Supporting Information

Figure 1S, PXRD stability data for dispersion system of CLF with different polymers stressed at 40°C 75%RH conditions (A: HPMCP; B: HPMC and C: PVPVA). Percentage in the legend indicates CLF loading

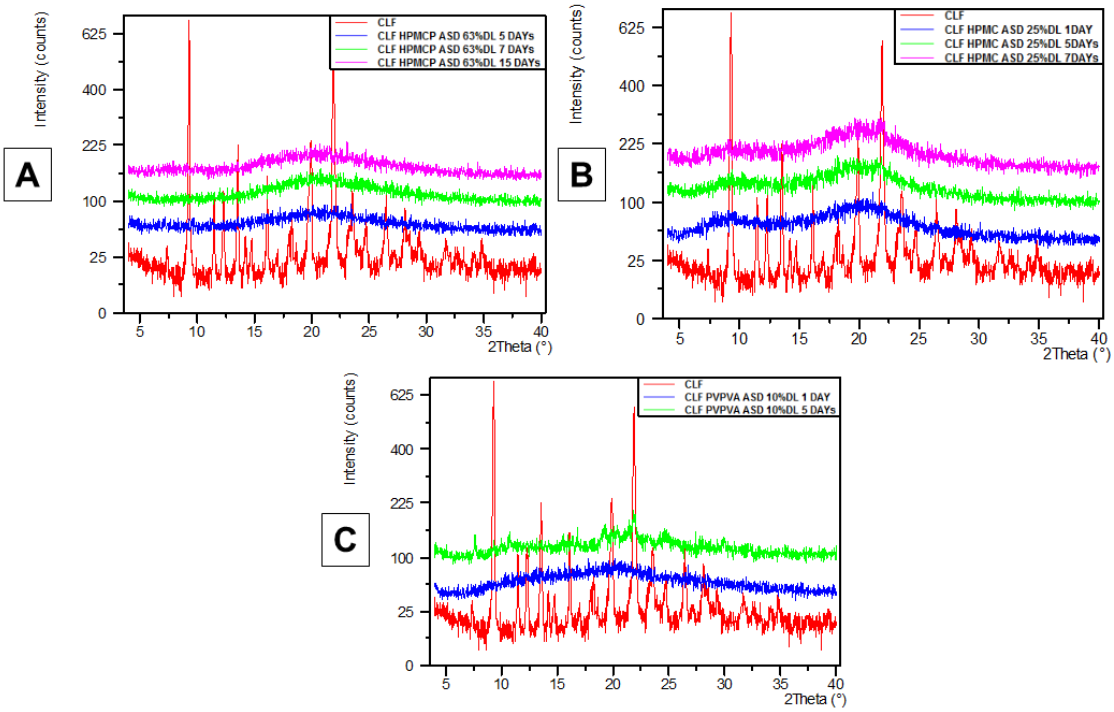
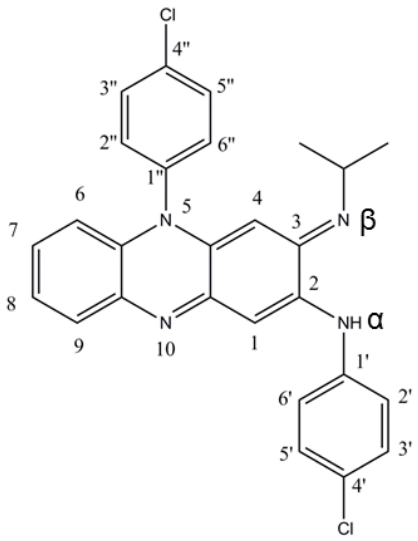


Figure 2S, Proton NMR assignment for CLF



Proton	Chemical shifts	Proton	Chemical shifts
1	6.72	**3'/5'**	7.45 (d, 8.6 Hz)
4	5.20	**2''/6''**	7.59 (d, 8.1 Hz)
6	6.45 (d, 7.5Hz)	**3''/5''**	7.86 (d, 8.2 Hz)
7/8	7.21 (m)	**(ipr-C)H**	3.37 (m, 6.1 Hz)
9	7.63 (d, 7.2Hz)	**Methyl-H**	1.05 (d, 6.1 Hz)
2'/6'	7.42 (d, 8.6 Hz)	**H_α**	8.62 (b)

