Electronic supplementary information

Electric Field Induced Tuning of Molecular Conformation to Acquire Spintronics Property in Biphenyl Systems

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Optimized Coordinate of Biphenyl

$E_{\parallel}$ = 0.00 a.u.

0 1

C	-0.74356500	0.00000100	0.00000000
C	-1.46641600	1.13206200	0.41656800
C	-2.86235200	1.13289400	0.41592000
C	-3.56719600	-0.00000100	0.00000000
C	-2.86235100	-1.13289500	-0.41592100
C	-1.46641500	-1.13206100	-0.41656800
C	0.74356500	0.00000100	0.00000000
C	1.46641600	1.13206200	-0.41656700
C	2.86235200	1.13289400	-0.41592100
C	3.56719600	-0.00000100	-0.00000100
C	2.86235100	-1.13289500	0.41592100
C	1.46641500	-1.13206100	0.41656900

H	-0.92997000	2.00919500	0.76662200
H	-3.39936700	2.01628800	0.74998700
H	-4.65331000	-0.00000200	0.00000100
H	-3.39936500	-2.01628900	-0.74998800
H	-0.92996800	-2.00919300	-0.76662400
H	0.92997000	2.00919600	-0.76662000
H	3.39936700	2.01628800	-0.74998800
H	4.65331000	-0.00000200	-0.00000200
H	3.39936500	-2.01628900	0.74998900
H	0.92996800	-2.00919300	0.76662400

$E_{\parallel}$ = 0.0015 a.u.

0 1

C	-0.74414000	-0.00000100	0.00000000
C	-1.46649300	-1.13265200	-0.41568600
C	-2.86232900	-1.13313500	-0.41563100
C	-3.56681300	0.00000000	0.00000000
C	-2.86232800	1.13313600	0.41563100
C	-1.46649200	1.13265200	0.41568600
C	0.74291000	-0.00000100	0.00000000
C	1.46652800	-1.13190600	0.41626500
C	2.86253900	-1.13306800	0.41514600
C	3.56782000	0.00000000	0.00000000
C	2.86253800	1.13306800	-0.41514600
C	1.46652800	1.13190600	-0.41626500

H	-0.93053900	-2.01032400	-0.76549200
H	-3.39983800	-2.01612700	-0.74932800
H	-4.65265400	0.00000100	0.00000000
H	-3.39983600	2.01612800	0.74932900
H	-0.93053800	2.01032300	0.76549200
H	0.92972500	-2.00893600	0.76565000
H	3.39905800	-2.01713100	0.74879600
H	4.65423000	0.00000100	0.00000000
H	3.39905700	2.01713100	-0.74879600
H	0.92972300	2.00893500	-0.76565000

$E_{\parallel}$ = 0.0030 a.u.

0 1

C	-0.74481900	0.00000000	0.00000000
C	-1.46651100	1.13378400	0.41352200
C	-2.86236700	1.13404500	0.41365000
C	-3.56648500	0.00000000	0.00000000
C	-2.86236700	-1.13404500	-0.41365100
C	-1.46651100	-1.13378400	-0.41352200
C	0.74202100	0.00000000	0.00000000
C	1.46681900	1.13233600	-0.41426000
C	2.86277000	1.13369600	-0.41295700
C	3.56865000	0.00000000	0.00000000
C	2.86277000	-1.13369600	0.41295800
C	1.46681900	-1.13233600	0.41426000

H	-0.93119900	2.01244400	0.76207700
H	-3.40081100	2.01685600	0.74575200
H	-4.65213900	0.00000000	0.00000000
H	-3.40081100	-2.01685600	-0.74575300
H	-0.93119900	-2.01244400	-0.76207700
H	0.92961600	2.00966600	-0.76204500
H	3.39839500	2.01912000	-0.74517300
H	4.65539200	0.00000000	0.00000000
H	3.39839500	-2.01912000	0.74517400
H	0.92961600	-2.00966600	0.76204500

$E_{\parallel}$ = 0.0045 a.u.

