707697466
H97	6.4833073706	3.4432319179	-0.2710372518
C98	5.2087152172	5.2653781353	8.6020892745
H99	5.2473158842	6.1221422283	9.2781932107
H100	4.7031307388	4.4313710369	9.0936347664
H101	4.6281198096	5.5487146087	7.7173795076
C102	13.7117136487	1.7883994478	5.6772842837
H103	13.1847655703	1.7078469837	6.6363305741
H104	14.5995312049	2.4048545185	5.8422272190
H105	14.0420869175	0.7819645362	5.4031936485
C106	10.2766472127	10.7161845764	4.3108502039
H107	9.5640767591	11.5452178942	4.2920427942
H108	10.6594851979	10.5896499809	3.2897286542

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H109          11.1248526387      11.0047872925       4.9386817483
C110          11.0163757651       5.0244518527      -1.9755967898
H111          11.3944521274       5.9685256195      -1.5719162412
H112          10.4172554674       5.2434483435      -2.8605378216
H113          11.8696283233       4.4030755003      -2.2509779648


Complex 2:
Optimized ground state
                                 angstroms
   atom            x                  y                   z
   Cu1         14.1477639896       4.2365645006      -1.0834114133
   Si2         14.6646753895       3.4377693737      -4.2169565163
   O3          14.8326090052       3.5275136467      -2.6077251317
   O4          14.4688440603       7.0398271425       3.2046870646
   O5          10.2665480595       5.1302051498       2.1375694439
   N6          12.1194008905       4.7467419890       0.8506025133
   N7          14.1840459522       5.7126427339       1.3625889711
   C8          13.4249104319       4.9542521215       0.5220217552
   C9          11.4615715341       5.2699854663       1.9948868605
   C10         12.3369725322       5.9420049282       3.0486131869
   C11         13.7387006049       6.3094370607       2.5702446407
   C12         11.3130930068       3.9767803387      -0.0913365843
   C13         10.7607602169       4.6290023022      -1.2022294120
   C14         10.0311351759       3.8573123517      -2.1120691321
   H15          9.6141974168       4.3441987081      -2.9901001776
   C16          9.8462638194       2.4839991669      -1.9368839137
   C17         10.3928432933       1.8783043503      -0.7992149463
   H18         10.2489656783       0.8118582143      -0.6417898784
   C19         11.1287749199       2.6040038953       0.1402412905
   C20         10.9681581758       6.1040239009      -1.4474137513
   H21         10.7278672392       6.7032063182      -0.5624361924
   H22         10.3378005180       6.4489737760      -2.2702174485
   H23         12.0084629366       6.3122628703      -1.7260968713
   C24          9.1128619115       1.6611264689      -2.9686501198
   H25          9.8282066320       1.1497572219      -3.6240365956
   H26          8.4725645869       2.2848365476      -3.5988354264
   H27          8.4884984549       0.8925279930      -2.5013312729
   C28         11.7129641528       1.9197342858       1.3530887421
   H29         11.4947481508       0.8490583549       1.3331088144
   H30         11.2974061849       2.3266471485       2.2824936606
   H31         12.8023452229       2.0361170743       1.3958426517
   C32         12.5132723126       4.9125700398       4.2051251078
   H33         13.0082024656       3.9977347884       3.8630092801
   H34         11.5300963791       4.6491488192       4.6027209670
   H35         13.1183085256       5.3626463470       4.9958570143
   C36         11.6277710479       7.2074233762       3.5737049210
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H37	12.2297783930	7.6611344111	4.3624478730
H38	10.6440072466	6.9389300263	3.9615016074
H39	11.4928066512	7.9450601107	2.7762892710
C40	15.5652207437	5.9577515861	0.9598530454
C41	16.5406779558	5.0078967971	1.2926394515
C42	17.8494847848	5.2396346210	0.8592461449
H43	18.6171810233	4.5081820080	1.1004983152
C44	18.1922917976	6.3742950844	0.1196054380
C45	17.1907532432	7.3069617903	-0.1694559653
H46	17.4433976949	8.2007199351	-0.7353799942
C47	15.8685388113	7.1238907637	0.2405166985
C48	16.2001990723	3.7589133533	2.0700392482
H49	17.1042784922	3.1888668939	2.2970633312
H50	15.5310499942	3.1059748277	1.4965653281
H51	15.7040688389	3.9920196804	3.0191999171
C52	19.6019659055	6.5783092677	-0.3830316706
H53	20.3265679805	6.0177804800	0.2146329204
H54	19.8867208277	7.6350915949	-0.3626709589
H55	19.6959143569	6.2357448419	-1.4205809714
C56	14.8125149929	8.1511273041	-0.0879385532
H57	13.9902525791	7.7142971737	-0.6660628350
H58	15.2386475181	8.9644124160	-0.6804610024
H59	14.3863797122	8.5877074736	0.8223290504
C60	13.5376245655	4.7954542306	-4.9457917308
C61	12.3614927147	4.5153733388	-5.6639993266
H62	12.0682222731	3.4810612743	-5.8264210732
C63	11.5624018386	5.5364371576	-6.1875006568
H64	10.6624171874	5.2874841978	-6.7456402394
C65	11.9206699073	6.8724007142	-6.0026379169
H66	11.3043298739	7.6680591344	-6.4139141773
C67	13.0859700586	7.1778081177	-5.2941765761
H68	13.3808708119	8.2156823142	-5.1550030571
C69	13.8795330635	6.1522463788	-4.7775018097
H70	14.7919627983	6.4117126742	-4.2432241692
C71	16.3511000650	3.6285792412	-5.0704953358
C72	16.4819154100	4.0913799344	-6.3928798280
H73	15.5982795522	4.4149304140	-6.9394672459
C74	17.7268464197	4.1592576941	-7.0234930844
H75	17.7975364250	4.5194839960	-8.0474068934
C76	18.8791893521	3.7698553862	-6.3386385641
H77	19.8495279290	3.8209981986	-6.8264266731
C78	18.7758299341	3.3184842841	-5.0207098253
H79	19.6696093409	3.0167898238	-4.4790690544
C80	17.5275729287	3.2499416783	-4.3984949218
H81	17.4576467326	2.9006600083	-3.3710153763
C82	13.9350538442	1.7511718993	-4.7170103465
C83	13.9910579458	1.2613946205	-6.0352479170