Figure 3S, 1D ^{1}H NMR for CLF in DMSO, 298K

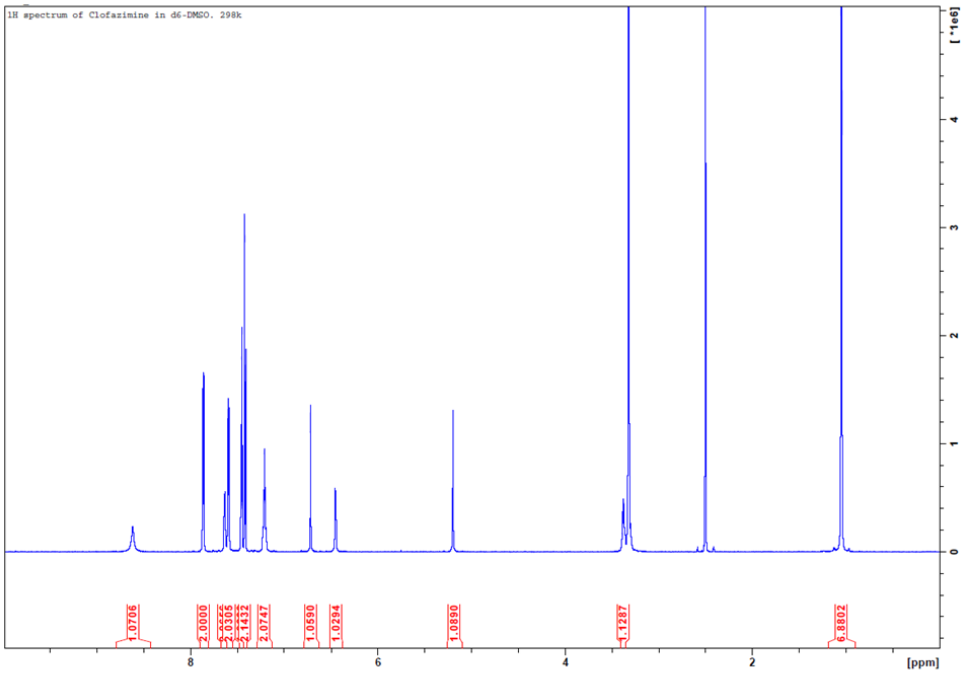


Figure 4S, 2D COSY for CLF in DMSO, 298K

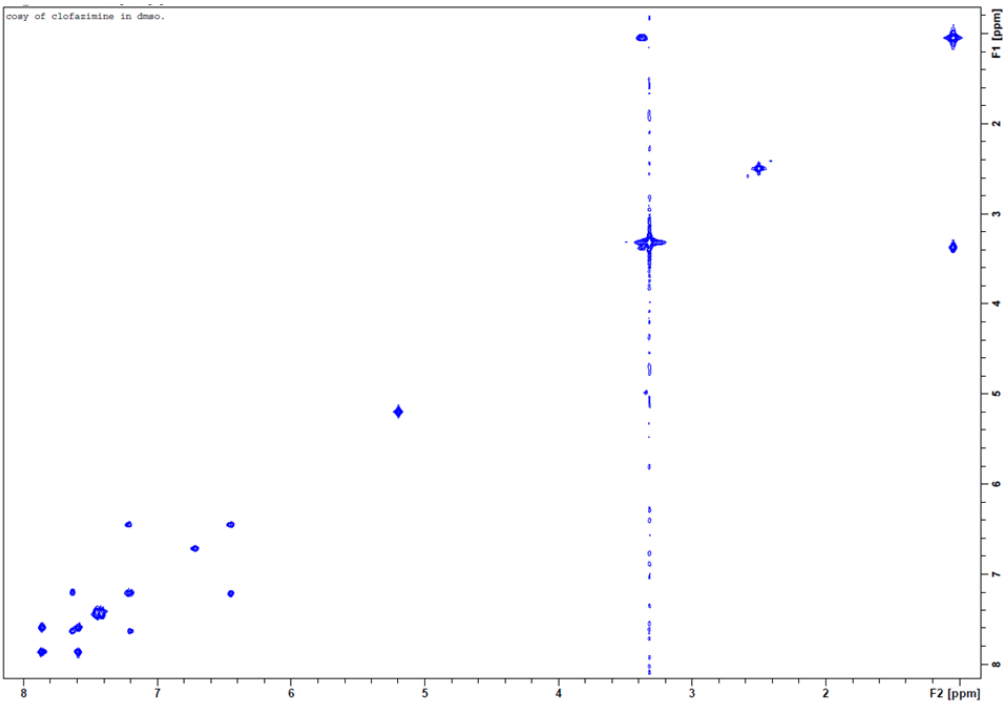


Figure 5S, 2D HSQC of CLF in DMSO, 298K

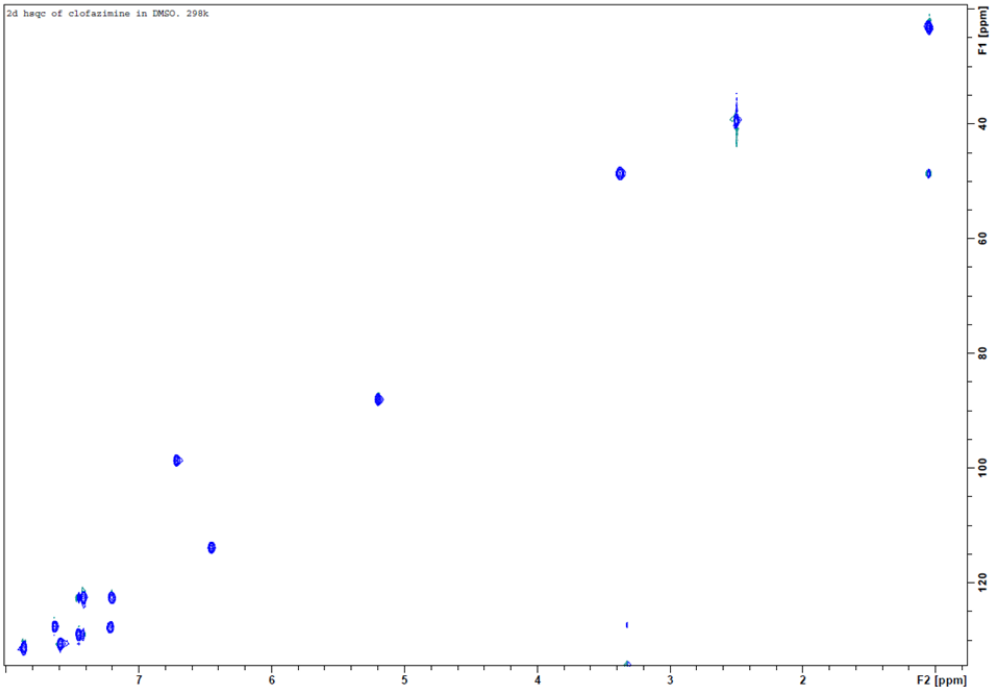


