Supporting information

for

Light emission mechanism in dimers of carbene-metal-amide complexes

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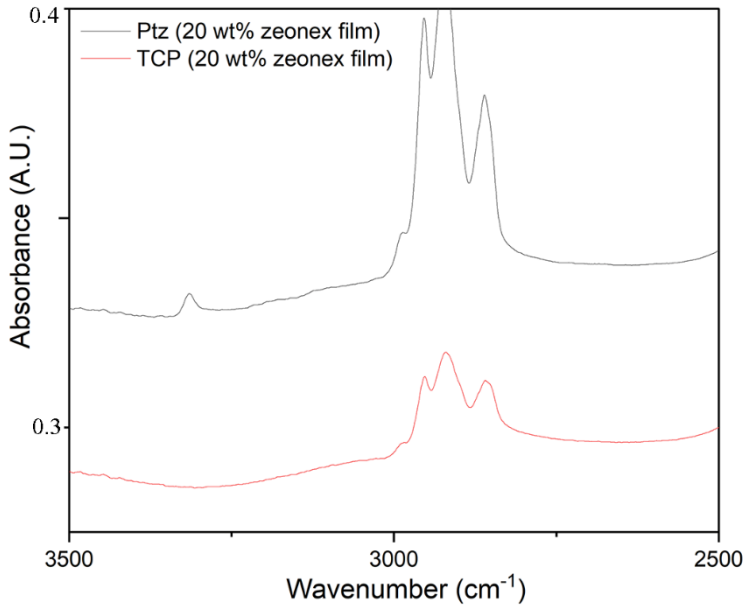

Figure S1. IR spectra of doped zeonex films containing 20 wt% of 10H-phenothiazine 5,5-dioxide (Ptz) or **TCP**. The first sample features a characteristic N-H stretching signal at 3310 cm^{-1}, while no such feature can be resolved for the complex-containing sample.

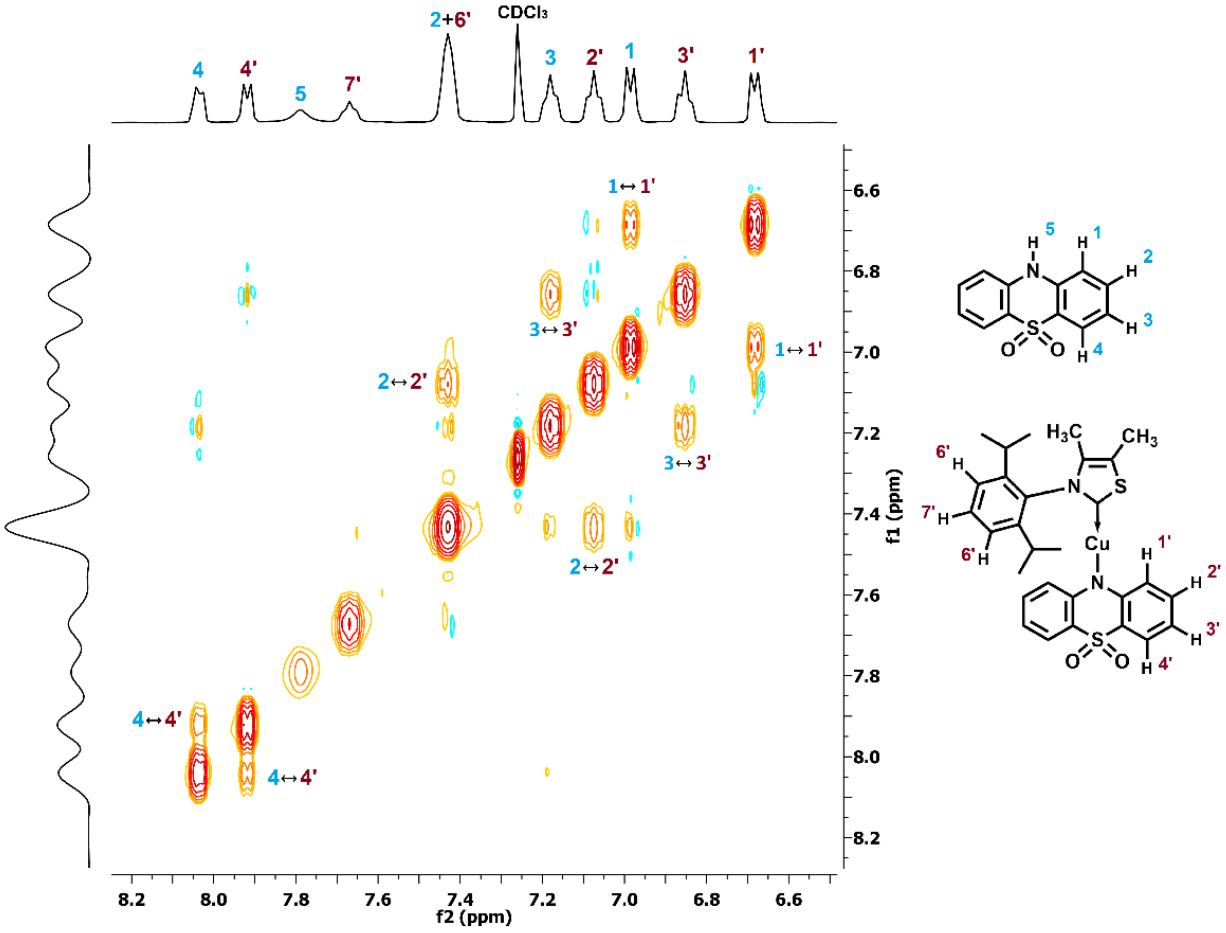

Figure S2. 2D NOESY spectra of mixture of Ptz and **TCP** in 1:1 molar ratio ($CDCl_3$). Close proximity between complexed and uncomplexed Ptz fragments is evident, suggesting a formation of hydrogen bond.

Table S1. Crystallographic data and structure refinement for crystal forms C1 and C2 of **TCP**.

	Crystal form C1	Crystal form C2
Empirical formula	$C_{121}H_{134}Cu_4N_8O_8S_8$	$C_{99}H_{102}Cu_3N_7O_8S_7$
Formula weight	2338.99	1933.06
Temperature/K	150.0(1)	150
Crystal system	monoclinic	Triclinic
Space group	$P2_1/c$	$P\ \bar{1}$
a/Å	13.1244(3)	12.2143(1)
b/Å	35.6810(5)	14.3299(1)
c/Å	14.4150(3)	28.9827(1)
α/°	90	94.412(1)
β/°	116.810(2)	100.883(1)
γ/°	90	110.808(1)
Volume/Å^3	6024.8(2)	4599.03(7)
Z	2	2
ρ_{calc}mg/mm^3	1.289	1.3958
μ/mm^{-1}	2.537	2.775
F(000)	2448.0	2016
Crystal size/mm^3	0.18 × 0.04 × 0.03	0.17 × 0.06 × 0.04
Radiation	CuKα (λ = 1.54184 Å)	Cu Kα (λ = 1.54184 Å)
2Θ max. for data collection	160.0°	160.0°
Index ranges	$-16 \le h \le 15$, $-45 \le k \le 45$, $-11 \le l \le 17$	$-15 \le h \le 15$, $-18 \le k \le 18$, $-37 \le l \le 36$
Reflections collected	37141	92885
Independent reflections	12061 [R_{int} = 0.0253, R_{sigma} = 0.0281]	19798 [R_{int} = 0.0319, R_{sigma} = 0.0256]
Data/restraints/parameters	12061/0/675	19798/0/1139
Goodness-of-fit on F^2	1.032	1.035
Final *R* indexes [$I > 2\sigma(I)$]	R_1 = 0.0450, wR_2 = 0.1256	R_1 = 0.0326, wR_2 = 0.0905
Final *R* indexes [all data]	R_1 = 0.0494, wR_2 = 0.1294	R_1 = 0.0339, wR_2 = 0.0916
Largest diff. peak/hole / e Å^{-3}	1.05/-0.65	0.36/-0.50
CCDC deposition number	2209354	2209353

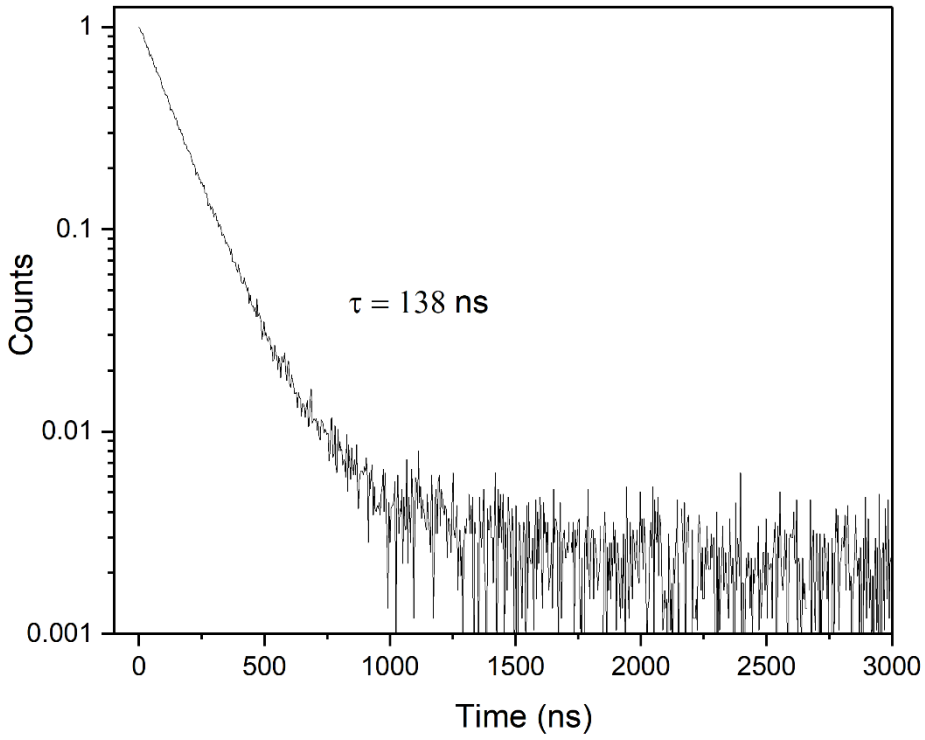

Figure S3. PL decay of **TCP** in toluene solution measured at 487 nm.

