Supporting Information for:

Incorporating BODIPY Fluorophores into Tetrakis(arylethynyl)benzenes

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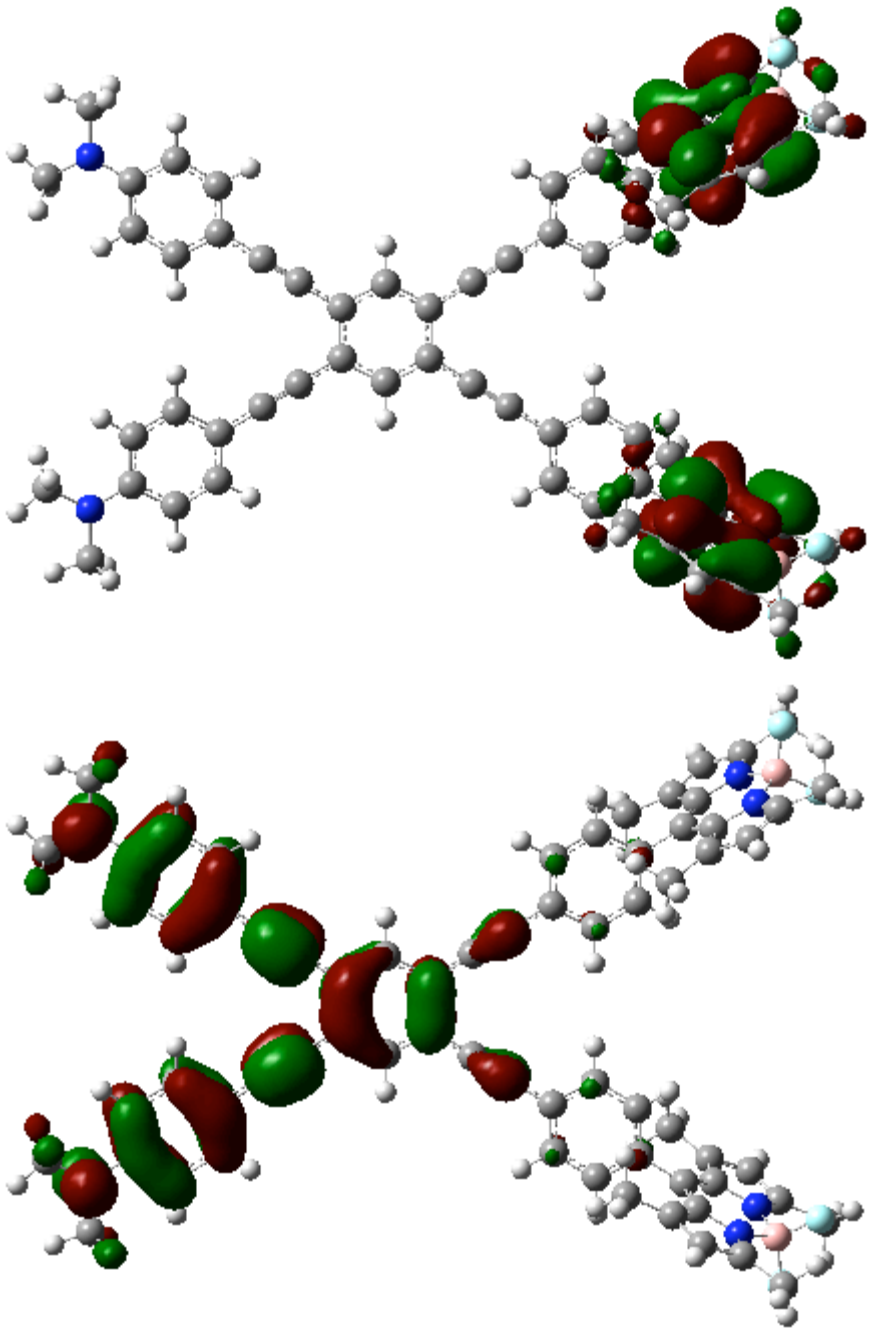


Figure S1. HOMO (bottom) and LUMO (top) maps of **1'**.

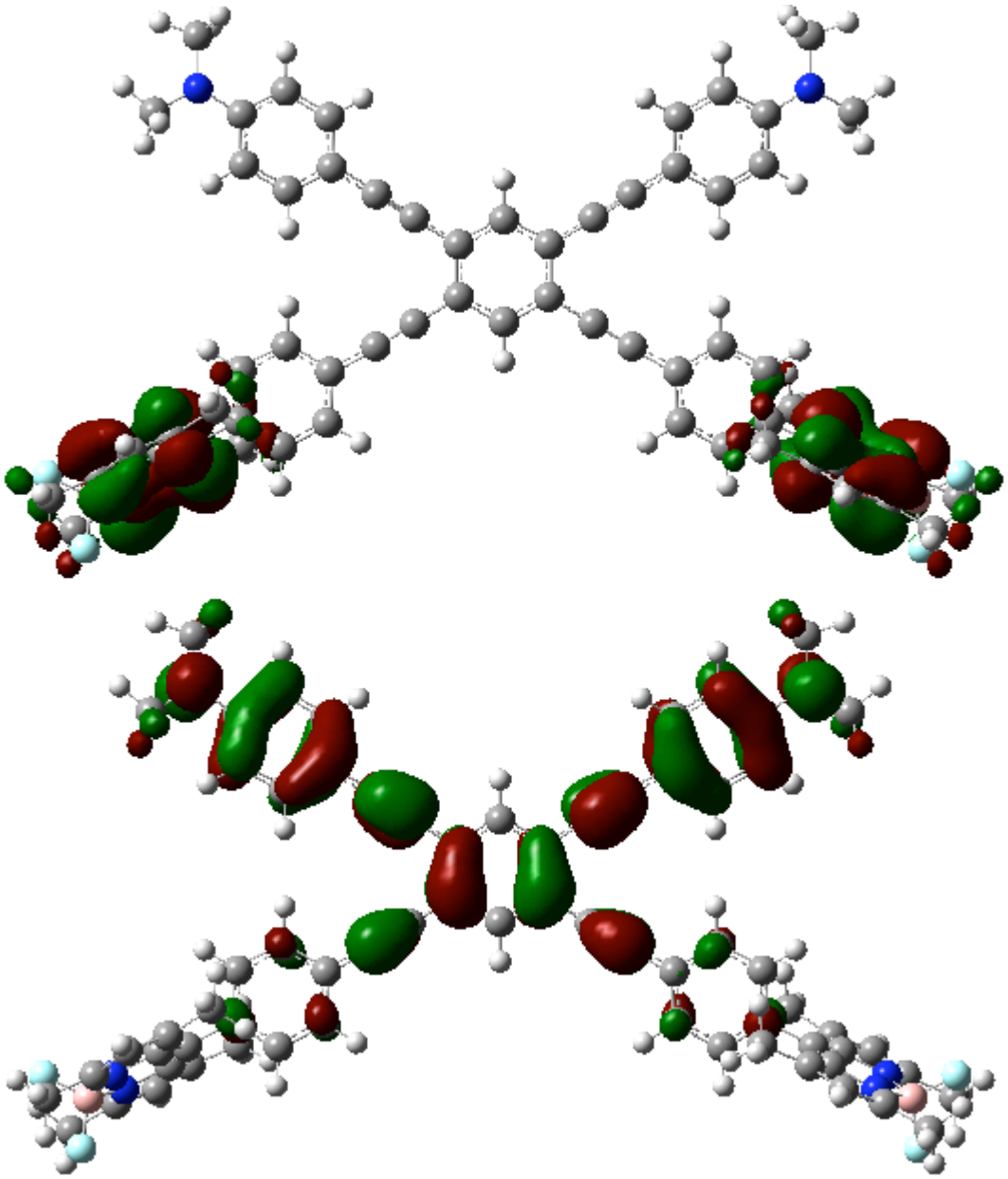


Figure S2. HOMO (bottom) and LUMO (top) maps of **2'**.

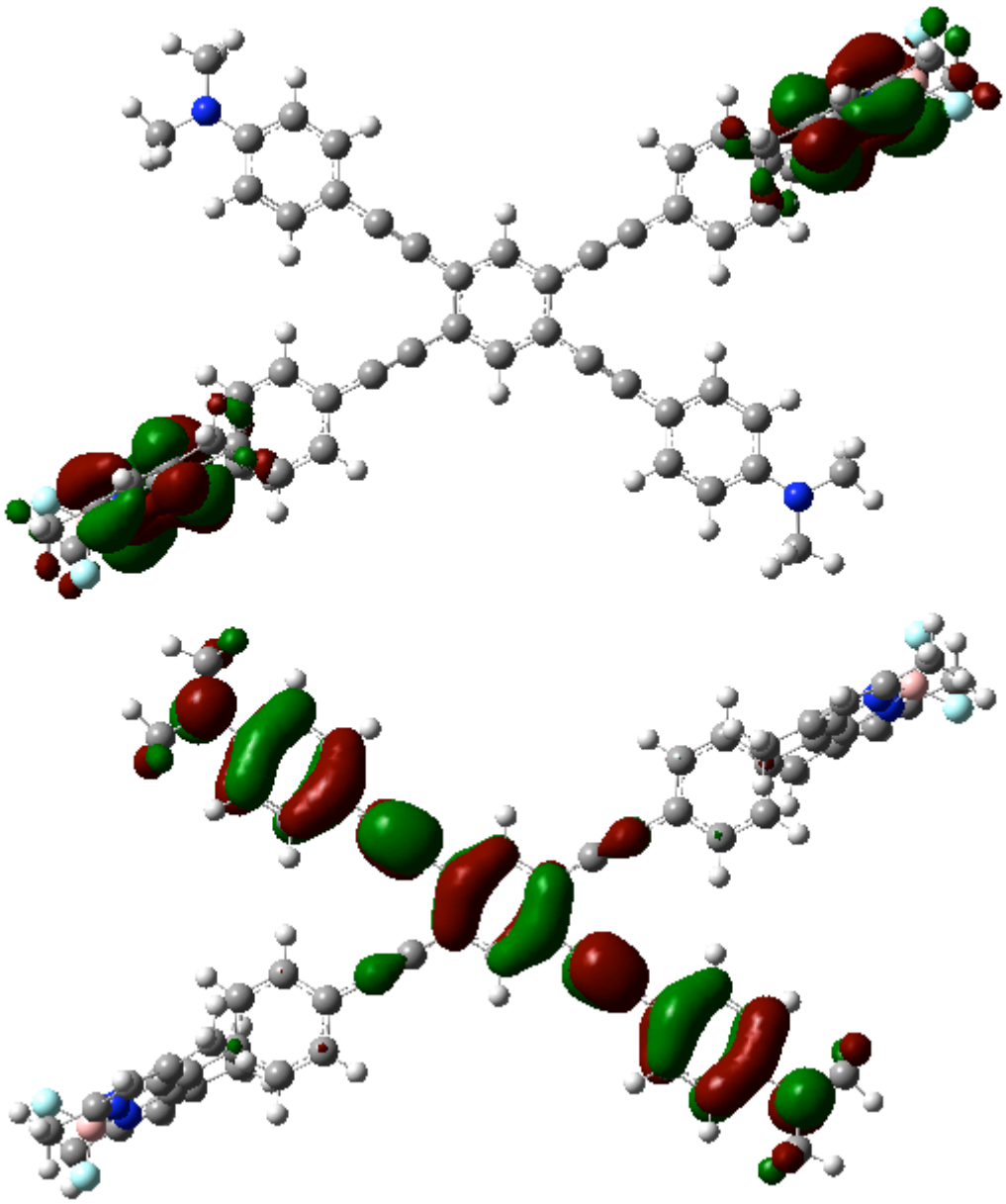


Figure S3. HOMO (bottom) and LUMO (top) maps of **3'**.

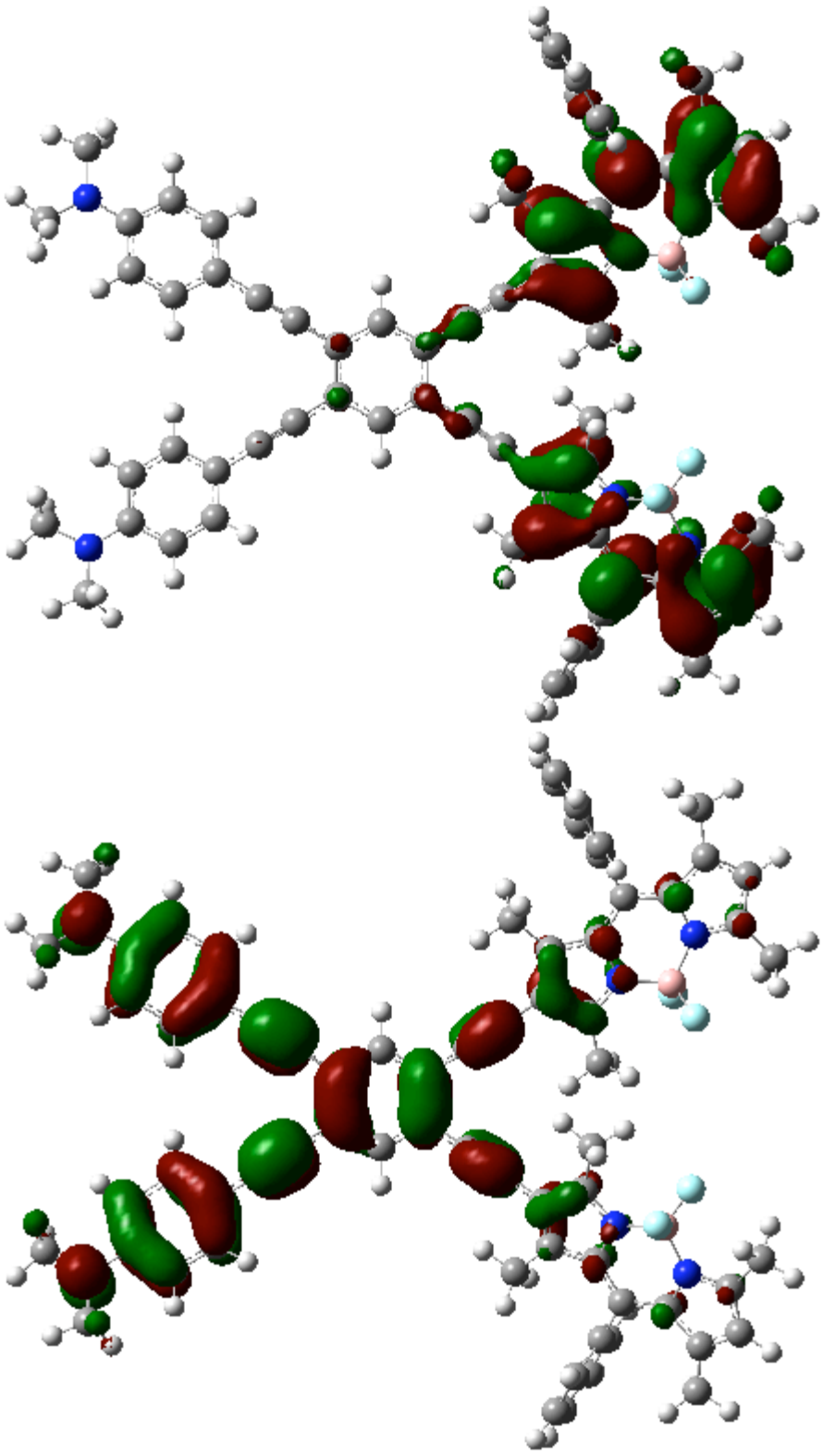


Figure S4. HOMO (bottom) and LUMO (top) maps of **4'**.

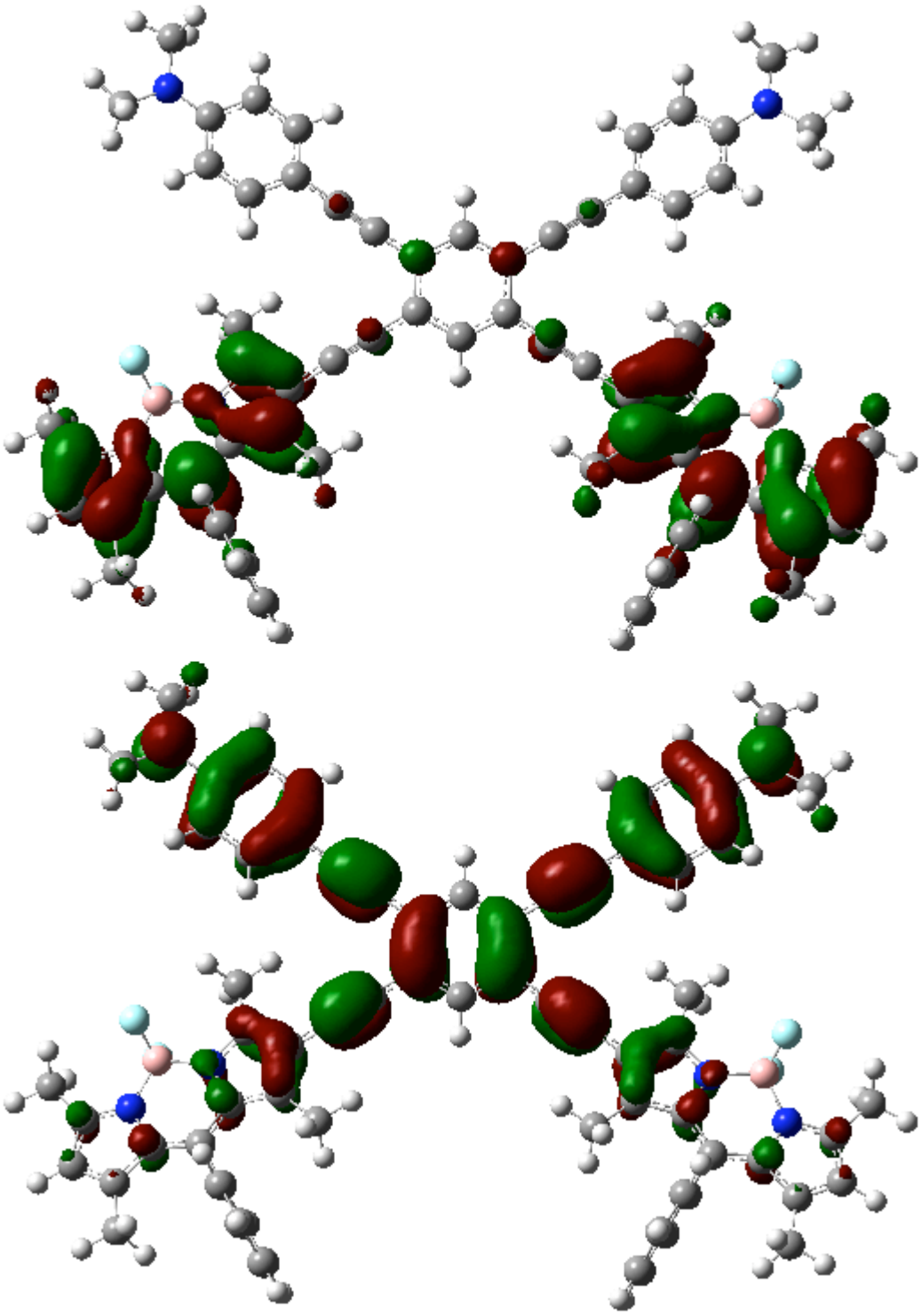


Figure S5. HOMO (bottom) and LUMO (top) maps of **5'**.

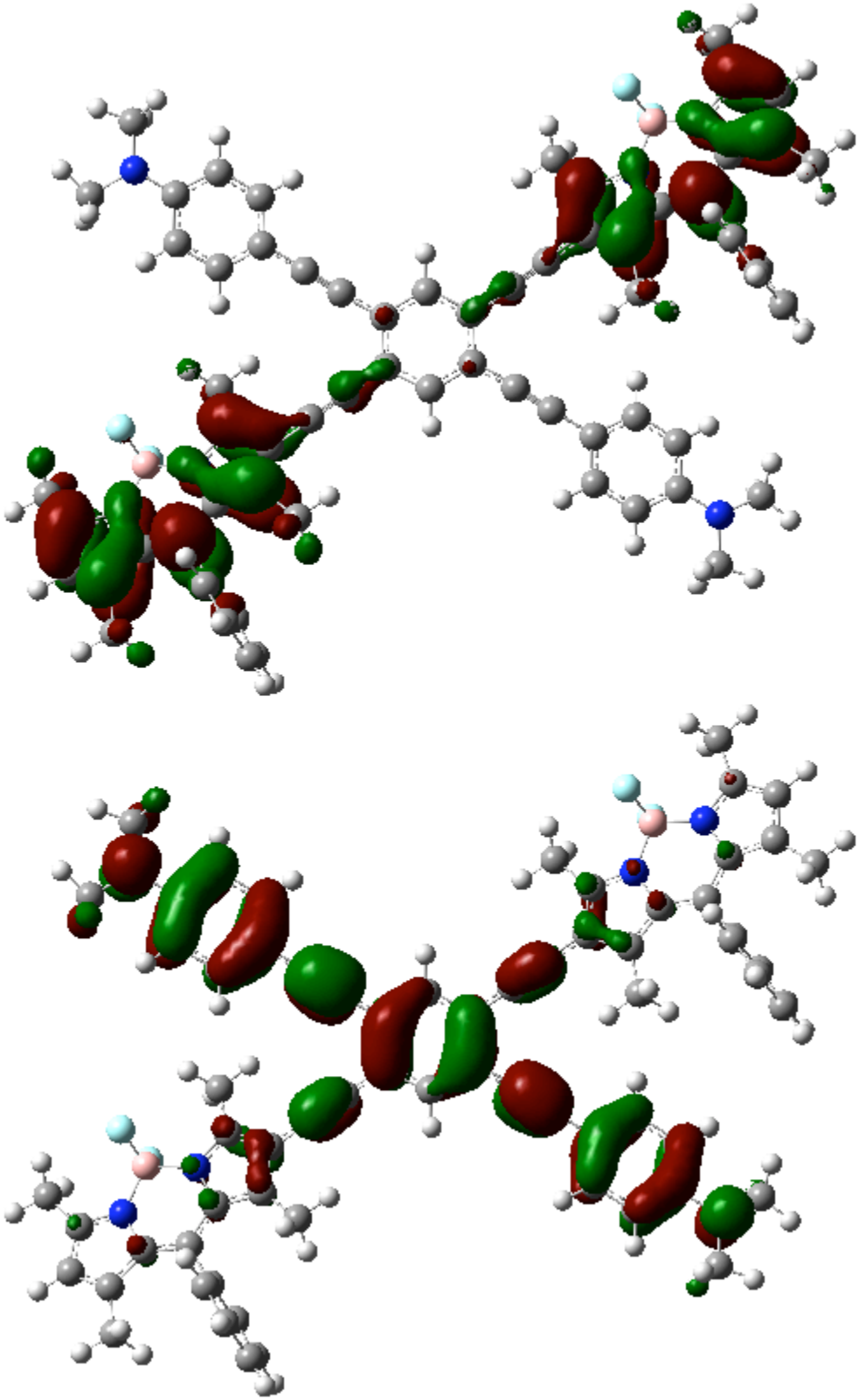


Figure S6. HOMO (bottom) and LUMO (top) maps of **6'**.

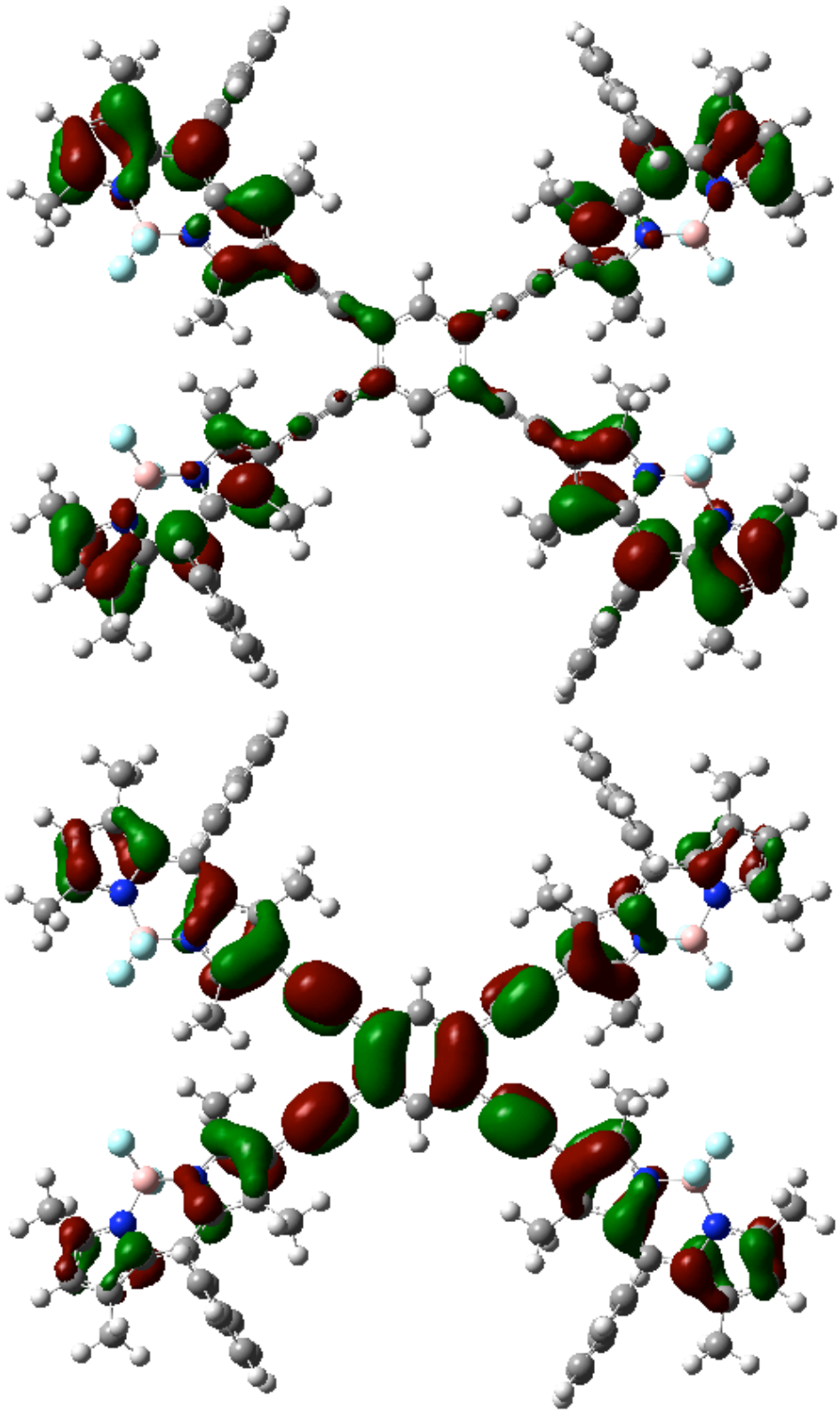


Figure S7. HOMO (bottom) and LUMO (top) maps of **7**.

