Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Experimental and Theoretical Investigation of Intramolecular Cooperativity in Cyclic Benzene Trimer Motif

Chakka Kiran Kumar, Shankar Deval Sathiyashivan, Dhanraj T. Masram, K. V. Jovan Jose, Malaichamy Sathiyendiran

Contents

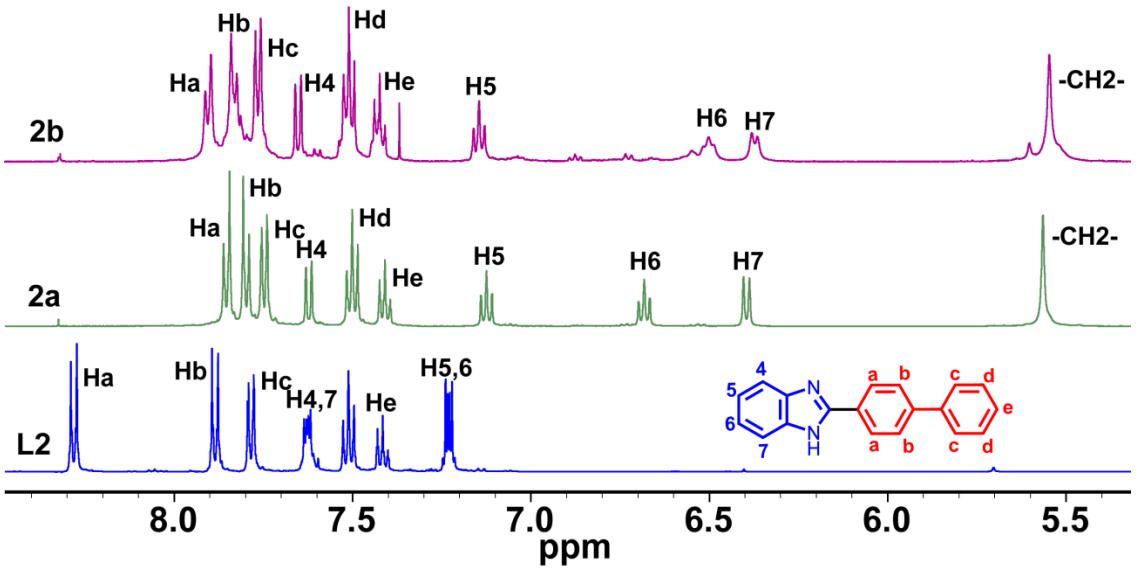

Fig. S1 Partial ^{1}H NMR spectra of L^{2}, **2a,** and **2b** in d_6-DMSO.

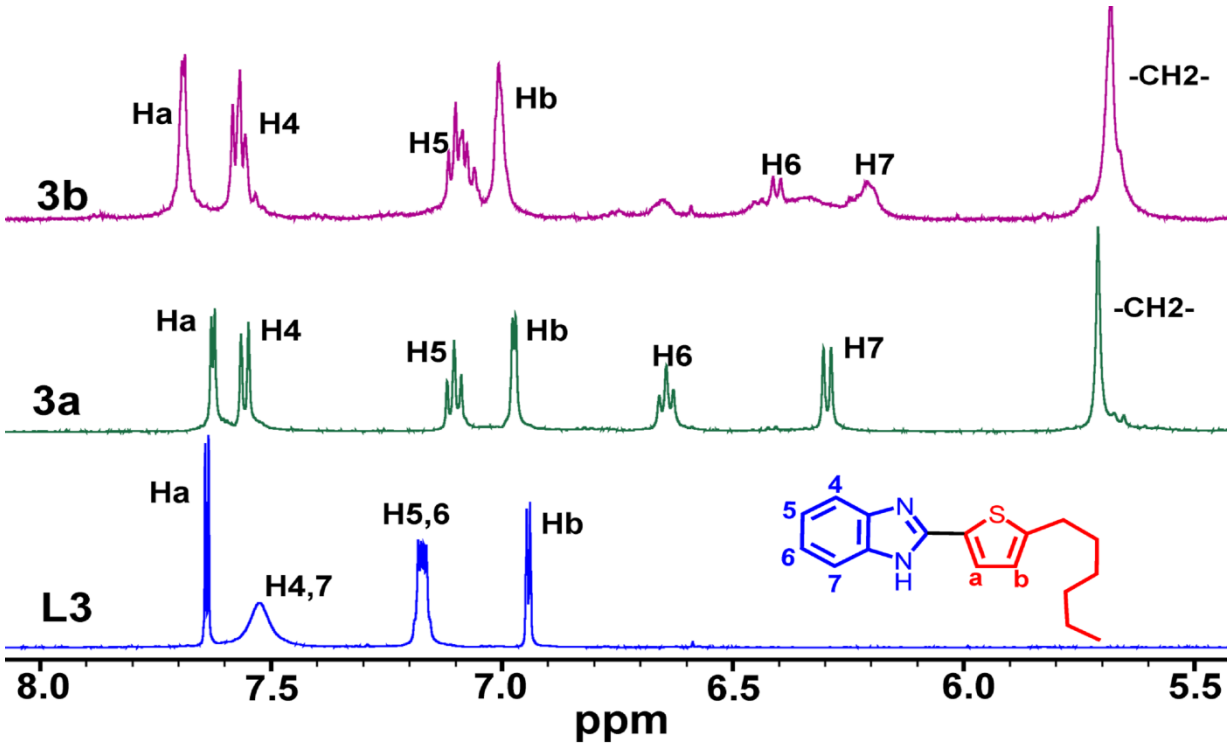

Fig. S2 Partial ^{1}H NMR spectra of L^{3}, **3a,** and **3b** in d_6-DMSO.

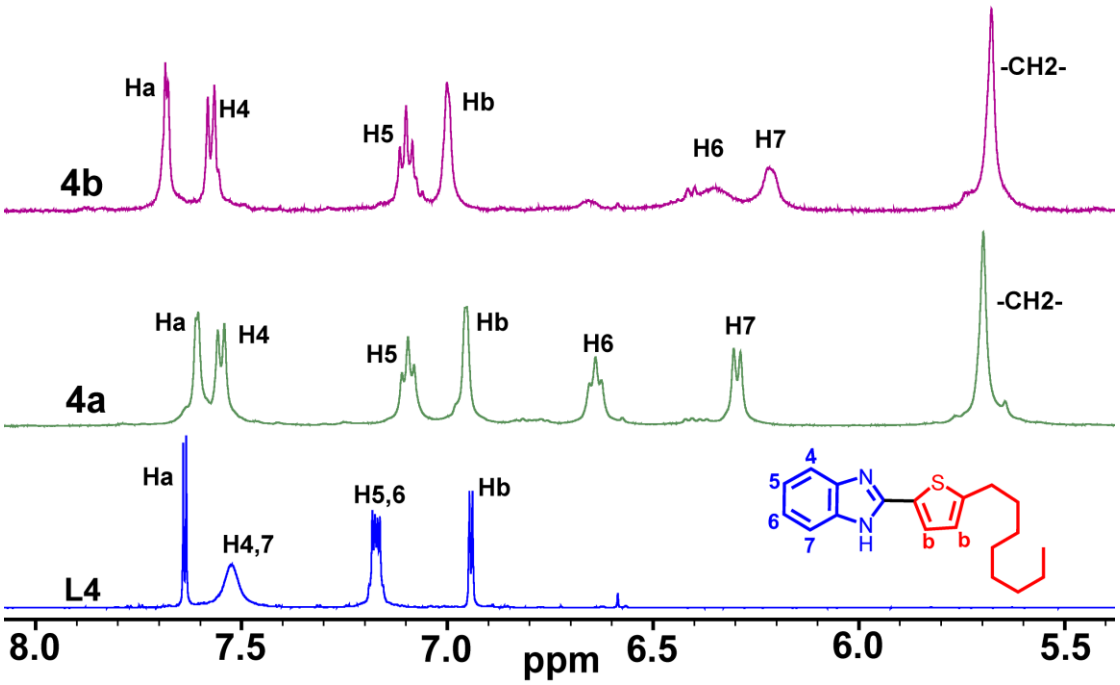

Fig. S3 Partial ^{1}H NMR spectra of L^{4}, **4a,** and **4b** in d_6-DMSO.

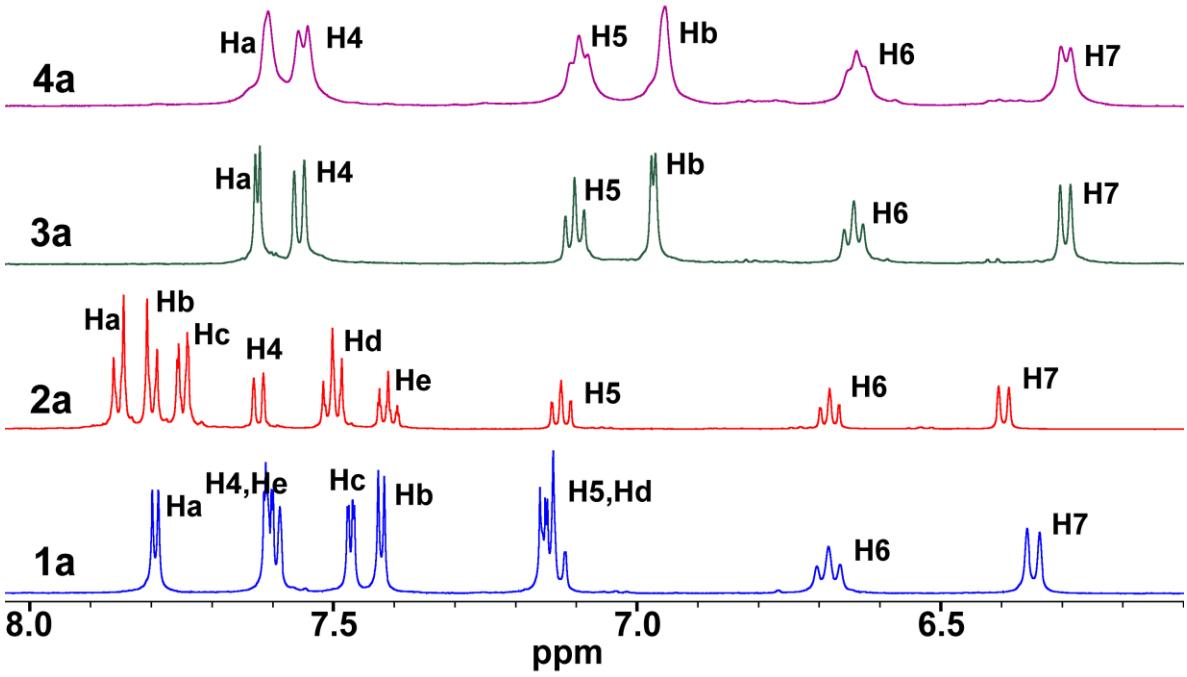

Fig. S4 Partial ^{1}H NMR spectra of **1a**, **2a**, **3a,** and **4a** in d_6-DMSO.

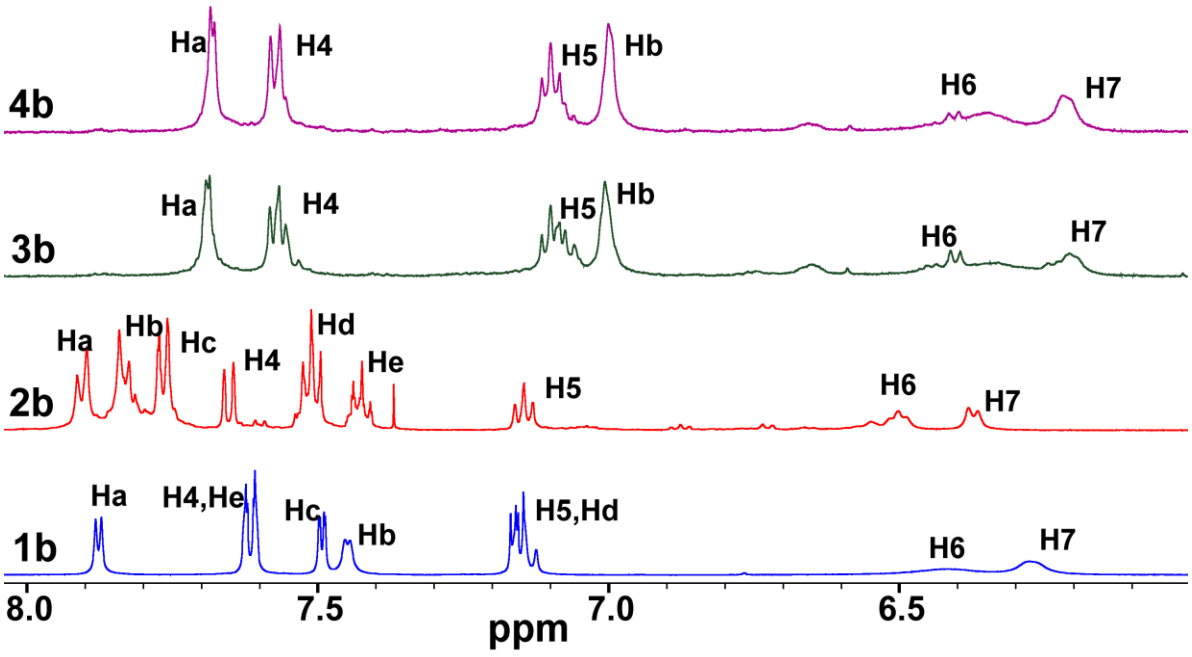

Fig. S5 Partial ^{1}H NMR spectra of **1b**, **2b**, **3b,** and **4b** in d_6-DMSO.