Table S2 Fitted PL decay components at different wavelength values for doped zeonex film (**TCP** content 5 wt%), using 375 nm excitation. The analysed spectral region covers the red emission peak of the dual-emitting sample.

	Wavelength, nm												
Parameter	550	570	590	610	630	650	670	690	710	730	750	770	790
a_1	53	383	254	318	208	170	126	73	46	18	10	8	-
τ_1, ns (contribution %)[a]	347 (2)	134 (6)	174 (6)	238 (10)	254 (9)	267 (10)	235 (8)	276 (8)	296 (9)	345 (7)	178 (3)	8 (0.5)	-
a_2	840	319	353	160	156	102	88	52	32	22	14	13	5
τ_2, ns (contribution %)[a]	346 (28)	542 (20)	432 (19)	869 (19)	654 (17)	717 (16)	801 (19)	667 (14)	579 (12)	476 (11)	649 (15)	464 (43)	352 (12)
a_3	231	160	158	106	105	85	53	42	27	17	10	2	3
τ_3, ns (contribution %)[a]	3183 (70)	3967 (74)	3746 (75)	4951 (71)	4218 (74)	4122 (74)	5025 (73)	4598 (78)	4359 (79)	4344 (82)	5273 (82)	4693 (56.5)	4910 (88)

[a] Contribution of individual decay components calculated using formula:

$a_i = (a_i \cdot \tau_i)/(a_1 \cdot \tau_1 + a_2 \cdot \tau_2 + a_3 \cdot \tau_3)$

Table S3 Fitted PL decay components at different wavelength values for doped zeonex film (**TCP** content 50 wt%), using 375 nm excitation. The analysed spectral region covers the red emission peak of the dual-emitting sample.

			Wavelength, nm												
Parameter	510	530	550	570	590	610	630	650	670	690	710	730	750	770	790
a_1	1680	1773	1678	1983	1743	2422	2082	1664	1098	744	434	220	100	43	20
τ_1, ns (contribution %)[a]	230 (3)	266 (3)	260 (3)	419 (5)	440 (5)	602 (12)	634 (13)	658 (14)	619 (13)	635 (13)	580 (11)	564 (10)	579 (9)	629 (8)	623 (8)
a_2	2706	2698	2741	1977	1986	1080	930	732	618	412	293	180	102	51	18
τ_2, ns (contribution %)[a]	739 (17)	875 (16)	784 (14)	1266 (15)	1272 (17)	2173 (19)	2189 (20)	2143 (21)	2040 (24)	1846 (21)	1725 (23)	1529 (22)	1347 (21)	1158 (18)	1013 (11)
a_3	1885	1867	2108	1680	1586	1336	1114	848	623	432	280	170	98	50	27
τ_3, ns (contribution %)[a]	4863 (80)	6535 (81)	6202 (83)	7898 (80)	7395 (78)	6274 (69)	5951 (67)	5871 (65)	5305 (63)	5533 (66)	5198 (66)	5016 (68)	4806 (70)	4843 (74)	5100 (81)

[a] Contribution of individual decay components calculated using formula:

$a_i = (a_i \cdot \tau_i)/(a_1 \cdot \tau_1 + a_2 \cdot \tau_2 + a_3 \cdot \tau_3)$

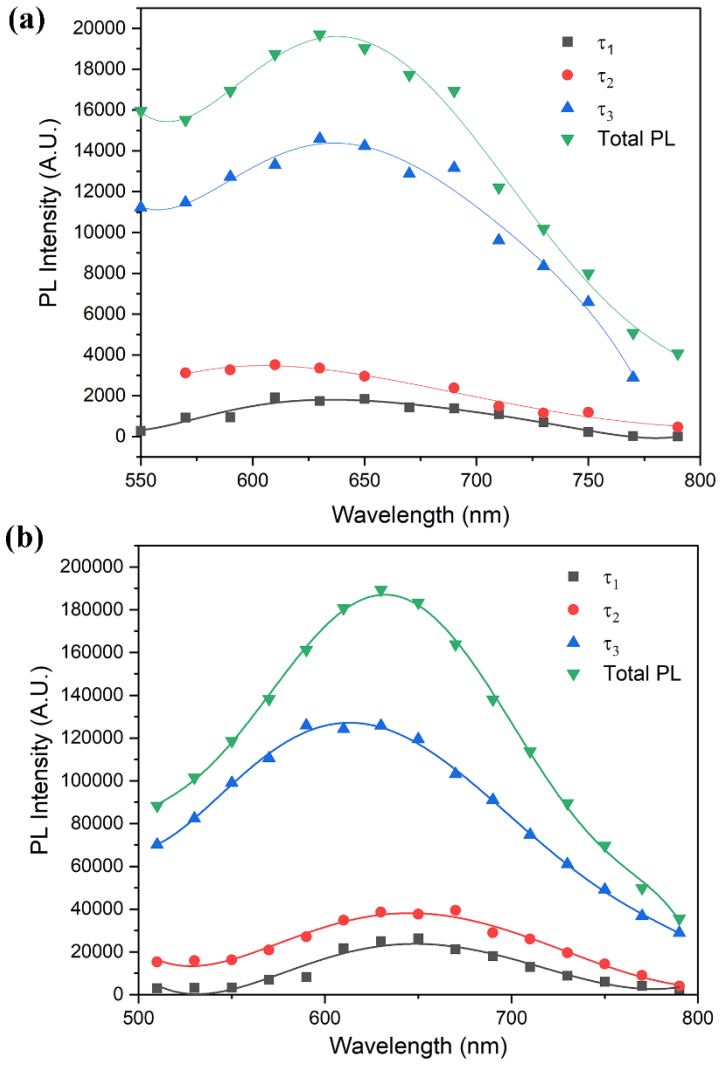

Figure S4. Deconvolution of the red emission peak for doped zeonex films containing (a) 5wt% or (b) 50 wt% of complex **TCP**. Deconvolution is performed using PL decay data given in Table S2 and S3 and illustrates a relative contribution towards total PL intensity for three individual components (τ_1, τ_2 and τ_3) of the fitted triexponential decay function.

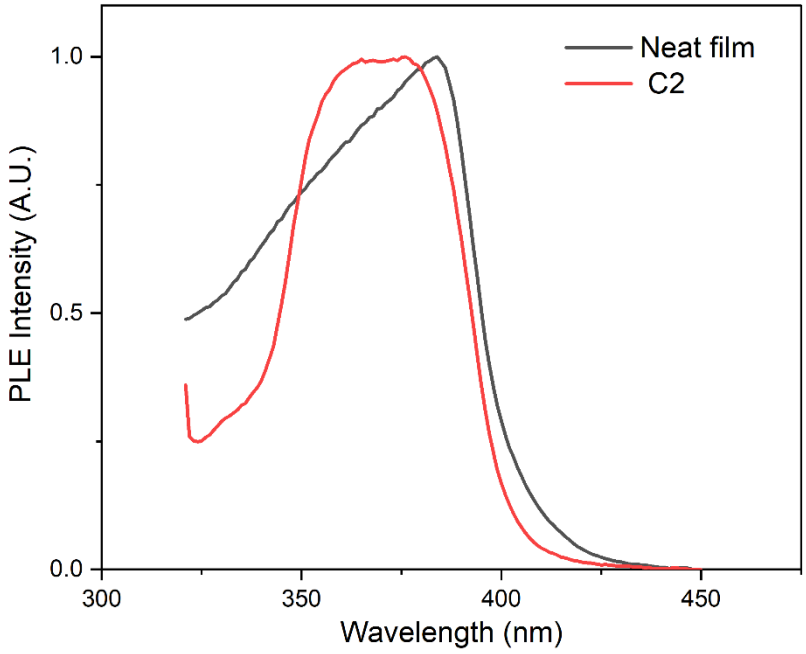

Figure S5. PLE spectra of neat film and crystal form C2 of **TCP**. Measured at the respective emission band maxima.