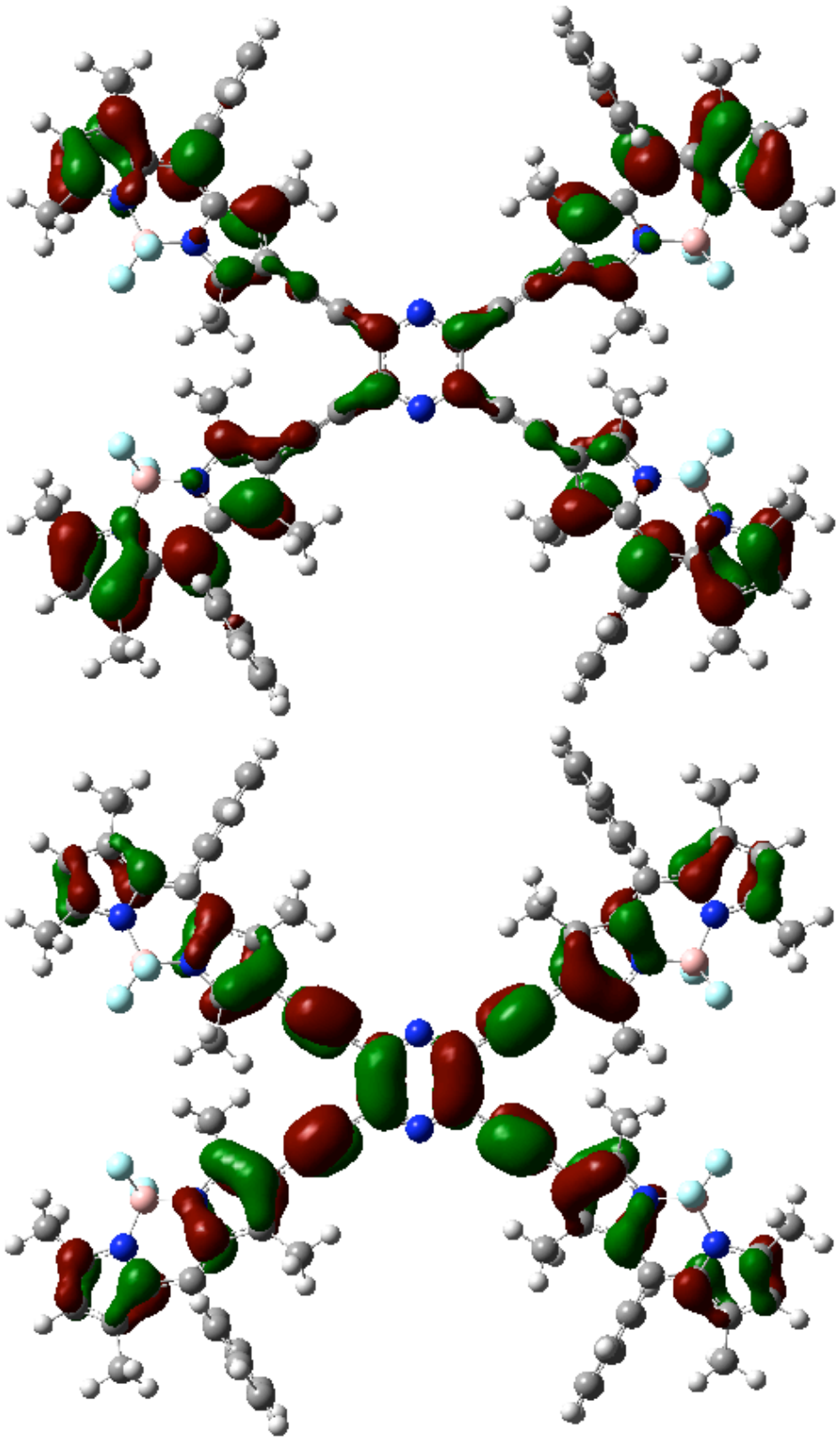


Figure S8. HOMO (bottom) and LUMO (top) maps of **8**.

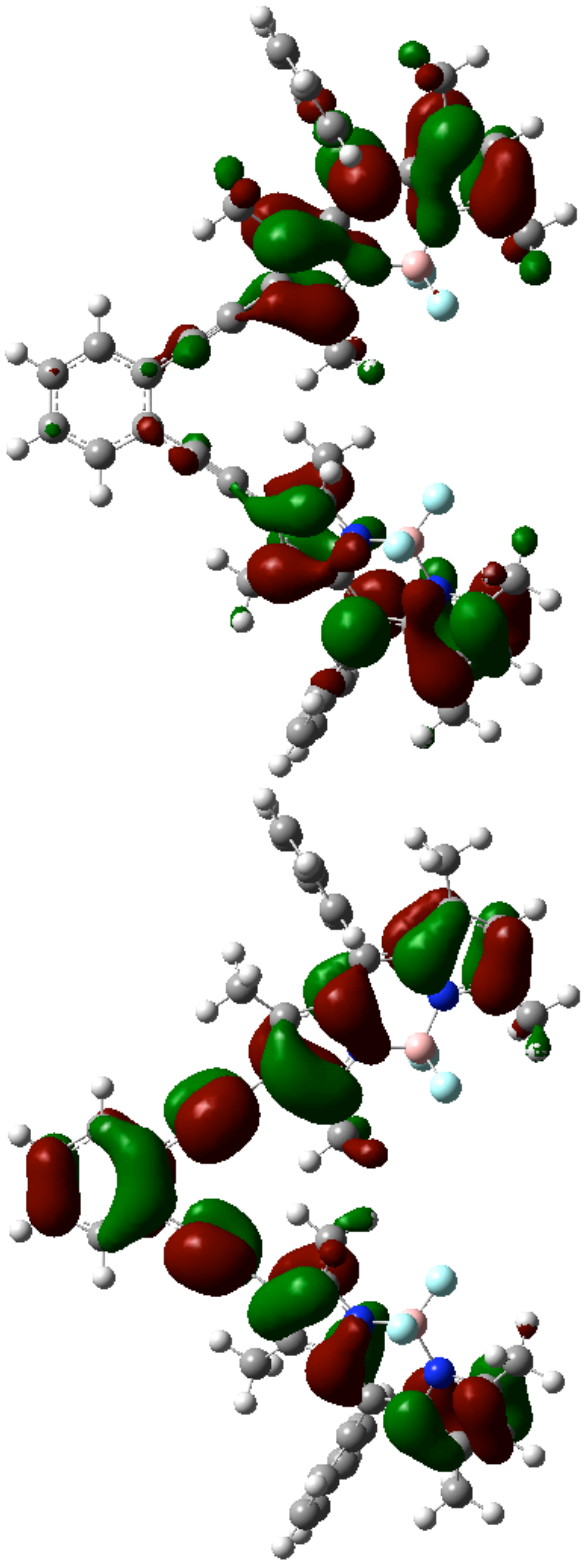


Figure S9. HOMO (bottom) and LUMO (top) maps of **9**.

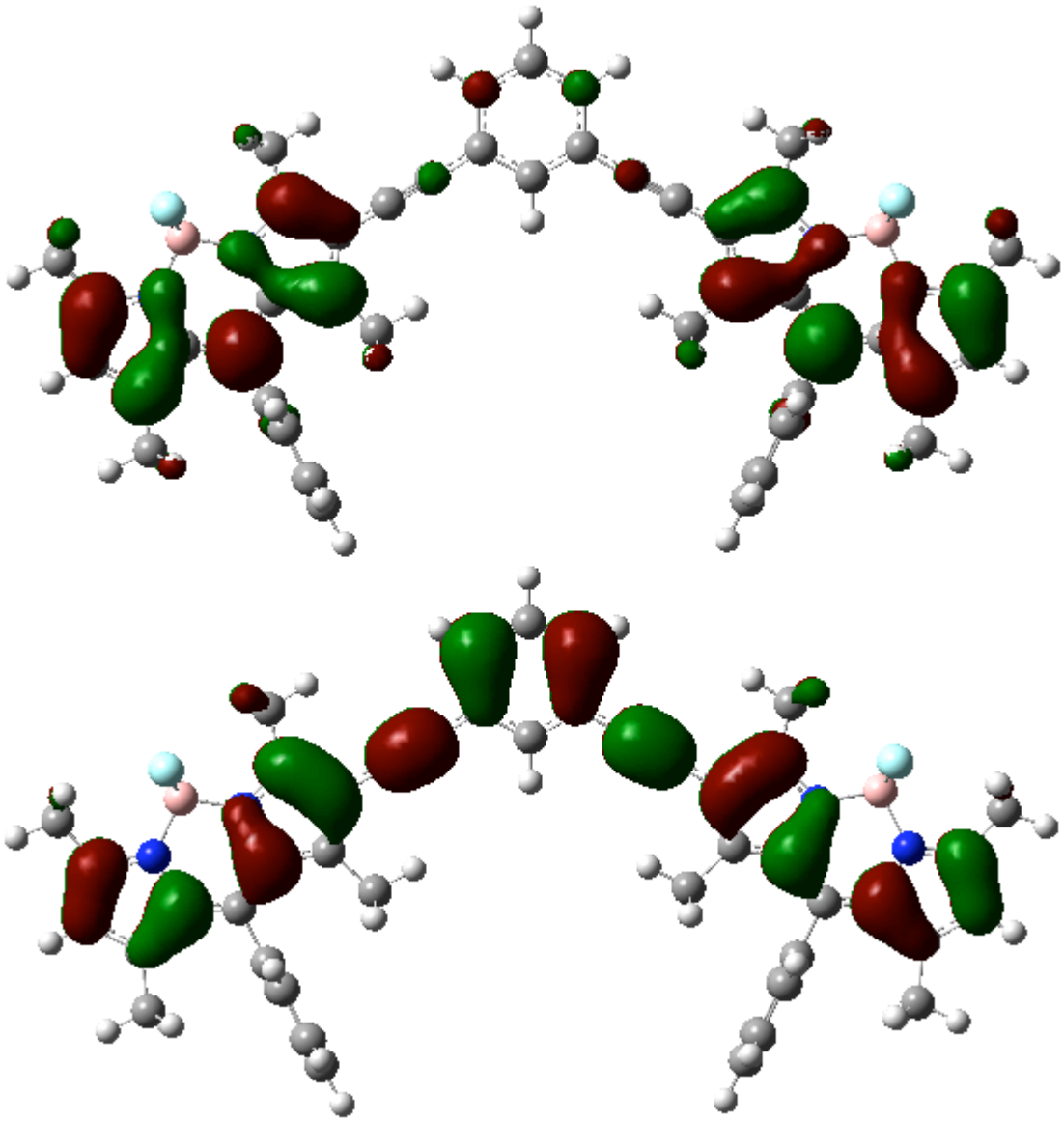


Figure S10. HOMO (bottom) and LUMO (top) of **10**.

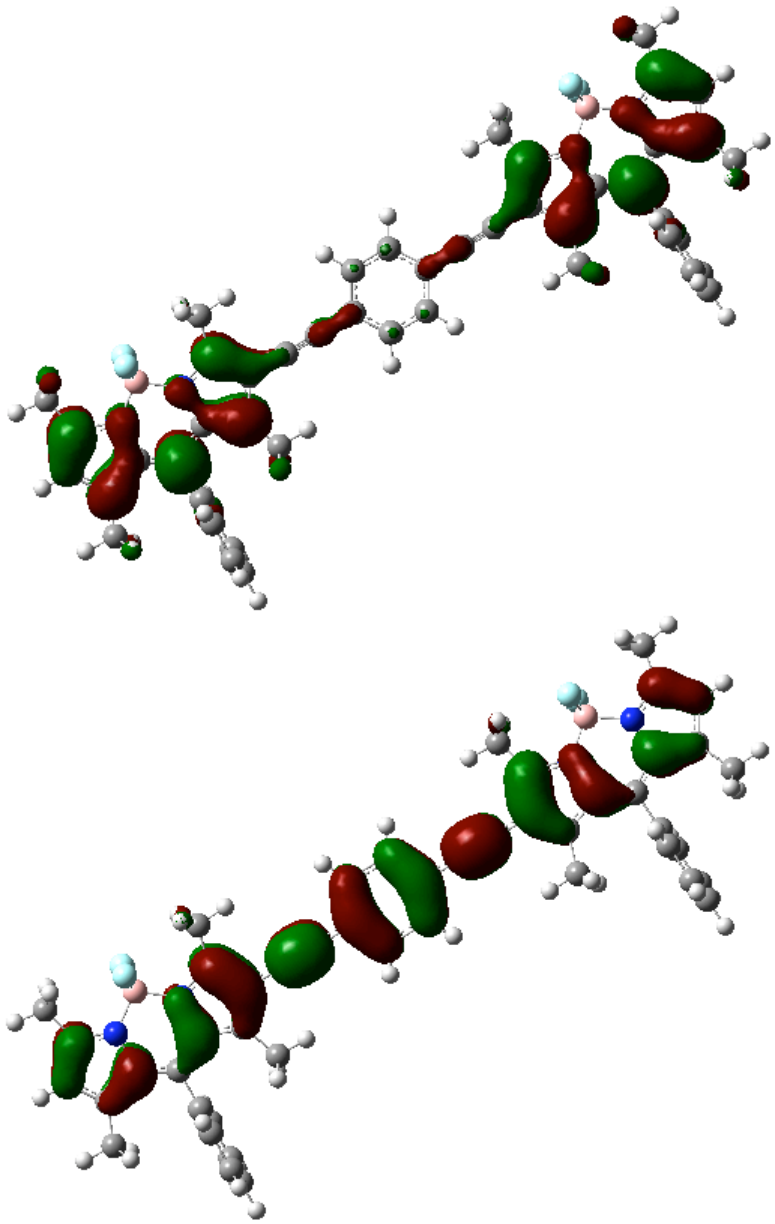


Figure S11. HOMO (bottom) and LUMO (top) maps of **11**.

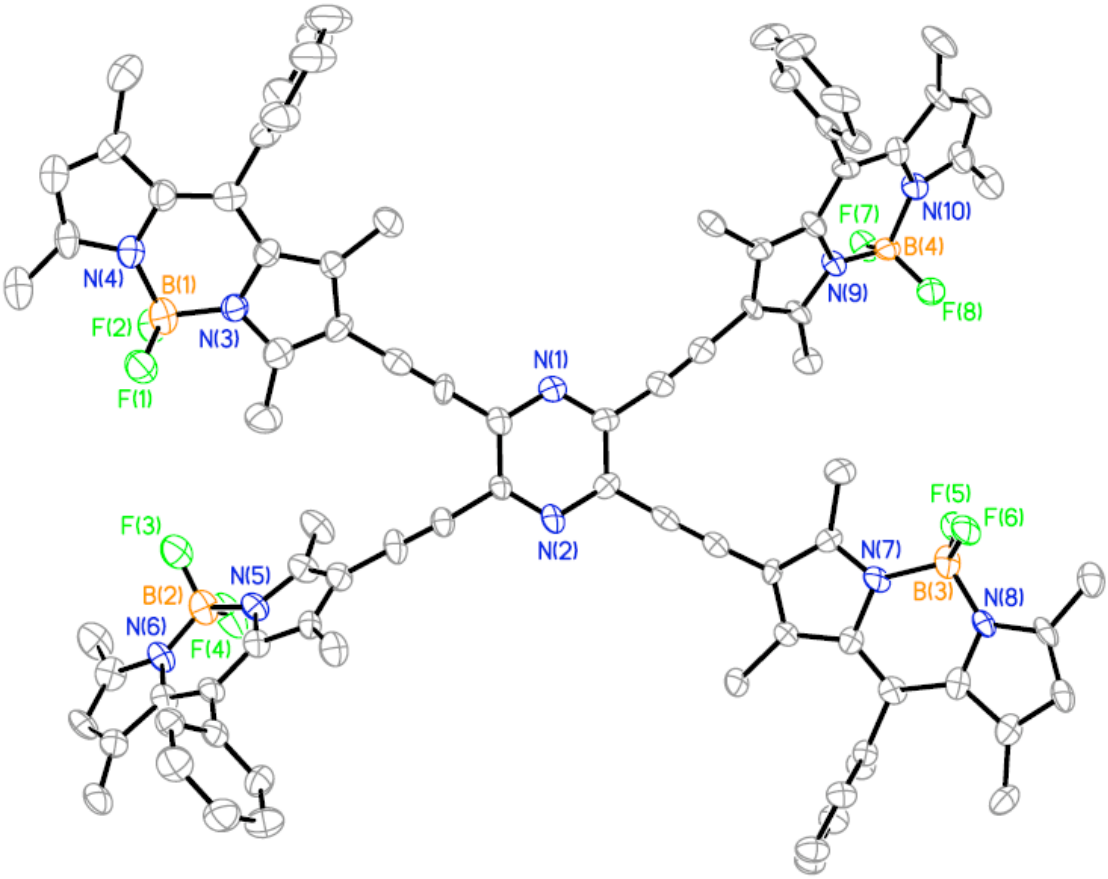


Figure S12. X-ray structure of **8**; ellipsoids drawn at the 30% level.

Cartesian Coordinates

1'
B3LYP/6-31G* = -3403.96398297 au
B3LYP/6-31G* Zero Point Corrected Energy = -3402.865410 au
NIMAG = 0

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C	-2.58838700	-0.71089800	-0.07076600
C	-2.58839000	0.71098000	0.06915100
C	-3.81486900	1.38444900	0.13842600
C	-6.25724600	1.44314800	0.12470600
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C	-1.37233600	-1.44259200	-0.11969700
C	-1.37234700	1.44268700	0.11805300
C	-7.29314800	2.08323400	0.15848700
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H	-14.19474300	-5.07565900	0.12382000
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2'
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B3LYP/6-31G* Zero Point Corrected Energy = -3402.866463 au
NIMAG = 0

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C	-1.22630700	1.39970700	0.02670100
C	-1.22796800	2.82990600	0.03928600
C	0.00001700	3.50605200	-0.00001600
C	2.44115700	3.56131500	-0.09676300
C	2.44461500	0.67121800	-0.02693800
C	-2.44460200	0.67123500	0.02689900
C	-2.44112400	3.56133000	0.09673500
C	3.47666600	4.19969000	-0.16312500
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C	4.73683300	-0.63506600	0.02844900
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C	-11.04910000	-3.45522800	2.24146200
C	-10.15207100	-2.79554300	3.10634100
C	-9.04816700	-2.38385900	2.36880200
C	-7.87333900	-1.64462800	2.93948800
C	-12.37085700	-4.06887400	2.57076100
C	-7.13106000	-2.63362200	-3.17879500
C	-11.69629700	-4.95724000	-3.13936100
C	9.00550000	-3.19329900	1.37976000
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N	10.53310100	-3.46283000	-0.99746100
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C	11.04914400	-3.45520200	-2.24144800
C	10.15213600	-2.79548500	-3.10632400
C	9.04822000	-2.38381900	-2.36879300
C	7.87341600	-1.64454400	-2.93947200
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C	7.13106600	-2.63362800	3.17878700
C	11.69627700	-4.95729600	3.13935900
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F	-12.43426800	-3.45387100	-0.49885300
F	-11.40827000	-5.45412900	-0.06399800
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C	-9.52162900	6.44135900	1.02514800
N	8.33681200	7.07918300	-0.47567700
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C	8.34603200	8.51525100	-0.25307800
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H	3.90711100	-2.57540400	-0.42512700
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H	-6.08821900	-3.74853000	0.35234300
H	-8.05705600	-0.04319900	-0.57119500
H	-5.87662400	1.13491600	-0.50328600
H	-9.26013900	-4.03138800	-4.57174200
H	-10.30756200	-2.64194700	4.16678000
H	-8.03359400	-1.46653200	4.00746200
H	-6.93808900	-2.20374000	2.82838700
H	-7.71728300	-0.67475500	2.45517600
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H	-12.57935900	-3.97848500	3.63988700
H	-13.17340700	-3.58247400	2.00564000
H	-7.01187200	-2.83967700	-4.24707000
H	-6.27473100	-3.06952100	-2.65337800
H	-7.06706400	-1.54946000	-3.03629600
H	-11.64461100	-5.21909200	-4.19925700
H	-11.83013900	-5.86797200	-2.54673900
H	-12.58207100	-4.33638500	-2.96551700
H	9.26012500	-4.03142100	4.57173600
H	10.30764700	-2.64185900	-4.16675500
H	8.03361700	-1.46655700	-4.00747200
H	7.71748200	-0.67461000	-2.45523700
H	6.93812300	-2.20355800	-2.82825500
H	12.38412400	-5.12645900	-2.28754100
H	13.17345800	-3.58241500	-2.00565300
H	12.57938900	-3.97849600	-3.63987500
H	7.01181200	-2.83980300	4.24703200
H	7.06715700	-1.54944200	3.03642200
H	6.27473200	-3.06939700	2.65327500
H	11.83014200	-5.86799900	2.54669700
H	12.58205300	-4.33642700	2.96557200
H	11.64456100	-5.21920000	4.19924000
H	-9.37209400	8.88065400	0.32099800
H	-7.73792200	9.06003500	0.99133000
H	-7.96952400	8.76435500	-0.74694300
H	-10.35921100	7.13904200	0.97523600
H	-9.38865700	6.13974200	2.07539500
H	-9.79705700	5.54943100	0.44826500
H	10.35914500	7.13928100	-0.97517100
H	9.79705000	5.54964500	-0.44821400
H	9.38862600	6.13995500	-2.07533900
H	7.73780600	9.06017000	-0.99130400
H	9.37196200	8.88085100	-0.32091100
H	7.96935900	8.76451200	0.74697900

3'

B3LYP/6-31G* = -3403.96460682 au

B3LYP/6-31G* Zero Point Corrected Energy = -3402.866010 au
NIMAG = 0

C	-0.82879700	1.15774100	-0.07312400
C	-1.40799900	-0.14344900	0.05135300
C	-0.56905700	-1.26345700	0.12394500
C	0.82861000	-1.15726200	0.07245700
C	1.40781400	0.14393200	-0.05203000
C	0.56887400	1.26393600	-0.12463600
C	-1.63603600	2.32159800	-0.13226300
C	-2.81748600	-0.31285300	0.08256200
C	1.63586900	-2.32110600	0.13162500
C	2.81730500	0.31331200	-0.08320700
C	-2.31764100	3.33056000	-0.17153300
C	-4.02407400	-0.46849200	0.09319300
C	4.02390200	0.46888300	-0.09375400
C	2.31753400	-3.33001900	0.17108900
C	-3.12573800	4.49698300	-0.21219900
C	5.43761000	0.62711700	-0.08920000
C	-5.43776000	-0.62691300	0.08878700
C	3.12577100	-4.49634600	0.21186600
C	-6.27672500	0.43773300	-0.29980200
C	-7.65907400	0.28145100	-0.31086500
C	-8.24622400	-0.93533700	0.06456200
C	-7.41532600	-1.99590600	0.45283400
C	-6.03189500	-1.84839600	0.46514700
C	-2.60813300	5.73595800	-0.64052100
C	-3.39713300	6.87458200	-0.68623500
C	-4.75825400	6.83949000	-0.29509700
C	-5.27878200	5.59270800	0.13141900
C	-4.48160800	4.45966800	0.17205900
C	6.27635400	-0.43752900	0.29988000
C	7.65872300	-0.28143800	0.31113900
C	8.24611400	0.93513400	-0.06460800
C	7.41543600	1.99569000	-0.45339100
C	6.03198400	1.84838600	-0.46586400
C	2.60838000	-5.73530000	0.64049500
C	3.39752900	-6.87381600	0.68631800
C	4.75859400	-6.83863900	0.29497200
C	5.27891800	-5.59185500	-0.13180700
C	4.48159100	-4.45892500	-0.17255900
C	-9.73126900	-1.10210800	0.04603300
C	9.73117700	1.10171300	-0.04589300
C	-10.47299600	-0.81894000	1.20509300
N	-11.86436200	-0.97511000	1.20890700
B	-12.73650100	-1.45327500	0.01023500
N	-11.75010600	-1.70739700	-1.16824400
C	-10.36023100	-1.54245400	-1.13016100
C	-10.07971500	-0.35898400	2.50702100