Figure 6S, 2D NOESY of CLF in DMSO, 298K

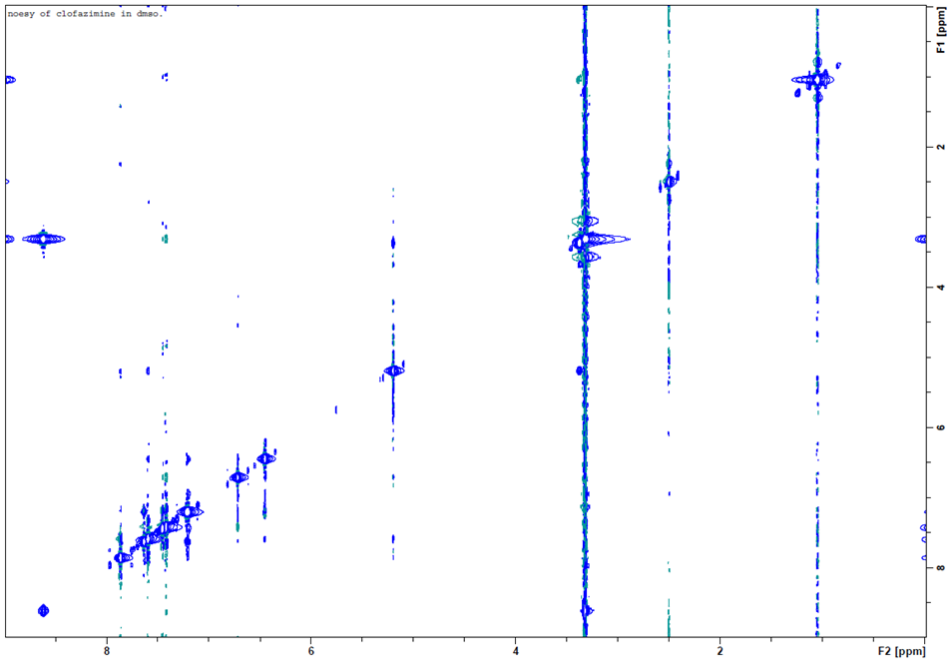


Figure 7S, 1D ^{1}H NMR of CLF with acetic acid and HPMCP in $CDCl_3$, 298K

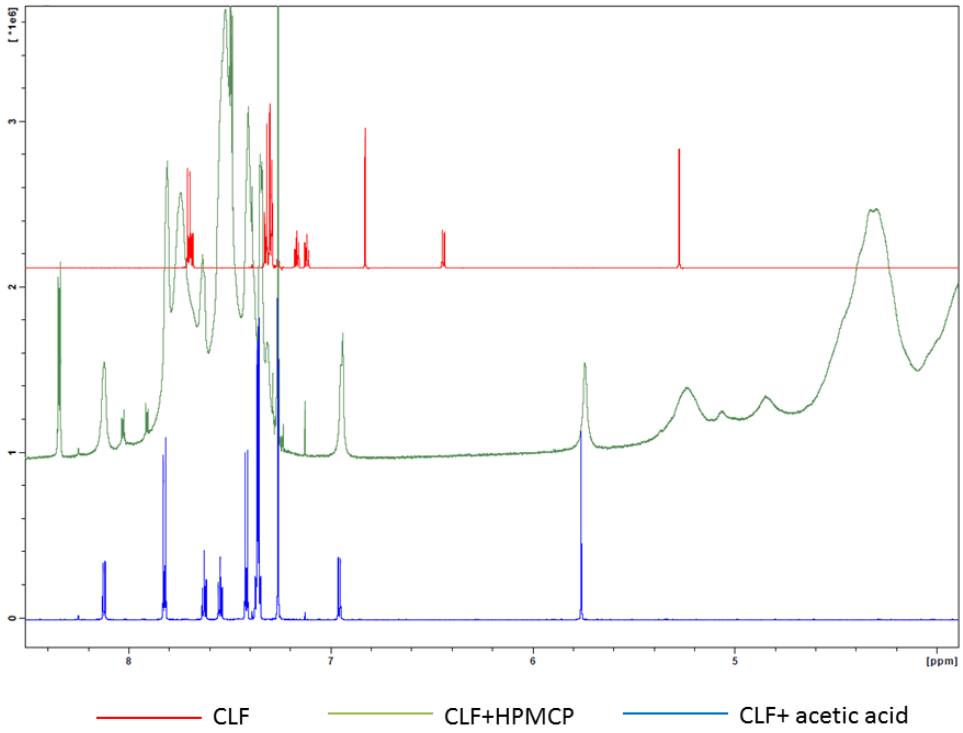


Figure 8S, 1D ^{1}H NMR of CLF with Phthalic acid and HPMCP in $CDCl_3$, 298K