0 1

C	-0.74538300	0.00000100	0.00000000
C	-1.46671600	1.13564000	0.40929300
C	-2.86251700	1.13558400	0.40991700
C	-3.56637800	-0.00000100	0.00000000
C	-2.86251500	-1.13558500	-0.40991700
C	-1.46671500	-1.13563900	-0.40929300
C	0.74115000	0.00000100	0.00000000
C	1.46717200	1.13323400	-0.41101000
C	2.86312100	1.13485600	-0.40922500
C	3.56967100	-0.00000100	0.00000000
C	2.86311900	-1.13485800	0.40922600

C	1.46717100	-1.13323300	0.41101000
H	-0.93207300	2.01579000	0.75533300
H	-3.40171400	2.01892500	0.73896700
H	-4.65190400	-0.00000200	0.00000000
H	-3.40171200	-2.01892600	-0.73896700
H	-0.93206900	-2.01578800	-0.75533300
H	0.92987600	2.01139000	-0.75632700
H	3.39794300	2.02199300	-0.73886400
H	4.65675500	-0.00000200	0.00000000
H	3.39794100	-2.02199500	0.73886400
H	0.92987200	-2.01138800	0.75632700

$E_{\parallel}$ = 0.0060 a.u.

0 1

C	-0.74574500	0.00000000	0.00000000
C	-1.46707000	-1.13782400	-0.40405100
C	-2.86273600	-1.13739800	-0.40529000
C	-3.56646200	0.00000000	0.00000000
C	-2.86273500	1.13739800	0.40528900
C	-1.46707000	1.13782400	0.40405100
C	0.74022400	0.00000000	0.00000000
C	1.46756600	-1.13457400	0.40658500
C	2.86354800	-1.13651800	0.40417400
C	3.57084000	0.00000000	0.00000000

C	2.86354800	1.13651800	-0.40417300
C	1.46756600	1.13457400	-0.40658500
H	-0.93313600	-2.01976600	-0.74699600
H	-3.40250700	-2.02159200	-0.73070200
H	-4.65186100	0.00000000	0.00000000
H	-3.40250600	2.02159300	0.73070100
H	-0.93313600	2.01976600	0.74699600
H	0.93011700	-2.01385600	0.74844700
H	3.39785300	-2.02561900	0.73017500
H	4.65836700	0.00000000	0.00000000
H	3.39785200	2.02561900	-0.73017500
H	0.93011600	2.01385600	-0.74844600

$E_{\|}$ = 0.0075 a.u.

0 1

C	-0.74537800	0.00000000	0.00000000
C	-1.46749700	1.13987000	0.39821500
C	-2.86318900	1.13957100	0.39916500
C	-3.56732700	0.00000000	0.00000000
C	-2.86318900	-1.13957100	-0.39916500
C	-1.46749700	-1.13987000	-0.39821500
C	0.74006100	0.00000000	0.00000000
C	1.46806400	1.13690100	-0.40036400
C	2.86393100	1.13862200	-0.39829600

C	3.57152200	0.00000000	0.00000000
C	2.86393100	-1.13862200	0.39829600
C	1.46806400	-1.13690100	0.40036400
H	-0.93390600	2.02356700	0.73700700
H	-3.40300800	2.02549500	0.72015100
H	-4.65301400	0.00000000	0.00000000
H	-3.40300800	-2.02549500	-0.72015100
H	-0.93390600	-2.02356700	-0.73700700
H	0.93110600	2.01811000	-0.73817600
H	3.39824300	2.02935900	-0.71991500
H	4.65916700	0.00000000	0.00000000
H	3.39824300	-2.02935900	0.71991500
H	0.93110600	-2.01811000	0.73817600

$E_{\|}$ = 0.0090 a.u.