H84	14.4915439043	1.8439689910	-6.8064652567
C85	13.4269842132	0.0318963216	-6.3820525575
H86	13.4845698759	-0.3200939393	-7.4095969941
C87	12.7958889358	-0.7478774791	-5.4106658293
H88	12.3598687819	-1.7074491415	-5.6774355319
C89	12.7395709309	-0.2887306097	-4.0929684294
H90	12.2621059230	-0.8961766810	-3.3269727514
C91	13.3022065736	0.9452115545	-3.7542463893
H92	13.2578058804	1.2929280813	-2.7251153757

Optimized triplet excited state

		angstroms	
atom	x	y	z
Cu1	14.5631714171	4.5072464766	-1.2092830486
Si2	14.8661219502	3.4538839255	-4.1878333981
O3	15.2620517241	3.5851548372	-2.5880027388
O4	14.4300313677	6.6848797559	3.2196052793
O5	10.2324692418	4.8126687222	1.9464123061
N6	12.0692802045	4.6200094586	0.6048930794
N7	14.1291889888	5.5422220260	1.2760919847
C8	13.4172773850	4.8150936397	0.3199436601
C9	11.4379670299	4.9896077201	1.7942789485
C10	12.2930487976	5.5698355981	2.9311020200
C11	13.6962305928	6.0006800207	2.5054797890
C12	11.2287683172	3.9906793040	-0.3917240142
C13	10.5542631258	4.7952037731	-1.3214492443
C14	9.6843737331	4.1728349828	-2.2230759505
H15	9.1553218593	4.7873299659	-2.9477252883
C16	9.4616774637	2.7943627278	-2.2014421376
C17	10.1390311441	2.0276602573	-1.2469054413
H18	9.9589628121	0.9553382077	-1.1985163955
C19	11.0232695975	2.6029165662	-0.3309806904
C20	10.7066492154	6.2969470296	-1.3158745523
H21	10.3276818377	6.7186592097	-0.3775854537
H22	10.1485209709	6.7464488136	-2.1409162369
H23	11.7548977771	6.5966619525	-1.4173452561
C24	8.5227603555	2.1390153358	-3.1867325000
H25	9.0810537023	1.6320358855	-3.9831115094
H26	7.8621702801	2.8716054030	-3.6593118409
H27	7.8964226313	1.3838024832	-2.6997291664
C28	11.6858681360	1.7606849446	0.7322276085
H29	11.5258213238	0.6961864460	0.5417211772