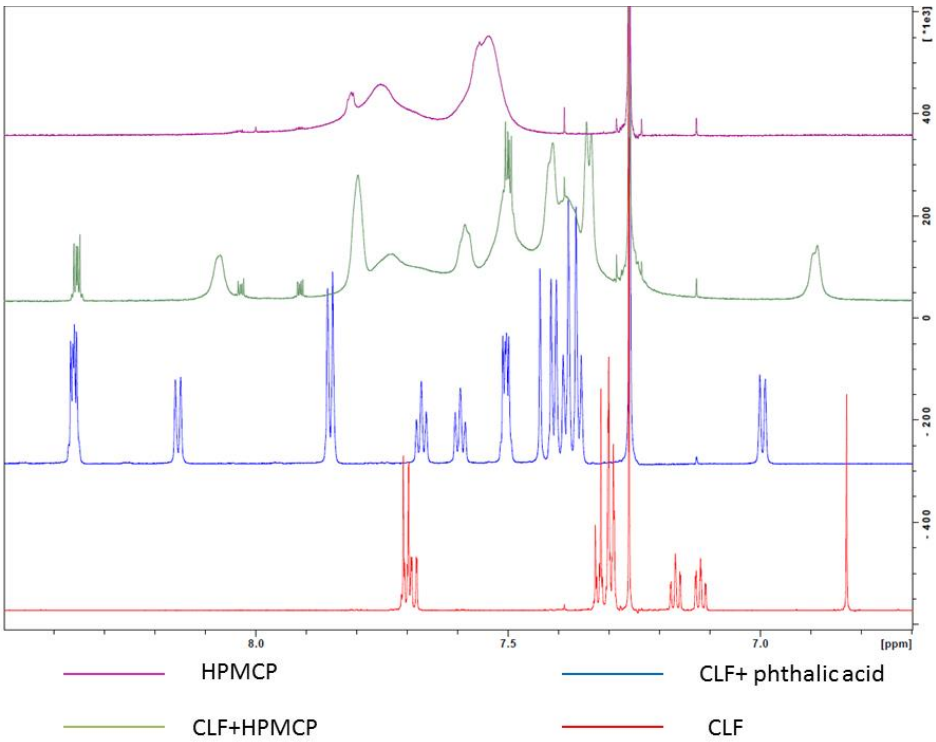


Figure 9S 2D DOSY of CLF with different polymers

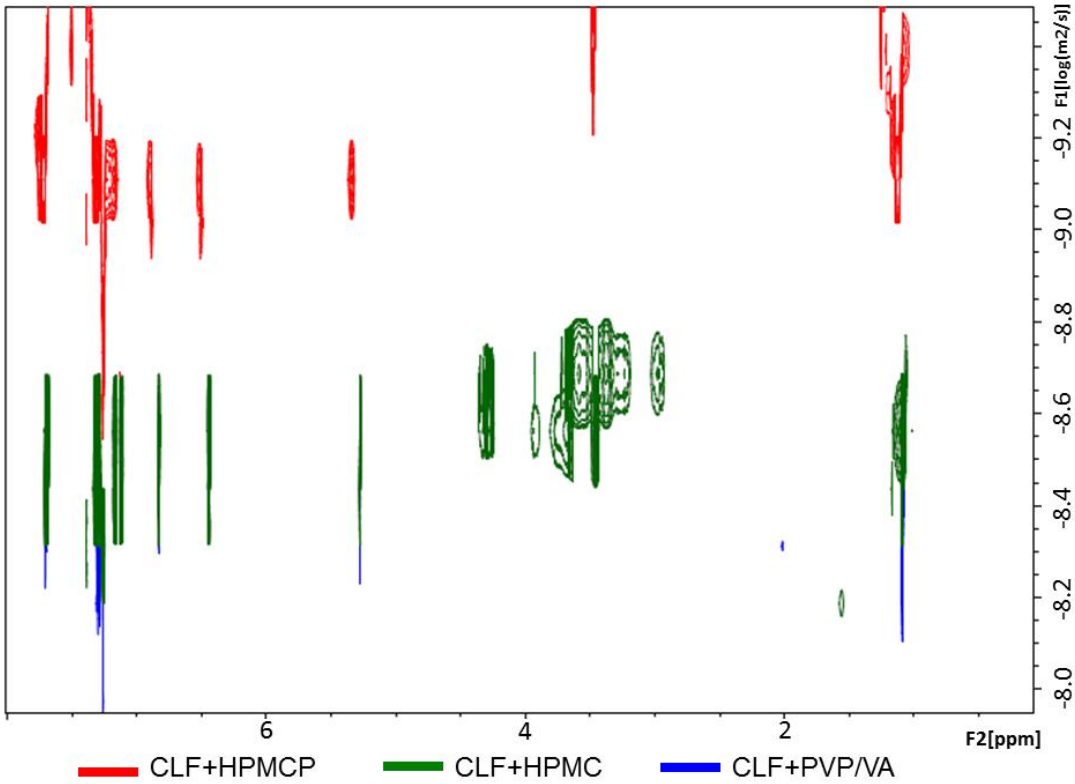


Figure 10S Simulated NMR spectrum for CLF and complex I and Complex II

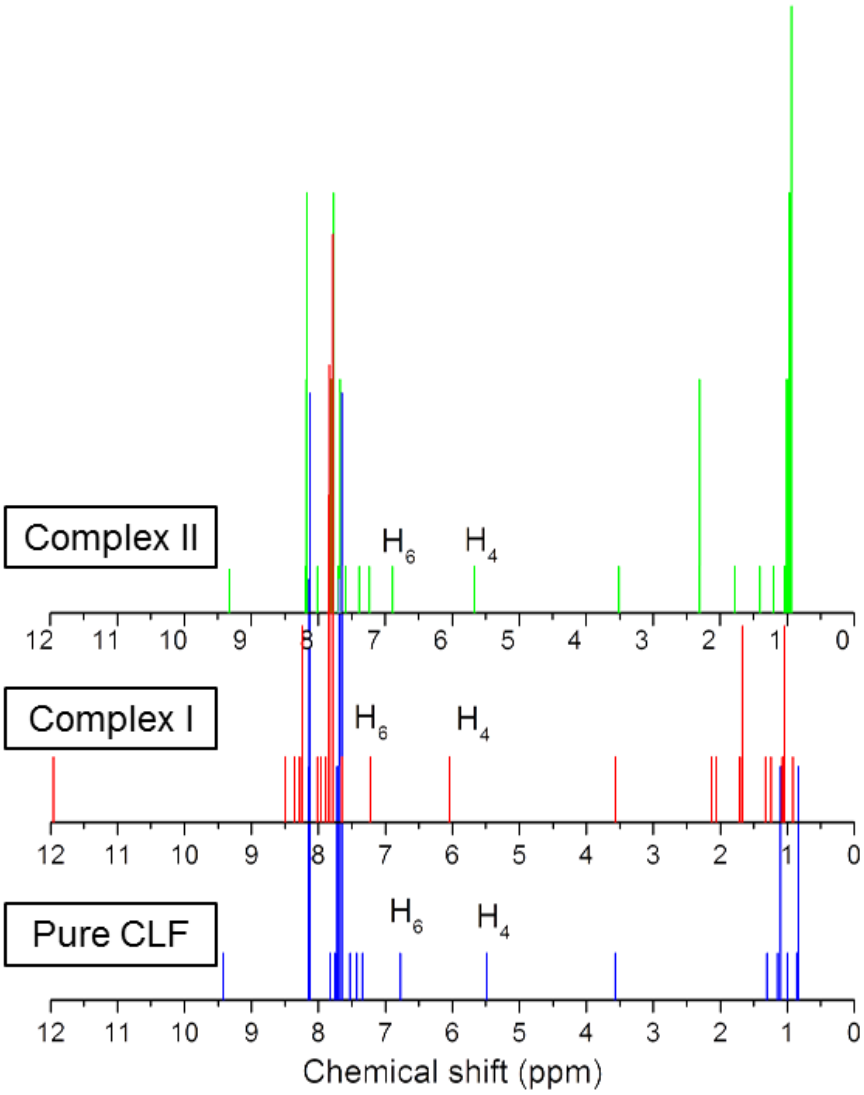


Figure 11S Simulated UV/Vis spectra for CLF and complex I and Complex II

