Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for

N-cyanomethylmethanimine tethered anthracene dimer: concise synthesis, conformational properties and photoinduced configurational isomerization

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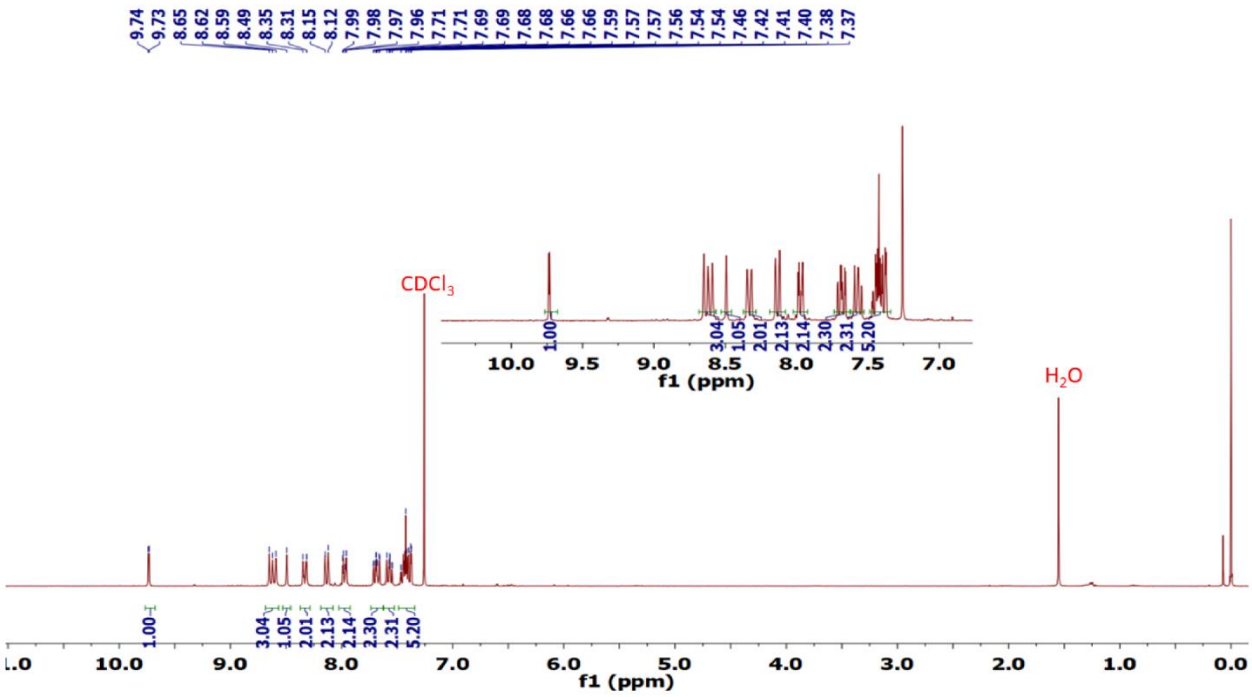

Fig. S-1 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **1**.

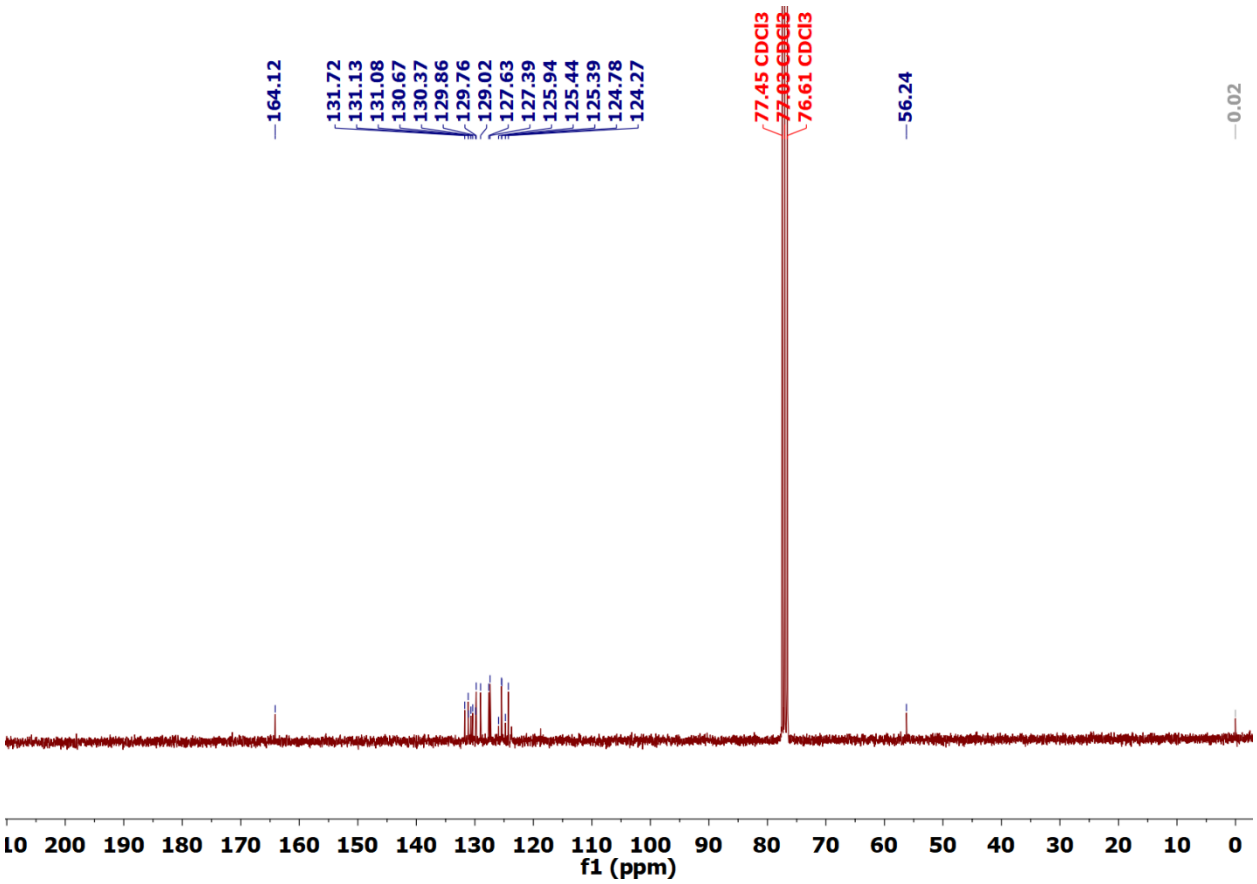

Fig. S-2 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **1**.