H30	11.2696214518	1.9926148723	1.7197257364
H31	12.7646978442	1.9411709913	0.7779920724
C32	12.4375700076	4.4695437594	4.0199793337
H33	12.9554052137	3.5853731533	3.6325383831
H34	11.4446989949	4.1658339400	4.3621984596
H35	13.0083159423	4.8632404692	4.8653170810
C36	11.5555018179	6.7844088741	3.5359110926
H37	12.1349711726	7.1867342603	4.3692279845
H38	10.5669874243	6.4757893728	3.8806201796
H39	11.4250819005	7.5793212146	2.7939272009
C40	15.4722668801	5.8472096585	0.8448029879
C41	16.5147774890	4.9368538967	1.1366093144
C42	17.8085058612	5.2746015981	0.7362523890
H43	18.6212707876	4.5872612503	0.9579040835
C44	18.0897782347	6.4820471155	0.0851980079
C45	17.0388354013	7.3727198004	-0.1660666426
H46	17.2508479981	8.3258395469	-0.6447116932
C47	15.7257996190	7.0866058909	0.2099089622
C48	16.2492973382	3.6806419557	1.9300692638
H49	17.1290477471	3.0326831991	1.9373678917
H50	15.4066539008	3.1137610973	1.5241395608
H51	16.0046000703	3.9358659219	2.9679518221
C52	19.4981134565	6.8165017210	-0.3403211540
H53	20.2357437108	6.3433822323	0.3145233543
H54	19.6718503979	7.8967000062	-0.3296586595
H55	19.6904286317	6.4634078450	-1.3607785677
C56	14.6276640559	8.1071996712	0.0413896112
H57	13.7235095698	7.6675046343	-0.3894832222
H58	14.9529176360	8.9290736390	-0.6013593075
H59	14.3568244443	8.5216955124	1.0194804790
C60	13.6429758862	4.8082603469	-4.7005030083
C61	12.4004842012	4.5293340212	-5.2969534688
H62	12.1199640037	3.4976830372	-5.4930620744
C63	11.5103057326	5.5518893744	-5.6361041166
H64	10.5566040365	5.3075427124	-6.0974606551
C65	11.8401997865	6.8834763300	-5.3791954449
H66	11.1477738250	7.6794822520	-5.6404899918
C67	13.0707629601	7.1872688596	-4.7910879928
H68	13.3390606671	8.2224730081	-4.5944650591
C69	13.9585117303	6.1615392839	-4.4611535295
H70	14.9185239383	6.4206808774	-4.0165758405
C71	16.4719390532	3.6590895956	-5.1584379069
C72	16.5133093253	4.2297443320	-6.4427809838
H73	15.5944364314	4.5821581279	-6.9064547578
C74	17.7189402920	4.3652337274	-7.1347882375
H75	17.7267780251	4.8090288057	-8.1271936159
C76	18.9128003675	3.9387525507	-6.5499824934

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H77        19.8524212941        4.0483214217       -7.0850942709
C78        18.8944808528        3.3773830766       -5.2710794669
H79        19.8214051692        3.0482771430       -4.8078747554
C80        17.6874234881        3.2402311696       -4.5848577560
H81        17.6829172909        2.8118849319       -3.5858064659
C82        14.0855935253        1.7525803059       -4.4492549868
C83        14.5093944230        0.8723645257       -5.4596321538
H84        15.3192823243        1.1646277755       -6.1240914789
C85        13.9109646319       -0.3789901922       -5.6254185881
H86        14.2555941683       -1.0425374304       -6.4146179440
C87        12.8770244472       -0.7795847745       -4.7779926350
H88        12.4131084242       -1.7544361145       -4.9042157964
C89        12.4454903267        0.0783020550       -3.7638582753
H90        11.6435256333       -0.2249337375       -3.0954300726
C91        13.0444398368        1.3276951522       -3.6012011587
H92        12.6924330724        1.9765573620       -2.8028443366
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Complex **3**:
Optimized ground state

