

## Borazine: Spin Blocker? Or Not?

Debojit Bhattacharya,<sup>a\*</sup> Suranjan Shil,<sup>b</sup> Anirban Misra<sup>b</sup>, Laimutis Bytautas<sup>c</sup>

and Douglas J. Klein<sup>a</sup>

<sup>a</sup>MARS, Texas A&M University at Galveston, Texas, 77553, USA

<sup>b</sup>Department of Chemistry, University of North Bengal, Darjeeling, Pin. 734013, West Bengal, India

<sup>c</sup> Galveston College, Department of Chemistry, 4015 Avenue Q, Galveston, Texas, 77550, USA.

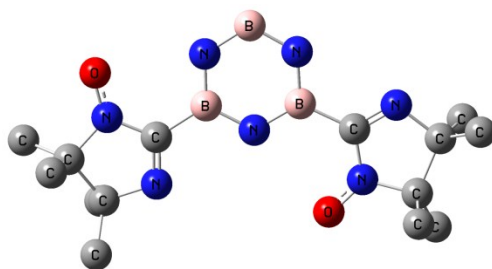
\*Telephone: (409) 740-4538, Email: debojitilora@gmail.com

### The Optimized XYZ Coordinates of All Borazine Bridged Diradicals and the Respective Optimized Structures in UB3LYP/6-311G(d,p) Level of Theory (Hydrogens are Omitted Due to Picture Clarity).

#### Diradical (IN-B B-IN)

H	0.07922100	-0.52977500	-0.07527800
H	2.09939800	3.12857300	-0.00296000
H	-0.04141800	4.54549100	0.01379500
H	-2.12350400	3.03127800	-0.01120900
N	-1.21817600	2.57915500	-0.02094800
N	1.21835700	2.63329600	-0.01460600
N	0.05033400	0.48320200	-0.05602200
B	-1.20724100	1.15608800	-0.04532100
B	-0.01530600	3.35445000	-0.00588800
B	1.27298800	1.20839300	-0.03722300
C	4.33012900	-1.19461700	0.19961300
C	4.95047700	0.21983400	-0.11940400
C	-4.83972400	-0.23193400	0.19204600
C	-3.95740300	-1.47566300	-0.20822500
O	1.97602400	-1.76155600	-0.05749400
O	-4.11214300	2.08682200	0.04102000
N	2.88170400	-0.87586900	-0.04289000
N	3.80776200	1.16841600	-0.01024000
N	-3.82149900	0.85386500	-0.01333400
N	-2.55272000	-0.99540400	-0.10060700
C	2.69422800	0.51352000	-0.03307100
C	-2.53411000	0.29481300	-0.05675300
C	6.06215400	0.66089000	0.83808000
C	4.43490300	-1.61402300	1.67694200

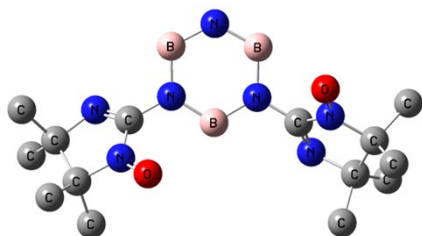
C	5.45888600	0.34452000	-1.56925600
C	4.75721400	-2.35741000	-0.69507000
C	-6.07216700	0.05185000	-0.66610000
C	-4.13967000	-1.90132900	-1.67867900
C	-4.13550500	-2.70342200	0.69087600
C	-5.22582400	-0.18359300	1.68143100
H	-3.38924500	-2.65575200	-1.92107500
H	-5.13068000	-2.32966900	-1.84901200
H	-3.99914400	-1.06082300	-2.36110000
H	-6.50652200	1.00650000	-0.36445700
H	-5.83258200	0.11349300	-1.72724300
H	-6.82195500	-0.72991700	-0.52192400
H	-3.89625400	-2.48599500	1.73169100
H	-5.15975200	-3.08427800	0.63981500
H	-3.45957000	-3.49128300	0.35324000
H	-4.36357600	-0.35210600	2.32900800
H	-5.63219500	0.80464200	1.90603700
H	-5.98567200	-0.93293500	1.91205300
H	5.80864800	-2.60047700	-0.52321700
H	4.15609200	-3.23562300	-0.45319200
H	4.61855000	-2.13834900	-1.75335400
H	5.45990200	-1.88843700	1.93392700
H	4.10866100	-0.81726900	2.34771900
H	3.79158400	-2.48100000	1.84026100
H	6.91601400	-0.02135800	0.79173100
H	6.40455800	1.65689600	0.55057700
H	5.71564100	0.71500800	1.87003900
H	6.34054800	-0.27920300	-1.73654300
H	4.68895200	0.06353200	-2.29048000
H	5.72920700	1.38480600	-1.75894400



### Diradical (IN-N $\square$ N-IN)

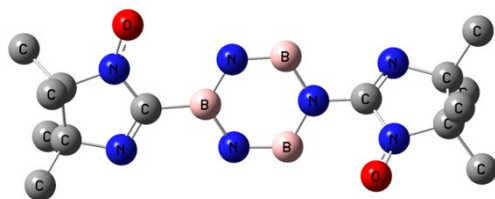
C	3.92272300	-1.25794900	-0.68727000
C	4.56357100	-0.23801200	0.33894900
C	-4.06736000	-1.13580800	0.41221800
C	-4.69605700	0.00038800	-0.49104100
N	-1.28652900	1.17757500	-0.23661100
N	-3.53407100	0.80244600	-0.96308000
N	-2.75858800	-0.47881600	0.72855300
N	3.33389900	0.54170300	0.68971300
N	2.65071700	-0.61981300	-1.12406200
B	-0.08367900	0.37978200	-0.28769900
B	-1.24189100	2.62260200	-0.19163700


B	1.27032900	2.51202800	-0.22990800
N	0.04333700	3.23261700	-0.19975400
N	1.18222700	1.06626800	-0.26651800
C	2.35868800	0.30881100	-0.29642800
C	-2.53042100	0.53786600	-0.21714600
O	3.26968800	1.38831700	1.62592600
O	-1.94479700	-0.89249200	1.60255700
C	5.54999000	0.76085600	-0.29186000
H	5.76416200	1.54727100	0.43494400
H	6.48768500	0.26902400	-0.55785800
H	5.13673400	1.22899600	-1.18707100
C	5.17266000	-0.82973500	1.60908500
H	6.07075300	-1.40269700	1.36608500
H	5.45315500	-0.01988200	2.28496300
H	4.47583300	-1.47994500	2.13701000
C	4.78417700	-1.53736400	-1.92245400
H	5.73630200	-1.99819400	-1.64354700
H	4.24945000	-2.22671700	-2.57866200
H	4.98860100	-0.63080300	-2.49189000
C	3.52806800	-2.59709700	-0.03624800
H	2.96690800	-3.18770300	-0.76258400
H	4.40843900	-3.16803100	0.26925200
H	2.88778800	-2.44786100	0.83544500
C	-4.80013100	-1.47198200	1.70937300
H	-5.76133300	-1.94235900	1.48868100
H	-4.19901100	-2.17267400	2.29152000
H	-4.97524600	-0.59079800	2.32554200
C	-3.73497900	-2.43179700	-0.34817500
H	-3.11413800	-3.06413500	0.29001800
H	-4.64457700	-2.98015300	-0.60081300
H	-3.18302000	-2.23139800	-1.26824800
C	-5.59221300	0.96923400	0.30266300
H	-5.85708600	1.80935900	-0.34179100
H	-6.51271000	0.48190300	0.63347600
H	-5.07506800	1.37019600	1.17678200
C	-5.47031300	-0.51551000	-1.70738600
H	-6.32394800	-1.12678200	-1.40053700
H	-5.84646400	0.33667700	-2.27682800
H	-4.83987200	-1.10517500	-2.37261200
H	-2.24049700	3.25800700	-0.12801000
H	0.08826200	4.24035600	-0.17836900
H	2.31613500	3.06545800	-0.29086400
H	-0.12751700	-0.79585200	-0.37905300