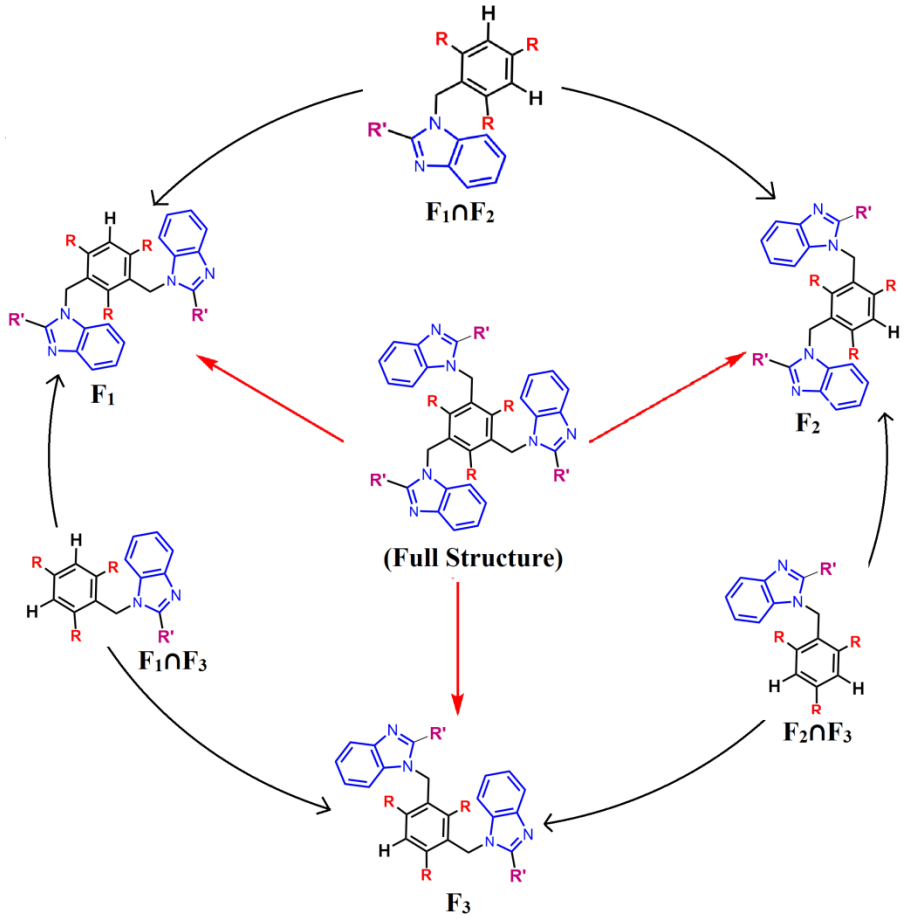

Fig. S6 The scheme followed for calculating the intramolecular C-H···π interaction energy between benzene C-H with the neighboring benzene π-electron cloud of **1a**, **1b**, **2a** and **2b** molecules. Here, F_1, F_2, and F_3 are the fragments generated from the full structure by removing one of the ligands and satisfying the carbon valency with a hydrogen atom. Fragment single point energies and total energies are calculated to evaluate the intramolecular energies at M062X [MPW1PW91]/6-311+G(d,p) levels of theory and basis function.

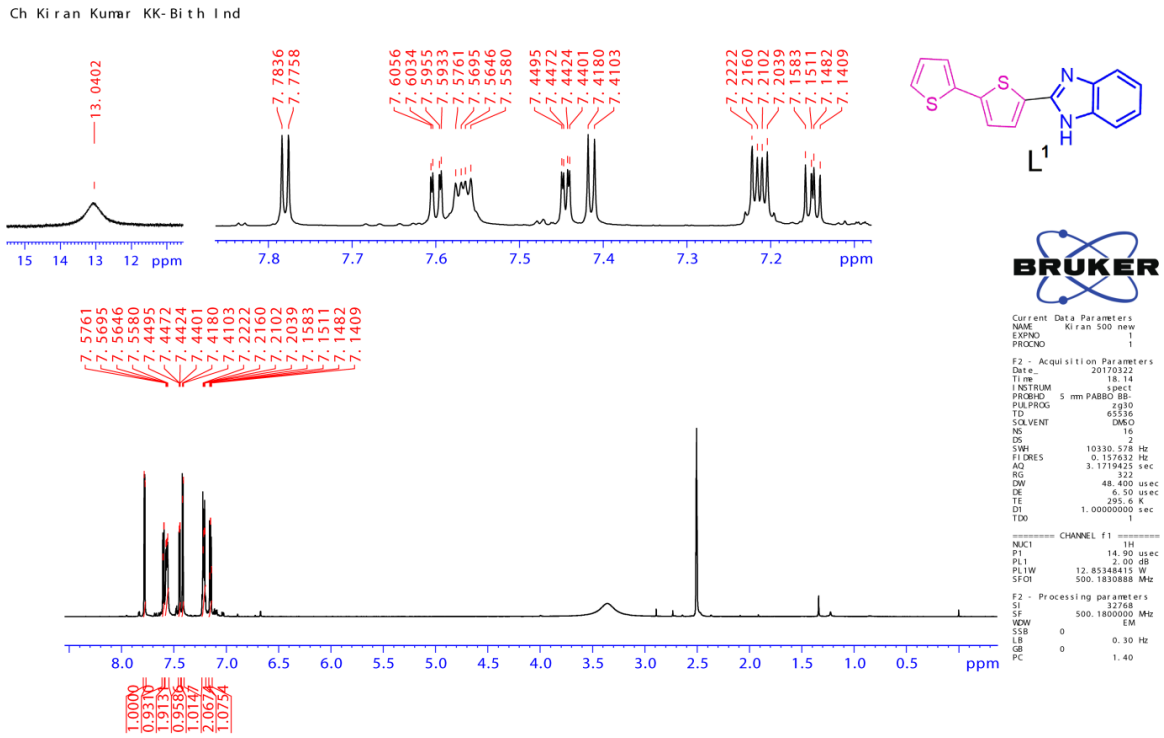

Fig. S7 ^{1}H NMR spectrum of L^{1} in d_6-DMSO.

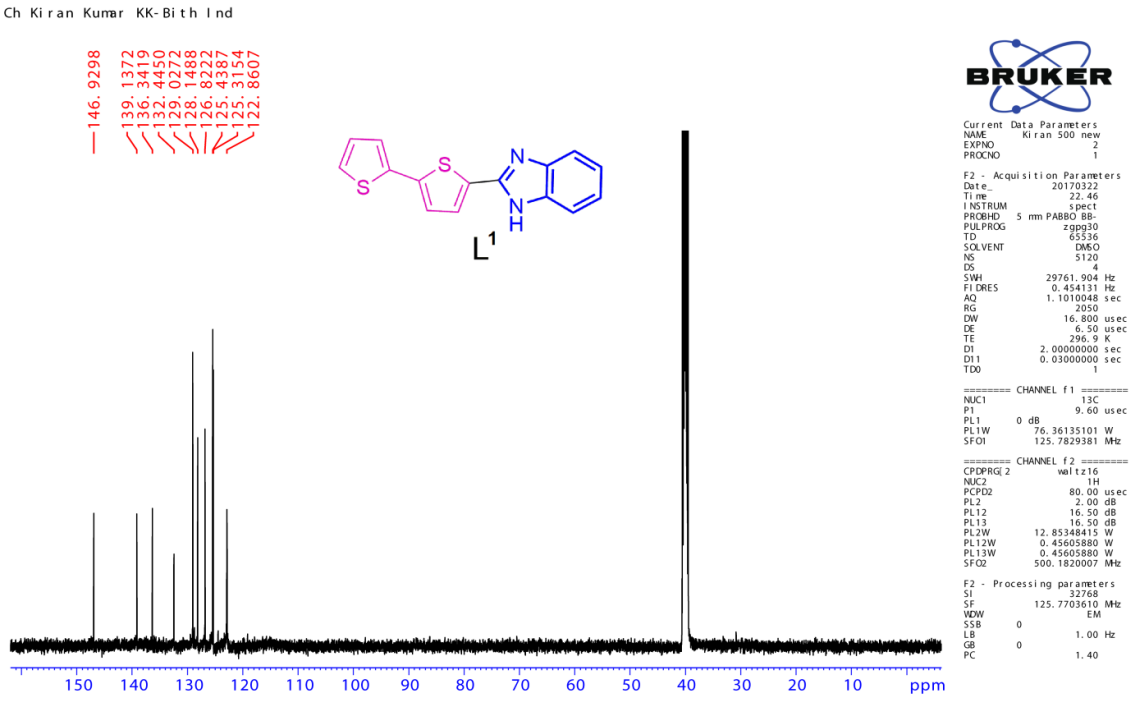

Fig. S8 ^{13}C NMR spectrum of L^{1} in d_6-DMSO.

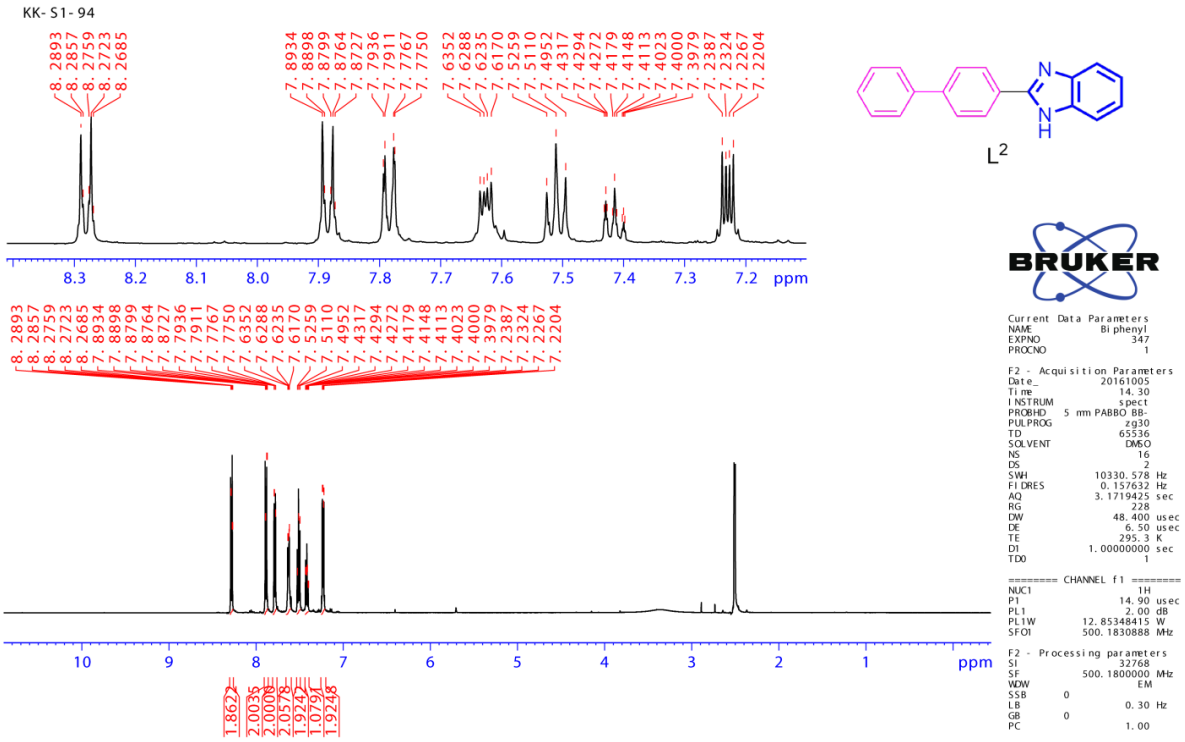

Fig. S9 ^{1}H NMR spectrum of L^2 in d_6-DMSO.

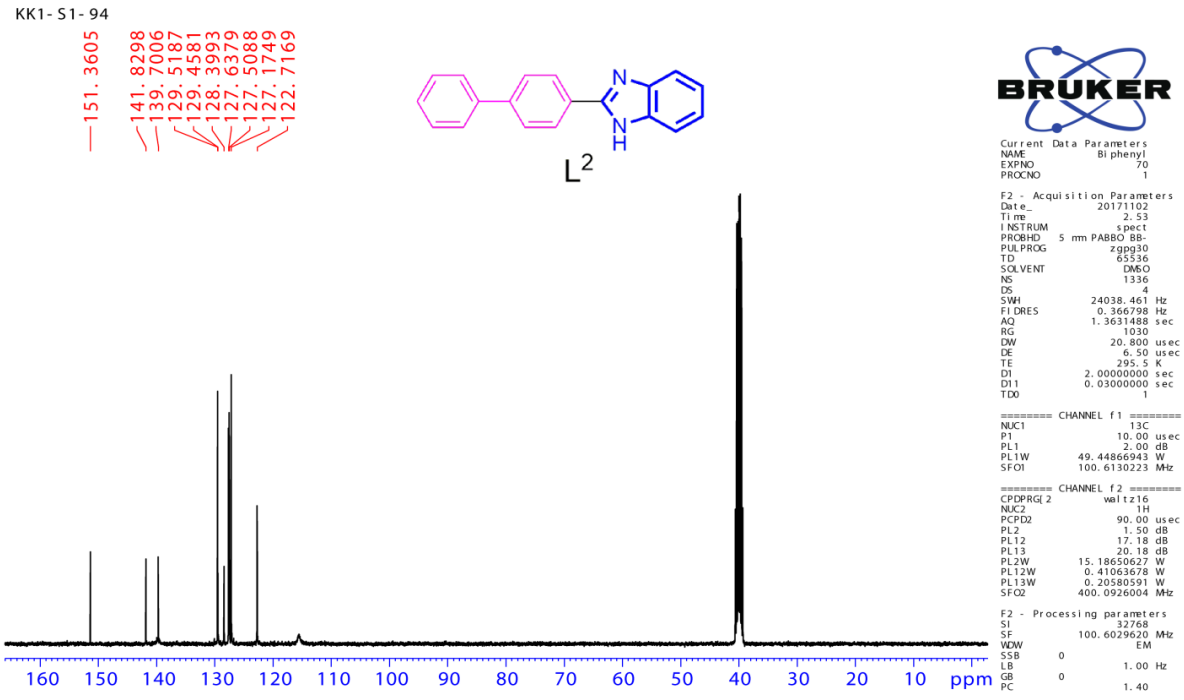

Fig. S10 ^{13}C NMR spectrum of L^2 in d_6-DMSO.

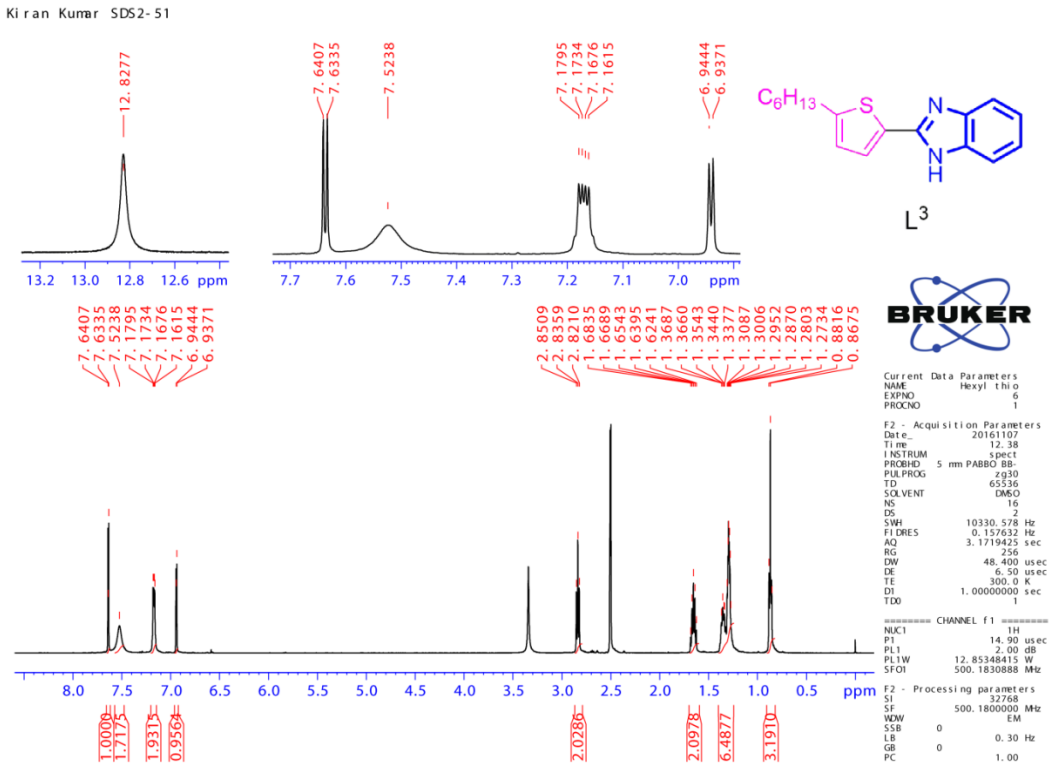

Fig. S11 ^{1}H NMR spectrum of L^3 in d_6-DMSO.