0 1

C	0.73808200	-0.00000600	-0.00003300
C	1.46881000	1.13869000	-0.39357900
C	2.86466300	1.14092000	-0.39056100
C	3.57379200	-0.00000400	0.00002400
C	2.86464900	-1.14093000	0.39057800
C	1.46879600	-1.13870200	0.39353800
C	-0.74660500	0.00000700	-0.00003200
C	-1.46790500	1.14340000	0.39009500

C	-2.86348200	1.14248700	0.39200700
C	-3.56700800	0.00000400	0.00002500
C	-2.86349500	-1.14247800	-0.39198900
C	-1.46791700	-1.14338800	-0.39013500
H	0.93143200	2.02145000	-0.72603100
H	3.39731700	2.03523600	-0.70675200
H	4.66228900	0.00000700	0.00007500
H	3.39729100	-2.03522000	0.70686500
H	0.93140500	-2.02143500	0.72604200
H	-0.93583800	2.03006300	0.72416200
H	-3.40496000	2.02904100	0.70734800
H	-4.65237000	-0.00000800	0.00007600
H	-3.40498500	-2.02905500	-0.70725100
H	-0.93586200	-2.03007200	-0.72417100

$E^{\perp}$ = 0.0015 a.u.

0 1

C	-0.74359300	0.00019700	-0.00041200
C	-1.46648000	1.13407800	0.41099100
C	-2.86243000	1.13476900	0.41057100
C	-3.56731400	-0.00000700	0.00000700
C	-2.86241600	-1.13483100	-0.41031600
C	-1.46651400	-1.13412600	-0.41058200
C	0.74359300	-0.00018500	-0.00040600
C	1.46652100	1.13413300	-0.41057300

C	2.86242500	1.13482500	-0.41031500
C	3.56731400	-0.00000600	0.00000100
C	2.86242100	-1.13477400	0.41057500
C	1.46647300	-1.13407200	0.41099800
H	-0.92991800	2.01262500	0.75756300
H	-3.39964700	2.02009800	0.73961000
H	-4.65348500	0.00002000	-0.00089200
H	-3.39932600	-2.01977400	-0.74041700
H	-0.93040300	-2.01265500	-0.75750200
H	0.93041900	2.01267600	-0.75746900
H	3.39933800	2.01976400	-0.74042100
H	4.65348500	-0.00004800	-0.00091200
H	3.39963400	-2.02010300	0.73962200
H	0.92990100	-2.01261100	0.75757600

$E^{\perp}$ = 0.0030 a.u.

0 1

C	-0.74349000	-0.00000100	-0.00003200
C	-1.46605800	-1.12978500	-0.42321000
C	-2.86193600	-1.13060900	-0.42265500
C	-3.56665700	0.00002400	0.00007600
C	-2.86188300	1.13064600	0.42266400
C	-1.46602300	1.12983300	0.42300400
C	0.74349000	0.00001400	-0.00003300
C	1.46601800	-1.12982900	0.42300700

C	2.86187300	-1.13065200	0.42266600
C	3.56665700	-0.00003000	0.00007600
C	2.86194700	1.13060300	-0.42265200
C	1.46606300	1.12978800	-0.42321000
H	-0.92896800	-2.00490400	-0.77743900
H	-3.39902100	-2.01184600	-0.76191700
H	-4.65266800	-0.00002300	0.00041800
H	-3.39883600	2.01170600	0.76241900
H	-0.92898500	2.00485400	0.77741000
H	0.92896700	-2.00484200	0.77741400
H	3.39882600	-2.01171300	0.76241800
H	4.65266800	0.00000100	0.00041600
H	3.39903100	2.01184300	-0.76191100
H	0.92898600	2.00491600	-0.77743600

Optimized Coordinate of Monoradical

$E_{\parallel}$ = 0.00 a.u.

0 2

C	0.32595100	0.00000300	0.00000000
C	1.06028500	-1.15544100	0.35638400
C	2.44336100	-1.16143400	0.35959600
C	3.19497300	0.00000000	0.00000300
C	2.44336400	1.16143400	-0.35959500
C	1.06028800	1.15544400	-0.35638600
C	-1.15398900	0.00000300	-0.00000200
C	-1.88100600	-1.14751600	-0.37294100
C	-3.27603200	-1.14764800	-0.37261700
C	-3.98183200	-0.00000200	-0.00000100
C	-3.27603500	1.14764500	0.37261700
C	-1.88101000	1.14751700	0.37294100
H	0.52703800	-2.05058600	0.66248200
H	2.97824900	-2.06137100	0.65167100
H	2.97825500	2.06137000	-0.65167000
H	0.52704400	2.05058900	-0.66248700
H	-1.34839800	-2.03797400	-0.69301400
H	-3.81266100	-2.04296800	-0.67387300
H	-5.06786800	-0.00000400	0.00000000
H	-3.81266800	2.04296300	0.67387600
H	-1.34840500	2.03797500	0.69301800
H	5.15954500	-0.88666800	0.27539600

H	5.15954800	0.88665600	-0.27541200
C	4.59840200	-0.00000200	0.00000300

$E_{\parallel}$ = 0.0015 a.u.