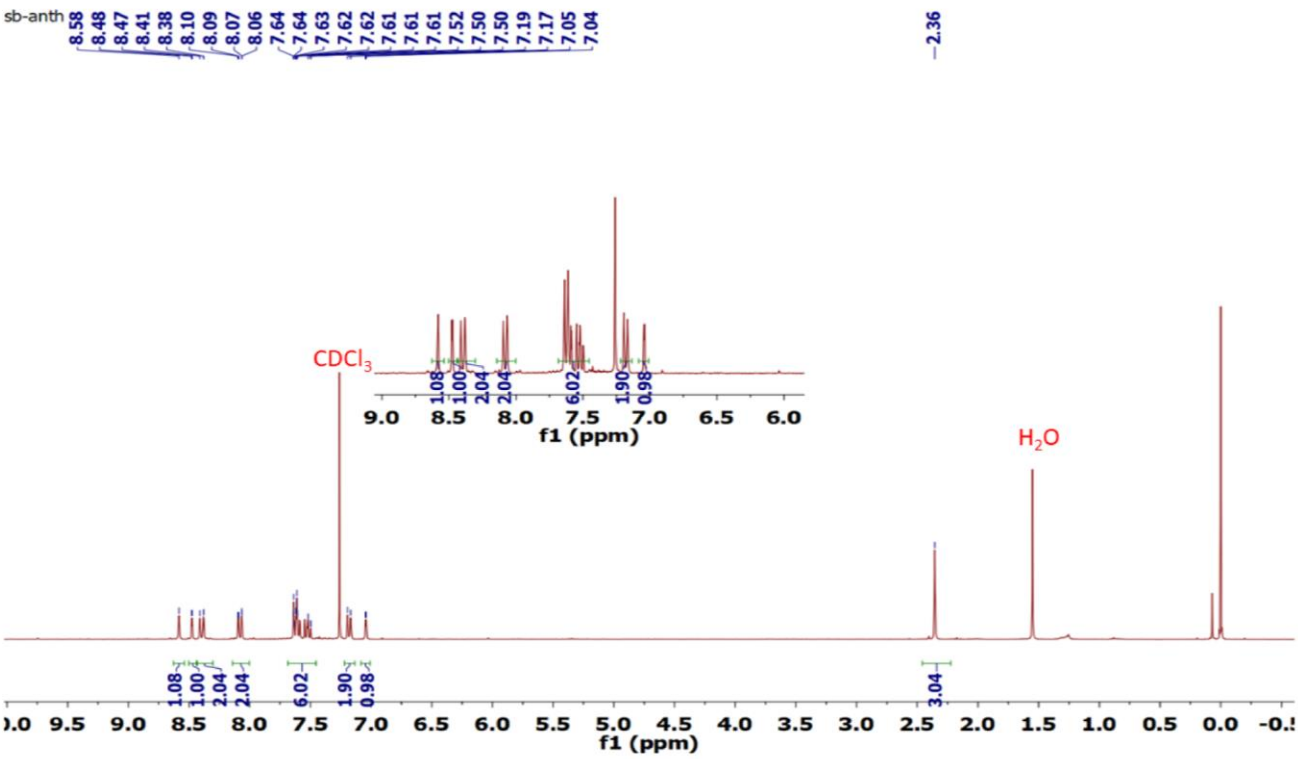

Fig. S-3 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **5a**.

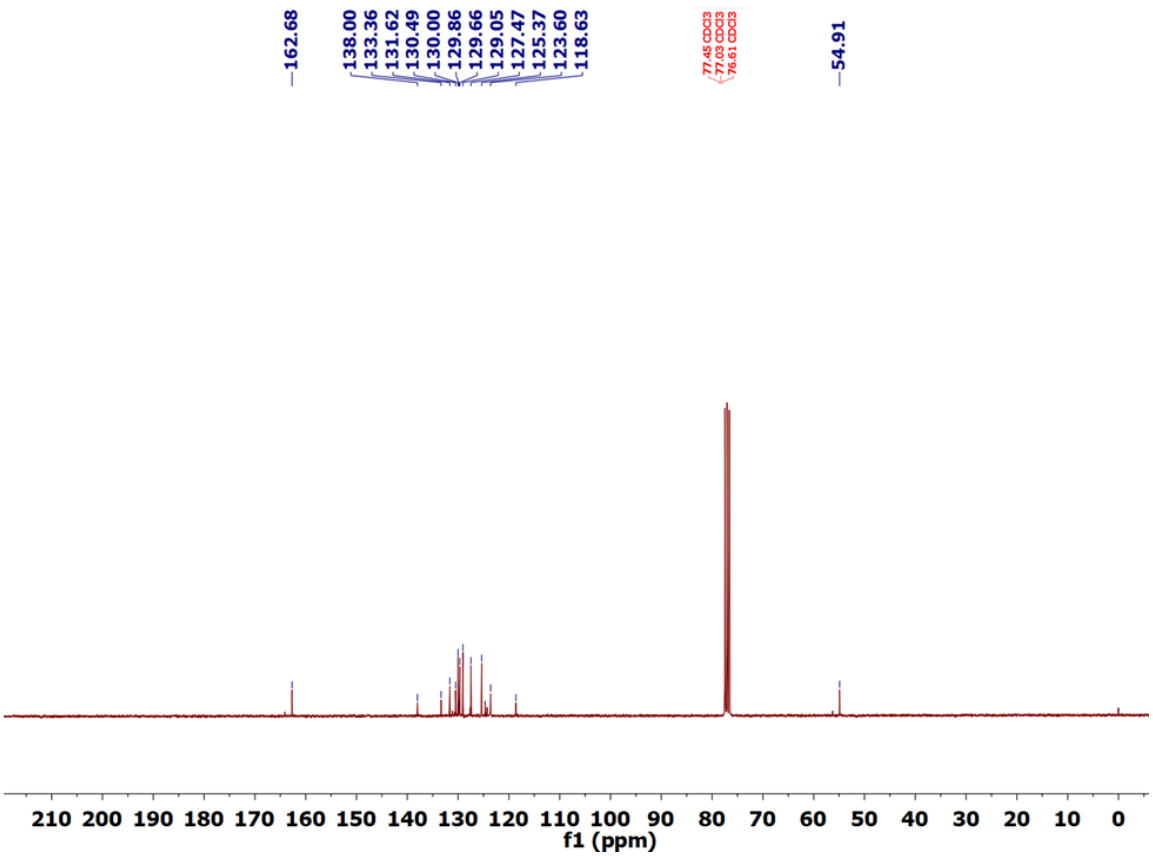

Fig. S-4 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **5a**.

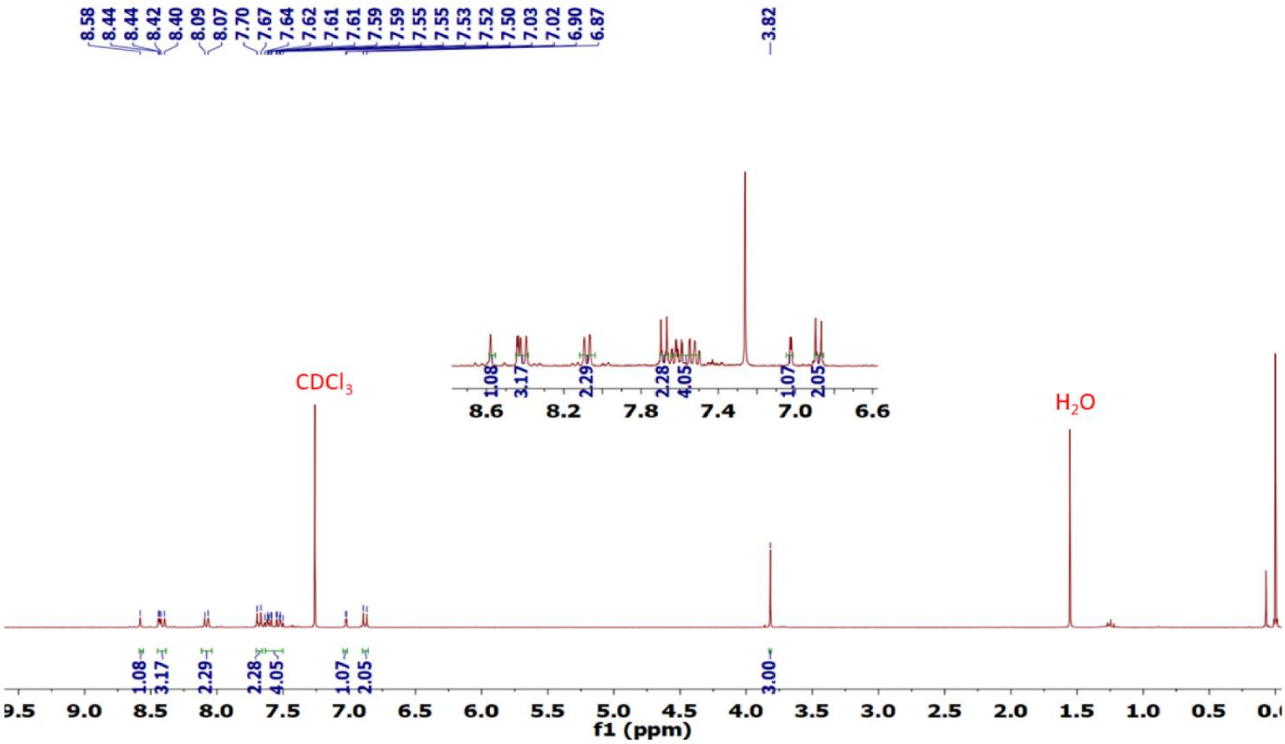

Fig. S-5 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **5b**.