Temperature, K	300	280	260	240	220	200	180	160
τ, μs	2.86	3.41	4.32	5.55	7.01	9.15	13.8	18.3

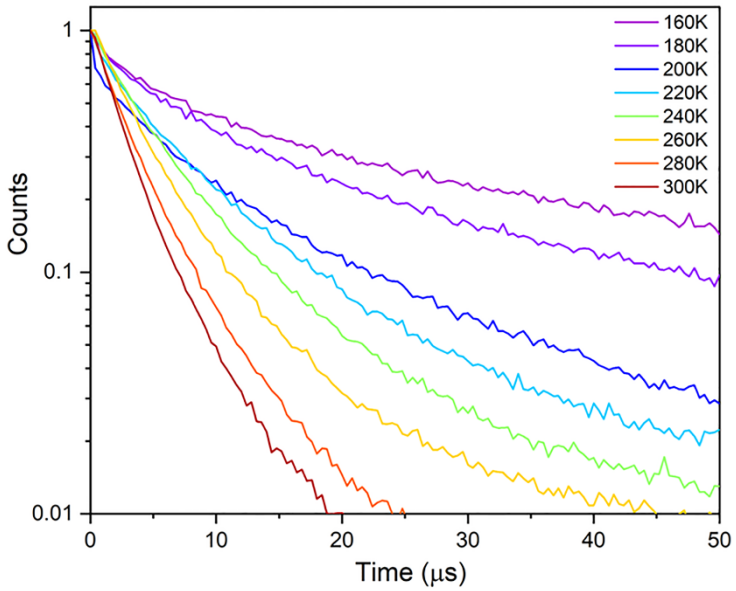

Figure S6. PL decays and corresponding τ values measured at 450 nm for doped zeonex film (**TCP** content 10 wt%) in 300 – 240 K temperature interval. Gradually increasing lifetimes of the monoexponential radiative decay process indicate TADF nature of LLCT emission.

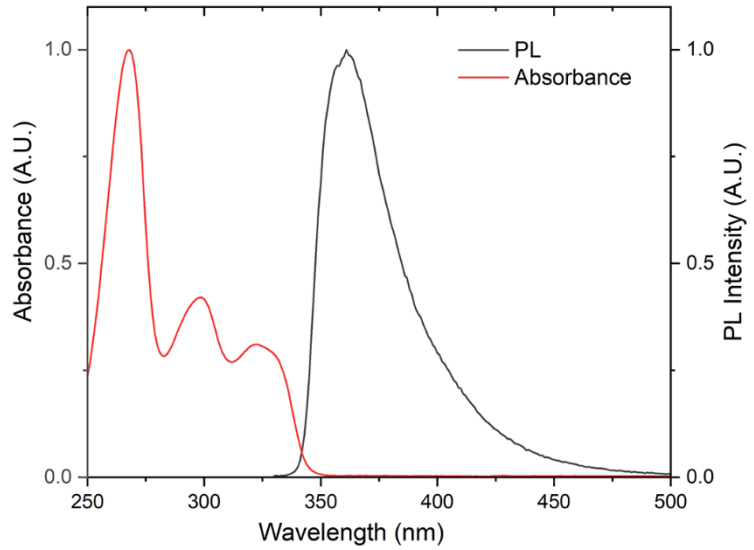

Figure S7. UV-Vis and PL spectra of Ptz in toluene (concentration $1 \cdot 10^{-5}$ mol L^{-1}).

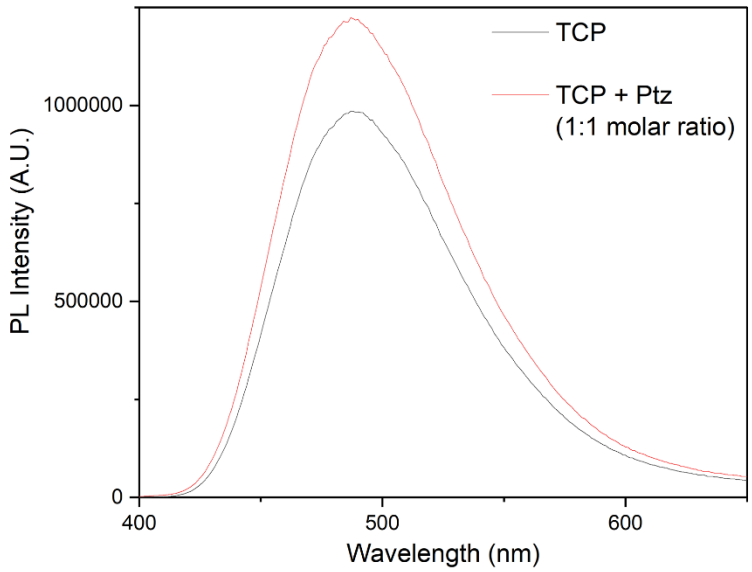

Figure S8. PL spectra of **TCP** and equimolar **TCP**:Ptz mixture in toluene (individual compound concentration $1 \cdot 10^{-3}$ mol L^{-1}) using 340 nm excitation. Increased PL intensity of the mixture is indicative of an antenna effect (excitation transfer from Ptz to **TCP**).

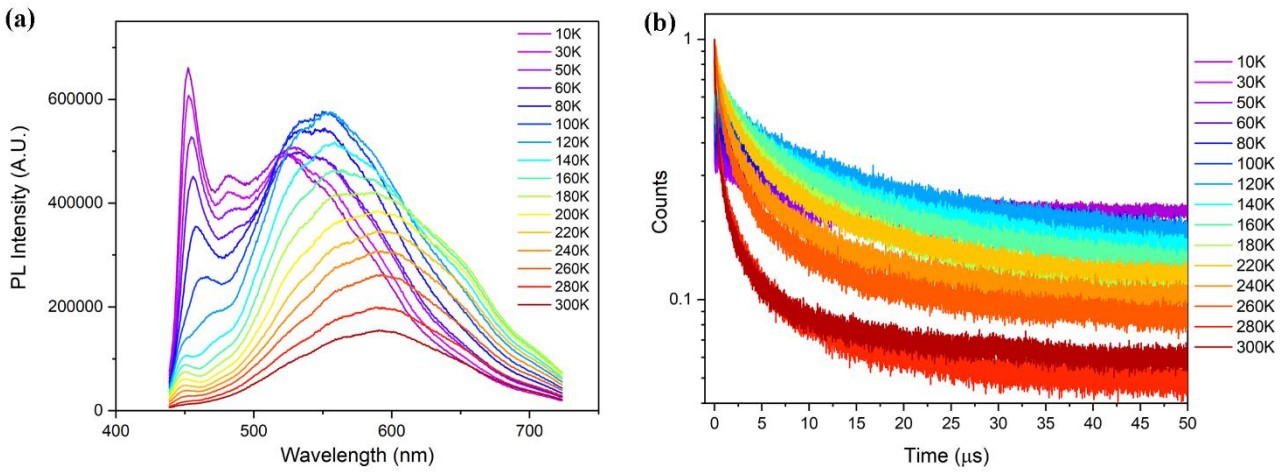

Figure S9. PL spectra (a) and decays (b) measured in neat film of **TCP** in 300 – 10 K temperature interval.

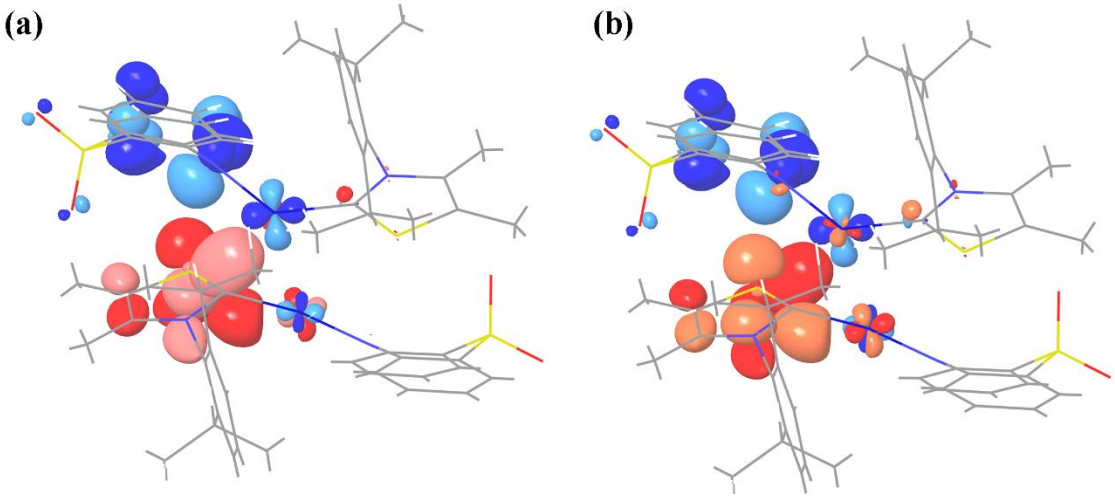

Figure S10. Natural transition orbitals (NTOs) of $S_0 \rightarrow S_1$ (a) and $S_0 \rightarrow T_1$ transition for and dimer of **TCP** at S_1 geometry. Blue NTOs correspond to a hole but red to a particle.