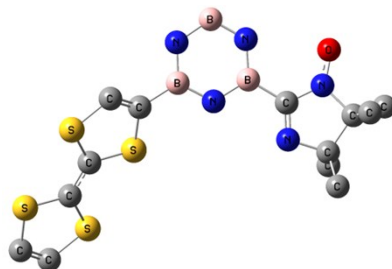
**Diradical (IN-B $\square$ N-IN)**

H	-1.09417700	-1.98841500	-0.68349100
H	1.44296600	-2.09966200	-0.88429500
H	1.35304500	2.31053800	0.36574600
H	-1.19665100	2.04661200	0.32721800
C	-5.02872300	-0.92138500	-0.32768700
C	-5.17771600	0.50904900	0.32298800
C	5.07456800	-0.44098200	0.52389500
C	5.07060200	0.66402000	-0.60884700
N	1.51624300	0.10060000	-0.21432600
N	3.64145100	1.03182400	-0.79184700
N	3.63188200	-0.84263000	0.47208000
N	-3.76508000	0.99361400	0.15763000
N	-3.56391300	-1.18694500	-0.33770800
B	0.83747300	-1.14519800	-0.52943000
B	0.77838500	1.30811000	0.09946700
B	-1.34330600	0.01988000	-0.15693500
N	-0.64254200	1.22858600	0.10809900
N	-0.58337900	-1.14229600	-0.47140700
C	-2.91925300	-0.08914000	-0.12048900
C	2.91227100	0.14702200	-0.22799400
O	-3.41043800	2.18192700	0.42007000
O	3.13612600	-1.76092500	1.18685000
C	-5.45189400	0.49418000	1.83760900
H	-5.32377800	1.50669000	2.22544300
H	-6.47275900	0.16826600	2.04613500
H	-4.76119400	-0.16314200	2.36872400
C	-6.13684300	1.48235500	-0.36157300
H	-7.16757900	1.13737000	-0.25028600
H	-6.04871300	2.46367300	0.10768700
H	-5.92110200	1.59809400	-1.42324100
C	-5.73409400	-2.04699400	0.43658100
H	-6.81528600	-1.88404600	0.46713600
H	-5.54514000	-2.99436400	-0.07183900
H	-5.36703800	-2.14052100	1.45839600
C	-5.47009300	-0.96899900	-1.80435500
H	-5.20070300	-1.94175600	-2.21945800
H	-6.55087100	-0.83852900	-1.90122400
H	-4.97040800	-0.20298800	-2.40036100
C	5.95661900	-1.66748800	0.29059900
H	7.01257500	-1.38943600	0.33192500
H	5.76268600	-2.40159600	1.07497200
H	5.75890700	-2.14209500	-0.66994400
C	5.31868200	0.10614900	1.94138000
H	5.08639100	-0.67913300	2.66339400
H	6.36125700	0.40246800	2.07094600
H	4.68238600	0.96589400	2.15864900
C	5.54576500	0.13033400	-1.97389000
H	5.37778500	0.90106000	-2.72821200
H	6.61065900	-0.11520700	-1.95941400
H	4.98588900	-0.75712200	-2.27569900
C	5.87040500	1.92450900	-0.26291100
H	6.92911400	1.69186500	-0.11608300
H	5.78634700	2.63468400	-1.08776400
H	5.49272100	2.41373900	0.63457900



**Diradical (IN-B  B-TTF)**

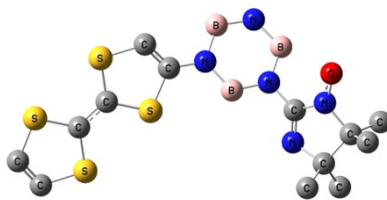
H	3.84359000	2.81467900	-0.73361700
H	0.89336100	0.05725500	0.21837700
B	2.49148100	1.30556600	-0.25897800
B	1.89707600	3.67707600	-0.75775500
H	2.20314200	4.78424500	-1.05692800
B	0.10565200	2.01168000	-0.19406400
N	2.85481100	2.63358000	-0.60171200
N	1.09726300	1.00713800	-0.06739300
N	0.51281300	3.32989700	-0.53937100
C	3.51695600	0.13045500	-0.06374000
C	4.35824700	-1.96082300	0.23934300
C	-1.43081400	1.68367800	0.05554900
C	-3.69612200	0.36432000	0.12245700
C	-2.33352100	2.48261800	0.66599200
C	-4.69905200	-0.59353600	-0.02297800
C	-6.05299100	-2.72029800	-0.58388400
C	-6.92608500	-1.90153600	0.02148000
H	-6.27711100	-3.70982100	-0.95831300
H	-7.96665200	-2.12490300	0.21355300
S	-2.06713200	0.13284500	-0.45246500
S	-3.96129000	1.90757100	0.88329300
S	-4.42307700	-2.14121400	-0.78352600
S	-6.33393400	-0.34859100	0.54030800
H	-2.11938500	3.46586700	1.06446000
H	-0.17688900	4.04982000	-0.69639400
N	4.89823400	0.28248400	-0.18976000
N	3.15780700	-1.07456000	0.23650900
C	5.59146200	-0.97189800	0.26892400
O	5.50820000	1.35466500	-0.47479900
C	6.13097000	-0.67460100	1.67909200
H	6.66023000	-1.54021900	2.08105000
H	6.83059200	0.16125600	1.61962100
H	5.33327500	-0.40261600	2.37277900
C	6.75362300	-1.28866000	-0.67108200
H	7.47256200	-0.46842400	-0.64353600
H	7.26114600	-2.20043800	-0.34837800
H	6.43012700	-1.41679100	-1.70344400
C	4.27077900	-2.78193100	-1.06252900
H	5.08805100	-3.50347200	-1.12862600
H	3.32693500	-3.33004800	-1.07275000
H	4.29760800	-2.14296000	-1.94727800
C	4.27489900	-2.91357000	1.43622300
H	3.37957700	-3.53090000	1.33960600
H	5.14286500	-3.57737400	1.46969800
H	4.21066100	-2.37894900	2.38373800



### Diradical (IN-N N-TTF)

H	3.98661000	2.60816100	-1.14269200
H	0.70102600	-0.27333400	0.19984500
H	2.14474100	4.32143300	-1.29049800
C	3.36625600	0.06440900	-0.23864600
C	4.44096800	-1.90276300	-0.14692600
C	-1.28017700	1.61989600	-0.04078400
C	-3.57994600	0.37585300	0.07815000
C	-2.16628100	2.48927300	0.50569800
C	-4.60327700	-0.56695900	0.02633700
C	-6.01125300	-2.70433600	-0.33239400
C	-6.85795100	-1.81718900	0.20859600
H	-6.26051300	-3.71770200	-0.61589500
H	-7.90044800	-1.99895200	0.43129700
S	-1.96084100	0.03846000	-0.46840400
S	-3.80836300	1.98249500	0.70329100
S	-4.37136400	-2.18043200	-0.60296700
S	-6.22682700	-0.23693300	0.58434600
H	-1.91858900	3.48644200	0.83848300
H	-0.33087600	4.04962600	-0.90226200
N	4.48378200	0.33346700	0.55728800
N	3.29985800	-1.11874700	-0.70974000
C	5.43917700	-0.81862300	0.43580200
O	4.72470500	1.41991500	1.15574300
C	6.06088100	-1.11701000	1.79834500
H	6.74849700	-1.96192700	1.71928200
H	6.62588900	-0.24692500	2.13657200
H	5.31251400	-1.34657500	2.55607600
C	6.53360500	-0.37302300	-0.54975300
H	7.03200700	0.51069200	-0.14656600
H	7.27931600	-1.15857300	-0.68235800
H	6.12273400	-0.11744100	-1.52817100
C	5.03469900	-2.77655500	-1.25528800
H	5.88577800	-3.35361600	-0.88418300
H	4.27394400	-3.47732100	-1.60399000
H	5.36125600	-2.18795100	-2.11227200
C	3.83330100	-2.80866700	0.94016400
H	3.05048800	-3.42147100	0.48970000
H	4.58549000	-3.47388300	1.36994500
H	3.38275600	-2.22711800	1.74744000
N	2.41495800	1.08895100	-0.41944400
N	0.05966200	1.85898800	-0.32452600
N	1.85398800	3.40740700	-0.97259400