C	-11.25270700	-0.25711600	3.24567900
C	-12.33383600	-0.64116100	2.42622600
C	-12.10145000	-2.13509400	-2.39579700
C	-10.94181100	-2.25880900	-3.18841900
C	-9.84109500	-1.89539200	-2.42182700
C	-8.42412500	-1.89701400	-2.91622100
C	-13.51884500	-2.41301100	-2.77702000
C	-8.71287900	-0.03307200	3.03440300
C	-13.78591500	-0.69594300	2.77345400
C	10.36008300	1.54176500	1.13044300
N	11.74998300	1.70639600	1.16873400
B	12.73645700	1.45236300	-0.00968300
N	11.86436000	0.97477300	-1.20861000
C	10.47298700	0.81868000	-1.20493600
C	9.84083200	1.89475600	2.42204800
C	10.94152200	2.25788400	3.18882300
C	12.10124600	2.13396400	2.39636700
C	12.33391700	0.64098300	-2.42593800
C	11.25283600	0.25712900	-3.24554200
C	10.07979000	0.35892200	-2.50695800
C	8.71298500	0.03317300	-3.03451800
C	13.78603100	0.69571200	-2.77303500
C	8.42378300	1.89675200	2.91621000
C	13.51863900	2.41163200	2.77777500
F	-13.39847300	-2.63402000	0.34145800
F	-13.65302200	-0.46273400	-0.33859500
F	13.39877100	2.63304000	-0.34046600
F	13.65269300	0.46148400	0.33895900
N	-5.54474200	7.97581400	-0.32278000
C	-6.96551300	7.88001800	-0.03437300
C	-5.01474000	9.20936800	-0.87834100
N	5.54520400	-7.97487400	0.32273600
C	5.01554100	-9.20826400	0.87897700
C	6.96585600	-7.87903600	0.03381000
H	-1.01557600	-2.24768200	0.21334600
H	1.01539000	2.24816300	-0.21404500
H	-5.82938200	1.38038000	-0.59970600
H	-8.29391900	1.10877900	-0.61616300
H	-7.86043000	-2.94316600	0.74470900
H	-5.39692600	-2.67582000	0.76608700
H	-1.56805700	5.79586100	-0.94717400
H	-2.95098500	7.79992100	-1.03003100
H	-6.31511500	5.50815100	0.43558900
H	-4.90657100	3.52029300	0.51384500
H	5.82882500	-1.38001700	0.60000400
H	8.29339400	-1.10875400	0.61683400
H	7.86073000	2.94278200	-0.74551900
H	5.39718500	2.67580700	-0.76717100
H	1.56835200	-5.79527600	0.94729600

H	2.95153800	-7.79914500	1.03033800
H	6.31522500	-5.50719800	-0.43603500
H	4.90639700	-3.51955100	-0.51454300
H	-11.33474700	0.06215200	4.27696200
H	-10.92438500	-2.58455300	-4.22078300
H	-8.39539500	-2.25496600	-3.95009300
H	-7.77555700	-2.54434400	-2.31664100
H	-7.97588700	-0.89766800	-2.89407200
H	-14.13414100	-1.51667000	-2.64571400
H	-13.94646700	-3.18489600	-2.12826900
H	-13.57869600	-2.74289500	-3.81727200
H	-8.78920800	0.30293000	4.07327700
H	-8.22434500	0.76024500	2.45860400
H	-8.04044000	-0.89730800	3.00914500
H	-14.36378300	-0.03849500	2.11514000
H	-14.17743500	-1.70830900	2.62814700
H	-13.94345400	-0.39417800	3.81209700
H	10.92401800	2.58355500	4.22121000
H	11.33494700	-0.06199500	-4.27686400
H	8.78949700	-0.30362500	-4.07312000
H	8.22390800	-0.75947900	-2.45827900
H	8.04092500	0.89773900	-3.01013800
H	13.94361800	0.39423400	-3.81175300
H	14.17765200	1.70798900	-2.62739100
H	14.36377300	0.03800200	-2.11487000
H	7.77550500	2.54428500	2.31652700
H	8.39497900	2.25470100	3.95008100
H	7.97525700	0.89754200	2.89396500
H	14.13400400	1.51548000	2.64555800
H	13.94615400	3.18420100	2.12976000
H	13.57851900	2.74052900	3.81834000
H	-7.49520800	7.22604000	-0.74381500
H	-7.41063800	8.87472400	-0.09198700
H	-7.14188800	7.49487000	0.97815400
H	-5.77139300	9.99177700	-0.79954900
H	-4.12815700	9.54619900	-0.32596400
H	-4.73626300	9.10731100	-1.93837600
H	5.77234100	-9.99055600	0.80044500
H	4.12893000	-9.54554500	0.32691500
H	4.73722300	-9.10574100	1.93900800
H	7.41094900	-8.87379100	0.09085200
H	7.49590800	-7.22533400	0.74325300
H	7.14180100	-7.49354800	-0.97865200

4'

B3LYP/6-31G* = -3403.97008022 au

B3LYP/6-31G* Zero Point Corrected Energy = -3402.871676 au

NIMAG = 0

C	-3.93163900	-0.71984900	0.04371800
C	-3.94479200	0.70812000	-0.03244500
C	-2.72225300	1.39347800	-0.07006500
C	-1.48692700	0.73060700	-0.02672100
C	-1.47409100	-0.69398200	0.07204200
C	-2.69611500	-1.38060400	0.09845400
C	-5.13741700	-1.46683200	0.06252400
C	-5.16660100	1.42811400	-0.06429300
C	-0.28302500	1.48061300	-0.09326400
C	-0.25794600	-1.42525200	0.15262700
C	-6.16374500	-2.12257700	0.06864100
C	-6.21272300	2.05158100	-0.07852000
C	0.75162400	-2.10029700	0.25223600
C	0.72666900	2.15720200	-0.18129300
C	-7.36852700	-2.87455600	0.07069300
C	1.91742100	-2.89036200	0.37394500
C	-7.44620800	2.75529000	-0.08560500
C	1.89708700	2.93947000	-0.29330600
C	-8.65145200	2.11351200	0.26409500
C	-9.86066800	2.79183600	0.26396700
C	-9.93438600	4.15891000	-0.09760400
C	-8.72121400	4.80556000	-0.43599400
C	-7.51620900	4.11931100	-0.43105700
C	-7.39021200	-4.22623100	0.46784100
C	-8.56565300	-4.96152200	0.47592200
C	-9.79413600	-4.38375300	0.07384300
C	-9.77260700	-3.02356100	-0.31901700
C	-8.59229500	-2.29565500	-0.32158400
C	3.07557600	-2.53859000	1.12777900
N	3.97472900	-3.52734100	1.03249600
C	3.45201200	-4.54862300	0.22452700
C	2.14614200	-4.15601200	-0.19550100
C	3.15128500	2.47377600	-0.78835500
N	4.03159500	3.48295900	-0.76280100
C	3.40142400	4.63133100	-0.25882700
C	2.04650000	4.29815800	0.03904800
B	5.51433100	3.38631100	-1.24514500
N	6.14087900	4.79043800	-0.99740100
C	5.47648000	5.91183100	-0.48592900
C	4.12269600	5.83191500	-0.12479300
B	5.36842900	-3.53734600	1.73768200
N	6.05247100	-4.87350100	1.32097100
C	5.49947000	-5.86309500	0.49922000
C	4.21321300	-5.70259800	-0.03800900
C	7.28339200	-5.26339800	1.70083300
C	7.56210000	-6.52369900	1.13108000
C	6.46549000	-6.92014500	0.37632700
C	7.41842800	5.12502200	-1.25796200

C	7.61617600	6.48028100	-0.91944900
C	6.41994200	6.99456400	-0.43562900
C	3.43374200	7.04397700	0.41577900
C	0.94576600	5.14962100	0.59420400
C	3.48397300	1.10741600	-1.28422000
C	8.40870600	4.15549000	-1.81528000
C	6.22945600	8.40845000	0.02946900
C	3.30172200	-1.29963000	1.92635200
C	1.15772300	-4.87391600	-1.06284200
C	3.64157900	-6.77637700	-0.90769000
C	6.38235000	-8.20806900	-0.38912500
C	8.15423400	-4.43185700	2.58449700
C	3.41408200	7.29299900	1.79465300
C	2.76808500	8.42306800	2.29863400
C	2.13576500	9.31520000	1.43047500
C	2.15224200	9.07320900	0.05550200
C	2.79810600	7.94380600	-0.45022100
C	3.82833700	-6.73865100	-2.29594300
C	3.29447300	-7.74118400	-3.10732700
C	2.56852200	-8.79025300	-2.54006100
C	2.37889200	-8.83365300	-1.15747200
C	2.91290500	-7.83250200	-0.34448000
F	6.12918900	-2.45740000	1.30309300
F	5.19961700	-3.49811300	3.11934700
F	6.19214800	2.42438400	-0.50387600
F	5.55001900	3.08066200	-2.60273100
N	-10.96672900	-5.12163000	0.05903600
C	-12.23147500	-4.45673800	-0.20248600
C	-10.98358900	-6.45466400	0.63664100
N	-11.14463800	4.83368000	-0.12512100
C	-11.16085000	6.27181500	-0.33178100
C	-12.33429800	4.19458800	0.41084600
H	-2.73269900	2.47581500	-0.13844200
H	-2.68570300	-2.46288500	0.16753600
H	-8.62583600	1.06651200	0.55178700
H	-10.75542000	2.25242800	0.55078000
H	-8.71650000	5.85530400	-0.70369500
H	-6.60330600	4.64393700	-0.69718700
H	-6.46402400	-4.69885900	0.78125200
H	-8.52630600	-5.99505800	0.79831800
H	-10.68593900	-2.52832800	-0.62634200
H	-8.60630800	-1.25624800	-0.63643600
H	8.48163000	-7.07911800	1.26602900
H	8.54987100	7.01852100	-1.02305900
H	1.18508300	5.53374000	1.59165700
H	0.03041200	4.55597100	0.66908300
H	0.74018100	6.02052600	-0.03694700
H	2.62628900	0.44199000	-1.16536600
H	4.34470800	0.70320100	-0.74196200

H	3.76977600	1.14681000	-2.34134400
H	8.04692500	3.73926000	-2.76139600
H	8.54570300	3.31008800	-1.13252600
H	9.37219900	4.64417300	-1.98086400
H	5.90597700	8.46079200	1.07437600
H	5.47325200	8.93924900	-0.55881500
H	7.17303300	8.95572000	-0.06071400
H	2.45242200	-0.62135200	1.82045000
H	4.21837700	-0.79730100	1.60123700
H	3.43852100	-1.54957700	2.98425900
H	0.88706900	-5.85371200	-0.65562000
H	0.24726600	-4.27430600	-1.14885000
H	1.54647800	-5.04891400	-2.07181900
H	7.31322400	-8.77024700	-0.26520400
H	6.22652500	-8.04300100	-1.46054100
H	5.55671200	-8.84119800	-0.04701100
H	7.63248700	-4.18947700	3.51596000
H	9.08279500	-4.95992900	2.81558700
H	8.39296500	-3.47813800	2.10133100
H	3.90504500	6.59741400	2.46993600
H	2.75868900	8.60493600	3.36993300
H	1.63224400	10.19417400	1.82346900
H	1.66156100	9.76310900	-0.62581200
H	2.80998300	7.75429100	-1.52019600
H	4.39196000	-5.92084300	-2.73683700
H	3.44547700	-7.70089100	-4.18268500
H	2.15209700	-9.56966800	-3.17224900
H	1.81436400	-9.64702700	-0.70953300
H	2.76548600	-7.86543700	0.73165600
H	-13.03332700	-5.19739700	-0.19401200
H	-12.46871000	-3.68445600	0.54631000
H	-12.23099300	-3.98093700	-1.19094100
H	-10.28328800	-7.12037200	0.11700000
H	-11.98349000	-6.87889100	0.52851400
H	-10.72320900	-6.45623000	1.70672900
H	-10.70578700	6.53657100	-1.29391000
H	-12.19584400	6.61826000	-0.35089000
H	-10.62789000	6.82235500	0.45962800
H	-13.18530600	4.86806600	0.29383200
H	-12.23775400	3.94422700	1.47912600
H	-12.56623800	3.27091600	-0.13361100

5'

B3LYP/6-31G* = -3403.97167389 au
B3LYP/6-31G* Zero Point Corrected Energy = -3402.872834 au
NIMAG = 0

C	-1.24232100	2.84677300	0.03613000

C	-1.24172100	1.41940200	-0.03871400
C	-0.01353800	0.74407600	-0.06980000
C	1.21521900	1.41772700	-0.03345100
C	1.21742400	2.84509000	0.04364000
C	-0.01196900	3.51961300	0.06915700
C	-2.45193300	3.58610300	0.09844700
C	-2.45324000	0.68142200	-0.09742100
C	2.42688000	0.67976800	-0.09054100
C	2.42881700	3.58045700	0.11728100
C	-3.46780700	4.25394000	0.18060100
C	-3.47640900	0.02360600	-0.16690700
C	3.44915800	4.23972900	0.21202800
C	3.45243900	0.02584000	-0.16130700
C	-4.65488400	5.02768700	0.28141700
C	4.64513300	4.99679600	0.33270600
C	4.65234200	-0.71394600	-0.24839500
C	-4.66277300	6.40159500	-0.03200500
C	-5.81886700	7.16063300	0.06394000
C	-7.04324200	6.58158400	0.47821800
C	-7.03041700	5.20464700	0.80927500
C	-5.86946000	4.45391700	0.70884200
C	4.68212200	6.36873200	0.01332200
C	5.84934000	7.10838600	0.12672800
C	7.05257000	6.51397100	0.57921300
C	7.01536300	5.13391300	0.89507000
C	5.84375600	4.40269400	0.77713000
C	-4.67218300	-0.72315900	-0.25032600
C	-4.87197600	-2.06062200	0.13453800
C	-6.24189800	-2.35185500	-0.14122200
N	-6.83160100	-1.19877900	-0.68256600
C	-5.91136000	-0.22808300	-0.75512200
C	5.88503100	-0.21281100	-0.76320200
N	6.81206400	-1.17718000	-0.69259300
C	6.23335400	-2.33187500	-0.14283700
C	4.86336500	-2.04837000	0.14071500
C	-7.00623000	-3.51867400	0.03659900
C	-8.36522600	-3.55938800	-0.31424800
N	-8.99202900	-2.42960900	-0.85398900
B	-8.32168100	-1.05102200	-1.12489200
B	8.29885900	-1.02090600	-1.14285900
N	8.97962400	-2.39424600	-0.87165500
C	8.36333400	-3.52631700	-0.32469700
C	7.00630600	-3.49304100	0.03456900
C	-9.34402100	-4.60759000	-0.23537300
C	-10.52336600	-4.06610100	-0.73231700
C	-10.28089800	-2.72812500	-1.10565000
C	10.26868500	-2.68550500	-1.13081500
C	10.52181500	-4.02088100	-0.75542300
C	9.34904900	-4.56825200	-0.24938500

C	-3.80146900	-2.93235600	0.71647800
C	-6.35803000	-4.73991300	0.60653700
C	-9.20103100	-6.01473500	0.26605900
C	-11.23880300	-1.74207100	-1.69037000
C	-6.19020100	1.12959100	-1.30418200
C	6.15134100	1.14443700	-1.31964400
C	3.80238800	-2.92461800	0.73322100
C	6.36981900	-4.71642300	0.61307700
C	9.21794800	-5.97506900	0.25624300
C	11.21666200	-1.69526300	-1.72458300
C	-6.35035900	-4.95960000	1.99041200
C	-5.74294400	-6.09891900	2.52092100
C	-5.13814800	-7.03000400	1.67432200
C	-5.14293200	-6.81739800	0.29437800
C	-5.74964500	-5.67847600	-0.23768800
C	6.37568400	-4.93288100	1.99746400
C	5.77981200	-6.07454900	2.53596600
C	5.17324100	-7.01127200	1.69688400
C	5.16445400	-6.80183600	0.31647600
C	5.75946100	-5.66048500	-0.22354900
F	-8.38589200	-0.74559800	-2.48094400
F	-8.94344600	-0.06099500	-0.36725500
F	8.91788000	-0.02471900	-0.39108200
F	8.35451000	-0.71889000	-2.50012400
N	8.21568400	7.25218700	0.71500500
C	8.26062900	8.62194600	0.23318500
C	9.46490700	6.57616400	1.02336400
N	-8.20526300	7.32942300	0.55196200
C	-9.40797000	6.73994900	1.11544200
C	-8.15117100	8.76762200	0.35544000
H	-0.01414900	-0.33849800	-0.13655600
H	-0.01147500	4.60209400	0.13424700
H	-3.74035500	6.87442600	-0.35613400
H	-5.76844600	8.21344700	-0.18647500
H	-7.93447600	4.71476100	1.15014300
H	-5.89146100	3.40137100	0.97350400
H	3.77585700	6.85403100	-0.33691900
H	5.82424200	8.15776400	-0.14143300
H	7.90912100	4.62530100	1.23566400
H	5.84616000	3.34791900	1.03374500
H	-11.47425100	-4.57586400	-0.82281700
H	11.47520200	-4.52504400	-0.85079000
H	-4.05787700	-3.28440600	1.72142900
H	-3.62028800	-3.82440000	0.10759400
H	-2.86831500	-2.36582800	0.78118500
H	-10.15922900	-6.53625000	0.17729200
H	-8.45364600	-6.58196700	-0.29881500
H	-8.89239500	-6.05054300	1.31625800
H	-10.87763000	-1.38455800	-2.66045300

H	-11.32793800	-0.86185600	-1.04458200
H	-12.22505300	-2.19556500	-1.81784500
H	-6.48323000	1.06098300	-2.35769500
H	-7.02978900	1.59234900	-0.77564000
H	-5.30538800	1.76318300	-1.21507600
H	6.44298800	1.07281100	-2.37331200
H	5.26148300	1.77104900	-1.23162600
H	6.98769200	1.61742500	-0.79499600
H	4.07013600	-3.27544300	1.73559500
H	3.61921400	-3.81756400	0.12618500
H	2.86737500	-2.36223100	0.80671200
H	8.46891300	-6.54755100	-0.30108900
H	8.91842200	-6.01036900	1.30909400
H	10.17817200	-6.49161900	0.16051300
H	12.20535300	-2.14246700	-1.85535100
H	10.84799000	-1.34431200	-2.69424500
H	11.30306400	-0.81176300	-1.08292800
H	-6.82018000	-4.23387200	2.64881000
H	-5.74228900	-6.25771200	3.59592800
H	-4.66515400	-7.91647700	2.08786300
H	-4.67367900	-7.53776300	-0.37028600
H	-5.75232500	-5.51170900	-1.31148000
H	6.84706400	-4.20286700	2.64998600
H	5.78958900	-6.23079200	3.61130000
H	4.70935000	-7.89963600	2.11663200
H	4.69368400	-7.52656800	-0.34234100
H	5.75158500	-5.49617400	-1.29769400
H	9.24377900	9.04429400	0.44851300
H	8.08429900	8.69645300	-0.85139600
H	7.51399000	9.24485400	0.74120100
H	9.40291400	6.04891300	1.98339900
H	9.75221500	5.84479800	0.25221800
H	10.26183800	7.31753300	1.10455800
H	-9.28030600	6.44232800	2.16789200
H	-10.22065200	7.46670400	1.06308600
H	-9.71750400	5.85358700	0.54803200
H	-7.51475300	9.27253100	1.09887100
H	-7.76918800	9.01777700	-0.64240800
H	-9.15942600	9.17779700	0.43562600

6'

B3LYP/6-31G* = -3403.97112859 au

B3LYP/6-31G* Zero Point Corrected Energy = -3402.872380 au

NIMAG = 0

C	-0.91046000	1.46815200	-0.02660400
C	-1.44239700	0.14326600	-0.09704800
C	-0.55715100	-0.94022900	-0.17954200

C	0.83527200	-0.77413300	-0.20708900
C	1.36742000	0.55043700	-0.14132800
C	0.48214500	1.63419200	-0.05556700
C	-1.75540100	2.60127200	0.09222800
C	-2.84365100	-0.08786600	-0.10515500
C	1.67664700	-1.91165600	-0.32118900
C	2.76816000	0.78328100	-0.14455400
C	-2.45144000	3.59285500	0.22312400
C	-4.04122100	-0.30877000	-0.13947700
C	3.96477500	1.01142600	-0.12603900
C	2.35727900	-2.91425600	-0.44671700
C	-3.26878000	4.74292000	0.38485400
C	5.35443200	1.26110900	-0.09636500
C	-5.43318100	-0.54314400	-0.19180000
C	3.14811400	-4.08441500	-0.60344400
C	-2.75827400	6.04049200	0.18078200
C	-3.55404100	7.16519200	0.33502200
C	-4.91454100	7.05397300	0.71283300
C	-5.42778400	5.74918400	0.91270200
C	-4.62404700	4.63084100	0.75612700
C	2.64753900	-5.35621300	-0.26075700
C	3.40982200	-6.50350900	-0.41992000
C	4.72886600	-6.44169900	-0.93035700
C	5.22525400	-5.16520400	-1.28856900
C	4.45606400	-4.02291600	-1.12409400
C	-6.12710200	-1.67600800	0.26840400
C	-7.50596600	-1.43755000	-0.01367300
N	-7.61275200	-0.18204900	-0.63252700
C	-6.39159900	0.35699100	-0.74533100
C	5.98142600	2.47007600	-0.51898800
N	7.30547200	2.35847800	-0.34964100
C	7.59498400	1.09278300	0.18449200
C	6.36419900	0.38883700	0.34911200
C	-8.65720200	-2.21181900	0.21602000
C	-9.92944000	-1.75502100	-0.16331300
N	-10.07886000	-0.50814000	-0.78255300
B	-8.93521800	0.49508800	-1.11191700
B	8.34776700	3.46440700	-0.70824800
N	9.74194800	2.88045800	-0.33620700
C	9.98814700	1.61184300	0.20259600
C	8.92612600	0.72999100	0.45787400
C	-11.23408600	-2.34464600	-0.04563700
C	-12.11840900	-1.42734800	-0.60001000
C	-11.38443900	-0.30855900	-1.04511900
C	10.91556300	3.52332900	-0.48518900
C	11.95857900	2.68287900	-0.04388000
C	11.40685200	1.48406400	0.39067000
C	-11.63733300	-3.66670600	0.53875200
C	-11.89417100	0.92995600	-1.70677500

C	-8.52387800	-3.54797900	0.87418100
C	-5.46695100	-2.85421400	0.91706700
C	-6.13264400	1.68253700	-1.37714100
C	5.32581400	3.68792900	-1.07669800
C	6.10296800	-0.98530100	0.88547700
C	9.21659700	-0.62046900	1.03041100
C	12.19974500	0.33291500	0.93634500
C	11.01156000	4.90793600	-1.03735700
C	-8.32359500	-4.70131200	0.10401700
C	-8.20066400	-5.94818900	0.71942200
C	-8.27674200	-6.05499200	2.10940300
C	-8.47615400	-4.90952800	2.88252100
C	-8.59912200	-3.66188400	2.26874400
C	9.46774500	-1.71006800	0.18586300
C	9.74353600	-2.96917400	0.72150400
C	9.77054500	-3.15252600	2.10526800
C	9.52010600	-2.07123000	2.95206500
C	9.24444300	-0.81136100	2.41823400
F	-9.13423100	1.68781000	-0.42040100
F	-8.88083000	0.72520200	-2.48320200
F	8.09787900	4.61335800	0.03708600
F	8.29349700	3.74130300	-2.07147100
N	5.50396500	-7.58311100	-1.06708700
C	6.77405000	-7.50778800	-1.76833400
C	4.89812200	-8.88882600	-0.86767700
N	-5.70855100	8.17421100	0.88673700
C	-7.13640700	8.01726900	1.10861700
C	-5.19445000	9.48477200	0.52810900
H	-0.96336800	-1.94398700	-0.24025300
H	0.88834600	2.63797600	0.00407600
H	-1.71880800	6.15925100	-0.11057000
H	-3.11289000	8.13853000	0.15698600
H	-6.46416900	5.60487000	1.19306600
H	-5.04504300	3.64454500	0.92435900
H	1.63921300	-5.43722800	0.13441400
H	2.97244900	-7.45617700	-0.14663200
H	6.22066900	-5.06169300	-1.70344300
H	4.86295700	-3.05876200	-1.41309900
H	-13.19191600	-1.54126800	-0.68248700
H	13.01019800	2.94029900	-0.04757400
H	-12.72300200	-3.78539600	0.46636500
H	-11.16990500	-4.50931800	0.01804500
H	-11.35646300	-3.75637400	1.59344700
H	-11.62934700	1.81602200	-1.11993500
H	-12.98030000	0.88477000	-1.82016800
H	-11.43318000	1.05663400	-2.69209900
H	-4.38937100	-2.67784100	0.97754900
H	-5.84206700	-3.03103100	1.93063100
H	-5.63146200	-3.77964700	0.35470800

H	-6.44158300	1.66963600	-2.42818600
H	-5.07105800	1.93045600	-1.31422200
H	-6.72206600	2.46426600	-0.88703900
H	4.24165400	3.55765200	-1.09104900
H	5.68211000	3.88100600	-2.09442000
H	5.58329300	4.56857200	-0.47934900
H	6.43633200	-1.09068600	1.92375900
H	6.62172700	-1.76023300	0.31123600
H	5.03034300	-1.19445200	0.84870000
H	13.26508100	0.58397600	0.93056600
H	11.91627900	0.08583000	1.96505700
H	12.06377300	-0.57985900	0.34678000
H	12.05486300	5.22969000	-1.08740500
H	10.44694600	5.60971100	-0.41421700
H	10.57066900	4.95284800	-2.03874300
H	-8.26351800	-4.61721400	-0.97772300
H	-8.04487600	-6.83549800	0.11173700
H	-8.18036400	-7.02574500	2.58783400
H	-8.53528200	-4.98531300	3.96492900
H	-8.75354000	-2.76989700	2.86990900
H	9.44655100	-1.56671400	-0.89115400
H	9.93702700	-3.80662900	0.05645800
H	9.98414300	-4.13304200	2.52177400
H	9.53754000	-2.20710200	4.03002700
H	9.04827000	0.03015600	3.07717000
H	7.24721400	-8.49145900	-1.75651200
H	7.45650600	-6.80653000	-1.27267700
H	6.66425700	-7.19087700	-2.81762700
H	4.08197800	-9.09304200	-1.57875600
H	5.66097900	-9.65960800	-0.99257000
H	4.49443700	-8.98473200	0.14754100
H	-7.33515200	7.44621900	2.02408000
H	-7.64042500	7.50643900	0.27372200
H	-7.58952500	9.00289900	1.22913100
H	-4.94356900	9.56426900	-0.54128900
H	-5.94846800	10.23964800	0.75833000
H	-4.29424400	9.72859400	1.10584900

7

B3LYP/6-31G* = -4810.96496931 au
B3LYP/6-31G* Zero Point Corrected Energy = -4809.524255 au
NIMAG = 0

C	1.21929200	-0.73147400	-0.03028000
C	1.23881000	0.69633200	-0.04302300
C	0.01979100	1.38859300	-0.03650900
C	-1.21940700	0.73149000	-0.03022000
C	-1.23892800	-0.69631600	-0.04299300