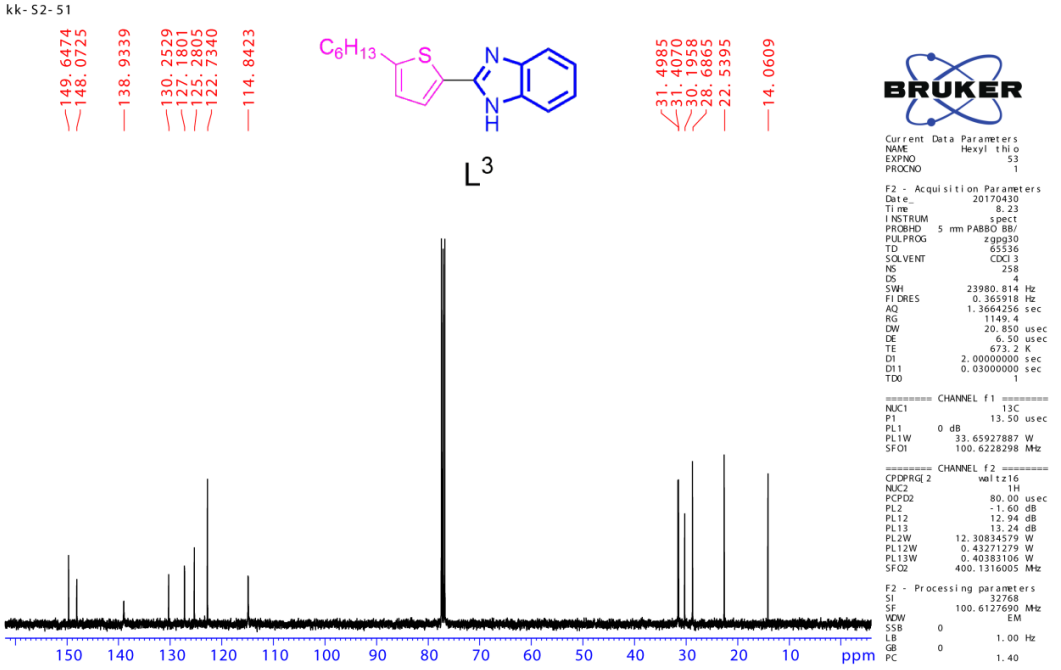

Fig. S12 ^{13}C NMR spectrum of L^3 in $CDCl_3$.

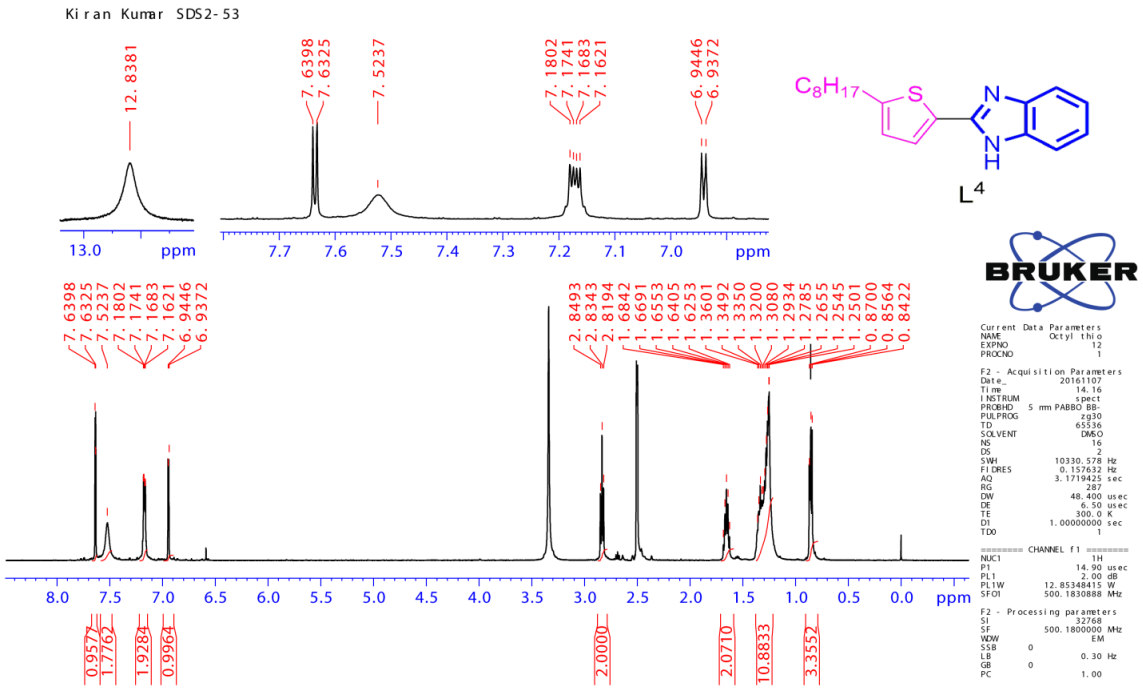

Fig. S13 ^{13}C NMR spectrum of L^4 in d_6-DMSO.

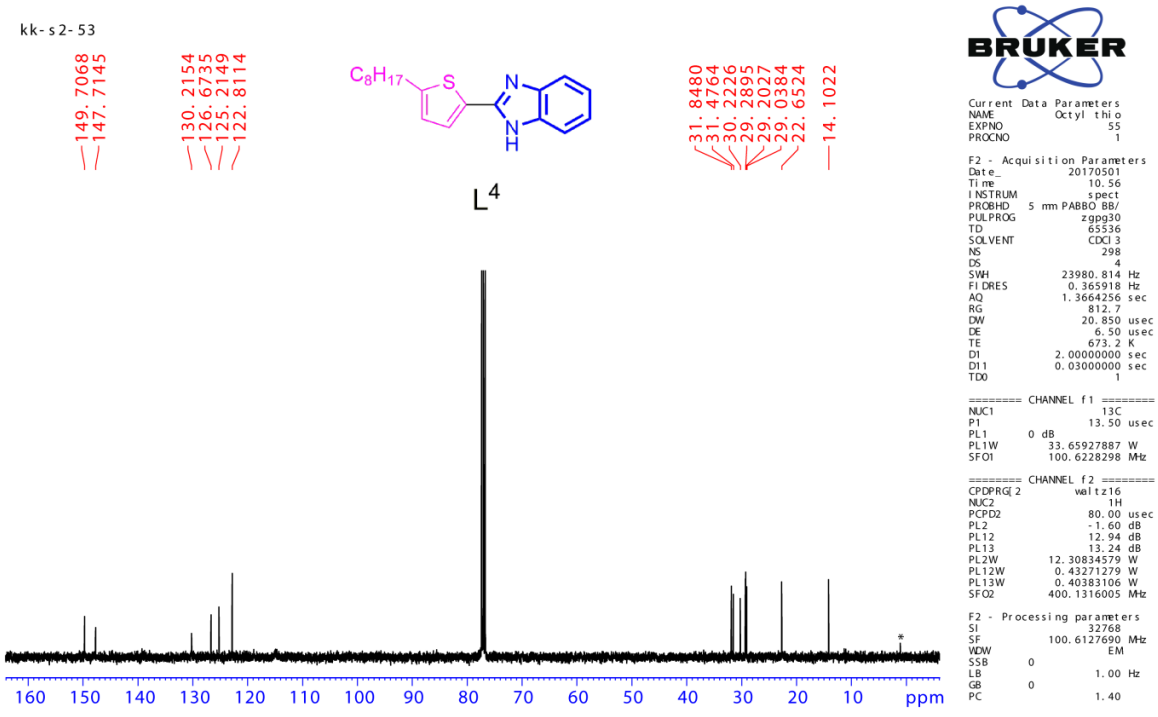

Fig. S14 ^{13}C NMR spectrum of L^4 in $CDCl_3$ (* = solvent residual peaks).

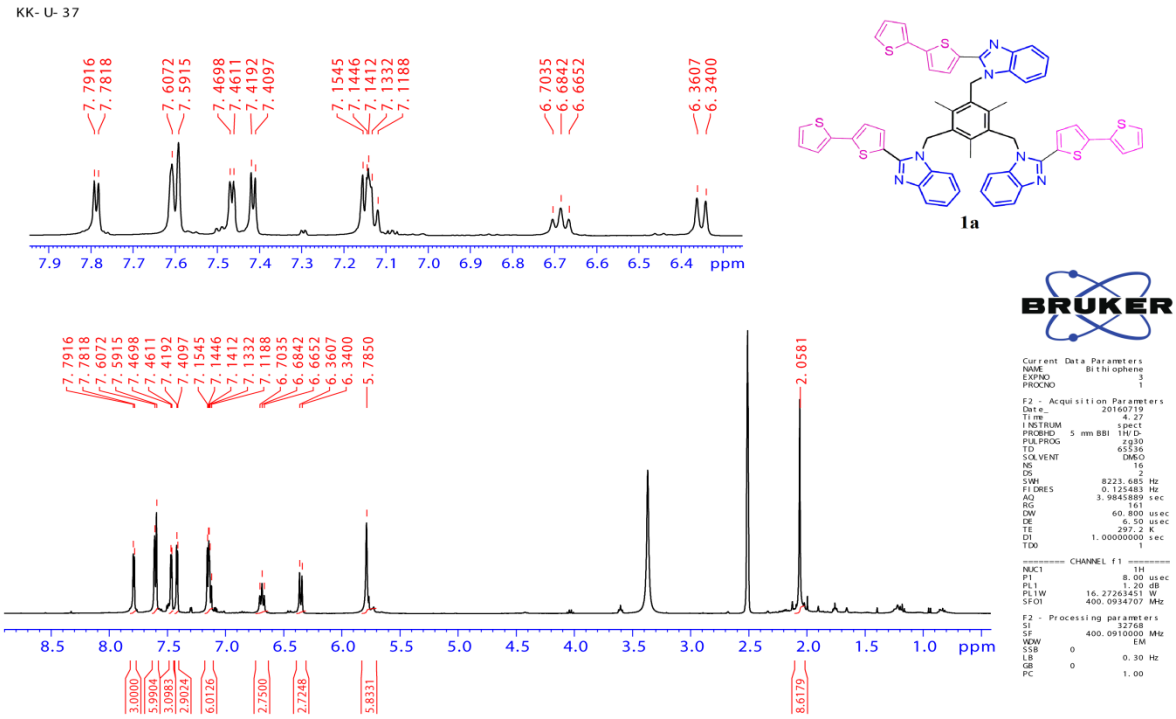

Fig. S15 ^{1}H NMR spectrum of **1a** in d_6-DMSO.

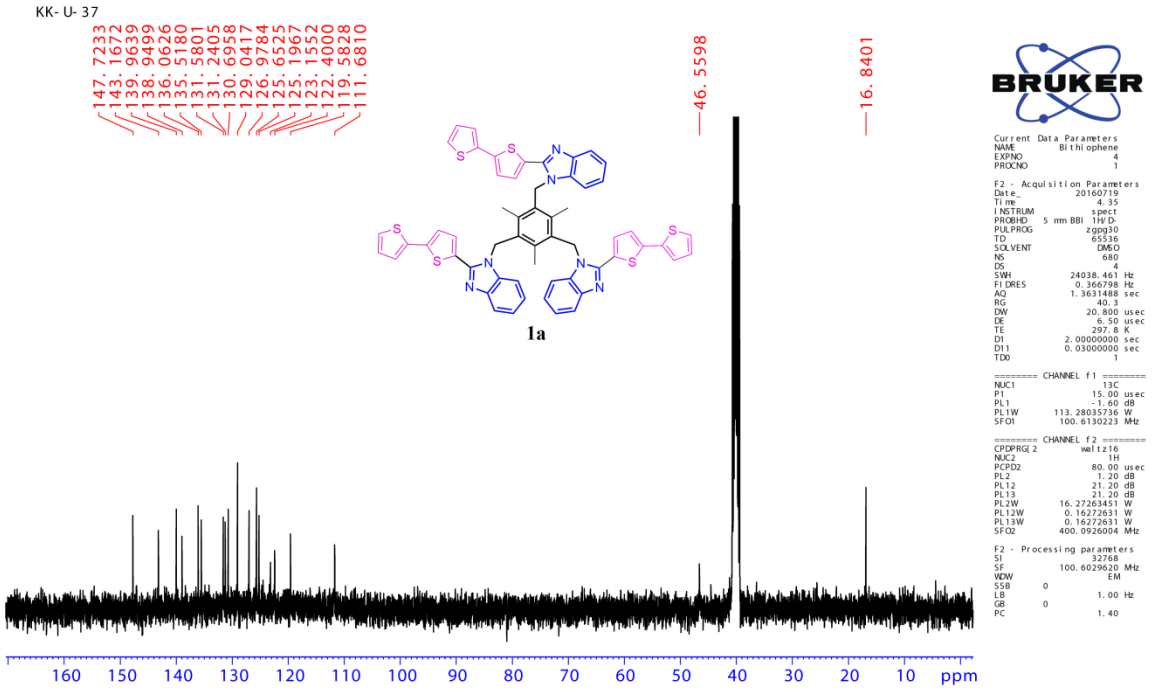

Fig. S16 ^{13}C NMR spectrum of **1a** in d_6-DMSO.