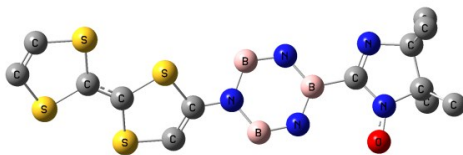
B	2.86340400	2.40233800	-0.84493400
B	0.47940500	3.19840300	-0.74617800
B	1.04765400	0.79793600	-0.16461800



### Diradical (IN-B $\square$ N-TTF)

H	-2.65525300	-2.01413600	-0.80771400
H	-2.12466700	1.73678200	0.90476000
B	-2.58732100	-0.11680600	0.05197600
B	-0.62256500	-1.57978700	-0.42546700
H	-0.15020600	-2.57745700	-0.85893100
B	-0.30516300	0.71741700	0.62255600
H	0.42198900	1.55168600	1.05460100
N	-2.00730900	-1.32872000	-0.43146800
N	-1.69995000	0.88178200	0.56645700
N	0.26085600	-0.54261200	0.12915000
C	-4.12932800	0.16486800	0.03687100
C	-6.12033900	1.24894700	0.20267400
C	1.62609800	-0.77916900	0.19106300
C	4.20573800	-0.33741300	0.05783600
C	2.24103500	-1.96786200	0.41892300
C	5.46703700	0.24147300	-0.04884700
C	7.44404300	1.87871400	-0.35527200
C	8.01226900	0.68619700	-0.12960500
H	7.97532800	2.80449700	-0.52844900
H	9.07583900	0.49440000	-0.09210800
S	2.73238600	0.57695700	-0.10847400
S	3.96841800	-2.03037200	0.37471400
S	5.70218600	1.94290900	-0.37211400
S	6.94860600	-0.67108700	0.12454600
H	1.72335800	-2.89105200	0.63347800
C	-6.45804200	-0.26252800	-0.12136000
O	-4.82092600	-1.90284200	-0.90439900
N	-5.07047000	-0.75193900	-0.43639000
N	-4.65200600	1.26690800	0.46278600
C	-6.33725100	2.19000600	-0.99927400
H	-7.39895900	2.28201800	-1.23811900
H	-5.95401800	3.18026100	-0.74772200
H	-5.80860400	1.84123000	-1.88844000
C	-6.85152400	1.81939800	1.42195000
H	-6.53347700	2.85168500	1.57827600
H	-7.93330900	1.81653000	1.26458100
H	-6.63188200	1.26144000	2.33186600
C	-7.37755400	-0.52268200	-1.31401800
H	-7.42816600	-1.59606500	-1.50337000
H	-8.38624300	-0.16592300	-1.09449700

H	-7.02693100	-0.03641600	-2.22376600
C	-6.93708200	-1.07944800	1.09172500
H	-7.94856400	-0.78746500	1.37871100
H	-6.94604800	-2.13748400	0.82316200
H	-6.28151700	-0.95138500	1.95504100

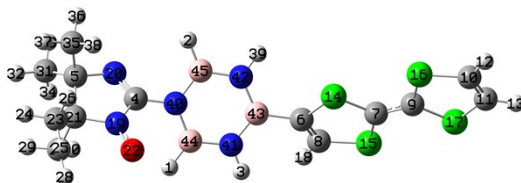


### Diradical (IN-N $\square$ B-TTF)

H	-2.91388100	-2.17238700	0.83260800
H	-2.34226400	1.74163900	-1.48633500
H	-0.41607700	-2.30017100	0.85952800
C	-4.13647900	0.04419300	-0.28011800
C	-6.24829500	0.61336200	-0.78526700
C	1.65863000	-0.82330900	-0.24531500
C	4.23297900	-0.34755000	-0.09344600
C	2.28784900	-2.00503300	-0.42649300
C	5.48307000	0.25081000	0.06107000
C	7.42060700	1.91719600	0.43317300
C	8.01411900	0.72769200	0.25290400
H	7.93222500	2.85197700	0.61780100
H	9.08073200	0.54959800	0.26853700
S	2.73335600	0.53543200	0.01630800
S	4.02698300	-2.05019400	-0.39309800
S	5.68159500	1.95876800	0.36456300
S	6.97988200	-0.64384000	-0.02910500
H	1.79134800	-2.94750500	-0.61835800
N	-4.80150800	-0.00193100	0.95281400
N	-4.87367800	0.31461200	-1.28500200
C	-6.27900400	0.04931600	0.69480500
O	-4.26947500	-0.21770100	2.07909800
C	-6.95514900	0.91971200	1.75199100
H	-8.03089100	0.96587900	1.56891500
H	-6.79436400	0.48010100	2.73783700
H	-6.56085800	1.93515800	1.76880700
C	-6.78920100	-1.39806400	0.80812500
H	-6.57130600	-1.77026500	1.81119600
H	-7.86799500	-1.44342100	0.65011800
H	-6.30559500	-2.05786800	0.08539900
C	-7.26795800	-0.03120300	-1.72807400
H	-8.28962700	0.15053600	-1.38367500
H	-7.16041700	0.40611800	-2.72230300
H	-7.11826000	-1.10663800	-1.82108500
C	-6.39904200	2.14441700	-0.84794200
H	-6.21928400	2.47443900	-1.87248200
H	-7.40458500	2.45603700	-0.55687600
H	-5.67742900	2.64935200	-0.20224700
H	0.10185400	1.19819100	-1.42362800

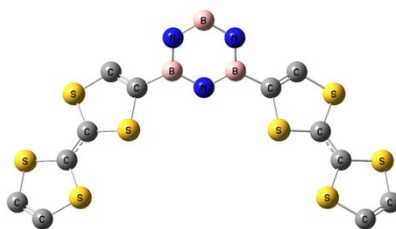


N	-2.74637500	-0.17421600	-0.29661000
N	-0.78731200	-1.50684000	0.35781800
N	-0.48029100	0.54413000	-0.92121100
B	0.08704400	-0.58275000	-0.26890100
B	-2.21528400	-1.34388700	0.36171500
B	-1.89880000	0.78237000	-0.95529100



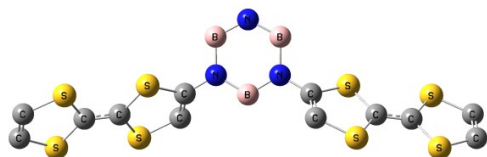
### Diradical (TTF-B-C<sub>6</sub>H<sub>4</sub>-B-TTF)

H	-2.08655900	4.16315600	1.14139100
H	-0.00000200	0.83173400	-0.34289700
B	-1.25194500	2.38768500	0.36624500
B	0.00000100	4.39681000	1.19741500
H	0.00000300	5.48378500	1.66647200
B	1.25194300	2.38768200	0.36624600
N	-1.22033600	3.70125400	0.90232700
N	-0.00000100	1.72641500	0.12641200
N	1.22033600	3.70125100	0.90232800
C	-2.64610600	1.71457600	0.02111100
C	-3.67226100	2.34720200	-0.58884300
C	-4.60361600	-0.02165000	-0.18584400
C	2.64610400	1.71457200	0.02111200
C	4.60361500	-0.02165200	-0.18584700
C	3.67226300	2.34720300	-0.58883000
C	-5.41578700	-1.15304600	-0.09714200
C	-6.37964600	-3.50038300	0.37965500
C	-7.37123700	-2.83243200	-0.23180700
H	-6.43308000	-4.52319000	0.72782000
H	-8.35160400	-3.23118900	-0.45635700
C	5.41578700	-1.15304800	-0.09714600
C	6.37964400	-3.50038800	0.37964100
C	7.37124000	-2.83243000	-0.23180500
H	6.43307600	-4.52319800	0.72779700
H	8.35161000	-3.23118300	-0.45635000
S	2.97031600	0.03847000	0.43264300
S	5.14345200	1.47402900	-0.89949600
S	4.88684700	-2.64503600	0.63470900
S	7.05252500	-1.18927400	-0.69990300
S	-4.88685100	-2.64502800	0.63472800
S	-7.05251700	-1.18928100	-0.69991800
S	-2.97032200	0.03847900	0.43265800
S	-5.14344900	1.47402600	-0.89950900
H	-3.65245100	3.37515700	-0.92819800
H	3.65245500	3.37516300	-0.92817200
H	2.08656000	4.16315300	1.14139000