0 2

C	-0.32562500	0.00000100	0.00000000
C	-1.06028000	1.15570600	0.35537600
C	-2.44330900	1.16169700	0.35849100
C	-3.19523500	0.00000000	-0.00000200
C	-2.44330800	-1.16169700	-0.35849200
C	-1.06027900	-1.15570500	-0.35537500
C	1.15417100	0.00000100	0.00000100
C	1.88099300	1.14804000	-0.37174400
C	3.27598700	1.14809200	-0.37151600
C	3.98166700	-0.00000100	0.00000100
C	3.27598600	-1.14809300	0.37151700
C	1.88099200	-1.14804000	0.37174500
H	-0.52696900	2.05110700	0.66048800
H	-2.97796700	2.06211600	0.64971700
H	-2.97796500	-2.06211600	-0.64971800
H	-0.52696700	-2.05110600	-0.66048600
H	1.34861300	2.03900100	-0.69089300
H	3.81281300	2.04351800	-0.67188600

H	5.06764000	-0.00000100	0.00000100
H	3.81281100	-2.04351900	0.67188700
H	1.34861000	-2.03900000	0.69089300
H	-5.15955800	0.88714200	0.27455800
H	-5.15955700	-0.88714500	-0.27455900
C	-4.59867600	-0.00000100	-0.00000200

$E_{\parallel}$ = 0.0030 a.u.

0 2

C	0.32474000	0.00000100	0.00000000
C	1.06050200	-1.15674900	0.35157600
C	2.44332900	-1.16272500	0.35447700
C	3.19594500	0.00000000	0.00000000
C	2.44333100	1.16272500	-0.35447900
C	1.06050300	1.15675000	-0.35157700
C	-1.15455600	0.00000100	-0.00000100
C	-1.88117000	-1.14980900	-0.36732500
C	-3.27603100	-1.14955700	-0.36762900
C	-3.98142200	-0.00000100	0.00000100
C	-3.27603200	1.14955500	0.36763100
C	-1.88117100	1.14981000	0.36732600
H	0.52714100	-2.05295200	0.65384500
H	2.97765500	-2.06442200	0.64290000
H	2.97765700	2.06442100	-0.64290200
H	0.52714300	2.05295400	-0.65384800

H	-1.34947100	-2.04219800	-0.68368600
H	-3.81352900	-2.04542400	-0.66497800
H	-5.06726600	-0.00000200	0.00000200
H	-3.81353200	2.04542200	0.66498100
H	-1.34947400	2.04219900	0.68368800
H	5.15997900	-0.88835300	0.27171000
H	5.15998000	0.88835000	-0.27171100
C	4.59931900	-0.00000100	-0.00000100

$E_{\|}$ = 0.0045 a.u.

0 2

C	0.32388700	0.00000100	0.00000000
C	1.06086600	-1.15861600	0.34537300
C	2.44343300	-1.16451400	0.34820600
C	3.19678600	0.00000000	0.00000000
C	2.44343400	1.16451400	-0.34820800
C	1.06086700	1.15861700	-0.34537400
C	-1.15461100	0.00000100	0.00000000
C	-1.88154500	-1.15230000	-0.36050700
C	-3.27623100	-1.15179600	-0.36117900
C	-3.98159300	-0.00000100	0.00000100
C	-3.27623200	1.15179500	0.36118100
C	-1.88154700	1.15230100	0.36050900
H	0.52769900	-2.05633400	0.64314900

H	2.97754000	-2.06790600	0.63213600
H	2.97754200	2.06790500	-0.63213900
H	0.52770100	2.05633600	-0.64315100
H	-1.35053800	-2.04671000	-0.67226400
H	-3.81424400	-2.04888900	-0.65365000
H	-5.06743500	-0.00000200	0.00000200
H	-3.81424700	2.04888700	0.65365300
H	-1.35054100	2.04671200	0.67226700
H	5.16067500	-0.88994500	0.26711900
H	5.16067600	0.88994200	-0.26711900
C	4.60001400	-0.00000100	-0.00000100

$E_{\parallel}$ = 0.0060 a.u.