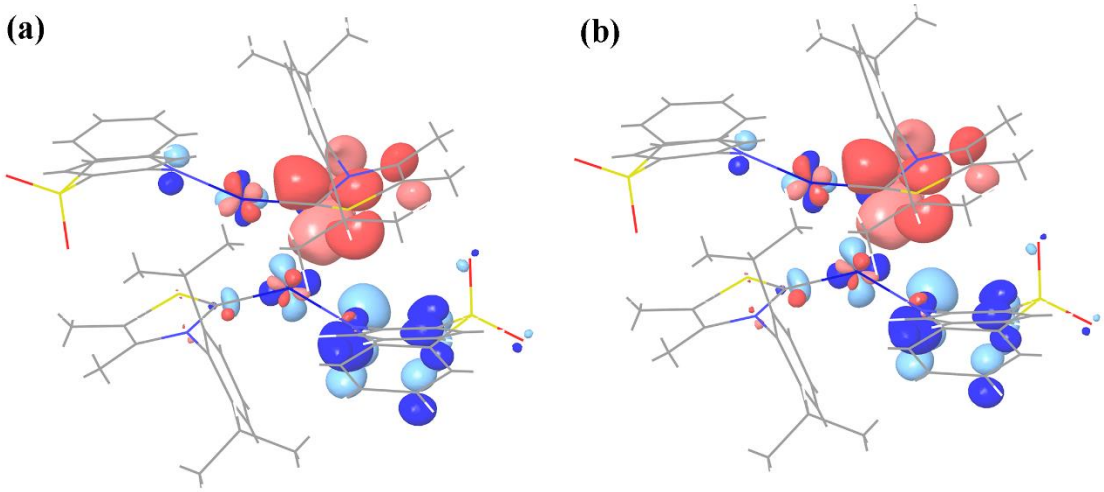

Figure S11. Natural transition orbitals (NTOs) of $S_0 \rightarrow S_1$ (a) and $S_0 \rightarrow T_1$ transition for and dimer of **TCP** at T_1 geometry. Blue NTOs correspond to a hole but red to a particle.

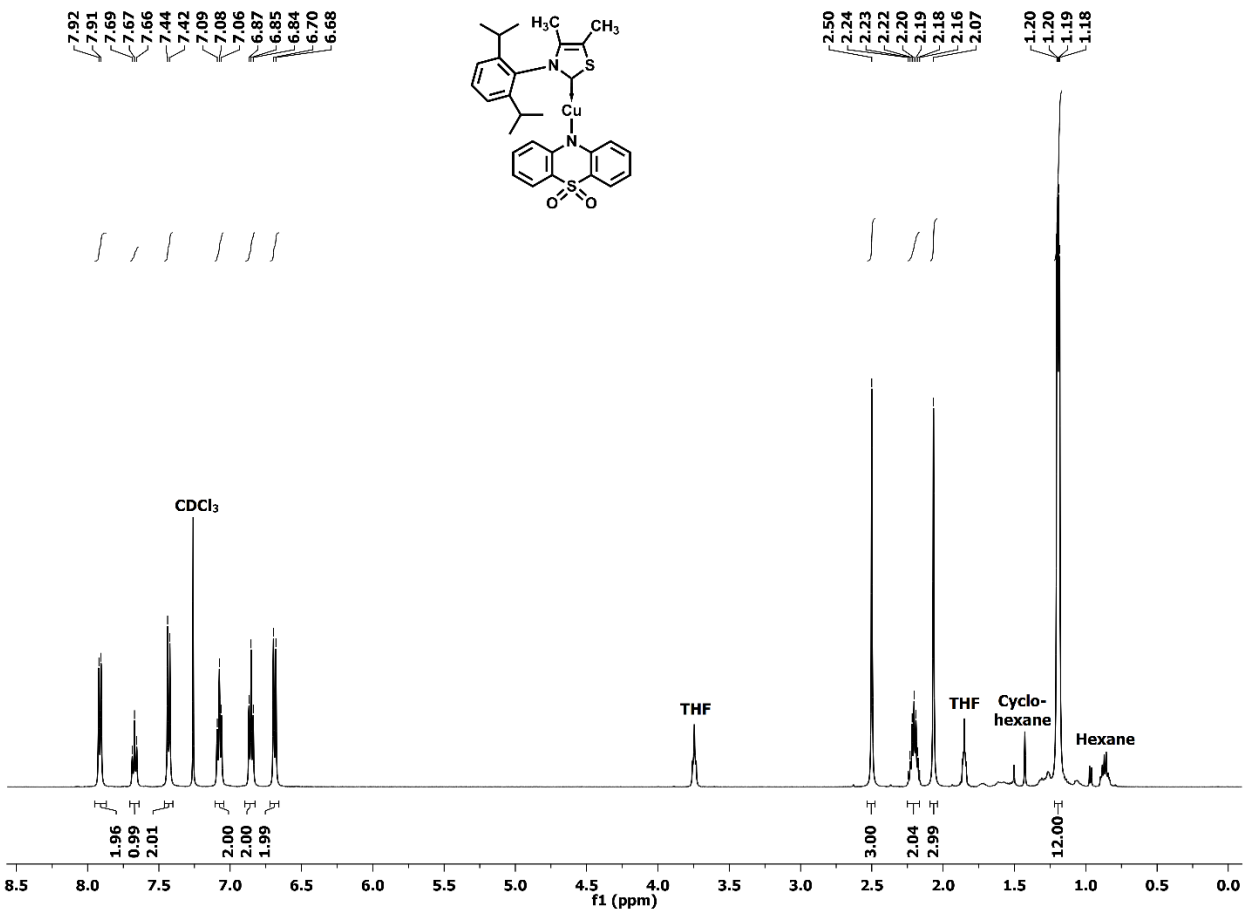

Figure S12. ^{1}H NMR spectra of **TCP** ($CDCl_3$).

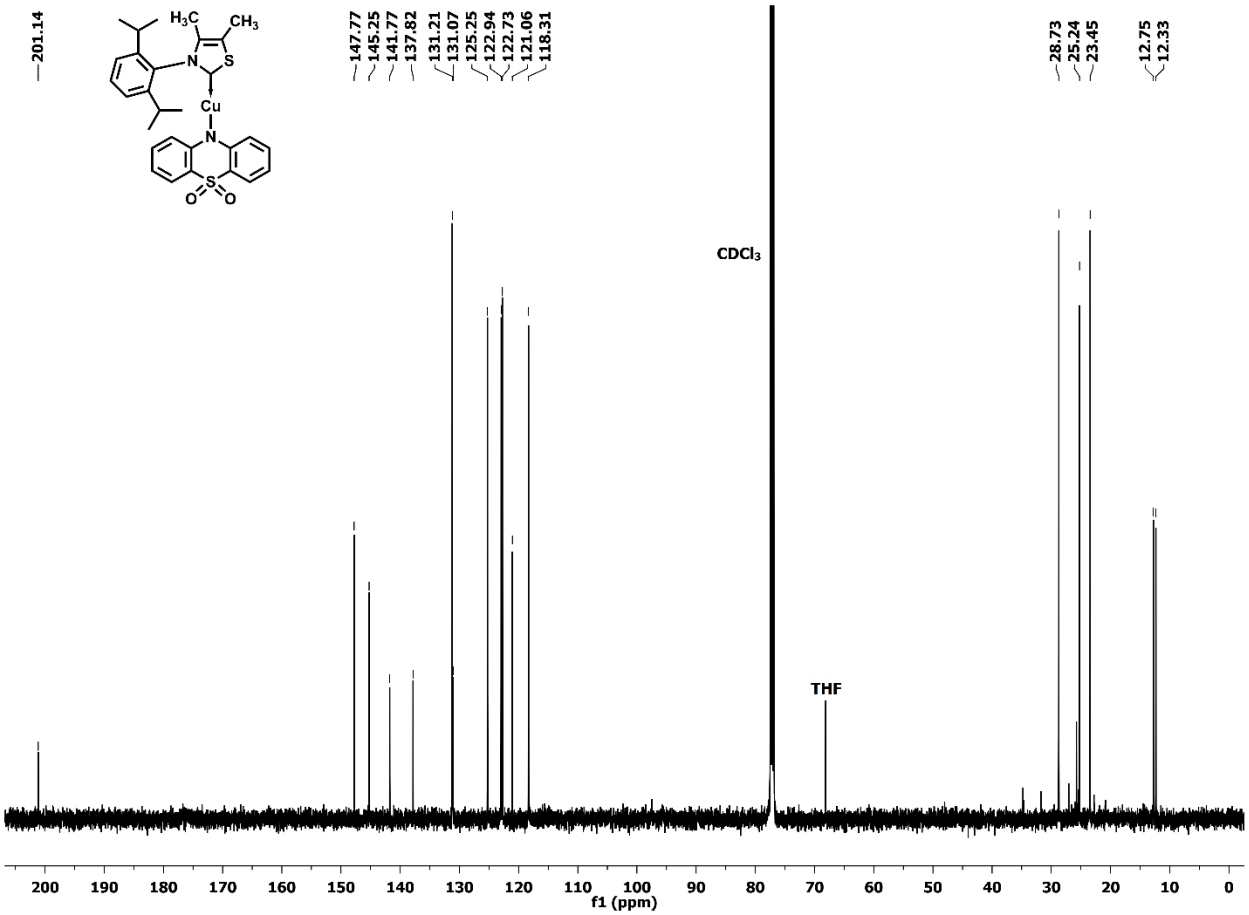

Figure S13. ^{13}C NMR spectra of **TCP** ($CDCl_3$).