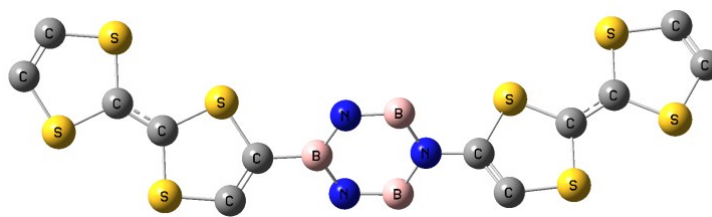
### Diradical (TTF-N-TTF)

H	0.00000200	4.32992200	-0.00009500
B	1.23198300	2.66018800	0.23898500
B	-0.00000100	0.46297300	0.00001900
H	0.00000100	-0.72070700	0.00004300
B	-1.23198200	2.66017500	-0.23907100
N	1.21782600	1.19988300	0.23940700
N	0.00000100	3.31833000	-0.00006300
N	-1.21782700	1.19986900	-0.23942000
C	2.40280000	0.49582200	0.52968500
C	2.57858300	-0.42190200	1.50048500
C	4.88302900	-0.29877300	0.33882400
C	-2.40279600	0.49579300	-0.52967700
C	-4.88302900	-0.29878800	-0.33881300
C	-2.57855500	-0.42200600	-1.50041000
C	6.22553700	-0.45894900	-0.00613500
C	8.55476800	-0.28273000	-1.10395100
C	8.69652300	-1.19287700	-0.12676200
H	9.33708300	0.04554300	-1.77522000
H	9.61157300	-1.71655400	0.11599700
C	-6.22554200	-0.45894500	0.00613400
C	-8.55479700	-0.28264600	1.10388700
C	-8.69652400	-1.19288700	0.12678000
H	-9.33713100	0.04568500	1.77510600
H	-9.61156400	-1.71659300	-0.11595200
S	-3.81715700	0.80280500	0.49182900
S	-4.13276700	-1.18264300	-1.64331600
S	-6.98046500	0.42752500	1.30408600
S	-7.29127800	-1.55915200	-0.82870200
S	6.98042700	0.42741400	-1.30417800
S	7.29130500	-1.55905600	0.82879200
S	3.81713800	0.80275800	-0.49187600
S	4.13279700	-1.18252800	1.64341200
H	1.82267000	-0.71056300	2.21754100
H	-1.82262600	-0.71072500	-2.21742500
H	-2.24167000	3.24504100	-0.43735400
H	2.24167500	3.24506400	0.43722000



## Diradical (TTF-B $\square$ N-TTF)

H	-1.05075800	-2.48334400	-1.45120400
H	-1.14902700	0.63232300	1.37568300
B	-1.36507900	-0.93733700	-0.03849700
B	0.83404400	-1.88453900	-0.79474200
H	1.44959700	-2.64125300	-1.46552900
B	0.77335400	0.01959700	0.86411200
H	1.33693900	0.78788400	1.56832500
N	-0.58951800	-1.85480300	-0.80818800
N	-0.64806900	-0.00690800	0.77403000
N	1.52347900	-0.93736400	0.06843400
C	-2.94526200	-0.97499100	-0.08135900
C	-3.70231500	-2.09132700	-0.15782600
C	-5.45357600	-0.20452100	-0.02756800
C	2.92561200	-0.98500500	0.14964400
C	5.41403800	-0.19471800	0.05418800
C	3.67891300	-2.07727000	0.39159900
C	-6.63335400	0.54029000	0.00650200
C	-8.38202700	2.43573400	0.10499600
C	-9.09860400	1.30235900	0.02508700
H	-8.79227700	3.43513300	0.16251800
H	-10.17872300	1.24231700	0.00837000
C	6.59111200	0.54824000	-0.03776300
C	8.33708600	2.42811900	-0.32654200
C	9.05370200	1.32041100	-0.07869000
H	8.74523200	3.41469500	-0.50040000
H	10.13281300	1.27032000	-0.02093600
S	3.83176800	0.50714400	-0.15197000
S	5.40529600	-1.90784600	0.38054200
S	6.60624000	2.25991900	-0.37240200
S	8.17302600	-0.15833600	0.17020700
S	-6.65069200	2.28039700	0.11651100
S	-8.21508200	-0.19154200	-0.05868700
S	-3.86511700	0.51962700	0.01650900
S	-5.43455100	-1.94525000	-0.13845700
H	-3.31628400	-3.10181600	-0.20350800
H	3.28349100	-3.06106900	0.60271400

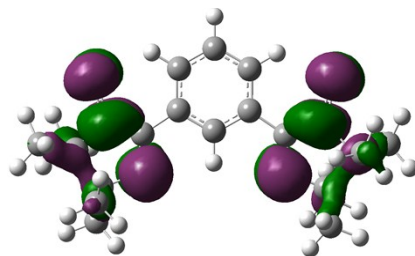
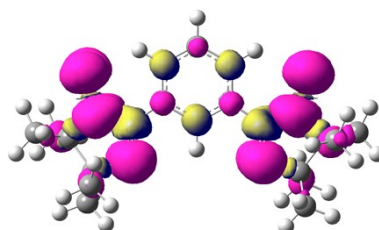
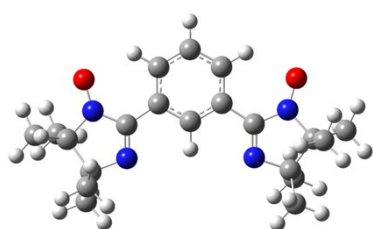


**The Optimized XYZ Coordinates of Relevant 6 Benzene Bridged Diradicals, Their Respective Optimized Structures, Spin Density Distribution Plots, Spatial distribution of Magnetic Orbitals and the Respective *J* Values (Table 1S) are Given in UB3LYP/6-311G(d,p) Level of Theory. The Different Colors Used for the Atoms in Their Optimized Structures, in Spin Density Distribution Plots and in the Plots of Magnetic Orbitals.**

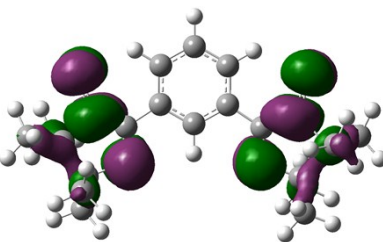
**Diradical (IN--IN)**

C	-1.21769200	1.11715900	0.02418800
C	0.00000000	0.42991900	-0.00000800
C	1.21769200	1.11715900	-0.02420700
C	1.21172700	2.52091600	-0.02357600
C	-0.00000100	3.20327400	-0.00001400
C	-1.21172700	2.52091600	0.02355100
H	0.00000100	-0.65099000	-0.00000700
H	2.14670100	3.05966800	-0.04336100
H	-0.00000100	4.28723700	-0.00001600
H	-2.14670200	3.05966700	0.04333600
C	-2.45193200	0.30316900	0.04711200
C	-3.83958200	-1.48727500	0.19703600
C	-4.74558100	-0.25640000	-0.17173400
C	2.45193200	0.30317000	-0.04713200
C	3.83958500	-1.48727300	-0.19704500
C	4.74557800	-0.25640100	0.17175100
N	-3.75182600	0.84808300	0.05926700
N	-2.45291900	-0.98588300	0.05167500
N	2.45292000	-0.98588100	-0.05170200
N	3.75182700	0.84808500	-0.05925300
C	5.13048600	-0.18220800	1.66031500
H	5.87891800	-0.93775000	1.90727400
H	5.55169900	0.80424100	1.86463900
H	4.26481000	-0.32521000	2.30958800
C	5.98350700	-0.01971900	-0.69152400
H	6.44364600	0.92844600	-0.40895200
H	6.71155800	-0.81873300	-0.53158700
H	5.74495100	0.02743200	-1.75363700
C	4.02769800	-2.71258200	0.70351900
H	3.33626800	-3.49562100	0.38646800
H	5.04662800	-3.10366000	0.62913500
H	3.81600500	-2.48725000	1.74857500
C	3.98208700	-1.92123400	-1.66988200
H	4.96208700	-2.36563700	-1.86106000
H	3.21446000	-2.66427900	-1.89285700
H	3.83987300	-1.08033900	-2.35168800
C	-3.98206100	-1.92125000	1.66987000
H	-4.96206000	-2.36565100	1.86106000
H	-3.21443300	-2.66430000	1.89282600
H	-3.83983200	-1.08036200	2.35168200
C	-4.02771000	-2.71257500	-0.70353800
H	-3.33628000	-3.49562000	-0.38650200
H	-5.04664000	-3.10365000	-0.62914600
H	-3.81602800	-2.48723500	-1.74859500