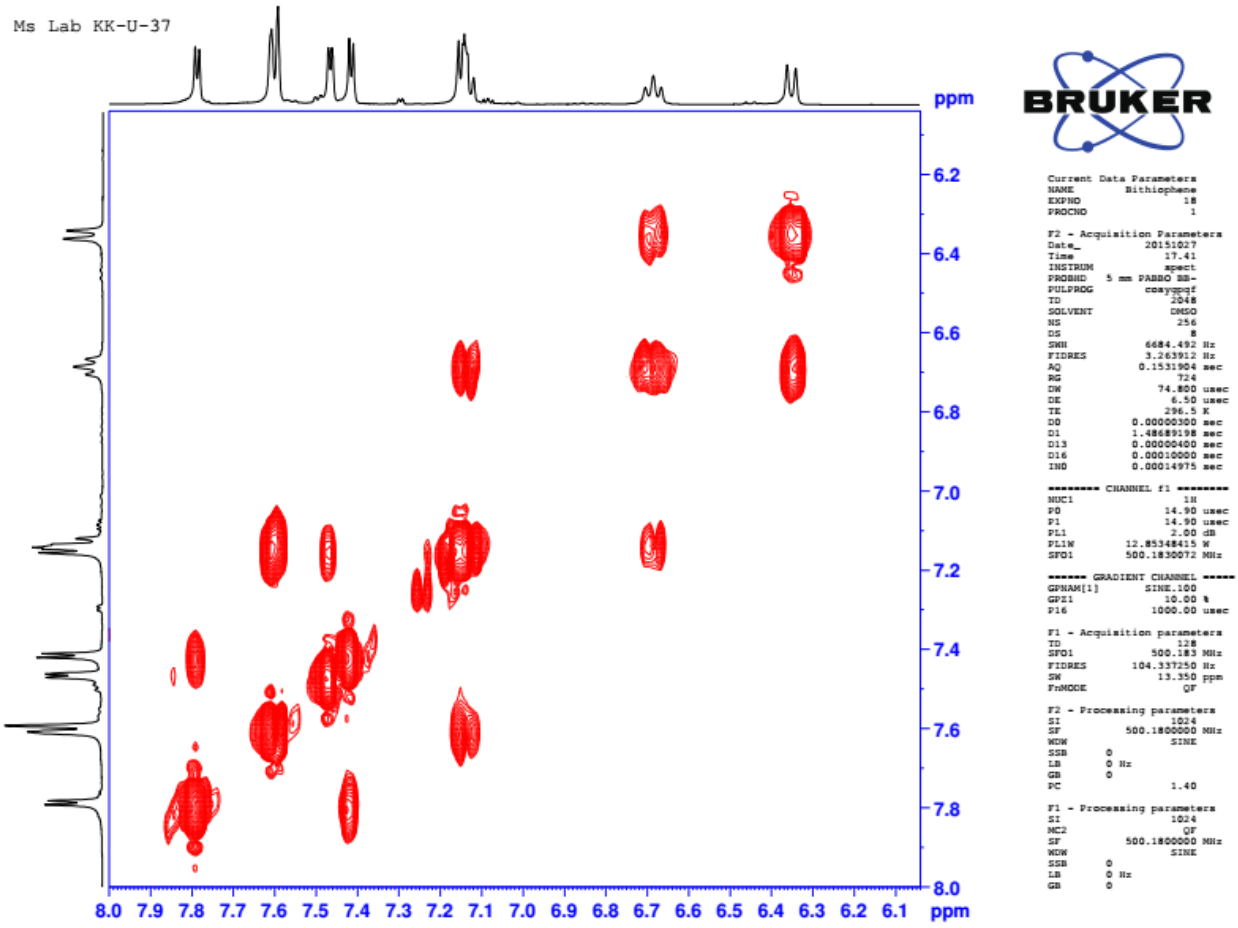

Fig. S17 Partial ^{1}H-^{1}H COSY NMR spectrum of **1a** in d_6-DMSO.

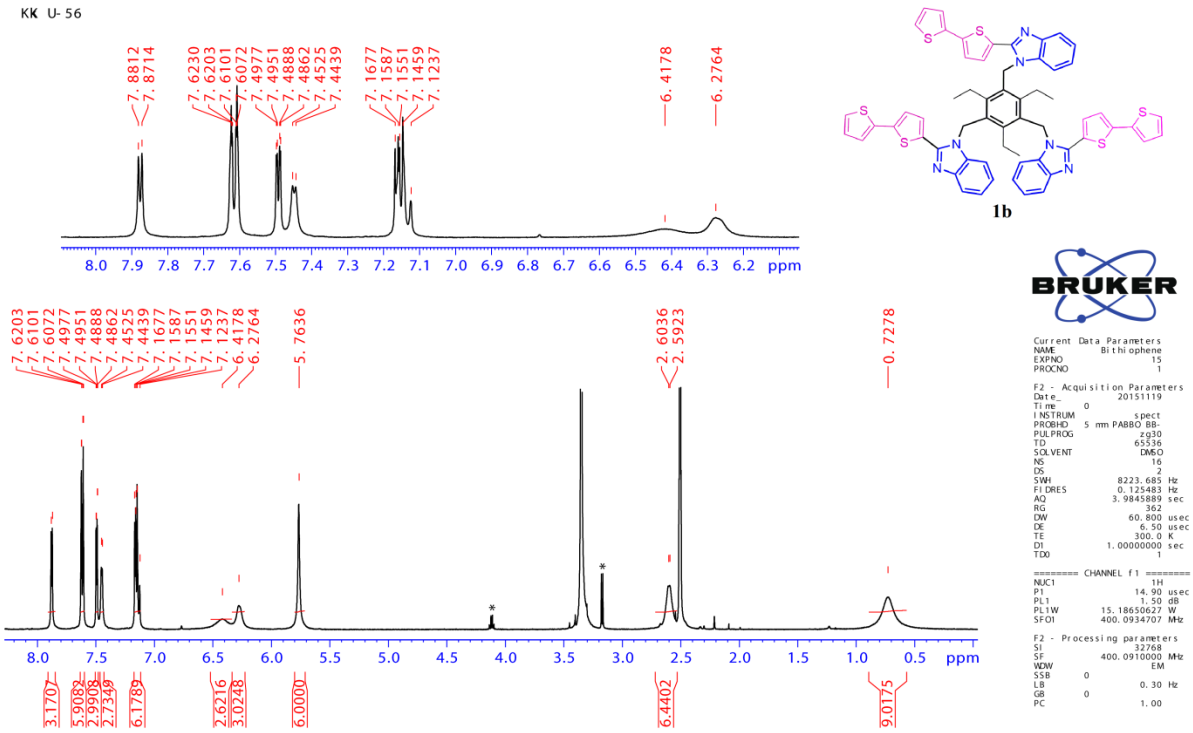

Fig. S18 ^{1}H NMR spectrum of **1b** in d_6-DMSO (* = solvent residual peaks).

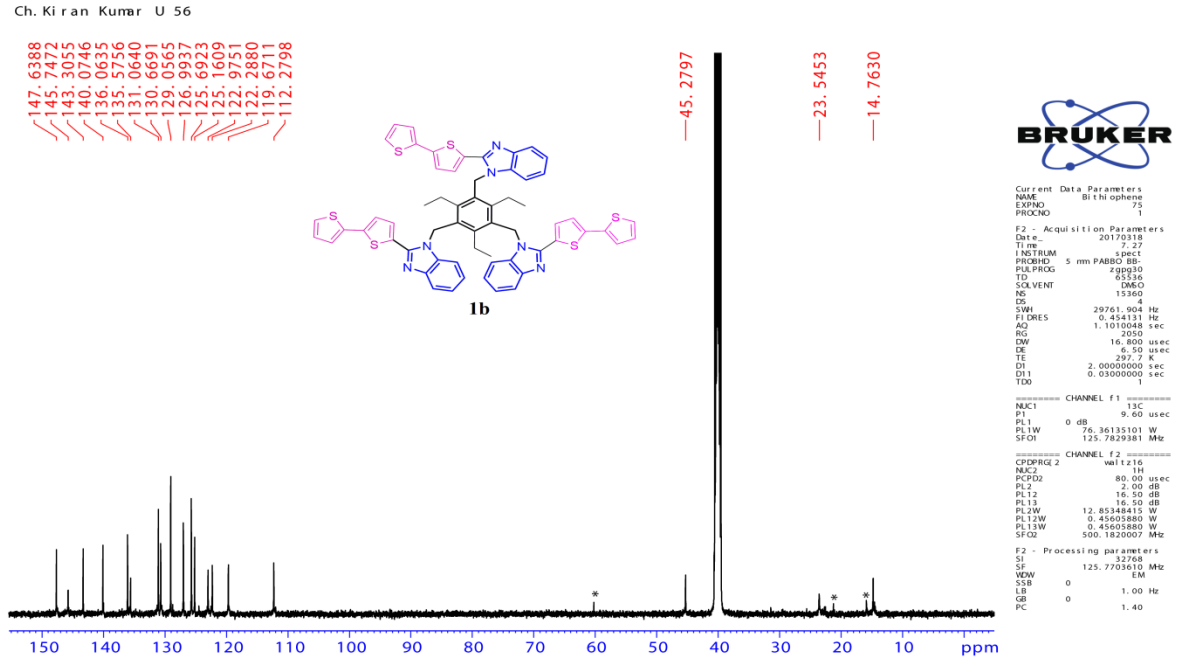

Fig. S19 ^{13}C NMR spectrum of **1b** in d_6-DMSO.

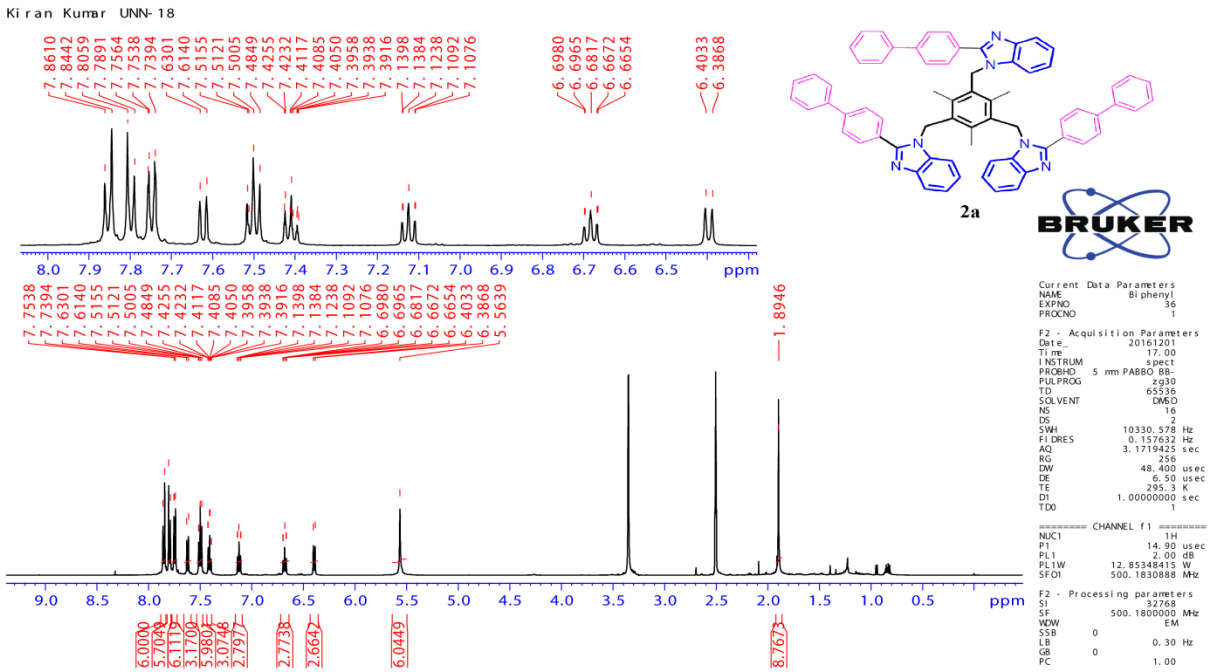

Fig. S20 ^{1}H NMR spectrum of **2a** in d_6-DMSO.

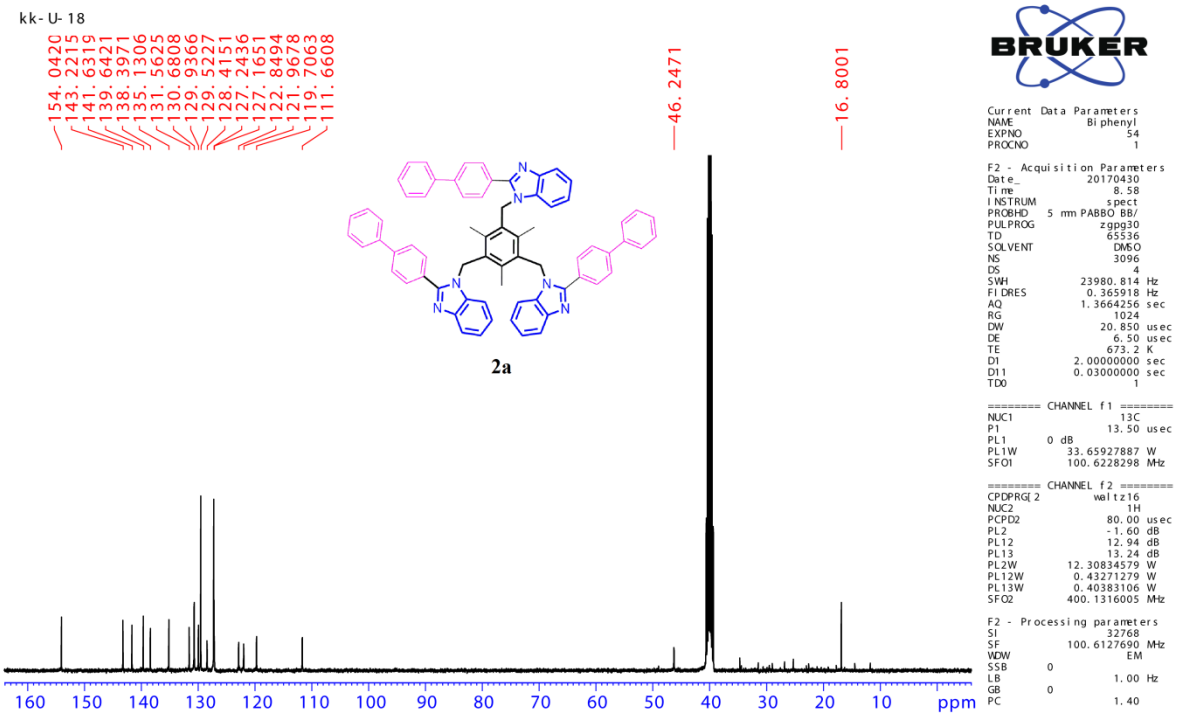

Fig. S21 ^{13}C NMR spectrum of **2a** in d_6-DMSO (* = solvent residual peaks).