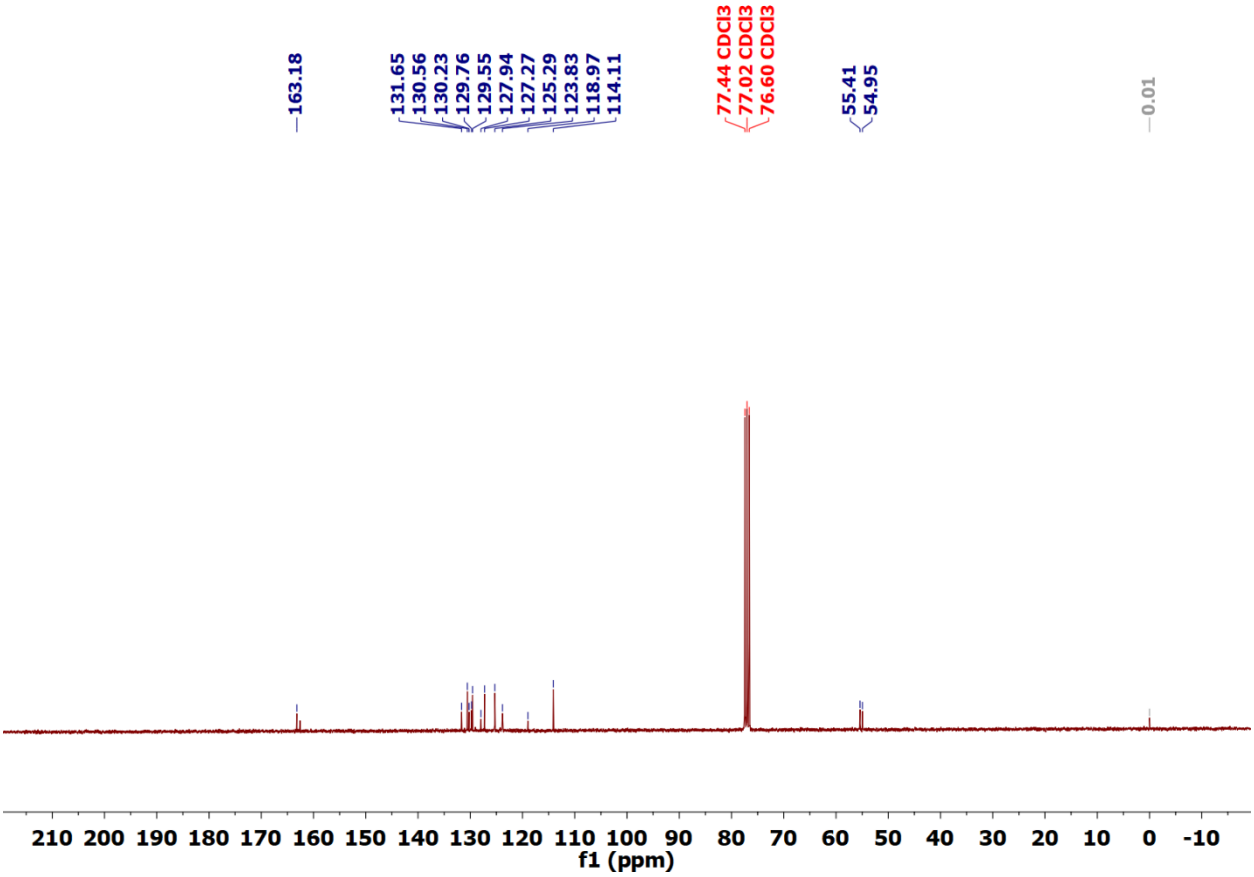

Fig. S-6 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **5b**.

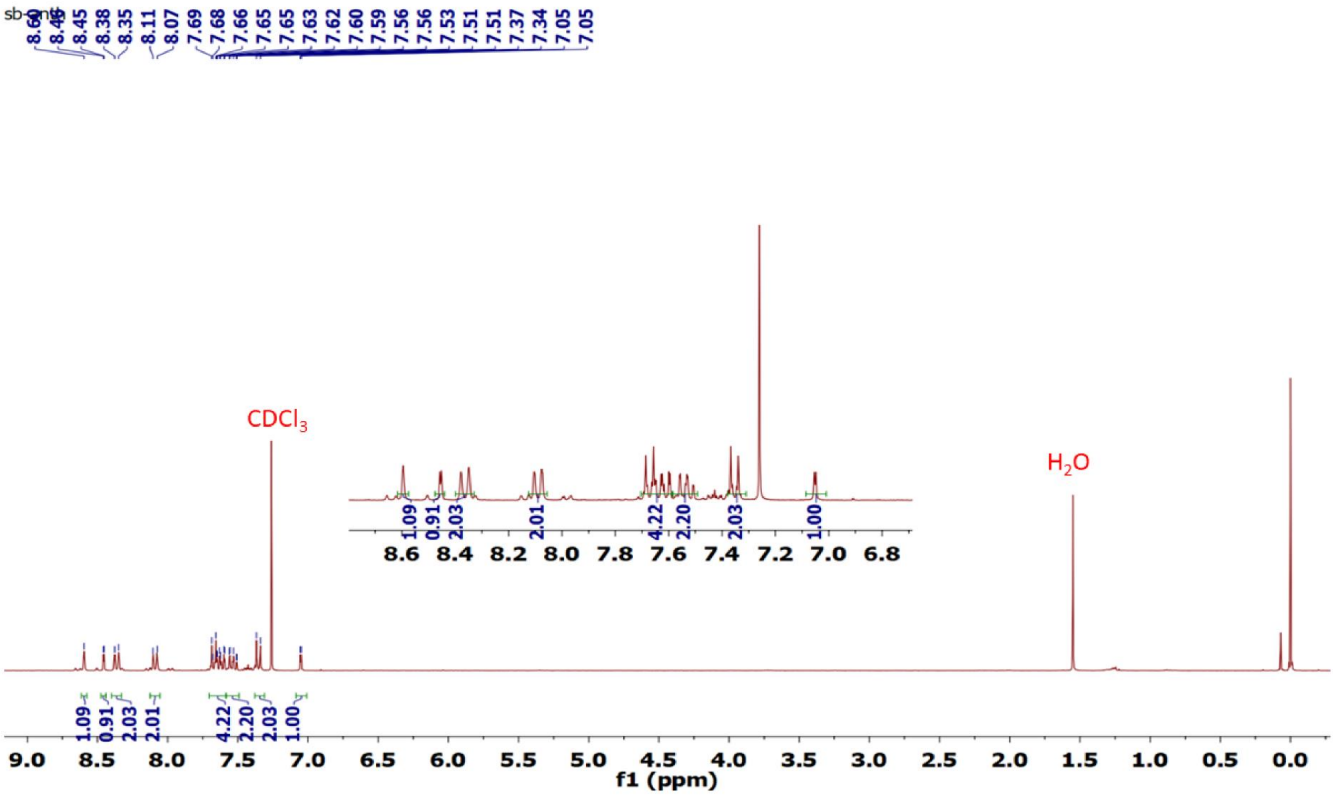

Fig. S-7 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **5c**.