C	-0.01990700	-1.38857800	-0.03653600
C	2.41756200	-1.49227200	-0.00605400
C	2.45843500	1.42515600	-0.06888400
C	-2.41768500	1.49227300	-0.00594800
C	-2.45855600	-1.42513700	-0.06882900
C	3.41944200	-2.18459900	0.03874400
C	3.47297300	2.09828300	-0.11796000
C	-3.47305200	-2.09832900	-0.11791000
C	-3.41958300	2.18457300	0.03886800
C	-4.64485300	-2.88597000	-0.17874900
C	-4.57948700	2.98785700	0.09480700
C	-5.81707600	-2.56209200	-0.92247300
N	-6.71866300	-3.53999900	-0.76136000
C	-6.18380200	-4.52584400	0.08164600
C	-4.86728600	-4.12309600	0.45395700
C	-5.83843700	2.57790400	0.62429400
N	-6.70546800	3.59360800	0.52038600
C	-6.06137700	4.69133200	-0.07078500
C	-4.71139600	4.31960700	-0.34094700
B	-8.18701900	3.55506600	1.01468100
N	-8.79647400	4.94315300	0.65667900
C	-8.11991600	6.01116700	0.05416000
C	-6.76841000	5.88705000	-0.29949200
B	-8.12911500	-3.57141700	-1.43180400
N	-8.81192100	-4.88087000	-0.93599500
C	-8.24489200	-5.83674300	-0.08380300
C	-6.94621300	-5.66146800	0.41536300
C	-10.05347600	-5.27901500	-1.26848200
C	-10.32597900	-6.51102600	-0.63618000
C	-9.21428800	-6.88105700	0.10891800
C	-10.06994400	5.31183100	0.88751000
C	-10.25383200	6.63633100	0.43627400
C	-9.05299100	7.09578000	-0.08816300
C	-6.06369100	7.04473600	-0.93134800
C	-3.59953500	5.11083000	-0.95960000
C	-6.18864400	1.25984600	1.22702300
C	-11.06954200	4.40325300	1.52483100
C	-8.84901800	8.46150600	-0.67486500
C	-6.05608000	-1.35976600	-1.77165000
C	-3.86309200	-4.80536400	1.33222800
C	-6.35990100	-6.69769000	1.31993300
C	-9.11906200	-8.13454900	0.92803300
C	-10.93919000	-4.48435700	-2.17094100
C	-6.02386100	7.17801000	-2.32563300
C	-5.36410700	8.25917200	-2.91255000
C	-4.73760000	9.21676300	-2.11270000
C	-4.77361600	9.08966600	-0.72272400
C	-5.43383700	8.00984900	-0.13409900
C	-6.51770400	-6.59841200	2.70868200

C	-5.96934200	-7.56619000	3.55206500
C	-5.25812700	-8.64165900	3.01641500
C	-5.09752200	-8.74632100	1.63341300
C	-5.64581300	-7.77992600	0.78851300
F	-8.87011100	-2.46552200	-1.02957200
F	-7.99490000	-3.59879600	-2.81731300
F	-8.22006200	3.35902600	2.39211500
F	-8.88034600	2.54584300	0.35474300
C	10.25378400	-6.63615700	0.43679800
C	10.06973700	-5.31175800	0.88826300
N	8.79630700	-4.94308300	0.65721100
C	8.11993200	-6.01100000	0.05431300
C	9.05308500	-7.09554500	-0.08801700
B	8.18671000	-3.55509700	1.01536300
N	6.70529100	-3.59358200	0.52067000
C	6.06137200	-4.69122000	-0.07084500
C	6.76850600	-5.88686300	-0.29963600
C	5.83819800	-2.57793000	0.62457700
C	4.57937600	-2.98783600	0.09474500
C	4.71143800	-4.31949600	-0.34124100
C	11.06913600	-4.40328600	1.52604500
C	8.84929700	-8.46117000	-0.67502000
C	6.06398500	-7.04444200	-0.93190700
C	3.59975000	-5.11063900	-0.96030600
C	6.18823100	-1.25996100	1.22760300
C	5.43412500	-8.00983900	-0.13499900
C	4.77410000	-9.08956800	-0.72400300
C	4.73828000	-9.21629200	-2.11401800
C	5.36479000	-8.25841700	-2.91352600
C	6.02435000	-7.17734400	-2.32622900
F	8.21939600	-3.35936700	2.39285000
F	8.88017000	-2.54570200	0.35583100
C	4.64479900	2.88588600	-0.17880300
C	5.81704800	2.56190300	-0.92244900
N	6.71865100	3.53980600	-0.76138300
C	6.18378900	4.52572700	0.08153300
C	4.86725200	4.12303900	0.45383200
B	8.12913500	3.57111500	-1.43175300
N	8.81195000	4.88061200	-0.93605600
C	8.24490400	5.83657600	-0.08397700
C	6.94621200	5.66136800	0.41517100
C	10.05353000	5.27869300	-1.26851900
C	10.32603100	6.51076200	-0.63632500
C	9.21431500	6.88089000	0.10868300
C	6.05606500	1.35948600	-1.77149300
C	3.86304800	4.80538600	1.33203000
C	6.35989800	6.69766600	1.31965400
C	9.11907800	8.13445700	0.92768200
C	10.93926800	4.48392600	-2.17085900

C	5.64583900	7.77986700	0.78811900
C	5.09755100	8.74635200	1.63291900
C	5.25812900	8.64181300	3.01593400
C	5.96931300	7.56638000	3.55169600
C	6.51767200	6.59851400	2.70841300
F	8.87008600	2.46525400	-1.02935400
F	7.99499900	3.59834200	-2.81727300
H	0.03586500	2.47294000	-0.03732400
H	-0.03597900	-2.47292400	-0.03736800
H	-11.25199000	-7.06495300	-0.72437400
H	-11.18221300	7.19041900	0.49310700
H	-3.39720900	6.03685000	-0.41151300
H	-2.68638200	4.50913800	-0.96691100
H	-3.82392300	5.39892200	-1.99242900
H	-5.34217900	0.57350800	1.15631800
H	-7.05911600	0.82824500	0.72293600
H	-6.46665500	1.38659300	2.27929400
H	-12.03455500	4.90589100	1.62739600
H	-11.19660700	3.49384800	0.92819800
H	-10.72183600	4.08379900	2.51314300
H	-8.08375200	9.03277200	-0.13877400
H	-9.78591100	9.02539400	-0.62915100
H	-8.53066000	8.41787100	-1.72190600
H	-6.25552100	-1.65962000	-2.80608600
H	-6.94201800	-0.81728900	-1.42572600
H	-5.18755400	-0.69827600	-1.74442000
H	-4.22857100	-4.92796600	2.35750300
H	-3.60816200	-5.80579800	0.96738100
H	-2.94710300	-4.20904100	1.36779500
H	-10.05513400	-8.69639300	0.85118000
H	-8.93635100	-7.92370200	1.98705900
H	-8.30471800	-8.78638500	0.59408400
H	-11.89567300	-4.99275100	-2.31597000
H	-11.11822200	-3.48825900	-1.75262900
H	-10.45802200	-4.33398400	-3.14321900
H	-6.51064900	6.43167300	-2.94762200
H	-5.33965300	8.35174600	-3.99496100
H	-4.22355500	10.05755300	-2.57026600
H	-4.28754300	9.83110800	-0.09431100
H	-5.46127900	7.90962800	0.94758800
H	-7.07024100	-5.76028500	3.12470700
H	-6.09780200	-7.47832900	4.62750000
H	-4.83082800	-9.39413100	3.67347800
H	-4.54492500	-9.58074700	1.21001100
H	-5.52105300	-7.86058300	-0.28797700
H	11.18217300	-7.19022000	0.49374600
H	10.72121800	-4.08417200	2.51439400
H	12.03417400	-4.90587000	1.62863900
H	11.19622800	-3.49368400	0.92972100

H	8.53115400	-8.41735400	-1.72211700
H	9.78620600	-9.02502400	-0.62921700
H	8.08394500	-9.03257100	-0.13919400
H	2.68652800	-4.50905000	-0.96753900
H	3.82431000	-5.39834400	-1.99320800
H	3.39746200	-6.03687100	-0.41256900
H	5.34169500	-0.57370000	1.15700000
H	7.05867400	-0.82814900	0.72364300
H	6.46621900	-1.38690300	2.27985500
H	5.46142600	-7.90991100	0.94671800
H	4.28802400	-9.83123400	-0.09585500
H	4.22438400	-10.05701300	-2.57188000
H	5.34049100	-8.35070100	-3.99596500
H	6.51114300	-6.43078800	-2.94795300
H	11.25206000	7.06465700	-0.72453100
H	6.94200400	0.81705600	-1.42549800
H	5.18754400	0.69799100	-1.74419100
H	6.25551200	1.65922400	-2.80596100
H	4.22854400	4.92815700	2.35727800
H	3.60806500	5.80575900	0.96704500
H	2.94708400	4.20903000	1.36769600
H	10.05515500	8.69628900	0.85080100
H	8.93634500	7.92370200	1.98672300
H	8.30474400	8.78626800	0.59366200
H	11.89576000	4.99229600	-2.31591500
H	11.11828300	3.48787200	-1.75243100
H	10.45812500	4.33344700	-3.14313300
H	5.52110600	7.86043000	-0.28838100
H	4.54498100	9.58075100	1.20942900
H	4.83083600	9.39435300	3.67292300
H	6.09775400	7.47861600	4.62714000
H	7.07018900	5.76041700	3.12452600

8

B3LYP/6-31G* = -4843.02969218 au
B3LYP/6-31G* Zero Point Corrected Energy = -4841.614190 au
NIMAG = 0

C	1.15653200	-0.70620800	0.08392900
C	1.14604300	0.72344300	0.03511100
N	-0.01076500	1.40398600	0.05953400
C	-1.15651900	0.70619800	0.08389600
C	-1.14602800	-0.72346500	0.03510500
N	0.01077400	-1.40400000	0.05956500
C	2.37226800	-1.43809400	0.16589600
C	2.34944600	1.47330800	-0.05092500
C	-2.37226100	1.43807300	0.16584600
C	-2.34943800	-1.47332100	-0.05092800

C	3.39397900	-2.09367200	0.26759700
C	3.36091700	2.14369000	-0.15948000
C	-3.36090800	-2.14369900	-0.15951900
C	-3.39398500	2.09363200	0.26752800
C	-4.51487500	-2.94448700	-0.28401600
C	-4.56186000	2.87726800	0.37953300
C	-5.76539800	-2.51634600	-0.81731200
N	-6.62539600	-3.54240100	-0.78255500
C	-5.98353800	-4.66469700	-0.23537000
C	-4.64254800	-4.29972700	0.07891100
C	-5.76560700	2.48031100	1.03119700
N	-6.65497300	3.47812500	0.94387500
C	-6.08004800	4.54914400	0.24186800
C	-4.74973700	4.18302700	-0.11419000
B	-8.09077200	3.44837700	1.55884200
N	-8.74808300	4.80977700	1.18299200
C	-8.14404500	5.84761400	0.46180300
C	-6.82565600	5.72041200	0.00310500
B	-8.09720300	-3.48942100	-1.30367300
N	-8.70393400	-4.89645600	-1.02265500
C	-8.02957900	-5.98997900	-0.46421500
C	-6.68608900	-5.87607100	-0.08120000
C	-9.97089800	-5.26010000	-1.29135500
C	-10.15338000	-6.60731200	-0.91050900
C	-8.95821400	-7.08605900	-0.39176600
C	-10.00427600	5.17427300	1.49714000
C	-10.25056900	6.46583300	0.98304700
C	-9.10729400	6.90813600	0.33186000
C	-6.20056200	6.84562700	-0.75791100
C	-3.70077200	4.95365800	-0.85624900
C	-6.04203500	1.19580800	1.73676200
C	-10.92987300	4.29241700	2.26903700
C	-8.98055300	8.23602500	-0.35478900
C	-6.11271900	-1.17354400	-1.36491000
C	-3.53349700	-5.11189100	0.67493900
C	-5.98418000	-7.05971200	0.50352600
C	-8.75356000	-8.47883800	0.12696800
C	-10.96716300	-4.32549400	-1.89509800
C	-6.26161700	6.87383300	-2.15747600
C	-5.68222200	7.92656700	-2.86759900
C	-5.03413600	8.95909600	-2.18704100
C	-4.96834400	8.93579600	-0.79254900
C	-5.54964700	7.88530800	-0.08051000
C	-5.96132000	-7.25878500	1.89031200
C	-5.30390500	-8.36390300	2.43347600
C	-4.66231300	-9.27928900	1.59702600
C	-4.68096900	-9.08610700	0.21434300
C	-5.33934900	-7.98269300	-0.33082700
F	-8.81008700	-2.51652700	-0.61101400

F	-8.10538000	-3.22989100	-2.67074500
F	-8.01135400	3.32165600	2.94221200
F	-8.82002000	2.40007300	1.00742100
C	10.25054500	-6.46590900	0.98308900
C	10.00420700	-5.17441000	1.49731500
N	8.74803700	-4.80988300	1.18311300
C	8.14406000	-5.84763600	0.46175200
C	9.10732000	-6.90814400	0.33176800
B	8.09064200	-3.44858400	1.55918600
N	6.65489700	-3.47826000	0.94410300
C	6.08006000	-4.54916500	0.24185200
C	6.82570500	-5.72038800	0.00297400
C	5.76551600	-2.48046100	1.03147900
C	4.56185000	-2.87731600	0.37961100
C	4.74979600	-4.18298900	-0.11431800
C	10.92973700	-4.29264100	2.26939200
C	8.98062800	-8.23595700	-0.35503400
C	6.20068900	-6.84549100	-0.75827400
C	3.70095100	-4.95347700	-0.85669600
C	6.04186900	-1.19606300	1.73726400
C	5.54942900	-7.88511200	-0.08110600
C	4.96819300	-8.93548900	-0.79335900
C	5.03437800	-8.95873000	-2.18783500
C	5.68280200	-7.92626200	-2.86815900
C	6.26214800	-6.87364500	-2.15781900
F	8.01111700	-3.32214700	2.94258000
F	8.81989700	-2.40014100	1.00803800
C	4.51488700	2.94447500	-0.28396300
C	5.76546700	2.51627900	-0.81708100
N	6.62544200	3.54235600	-0.78239400
C	5.98351500	4.66471800	-0.23542400
C	4.64250700	4.29976600	0.07879500
B	8.09728500	3.48933500	-1.30339200
N	8.70400300	4.89638900	-1.02242300
C	8.02957300	5.98998400	-0.46421200
C	6.68603900	5.87612000	-0.08134400
C	9.97099100	5.26000700	-1.29103100
C	10.15341800	6.60727600	-0.91035100
C	8.95819000	7.08608400	-0.39181300
C	6.11286800	1.17339800	-1.36443100
C	3.53339300	5.11198000	0.67464200
C	5.98405800	7.05983200	0.50315400
C	8.75346700	8.47892700	0.12672000
C	10.96734800	4.32532900	-1.89451200
C	5.33923500	7.98266800	-0.33136300
C	4.68079600	9.08614100	0.21361500
C	4.66206900	9.27952600	1.59626900
C	5.30365300	8.36428500	2.43288300
C	5.96113200	7.25911100	1.88991100

F	8.81011400	2.51648900	-0.61061400
F	8.10556700	3.22971600	-2.67044800
H	-11.07736000	-7.16276800	-1.00972600
H	-11.18154200	7.00921700	1.08379900
H	-3.50141400	5.92567500	-0.39417900
H	-2.76894800	4.38163200	-0.86994600
H	-3.99343200	5.15147600	-1.89344100
H	-5.20068700	0.50953900	1.61942900
H	-6.95422600	0.73387800	1.34685500
H	-6.21327200	1.37901000	2.80349400
H	-11.89029000	4.78893000	2.42821700
H	-11.09360300	3.34942400	1.73683500
H	-10.49122400	4.03290700	3.23839300
H	-8.19860600	8.85999500	0.09087400
H	-9.92803300	8.77911400	-0.28334200
H	-8.72924800	8.12966200	-1.41538000
H	-6.35582600	-1.25083500	-2.43066800
H	-7.00332200	-0.77655500	-0.86804400
H	-5.27690300	-0.48273900	-1.23490300
H	-3.76028200	-5.42559500	1.70008100
H	-3.33828400	-6.02419700	0.10262000
H	-2.61656200	-4.51654000	0.69765600
H	-9.69016300	-9.04025300	0.05377400
H	-8.43371300	-8.48676000	1.17421800
H	-7.98842000	-9.02215600	-0.43779400
H	-11.92017100	-4.83431100	-2.06004600
H	-11.12715000	-3.46116300	-1.24183300
H	-10.59610900	-3.93389000	-2.84813700
H	-6.76537200	6.06939500	-2.68657100
H	-5.73673300	7.93826800	-3.95279700
H	-4.58199500	9.77734100	-2.74070500
H	-4.46439000	9.73552700	-0.25654300
H	-5.49932900	7.86631000	1.00481000
H	-6.45929200	-6.54494400	2.54093700
H	-5.29257300	-8.50775900	3.51046700
H	-4.14951200	-10.13841500	2.02063000
H	-4.18240500	-9.79403200	-0.44225600
H	-5.35282300	-7.83091700	-1.40675600
H	11.18151100	-7.00930300	1.08385400
H	10.49100600	-4.03325300	3.23874400
H	11.89014400	-4.78916500	2.42858900
H	11.09350000	-3.34958100	1.73731800
H	8.72979400	-8.12945900	-1.41572600
H	9.92798200	-8.77922100	-0.28323700
H	8.19837800	-8.85982100	0.09024000
H	2.76919500	-4.38134800	-0.87063300
H	3.99388900	-5.15129400	-1.89380900
H	3.50134800	-5.92548600	-0.39471600
H	5.20047900	-0.50982600	1.62005200

H	6.95402800	-0.73400900	1.34742600
H	6.21313100	-1.37943900	2.80396100
H	5.49880400	-7.86615300	1.00420100
H	4.46397900	-9.73517900	-0.25753600
H	4.58227900	-9.77688700	-2.74166500
H	5.73761800	-7.93791600	-3.95334100
H	6.76616800	-6.06925400	-2.68673400
H	11.07740300	7.16272600	-1.00955100
H	7.00333400	0.77643200	-0.86729900
H	5.27699500	0.48264000	-1.23453600
H	6.35624200	1.25054700	-2.43013800
H	3.76005700	5.42572500	1.69979900
H	3.33826800	6.02426200	0.10225800
H	2.61644800	4.51664200	0.69727900
H	9.69002400	9.04040100	0.05337500
H	8.43370600	8.48697800	1.17399800
H	7.98824100	9.02210400	-0.43805600
H	11.92029500	4.83420600	-2.05963000
H	11.12745900	3.46121500	-1.24098700
H	10.59632100	3.93339400	-2.84742400
H	5.35276400	7.83073700	-1.40727000
H	4.18223900	9.79395400	-0.44311000
H	4.14921900	10.13869800	2.01972100
H	5.29226700	8.50829800	3.50985300
H	6.45909900	6.54538400	2.54066400

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B3LYP/6-31G* = -2521.60663907 au
B3LYP/6-31G* Zero Point Corrected Energy = -2520.836245 au
NIMAG = 0

C	-0.57324900	7.40197000	0.21704200
C	0.82332400	7.37864200	0.14239800
C	1.49540300	6.16307200	0.08497700
C	0.79458700	4.94109100	0.10266900
C	-0.62763200	4.96463800	0.19551600
C	-1.28608900	6.20852000	0.24477000
C	1.51161700	3.71717600	0.01079400
C	-1.38821900	3.76353700	0.25251600
C	-2.08552800	2.76808700	0.33602400
C	2.16622600	2.69617300	-0.10500400
C	-2.89519200	1.61400000	0.44341600
C	2.92262100	1.51245300	-0.25296700
C	-2.56721500	0.44744900	1.19421200
N	-3.56828600	-0.43644700	1.08511300
C	-4.57414900	0.10486200	0.27056600
C	-4.15888200	1.40672500	-0.13891400
C	2.42453600	0.27834900	-0.76550900

N	3.41797600	-0.62021600	-0.77815500
C	4.58675700	-0.02214200	-0.28295800
C	4.28428600	1.33105200	0.05119100
B	3.28421800	-2.09118900	-1.28697200
N	4.68143300	-2.74747800	-1.08044900
C	5.82562800	-2.11323900	-0.58047200
C	5.77733200	-0.76721600	-0.18860500
B	-3.60572900	-1.83194600	1.78568300
N	-4.94834100	-2.49389100	1.35468200
C	-5.92211400	-1.92301700	0.52582100
C	-5.73756500	-0.63812500	-0.00542100
C	-5.35963300	-3.72030500	1.72548200
C	-6.61859400	-3.97858900	1.14250600
C	-6.99195500	-2.87365700	0.38878100
C	4.98796900	-4.02413900	-1.37606000
C	6.34744000	-4.25187300	-1.07389200
C	6.89330300	-3.07565800	-0.57693600
C	7.01177700	-0.11142900	0.34273300
C	5.16651600	2.40342400	0.61370000
C	1.04237700	-0.02010000	-1.23931900
C	3.98947500	-4.98627200	-1.93145100
C	8.32162900	-2.91873600	-0.14476900
C	-1.33948900	0.19826300	2.00330600
C	-4.85384500	2.41009800	-1.00802300
C	-6.79422500	-0.04699000	-0.88291200
C	-8.27123100	-2.76835600	-0.38817100
C	-4.54927700	-4.60673300	2.61316100
C	7.29450300	-0.13912500	1.71495200
C	8.44446800	0.47706500	2.21117900
C	9.32339600	1.12590400	1.34171300
C	9.04801300	1.15619200	-0.02673500
C	7.89821700	0.54086800	-0.52464100
C	-6.74154800	-0.22167200	-2.27223200
C	-7.72886500	0.32961600	-3.09063700
C	-8.77706600	1.06149700	-2.52938400
C	-8.83504900	1.23948100	-1.14576600
C	-7.84948300	0.68760000	-0.32570300
F	-2.53357100	-2.60789000	1.35835500
F	-3.57612000	-1.66769600	3.16807100
F	2.32544600	-2.76566100	-0.53955600
F	2.95130300	-2.09482900	-2.63875400
H	2.57853900	6.13737300	0.01652800
H	-2.36946400	6.21736100	0.31366600
H	-7.18818600	-4.89066200	1.26835700
H	6.86695300	-5.19173500	-1.21142200
H	5.58757500	2.12349100	1.58506200
H	4.58480300	3.32015100	0.74492900
H	6.01383800	2.62579900	-0.04362500
H	0.40133100	0.85484700	-1.11260700

H	0.62339400	-0.86764900	-0.68715700
H	1.05783300	-0.31117600	-2.29541400
H	3.54670400	-4.59041500	-2.85137600
H	3.16531400	-5.13660300	-1.22570700
H	4.46147200	-5.94913300	-2.14266500
H	8.40745300	-2.63459700	0.90940100
H	8.84545600	-2.14796600	-0.72007800
H	8.85417400	-3.86476500	-0.28396400
H	-0.64382700	1.03402500	1.90251600
H	-0.85281300	-0.72840200	1.68307600
H	-1.60089300	0.06730900	3.05920900
H	-5.84123500	2.67943900	-0.61909300
H	-4.24819100	3.31865900	-1.06902700
H	-5.00782500	2.03594200	-2.02603800
H	-8.84177600	-3.69660300	-0.28493300
H	-8.09419200	-2.59589800	-1.45500800
H	-8.90151100	-1.94361000	-0.03844800
H	-4.31121100	-4.09354900	3.55051100
H	-5.09122000	-5.53008300	2.83252300
H	-3.59307800	-4.85384000	2.13929300
H	6.60912400	-0.64289300	2.39122900
H	8.65243500	0.44994300	3.27740900
H	10.21814500	1.60576100	1.72861900
H	9.72770100	1.65960000	-0.70900200
H	7.68270700	0.56551000	-1.58947600
H	-5.92470900	-0.79039600	-2.70833500
H	-7.67758400	0.18721900	-4.16669300
H	-9.54471800	1.49127000	-3.16698800
H	-9.64797600	1.80832100	-0.70252500
H	-7.89413000	0.82538500	0.75129100
H	1.38637400	8.30761200	0.12447400
H	-1.10403900	8.34893500	0.25891000

10

B3LYP/6-31G* = -2521.60798242 au
B3LYP/6-31G* Zero Point Corrected Energy = -2520.837821 au
NIMAG = 0

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C	-1.22298700	-3.57279600	0.00066100
C	0.00000500	-2.88003000	0.00057200
C	1.22299500	-3.57280500	0.00064600
C	1.21044000	-4.98319200	0.00081900
C	-0.00000400	-5.67161800	0.00090200
C	-2.45640000	-2.85985600	0.00054600
C	2.45640900	-2.85986800	0.00051500
C	-3.51486100	-2.25739600	0.00039600
C	3.51487000	-2.25740800	0.00035500