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                                  angstroms
   atom             x                   y                   z
   Cu1        5.4136239688        5.0694737608        2.6556833940
   F2         2.3251689873        5.4749853745        2.4246084118
   F3         0.7546939338        7.5509151280        3.1557937764
   F4         1.8559375620        9.7564779288        4.3293617147
   F5         4.5467679686        9.8682636724        4.7795958340
   F6         6.1307460215        7.7996330526        4.0706644627
   O7         9.9717760899        3.2032683289        1.1573345801
   O8         6.3782195731        0.1487623298        1.3479275315
   N9         7.8628796732        3.8727467442        1.7435361475
   N10        6.0806028022        2.3698102954        1.8199377151
   C11        6.5518211016        3.6297284307        2.0161272220
   C12        8.7979192535        2.9220094263        1.2568141328
   C13        8.2354623894        1.5772339107        0.8077586177
   C14        6.8461846805        1.2655215336        1.3550272988
   C15        8.0956209829        1.6509406705       -0.7439556017
   H16        7.7202362754        0.6942047102       -1.1156216204
   H17        9.0768275274        1.8502401696       -1.1819668772
   H18        7.4061677003        2.4423114349       -1.0544753097
   C19        9.2118888695        0.4505589448        1.1960040561
   H20        9.3235651424        0.3822250238        2.2824719440
   H21       10.1927688362        0.6527670805        0.7635392804
   H22        8.8317443144       -0.5044928275        0.8308528397
   C23        8.3477270106        5.2195144238        2.0329080735
   C24        8.2356686496        6.2024456960        1.0402623107
   C25        8.6216762893        7.5049626783        1.3688589754
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H26               8.5224308671        8.2849239011        0.6175922274
C27               9.1038143852        7.8335214923        2.6382056053
C28               9.2437519229        6.8112151355        3.5815121456
H29               9.6307004289        7.0488133235        4.5695772588
C30               8.8711253468        5.4947543814        3.3048011341
C31               7.6888231158        5.8869079972       -0.3311710753
H32               8.2546345627        5.0856630152       -0.8200473362
H33               7.7355520785        6.7679955592       -0.9755479829
H34               6.6401801933        5.5700697407       -0.2786697842
C35               9.4121126028        9.2646655622        3.0051914955
H36               9.6279754407        9.8706760007        2.1208345687
H37              10.2660588687        9.3337237624        3.6863855002
H38               8.5494185126        9.7135393331        3.5128715552
C39               9.0079194913        4.4196566808        4.3555241581
H40               9.4565691726        4.8265209866        5.2648357985
H41               9.6412906584        3.5961852415        4.0075810858
H42               8.0329600047        3.9986514502        4.6283154079
C43               4.6895364302        2.1183489353        2.1846047776
C44               3.7008072829        2.2378328795        1.1969656992
C45               2.3736058882        2.0301439619        1.5773406310
H46               1.5926330694        2.1330167848        0.8277269918
C47               2.0225592862        1.7112448620        2.8927512505
C48               3.0425260385        1.5778762984        3.8384746960
H49               2.7881166643        1.3188829776        4.8635447420
C50               4.3866722585        1.7758932794        3.5093919949
C51               4.0434867468        2.6006617478       -0.2277769578
H52               3.1416716030        2.6332444777       -0.8437227413
H53               4.7283616574        1.8729253561       -0.6782384801
H54               4.5198506591        3.5865975371       -0.2848351150
C55               0.5728423068        1.5494115894        3.2835296788
H56               0.1068630666        2.5282451826        3.4506850281
H57               0.4672458158        0.9718195773        4.2062472678
H58              -0.0008197092        1.0467038720        2.4983299765
C59               5.4624068488        1.6363479547        4.5591327526
H60               6.2289715567        0.9134486774        4.2590043366
H61               5.0344829057        1.2965767386        5.5052449609
H62               5.9620218724        2.5942660223        4.7467316412
C63               4.2944029015        6.5479232438        3.2149738648
C64               2.9199771499        6.5468117779        3.0128518611
C65               2.0816787751        7.5989612196        3.3741267420
C66               2.6380307006        8.7263072410        3.9730068880
C67               4.0109654289        8.7780888474        4.1997597374
C68               4.7981869485        7.6936266701        3.8184597393
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Optimized triplet excited state