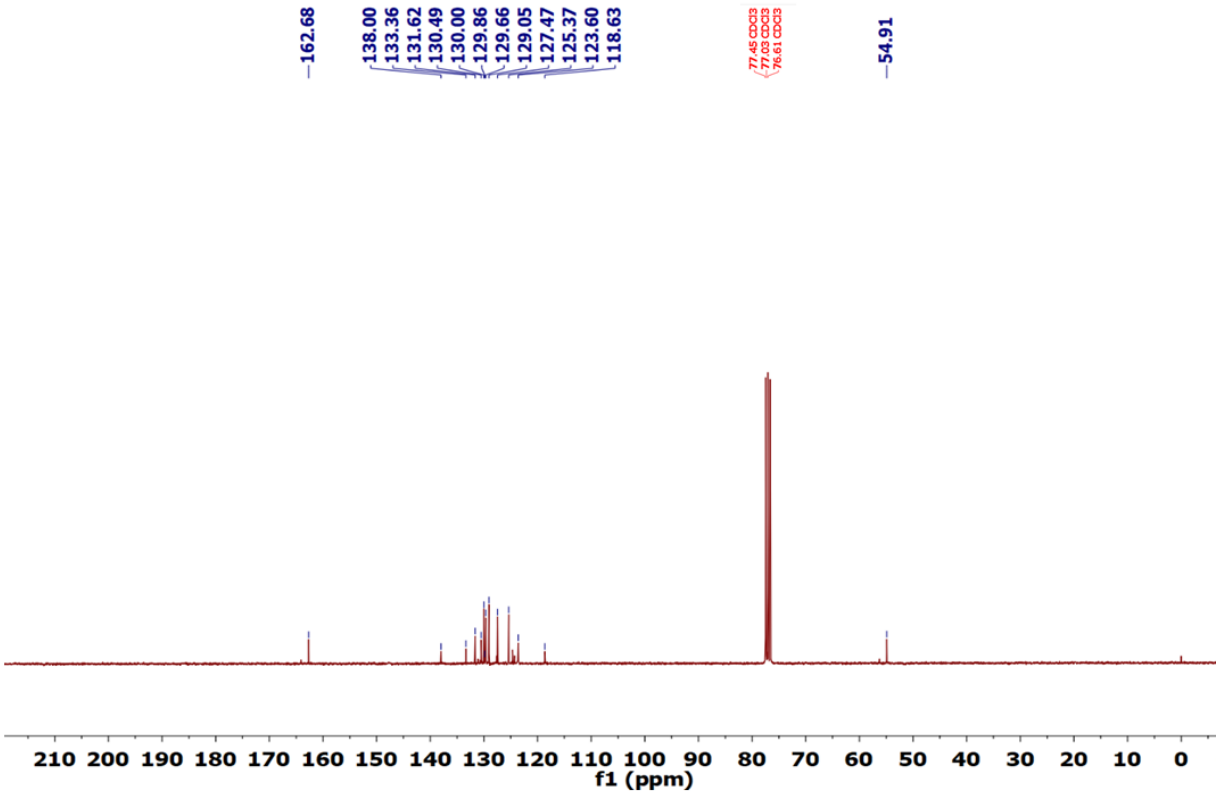

Fig. S-8 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **5c**.

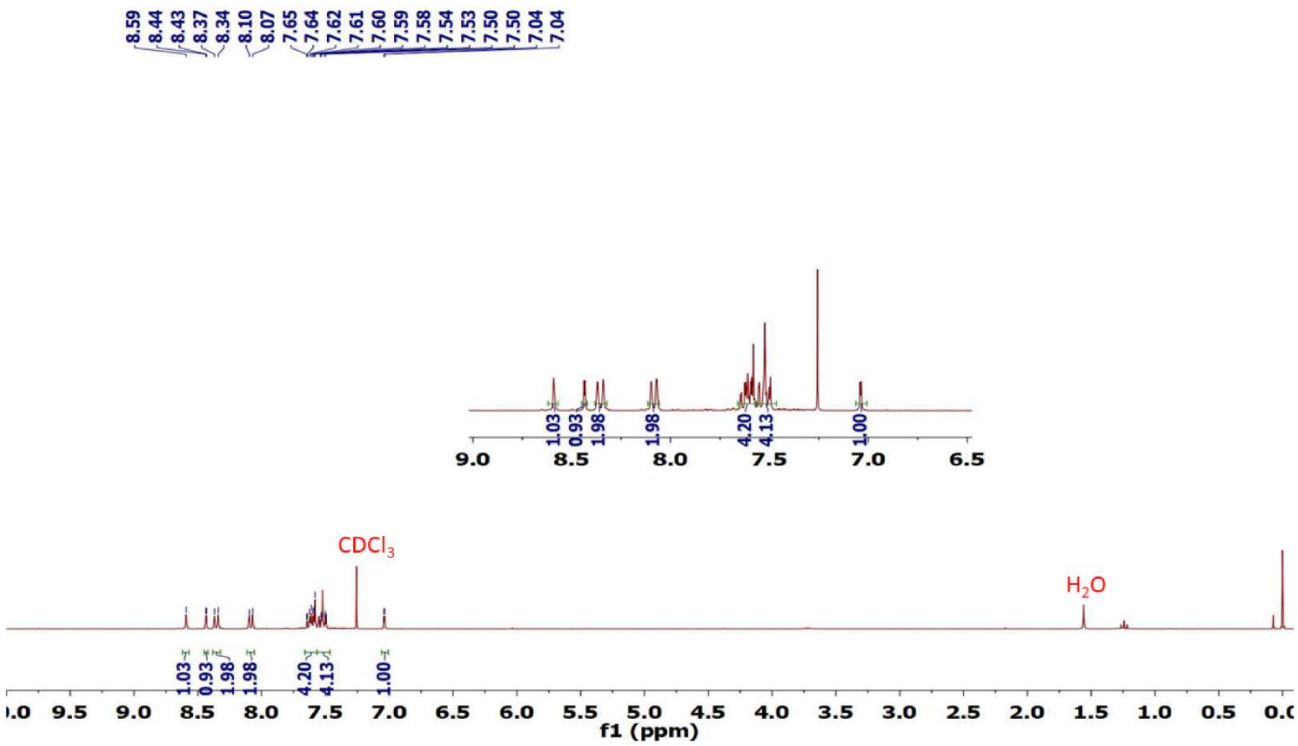

Fig. S-9 ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **5d**.

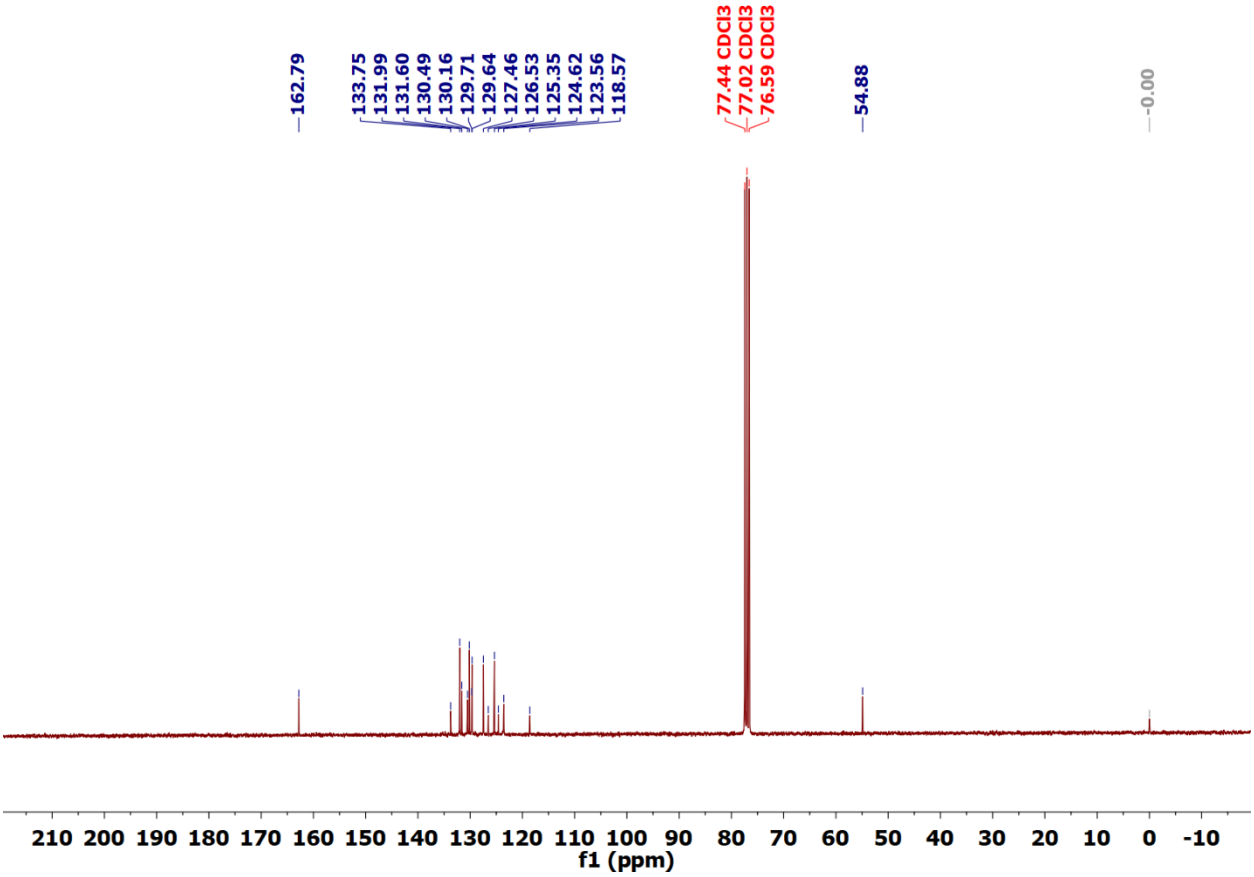

Fig. S-10 ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **5d**.