C	4.74452200	-1.56144700	0.00016900
C	-4.74451600	-1.56143900	0.00022900
C	-4.93473100	-0.16728400	0.00022500
C	-6.34614200	0.03887900	-0.00002300
N	-6.97017400	-1.21771500	-0.00016500
C	-6.03170500	-2.17370500	-0.00001000
C	6.03171300	-2.17370800	-0.00021300
N	6.97017900	-1.21771500	-0.00034900
C	6.34614300	0.03887800	-0.00005700
C	4.93473200	-0.16729200	0.00027600
C	-7.12221300	1.21341400	-0.00008700
C	-8.52365100	1.15829500	-0.00032000
N	-9.18500400	-0.07649900	-0.00045100
B	-8.50994200	-1.47923800	-0.00029200
B	8.50994900	-1.47923400	-0.00059000
N	9.18500600	-0.07649200	-0.00044900
C	8.52364900	1.15829900	-0.00023000
C	7.12221000	1.21341500	-0.00001500
C	-9.52434400	2.19041600	-0.00039600
C	-10.74832900	1.53454400	-0.00060700
C	-10.51287000	0.14338800	-0.00063900
C	10.51287000	0.14339900	-0.00061100
C	10.74832500	1.53455600	-0.00046500
C	9.52433800	2.19042400	-0.00021900
C	-3.81666200	0.83014400	0.00041700
C	-6.43894900	2.54342900	0.00003100
C	-9.36046500	3.68190600	-0.00028700
C	-11.51411300	-0.96494600	-0.00095200
C	-6.34842100	-3.63103500	-0.00005900
C	6.34843500	-3.63103700	-0.00035500
C	3.81665900	0.83013200	0.00067500
C	6.43894300	2.54342800	0.00019500
C	9.36045400	3.68191300	0.00004900
C	11.51411800	-0.96493000	-0.00105300
C	-6.11509800	3.17425100	-1.20852400
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C	-5.15903000	5.03994100	0.00031700
C	-5.47863700	4.41635700	1.20793000
C	-6.11565200	3.17426100	1.20873000
C	6.11482000	3.17417900	-1.20832600
C	5.47782400	4.41628000	-1.20717200
C	5.15901500	5.03993500	0.00061900
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C	6.11591300	3.17432900	1.20892800
F	-8.87062000	-2.18333600	1.14506500
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F	8.87045200	-2.18322600	-1.14605100
F	8.87065100	-2.18360200	1.14458700
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H	-0.00000700	-6.75817600	0.00104500
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H	11.72549900	2.00056800	-0.00057400
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H	-3.84732100	1.48324800	0.87908400
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H	-10.34476900	4.16048400	-0.00110800
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H	-11.37871100	-1.60421300	-0.87982700
H	-12.53066700	-0.56374600	-0.00016100
H	-6.94728900	-3.89158000	0.87894400
H	-6.94777600	-3.89141600	-0.87876700
H	-5.42646300	-4.21626600	-0.00033900
H	6.94665200	-3.89178500	0.87903700
H	5.42647900	-4.21627000	-0.00141200
H	6.94844300	-3.89121100	-0.87867300
H	3.84705100	1.48346500	-0.87782300
H	3.84750400	1.48326100	0.87931700
H	2.85912500	0.30193200	0.00086300
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H	10.34475500	4.16049500	-0.00144200
H	12.53067100	-0.56372700	-0.00010300
H	11.37772200	-1.60568700	0.87656500
H	11.37879300	-1.60402200	-0.88006800
H	-6.36303900	2.68798700	-2.14817400
H	-5.23148400	4.89577200	-2.15092000
H	-4.66336900	6.00682000	0.00042000
H	-5.23245400	4.89578000	2.15152300
H	-6.36402600	2.68800100	2.14826800
H	6.36255800	2.68786200	-2.14800200
H	5.23101000	4.89565000	-2.15062700
H	4.66335000	6.00681300	0.00077700
H	5.23290100	4.89589100	2.15181600
H	6.36449600	2.68812400	2.14843900
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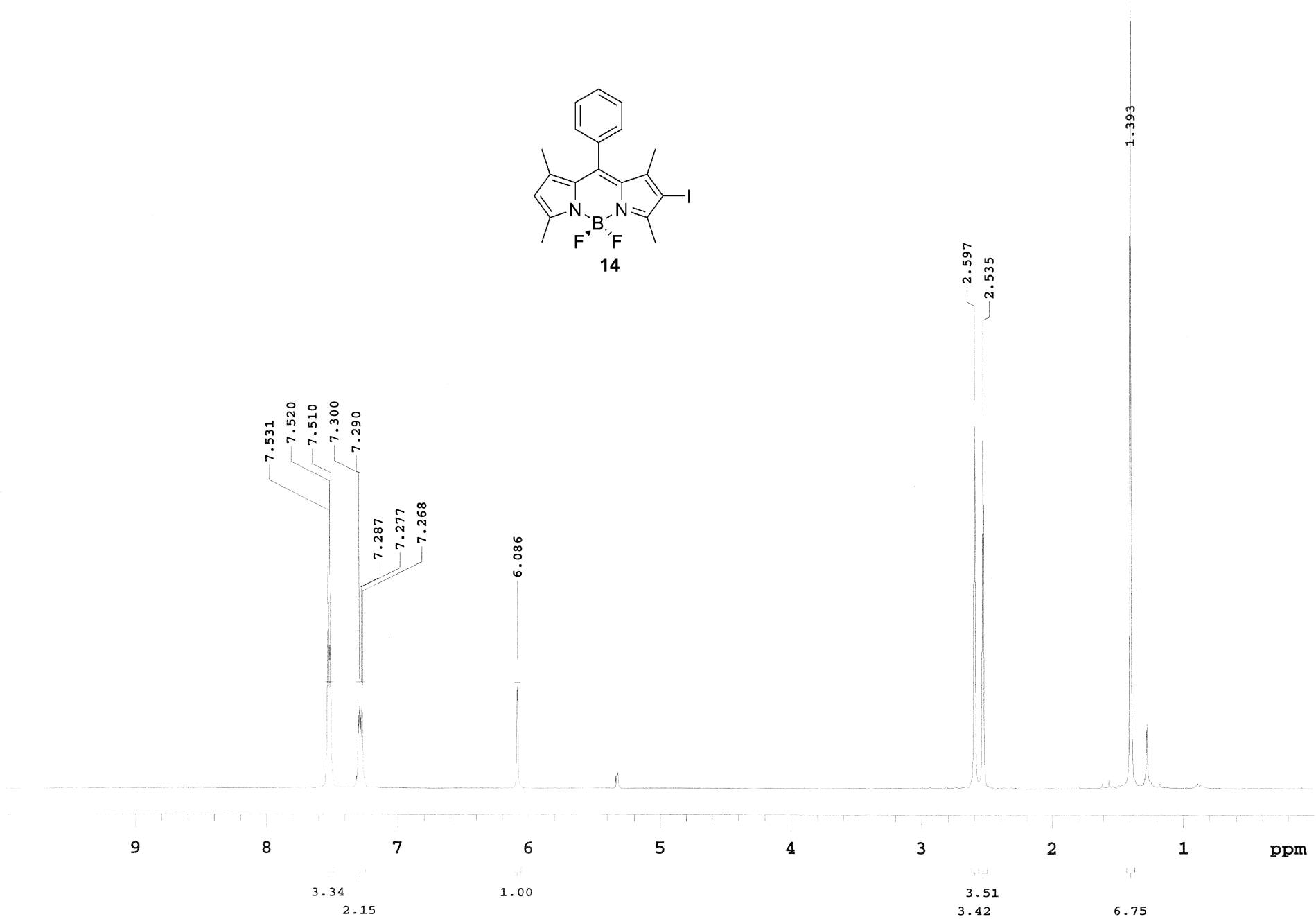
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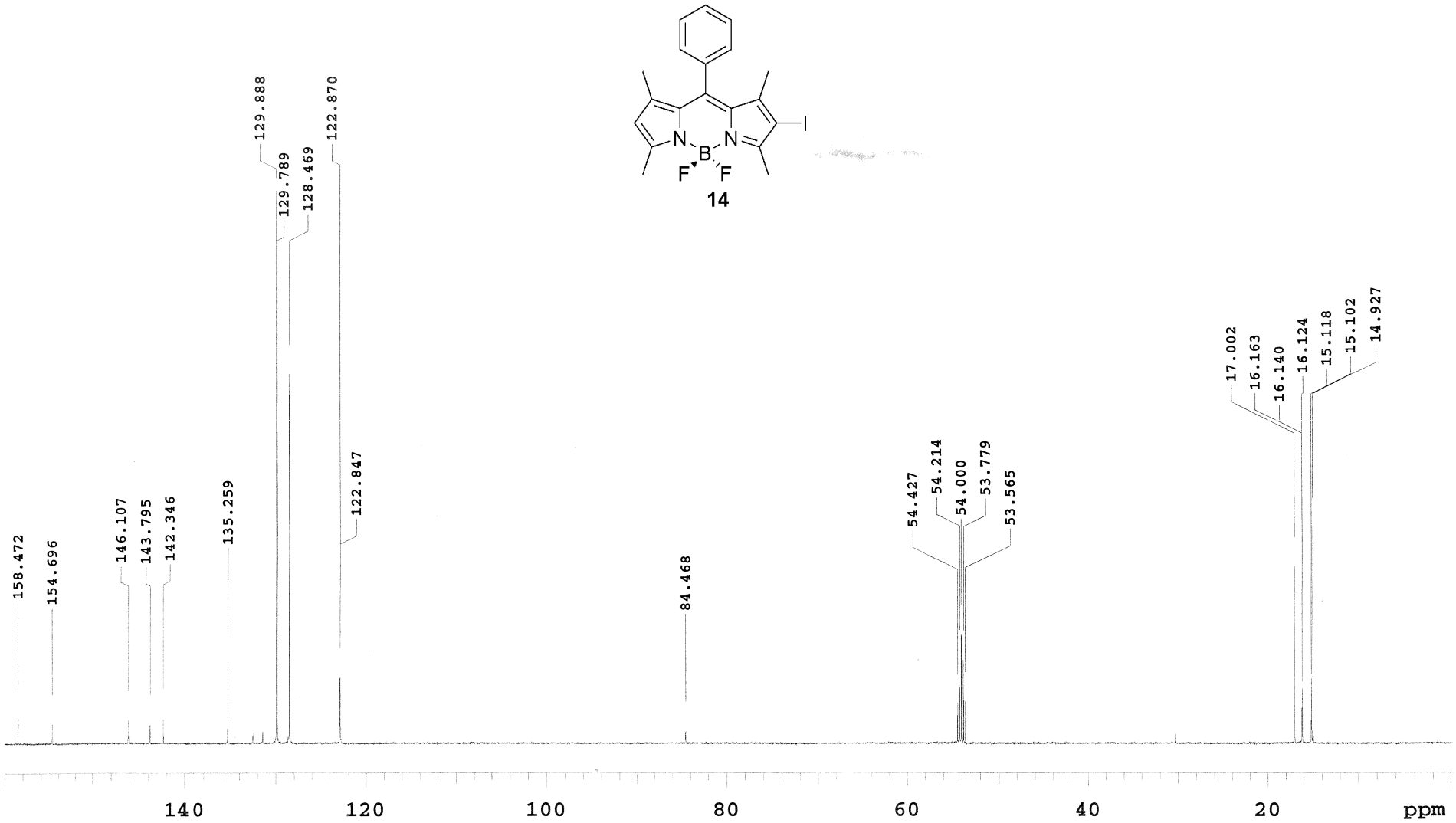
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B3LYP/6-31G* Zero Point Corrected Energy = -2520.838727 au
NIMAG = 0

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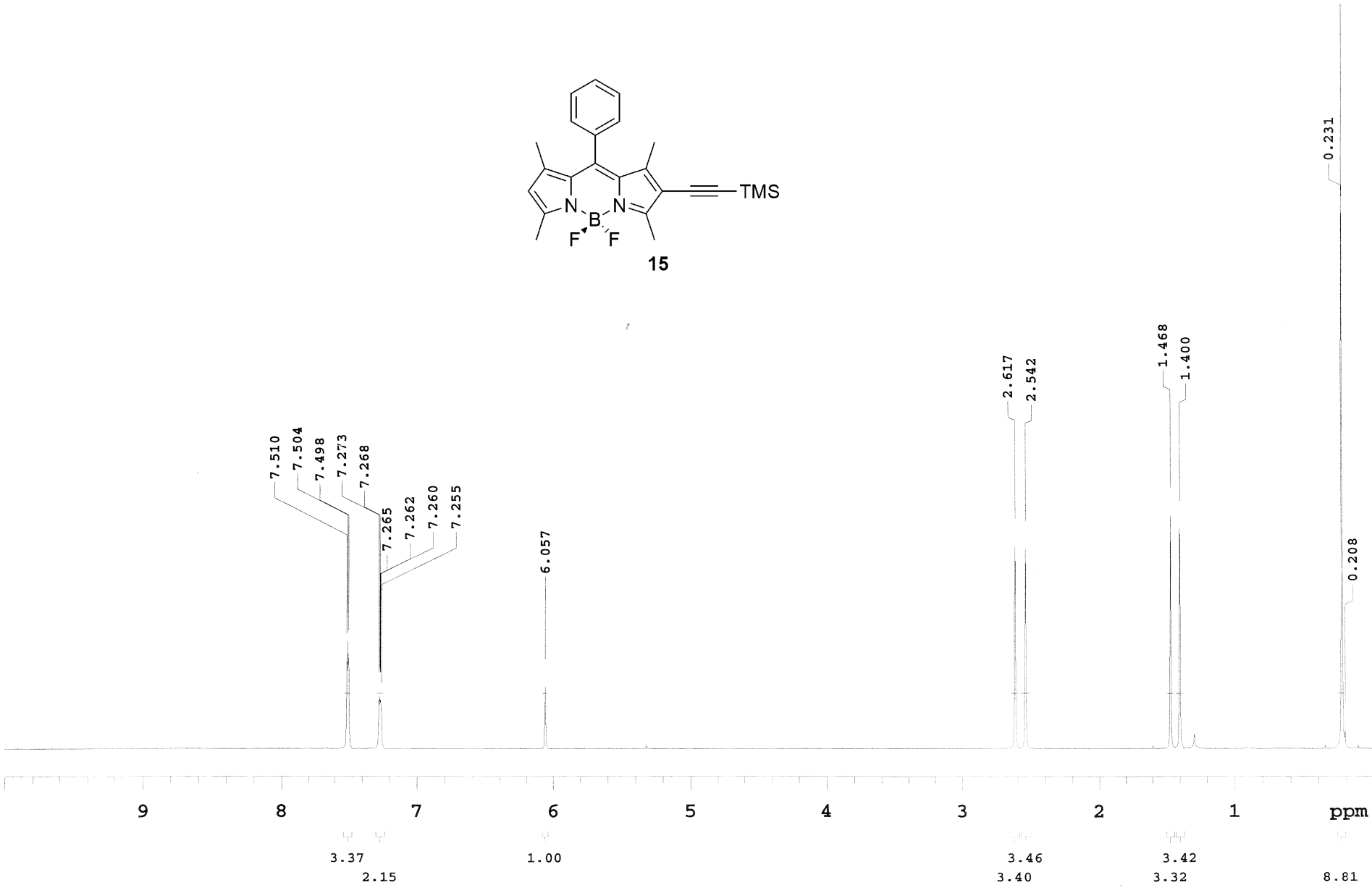
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C	2.83801300	-0.51899700	0.01913400
C	-4.05683200	-0.52185900	-0.02808200
C	4.05684200	-0.52186600	0.02783000
C	5.46875400	-0.52824700	0.03916700
C	-5.46874100	-0.52823100	-0.03938000
C	-6.32743500	0.58047300	0.08146900
C	-7.65415400	0.06224300	0.01172400
N	-7.57065900	-1.32919200	-0.14970400
C	-6.28149300	-1.69112200	-0.18061300
C	6.28149800	-1.69113700	0.18042300
N	7.57066600	-1.32920900	0.14956200
C	7.65416900	0.06222700	-0.01183200
C	6.32745500	0.58046000	-0.08163400
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C	-10.09997000	-0.04759500	-0.02233300
N	-10.05957700	-1.43736100	-0.19284000
B	-8.77598900	-2.31270300	-0.28897400
B	8.77598600	-2.31268900	0.28909500
N	10.05958300	-1.43735600	0.19296500
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C	8.91194200	0.69147600	-0.07548400
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C	11.32092900	-1.90275000	0.25638400
C	12.21718400	-0.82069500	0.12691900
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C	-12.08058900	1.71293400	0.19096300
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C	9.09899600	4.40190200	0.70812200
C	9.11321300	4.95884400	-0.57222200

C	9.06121400	4.12531400	-1.69114500
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F	-8.75225400	-3.24137300	0.74741800
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F	8.72302800	-2.95216100	1.52437600
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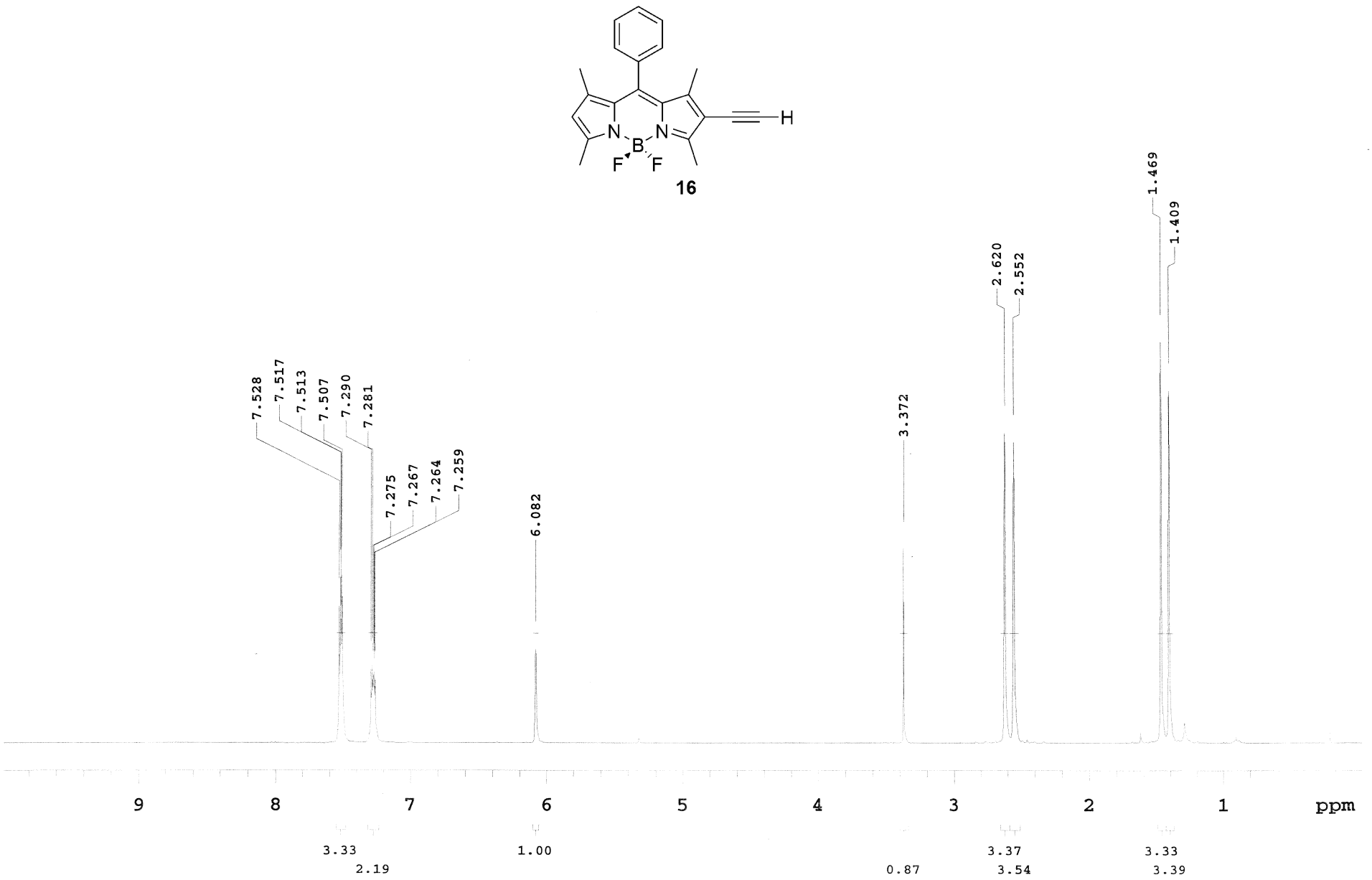
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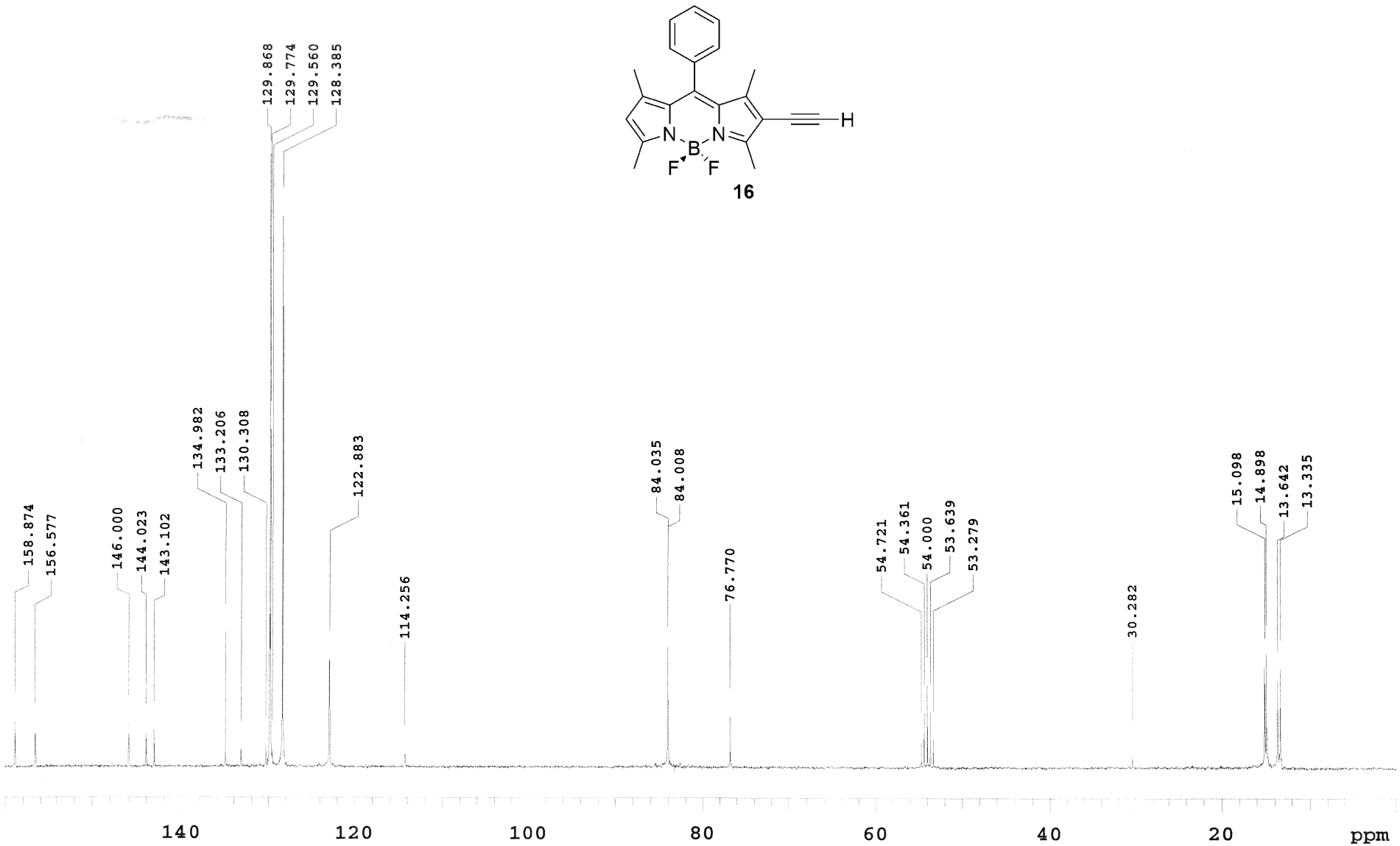