		angstroms	
atom	x	y	z
Cu1	5.5116730463	5.0177151665	2.6116349140
F2	2.4906534970	5.5407659260	2.2681739870
F3	0.8819548955	7.5086719197	3.2175553250
F4	1.9277215143	9.4985581375	4.7668021105
F5	4.5899732415	9.5045275490	5.3743727744
F6	6.1970683763	7.5351705547	4.4573576221
O7	9.9673151356	3.2737006122	0.9197954715
O8	6.3054132788	0.1484342321	1.0918724341
N9	7.8808514168	3.8587052514	1.6116694426
N10	6.0850833914	2.3191871192	1.7364553734
C11	6.5571033572	3.6040843985	1.9225849984
C12	8.7975232168	2.9516176306	1.1184363597
C13	8.2761549538	1.5329677363	0.8270155253
C14	6.8143329241	1.2576370211	1.2318609844
C15	8.3918628629	1.2944903051	-0.7015597566
H16	8.0709471305	0.2772735784	-0.9372176789
H17	9.4284242089	1.4375014786	-1.0156018508
H18	7.7619624239	1.9937213658	-1.2625915700
C19	9.1797046164	0.5223065532	1.5725418004
H20	9.1220455286	0.6638093430	2.6573276323
H21	10.2172711116	0.6627782716	1.2628648323
H22	8.8553804789	-0.4944506316	1.3417222006
C23	8.2429019661	5.2244120555	1.9313340610
C24	7.8903488982	6.2571399745	1.0271865648
C25	8.1543230903	7.5765676641	1.4046144201
H26	7.8761866725	8.3803697443	0.7274386813
C27	8.7587623302	7.8865043573	2.6256783308
C28	9.1531956449	6.8342951598	3.4662095544
H29	9.6452589783	7.0655618173	4.4077065629
C30	8.9059111368	5.5017092897	3.1480833302
C31	7.3325949649	5.9531503035	-0.3436797731
H32	8.1024506720	5.4879405213	-0.9704432682
H33	7.0043979369	6.8714604829	-0.8366854316
H34	6.4837317310	5.2654547027	-0.3034763192
C35	8.9355942685	9.3177256481	3.0625517585
H36	8.9404416305	10.0047557514	2.2117806646
H37	9.8624540123	9.4575946916	3.6274454204
H38	8.1046656276	9.6048225813	3.7195962952
C39	9.3508082347	4.3876717952	4.0611791867
H40	9.7391712510	4.7881639912	5.0007811605
H41	10.1395915500	3.7977125328	3.5819898176
H42	8.5261069804	3.7063798029	4.2956744797
C43	4.6825441091	2.1850055519	2.0822163201

C44	3.7100038829	2.2773317159	1.0649090291
C45	2.3672577534	2.2496604256	1.4386721399
H46	1.6064040542	2.3338743105	0.6662862655
C47	1.9716012611	2.1354725754	2.7780576522
C48	2.9613130130	1.9988106262	3.7559478216
H49	2.6690034079	1.8760512484	4.7961074689
C50	4.3220625782	2.0162235679	3.4367181061
C51	4.1068151499	2.3761486501	-0.3870262156
H52	3.2297568296	2.5406832091	-1.0180148420
H53	4.5969646828	1.4518657742	-0.7121639526
H54	4.8082399460	3.1995079166	-0.5588883969
C55	0.5110529191	2.1929318454	3.1515557621
H56	0.1671432630	3.2346404156	3.1807508079
H57	0.3285134057	1.7567686337	4.1376428873
H58	-0.1121068657	1.6663071294	2.4216742207
C59	5.3637992404	1.7936238249	4.5082657021
H60	5.9179888199	0.8674273001	4.3185664798
H61	4.8929254730	1.7126854126	5.4912620534
H62	6.0930979317	2.6088718070	4.5478912854
C63	4.4029411906	6.4628837852	3.3252379142
C64	3.0439393358	6.5098337587	3.0444146363
C65	2.1922346775	7.5071226992	3.5125131787
C66	2.7214449171	8.5243950553	4.3038714628
C67	4.0798927946	8.5232170743	4.6117014887
C68	4.8813000794	7.4956390603	4.1197814401

Complex **4:**

Optimized ground state

atom	x	y	z
Cu1	6.2185268362	15.3707726626	8.7791210555
O2	6.6528768447	20.1796722695	6.8839655283
O3	10.5362931531	17.4359293461	6.7915396599
N4	6.6315610624	18.0222908312	7.6466128710
N5	8.5227305111	16.6647261312	7.5578057199
C6	7.2117718165	16.8149152469	7.8988664789
C7	7.2663510110	19.1496478839	7.0648063328
C8	8.7333042632	19.0114744354	6.6735501566
C9	9.3642097429	17.6637005009	7.0033709309
C10	5.2213253905	18.1712129266	7.9930573845
C11	4.2530705568	17.7623968606	7.0649407266
C12	2.9084718063	17.8943614615	7.4231134734