DFT-optimized molecular geometries

Monomer S_0 geometry:

atom	x	y	z
Cu1	-2.1752618652	19.2409259482	4.5062590361
C1	-4.8044427191	20.3820993787	3.2927086731
H1	-4.3694835412	20.6382767657	4.2576966635
C2	-6.0866230399	20.7902461943	2.9765304800
H2	-6.6614754252	21.3441095385	3.7142432754
C3	-6.6405242209	20.5324221374	1.7150276526
H3	-7.6389881734	20.8783049523	1.4675523721
C4	-5.8929141232	19.8254543453	0.7904224082
H4	-6.2831052713	19.5895424298	-0.1957910962
C4A	-4.6101520937	19.3883657454	1.1237039874
S5	-3.7685683479	18.3129042950	0.0340416346
O1	-4.1370179700	18.5960928338	-1.3614397537
O2	-3.9431400497	16.9280231557	0.5046332979
C5A	-2.1246009337	18.8110538880	0.3489233397
C6	-1.1856552711	18.7249842014	-0.6799158800
H6	-1.5304048061	18.4750784405	-1.6795736256
C7	0.1527122470	18.9464123883	-0.4091858908
H7	0.8931992241	18.8831791788	-1.2003974297
C8	0.5324784481	19.2488393269	0.9050259745
H8	1.5790213800	19.4224457063	1.1400832745
C9	-0.4026265149	19.3599650367	1.9172039877
H9	-0.0857568231	19.6416847926	2.9186475671
C9A	-1.7807998642	19.1657959893	1.6741047994
N10	-2.6930074993	19.3925170619	2.6811415627
C10A	-4.0008634967	19.6819377180	2.3649003604
S11	-2.4327567172	19.2259200014	7.7430544016
C12	-1.5376006807	19.2171852633	6.2902908021
N13	-0.2383116497	19.2407106272	6.6204337390
C14	0.0913149404	19.2581346351	7.9796509840
C15	-1.0204480509	19.2566746811	8.7615068555
C16	0.7807146159	19.2542293467	5.6006987799
C17	1.1690360305	18.0392280053	5.0197687451
C18	2.1879612236	18.0865814355	4.0645173474
H18	2.5139141163	17.1660784964	3.5887063379
C19	2.7768987893	19.2906830415	3.7044130872
H19	3.5704408523	19.3036452866	2.9619157562
C20	2.3397227362	20.4839344826	4.2688273137
H20	2.7831106638	21.4214121745	3.9473016249
C21	1.3278157465	20.4940807034	5.2298044457
C22	0.5118566662	16.7162653478	5.3581211530
H22	-0.2303119406	16.8900508221	6.1440348329
C23	-0.2330629573	16.1703634286	4.1345096666
H23A	0.4583335430	15.9530329466	3.3132461898
H23B	-0.9710967898	16.8892842205	3.7615025169
H23C	-0.7577153651	15.2438105619	4.3893295825
C24	1.5257788267	15.7014981293	5.8904212555
H24A	2.0482683603	16.0828337206	6.7739030626
H24B	2.2792325628	15.4552230184	5.1345817305
H24C	1.0194030216	14.7716663389	6.1682918589
C25	0.7816236304	21.8040616949	5.7649188590
H25	0.2375869387	21.5972940437	6.6939779110
C26	-0.2215604096	22.3813653528	4.7579305001
H26A	-1.0359885370	21.6757183111	4.5574175637
H26B	0.2730175750	22.5973634247	3.8041553987
H26C	-0.6576992779	23.3120172146	5.1364658111
C27	1.8777429110	22.8186778878	6.0921907579
H27A	2.3972523504	23.1605314378	5.1909326345
H27B	2.6252980128	22.4004171796	6.7743003291
H27C	1.4388429189	23.7019209776	6.5666394970
C28	1.5240647709	19.2793882768	8.3846246195
H28A	2.0217748423	20.1871058882	8.0273738693

H28B	2.0621136574	18.4248212813	7.9619411901
H28C	1.6147091991	19.2428810917	9.4703807299
C29	-1.1296690640	19.2837668179	10.2471687640
H29A	-1.6656595438	18.4058173391	10.6212676335
H29B	-1.6694215454	20.1741557199	10.5844453969
H29C	-0.1396489932	19.2963815254	10.7080942542

Dimer S_0 geometry**:**

atom	x	y	z
Cu3	3.0173198415	4.0779783317	3.4212791035
S71	4.2254943083	1.0689286474	3.4704917054
S65	-0.7571353476	7.0361200172	4.1696068136
N73	5.6485835456	3.0208992126	2.9772969112
N70	1.6735941981	5.4214611029	3.2477220174
O91	-0.9817907018	6.2803978227	5.4182397975
O92	-1.6777462152	8.1439802701	3.8927246880
C65A	0.9033007231	7.5879542566	4.1406028972
C69A	1.9101178139	6.6666521525	3.7759578206
C75	5.8588492473	0.7565017704	2.9918722011
C81	5.8403461881	4.9071972021	1.4427303648
C72	4.3832541054	2.7613213626	3.3489314812
C77	6.6530016004	5.1111142864	3.7620494003
C76	6.0616127542	4.3781884448	2.7244740695
C74	6.4967788690	1.9366667752	2.7692297006
C64A	-0.7171591589	5.8940049160	2.8514012772
C78	7.0607734762	6.4155273949	3.4680796125
H78	7.5223196619	7.0122952519	4.2496306976
C70A	0.4660872425	5.1478689910	2.6548840616
C66	1.1944797400	8.8789620212	4.5875470409
H66	0.3679903008	9.5463642894	4.8151789939
C69	3.2441590252	7.1125577597	3.9270948599
H69	4.0517829634	6.4487867061	3.6235824975
C82	6.7715827122	4.5827651802	5.1771565822
H82	6.4536287262	3.5355470789	5.1971287583
C64	-1.8971945127	5.6420038112	2.1506715154
H64	-2.7587629687	6.2751383331	2.3426047435
C67	2.5116770538	9.2794258877	4.7312191601
H67	2.7481418045	10.2806912170	5.0765741569
C68	3.5332889505	8.3772203739	4.4000748134
H68	4.5741473393	8.6766482284	4.4896940512
C80	6.2604269657	6.2168395308	1.2058841832
H80	6.0980315855	6.6587349371	0.2271280474
C61	0.3702865981	4.0831147803	1.7301512040
H61	1.2652469589	3.4966530946	1.5302174776
C85	5.1445082108	4.1243625860	0.3460369974
H85	4.8852054751	3.1368981687	0.7414507843
C62	-0.8054613042	3.8110278248	1.0564880418
H62	-0.8287769136	2.9863926410	0.3490763950
C88	7.9331916431	2.1317184535	2.4407964589
H88a	8.3368763827	1.2265502283	1.9836742186
H88b	8.0837543451	2.9706775177	1.7566848401
H88c	8.4943546374	2.3170151645	3.3620874929
C79	6.8738525099	6.9619171259	2.2052808758
H79	7.1969661475	7.9787455814	2.0011636890
C63	-1.9510902088	4.5948103522	1.2483402034
H63	-2.8631933878	4.3852582747	0.6995764646
C89	6.4572319868	-0.6084461359	2.9524928872
H89a	6.8240246591	-0.8506951712	1.9498434975
H89b	7.2958102207	-0.6526949801	3.6536410261
H89c	5.7315000707	-1.3698290635	3.2432745353
C84	8.2044770640	4.6254669858	5.7084856807
H84b	8.2370523569	4.2013397193	6.7165374687
H84c	8.8781725127	4.0373985070	5.0798279784
C83	5.8236013971	5.3813993075	6.0764168986
H83a	5.8847594963	5.0158320169	7.1058705817