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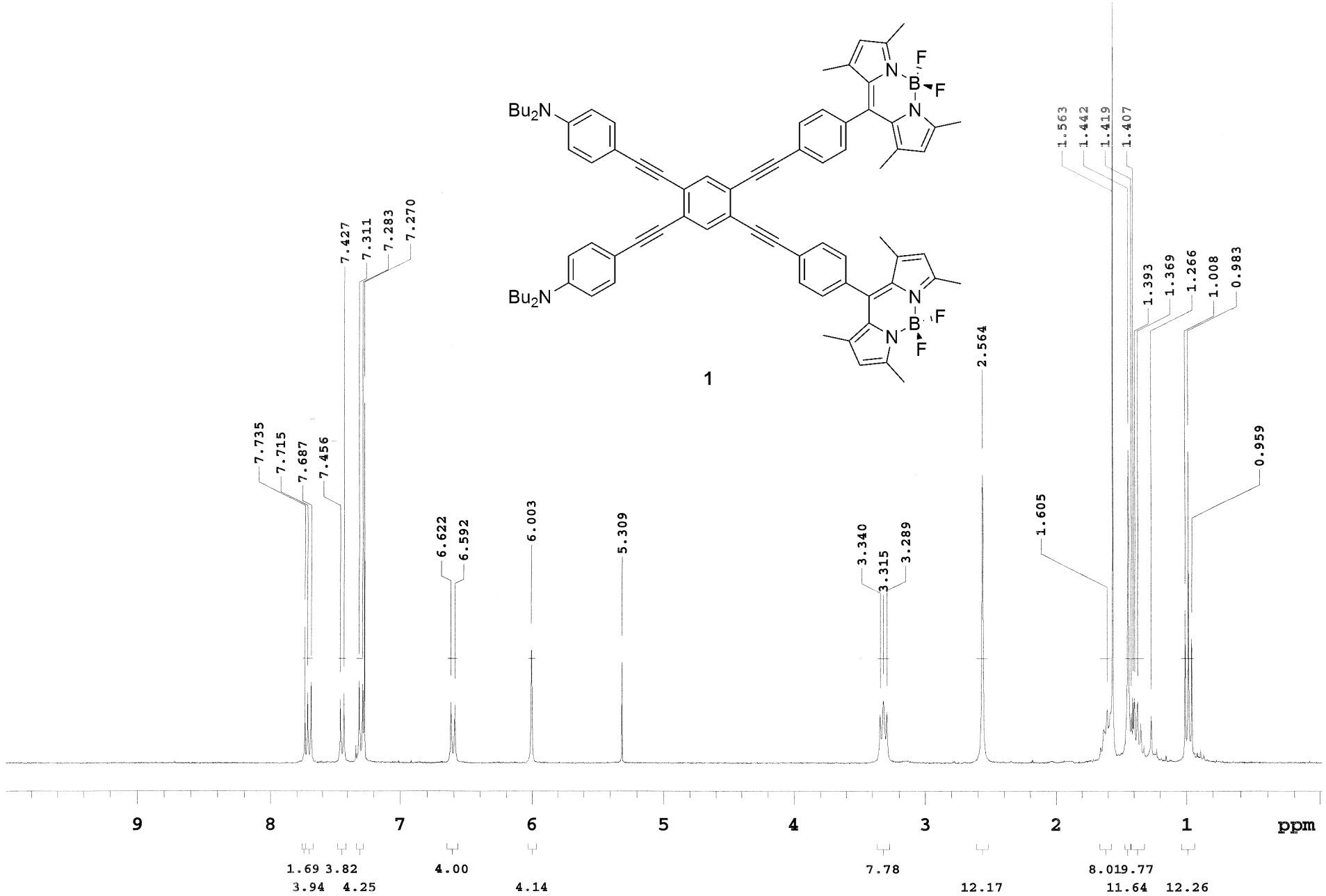
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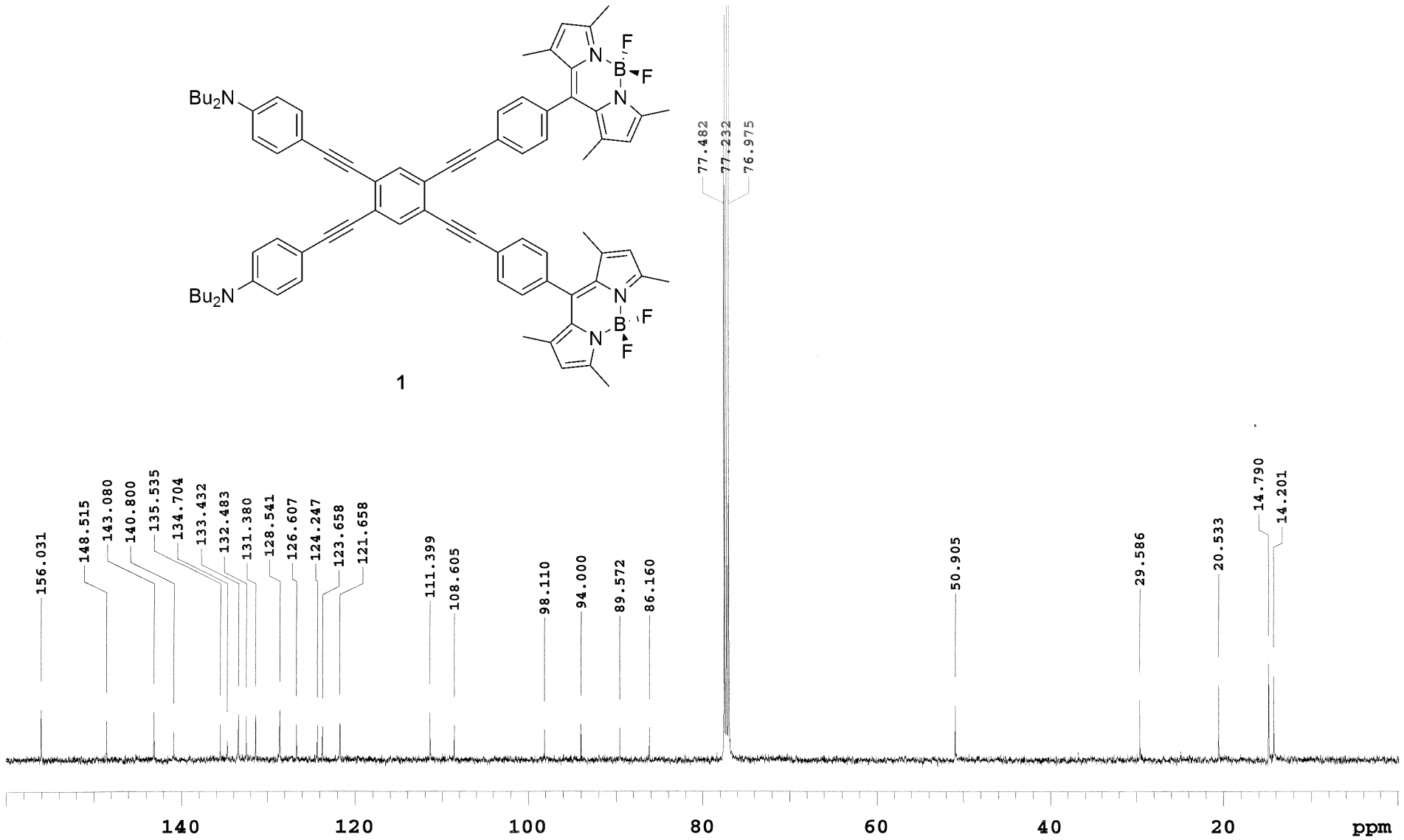
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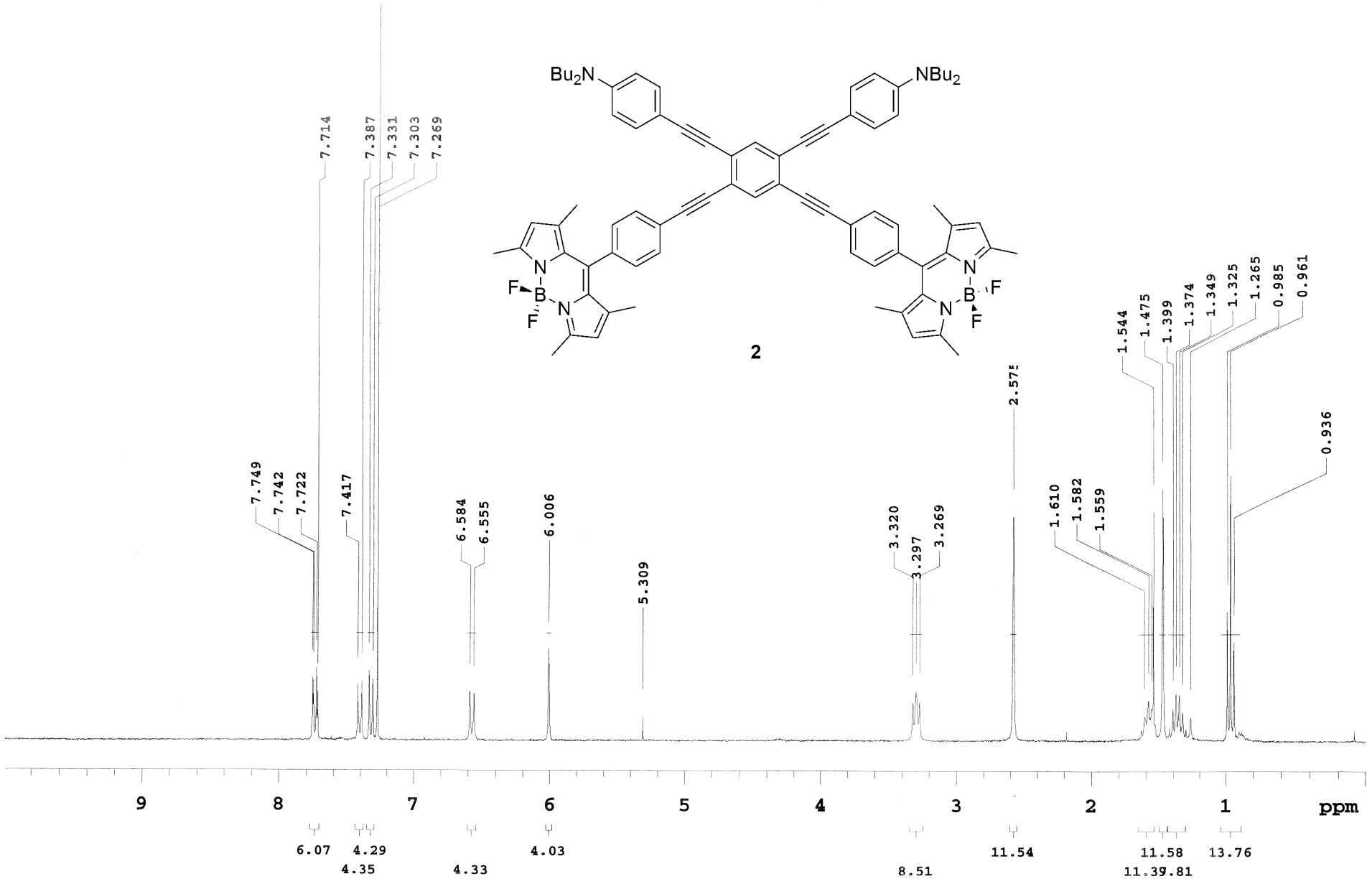

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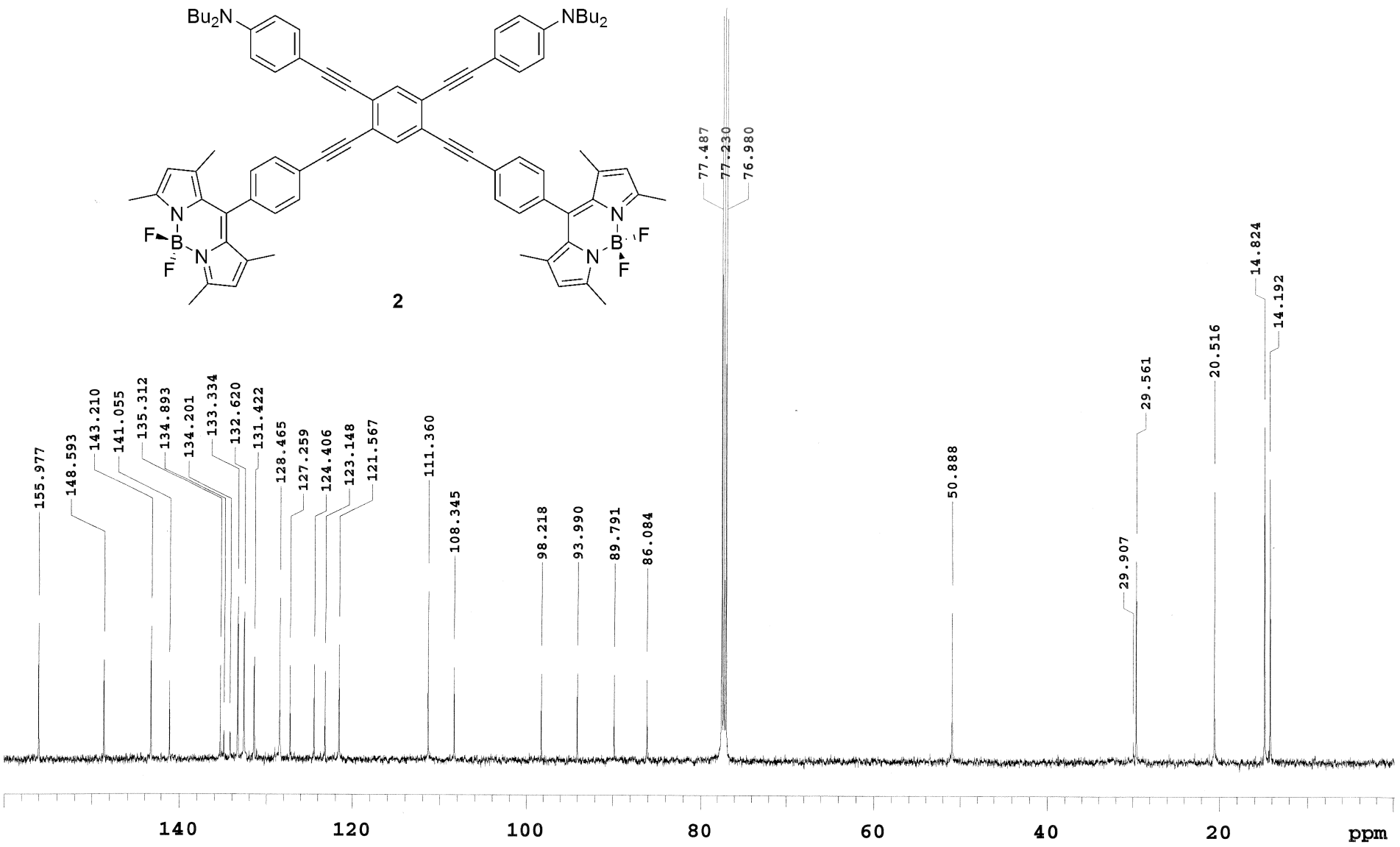

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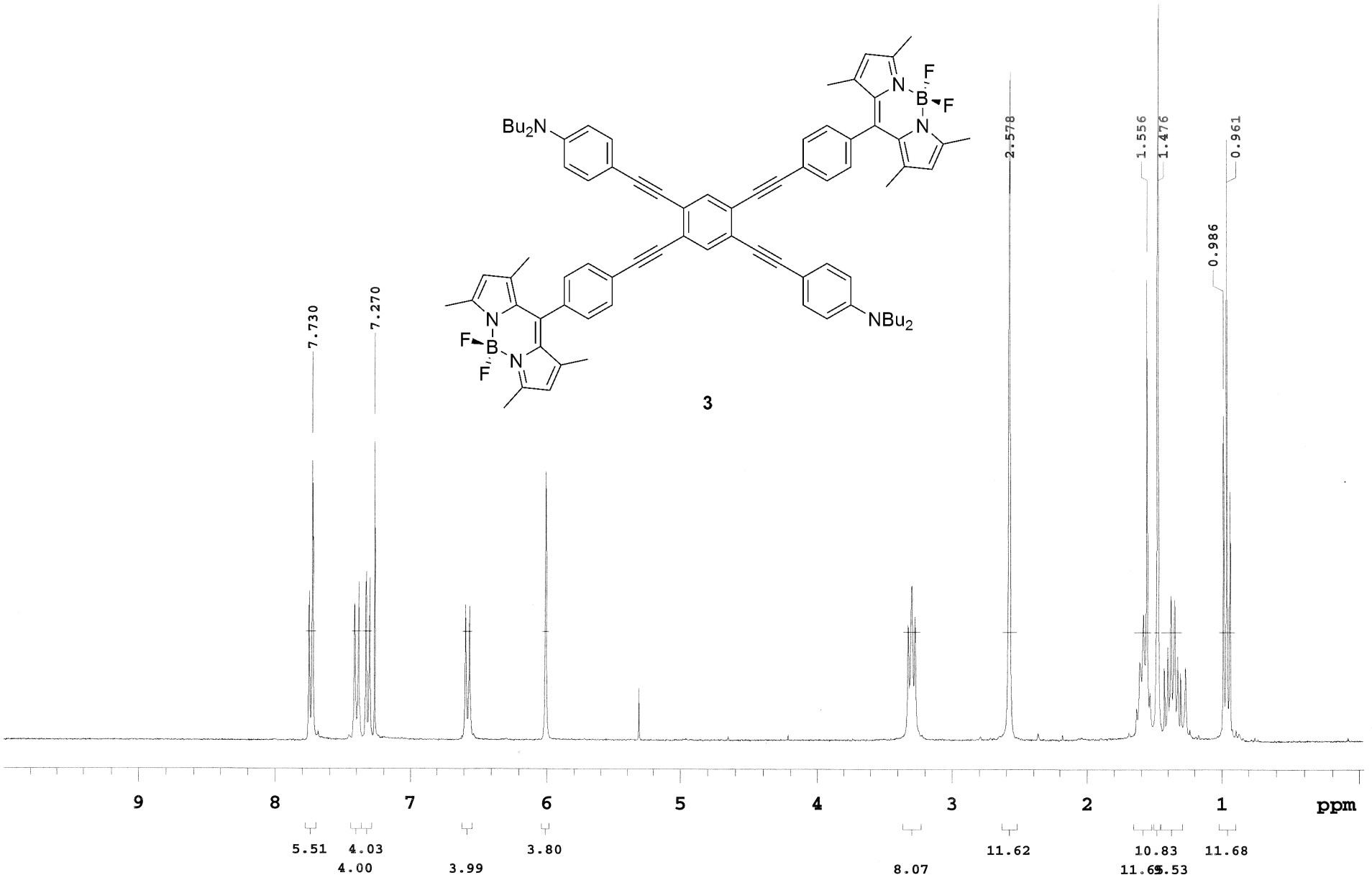
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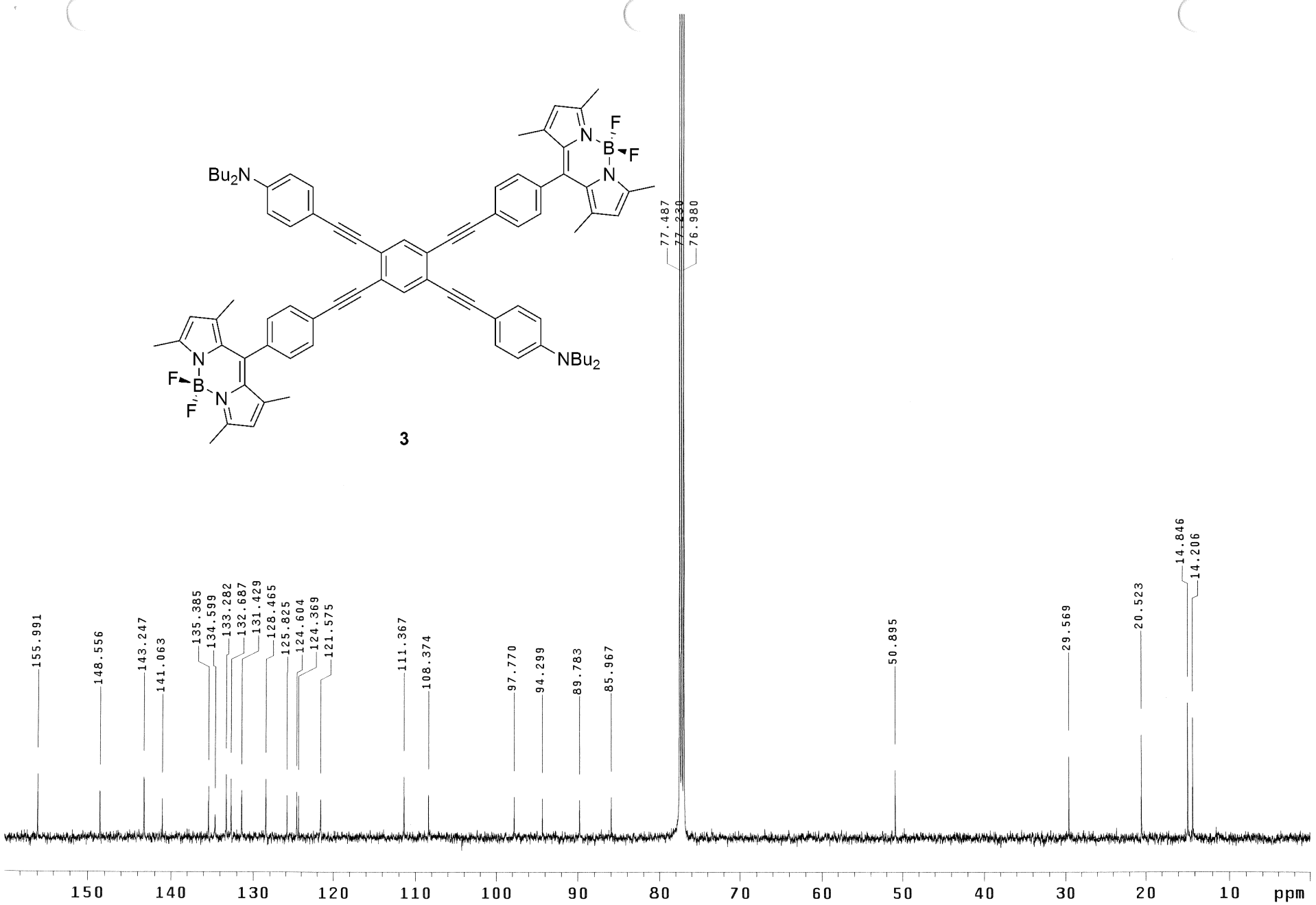

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8
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5
4
3
2
1
ppm
1.69 3.82
3.94 4.25
4.00
4.14
7.78
12.17
8.01 9.77
11.64 12.26


Bu2N
Bu2N
N
B
F
F
F
N
N
B
F
F
1
156.031
148.515
143.080
140.800
135.535
134.704
133.432
132.483
131.380
128.541
126.607
124.247
123.658
121.658
111.399
108.605
98.110
94.000
89.572
86.160
77.482
77.232
76.975
50.905
29.586
20.533
14.790
14.201
140
120
100
80
60
40
20
ppm

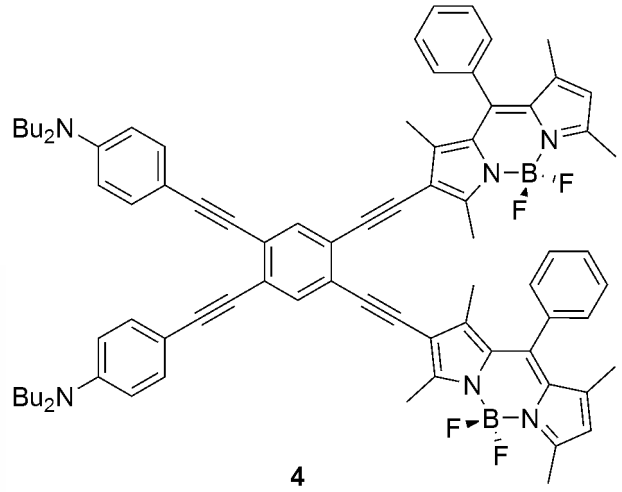

Bu2N
NBu2
N
F
B
F
N
2
7.749
7.742
7.722
7.714
7.417
7.387
7.331
7.303
7.269
6.584
6.555
6.006
5.309
3.320
3.297
3.269
2.575
1.610
1.582
1.559
1.544
1.475
1.399
1.374
1.349
1.325
1.265
0.985
0.961
0.936
9
8
7
6
5
4
3
2
1
ppm
6.07
4.29
4.35
4.33
4.03
8.51
11.54
11.58
11.39
9.81
13.76


Bu2N
NBu2
N
F
B
F
N
2
77.487
77.230
76.980
155.977
148.593
143.210
141.055
135.312
134.893
134.201
133.334
132.620
131.422
128.465
127.259
124.406
123.148
121.567
111.360
108.345
98.218
93.990
89.791
86.084
50.888
29.907
29.561
20.516
14.824
14.192
140
120
100
80
60
40
20
ppm

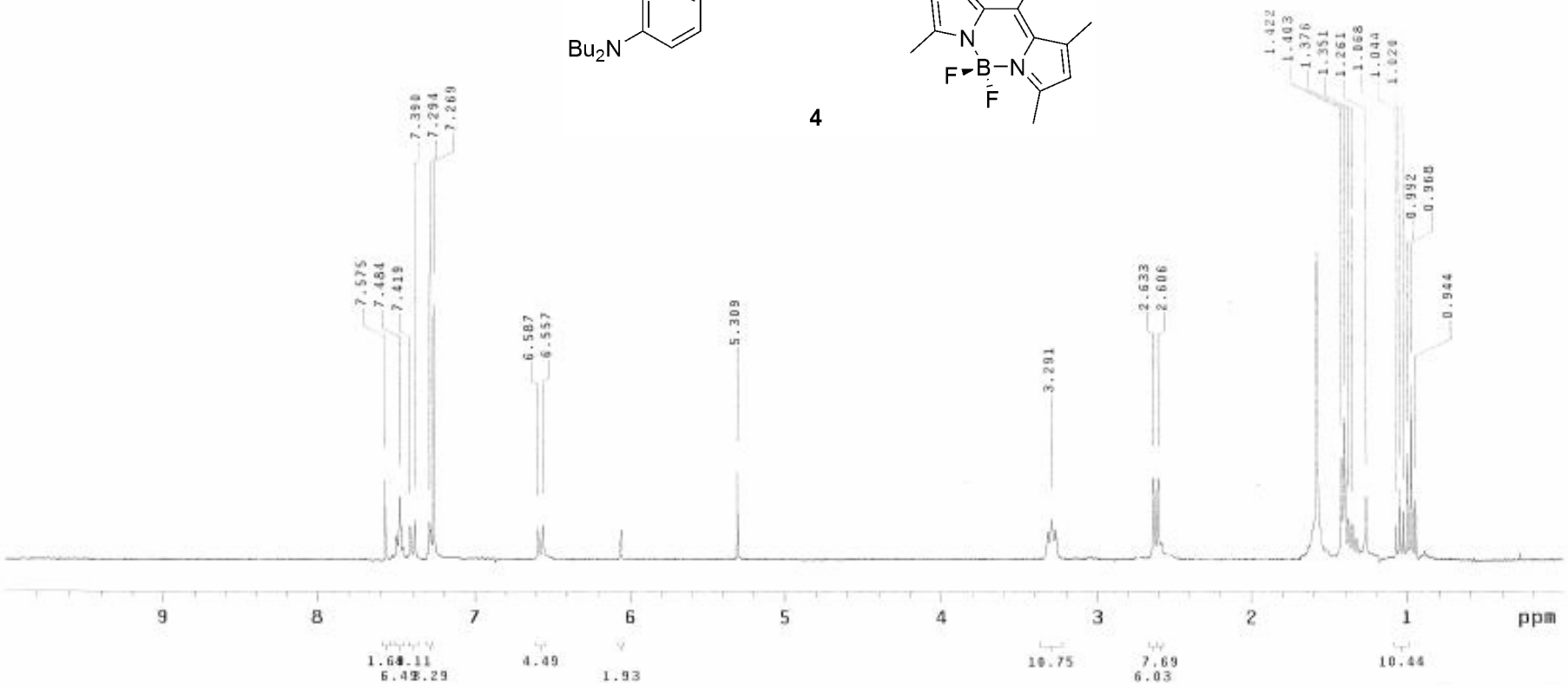

7.730
7.270
2.578
1.556
1.476
0.986
0.961
Bu2N
NBu2
F
B
N
3
9
8
7
6
5
4
3
2
1
ppm
5.51
4.03
4.00
3.99
3.80
8.07
11.62
10.83
11.68