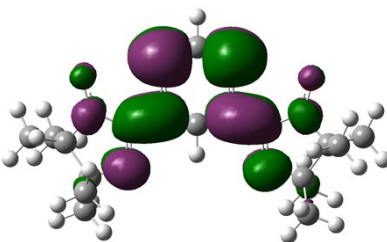
C	-5.98349600	-0.01972800	0.69156200
H	-6.44364200	0.92843900	0.40900700
H	-6.71154900	-0.81874100	0.53163000
H	-5.74492400	0.02741400	1.75367300
C	-5.13051100	-0.18219000	-1.66029100
H	-5.87894500	-0.93773200	-1.90724700
H	-5.55172900	0.80426000	-1.86459800
H	-4.26484400	-0.32518500	-2.30957900
O	-4.09228500	2.06682600	0.06365000
O	4.09228600	2.06682800	-0.06361200



HOMO-1(SOMO1)



HOMO (SOMO2)

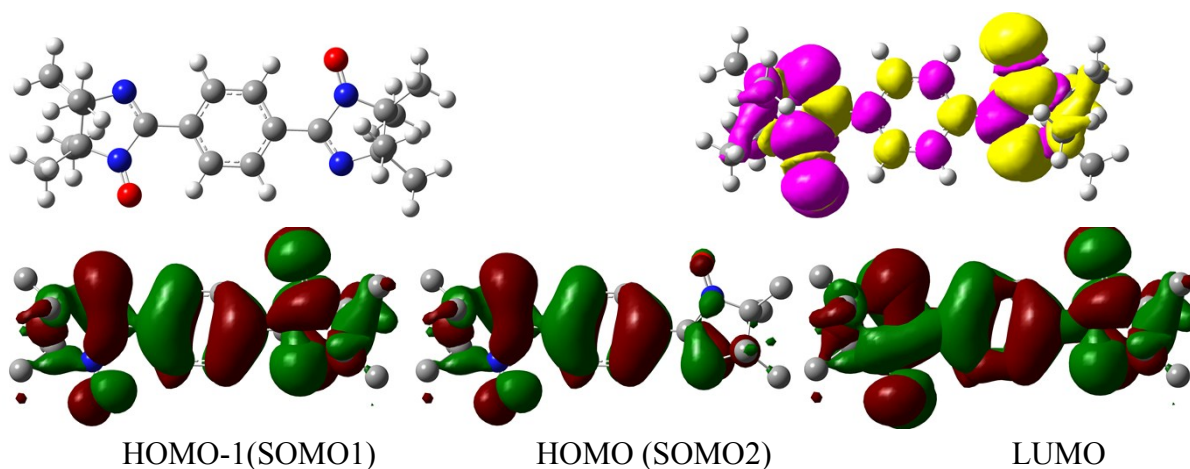


LUMO

### Diradical ( $^{\text{IN}}-\text{C}_6\text{H}_4-\text{IN}$ )

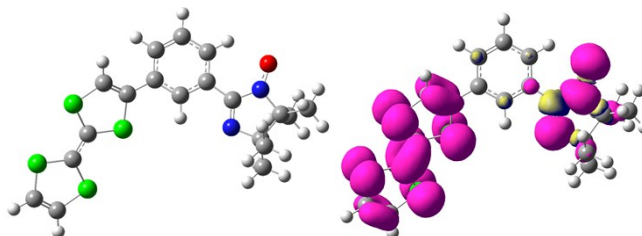
H	-1.23605400	-2.13765900	-0.11069000
H	1.23882600	-2.14428700	-0.09230800
H	1.23605400	2.13765900	-0.11068900
H	-1.23882600	2.14428700	-0.09230800
C	-4.98468600	-0.92978200	-0.25967900
C	-5.13748000	0.53605200	0.29034800
C	5.13748000	-0.53605200	0.29034800
C	4.98468600	0.92978200	-0.25967900
N	3.52865600	1.19951100	-0.20380900
N	3.73374700	-1.02385800	0.06199800
N	-3.73374700	1.02385800	0.06199700
N	-3.52865600	-1.19951100	-0.20381000
C	-2.88253200	-0.08971100	-0.08930700
C	2.88253200	0.08971100	-0.08930600
O	-3.41481100	2.24025600	0.19984100
O	3.41481200	-2.24025600	0.19984100
C	-5.37830800	0.61645400	1.80834100
H	-5.24458300	1.65130800	2.12977300
H	-6.39366900	0.30281400	2.05832300
H	-4.67487300	-0.00718000	2.36295300

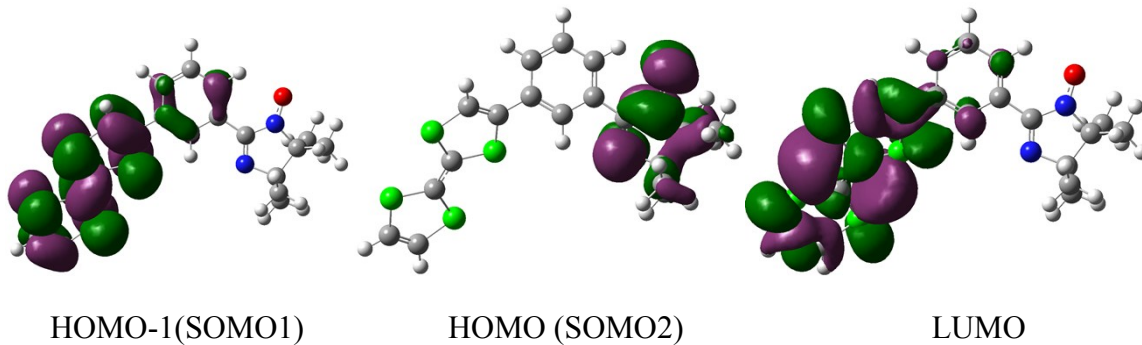
C	-6.12192700	1.45034100	-0.43619800
H	-7.14496300	1.09924800	-0.28101400
H	-6.03919000	2.46157800	-0.03463300
H	-5.92862600	1.49795200	-1.50743700
C	-5.72453000	-1.99793100	0.55296900
H	-6.80423700	-1.82251700	0.54314500
H	-5.53295600	-2.97704700	0.10965200
H	-5.38608200	-2.03138600	1.58842800
C	-5.38731200	-1.06194300	-1.74238100
H	-5.10956200	-2.05685600	-2.09472200
H	-6.46477500	-0.93503100	-1.87393500
H	-4.86970200	-0.33084800	-2.36660500
C	6.12192700	-1.45034100	-0.43619800
H	7.14496300	-1.09924700	-0.28101500
H	6.03919100	-2.46157800	-0.03463300
H	5.92862600	-1.49795200	-1.50743700
C	5.37830800	-0.61645400	1.80834100
H	5.24458400	-1.65130800	2.12977300
H	6.39367000	-0.30281300	2.05832200
H	4.67487300	0.00718000	2.36295300
C	5.38731100	1.06194300	-1.74238100
H	5.10956000	2.05685500	-2.09472300
H	6.46477500	0.93503200	-1.87393600
H	4.86970200	0.33084700	-2.36660500
C	5.72453000	1.99793100	0.55296800
H	6.80423700	1.82251700	0.54314300
H	5.53295600	2.97704700	0.10965200
H	5.38608300	2.03138600	1.58842700
C	-1.40812600	-0.00226400	-0.09561400
C	-0.69971900	1.20953700	-0.09776000
C	0.68741500	1.20495300	-0.10354700
C	1.40812600	0.00226400	-0.09561400
C	0.69971900	-1.20953700	-0.09776000
C	-0.68741600	-1.20495300	-0.10354800