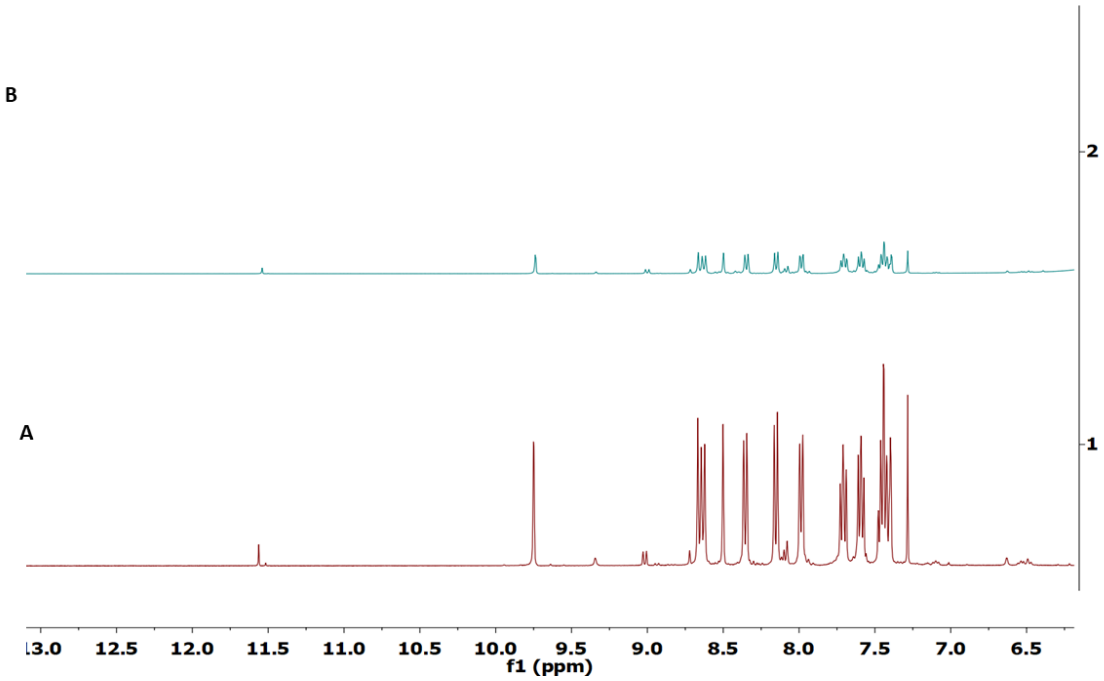

Fig. S-11 ^{1}H NMR (400 MHz, $CDCl_3$) spectra of (A) anthracene dimer **1.** (B) A mixture of **1** and hydrogen peroxide in $CDCl_3$ after mixing for 24 hours.

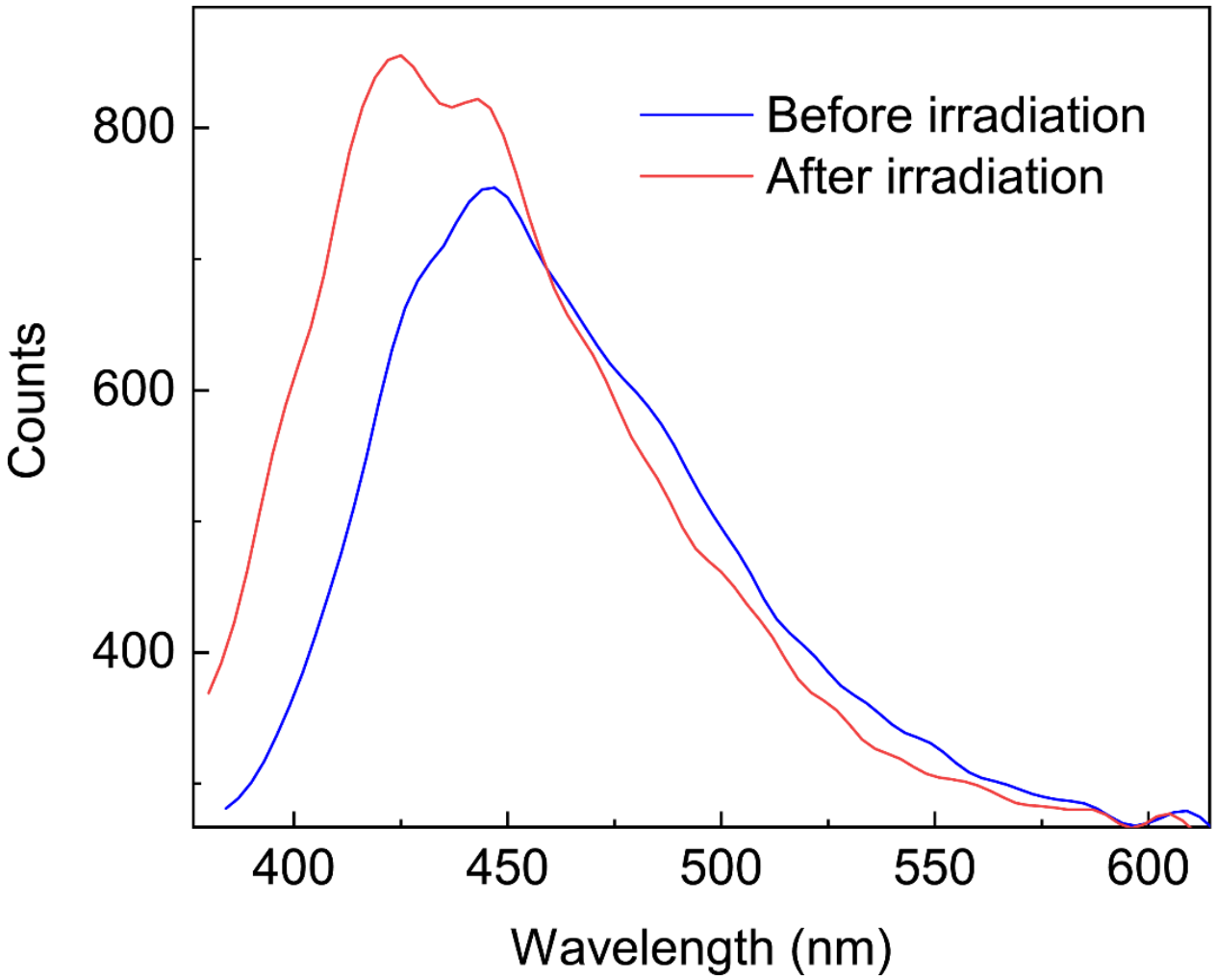

Figure S-12: Fluorescence spectra of compound **1** (2.0 mM in CH_2Cl_2, rt) measured before and after photoirradiation at 365 nm for 1 h.

Detailed Results of DFT Calculations

Cartesian coordinates and optimized *cis*-1-conformer-1 in gas phase: *E*(RM062X) = -1301.363980 hartees; Dipole Moment = 5. 6.283323 Debye; Basis Set = def2SVP.