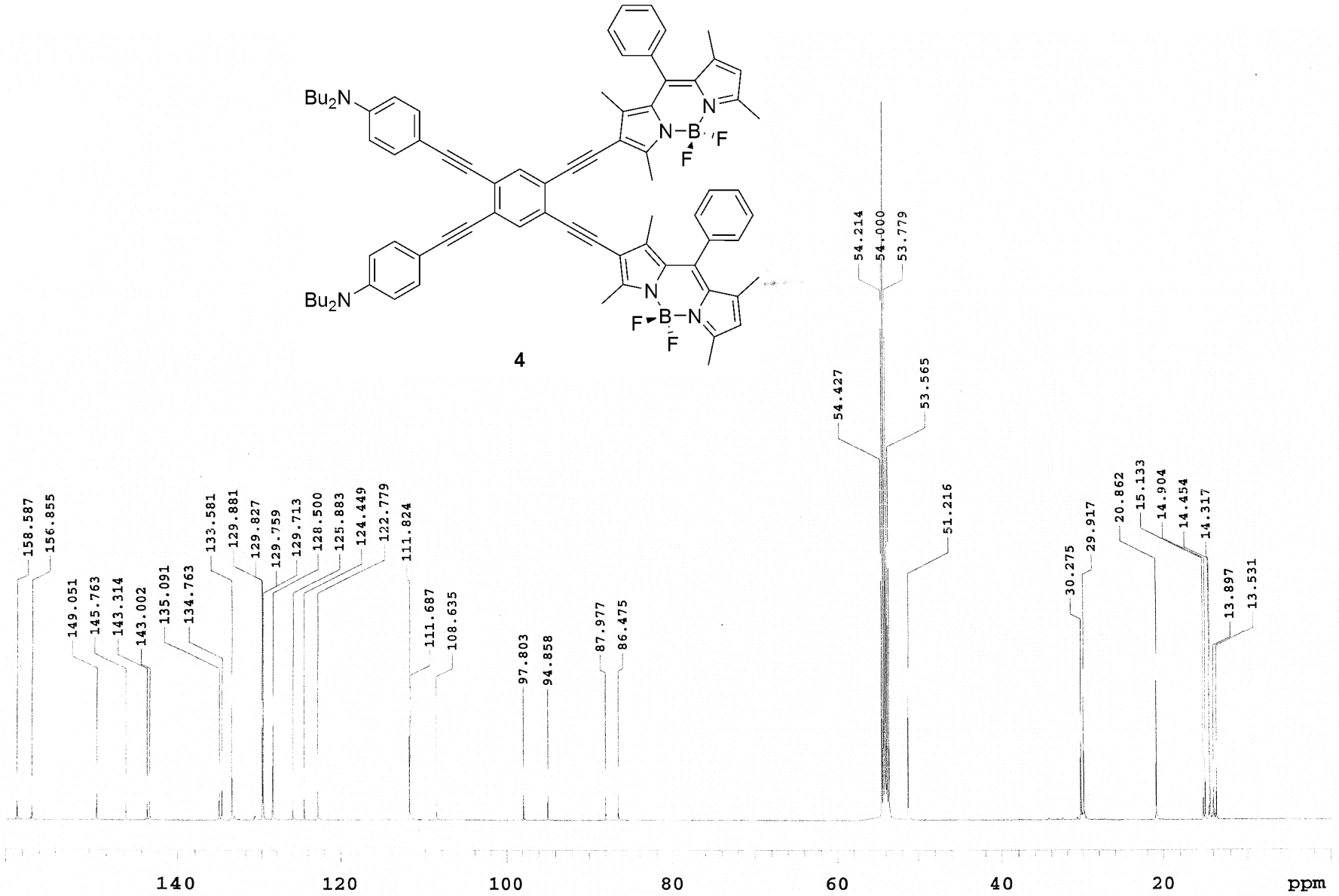


PULSE SEQUENCE Relax. delay 4.000 sec Pulse 67.5 degrees Acq. time 0.540 sec Width 30303.0 Hz 632 repetitions	OBSERVE C13, 125.7512880 DECOUPLE H1, 500.1042349 Power 40 dB on during acquisition off during delay waltz16 modulated	DATA PROCESSING Line broadening 2.0 Hz FT size 65536 Total time 47 minutes			DBG-5mm 13C Pulse Sequence: s2pul Solvent: CDCl3 Temp. 25.0 C / 298.1 K User: 1-15-87 INOVA-500 "fourier"

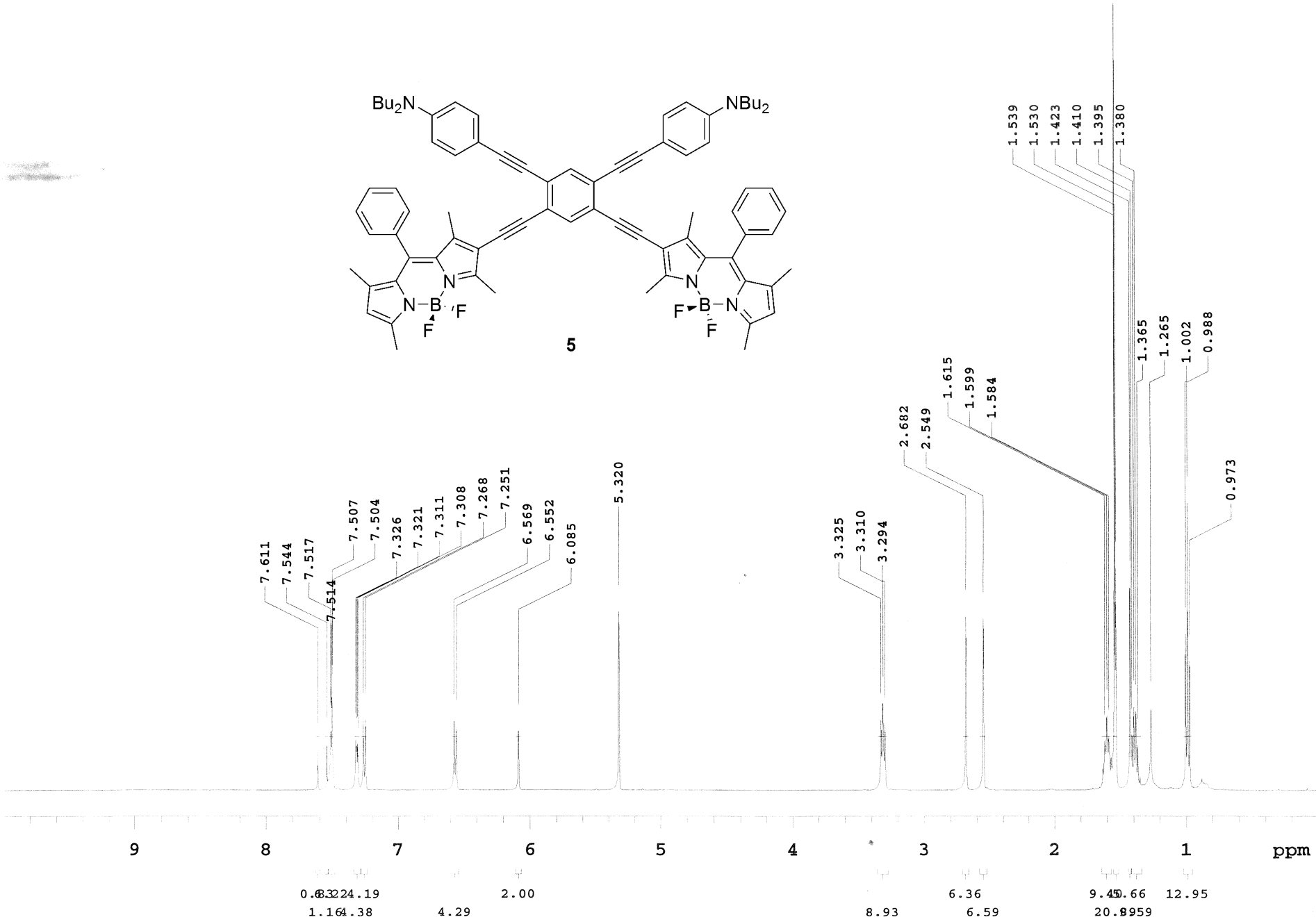

Bu2N
Bu2N
N
N–B
F
F
N
F–B–N
F

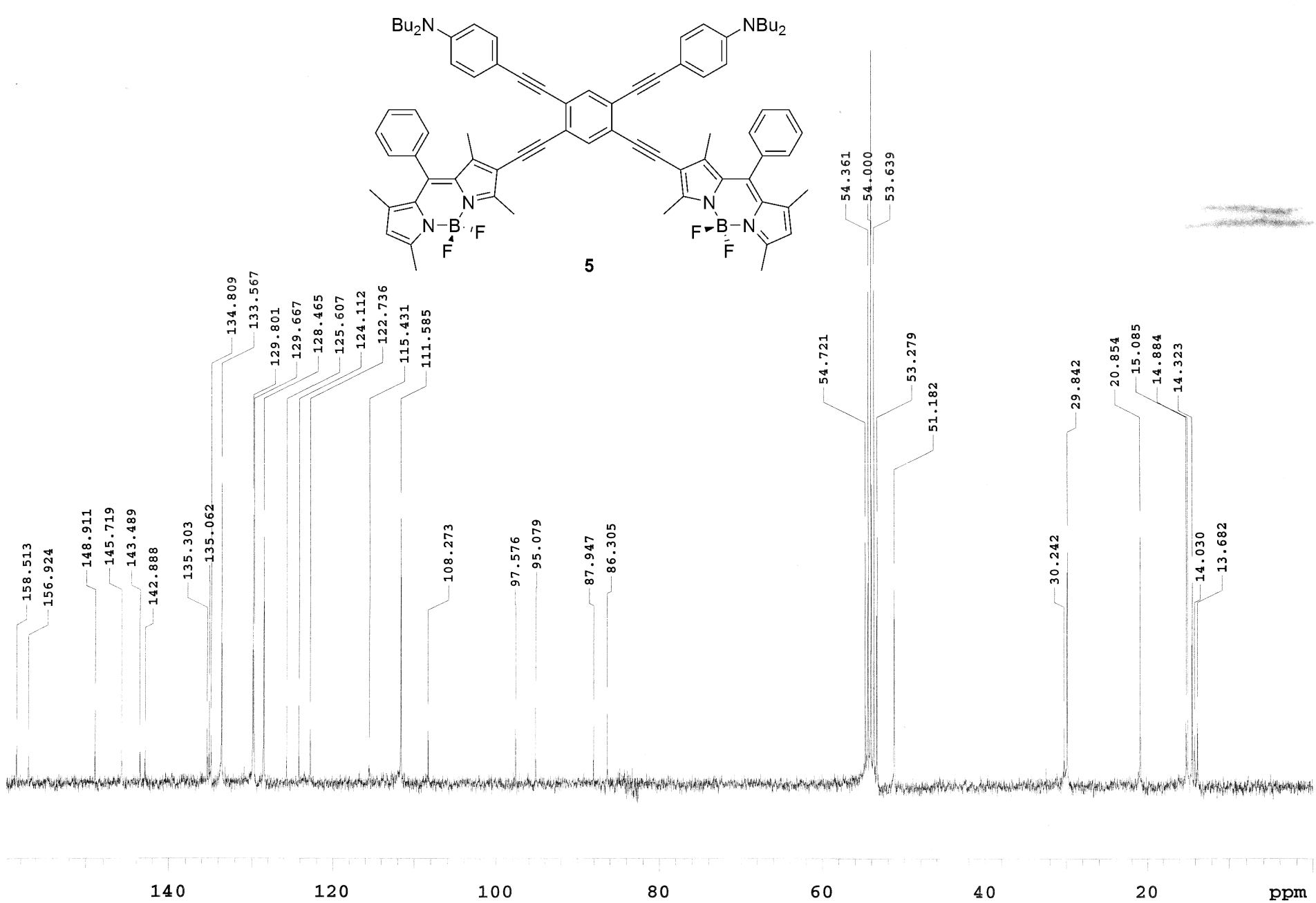
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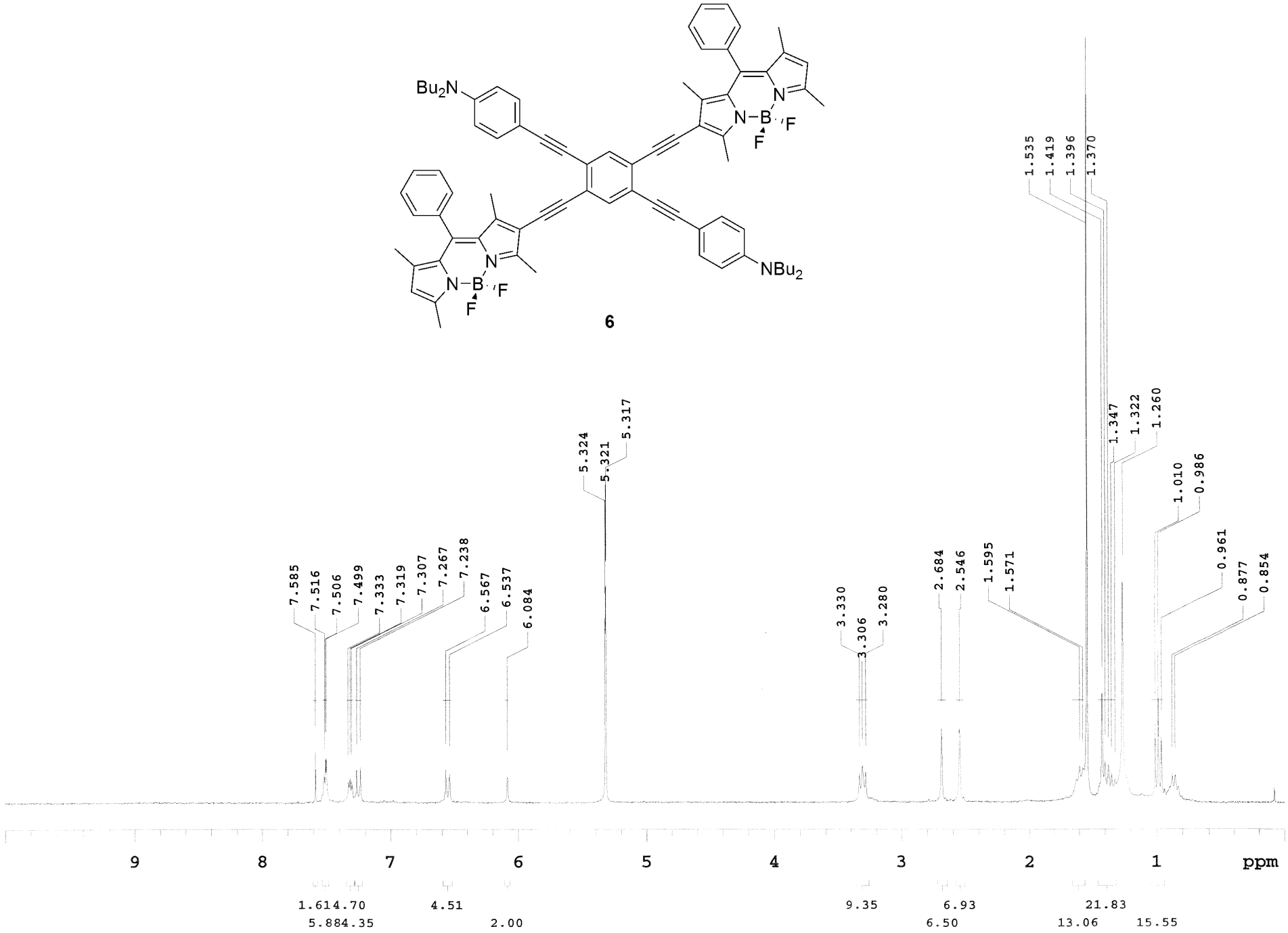

7.575
7.484
7.419
7.390
7.294
7.269
6.587
6.557
5.309
3.291
2.633
2.606
1.422
1.403
1.376
1.351
1.261
1.068
1.044
1.020
0.992
0.968
0.944
9
8
7
6
5
4
3
2
1
ppm
1.64
6.49
4.11
8.29
4.49
1.93
10.75
7.69
6.03
10.44

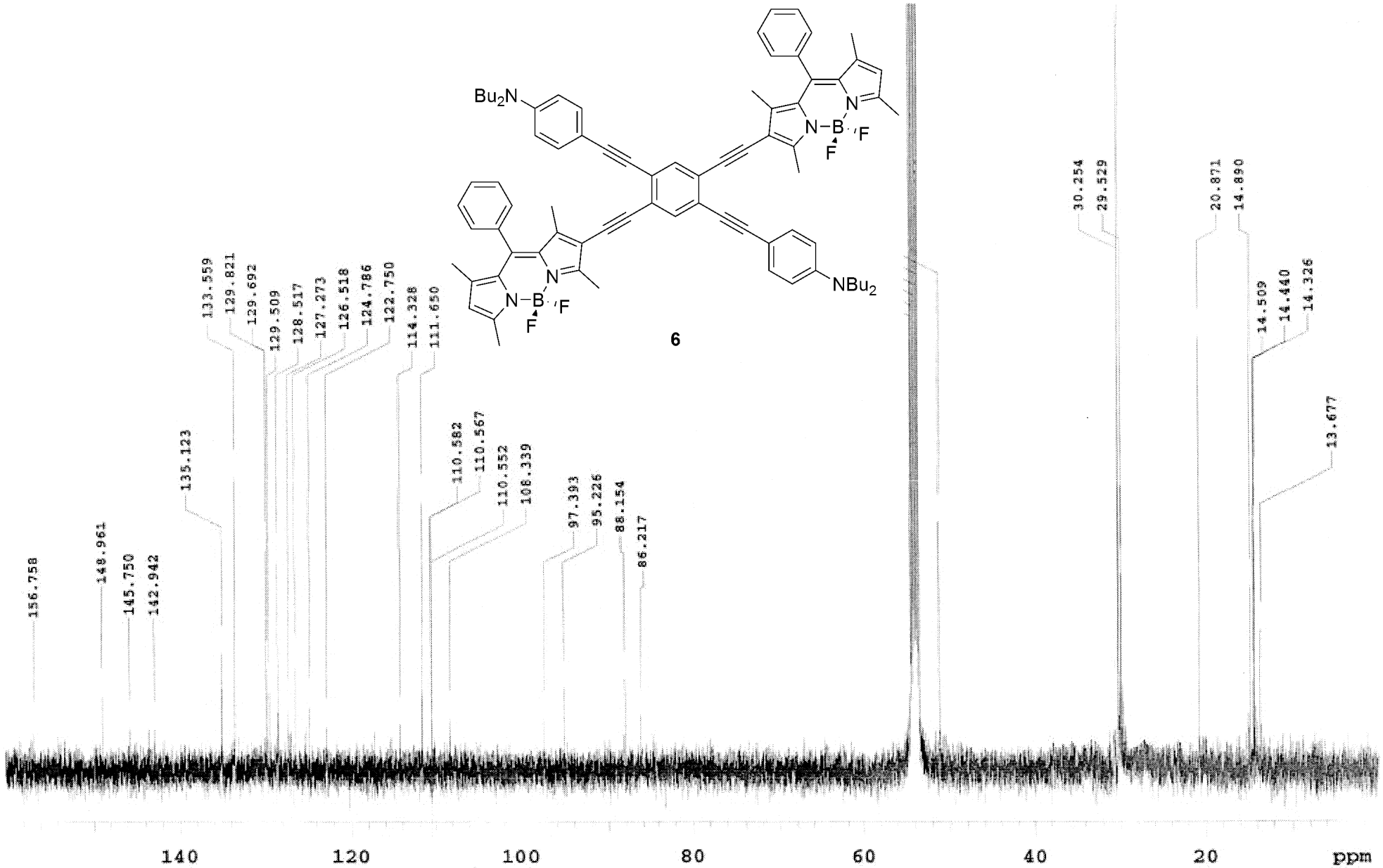

Bu2N
Bu2N
N
N
B
F
F
F
B
N
F
158.587
156.855
149.051
145.763
143.314
143.002
135.091
134.763
133.581
129.881
129.827
129.759
129.713
128.500
125.883
124.449
122.779
111.824
111.687
108.635
97.803
94.858
87.977
86.475
54.427
54.214
54.000
53.779
53.565
51.216
30.275
29.917
20.862
15.133
14.904
14.454
14.317
13.897
13.531
140
120
100
80
60
40
20
ppm

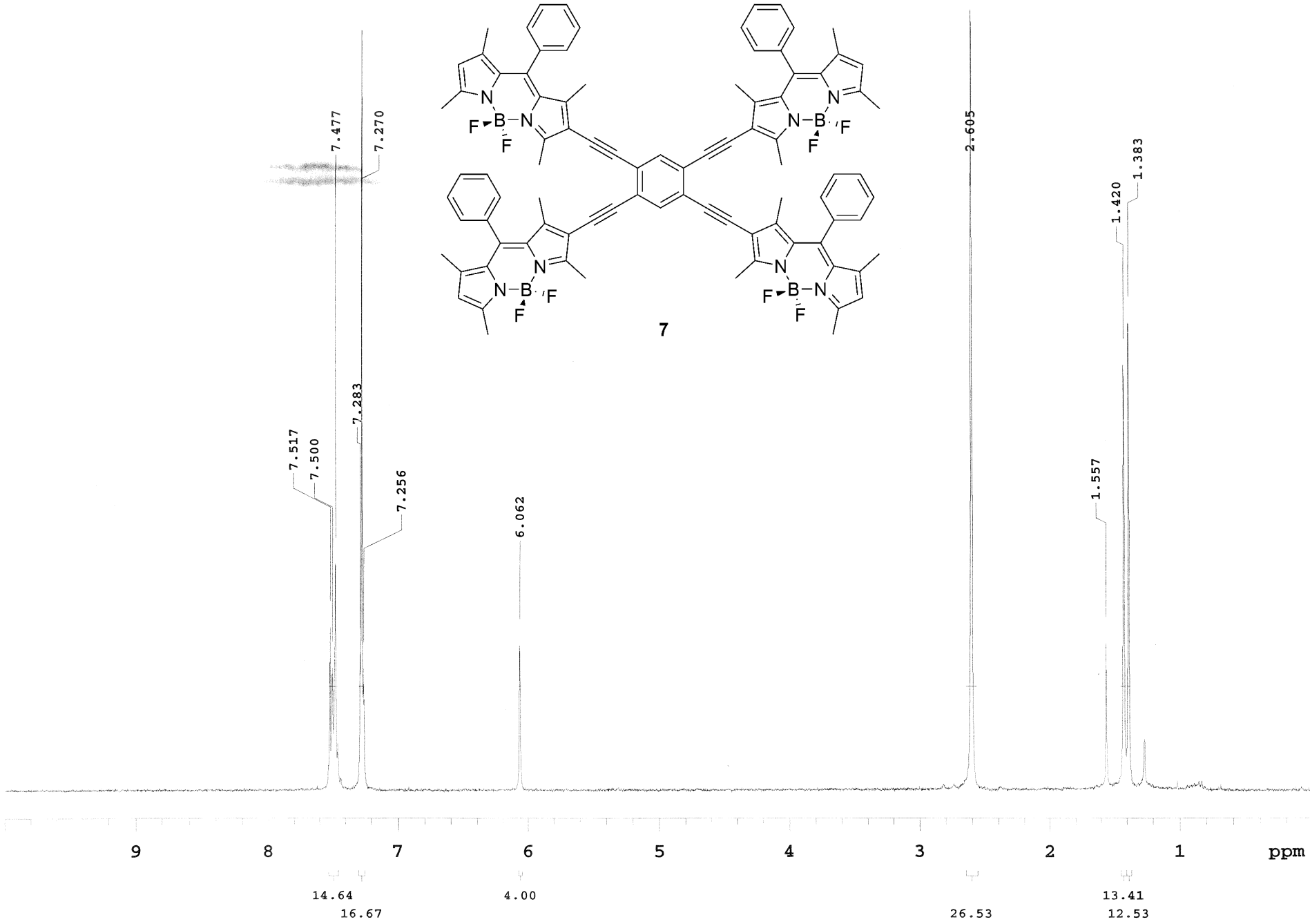
4


Bu2N
NBu2
N
N
B
F
F
F
B
N
F
5
1.539
1.530
1.423
1.410
1.395
1.380
1.365
1.265
1.002
0.988
0.973
1.615
1.599
1.584
2.682
2.549
3.325
3.310
3.294
5.320
6.569
6.552
6.085
7.611
7.544
7.517
7.514
7.507
7.504
7.326
7.321
7.311
7.308
7.268
7.251
9
8
7
6
5
4
3
2
1
ppm
0.63
3.32
4.19
2.00
6.36
9.45
0.66
12.95
1.16
4.38
4.29
8.93
6.59
20.89

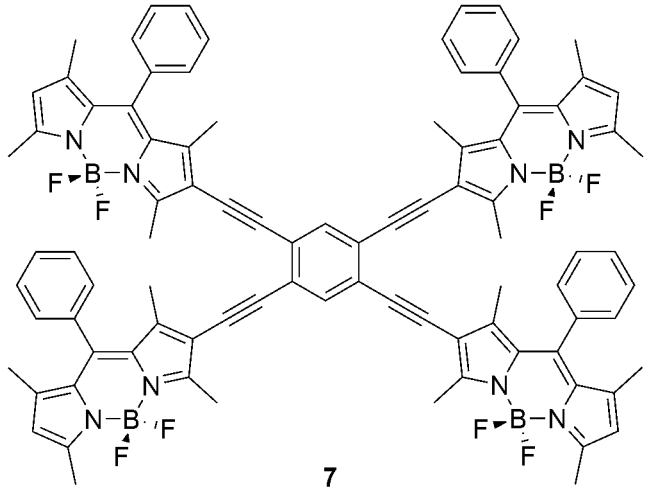

Bu2N
NBu2
N
B
F
F
5
158.513
156.924
148.911
145.719
143.489
142.888
135.303
135.062
134.809
133.567
129.801
129.667
128.465
125.607
124.112
122.736
115.431
111.585
108.273
97.576
95.079
87.947
86.305
54.721
54.361
54.000
53.639
53.279
51.182
30.242
29.842
20.854
15.085
14.884
14.323
14.030
13.682
140
120
100
80
60
40
20
ppm


Bu2N
NBu2
N
N–B
F
F
6
1.535
1.419
1.396
1.370
1.347
1.322
1.260
1.010
0.986
0.961
0.877
0.854
1.595
1.571
2.684
2.546
3.330
3.306
3.280
5.324
5.321
5.317
7.585
7.516
7.506
7.499
7.333
7.319
7.307
7.267
7.238
6.567
6.537
6.084
9
8
7
6
5
4
3
2
1
ppm
1.614.70
5.884.35
4.51
2.00
9.35
6.50
6.93
13.06
21.83
15.55