## Diradical (IN--TTF)

H	3.86663500	2.84156900	-0.59607000
H	0.80373800	0.00556300	0.29138800
H	2.16219200	4.61720700	-0.87030900
C	3.37853400	0.17901000	0.01436200
C	4.18059000	-1.89103200	0.47637300
C	-1.31536700	1.71573600	0.07855500
C	-3.56784000	0.38130600	0.07900900
C	-2.25850000	2.53869800	0.59891100
C	-4.55142600	-0.59616500	-0.05077700
C	-5.85558900	-2.77331800	-0.53687200
C	-6.76452200	-1.93030400	-0.02634600
H	-6.05057300	-3.78768000	-0.85699200
H	-7.81054300	-2.15492100	0.13130300
S	-1.91508600	0.13181700	-0.41266700
S	-3.88699300	1.96429300	0.72877700
S	-4.22366500	-2.18545100	-0.69851500
S	-6.21500900	-0.33824300	0.41898100
H	-2.06376000	3.53278200	0.97675800
H	-0.23272400	4.10412500	-0.59740900
N	4.76959400	0.31581900	-0.06469000
N	2.99228900	-1.02970900	0.24152600
C	5.39542700	-1.05439400	-0.07989600
O	5.43369700	1.37212800	-0.26148800
C	6.67070100	-1.04345300	0.76066500
H	7.12592800	-2.03625800	0.76137500
H	7.38354600	-0.34032100	0.32763800
H	6.48760800	-0.74301400	1.79170300
C	5.74439500	-1.34748400	-1.55010100
H	6.43497500	-0.58140100	-1.90753500
H	6.22993300	-2.32015300	-1.64501900
H	4.86023700	-1.33685800	-2.19040600
C	3.96854600	-3.24114600	-0.21533600
H	4.83125600	-3.89585500	-0.06672600
H	3.09323200	-3.73025000	0.21645200
H	3.79687900	-3.13149100	-1.28583600
C	4.24565700	-2.11170900	2.00088400
H	3.31127000	-2.56777100	2.33288600
H	5.06775500	-2.77947300	2.26706900
H	4.37082200	-1.17166700	2.54172100
C	0.50750500	3.32733800	-0.44663200
C	2.81905600	2.61421800	-0.46715600
C	1.07285300	1.02000900	0.02222800
C	2.43230200	1.30513900	-0.15141700
C	0.10735800	2.01912700	-0.11940100
C	1.85379600	3.61132700	-0.61257700



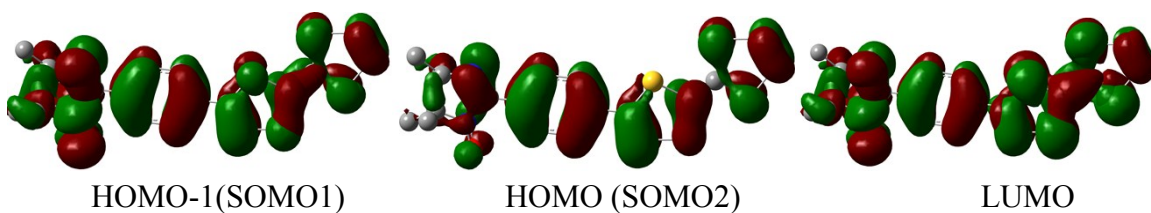
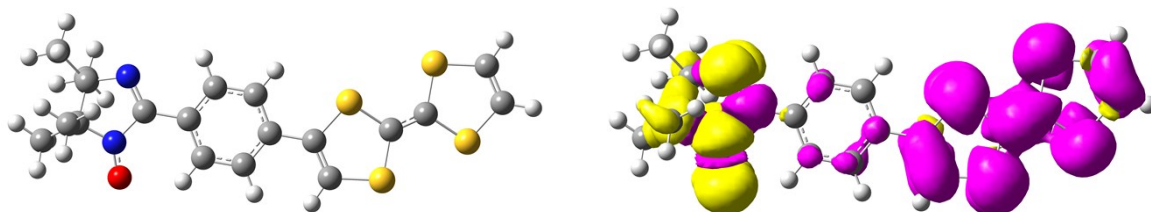


**Diradical (IN--TTF)**

H	-2.72115000	-2.19824400	0.65364200
H	-2.19059400	1.78047800	-0.83438900
H	-0.28587600	-2.54318600	0.63393300
H	0.25074500	1.44506300	-0.91225900
C	-4.06645700	0.10577200	-0.08171300
C	-6.03509900	1.17214300	-0.43924600
C	1.61228200	-0.81025600	-0.18983600
C	4.18681400	-0.33813500	-0.06483500
C	2.24173500	-1.98059700	-0.46370600
C	5.43967800	0.25441600	0.06209600
C	7.39138400	1.91091300	0.41897700
C	7.97766300	0.73463800	0.15518900
H	7.90873400	2.83870100	0.62137800
H	9.04404500	0.56046000	0.11091000
S	2.69609800	0.53659200	0.16558800
S	3.97096200	-2.02272900	-0.44675600
S	5.64949500	1.94811200	0.43831100
S	6.93454300	-0.62963300	-0.13893200
H	1.73697800	-2.89884200	-0.73004400
C	-6.36738600	-0.09944500	0.43047700
O	-4.87182000	-1.99635500	0.73306700
N	-5.04244000	-0.81020700	0.33209700
N	-4.55198600	1.24146900	-0.45325200
C	-6.45908400	1.02516500	-1.91532500
H	-7.54684700	1.02724200	-2.01350800
H	-6.06092900	1.86785100	-2.48280800
H	-6.07046800	0.10687800	-2.36014800
C	-6.59529900	2.48706000	0.11230200
H	-6.29223000	3.30690400	-0.54133200
H	-7.68777600	2.46170800	0.14317100
H	-6.22411500	2.70403300	1.11358800
C	-7.47839100	-1.01490200	-0.07944000
H	-7.52890000	-1.90693400	0.54655200
H	-8.44074300	-0.50137500	-0.02287400
H	-7.31461900	-1.33442700	-1.10800600
C	-6.58162400	0.19720800	1.92544700
H	-7.53905100	0.69527900	2.08648900
H	-6.58645600	-0.74635300	2.47434300



H	-5.78977600	0.82780200	2.33412200
C	-2.61763800	-0.18302400	-0.08830800
C	-1.75693800	0.84079900	-0.51869700
C	-0.38782700	0.64810000	-0.54763100
C	0.16604800	-0.58183600	-0.15010800
C	-0.69297200	-1.60170700	0.28447800
C	-2.06738600	-1.40939500	0.31311400



HOMO-1(SOMO1)