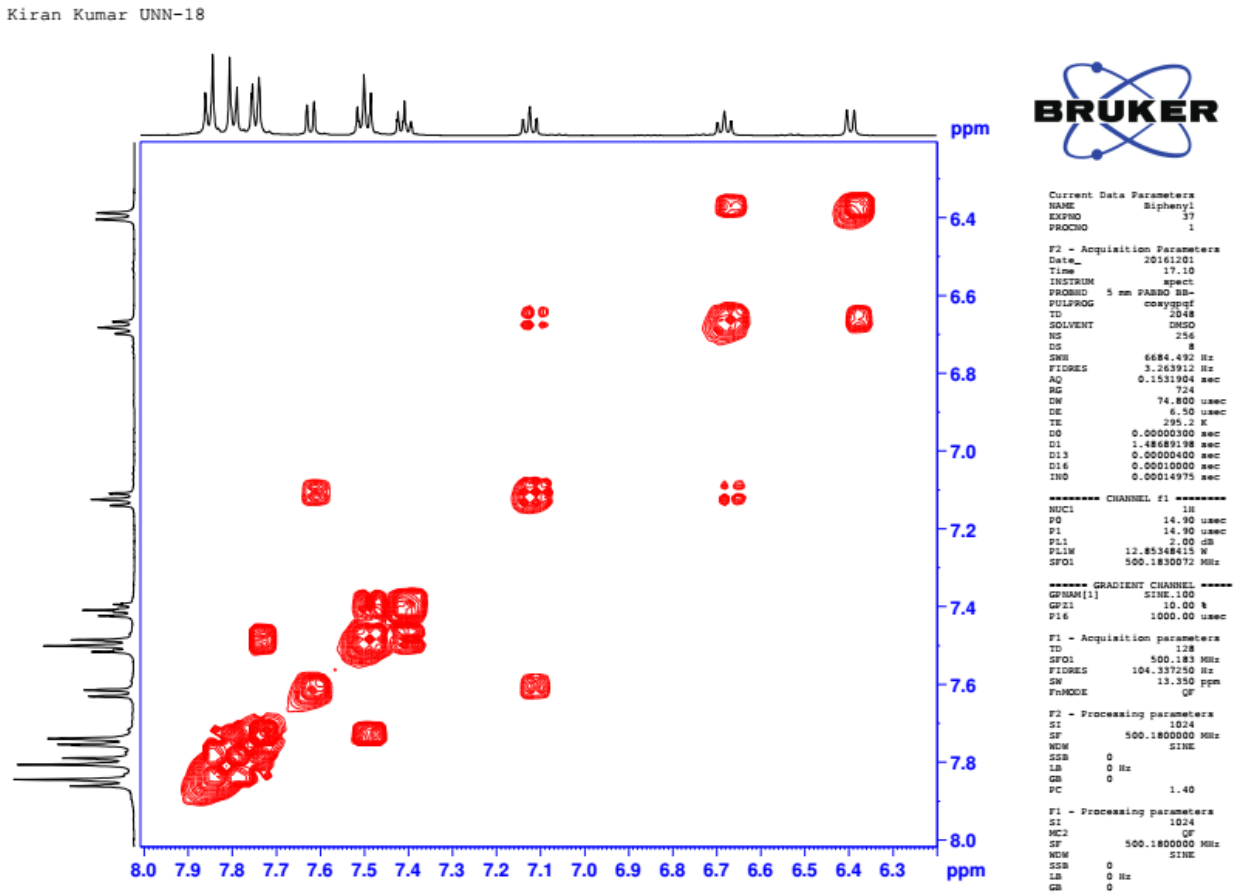

Fig. S22 Partial ^{1}H-^{1}H COSY NMR spectrum of **2a** in d_6-DMSO.

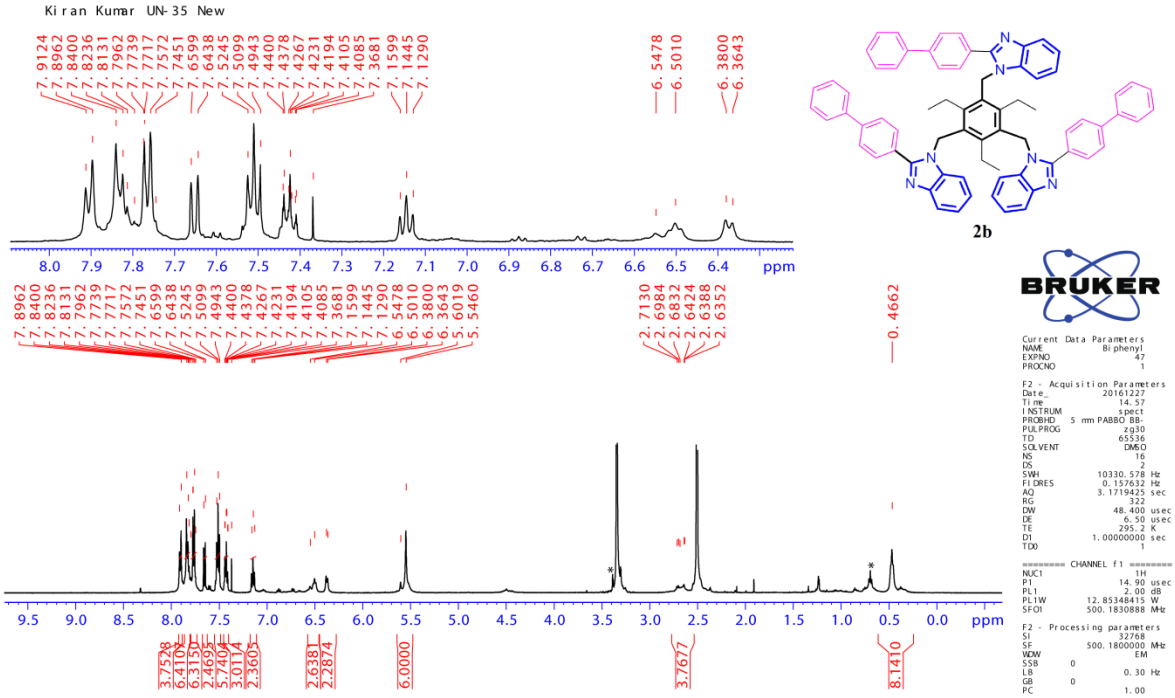

Fig. S23 ^{1}H NMR spectrum of **2b** in d_6-DMSO (* = solvent residual peaks).

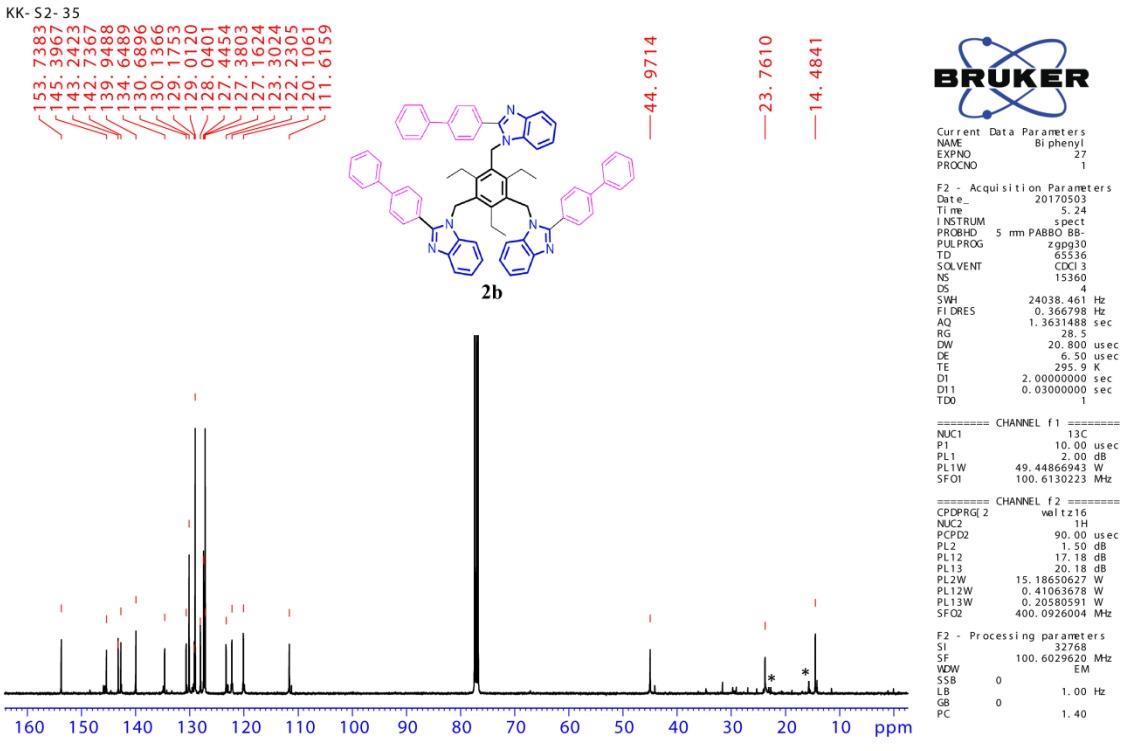

Fig. S24 ^{13}C NMR spectrum of **2b** in $CDCl_3$ (* = solvent residual peaks).

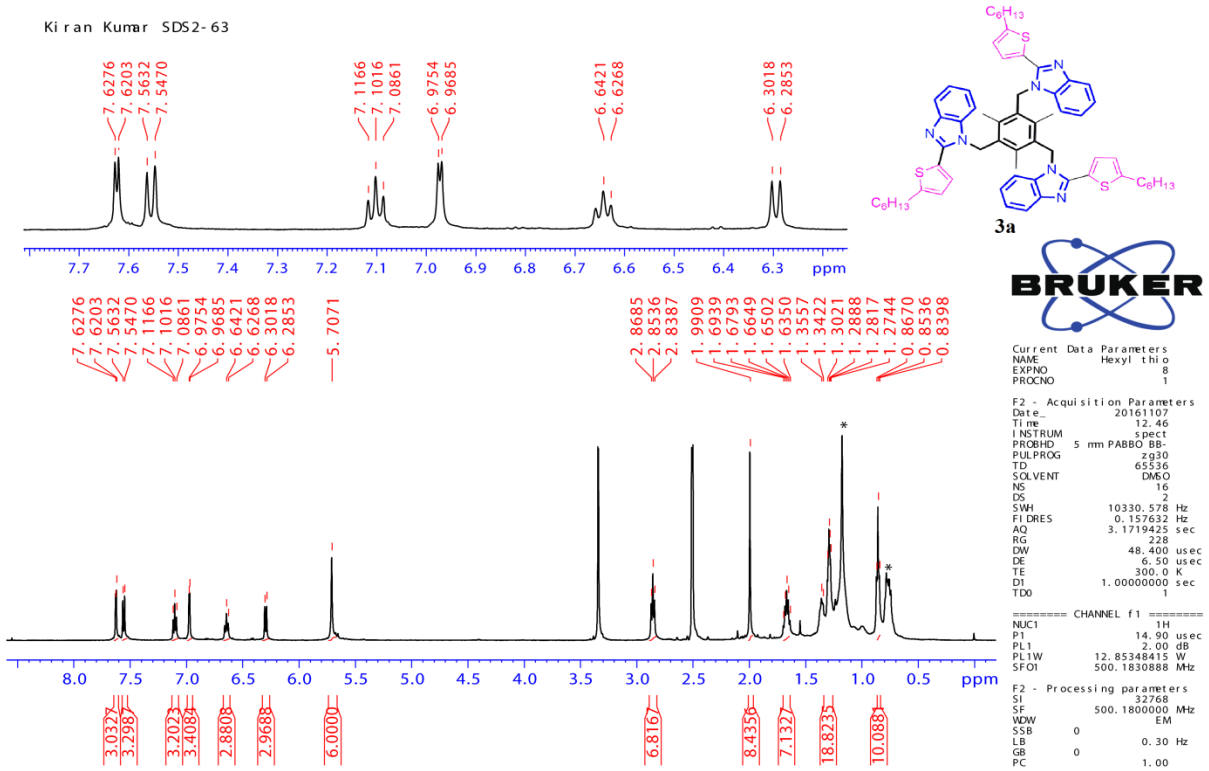

Fig. S25 ^{1}H NMR spectrum of **3a** in d_6-DMSO (* = solvent residual peaks).

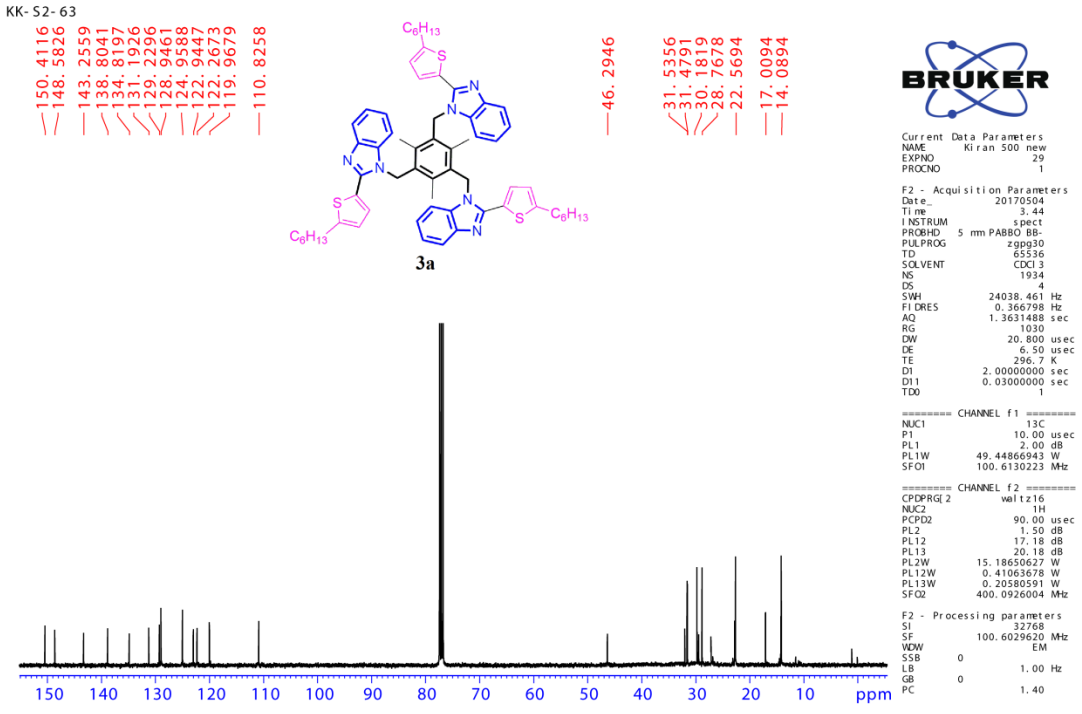

Fig. S26 ^{13}C NMR spectrum of **3a** in $CDCl_3$.