N	1.032300	4.734600	0.653300
N	0.411500	2.327000	-1.679300
C	0.511400	1.296700	0.640000
C	-0.431900	0.629400	1.452300
C	-1.780200	1.081900	1.647900
H	-2.109700	2.030600	1.226300
C	-2.676400	0.357200	2.382700
H	-3.692400	0.732600	2.513100
C	-2.301500	-0.881200	2.980000
H	-3.035000	-1.451300	3.551800
C	-1.019800	-1.332500	2.851800
H	-0.706000	-2.267000	3.322000
C	-0.044100	-0.590500	2.110900
C	1.270200	-1.047900	2.002800
H	1.553600	-1.981400	2.494900
C	2.233900	-0.333200	1.288500
C	3.587100	-0.792900	1.212600
H	3.851500	-1.708100	1.746400
C	4.522200	-0.105300	0.493900
H	5.553000	-0.459400	0.446700
C	4.152900	1.086300	-0.196000
H	4.907800	1.637200	-0.758700
C	2.867600	1.552600	-0.156900
H	2.614400	2.464500	-0.698200
C	1.853500	0.864500	0.591100
C	0.077900	2.456500	-0.256200
H	-1.015600	2.558000	-0.196700
C	0.619400	3.740000	0.242300
C	0.144800	1.250700	-2.297400
H	0.433100	1.229700	-3.360600
C	-0.493500	0.017400	-1.746200
C	-1.860300	0.016700	-1.409500
C	-2.715200	1.143400	-1.647200
H	-2.302100	2.026300	-2.140800
C	-4.034400	1.115200	-1.287000
H	-4.669800	1.979600	-1.485300
C	-4.593700	-0.039500	-0.663400
H	-5.648300	-0.042900	-0.384600
C	-3.812800	-1.133600	-0.421500
H	-4.229800	-2.022700	0.056200
C	-2.427800	-1.146800	-0.784100
C	-1.615300	-2.252800	-0.520200
H	-2.044700	-3.120900	-0.014100
C	-0.266200	-2.272000	-0.887300
C	0.575800	-3.394400	-0.601400

H	0.136400	-4.255600	-0.093600
C	1.895000	-3.391000	-0.957600
H	2.526000	-4.253000	-0.735700
C	2.455800	-2.262800	-1.626600
H	3.509900	-2.272000	-1.906900
C	1.688800	-1.165500	-1.902300
H	2.137300	-0.297600	-2.389100
C	0.304000	-1.126200	-1.537800

Cartesian coordinates and optimized *cis*-1-conformer-2 in gas phase: *E*(RM062X) = - -1301.359965 hartees; Dipole Moment = 6.143276Debye; Basis Set = def2SVP.

N	1.436200	4.188000	1.682500
N	0.374300	2.435800	-1.049600
C	1.131600	0.845700	0.722300
C	0.463000	-0.192700	1.407000
C	-0.867700	-0.082900	1.937900
H	-1.415800	0.856500	1.877000
C	-1.487500	-1.143500	2.536200
H	-2.501300	-1.021300	2.921600
C	-0.834500	-2.404400	2.658300
H	-1.350800	-3.239900	3.132700
C	0.439100	-2.550300	2.192500
H	0.964100	-3.503100	2.285600
C	1.128000	-1.460500	1.568500
C	2.435400	-1.620600	1.107300
H	2.931000	-2.586000	1.237200
C	3.121300	-0.580700	0.479100
C	4.462500	-0.759600	0.010300
H	4.945700	-1.723300	0.184000
C	5.119200	0.246800	-0.635500
H	6.141400	0.103200	-0.988200
C	4.466200	1.496800	-0.850100
H	4.997900	2.298100	-1.364900
C	3.186200	1.707400	-0.419500
H	2.709300	2.667400	-0.613200
C	2.457800	0.677400	0.268500
C	0.397400	2.145000	0.389400
H	-0.636000	2.075800	0.754100
C	0.989900	3.296100	1.104600
C	-0.342200	1.706900	-1.800700
H	-0.312900	1.948600	-2.875500
C	-1.207100	0.555600	-1.391900
C	-2.493200	0.791300	-0.871500
C	-3.019500	2.114300	-0.689500
H	-2.412300	2.972000	-0.986900
C	-4.258400	2.308000	-0.146400
H	-4.639000	3.321300	-0.010700

C	-5.066400	1.196500	0.242300
H	-6.053600	1.373300	0.670900
C	-4.604800	-0.077700	0.076600
H	-5.214500	-0.934300	0.371300
C	-3.307000	-0.326900	-0.476000
C	-2.799900	-1.622600	-0.597000
H	-3.412000	-2.468100	-0.273100
C	-1.513200	-1.861200	-1.089500
C	-0.966500	-3.183200	-1.155000
H	-1.586200	-4.017400	-0.819800
C	0.302600	-3.394000	-1.612800
H	0.711800	-4.404600	-1.651200
C	1.103900	-2.293900	-2.042900
H	2.120100	-2.473700	-2.397700
C	0.617700	-1.017600	-2.000900
H	1.249500	-0.182300	-2.310600
C	-0.705500	-0.753400	-1.517000

Cartesian coordinates and optimized *cis*-1-conformer-3 in gas phase: *E*(RM062X) = -1301.356251 hartees; Dipole Moment = 4.874153 Debye; Basis Set = def2SVP.

N	2.428000	3.725900	0.505900
N	-0.085600	2.630200	-1.369800
C	-0.382600	1.366900	0.845500
C	0.443500	0.434900	1.521100
C	1.862000	0.576700	1.700500
H	2.377500	1.462700	1.348300
C	2.609500	-0.389000	2.315400
H	3.683900	-0.236500	2.427300
C	2.014100	-1.587800	2.800200
H	2.631400	-2.349900	3.277800
C	0.668200	-1.763500	2.670800
H	0.181100	-2.666500	3.045000
C	-0.154200	-0.767000	2.051300
C	-1.528700	-0.972100	1.946100
H	-1.964200	-1.890800	2.346200
C	-2.360600	-0.029000	1.343700
C	-3.772000	-0.249700	1.262400
H	-4.174600	-1.162700	1.705800
C	-4.591500	0.651500	0.647000
H	-5.667100	0.478400	0.592800
C	-4.031300	1.823700	0.064000
H	-4.684400	2.539300	-0.437900
C	-2.685500	2.064800	0.117000
H	-2.303700	2.956900	-0.378800
C	-1.784200	1.157400	0.775100
C	0.083700	2.619900	0.098300
H	-0.572100	3.432300	0.449100
C	1.418700	3.187100	0.363000
C	0.040500	1.585500	-2.078800
H	-0.140600	1.735400	-3.156600

C	0.395800	0.193400	-1.668100
C	-0.621000	-0.779800	-1.599700
C	-1.980000	-0.489500	-1.947700
H	-2.234500	0.506100	-2.316100
C	-2.958100	-1.433800	-1.806700
H	-3.988100	-1.192400	-2.073200
C	-2.647200	-2.729600	-1.297400
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C	1.021400	-2.405600	-0.796400
H	1.261100	-3.405100	-0.425300
C	2.047100	-1.466700	-0.937400
C	3.405800	-1.791300	-0.624900
H	3.630000	-2.805100	-0.286400
C	4.396300	-0.858000	-0.743600
H	5.428300	-1.117900	-0.503400
C	4.087500	0.464100	-1.180700
H	4.884400	1.203900	-1.267700
C	2.802300	0.814800	-1.487900
H	2.583700	1.831200	-1.820300
C	1.733800	-0.134800	-1.379800

Cartesian coordinates and optimized *cis*-1-conformer-4 in gas phase: *E*(RM062X) -1301.353049 hartees; Dipole Moment = 6.205087 Debye; Basis Set = def2SVP.

N	-1.396600	4.719400	-0.481800
N	0.029100	2.092400	-2.069200
C	-0.982400	1.355900	0.211400
C	-2.106500	0.606300	0.619000
C	-3.416300	0.760900	0.049900
H	-3.595800	1.523400	-0.708400
C	-4.471800	0.005200	0.474900
H	-5.459400	0.164800	0.039500
C	-4.303300	-0.982400	1.490600
H	-5.156500	-1.582900	1.808700
C	-3.081100	-1.154100	2.070800
H	-2.936500	-1.892800	2.861900
C	-1.955700	-0.359900	1.675300
C	-0.713200	-0.515100	2.293000
H	-0.589500	-1.283600	3.060100
C	0.365300	0.315100	1.977700
C	1.625300	0.189100	2.646500
H	1.737400	-0.597600	3.395600
C	2.656000	1.037900	2.364600
H	3.612300	0.934500	2.879100
C	2.479400	2.080200	1.406400
H	3.296700	2.778100	1.217900
C	1.308700	2.206100	0.714300

H	1.200200	3.005800	-0.019400
C	0.213800	1.310100	0.952500
C	-1.036800	2.178000	-1.075300
H	-1.942700	1.878600	-1.624500
C	-1.233600	3.612000	-0.757600
C	0.811400	1.112300	-2.274000
H	1.538400	1.282400	-3.084900
C	0.939800	-0.204900	-1.587000
C	-0.158500	-1.081200	-1.490200
C	-1.392500	-0.847900	-2.180900
H	-1.466600	0.009000	-2.853100
C	-2.456900	-1.688800	-2.022200
H	-3.389300	-1.493000	-2.553600
C	-2.367000	-2.822000	-1.159400
H	-3.236800	-3.466200	-1.024900
C	-1.192500	-3.107800	-0.525200
H	-1.103500	-3.988500	0.114400
C	-0.044800	-2.266700	-0.686300
C	1.178000	-2.572800	-0.082800
H	1.259200	-3.473400	0.531000
C	2.303800	-1.764900	-0.262400
C	3.567300	-2.108200	0.319200
H	3.633800	-3.027100	0.905200
C	4.661900	-1.313700	0.139100
H	5.621500	-1.589100	0.578700
C	4.554500	-0.113600	-0.625400
H	5.434800	0.516300	-0.761900
C	3.361100	0.260300	-1.175600
H	3.295300	1.198500	-1.727400
C	2.189900	-0.555200	-1.030700

Cartesian coordinates and optimized *trans-conformer* in gas phase: *E*(RM062X)= -1301.349754 hartees; Dipole Moment = 6. 4.959290 Debye; Basis Set = def2SVP.