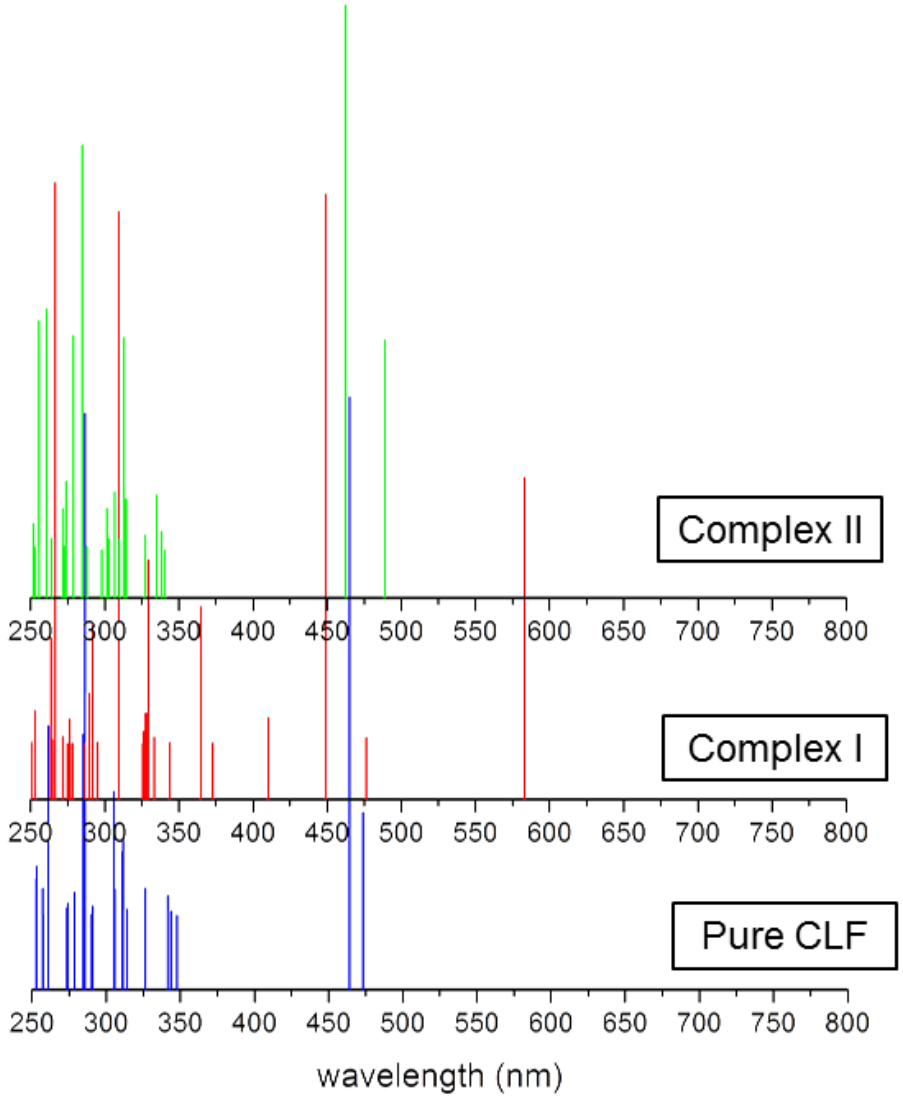


Table 1S: Optimized Cartesian coordinates, natural population analysis, and isotropic magnetic shielding tensors of **pure CLF**, calculated at the level of B3PW91 with 6-311++G (2d, 2p) basis sets.