H13	2.1448741690	17.5735175077	6.7187335049
C14	2.5236772953	18.4236037107	8.6586132565
C15	3.5226286635	18.8477278832	9.5406016903
H16	3.2391497592	19.2753882766	10.4994984432
C17	4.8809167263	18.7342214937	9.2310175457
C18	4.6373057259	17.1869953526	5.7230790712
H19	3.7482527292	16.9950456466	5.1172578295
H20	5.1740585718	16.2377117162	5.8376315668
H21	5.2846109537	17.8694107703	5.1600485868
C22	1.0653989743	18.5109586036	9.0437893386
H23	0.4253874992	18.6410600618	8.1658401267
H24	0.8804239230	19.3447987097	9.7278277666
H25	0.7415888739	17.5936700835	9.5512795842
C26	5.9348758280	19.1992564223	10.2068519634
H27	6.5564939093	19.9922936966	9.7757599960
H28	6.5962992738	18.3770542823	10.5028488453
H29	5.4717930182	19.5952900293	11.1139789190
C30	9.5368672783	20.1196283408	7.3997085837
H31	9.4834470364	20.0051227816	8.4874749061
H32	9.1255611906	21.0953582371	7.1344775933
H33	10.5842111508	20.0614286923	7.0976611935
C34	8.8326718056	19.2140520397	5.1373241355
H35	9.8808205212	19.1632307868	4.8355399272
H36	8.4175763256	20.1898513783	4.8771300110
H37	8.2763010263	18.4436272015	4.5930530243
C38	9.1324666402	15.3598726404	7.7930900144
C39	9.1336117717	14.4239355365	6.7491472309
C40	9.7191363549	13.1783570210	6.9925017075
H41	9.7242915501	12.4382523964	6.1957332086
C42	10.2914077578	12.8597045174	8.2276477539
C43	10.2890565920	13.8325869925	9.2317113135
H44	10.7404943300	13.6053533814	10.1945766777
C45	9.7198745095	15.0937288288	9.0377550810
C46	8.5230595134	14.7361152681	5.4036874666
H47	8.6013817136	13.8747401473	4.7358100811
H48	9.0282523073	15.5801946504	4.9193612461
H49	7.4609738821	14.9912243639	5.4936271816
C50	10.8734756088	11.4891559764	8.4817748118
H51	11.2174270091	11.0212274648	7.5545776071
H52	10.1226144418	10.8240484545	8.9261948919
H53	11.7187026844	11.5347600118	9.1754477977
C54	9.7327485253	16.1220551859	10.1416620397
H55	8.7148654605	16.3559293458	10.4741862711
H56	10.2029315262	17.0570076049	9.8165209874
H57	10.2881677339	15.7518059461	11.0066673471
C58	5.2766170701	13.9521414314	9.7145045324
C59	5.0977797614	12.6749436192	9.1278711271

C60	4.4436134131	11.6444773338	9.8151565534
H61	4.3257191904	10.6712682974	9.3373329016
C62	3.9361873829	11.8317651665	11.1049941516
C63	4.1048349759	13.0880503115	11.6912613794
H64	3.7215085138	13.2561729660	12.6980765557
C65	4.7579308341	14.1313591094	11.0182262735
C66	5.6046572460	12.3954758945	7.7244761151
H67	6.6613937603	12.6688277444	7.6211211444
H68	5.0468546183	12.9765373127	6.9778601035
H69	5.5035418283	11.3373918613	7.4570104331
C70	3.2116420370	10.7175142012	11.8254138495
H71	2.1862082099	10.5951697311	11.4521530309
H72	3.1452912623	10.9122828026	12.9006760836
H73	3.7163420354	9.7540822015	11.6890838846
C74	4.9158917056	15.4596407765	11.7351282610
H75	4.5538963171	16.2887915204	11.1160860135
H76	5.9696977315	15.6651767054	11.9665833906
H77	4.3634516350	15.4807086454	12.6815456732