N	1.701600	-3.018900	-2.826800
N	-0.116900	-0.866800	-0.901600
C	2.273600	-0.388600	-0.567500
C	2.581800	-1.271300	0.491800
C	1.899300	-2.518400	0.696600
H	1.073100	-2.793500	0.044500
C	2.247000	-3.350600	1.722800
H	1.710100	-4.290500	1.856400
C	3.293700	-3.006400	2.628300
H	3.554200	-3.688900	3.438200
C	3.955000	-1.822600	2.482800
H	4.751400	-1.535900	3.172200
C	3.619600	-0.920300	1.422500
C	4.282300	0.300000	1.283100
H	5.068800	0.564300	1.994000

C	3.959400	1.195500	0.263800
C	4.642000	2.451200	0.160100
H	5.415700	2.675400	0.897100
C	4.336800	3.343000	-0.824400
H	4.861300	4.296600	-0.893300
C	3.322900	3.020000	-1.772900
H	3.080100	3.731900	-2.563200
C	2.654400	1.829800	-1.713000
H	1.897200	1.639300	-2.471300
C	2.933600	0.854800	-0.691200
C	1.180000	-0.770600	-1.561900
H	1.148700	-0.021500	-2.365200
C	1.479600	-2.043100	-2.254800
C	-0.869200	0.151500	-0.991300
H	-0.539900	1.039400	-1.563800
C	-2.204100	0.268100	-0.367100
C	-2.567800	1.533200	0.156400
C	-1.665500	2.649600	0.202100
H	-0.639500	2.536700	-0.147800
C	-2.055200	3.855700	0.714200
H	-1.345800	4.684100	0.739700
C	-3.371000	4.043100	1.230600
H	-3.660700	5.013900	1.634400
C	-4.253100	3.002400	1.229600
H	-5.259800	3.121700	1.634800
C	-3.882500	1.722900	0.704000
C	-4.775800	0.650300	0.723300
H	-5.775000	0.797200	1.140800
C	-4.425700	-0.606500	0.225600
C	-5.364600	-1.688000	0.257200
H	-6.349200	-1.503200	0.691100
C	-5.038600	-2.913200	-0.244900
H	-5.759100	-3.731700	-0.217900
C	-3.748900	-3.122900	-0.815500
H	-3.497300	-4.102400	-1.224800
C	-2.821500	-2.119500	-0.858900
H	-1.840100	-2.308800	-1.284800
C	-3.115500	-0.816500	-0.333300

Cartesian coordinates and optimized *TS1* in gas phase: *E*(RM062X)= -1301.306319 hartees; Dipole Moment = 3.787525 Debye; Basis Set = def2SVP.

C	0.995200	-0.633200	1.415800
H	1.213600	-1.541700	2.007700
C	0.702300	0.361600	2.498200
N	0.405600	1.036100	3.385300
N	-0.083000	-0.893800	0.578300
C	-1.042000	-1.170900	-0.164500
H	-1.008800	-2.065500	-0.827600
H	-0.166500	3.663800	-0.859900
C	-1.106600	3.123200	-0.734900

H	-0.129000	1.241600	-0.601100
C	-1.082700	1.765900	-0.580500
C	-3.520200	3.159600	-0.631500
C	-2.295000	1.015000	-0.422800
C	-2.342000	3.837300	-0.746700
C	-3.539400	1.734900	-0.479400
C	-2.315600	-0.387600	-0.260900
H	-2.338500	4.921900	-0.862900
H	-5.686900	1.588600	-0.442500
H	-4.474900	3.688600	-0.658600
C	-3.541400	-1.084900	-0.193500
C	-3.615400	-2.508000	-0.018000
C	-4.777700	-0.355200	-0.267800
H	-6.946600	-0.494100	-0.248700
C	-4.745600	1.035100	-0.398500
C	-4.819400	-3.150900	0.048700
H	-2.696900	-3.086600	0.077300
H	-4.848600	-4.233500	0.180800
C	-6.042900	-2.422700	-0.042000
H	-6.993200	-2.954600	0.016500
C	-6.018600	-1.066400	-0.189900
H	2.662000	-4.936700	-0.081900
C	3.089400	-3.940600	-0.205900
H	1.438300	-3.003500	0.733500
C	2.411800	-2.852200	0.268500
C	4.864500	-2.547900	-1.057600
C	2.934600	-1.522600	0.115200
C	4.341800	-3.793900	-0.870500
C	4.178600	-1.382000	-0.587800
C	2.276300	-0.370800	0.608100
H	4.868700	-4.676600	-1.234600
H	5.654200	-0.000700	-1.328700
H	5.815900	-2.411900	-1.575600
C	2.773600	0.919500	0.323500
C	2.105400	2.146200	0.670200
C	4.026000	1.038900	-0.385400
H	5.521700	2.391400	-1.191100
C	4.701900	-0.105800	-0.803600
C	2.648000	3.363200	0.368600
H	1.140500	2.125000	1.169600
H	2.108500	4.269800	0.648000
C	3.903500	3.469500	-0.299700
H	4.320600	4.452800	-0.520000
C	4.566000	2.336900	-0.666100

Cartesian coordinates and optimized *TS2* in gas phase: *E*(RM062X)= -1301.349754 hartees; Dipole Moment = 4.787560 Debye; Basis Set = def2SVP.

H	-0.481500	2.730500	-2.854900
C	0.420200	2.440400	-2.314000
H	-0.165500	0.409000	-2.225500

C	0.612500	1.130600	-1.976700
C	2.482600	3.089500	-1.238900
C	1.764800	0.717000	-1.226200
C	1.374200	3.437600	-1.954100
C	2.700400	1.733900	-0.831100
C	1.966900	-0.610000	-0.791900
H	1.206200	4.475600	-2.243700
H	4.505600	2.164500	0.261200
H	3.217000	3.841600	-0.943600
C	2.981000	-0.917700	0.137300
C	3.097900	-2.190300	0.794300
C	3.929800	0.104500	0.497800
H	5.715700	0.574600	1.643100
C	3.782600	1.393600	-0.016700
C	4.108600	-2.438600	1.679000
H	2.356900	-2.966000	0.610100
H	4.165700	-3.411000	2.169700
C	5.086700	-1.443400	1.976700
H	5.894300	-1.670600	2.673600
C	4.992500	-0.208400	1.406600
C	0.965600	-1.669600	-1.259600
H	0.610700	-1.339100	-2.251200
C	1.601700	-2.991900	-1.580800
N	2.006000	-4.029200	-1.881900
N	-0.121500	-1.744000	-0.397500
C	-1.125600	-1.813600	0.334700
H	-1.389100	-2.753400	0.868300
H	-5.680700	-3.408800	-0.508600
C	-5.313000	-2.412200	-0.260200
H	-3.295300	-3.061400	-0.130800
C	-3.978600	-2.217100	-0.041300
C	-5.784000	-0.071700	0.118700
C	-3.462800	-0.919500	0.294700
C	-6.234300	-1.325600	-0.175800
C	-4.393400	0.175200	0.359000
C	-2.090800	-0.679400	0.524800
H	-7.295300	-1.502800	-0.355900
H	-4.626900	2.296000	0.646500
H	-6.475600	0.771400	0.174500
C	-1.632900	0.615100	0.855700
C	-0.272100	0.894200	1.213800
C	-2.567700	1.708500	0.873400
H	-2.813200	3.852300	1.136900
C	-3.920800	1.462200	0.626500
C	0.139000	2.167800	1.490200
H	0.442900	0.074900	1.274800
H	1.181600	2.350500	1.756600
C	-0.777800	3.259400	1.435200
H	-0.425300	4.270800	1.642300
C	-2.093100	3.031700	1.150900