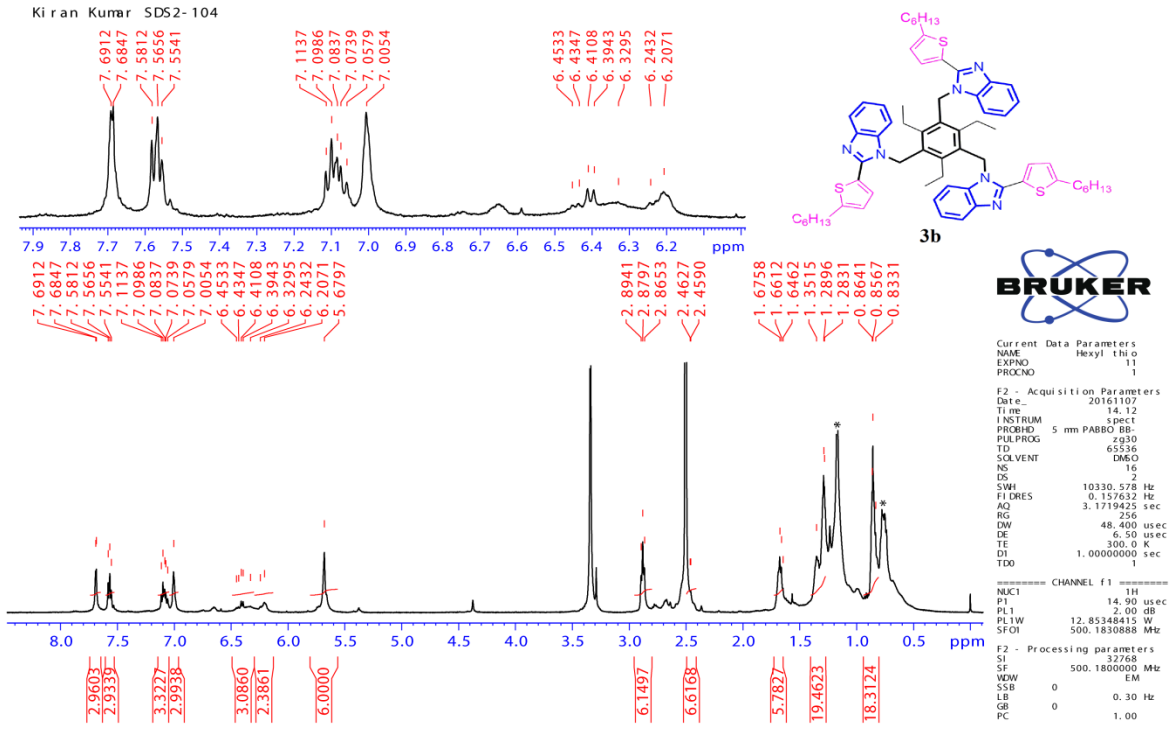

Fig. S27 ^{1}H NMR spectrum of **3b** in d_6-DMSO (* = solvent residual peaks).

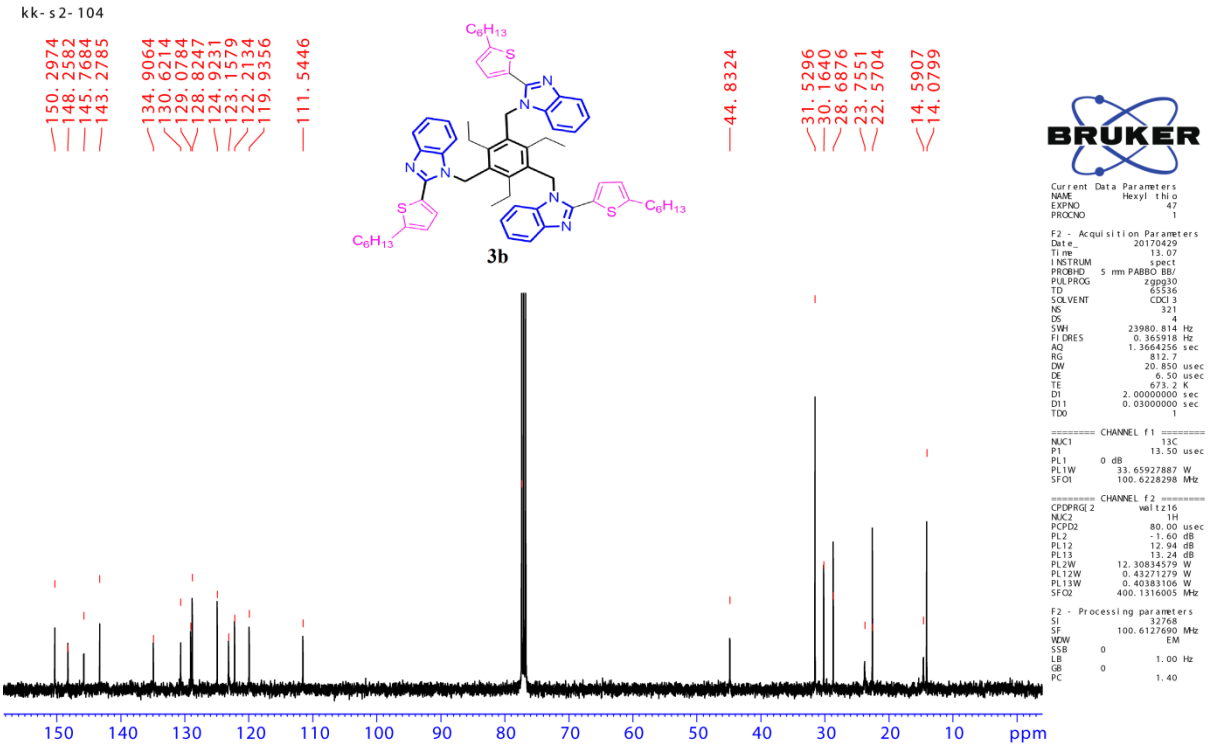

Fig. S28 ^{13}C NMR spectrum of **3b** in $CDCl_3$.

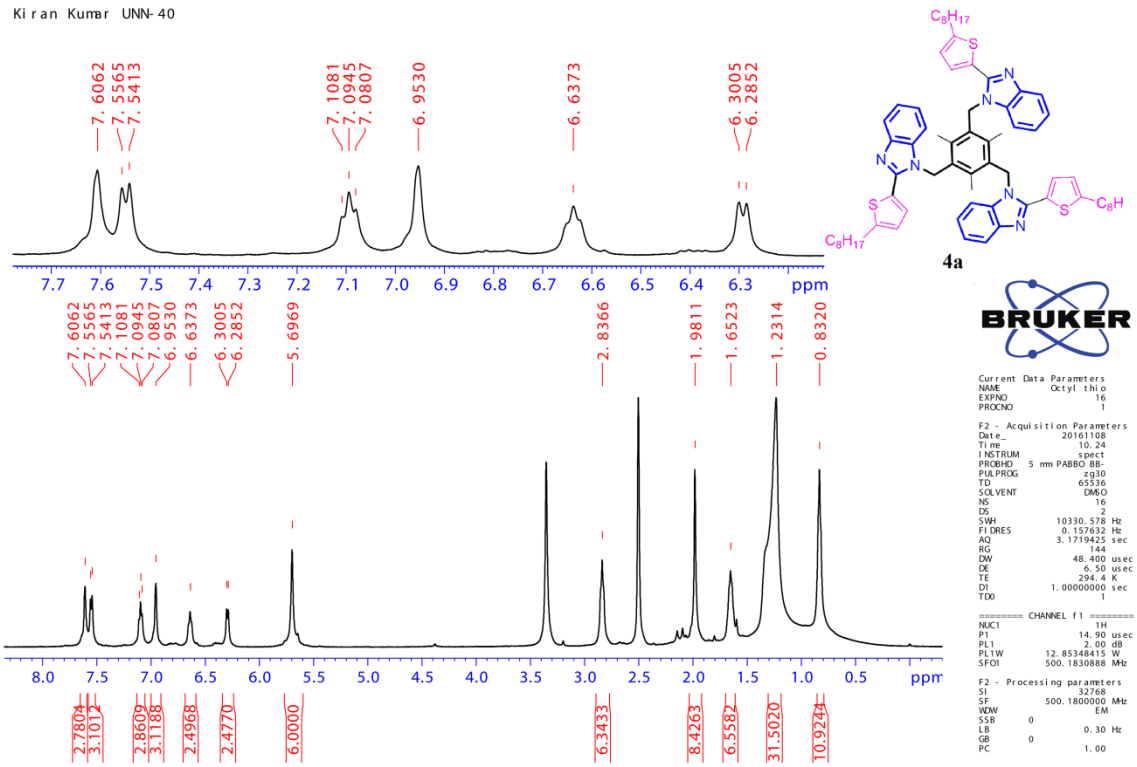

Fig. S29 ^{1}H NMR spectrum of **4a** in d_6-DMSO.

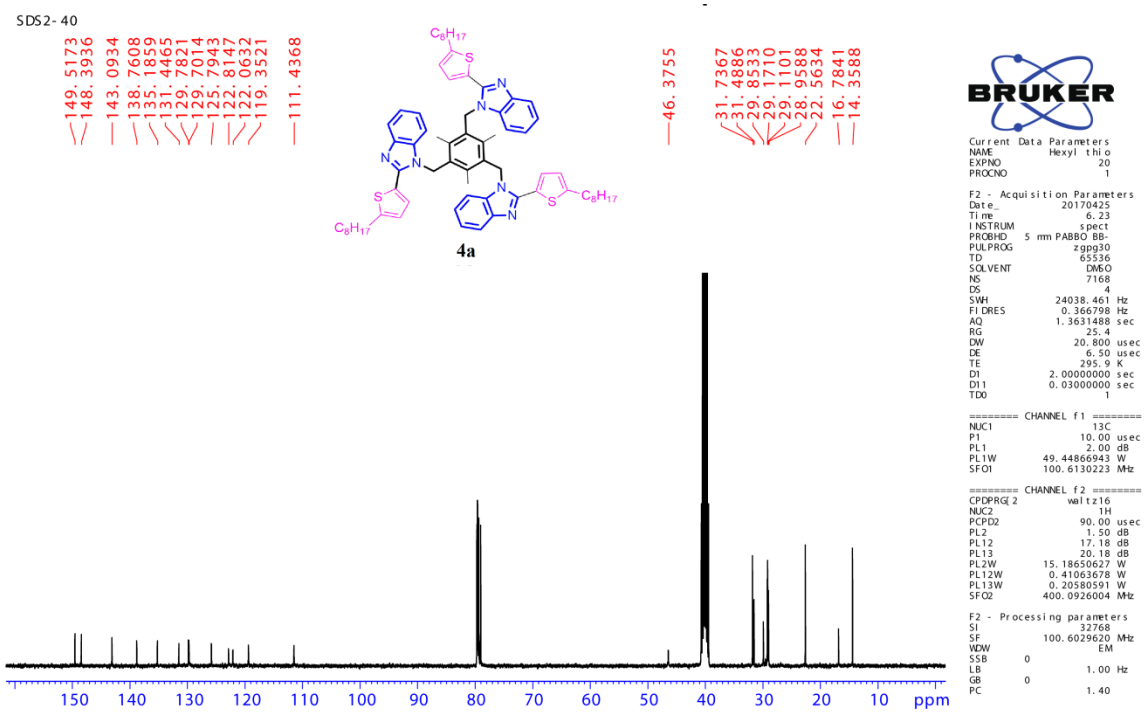

Fig. S30 ^{13}C NMR spectrum of **4a** in $CDCl_3$+d_6-DMSO.

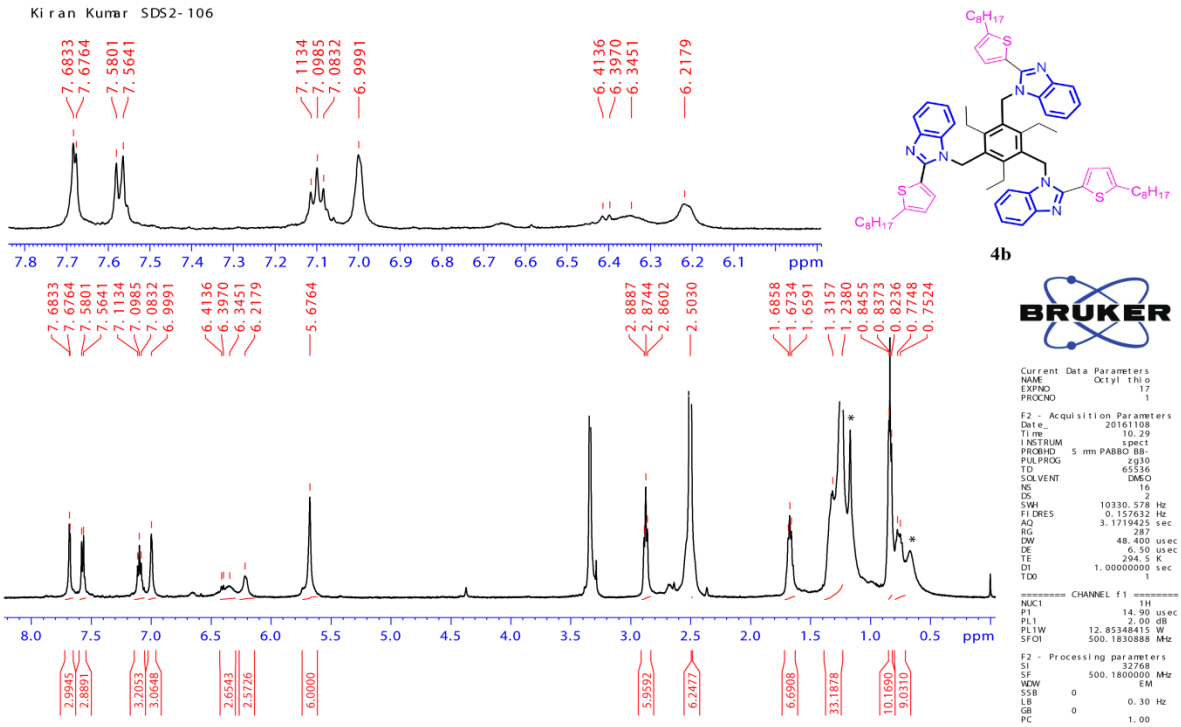

Fig. S31 ^{1}H NMR spectrum of **4b** in d_6-DMSO (* = solvent residual peaks).