H83b	6.0788362782	6.4471048119	6.0841647350
H83c	4.7880064847	5.2941537675	5.7287347010
C86	3.8372885406	4.8116708075	-0.0610609291
H86a	3.1862199299	4.9727794758	0.8047948460
H86b	4.0269990176	5.7883204493	-0.5188906291
H86c	3.2962316475	4.2006492076	-0.7912138508
C87	6.0635434378	3.9123437881	-0.8592984088
H87a	6.3496379904	4.8663486967	-1.3147088895
H87b	6.9817458639	3.3886974384	-0.5750404838
H87c	5.5560574781	3.3173305276	-1.6254777655
Cu2	3.6564545525	3.4180262889	7.3902141186
S35	7.4357428684	0.4638932028	6.6537835973
S41	2.4471789668	6.4266699311	7.3452281198
O3	7.6613121968	1.2176447010	5.4043359118
N43	1.0254762813	4.4735835712	7.8379590312
O4	8.3580959766	-0.6416325883	6.9346658799
N40	5.0008183260	2.0758018698	7.5679991402
C46	0.6127106931	3.1157263632	8.0882386150
C39A	4.7672301069	0.8289295976	7.0422153122
C51	0.0203483876	2.3845495693	7.0495521308
C44	0.1783709507	5.5574006313	8.0521561150
C36	6.2065942155	2.3521842094	8.1633759300
C45	0.8161038530	6.7379284353	7.8311431385
C39	3.4341415698	0.3801717767	6.8900313354
H39	2.6247848936	1.0434745518	7.1902503801
C47	0.8342703889	2.5844721419	9.3691056908
C50	-0.3887136364	1.0802179219	7.3419781120
H50	-0.8510174678	0.4850195860	6.5596731003
C34A	7.3914945546	1.6079225559	7.9702374703
C42	2.2899722713	4.7340367228	7.4637709002
C35A	5.7763733718	-0.0914607314	6.6817552115
C38	3.1481612433	-0.8865470290	6.4202342004
H38	2.1080106053	-1.1882364735	6.3296784043
C55	-0.0974196726	2.9146589553	5.6350491113
H55	0.2226322365	3.9613299839	5.6163490428
C49	-0.2021316957	0.5320892920	8.6039931625
H49	-0.5264083437	-0.4845727560	8.8068319763
C48	0.4126286500	1.2749882556	9.6041663040
H48	0.5750453514	0.8315349514	10.5821896951
C52	1.5323629163	3.3647542242	10.4660264380
H52	1.7966845193	4.3508373550	10.0699687469
C31	6.2983108496	3.4178595777	9.0876207858
H31	5.4016246954	4.0023927920	9.2857835827
C3	5.4883341479	-1.3845085592	6.2384601589
H3	6.3164493383	-2.0511044130	6.0143313957
C37	4.1720718150	-1.7879197427	6.0938403876
H37	3.9380427904	-2.7907577186	5.7512592462
C58	-1.2574698415	5.3622069538	8.3834673563
H58a	-1.8228979719	5.1920490706	7.4607331944
H58b	-1.4076918249	4.5134140516	9.0561931484
H58c	-1.6567071855	6.2626197034	8.8556518593
C59	0.2176730103	8.1024222709	7.8756671036
H59a	0.9460846146	8.8663457069	7.5976771844
H59b	-0.6151914429	8.1519479227	7.1676155521
H59c	-0.1584972021	8.3365487279	8.8771016626
C34	8.5694806276	1.8625818213	8.6735302968
H34	9.4324975103	1.2306593419	8.4843008002
C56	0.8493405037	2.1148471363	4.7354613137
H56a	0.5903720084	1.0499642018	4.7244452767
H56b	0.7922149680	2.4831272091	3.7067472718
H56c	1.8846262545	2.1976612573	5.0855791704
C32	7.4721579676	3.6925954276	9.7637053978
H32	7.4924196995	4.5177047171	10.4706640027
C54	0.6127361694	3.5819783096	11.6701864114
H54a	0.3205894974	2.6295786828	12.1253781585
H54b	1.1223351262	4.1742285850	12.4370070480
H54c	-0.3021829247	4.1108410701	11.3845152329

C33	8.6195127441	2.9106848716	9.5750232376
H33	9.5299206225	3.1221804653	10.1258488916
C57	-1.5305258785	2.8755439859	5.1039989786
H57a	-1.5624875651	3.3000696472	4.0960730449
H57b	-1.9171687149	1.8514752367	5.0527559198
H57c	-2.2023782046	3.4653658683	5.7331581718
C53	2.8359102970	2.6712336381	10.8746629098
H53a	3.3798480694	3.2803344660	11.6041850070
H53b	2.6409458554	1.6961819428	11.3337635948
H53c	3.4865231245	2.5055610743	10.0092273243
H134	8.5885070537	5.6505108608	5.7595546643

Monomer S_1 geometry**:**

atom	x	y	z
Cu1	-2.1386103691	19.1737669002	4.4503250247
C1	-4.6245855526	20.5484823309	3.3841290984
H1	-4.1560240307	20.6192560452	4.3628834005
C2	-5.8530927595	21.1409761900	3.1441705898
H2	-6.3604283139	21.6605473064	3.9505948600
C3	-6.4331746829	21.0897941217	1.8743764761
H3	-7.3904705203	21.5672889485	1.6861067924
C4	-5.7810679264	20.4129547497	0.8435480317
H4	-6.2208537401	20.3463869894	-0.1476394164
C4A	-4.5578574017	19.8082976539	1.0856737668
S5	-3.8889881087	18.7774779858	-0.1718409896
O1	-4.0652911288	19.4040947715	-1.4829910228
O2	-4.4045426378	17.4194906379	0.0233774912
C5A	-2.1903923334	18.7988441909	0.2808439259
C6	-1.2563627909	18.4901010663	-0.6928829213
H6	-1.5810423274	18.3666470555	-1.7224321655
C7	0.0832914424	18.3354483659	-0.3381747441
H7	0.8177699244	18.0964524852	-1.1003487499
C8	0.4687947232	18.4904032593	0.9948536928
H8	1.5073885364	18.3750292312	1.2833316148
C9	-0.4600445022	18.8192876975	1.9655090222
H9	-0.1422723587	18.9860009851	2.9916519003
C9A	-1.8251905517	18.9915140394	1.6390776039
N10	-2.6721195888	19.3924545582	2.6373710349
C10A	-3.9232083304	19.8744726050	2.3544532461
S11	-2.4455587946	18.8304917593	7.7592669017
C12	-1.5503535183	19.1030257000	6.2686904669
N13	-0.2057692573	19.2298225720	6.6437239720
C14	0.0951217411	19.1620538937	7.9908587203
C15	-0.9954487932	18.9547735380	8.7702706384
C16	0.7822666801	19.3025348588	5.6229633249
C17	1.3487202050	18.1078582284	5.1401100120
C18	2.3434068460	18.2008074388	4.1611664105
H18	2.8085582873	17.2934825569	3.7826534685
C19	2.7394132276	19.4375445126	3.6603269796
H19	3.5211341081	19.4926406707	2.9060949507
C20	2.1253959164	20.6011275780	4.1081238191
H20	2.4196966871	21.5606655592	3.6883468313
C21	1.1301117953	20.5553844708	5.0901307788
C22	0.8696631323	16.7520239814	5.6214751410
H22	0.1738500044	16.9198026693	6.4492239448
C23	0.0919195148	16.0472495256	4.5040767924
H23A	0.7261415530	15.8739834457	3.6270224958
H23B	-0.7642672953	16.6547946635	4.1936231736
H23C	-0.2845620645	15.0778400299	4.8469787329
C24	2.0150289936	15.8756716904	6.1310702941
H24A	2.5738024511	16.3716039288	6.9316003609
H24B	2.7223245750	15.6279115317	5.3319889073
H24C	1.6222745387	14.9326648740	6.5252718825
C25	0.4290678389	21.8259749765	5.5257835120
H25	-0.2760226134	21.5557787078	6.3181087956

C26	-0.3846496459	22.4054130118	4.3631729880
H26A	-1.1114528327	21.6707768523	3.9959772486
H26B	0.2621559556	22.6916474822	3.5263655709
H26C	-0.9343443330	23.2976630170	4.6849073296
C27	1.4093813267	22.8633836773	6.0804871265
H27A	2.1207255845	23.1936853752	5.3156742366
H27B	1.9843879229	22.4601937925	6.9202160331
H27C	0.8695716006	23.7491665887	6.4327455008
C28	1.5142467754	19.3195611917	8.4261506944
H28A	1.9167700569	20.2888634766	8.1105319726
H28B	2.1528070154	18.5469299241	7.9838094562
H28C	1.5978510941	19.2510858522	9.5113182189
C29	-1.0972785638	18.8271529492	10.2484622962
H29A	-1.5357778972	17.8641065649	10.5378083587
H29B	-1.7316870309	19.6117013093	10.6780832507
H29C	-0.1134497352	18.8991114199	10.7210225626

Dimer S_1 geometry**:**

	atom	x	y	z
Cu3	2.8322210000	4.1272650000	4.1005710000
S71	3.8772370000	1.0988520000	3.7268840000
S65	-0.7211970000	7.2623320000	4.1315660000
N73	5.5128770000	3.0445090000	3.5645230000
N70	1.6527720000	5.5008550000	3.5063650000
O91	-0.9580080000	6.6056880000	5.4331360000
O92	-1.6353070000	8.3528310000	3.7629500000
C65A	0.9433540000	7.7952770000	4.0650430000
C69A	1.9270610000	6.8024130000	3.8597400000
C75	5.4984460000	0.7873000000	3.1302840000
C81	5.4448780000	4.8468020000	1.9074680000
C72	4.2300600000	2.7862690000	4.0842680000
C77	6.6554210000	5.1703980000	4.0185420000
C76	5.8688010000	4.3777590000	3.1700440000
C74	6.2124460000	1.9407110000	3.0925500000
C64A	-0.6750370000	6.0323930000	2.8909850000
C78	7.0490170000	6.4368990000	3.5672040000
H78	7.6685970000	7.0607310000	4.2062820000
C70A	0.4874940000	5.2313870000	2.8243260000
C66	1.2617310000	9.1298270000	4.3207550000
H66	0.4553840000	9.8475400000	4.4453210000
C69	3.2709440000	7.2205890000	3.9766000000
H69	4.0565030000	6.4872060000	3.8078960000
C82	7.0738150000	4.7159390000	5.3992920000
H82	6.6318450000	3.7288130000	5.5770270000
C64	-1.7870620000	5.8182040000	2.0768560000
H64	-2.6356390000	6.4916490000	2.1607670000
C67	2.5906300000	9.5075180000	4.4183760000
H67	2.8531060000	10.5422670000	4.6163340000
C68	3.5892130000	8.5370280000	4.2519500000
H68	4.6371060000	8.8194370000	4.3170660000
C80	5.8714470000	6.1103600000	1.4973440000
H80	5.5730800000	6.4833320000	0.5216220000
C61	0.4419340000	4.1482360000	1.9198010000
H61	1.3266900000	3.5220360000	1.8360120000
C85	4.5791580000	4.0103210000	0.9842370000
H85	4.1293320000	3.2126230000	1.5855570000
C62	-0.6681700000	3.9147670000	1.1277790000
H62	-0.6544810000	3.0809210000	0.4305440000
C88	7.6333450000	2.0968730000	2.6656290000
H88a	7.9410810000	1.2670500000	2.0274530000
H88b	7.7805490000	3.0284280000	2.1125070000
H88c	8.2846850000	2.1108480000	3.5443400000
C79	6.6731200000	6.8997320000	2.3152450000
H79	6.9989130000	7.8796130000	1.9750300000
C63	-1.7894210000	4.7544150000	1.1894250000