Atomic Type	Coordinates(Angstroms)			Natural Charge(e)	Isotropic magnetic shielding tensor(ppm)
	X	Y	Z		
Cl	8.57929	0.70438	0.20117	-0.00125	708.9403
Cl	-6.96678	-2.33405	0.30340	0.01827	690.4833
N	0.08787	2.77828	-0.16436	-0.45669	-60.7806
N	-2.17413	1.14860	-0.02273	-0.38952	103.7129
C	-0.92483	0.56464	-0.04051	0.31490	47.4209
C	1.52816	0.91705	-0.11050	-0.27753	84.1422
N	2.93334	-1.07215	-0.07029	-0.53210	136.1622
C	0.21950	1.47720	-0.10523	0.15735	31.1400
C	-2.33307	2.52604	-0.08258	0.28526	51.4044
C	5.25061	-1.37969	-0.56999	-0.14170	60.0886
N	0.88340	-2.62405	-0.02109	-0.54172	-52.8164
C	0.57893	-1.36804	-0.02587	0.23097	30.7503
C	1.73853	-0.42938	-0.05779	0.18777	40.4934
C	4.23871	-0.59566	-0.00222	0.12600	43.0956
C	-3.83940	-0.05297	1.29676	-0.14130	49.6256
C	-1.16773	3.32165	-0.15777	0.06111	44.9712
C	-3.33343	0.30745	0.05487	0.09306	45.0816
C	-0.73263	-0.78672	-0.01272	-0.40698	94.4555
C	-4.96075	-0.86602	1.37776	-0.23558	49.9542
C	5.92598	0.98447	0.70899	-0.22138	52.6299
C	4.59800	0.58765	0.64988	-0.22382	63.8541
C	-1.30440	4.71687	-0.22263	-0.18716	53.0886
C	-2.54884	5.31069	-0.21148	-0.22846	59.6242
C	6.90764	0.19823	0.12901	-0.07236	49.7895
C	-3.59224	3.13477	-0.06974	-0.29401	68.8093
C	-5.55877	-1.31023	0.20735	-0.04361	38.7639
C	-0.13835	-3.65427	-0.00754	-0.07321	133.2955
C	6.57683	-0.99110	-0.50432	-0.24630	52.2951
C	-3.69331	4.51268	-0.13382	-0.18715	55.1051
C	-3.93856	-0.14334	-1.11078	-0.19026	49.5801
C	-5.06015	-0.95700	-1.03814	-0.21844	50.0098
C	-0.52460	-4.02093	-1.44221	-0.57691	164.3251
C	0.39540	-4.86815	0.74601	-0.54806	161.0774
H	1.28777	-5.26013	0.25364	0.19533	30.3906

H	-0.35451	-5.66062	0.78141	0.19683	30.5956
H	0.66214	-4.60308	1.77003	0.20628	30.5534
H	-1.58611	-1.44538	0.01012	0.22822	26.2069
H	2.34094	1.62215	-0.18724	0.22782	24.2707
H	-0.39768	5.30516	-0.28056	0.22595	23.5507
H	-4.48607	2.53033	-0.01053	0.22748	24.9227
H	7.34686	-1.60505	-0.95025	0.22989	24.0039
H	-1.04025	-3.30939	0.51360	0.17123	28.1268
H	6.19296	1.89939	1.21954	0.23000	23.8707
H	-3.53510	0.14234	-2.07321	0.23669	23.9729
H	-5.36488	-1.15025	2.33901	0.23575	23.5576
H	3.85293	1.18866	1.14832	0.22732	23.5758
H	-2.63930	6.38780	-0.26157	0.21693	24.0465
H	-3.35890	0.30274	2.19856	0.22912	23.9343
H	-4.67402	4.97063	-0.12331	0.21620	24.1657
H	4.98938	-2.30260	-1.07268	0.21225	24.3498
H	-5.54039	-1.31191	-1.93897	0.23652	23.5464
H	2.78999	-2.07853	-0.14492	0.42531	22.2766
H	-0.92438	-3.15754	-1.97566	0.20332	30.8624
H	-1.28074	-4.80821	-1.44536	0.20497	30.6935
H	0.34957	-4.38237	-1.98743	0.20567	30.8371

Table 2S: Calculated energies of the **pure CLF** under temperature of 298.15 Kelvin and pressure of 1.00 atm

Zero-point correction	0.429324 (Hartree/Particle)
Thermal correction to Energy	0.457493
Thermal correction to Enthalpy	0.458437
Thermal correction to Gibbs Free Energy	0.366616
E(RB3PW91)	-2181.35315634
Sum of electronic and zero-point Energies	-2180.923832
Sum of electronic and thermal Energies	-2180.895663
Sum of electronic and thermal Enthalpies	-2180.894719
Sum of electronic and thermal Free Energies	-2180.986540

Table 3S: Optimized Cartesian coordinates, natural population analysis, and isotropic magnetic shielding tensors of the **complex *I***, calculated at the level of B3PW91 with 6-311++G (2d, 2p) basis sets.

Atomic Type	Coordinates(Angstroms)			Natural Charge(e)	Isotropic magnetic shielding tensor(ppm)
	X	Y	Z		
Cl	-7.68268	2.64768	-0.45174	-0.00075	705.2324
Cl	7.17515	-2.48455	-0.40050	0.02692	684.9506
N	0.51282	3.09341	0.30079	-0.39130	-81.9411
N	2.63927	1.30794	0.07801	-0.34344	77.7577
C	1.36211	0.83669	0.00573	0.35090	48.3249
C	-1.04231	1.33572	0.05530	-0.29844	81.8958
N	-2.63278	-0.44875	-0.21798	-0.60517	120.4140
C	0.28504	1.80723	0.12344	0.13202	35.6761
C	2.90156	2.65391	0.26316	0.28644	53.1113
C	-4.88142	-0.04005	0.52789	-0.20570	54.4976
N	-0.53641	-2.25168	-0.38380	-0.50466	92.1246
C	-0.25735	-0.96541	-0.21961	0.27256	30.0124
C	-1.36257	0.01151	-0.12317	0.21630	39.3163
C	-3.79630	0.34009	-0.26384	0.14992	41.9198
C	4.26926	0.10794	-1.28879	-0.19059	51.0405
C	1.79247	3.53023	0.37386	0.06702	42.5922
C	3.73947	0.38496	-0.03665	0.09557	45.7090
C	1.06770	-0.50154	-0.15360	-0.39590	92.8903
C	5.33132	-0.77703	-1.40377	-0.21410	49.9191
C	-5.11964	2.13798	-1.18354	-0.22338	53.6051
C	-3.93024	1.42845	-1.12795	-0.21341	58.8601
C	2.03534	4.90627	0.56499	-0.18075	51.1835
C	3.31770	5.38915	0.64194	-0.21137	55.8608
C	-6.18354	1.75042	-0.38271	-0.05897	46.5212
C	4.20657	3.15780	0.34257	-0.28432	66.0951
C	5.84363	-1.37176	-0.25938	-0.04011	37.4957
C	0.45578	-3.32092	-0.51204	-0.05234	135.8688
C	-6.07604	0.66094	0.46761	-0.21900	51.3938
C	4.40499	4.50843	0.52971	-0.17345	52.3668
C	4.25530	-0.21192	1.10505	-0.19075	51.7584
C	5.31660	-1.09852	0.99496	-0.21349	49.3221
C	0.90767	-3.81564	0.86104	-0.58829	166.1825
C	-0.13119	-4.44234	-1.35932	-0.58488	165.5475
H	-1.01868	-4.86459	-0.88703	0.21843	29.9838
H	0.60687	-5.23563	-1.47809	0.21370	30.6200