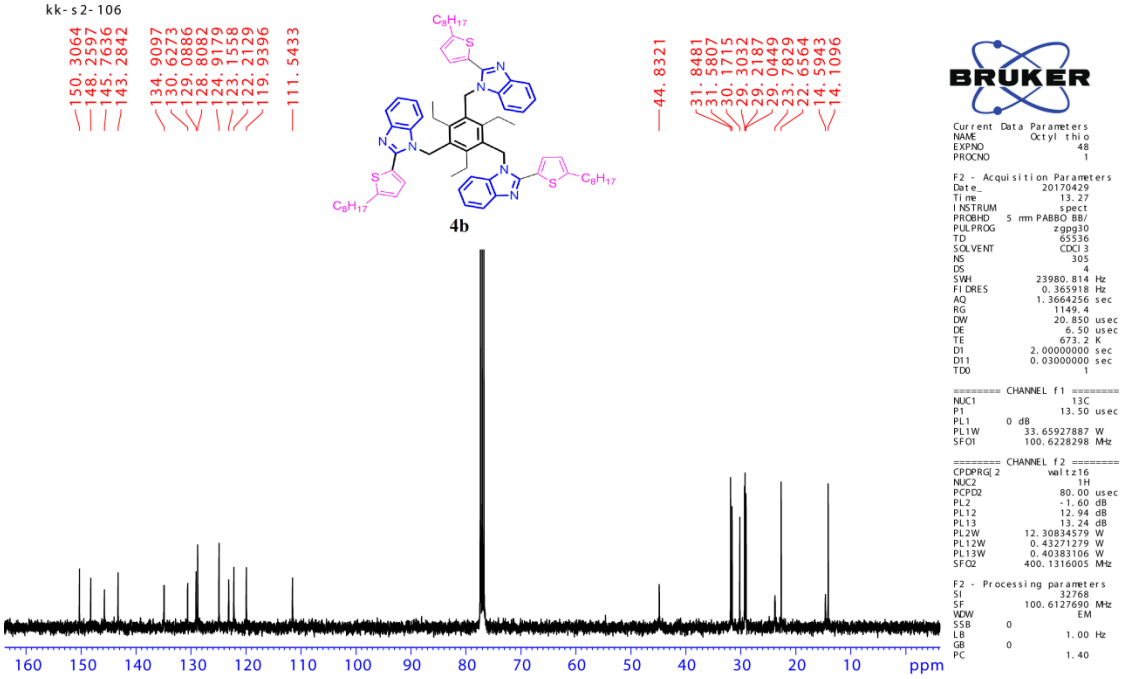

Fig. S32 ^{13}C NMR spectrum of **4b** in $CDCl_3$.

Table S1. The energy and optimized cartesian coordinates (in Å) of **1a** at MPW1PW91/6-31G(d,p) level of theory and basis function.

Energy@MPW1PW91/6-31G(d,p)= −4914.56353 Hartree

Atomic Symbol	X	Y	Z
S	2.05068700	6.79741600	-0.09578100
S	-6.91207900	-1.62276200	-0.09578100
S	4.86139200	-5.17465500	-0.09578100
N	2.15634200	2.94320900	0.97085600
N	2.37342500	4.83068400	2.18636600
N	-3.62706400	0.39584200	0.97085600
N	-5.37020700	-0.35989600	2.18636600
N	1.47072300	-3.33905100	0.97085600
N	2.99678300	-4.47078800	2.18636600
C	0.96615100	1.01483600	-0.13250100
C	-0.39635300	1.35252700	-0.13608400
C	-1.36194900	0.32929300	-0.13250100
C	-0.97314600	-1.01951500	-0.13608400
C	0.39579900	-1.34412900	-0.13250100
C	1.36949900	-0.33301200	-0.13608400
C	-0.82976000	2.79950200	-0.16225600
H	0.00000000	3.48723400	-0.02587200
H	-1.54636500	3.01833100	0.63350800
C	-2.00955900	-2.11834400	-0.16225600
C	2.83931900	-0.68115700	-0.16225600
H	3.02003300	-1.74361700	-0.02587200
H	3.38713400	-0.16997400	0.63350800
C	2.01634500	2.10553300	-0.21573600
H	2.98730300	1.67385900	-0.46167600
H	1.75911500	2.77772400	-1.03643900
C	2.05940300	2.56608300	2.30049100
C	1.88660800	1.33546000	2.93715900
H	1.77791500	0.40622300	2.39484700
C	1.84901300	1.34365900	4.32514500
H	1.72340400	0.39996200	4.84434300
C	1.97466000	2.53340900	5.06328900
H	1.94360900	2.48999300	6.14659600
C	2.14426600	3.75303000	4.43040100
H	2.24735200	4.67867400	4.98433400
C	2.18945600	3.76752200	3.03319000
C	2.36523500	4.31382100	0.97851100
C	2.53587400	5.13454100	-0.20575000
C	3.09054600	4.86979100	-1.43907400
H	3.51845700	3.91440800	-1.71170000
C	3.12180000	5.99700200	-2.28927300
H	3.54946400	5.98765800	-3.28411000
C	-2.83161700	0.69344000	-0.21573600
H	-2.94325600	1.75015000	-0.46167600
H	-3.28513700	0.13457600	-1.03643900
C	-3.25199500	0.50045300	2.30049100
C	-2.09984600	0.96612000	2.93715900
H	-1.24075700	1.33660800	2.39484700
C	-2.08814900	0.92946300	4.32514500
H	-1.20807900	1.29253000	4.84434300
C	-3.18132700	0.44340100	5.06328900
H	-3.12820100	0.43821800	6.14659600
C	-4.32235200	-0.01952700	4.43040100
H	-5.17552600	-0.39307300	4.98433400

C	-4.35749800	0.01236300	3.03319000
C	-4.91849600	-0.10855700	0.97851100
C	-5.71458000	-0.37113900	-0.20575000
C	-5.76263600	0.24159600	-1.43907400
H	-5.14920500	1.08986900	-1.71170000
C	-6.75445600	-0.29494300	-2.28927300
H	-6.96019600	0.08009700	-3.28411000
C	-7.47250300	-1.31675400	-1.70895100
C	0.81527200	-2.79897200	-0.21573600
H	-0.04404700	-3.42400900	-0.46167600
H	1.52602200	-2.91230100	-1.03643900
C	1.19259200	-3.06653700	2.30049100
C	0.21323900	-2.30158000	2.93715900
H	-0.53715800	-1.74283100	2.39484700
C	0.23913600	-2.27312200	4.32514500
H	-0.51532400	-1.69249200	4.84434300
C	1.20666700	-2.97681000	5.06328900
H	1.18459200	-2.92821100	6.14659600
C	2.17808700	-3.73350400	4.43040100
H	2.92817400	-4.28560100	4.98433400
C	2.16804200	-3.77988500	3.03319000
C	2.55326100	-4.20526400	0.97851100
C	3.17870600	-4.76340100	-0.20575000
C	2.67209000	-5.11138700	-1.43907400
H	1.63074800	-5.00427700	-1.71170000
C	3.63265700	-5.70205900	-2.28927300
H	3.41073200	-6.06775500	-3.28411000
C	4.87659400	-5.81300100	-1.70895100
C	2.59590900	7.12975500	-1.70895100
H	-1.84076900	-2.84835700	0.63350800
H	-3.02003300	-1.74361700	-0.02587200
C	6.08765000	-6.36794700	-2.27234900
C	7.20216800	-6.84323500	-1.62139700
S	6.28984900	-6.50390000	-3.99500700
C	8.20483400	-7.32096600	-2.50316600
H	7.28452300	-6.86816300	-0.54178300
C	7.84945600	-7.20825900	-3.81665200
H	9.14772300	-7.73926700	-2.17542200
H	8.41360800	-7.49570100	-4.69148300
C	-8.55862800	-2.08808600	-2.27234900
C	-9.52749900	-2.81564300	-1.62139700
S	-8.77746700	-2.19521800	-3.99500700
C	-10.44256000	-3.44511200	-2.50316600
H	-9.59026500	-2.87450000	-0.54178300
C	-10.16726300	-3.19369900	-3.81665200
H	-11.27626300	-4.05252700	-2.17542200
H	-10.69827100	-3.53854700	-4.69148300
C	2.47097900	8.45603200	-2.27234900
C	2.32533100	9.65887800	-1.62139700
S	2.48761900	8.69911900	-3.99500700
C	2.23772500	10.76607800	-2.50316600
H	2.30574200	9.74266300	-0.54178300
C	2.31780700	10.40195700	-3.81665200
H	2.12854100	11.79179400	-2.17542200
H	2.28466400	11.03424800	-4.69148300
H	-1.30878800	3.05542600	-1.11306400
H	3.30047100	-0.39426900	-1.11306400
H	-1.99168300	-2.66115700	-1.11306400

Table S2. The energy and optimized cartesian coordinates (in Å) of **1b** at MPW1PW91/6-31G(d,p) level of theory and basis function.

Energy@ MPW1PW91/6-31G(d,p)= −5032.48197 Hartree

Atomic Symbol	X	Y	Z
S	1.00529300	7.03029200	0.04569100
S	-6.59105800	-2.64453700	0.04569100
S	5.58576500	-4.38575500	0.04569100
N	1.70800200	3.20766800	0.99008200
N	1.68008700	5.07415000	2.25679000
N	-3.63192300	-0.12466200	0.99008200
N	-5.23438700	-1.08207800	2.25679000
N	1.92392100	-3.08300700	0.99008200
N	3.55430000	-3.99207400	2.25679000
C	0.80123100	1.15011800	-0.15898200
C	-0.60014200	1.27672700	-0.16276400
C	-1.39664600	0.11882700	-0.15898200
C	-0.80560700	-1.15810100	-0.16276400
C	0.59541600	-1.26894500	-0.15898200
C	1.40574800	-0.11862500	-0.16276400
C	-1.23152500	2.65407700	-0.21153000
H	-0.57234800	3.38201000	0.26097400
H	-2.14113600	2.67290000	0.39421700
C	-1.55112700	3.12097900	-1.63620600
H	-2.25670000	2.45111000	-2.13560400
H	-0.65165800	3.15699800	-2.25624100
H	-1.98601600	4.12305400	-1.62337700
C	-1.68273600	-2.39357100	-0.21153000
C	-1.92728400	-2.90380500	-1.63620600
H	-0.99437300	-3.17991400	-2.13560400
H	-2.40821100	-2.14285200	-2.25624100
H	-2.57766200	-3.78146800	-1.62337700
C	2.91426100	-0.26050600	-0.21153000
H	3.21508000	-1.19533700	0.26097400
H	3.38536700	0.51782800	0.39421700
C	3.47841100	-0.21717400	-1.63620600
H	3.05987000	-1.01414600	-2.25624100
H	4.56367800	-0.34158700	-1.62337700
H	3.25107400	0.72880500	-2.13560400
C	1.66115500	2.39872400	-0.22463400
H	2.67929500	2.14219100	-0.51879100
H	1.27077800	3.05220200	-1.00585200
C	1.70345900	2.78521900	2.31034100
C	1.72604400	1.52706900	2.91592000
H	1.73979700	0.60607800	2.34993000
C	1.72138700	1.49451400	4.30389300
H	1.74230300	0.52971900	4.79842000
C	1.69276500	2.67079400	5.07329800
H	1.69499100	2.59575800	6.15533900
C	1.66872000	3.91759600	4.47205400
H	1.65047300	4.83442900	5.04947900
C	1.67596800	3.97357000	3.07516600
C	1.71466800	4.59373200	1.03463800
C	1.72938000	5.46239000	-0.12762300
C	2.28234000	5.31767300	-1.38146600
H	2.84022100	4.44509600	-1.69391000
C	2.12189700	6.45999300	-2.19644900
H	2.51868400	6.54255100	-3.20068200
C	-2.90793400	0.23924100	-0.22463400

H	-3.19484000	1.24924200	-0.51879100
H	-3.27867400	-0.42557500	-1.00585200
C	-3.26380000	0.08262800	2.31034100
C	-2.18550300	0.73126300	2.91592000
H	-1.39477800	1.20367000	2.34993000
C	-2.15498100	0.74350800	4.30389300
H	-1.32990200	1.24401900	4.79842000
C	-3.15935800	0.13058100	5.07329800
H	-3.09548800	0.17002700	6.15533900
C	-4.22709800	-0.51364400	4.47205400
H	-5.01197500	-0.98786300	5.04947900
C	-4.27919700	-0.53535400	3.07516600
C	-4.83562200	-0.81192000	1.03463800
C	-5.59525800	-1.23350800	-0.12762300
C	-5.74640900	-0.68227200	-1.38146600
H	-5.26967700	0.23715600	-1.69391000
C	-6.65546700	-1.39238000	-2.19644900
H	-6.92535700	-1.09003200	-3.20068200
C	-7.20714500	-2.48675600	-1.56858200
C	1.24677700	-2.63796500	-0.22463400
H	0.51554400	-3.39143400	-0.51879100
H	2.00789600	-2.62662700	-1.00585200
C	1.56034200	-2.86784800	2.31034100
C	0.45945900	-2.25833300	2.91592000
H	-0.34502000	-1.80974800	2.34993000
C	0.43359300	-2.23802200	4.30389300
H	-0.41240100	-1.77373800	4.79842000
C	1.46659300	-2.80137400	5.07329800
H	1.40049700	-2.76578500	6.15533900
C	2.55837800	-3.40395100	4.47205400
H	3.36150200	-3.84656600	5.04947900
C	2.60322800	-3.43821600	3.07516600
C	3.12095400	-3.78181100	1.03463800
C	3.86587800	-4.22888300	-0.12762300
C	3.46407000	-4.63540000	-1.38146600
H	2.42945500	-4.68225200	-1.69391000
C	4.53357000	-5.06761400	-2.19644900
H	4.40667400	-5.45251900	-3.20068200
C	5.75716700	-4.99819300	-1.56858200
C	1.44997800	7.48494900	-1.56858200
H	-1.24423200	-3.19072800	0.39421700
H	-2.64273200	-2.18667300	0.26097400
C	7.05809000	-5.36102100	-2.08658700
C	8.20251100	-5.68274200	-1.39483400
S	7.34763100	-5.43220200	-3.80078400
C	9.29895000	-5.99301900	-2.23918100
H	8.24346300	-5.71701500	-0.31311000
C	8.98456800	-5.90714100	-3.56511800
H	10.27850200	-6.27698300	-1.87683300
H	9.61950000	-6.09286100	-4.41871600
C	-8.17182500	-3.43197500	-2.08658700
C	-9.02265400	-4.26221200	-1.39483400
S	-8.37824100	-3.64713400	-3.80078400
C	-9.83958100	-5.05661800	-2.23918100
H	-9.07281200	-4.28054100	-0.31311000
C	-9.60801800	-4.82729300	-3.56511800
H	-10.57527800	-5.76295200	-1.87683300
H	-10.08632200	-5.28430100	-4.41871600
C	1.11373600	8.79299600	-2.08658700
C	0.82014300	9.94495300	-1.39483400
S	1.03060900	9.07933600	-3.80078400

C	0.54063200	11.04963700	-2.23918100
H	0.82934900	9.99755600	-0.31311000
C	0.62345000	10.73443400	-3.56511800
H	0.29677500	12.03993600	-1.87683300
H	0.46682200	11.37716100	-4.41871600

Table S3. The energy and optimized cartesian coordinates (in Å) of **2a** at MPW1PW91/6-31G(d,p) level of theory and basis function.