H63	-2.6477010000	4.5774550000	0.5486190000
C89	5.9171900000	-0.5941060000	2.7671940000
H89a	6.9107000000	-0.5935840000	2.3124060000
H89b	5.9529110000	-1.2453160000	3.6496010000
H89c	5.2185010000	-1.0472670000	2.0528920000
C84	8.5925570000	4.5771940000	5.5206150000
H84b	8.8552640000	4.1931760000	6.5119350000
H84c	8.9924820000	3.8840190000	4.7754120000
C83	6.5344410000	5.6922310000	6.4474730000
H83a	6.8434350000	5.3916650000	7.4510400000
H83b	6.9013240000	6.7098620000	6.2727920000
H83c	5.4396470000	5.7271130000	6.4235170000
C86	3.4372860000	4.8349530000	0.3837110000
H86a	2.8671590000	5.3411390000	1.1686320000
H86b	3.8057730000	5.5914000000	-0.3186140000
H86c	2.7528820000	4.1841170000	-0.1709570000
C87	5.4227220000	3.3651070000	-0.1208550000
H87a	5.9112420000	4.1324660000	-0.7333930000
H87b	6.2001110000	2.7149560000	0.2915640000
H87c	4.7906340000	2.7592520000	-0.7798820000
Cu2	3.8518030000	3.2086340000	6.2520550000
S35	7.6451780000	0.6029980000	7.1764360000
S41	2.7410900000	6.0955460000	7.0740560000
O3	7.9779180000	1.1950830000	5.8740830000
N43	1.2483780000	4.1488540000	7.3613250000
O4	8.6171160000	-0.3072720000	7.7886990000
N40	4.9845430000	2.0267430000	7.3091260000
C46	0.8099240000	2.7906330000	7.5794240000
C39A	4.9302230000	0.6686420000	7.0888830000
C51	-0.0064770000	2.1569520000	6.6344960000
C44	0.4915860000	5.2296560000	7.8276750000
C36	5.9727300000	2.5210380000	8.1226770000
C45	1.1767130000	6.3998460000	7.7481640000
C39	3.6739830000	0.0598360000	6.9076240000
H39	2.7877320000	0.6877290000	6.9379040000
C47	1.1817990000	2.1780270000	8.7922840000
C50	-0.4939560000	0.8838600000	6.9527640000
H50	-1.1373330000	0.3716900000	6.2429020000
C34A	7.2342280000	1.9016390000	8.2886290000
C42	2.4828540000	4.4183920000	6.8924810000
C35A	6.0680780000	-0.1663300000	7.0738940000
C38	3.5727730000	-1.3080030000	6.7336050000
H38	2.5903100000	-1.7539830000	6.6099320000
C55	-0.3285520000	2.7495760000	5.2798490000
H55	0.1934850000	3.7086490000	5.1846270000
C49	-0.1692910000	0.2688150000	8.1523820000
H49	-0.5657220000	-0.7166900000	8.3821730000
C48	0.6730120000	0.9064280000	9.0561750000
H48	0.9361730000	0.4094200000	9.9850740000
C52	2.0734760000	2.8622810000	9.8106550000
H52	2.5959170000	3.6789770000	9.3029830000
C31	5.7076750000	3.6658230000	8.9021920000
H31	4.7435220000	4.1512930000	8.7788190000
C3	5.9704500000	-1.5388200000	6.8822630000
H3	6.8756890000	-2.1387530000	6.8702300000
C37	4.7163340000	-2.1142520000	6.7110690000
H37	4.6290550000	-3.1864210000	6.5658700000
C58	-0.9253200000	5.0639190000	8.2514890000
H58a	-1.5789650000	5.1881620000	7.3825410000
H58b	-1.1082830000	4.0835050000	8.6963350000
H58c	-1.1909300000	5.8352050000	8.9777680000
C59	0.6786330000	7.7718770000	8.0473550000
H59a	1.4945820000	8.4974230000	8.0791060000
H59b	-0.0253970000	8.0756650000	7.2653050000
H59c	0.1573880000	7.7984390000	9.0094700000
C34	8.1650050000	2.3635740000	9.2073490000
H34	9.1184790000	1.8512110000	9.2980310000

C56	0.1937910000	1.8066620000	4.1927670000
H56a	-0.2357990000	0.8043990000	4.2912800000
H56b	-0.0667670000	2.1855970000	3.2041630000
H56c	1.2826560000	1.7114390000	4.2485220000
C32	6.6312260000	4.1216270000	9.8298860000
H32	6.3909150000	4.9889710000	10.4374130000
C54	1.2375170000	3.4704070000	10.9419360000
H54a	0.6784480000	2.6889740000	11.4692950000
H54b	1.8857820000	3.9732730000	11.6679350000
H54c	0.5189250000	4.2042230000	10.5648300000
C33	7.8595420000	3.4726450000	9.9924210000
H33	8.5775430000	3.8316990000	10.7228490000
C57	-1.8237750000	3.0145720000	5.0939460000
H57a	-1.9916030000	3.4973220000	4.1259650000
H57b	-2.3997930000	2.0819650000	5.1139330000
H57c	-2.2177620000	3.6747620000	5.8709740000
C53	3.1387600000	1.9159350000	10.3682300000
H53a	3.8554820000	2.4749600000	10.9783890000
H53b	2.7003110000	1.1406860000	11.0057390000
H53c	3.6886170000	1.4232660000	9.5628710000
H134	9.0906040000	5.5451830000	5.3873260000

Monomer T_1 geometry**:**

atom	x	y	z
Cu1	-2.1754075769	19.0575535012	4.4690232872
C1	-4.7086578038	20.3108624346	3.4586818854
H1	-4.2604283511	20.3430199300	4.4499533406
C2	-5.9601831384	20.8701101124	3.2309089330
H2	-6.5056046566	21.3170054877	4.0617769016
C3	-6.5163991907	20.8838243968	1.9439729030
H3	-7.4924380574	21.3406492339	1.7645464081
C4	-5.8156585013	20.3012149595	0.8790235674
H4	-6.2344093059	20.2835902548	-0.1316446397
C4A	-4.5681010450	19.7281733941	1.1101482283
S5	-3.8207969077	18.8173410784	-0.2007565049
O1	-4.0315301853	19.5095481594	-1.4841341590
O2	-4.2447524603	17.4100160310	-0.0823311830
C5A	-2.1299715787	18.9297876132	0.2819682735
C6	-1.1603194960	18.7714605555	-0.7063875094
H6	-1.4685756556	18.7072799674	-1.7539285131
C7	0.1894994933	18.6923806166	-0.3398743278
H7	0.9538512224	18.5740628231	-1.1109095996
C8	0.5468232535	18.7645730704	1.0120112311
H8	1.5908487281	18.7016679556	1.3090922490
C9	-0.4186584242	18.9368659212	1.9954314513
H9	-0.1201901200	19.0326569865	3.0356595531
C9A	-1.7937293833	19.0388435007	1.6620486918
N10	-2.6846281527	19.2978128228	2.6833333333
C10A	-3.9557101138	19.7371388925	2.3983150616
S11	-2.4445171425	19.0002826656	7.7919293043
C12	-1.5582205844	19.0460179909	6.2912845667
N13	-0.2068522767	19.1415471560	6.6372398403
C14	0.1020508967	19.2123303528	7.9792929245
C15	-0.9897340380	19.1534989492	8.7710042203
C16	0.7811427495	19.1934677050	5.6182239920
C17	1.3113880131	17.9936920852	5.1234916981
C18	2.3285423143	18.0654404197	4.1692980896
H18	2.7676227447	17.1502051943	3.7856718526
C19	2.7879027751	19.2929997701	3.7090983665
H19	3.5924003586	19.3329682569	2.9801308317
C20	2.2081087787	20.4689210575	4.1656435724
H20	2.5497829967	21.4216585016	3.7746147161
C21	1.1893744040	20.4402750597	5.1199371406
C22	0.7949555137	16.6449860801	5.5860567657
H22	0.0472659600	16.8209898269	6.3544734121