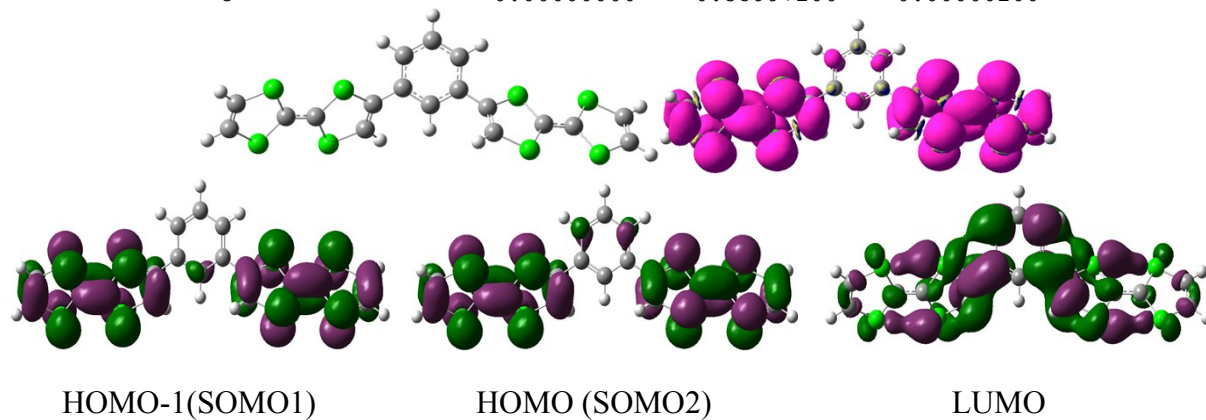
HOMO (SOMO2)

LUMO

### Diradical (TTF- $\square$ -TTF)

H	0.00000000	4.23206800	-0.00000200
H	0.00000000	-0.72344400	0.00000300
C	2.45797600	0.31318500	0.41326500
C	2.62454700	-0.77036300	1.20200800
C	4.99188900	-0.32508300	0.27819900
C	-2.45797500	0.31318400	-0.41326300
C	-4.99188900	-0.32508400	-0.27819800
C	-2.62454600	-0.77036500	-1.20200300
C	6.35847900	-0.36540000	-0.00073100
C	8.73626900	0.10870000	-0.88527900
C	8.86497800	-0.97165400	-0.09783600
H	9.53940800	0.59109200	-1.42626500
H	9.78865700	-1.49989200	0.09779000
C	-6.35847900	-0.36540000	0.00073000
C	-8.73627100	0.10870100	0.88527400
C	-8.86497800	-0.97165400	0.09783300
H	-9.53941000	0.59109500	1.42625800
H	-9.78865700	-1.49989200	-0.09779300
S	-3.91943600	0.86890000	0.40669400
S	-4.20658800	-1.47226600	-1.33200500
S	-7.14421100	0.78785100	1.04649100
S	-7.42575000	-1.57059900	-0.67091900
S	7.14421000	0.78784900	-1.04649600
S	7.42575100	-1.57059800	0.67091900
S	3.91943500	0.86889900	-0.40669500
S	4.20658900	-1.47226200	1.33200900
H	1.84638300	-1.22044200	1.80349900
H	-1.84638100	-1.22044600	-1.80349200
H	-2.10964800	3.01055100	-0.34457900
H	2.10964800	3.01055200	0.34457800

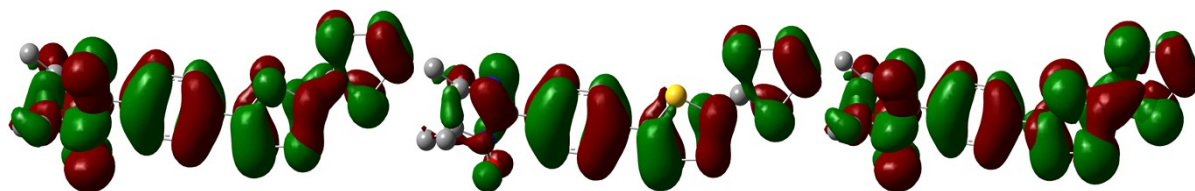
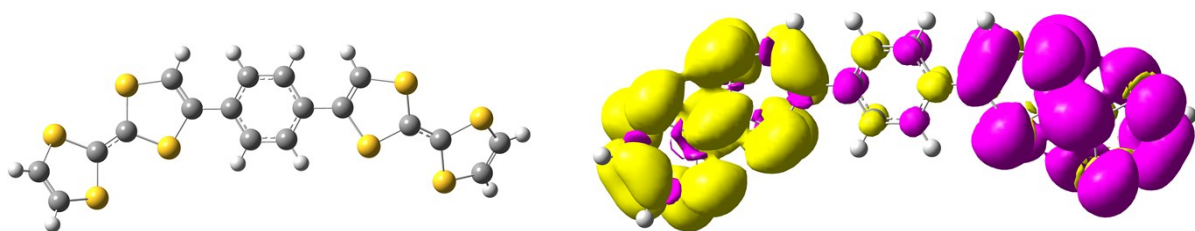
C	-1.20118500	1.05519200	-0.18674400
C	-1.19225200	2.45784900	-0.17998700
C	0.00000000	3.14924200	0.00000000
C	1.19225200	2.45784900	0.17998700
C	1.20118500	1.05519200	0.18674700
C	0.00000000	0.35997200	0.00000200



### Diradical (TTF TTF)

H	1.21555900	2.93385900	-0.13558100
H	1.20567100	-1.37308800	-0.18341200
H	-1.21555900	2.93385900	0.13558100
H	-1.20567100	-1.37308800	0.18341200
C	2.85276500	0.80110600	-0.41205200
C	3.52784900	1.66203900	-1.20573000
C	5.38182100	0.15430000	-0.23767600
C	-2.85276500	0.80110600	0.41205200
C	-5.38182100	0.15430000	0.23767600
C	-3.52784900	1.66203900	1.20573000
C	6.60111900	-0.44719800	0.07547400
C	8.46281400	-1.95899000	1.03012200
C	9.09781000	-1.07987900	0.23807800
H	8.93604600	-2.74879600	1.59804600
H	10.16526900	-1.04741500	0.06497100
C	-6.60111900	-0.44719800	-0.07547400
C	-8.46281400	-1.95899000	-1.03012200
C	-9.09781000	-1.07987900	-0.23807800
H	-8.93604600	-2.74879600	-1.59804600
H	-10.16526900	-1.04741400	-0.06497100
S	-3.86057200	-0.37801500	-0.43131500
S	-5.25183200	1.51897000	1.31598700
S	-6.73450400	-1.81279600	-1.15184500

S	-8.12196000	0.10598300	0.57598400
S	6.73450400	-1.81279600	1.15184500
S	8.12196000	0.10598300	-0.57598400
S	3.86057200	-0.37801500	0.43131500
S	5.25183200	1.51897000	-1.31598700
H	3.06762700	2.42833700	-1.81484300
H	-3.06762700	2.42833700	1.81484300
C	0.68775600	-0.42542100	-0.09403200
C	1.39495500	0.78163700	-0.19112100
C	-0.68775600	-0.42542100	0.09403200
C	-1.39495500	0.78163700	0.19112100
C	-0.68769700	1.98920900	0.08874900
C	0.68769700	1.98920900	-0.08874900









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









HOMO (SOMO2)