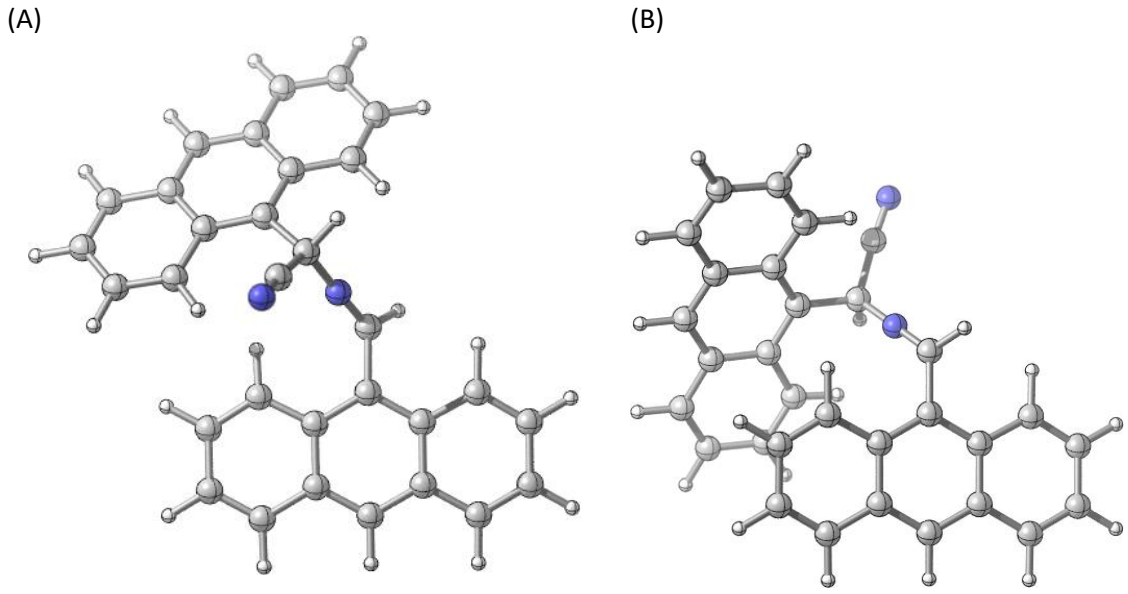

Figure S13: Comparison of the molecular structures of (A) **TS-1** and (B) **TS-2**.

Table 1. Crystal data and structure refinement of **1**

Identification code	SOH
Empirical formula	$C_{31}H_{20}N_2$
Formula weight	420.49
Temperature/K	293(2)
Crystal system	triclinic
Space group	*P*1
a/Å	5.18100(10)
b/Å	9.6048(2)
c/Å	11.9887(3)
α/°	67.824(2)
β/°	85.664(2)
γ/°	78.436(2)
Volume/Å^3	541.24(2)
Z	1
ρ_{calc}g/cm^3	1.290
μ/mm^{-1}	0.581
F(000)	220.0
Crystal size/mm^3	0.113 × 0.062 × 0.053
Radiation	Cu *K*α (λ = 1.54184)
2θ range for data collection/°	7.964 to 158.56
Index ranges	$-6 \le h \le 6$, $-12 \le k \le 12$, $-15 \le l \le 15$
Reflections collected	17194
Independent reflections	4253 [R_{int} = 0.0495, R_{sigma} = 0.0328]
Data/restraints/parameters	4253/3/299
Goodness-of-fit on F^2	1.145
Final *R* indexes [*I*>=2σ (I)]	R_1 = 0.0344, wR_2 = 0.0952
Final *R* indexes [all data]	R_1 = 0.0437, wR_2 = 0.1086
Largest diff. peak/hole / e Å^{-3}	0.09/-0.14

Table 2. Crystal data and structure refinement of **5d**

Empirical formula	$C_{23}H_{15}BrN_2$
Formula weight	399.28
Temperature/K	100(2)
Crystal system	monoclinic
Space group	*C*2/*c*
a/Å	45.2994(6)
b/Å	6.08550(10)
c/Å	12.8728(2)
β/°	92.7350(10)
Volume/Å^3	3544.60(9)
Z	8
ρ_{calc}g/cm^3	1.496
μ/mm^{-1}	3.210
F(000)	1616.0
Crystal size/mm^3	0.133 × 0.066 × 0.052
Radiation	Cu *K*α (λ = 1.54184)
2θ range for data collection/°	7.816 to 159.118
Index ranges	$-56 \le h \le 57$, $-7 \le k \le 7$, $-16 \le l \le 15$
Reflections collected	24198
Independent reflections	3794 [R_{int} = 0.0485, R_{sigma} = 0.0271]
Data/restraints/parameters	3794/1/295
Goodness-of-fit on F^2	1.057
Final *R* indexes [*I*>=2σ (I)]	R_1 = 0.0489, wR_2 = 0.1301
Final *R* indexes [all data]	R_1 = 0.0541, wR_2 = 0.1341
Largest diff. peak/hole / e Å^{-3}	0.58/-0.79

Halogen bonding in compound 5d

In the recent decades, halogen bonding (XB) has been attracted the attention of many researchers due to its contribution in many fields of science and engineering. Not long ago, it has been recognized as an important key in supramolecular interaction in crystal engineering as it is more directional than other non-covalent interactions.[1-3] Desiraju and coworkers have classified XB based on the values of the two C–X···X angles θ_1 and θ_2 in two categories, type I and type II (Please see Fig. S-14).[4]

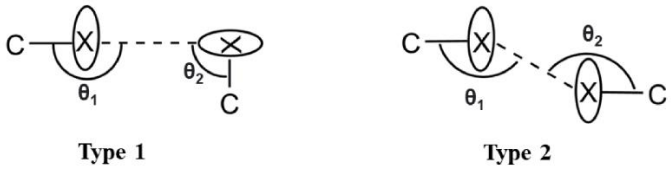

Fig. S-14 Types of halogen...halogen interactions. Type I, $\theta 1 \approx 180^\circ$ and $\theta_2 \approx 90^\circ$. Type II, $\theta 1 = \theta_2$

Figure S-15 highlights the Br···Br interaction in two independent molecules of **5d**. The distance of Br···Br is 3.54 Å which is less than the sum of the van der Waals radii and consents with the values found in the CSD.[5] The C–Br···Br angle is 139.6°. Subsequently, the halogen bonding in compound **5d** falls under the category of type II.

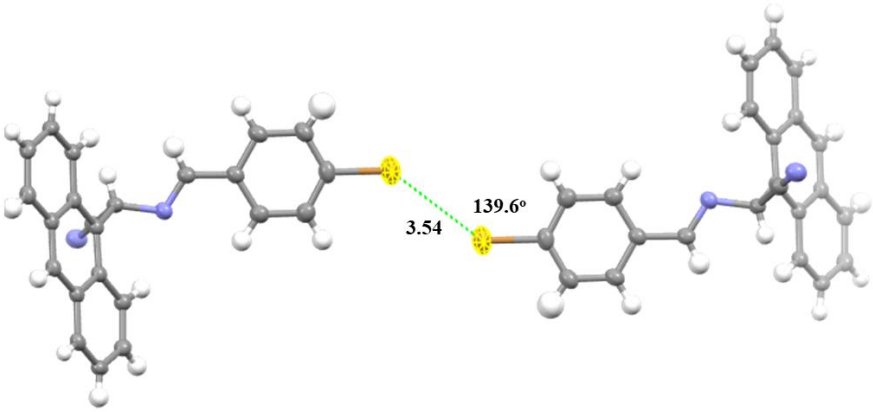

Fig. S-15 Halogen bonding interaction between the two crystallographically independent molecules of 5d (Hydrogen atoms are omitted for clarity).

Notes and references

1 P. Metrangolo, F. Meyer, T. Pilati, G. Resnati and G. Terraneo, Angewandte Chemie International Edition, 2008, 47, 6114–6127.

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4 D. ShekharáReddy, B. SatisháGoud, A. DavidáRae et al., Journal of the Chemical Society, Perkin Transactions 2, 1994, 2353–2360.

5 A. v. Bondi, The Journal of physical chemistry, 1964, 68, 441–451.