C23	0.1006459622	15.9229173183	4.4257463536
H23A	0.7962941745	15.7329102075	3.6006775684
H23B	-0.7297406751	16.5226971490	4.0391177773
H23C	-0.3017697704	14.9612257881	4.7539006410
C24	1.9112299867	15.7807867182	6.1799984475
H24A	2.4033798644	16.2827971652	7.0126148015
H24B	2.6734540307	15.5448511512	5.4333004173
H24C	1.5051822913	14.8360944375	6.5463559717
C25	0.5188083858	21.7291873582	5.5547922742
H25	-0.1601329241	21.4935256142	6.3715374311
C26	-0.3206086375	22.2866108995	4.3984999239
H26A	-1.0695843109	21.5532926229	4.0758617941
H26B	0.3098053353	22.5311922708	3.5350506284
H26C	-0.8445217625	23.1976687777	4.7014189813
C27	1.5259183872	22.7748955317	6.0452455885
H27A	2.1944795577	23.0958124115	5.2419993132
H27B	2.1414350528	22.3896457816	6.8582495317
H27C	1.0026442579	23.6619419851	6.4074074281
C28	1.5290461493	19.3395975458	8.3899702063
H28A	1.9719217647	20.2537847164	7.9959164825
H28B	2.1228544856	18.5089358194	8.0110394186
H28C	1.6183770944	19.3577942883	9.4693726768
C29	-1.0740792678	19.1885838656	10.2546325425
H29A	-1.5401580737	18.2873615898	10.6495498259
H29B	-1.6661108870	20.0346183308	10.5993298412
H29C	-0.0873146653	19.2731503459	10.6996009876

Dimer T_1 geometry**:**

atom	x	y	z
Cu3	2.7604400000	4.1704540000	4.2357940000
S71	3.7345740000	1.1308340000	3.8640400000
S65	-0.6379650000	7.4103700000	4.1366810000
N73	5.4037470000	3.0354300000	3.5868640000
N70	1.6869450000	5.5759670000	3.5280390000
O91	-0.9138520000	6.7518890000	5.4299430000
O92	-1.5080990000	8.5334940000	3.7597770000
C65A	1.0469750000	7.8887810000	4.0938950000
C69A	2.0016300000	6.8703120000	3.8814280000
C75	5.3503540000	0.7594970000	3.2964810000
C81	5.3779780000	4.7698240000	1.8611140000
C72	4.1273370000	2.8202670000	4.1342480000
C77	6.6092900000	5.1393670000	3.9494830000
C76	5.7960710000	4.3377610000	3.1364680000
C74	6.0828360000	1.8913350000	3.1858620000
C64A	-0.6194400000	6.1799460000	2.8938470000
C78	7.0378980000	6.3737350000	3.4494740000
H78	7.6772580000	7.0026760000	4.0615030000
C70A	0.5154060000	5.3396870000	2.8395300000
C66	1.4068930000	9.2078610000	4.3721300000
H66	0.6241210000	9.9508720000	4.5052700000
C69	3.3578050000	7.2410610000	3.9995310000
H69	4.1180460000	6.4862710000	3.8147790000
C82	7.0009720000	4.7358880000	5.3530660000
H82	6.5530150000	3.7585200000	5.5611770000
C64	-1.7340180000	5.9947770000	2.0762030000
H64	-2.5630140000	6.6944300000	2.1500990000
C67	2.7491570000	9.5395500000	4.4789210000
H67	3.0438920000	10.5626880000	4.6939680000
C68	3.7180680000	8.5426850000	4.2965660000
H68	4.7741000000	8.7909650000	4.3647150000
C80	5.8392950000	6.0016150000	1.4012050000
H80	5.5475480000	6.3455540000	0.4154610000
C61	0.4406540000	4.2482800000	1.9498600000
H61	1.3009350000	3.5895880000	1.8842350000
C85	4.4810190000	3.9210140000	0.9786110000

H85	3.9884240000	3.1853680000	1.6191290000
C62	-0.6721040000	4.0450480000	1.1512900000
H62	-0.6835530000	3.2039140000	0.4634050000
C88	7.4988620000	2.0022390000	2.7323710000
H88a	7.7939160000	1.1157270000	2.1746580000
H88b	7.6411020000	2.8750330000	2.0933890000
H88c	8.1608850000	2.0955570000	3.5952470000
C79	6.6692390000	6.7957770000	2.1828430000
H79	7.0210830000	7.7498470000	1.8035020000
C63	-1.7633510000	4.9235110000	1.1957620000
H63	-2.6225710000	4.7704200000	0.5490980000
C89	5.7464190000	-0.6482520000	3.0258600000
H89a	6.7251100000	-0.6886710000	2.5491710000
H89b	5.8011530000	-1.2296550000	3.9514100000
H89c	5.0287560000	-1.1436150000	2.3673550000
C84	8.5145850000	4.6010140000	5.5179710000
H84b	8.7491670000	4.2536600000	6.5291820000
H84c	8.9290850000	3.8793450000	4.8126470000
C83	6.4358030000	5.7532300000	6.3482530000
H83a	6.7064730000	5.4869670000	7.3720750000
H83b	6.8150290000	6.7608930000	6.1504410000
H83c	5.3437720000	5.7935590000	6.2826330000
C86	3.3902500000	4.7619920000	0.3077780000
H86a	2.8438160000	5.3585970000	1.0435060000
H86b	3.8043930000	5.4411830000	-0.4437180000
H86c	2.6746570000	4.1120660000	-0.2045140000
C87	5.3017590000	3.1695940000	-0.0769160000
H87a	5.8355310000	3.8758110000	-0.7207280000
H87b	6.0350250000	2.5033360000	0.3783150000
H87c	4.6453200000	2.5660830000	-0.7094740000
Cu2	3.8613570000	3.1859270000	6.3308920000
S35	7.7385610000	0.6784710000	7.1606570000
S41	2.6953560000	6.0478250000	7.1197730000
O3	8.0187500000	1.2467520000	5.8344620000
N43	1.1998200000	4.0729150000	7.2639810000
O4	8.7588520000	-0.1913600000	7.7608060000
N40	5.0408700000	2.0320940000	7.3269290000
C46	0.7990760000	2.6946140000	7.4395420000
C39A	5.0276630000	0.6674670000	7.1171260000
C51	0.0238740000	2.0504280000	6.4654720000
C44	0.4339990000	5.1245750000	7.7784510000
C36	6.0378270000	2.5646670000	8.1125590000
C45	1.1173270000	6.2996580000	7.7835620000
C39	3.7947450000	0.0100600000	6.9439310000
H39	2.8873090000	0.6074640000	6.9535340000
C47	1.1834710000	2.0669630000	8.6425500000
C50	-0.4135420000	0.7511690000	6.7494790000
H50	-1.0347390000	0.2317680000	6.0259050000
C34A	7.3217010000	1.9873360000	8.2556050000
C42	2.4451070000	4.3782020000	6.8396750000
C35A	6.1867270000	-0.1380610000	7.1163770000
C38	3.7343890000	-1.3658460000	6.8099020000
H38	2.7642170000	-1.8422800000	6.6929080000
C55	-0.3582300000	2.6803690000	5.1421980000
H55	0.1874440000	3.6261890000	5.0379390000
C49	-0.0793020000	0.1198600000	7.9378980000
H49	-0.4384270000	-0.8870290000	8.1372320000
C48	0.7238050000	0.7686100000	8.8692110000
H48	0.9984480000	0.2582300000	9.7885560000
C52	2.0280170000	2.7633690000	9.6928740000
H52	2.5470670000	3.5985060000	9.2080510000
C31	5.7660950000	3.7123620000	8.8886400000
H31	4.7826190000	4.1702910000	8.7927510000
C3	6.1312220000	-1.5230010000	6.9827550000
H3	7.0571390000	-2.0927450000	6.9968670000
C37	4.8980790000	-2.1432140000	6.8311020000
H37	4.8409570000	-3.2234860000	6.7291720000

C58	-0.9903230000	4.9393250000	8.1687050000
H58a	-1.6335510000	5.2335130000	7.3304940000
H58b	-1.2081560000	3.9019020000	8.4401090000
H58c	-1.2347370000	5.5830340000	9.0197010000
C59	0.6134910000	7.6501770000	8.1591280000
H59a	1.4332250000	8.3432340000	8.3626510000
H59b	0.0104520000	8.0506250000	7.3367920000
H59c	-0.0184130000	7.5958010000	9.0513950000
C34	8.2643130000	2.4828850000	9.1515040000
H34	9.2299130000	1.9866140000	9.2294460000
C56	0.0352710000	1.7593310000	3.9852890000
H56a	-0.4119800000	0.7671340000	4.0932850000
H56b	-0.3163890000	2.1764620000	3.0419340000
H56c	1.1163280000	1.6344090000	3.9207680000
C32	6.7058060000	4.2153700000	9.7762330000
H32	6.4579910000	5.0899740000	10.3748880000
C54	1.1430200000	3.3331340000	10.8053060000
H54a	0.5949100000	2.5279470000	11.3096880000
H54b	1.7567970000	3.8477830000	11.5538120000
H54c	0.4111520000	4.0481330000	10.4164140000
C33	7.9569760000	3.6001450000	9.9216210000
H33	8.6850280000	3.9909300000	10.6288050000
C57	-1.8546800000	3.0019860000	5.0780540000
H57a	-2.0768270000	3.5289260000	4.1439590000
H57b	-2.4530660000	2.0836460000	5.1030040000
H57c	-2.1747850000	3.6367300000	5.9080820000
C53	3.1053320000	1.8451910000	10.2719400000
H53a	3.7857470000	2.4237380000	10.9073530000
H53b	2.6765850000	1.0483410000	10.8909660000
H53c	3.6971830000	1.3830390000	9.4757810000
H134	9.0195240000	5.5606540000	5.3641540000