LUMO

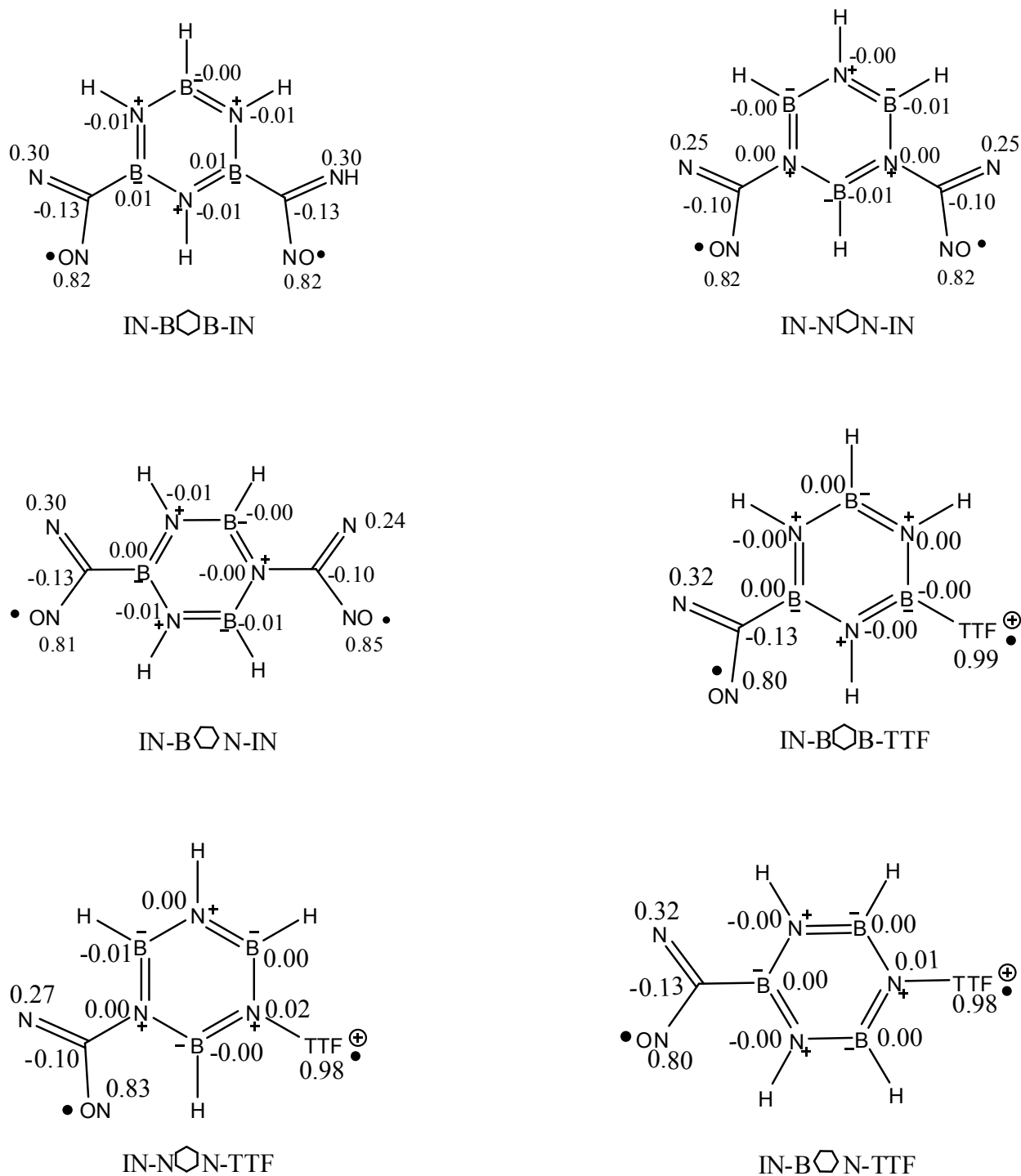
**Table 1S.** Optimized UB3LYP-level absolute energies ( $E$ , au),  $\langle S^2 \rangle$ , and intramolecular exchange-coupling constants ( $J$ , cm<sup>-1</sup>) using the 6-311G(d,p) basis set for corresponding benzene bridged diradicals.

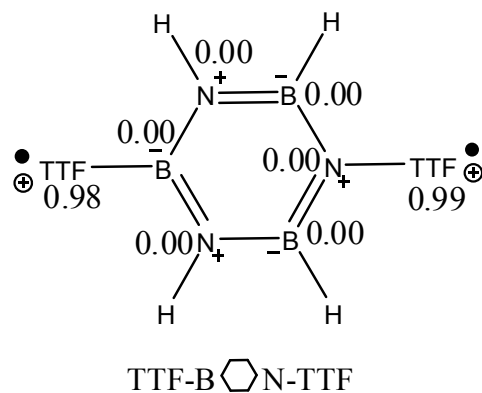
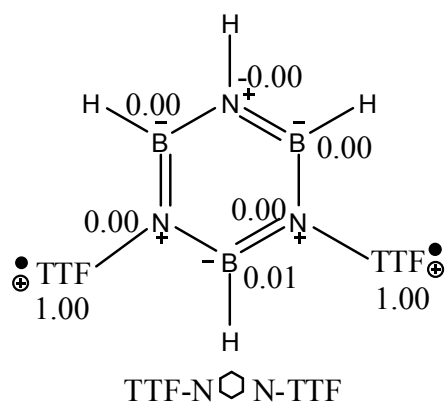
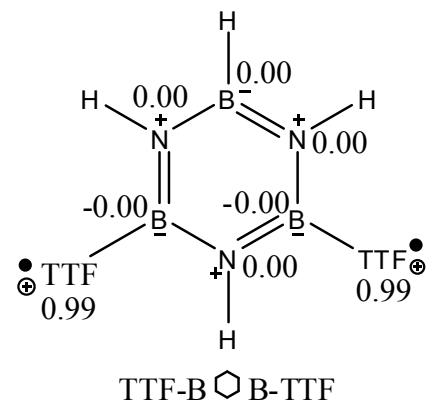
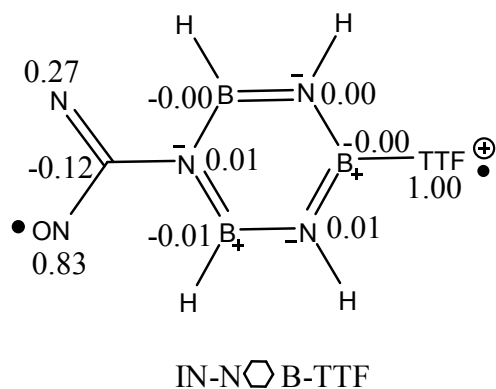
System	Spin State	UB3LYP/6-311G(d,p) level of theory		
		$E$ (a.u.)	$\langle S^2 \rangle$	$J$ (cm <sup>-1</sup> )
IN  IN	Triplet	-1148.61972	2.039	26.24
	BS	-1148.61960	1.035	
IN  IN	Triplet	-1148.62029	2.033	-42.16
	BS	-1148.62048	1.041	
IN  TTF	Triplet	-2512.93673	2.023	-20.16
	BS	-2512.93682	1.020	
IN  TTF	Triplet	-2512.93686	2.026	32.18
	BS	-2512.93871	1.003	
TTF  TTF	Triplet	-3877.18635	2.007	0.92
	BS	-3877.18635	1.007	
TTF  TTF	Triplet	-3877.18924	2.006	-8.76
	BS	-3877.18928	1.004	

**Table 2S.** Calculated NICS values at the UB3LYP level using a 6-311G(d, p) basis set for each diradical. NICS values along the central axis normal to the ring plane are obtained by placing the probe atom at regular 0.5Å increments from the ring plane. In the last row we list the NICS(X) values of free borazine and benzene at the same level of theory. The NICS values are expressed in ppm units.

System	NICS(0)	NICS(0.5Å)	NICS(1Å)	NICS(1.5Å)	NICS(2Å)
IN-B  B-IN	-2.17	-2.77	-2.93	-2.26	-1.55
IN-N  N-IN	-1.57	-2.36	-2.61	-2.02	-1.36
IN-B  N-IN	-1.85	-2.60	-2.85	-2.20	-1.49
IN-B  B-TTF	-2.02	-2.62	-2.78	-2.11	-1.40
IN-N  N-TTF	-1.57	-2.39	-2.69	-2.10	-1.43
IN-B  N-TTF	-1.55	-2.17	-2.49	-1.97	-1.36
IN-N  B-TTF	-1.92	-2.55	-2.64	-2.00	-1.34
TTF-B  B-TTF	-1.99	-2.44	-2.50	-1.89	-1.25
TTF-N  N-TTF	-2.01	-2.60	-2.74	-2.09	-1.39
TTF-B  N-TTF	-1.96	-2.48	-2.59	-1.96	-1.29
Benzene	-8.87	-10.80	-11.12	-8.23	-5.18
Borazine	-2.05	-2.75	-3.01	-2.34	-1.57

**Scheme 1S:** Schematic representation of different linkage specific borazine coupled (*meta*-B-B, *meta*-N-N and *para*-B-N connected) diradicals is investigated showing their atomic spin-populations in their triplet states. We depict only the  $\pi$ -network, neglecting the network which is purely  $\sigma$ , and the non-alternant TTF moieties are represented as a single node.





### The complete reference of 30.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene,

M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian'09W, Revision A.02; Gaussian, Inc.: Wallingford CT, 2009.