H	-0.41083	-4.08107	-2.34916	0.21350	30.3694
H	1.87454	-1.21230	-0.21129	0.23982	25.6546
H	-1.82017	2.07560	0.16438	0.24890	23.8469
H	1.17551	5.55772	0.64793	0.23204	23.2013
H	5.05260	2.49144	0.25865	0.23294	24.4683
H	-6.91316	0.36559	1.08478	0.23081	23.8628
H	1.31343	-2.91120	-1.04810	0.19810	28.1313
H	-5.22168	2.97850	-1.85578	0.22979	23.9119
H	3.83194	0.01344	2.07483	0.24060	24.0498
H	5.75562	-1.00064	-2.37218	0.23923	23.4544
H	-3.11358	1.71269	-1.77727	0.22825	23.7395
H	-1.51532	-2.58537	-0.31011	0.44172	19.7410
H	3.49355	6.44646	0.78904	0.22192	23.6783
H	3.85665	0.58121	-2.16976	0.23951	23.8431
H	5.41579	4.88992	0.59048	0.22106	23.7955
H	-4.77370	-0.88898	1.19281	0.24937	23.3384
H	5.72905	-1.57063	1.87516	0.23968	23.4162
H	-2.82566	-1.46574	-0.10169	0.44616	17.9317
H	1.31447	-3.00405	1.46488	0.21122	30.4587
H	1.67948	-4.57799	0.74726	0.21224	30.7786
H	0.06889	-4.25416	1.40305	0.21621	30.6544
O	-3.12998	-3.13781	-0.17097	-0.84572	12.6727
O	-3.67180	-2.93390	1.99006	-0.75581	-53.5009
C	-3.69265	-3.54152	0.90946	0.79687	2.6289
C	-4.44041	-4.86116	0.79853	-0.69004	160.8492
H	-3.75885	-5.64702	0.46829	0.21453	29.6330
H	-4.88711	-5.14224	1.74960	0.20817	30.0257
H	-5.22071	-4.77634	0.04027	0.21820	29.5726

Table 4S: Calculated energies of **complex I** under temperature of 298.15 Kelvin and pressure of 1.00 atm

Zero-point correction	0.493224 (Hartree/Particle)
Thermal correction to Energy	0.527141
Thermal correction to Enthalpy	0.528085
Thermal correction to Gibbs Free Energy	0.423258
E(RB3PW91)	-2410.44999132
Sum of electronic and zero-point Energies	-2409.956767
Sum of electronic and thermal Energies	-2409.922850
Sum of electronic and thermal Enthalpies	-2409.921906
Sum of electronic and thermal Free Energies	-2410.026733

Table 5S: Optimized Cartesian coordinates, natural population analysis, and isotropic magnetic shielding tensors of the **complex *II***, calculated at the level of B3PW91 with 6-311++G (2d, 2p) basis sets.

Atomic Type	Coordinates(Angstroms)			Natural Charge(e)	Isotropic magnetic shielding tensor(ppm)
	X	Y	Z		
Cl	-7.62533	-2.75090	0.73472	0.00098	706.8703
Cl	7.15649	2.40229	0.80066	0.02011	689.2134
N	0.48551	-3.05212	-0.56459	-0.45022	-63.1730
N	2.61988	-1.30663	-0.12907	-0.37890	97.3801
C	1.33530	-0.81785	-0.09539	0.32393	47.5082
C	-1.07402	-1.31372	-0.24807	-0.31041	83.7448
N	-2.65550	0.44474	0.17418	-0.64242	138.6902
C	0.26094	-1.78336	-0.31906	0.14526	32.5930
C	2.87903	-2.64530	-0.38608	0.28257	51.6839
C	-4.96503	0.01516	-0.40207	-0.19617	54.6151
N	-0.63826	2.25853	0.18023	-0.55326	-21.8689
C	-0.29773	1.00316	0.09816	0.19885	25.9122
C	-1.38680	-0.00482	-0.00070	0.34719	35.7815
C	-3.81324	-0.34951	0.29421	0.14634	42.9609
C	4.16476	-0.18059	1.38923	-0.14319	50.1542
C	1.77398	-3.49993	-0.60624	0.06369	44.4889
C	3.71606	-0.40693	0.09505	0.07859	44.7204
C	1.04321	0.50332	0.10699	-0.40931	92.3096
C	5.22649	0.68471	1.61068	-0.23392	50.0142
C	-5.02333	-2.19763	1.27444	-0.22371	53.3444
C	-3.85878	-1.45829	1.14143	-0.20866	56.2635
C	2.01356	-4.85892	-0.87169	-0.18315	52.6240
C	3.29663	-5.35756	-0.91679	-0.22470	58.9171
C	-6.15559	-1.81960	0.56847	-0.05788	46.5206
C	4.17942	-3.15989	-0.43076	-0.29135	67.8840
C	5.82303	1.31357	0.52735	-0.04408	38.5555
C	0.38586	3.27434	0.42886	-0.06536	131.4664
C	-6.13773	-0.71180	-0.26351	-0.22142	52.2908
C	4.38027	-4.50158	-0.69379	-0.18571	54.7453
C	4.31783	0.22812	-0.98302	-0.14709	50.4861
C	5.38032	1.09442	-0.76914	-0.23324	49.8214
C	1.00085	3.78026	-0.87860	-0.59412	166.0610
C	-0.22971	4.41810	1.22974	-0.58205	162.8510
H	-1.01322	4.92035	0.66063	0.20447	30.2959
H	0.53484	5.15648	1.47779	0.20614	30.6565