Energy@ MPW1PW91/6-31G(d,p)= −2989.88808 Hartree

Atomic Symbol	**X**	**Y**	**Z**
C	0.86125900	2.78912900	-0.24890900
H	0.00000000	3.43436100	-0.07601800
H	1.52816200	2.93151200	0.60354300
N	1.57866700	3.27278100	-1.42463100
C	0.41994900	1.33762000	-0.30026800
N	3.21053500	4.24900700	-2.63311200
C	1.37492500	0.30899000	-0.28995800
C	-0.95505600	1.03622500	-0.28995800
N	2.04497800	-3.00355700	-1.42463100
C	0.94843900	-1.03249600	-0.30026800
C	-1.36838700	-0.30512400	-0.30026800
C	-0.87902800	-2.78379200	-0.24119000
H	-0.05278700	-3.48823400	-0.24799900
H	-1.51027900	-3.03581700	-1.09826500
N	-3.62364500	-0.26922400	-1.42463100
C	2.33198700	3.62098500	-3.48269200
C	1.95170900	-2.62168200	-2.75232800
N	2.07448100	-4.90490800	-2.63311200
C	-0.41986900	-1.34521500	-0.28995800
C	-1.97132000	2.15315600	-0.24119000
H	-2.99450600	1.78983200	-0.24799900
H	-1.87395500	2.82584900	-1.09826500
C	2.73405900	4.04066700	-1.42912600
C	1.29458900	3.00107100	-2.75232800
C	-3.24629800	-0.37938900	-2.75232800
C	1.98482700	-2.14043700	-0.24890900
H	2.97424400	-1.71718000	-0.07601800
H	1.77468300	-2.78918400	0.60354300
C	-2.84608600	-0.64869200	-0.24890900
H	-2.97424400	-1.71718000	-0.07601800
H	-3.30284500	-0.14232900	0.60354300
C	1.96987200	-3.83005200	-3.48269200
C	2.85034800	0.63063500	-0.24119000
H	3.38423500	0.20996900	-1.09826500
H	3.04729300	1.69840300	-0.24799900
C	2.13229100	-4.38809800	-1.42912600
C	2.35031900	3.55524500	-4.87858500
H	3.14694200	4.03757200	-5.43296200
C	-2.12741100	-0.92204100	-3.38702200
H	-1.30232700	-1.36175400	-2.84306400
C	1.86221700	-1.38137100	-3.38702200
H	1.83047700	-0.44697100	-2.84306400
N	-5.28501600	0.65590100	-2.63311200
C	1.32679600	2.86946000	-5.51140600
H	1.31055700	2.80793900	-6.59425500
C	-2.10160900	-0.86604900	-4.77413200
H	-1.24715800	-1.28582000	-5.29328800
C	-4.30185900	0.20906700	-3.48269200
C	-4.25409300	0.25781300	-4.87858500
H	-5.07011100	0.70654500	-5.43296200
C	0.30078400	2.25307100	-4.77413200
H	-0.48997300	1.72298100	-5.29328800
C	0.26519400	2.30341200	-3.38702200
H	-0.52815000	1.80872500	-2.84306400
C	1.80082500	-1.38702200	-4.77413200

H	1.73713200	-0.43716100	-5.29328800
C	-3.14842300	-0.28569100	-5.51140600
H	-3.08702500	-0.26899400	-6.59425500
C	1.82162700	-2.58376900	-5.51140600
H	1.77646800	-2.53894500	-6.59425500
C	1.90377300	-3.81305900	-4.87858500
H	1.92316900	-4.74411700	-5.43296200
C	-4.86635000	0.34743100	-1.42912600
C	3.38818300	4.57315100	-0.22578600
C	4.78808200	4.56969000	-0.17805600
C	2.68831500	5.14796800	0.84187000
C	5.46090600	5.09384800	0.91378900
H	5.33325500	4.16466900	-1.02252800
C	3.36705900	5.67094400	1.93434400
H	1.60655100	5.21649300	0.81094000
C	4.76500300	5.64795100	1.99715200
H	6.54565800	5.09970100	0.91860500
H	2.80245000	6.09262800	2.75900400
C	2.26637300	-5.22082800	-0.22578600
C	1.56342600	-6.43144600	-0.17805600
C	3.11411300	-4.90213300	0.84187000
C	1.68094900	-7.27620700	0.91378900
H	0.94008100	-6.70106900	-1.02252800
C	3.22765200	-5.75143100	1.93434400
H	3.71434000	-3.99956000	0.81094000
C	2.50876800	-6.95058900	1.99715200
H	1.14364100	-8.21855700	0.91860500
H	3.87514600	-5.47330700	2.75900400
C	-5.65455600	0.64767700	-0.22578600
C	-6.35150800	1.86175600	-0.17805600
C	-5.80242800	-0.24583500	0.84187000
C	-7.14185500	2.18235900	0.91378900
H	-6.27333600	2.53640000	-1.02252800
C	-6.59471100	0.08048700	1.93434400
H	-5.32089100	-1.21693200	0.81094000
C	-7.27377100	1.30263800	1.99715200
H	-7.68930000	3.11885600	0.91860500
H	-6.67759500	-0.61932100	2.75900400
C	-8.11206400	1.65086300	3.16444800
C	-8.89400800	0.68068400	3.80403800
C	-8.14444100	2.96126700	3.65786900
C	-9.68121800	1.00986100	4.90100400
H	-8.90629100	-0.33342200	3.41849600
C	-8.93165900	3.29052700	4.75484600
H	-7.52648200	3.72155700	3.19165100
C	-9.70320300	2.31610300	5.38132100
H	-10.28713400	0.24551400	5.37590100
H	-8.93623100	4.30983400	5.12619100
H	-10.31813900	2.57302700	6.23700000
C	2.62634300	-7.85068600	3.16444800
C	3.85751500	-8.04277800	3.80403800
C	1.50768800	-8.53392600	3.65786900
C	3.96604300	-8.88911100	4.90100400
H	4.74189700	-7.54636400	3.41849600
C	1.61615000	-9.38030700	4.75484600
H	0.54027900	-8.37890300	3.19165100
C	2.84579800	-9.56127200	5.38132100
H	4.93094600	-9.03167600	5.37590100
H	0.73569000	-9.89392000	5.12619100
H	2.93076300	-10.22228400	6.23700000
C	5.48572200	6.19982200	3.16444800
C	5.03649300	7.36209500	3.80403800
C	6.63675300	5.57265900	3.65786900
C	5.71517400	7.87925000	4.90100400
H	4.16439400	7.87978500	3.41849600
C	7.31550900	6.08978000	4.75484600
H	6.98620400	4.65734700	3.19165100
C	6.85740500	7.24516900	5.38132100
H	5.35618800	8.78616200	5.37590100
H	8.20054100	5.58408600	5.12619100

H	7.38737600	7.64925700	6.23700000
H	3.31471900	0.22756300	0.66392100
H	-1.46028500	-2.98441200	0.66392100
H	-1.85443500	2.75685000	0.66392100

Table S4. The energy and optimized cartesian coordinates (in Å) of **2b** at MPW1PW91/6-31G(d,p) level of theory and basis function.

Energy@ MPW1PW91/6-31G(d,p)= −3107.80643 Hartree

Atomic Symbol	**X**	**Y**	**Z**
C	-0.84229500	2.79517100	0.21643400
H	0.00000000	3.43122600	-0.05582700
H	-1.57960700	2.91066100	-0.57905000
N	-1.46327400	3.32492700	1.42858600
C	-0.40212300	1.34331900	0.27609500
N	-2.99848400	4.37562900	2.70091700
C	-1.37263800	0.32427800	0.27076000
C	0.96715200	1.02660100	0.27076000
N	-2.14783500	-2.92969600	1.42858600
C	-0.96228700	-1.01990900	0.27609500
C	1.36441000	-0.32341000	0.27609500
C	0.82478400	-2.80646300	0.20956300
H	0.06447000	-3.43219800	0.67553500
H	1.72175600	-2.96804600	0.81283800
N	3.61110800	-0.39523100	1.42858600
C	-2.09901200	3.73214300	3.51594800
C	-2.09397400	-2.50303000	2.74620700
N	-2.29016400	-4.78457800	2.70091700
C	0.40548700	-1.35087800	0.27076000
C	2.01807600	2.11751600	0.20956300
H	2.94013500	1.77193200	0.67553500
H	1.70952600	2.97510700	0.81283800
C	-2.59284300	4.13027500	1.47840700
C	-1.12070100	3.06494900	2.74620700
C	3.21467500	-0.56191900	2.74620700
C	-1.99954100	-2.12703400	0.21643400
H	-2.97152800	-1.71561300	-0.05582700
H	-1.73090300	-2.82331000	-0.57905000
C	2.84183700	-0.66813700	0.21643400
H	2.97152800	-1.71561300	-0.05582700
H	3.31051000	-0.08735100	-0.57905000
C	-2.18262500	-3.68387000	3.51594800
C	-2.84286000	0.68894800	0.20956300
H	-3.43128100	-0.00706100	0.81283800
H	-3.00460500	1.66026600	0.67553500
C	-2.28050200	-4.31060600	1.47840700
C	-2.05387300	3.68723100	4.91213600
H	-2.80605200	4.20655600	5.49447900
C	2.06997200	-1.09229900	3.34524300
H	1.23608900	-1.47599000	2.77410500
C	-1.98094400	-1.24649900	3.34524300
H	-1.89628900	-0.33249000	2.77410500
N	5.28864800	0.40894900	2.70091700
C	-1.02878300	2.97157200	5.50773900
H	-0.96474100	2.92305200	6.58946800
C	2.02910500	-1.09938200	4.73282100
H	1.15167800	-1.50635900	5.22300000
C	4.28163700	-0.04827400	3.51594800
C	4.22017200	-0.06491000	4.91213600
H	5.04601000	0.32683500	5.49447900
C	-0.06246000	2.30694800	4.73282100
H	0.72870600	1.75056200	5.22300000
C	-0.08902800	2.33879700	3.34524300
H	0.66020000	1.80847900	2.77410500
C	-1.96664600	-1.20756600	4.73282100

H	-1.88038400	-0.24420300	5.22300000
C	3.08784800	-0.59483400	5.50773900
H	3.01380800	-0.62603600	6.58946800
C	-2.05906500	-2.37673800	5.50773900
H	-2.04906700	-2.29701600	6.58946800
C	2.32401700	2.57625500	-1.22065000
H	3.10524800	3.34003300	-1.22068000
H	2.67182000	1.74567800	-1.84026400
H	1.44057700	2.99360500	-1.71179700
C	-3.39311000	0.72453100	-1.22065000
H	-4.44517700	1.01920700	-1.22068000
H	-2.84771200	1.44102500	-1.84026400
H	-3.31282700	-0.24922600	-1.71179700
C	-2.16630000	-3.62232200	4.91213600
H	-2.23995800	-4.53339000	5.49447900
C	1.06909300	-3.30078500	-1.22065000
H	1.33992900	-4.35924000	-1.22068000
H	0.17589200	-3.18670300	-1.84026400
H	1.87225000	-2.74437900	-1.71179700
C	4.87334500	0.18033000	1.47840700
C	-3.29673600	4.65626000	0.30054800
C	-4.69647500	4.69816800	0.33296100
C	-2.64247000	5.17967600	-0.82096700
C	-5.41476700	5.21534400	-0.73291900
H	-5.20411100	4.33369800	1.21833500
C	-3.36668000	5.69595600	-1.88724700
H	-1.55914200	5.21223000	-0.85453200
C	-4.76592000	5.71721100	-1.86969100
H	-6.49724900	5.25703400	-0.67573800
H	-2.83775300	6.07685500	-2.75435200
C	-2.38407200	-5.18318700	0.30054800
C	-1.72049500	-6.41635000	0.33296100
C	-3.16449600	-4.87828400	-0.82096700
C	-1.80923700	-7.29699800	-0.73291900
H	-1.15103800	-6.67374100	1.21833500
C	-3.24950300	-5.76360800	-1.88724700
H	-3.73435300	-3.95637200	-0.85453200
C	-2.56829000	-6.98601300	-1.86969100
H	-1.30410100	-8.25530000	-0.67573800
H	-3.84383500	-5.49599400	-2.75435200
C	5.68080700	0.52692700	0.30054800
C	6.41697000	1.71818300	0.33296100
C	5.80696600	-0.30139200	-0.82096700
C	7.22400400	2.08165400	-0.73291900
H	6.35514800	2.34004300	1.21833500
C	6.61618200	0.06765200	-1.88724700
H	5.29349500	-1.25585800	-0.85453200
C	7.33421000	1.26880200	-1.86969100
H	7.80135000	2.99826600	-0.67573800
H	6.68158800	-0.58086100	-2.75435200
C	8.18913700	1.66390800	-3.00967900
C	8.94228600	0.71222000	-3.70885700
C	8.26607200	3.00168800	-3.41728200
C	9.74449600	1.08581200	-4.78044900
H	8.92019100	-0.32451900	-3.38965800
C	9.06836800	3.37541700	-4.48876300
H	7.67095500	3.75002400	-2.90434100
C	9.81076400	2.41893900	-5.17524000
H	10.32753300	0.33444600	-5.30238200
H	9.10752900	4.41591400	-4.79329700
H	10.43744600	2.71043900	-6.01108500
C	-2.65358200	-7.92395500	-3.00967900
C	-3.85434300	-8.10035700	-3.70885700
C	-1.53349800	-8.65947200	-3.41728200
C	-3.93190700	-8.98188800	-4.78044900
H	-4.74113700	-7.56285200	-3.38965800
C	-1.61098700	-9.54114600	-4.48876300
H	-0.58786100	-8.51825400	-2.90434100
C	-2.81051900	-9.70584100	-5.17524000
H	-4.87412800	-9.11112900	-5.30238200

H	-0.72947100	-10.09530900	-4.79329700
H	-2.87141400	-10.39431300	-6.01108500
C	-5.53555500	6.26004700	-3.00967900
C	-5.08794300	7.38813700	-3.70885700
C	-6.73257400	5.65778400	-3.41728200
C	-5.81258900	7.89607500	-4.78044900
H	-4.17905400	7.88737100	-3.38965800
C	-7.45738100	6.16572800	-4.48876300
H	-7.08309300	4.76823000	-2.90434100
C	-7.00024500	7.28690100	-5.17524000
H	-5.45340500	8.77668300	-5.30238200
H	-8.37805800	5.67939500	-4.79329700
H	-7.56603200	7.68387400	-6.01108500