Bu2N
NBu2
N
N
B
F
F
6
156.758
149.961
145.750
142.942
135.123
133.559
129.821
129.692
129.509
128.517
127.273
126.518
124.786
122.750
114.328
111.650
110.582
110.567
110.552
108.339
97.393
95.226
88.154
86.217
30.254
29.529
20.871
14.890
14.509
14.440
14.326
13.677
140
120
100
80
60
40
20
ppm

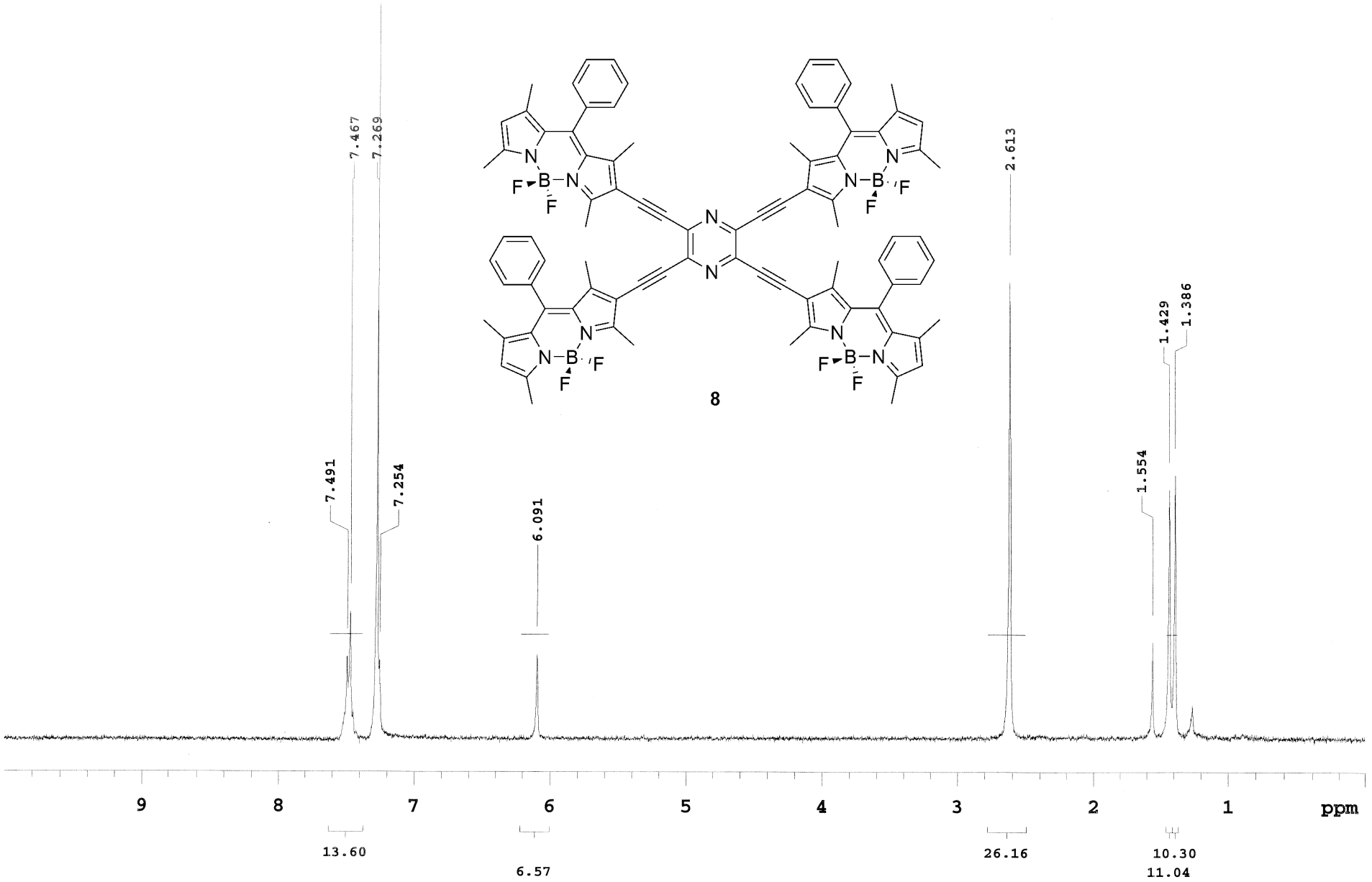

7.517
7.500
7.477
7.283
7.270
7.256
6.062
2.605
1.557
1.420
1.383
9
8
7
6
5
4
3
2
1
ppm
14.64
16.67
4.00
26.53
13.41
12.53

7



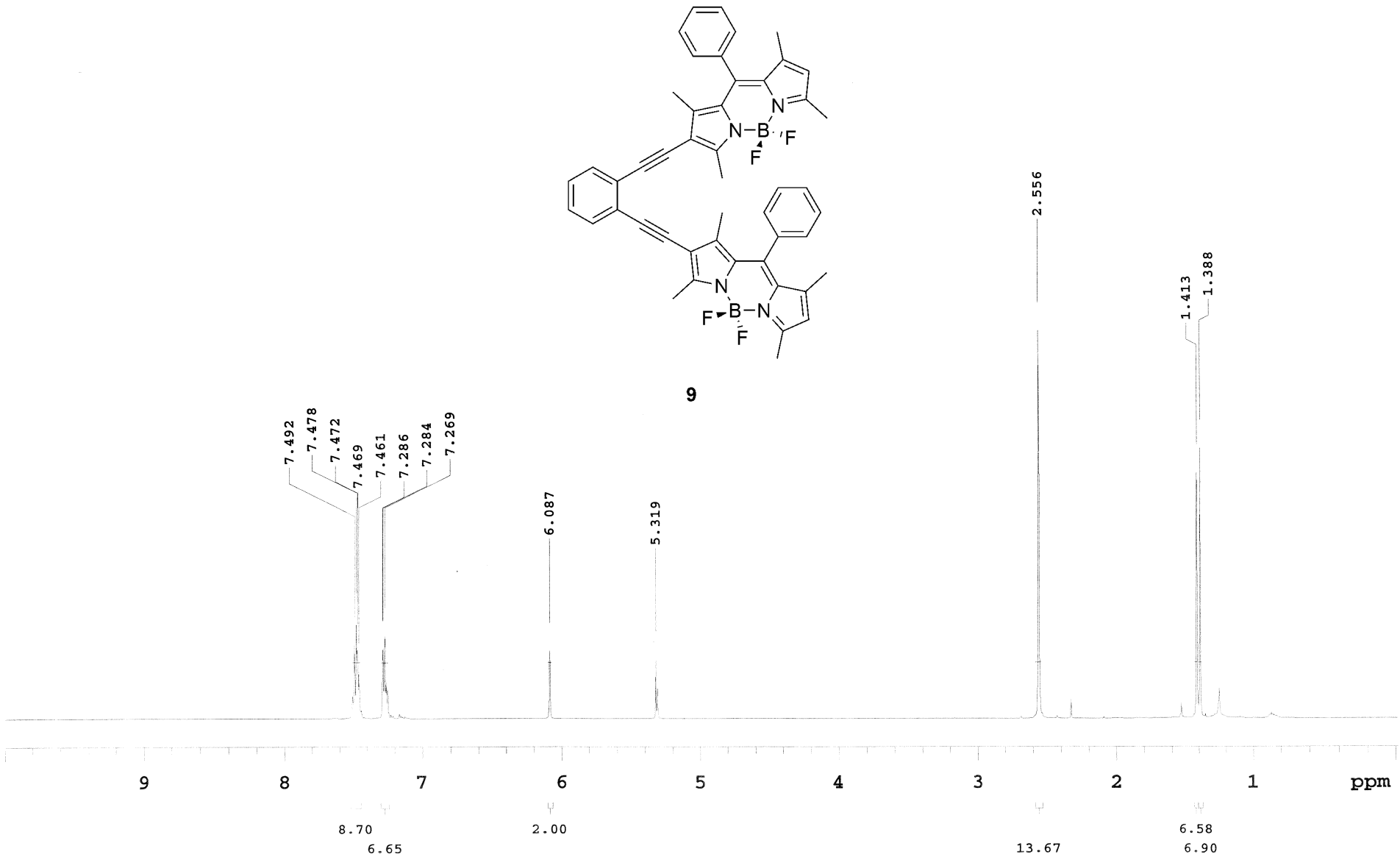
7

158.130
156.806
145.065
143.078
142.387
134.971
134.780
132.823
130.484
129.483
129.439
128.026
124.907
122.421
115.020
94.259
88.226
77.485
77.220
76.970
15.026
14.776
13.775
13.378
140
120
100
80
60
40
20
ppm

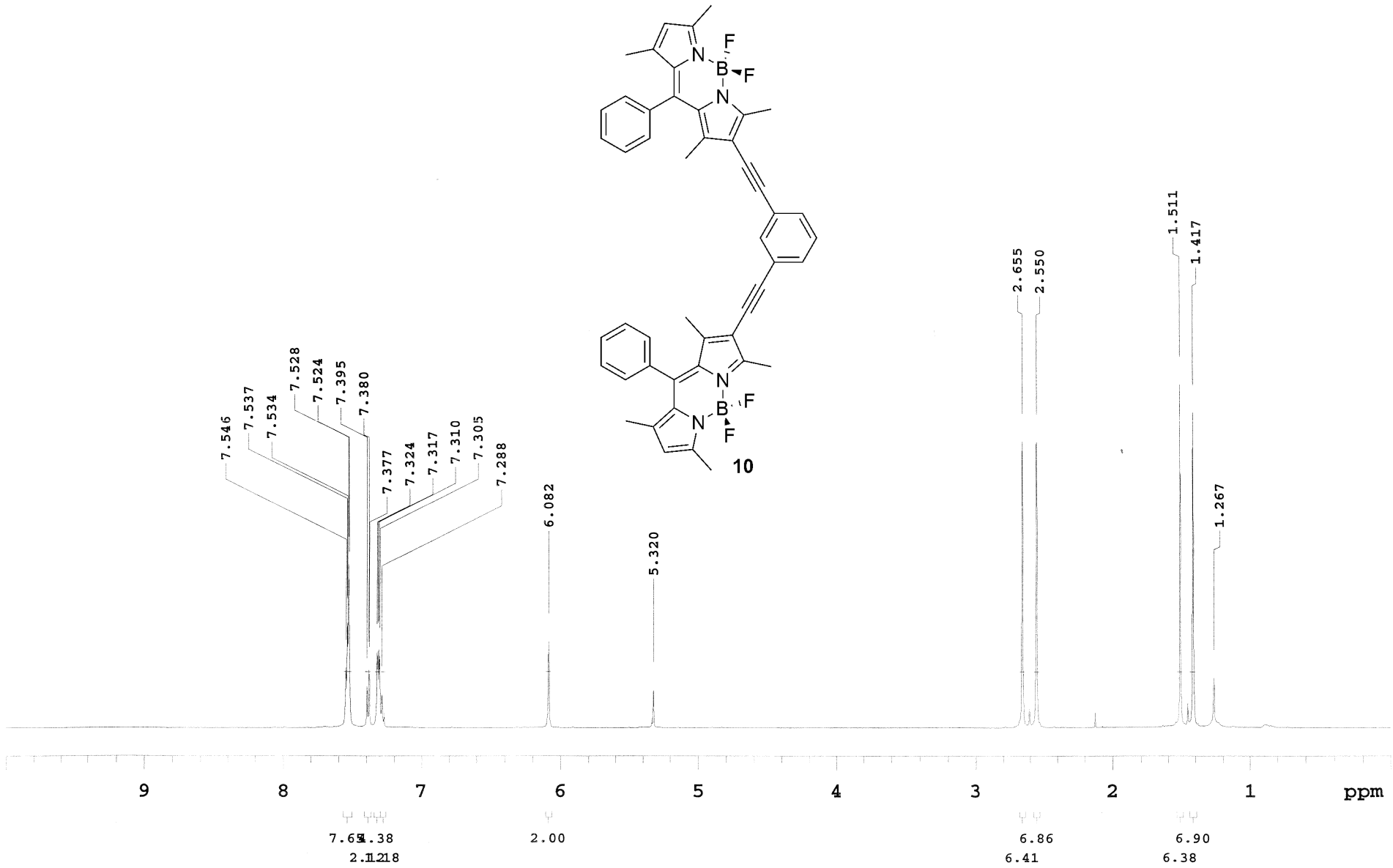

7.467
7.269
7.491
7.254
6.091
2.613
1.554
1.429
1.386
9
8
7
6
5
4
3
2
1
ppm
13.60
6.57
26.16
10.30
11.04

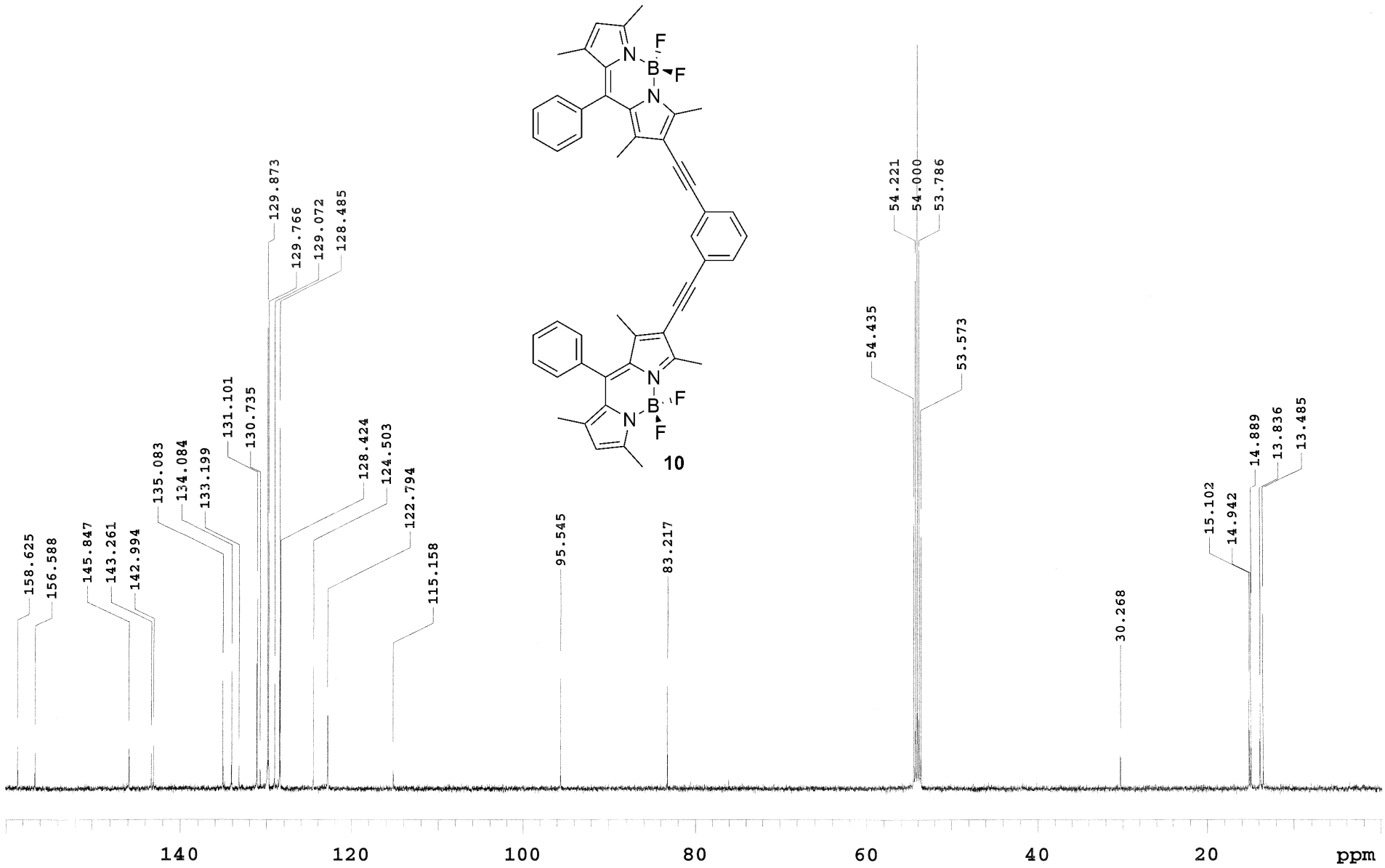
8

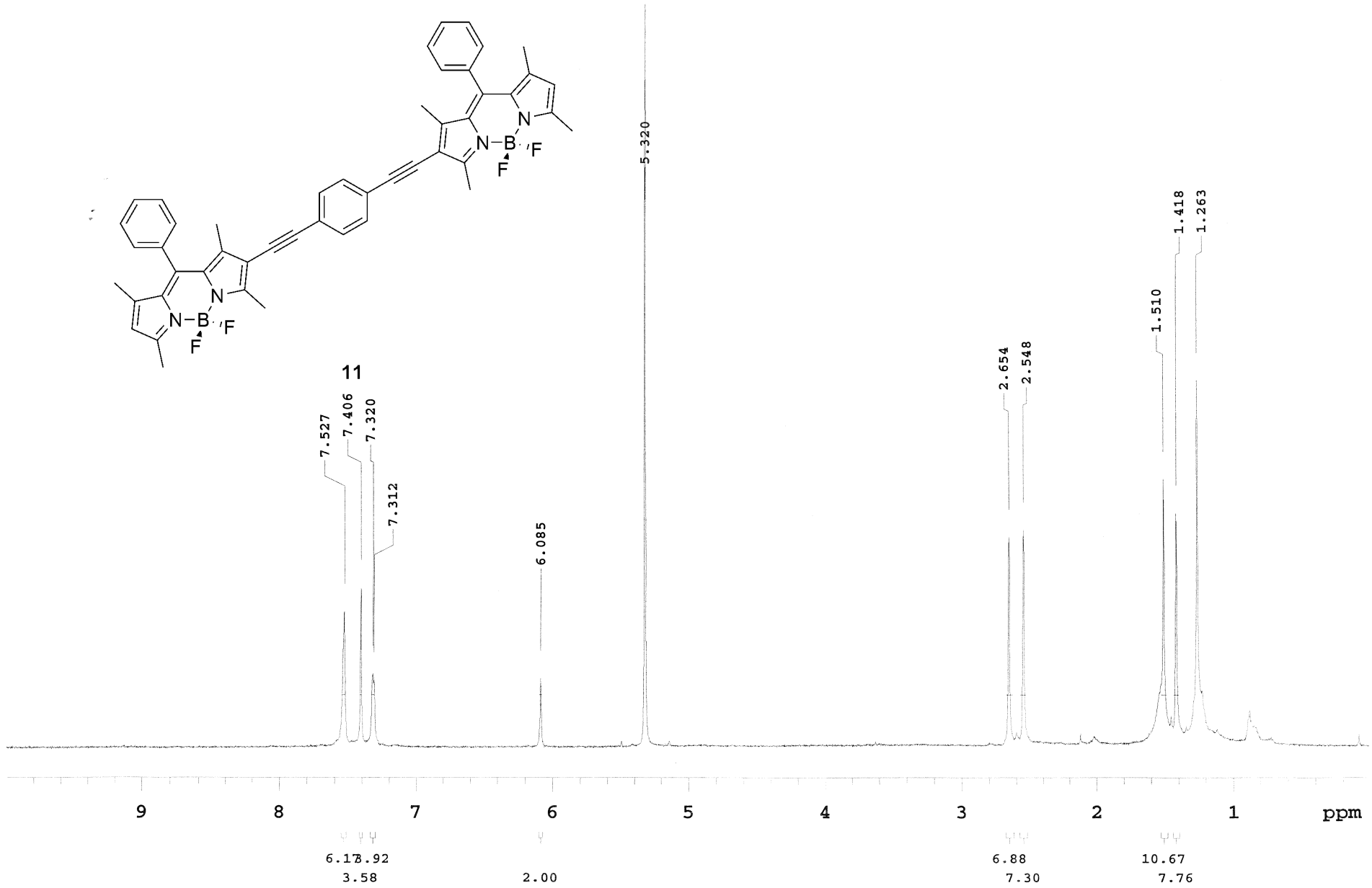
159.133
157.022
145.744
143.640
142.639
138.667
134.584
133.215
130.317
129.544
127.977
122.864
113.668
93.040
91.090
77.480
77.230
76.973
15.102
14.837
13.851
13.410
160
140
120
100
80
60
40
20
ppm
8

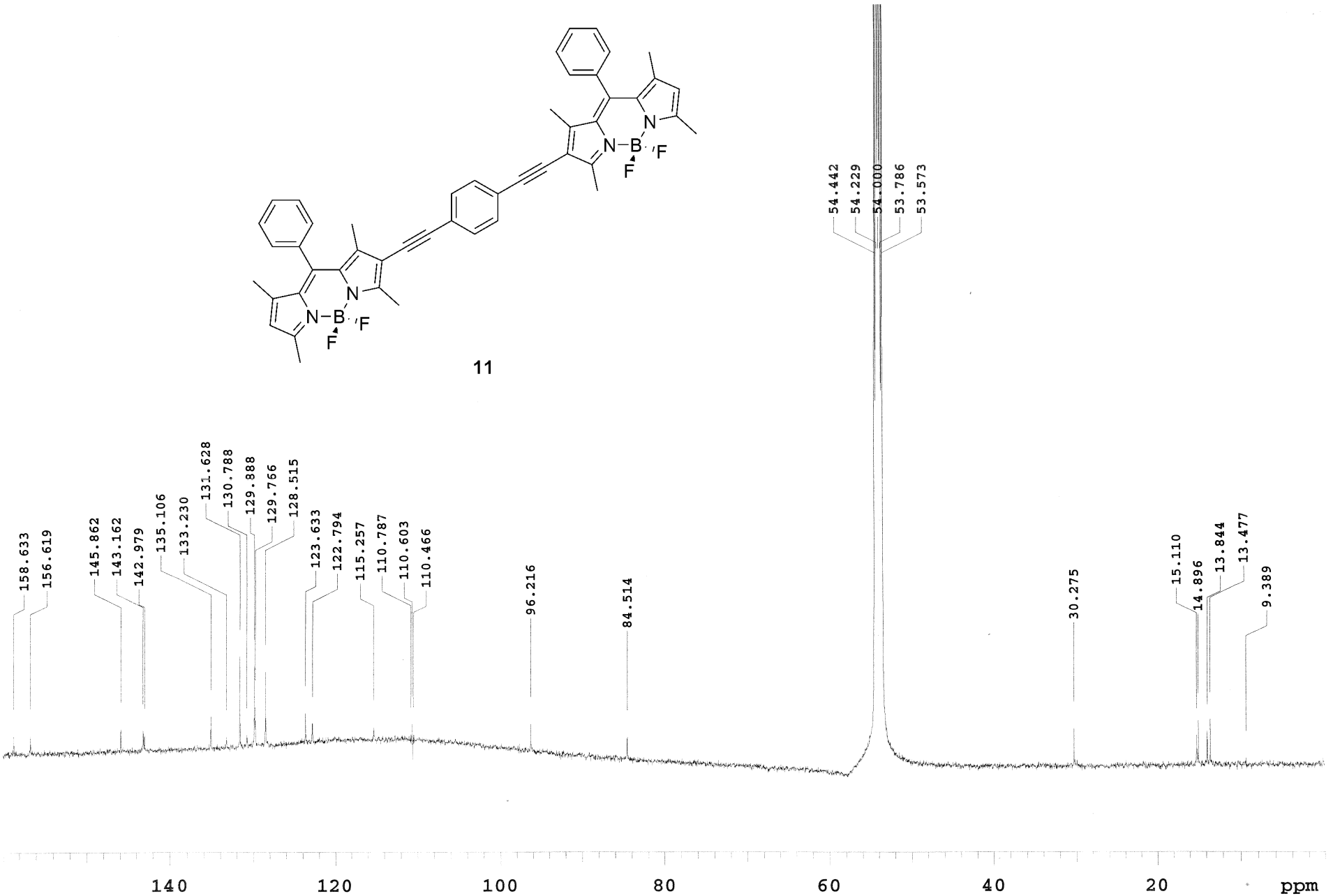

9
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7.478
7.472
7.469
7.461
7.286
7.284
7.269
6.087
5.319
2.556
1.413
1.388
9
8
7
6
5
4
3
2
1
ppm
8.70
6.65
2.00
13.67
6.58
6.90

158.419
156.626
145.656
143.200
142.903
134.977
133.092
132.215
130.674
129.812
129.667
128.668
128.363
128.302
125.998
122.656
115.333
95.072
86.566
54.427
54.214
54.000
53.779
53.565
30.222
15.087
14.866
13.805
13.439
140
120
100
80
60
40
20
ppm
9


F
N
B
F
N
10
7.546
7.537
7.534
7.528
7.524
7.395
7.380
7.377
7.324
7.317
7.310
7.305
7.288
6.082
5.320
2.655
2.550
1.511
1.417
1.267
9
8
7
6
5
4
3
2
1
ppm
7.65
1.38
2.11
2.18
2.00
6.86
6.41
6.90
6.38


F
B
F
N
N
10
158.625
156.588
145.847
143.261
142.994
135.083
134.084
133.199
131.101
130.735
129.873
129.766
129.072
128.485
128.424
124.503
122.794
115.158
95.545
83.217
54.435
54.221
54.000
53.786
53.573
30.268
15.102
14.942
14.889
13.836
13.485
140
120
100
80
60
40
20
ppm


11
7.527
7.406
7.320
7.312
6.085
5.320
2.654
2.548
1.510
1.418
1.263
9
8
7
6
5
4
3
2
1
ppm
6.17
3.92
3.58
2.00
6.88
7.30
10.67
7.76


11
158.633
156.619
145.862
143.162
142.979
135.106
133.230
131.628
130.788
129.888
129.766
128.515
123.633
122.794
115.257
110.787
110.603
110.466
96.216
84.514
54.442
54.229
54.000
53.786
53.573
30.275
15.110
14.896
13.844
13.477
9.389
140
120
100
80
60
40
20
ppm