H	-0.66586	4.04998	2.15882	0.21029	30.4883
H	1.85317	1.20502	0.21699	0.23028	26.0279
H	-1.84824	-2.05561	-0.37381	0.23146	24.4635
H	1.15316	-5.49421	-1.03751	0.22426	23.5290
H	5.02564	-2.51005	-0.26008	0.22802	24.8067
H	-7.02677	-0.42198	-0.80601	0.23035	23.8821
H	1.18545	2.84713	1.04285	0.18177	28.1862
H	-5.05277	-3.05340	1.93442	0.23060	23.9296
H	3.95885	0.04503	-1.98710	0.23026	24.0234
H	5.58601	0.86667	2.61353	0.23639	23.5191
H	-2.98521	-1.73741	1.71406	0.23072	23.6848
H	-1.81525	3.02184	-0.72985	0.49902	17.0173
H	3.46678	-6.40618	-1.12237	0.21782	23.9939
H	3.68694	-0.68004	2.22161	0.22991	23.8960
H	5.39097	-4.88751	-0.72561	0.21708	24.1064
H	-4.94313	0.87896	-1.05121	0.23016	24.3045
H	5.85804	1.59271	-1.60069	0.23644	23.5051
H	-2.79620	1.44815	0.25272	0.44157	22.3667
H	1.44303	2.96524	-1.45270	0.20634	30.7271
H	1.78168	4.51325	-0.66834	0.20898	30.7645
H	0.24291	4.26019	-1.49930	0.21016	30.6897
O	-2.37996	3.60819	-1.34706	-0.73162	81.7044
O	-3.98548	3.13516	0.12970	-0.67013	-73.1908
C	-3.59931	3.74262	-0.85437	0.81942	3.1301
C	-4.44833	4.70749	-1.62740	-0.68713	164.1599
H	-4.46325	4.42834	-2.68122	0.23493	29.3933
H	-5.45840	4.72086	-1.22948	0.22666	29.9144
H	-4.01436	5.70635	-1.56344	0.23693	29.3837

Table 6S: Calculated energies of the **complex *II*** under temperature of 298.15 Kelvin and pressure of 1.00 atm

Zero-point correction	0.492050 (Hartree/Particle)
Thermal correction to Energy	0.526187
Thermal correction to Enthalpy	0.527132
Thermal correction to Gibbs Free Energy	0.420792
E(RB3PW91)	-2410.44555476
Sum of electronic and zero-point Energies	-2409.953505
Sum of electronic and thermal Energies	-2409.919367
Sum of electronic and thermal Enthalpies	-2409.918423
Sum of electronic and thermal Free Energies	-2410.024763

Table 7S: Optimized Cartesian coordinates and isotropic magnetic shielding tensors of TMS, calculated at the level of B3PW91 with 6-311++G (2d, 2p) basis sets.

Atomic Type	Coordinates(Angstroms)			Isotropic magnetic shielding tensor(ppm)
	X	Y	Z	
Si	0.000000	0.000000	0.000000	339.1847
C	0.000000	0.000000	1.881823	186.9601
H	0.882586	-0.509561	2.275011	31.6975
H	0.000000	1.019123	2.275011	31.6975
H	-0.882586	-0.509561	2.275011	31.6975
C	0.000000	-1.774199	-0.627274	186.9601
H	-0.882586	-2.314755	-0.277918	31.6975
H	0.000000	-1.805193	-1.719175	31.6975
H	0.882586	-2.314755	-0.277918	31.6975
C	-1.536502	0.887100	-0.627274	186.9601
H	-1.563343	1.921719	-0.277918	31.6975
H	-1.563343	0.902597	-1.719175	31.6975
H	-2.445930	0.393035	-0.277918	31.6975
C	1.536502	0.887100	-0.627274	186.9601
H	2.445930	0.393035	-0.277918	31.6975
H	1.563343	0.902597	-1.719175	31.6975
H	1.563343	1.921719	-0.277918	31.6975

Table 8S: Changes of calculated NMR chemical shifts (ppm) and experimental chemical shifts (ppm) for H_4 and H_6

	Experimental chemical Shifts		**Calculated chemical Shifts**		
	Pure CLF	CLF+HPMCP	Pure CLF	Complex I	Complex II
H_4	5.27	5.76	5.49	6.04	5.67
H_6	6.44	6.94	7.43	7.85	7.23

Table 9S Details of dynamic NMR calculations for H_4 at 5.27 ppm

CLF (mg/ml)	HPMCP (mg/ml)	CLF (M)	HPMCP (M)	k_d (M)	k_{off} (s^{-1})	complex (ion-pair) concentration	frequency difference	calculated line width (Hz)	measured line width (Hz)	Measured chemical shift (ppm)	calculated chemical shift (ppm)
2	0.2	0.0042	0.00045	0.009	12000	0.00014	480	7.5	4.5	5.28	5.29
2	0.5	0.0042	0.00112	0.009	12000	0.00034	480	16.3	10.5	5.3	5.32
2	1.0	0.0042	0.00224	0.009	12000	0.00064	480	26.2	22.1	5.34	5.36
2	2.0	0.0042	0.00447	0.009	12000	0.00114	480	34.7	36.5	5.41	5.43
2	4.0	0.0042	0.00894	0.009	12000	0.00186	480	33.3	30.5	5.52	5.53
2	6.0	0.0042	0.01341	0.009	12000	0.00233	480	26.7	21.5	5.61	5.60
2	10.0	0.0042	0.02235	0.009	12000	0.00289	480	16.5	16.9	5.69	5.68