Optimized triplet excited state

angstroms

atom	x	y	z
Cu1	6.1295281312	15.4557262909	8.8269818533
O2	6.7361101729	20.1716045362	6.7962556842
O3	10.5187182506	17.2810323669	6.6002720125
N4	6.6713694490	18.0459165122	7.6253864522
N5	8.5526054642	16.6186524218	7.5554072957
C6	7.2193229000	16.7958227535	7.9475987845
C7	7.3321181230	19.1319915678	7.0774885472
C8	8.8490001873	19.0025838576	6.8914244138
C9	9.3835140112	17.5667961521	6.9804684564
C10	5.2599048787	18.1778206245	7.9177430706
C11	4.3132796894	17.7253600788	6.9780797266
C12	2.9558897619	17.8126762351	7.3056797463
H13	2.2189641547	17.4670793218	6.5838655868
C14	2.5243246962	18.3501181808	8.5223632824
C15	3.4898481439	18.8247478153	9.4171417395
H16	3.1705322065	19.2726489777	10.3561143294
C17	4.8583881915	18.7528574432	9.1370891630
C18	4.7441836852	17.2130964571	5.6252167132
H19	3.8839981178	16.8597398015	5.0500647026
H20	5.4603322273	16.3903966730	5.7179409143
H21	5.2344775776	18.0090657687	5.0536556310
C22	1.0540515064	18.4055885338	8.8688740071
H23	0.4343032093	18.4927728618	7.9711765950
H24	0.8283621713	19.2548306887	9.5213228251

H25	0.7360075689	17.4967106457	9.3962201830
C26	5.8738219363	19.3184278898	10.0997998061
H27	6.3410951478	20.2137866547	9.6746032411
H28	6.6723850412	18.5988150442	10.3079016039
H29	5.4028089799	19.5963206155	11.0468107523
C30	9.5331183743	19.8270482888	8.0177840921
H31	9.2827288964	19.4351468104	9.0097594547
H32	9.2013399939	20.8674587603	7.9629877157
H33	10.6186404058	19.7844211371	7.8936961881
C34	9.2349667947	19.5953349212	5.5203530496
H35	10.3175101777	19.5436256961	5.3913961867
H36	8.8954319621	20.6309332309	5.4607850034
H37	8.7669922609	19.0352470725	4.7036676356
C38	9.0799029404	15.2862038856	7.7589868749
C39	8.9870583959	14.3424521343	6.7228788279
C40	9.4350302250	13.0401780395	6.9699772084
H41	9.3681441073	12.3026079789	6.1724203426
C42	9.9761534904	12.6666593915	8.2046727816
C43	10.0784616475	13.6392630194	9.2031694797
H44	10.5116844823	13.3721593373	10.1650255460
C45	9.6485810535	14.9550279784	8.9998408072
C46	8.4568684488	14.7305456667	5.3645120236
H47	8.3683978314	13.8559360049	4.7138650741
H48	9.1331856523	15.4475837081	4.8861061753
H49	7.4739009479	15.2071503556	5.4370258156
C50	10.4762710740	11.2595191685	8.4400477730
H51	9.9283336909	10.5315104370	7.8335283416
H52	10.3767661324	10.9694076313	9.4908600606
H53	11.5376836234	11.1685124419	8.1770139420
C54	9.8236911495	15.9949263492	10.0802855334
H55	8.8822992671	16.5104300479	10.2947114875
H56	10.5494875073	16.7550373129	9.7692141777
H57	10.1867795625	15.5384848770	11.0052557219
C58	5.0751780607	14.0909250090	9.7007891335
C59	5.0406849524	12.8180106805	9.0893174406
C60	4.8210776407	11.7049392742	9.9085908597
H61	4.8458705182	10.7096388241	9.4675750969
C62	4.5285677849	11.8444747634	11.2721292217
C63	4.4378144787	13.1363814462	11.8150658874
H64	4.1674125866	13.2549672054	12.8632809911
C65	4.6514094942	14.2759127897	11.0358282763
C66	5.2747402633	12.6403238915	7.6060596597
H67	6.3454356717	12.5860901013	7.3768196584
H68	4.8619380848	13.4805537984	7.0372249006
H69	4.8074691317	11.7192257219	7.2446193667
C70	4.2826947654	10.6338619245	12.1383353597
H71	3.9642842109	9.7715175437	11.5455787596

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H72          3.5190153114      10.8312839930      12.8973307937
H73          5.1987627981      10.3454986060      12.6699431733
C74          4.4810511923      15.6549067701      11.6315892986
H75          4.0786756856      16.3617488133      10.8991155524
H76          5.4413217080      16.0571539534      11.9764712457
H77          3.8059341191      15.6278539406      12.4922777482
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