0 2

C	-0.32757600	0.00000000	0.00000000
C	-1.06232600	1.16360600	0.33244300
C	-2.44475300	1.16929100	0.33719200
C	-3.19636600	0.00000000	0.00000000
C	-2.44475200	-1.16929100	-0.33719200
C	-1.06232600	-1.16360600	-0.33244200
C	1.14971500	0.00000000	0.00000000
C	1.88345300	1.15331000	-0.35044500
C	3.27824700	1.15428800	-0.34788900
C	3.98790900	0.00000000	0.00000000

C	3.27824600	-1.15428800	0.34788900
C	1.88345300	-1.15331000	0.35044500
H	-0.53303400	2.06657500	0.62325900
H	-2.98072200	2.07327500	0.61239800
H	-2.98072200	-2.07327500	-0.61239800
H	-0.53303300	-2.06657500	-0.62325800
H	1.35139300	2.04955400	-0.65355500
H	3.81132300	2.05877800	-0.63121700
H	5.07532900	-0.00000100	0.00000000
H	3.81132200	-2.05877900	0.63121700
H	1.35139200	-2.04955300	0.65355400
H	-5.16091400	0.89070900	0.25723900
H	-5.16091400	-0.89071000	-0.25723900
C	-4.59816200	0.00000000	0.00000000

$E_{\parallel}$ = 0.0075 a.u.

0 2

C	0.31925700	0.00000000	0.00000000
C	1.06154100	-1.16349100	0.32642400
C	2.44319700	-1.16924600	0.32827500
C	3.20029000	0.00000000	0.00000000
C	2.44319700	1.16924600	-0.32827500
C	1.06154100	1.16349100	-0.32642400
C	-1.15642100	0.00000000	0.00000000

C	-1.88226500	-1.16093400	-0.33802400
C	-3.27618200	-1.15919900	-0.34124900
C	-3.97994500	0.00000000	0.00000000
C	-3.27618200	1.15919900	0.34124900
C	-1.88226500	1.16093400	0.33802400
H	0.52822300	-2.06539200	0.60933000
H	2.97549800	-2.07899200	0.59767700
H	2.97549800	2.07899200	-0.59767700
H	0.52822300	2.06539200	-0.60933000
H	-1.35438800	-2.06245900	-0.63483600
H	-3.81745100	-2.05855500	-0.61785800
H	-5.06516000	0.00000000	0.00000000
H	-3.81745100	2.05855500	0.61785800
H	-1.35438800	2.06245900	0.63483700
H	5.16332900	-0.89552400	0.25279700
H	5.16332900	0.89552400	-0.25279700
C	4.60336000	0.00000000	0.00000000

$E_{\parallel}$ = 0.0090 a.u.

0 2

C	0.31815800	0.00000000	0.00000000
C	1.06249700	-1.16759800	0.31186800
C	2.44363800	-1.17311000	0.31400400
C	3.20210300	0.00000000	-0.00000100

C	2.44363800	1.17311000	-0.31400500
C	1.06249700	1.16759800	-0.31186900
C	-1.15559100	0.00000000	0.00000000
C	-1.88350900	-1.16547400	-0.32310600
C	-3.27699900	-1.16367700	-0.32640400
C	-3.98151500	0.00000000	0.00000100
C	-3.27699900	1.16367700	0.32640500
C	-1.88350900	1.16547400	0.32310700
H	0.53055900	-2.07344500	0.58443200
H	2.97568200	-2.08615500	0.57281700
H	2.97568200	2.08615500	-0.57281900
H	0.53055900	2.07344400	-0.58443200
H	-1.35684600	-2.07101100	-0.60927800
H	-3.81833800	-2.06650000	-0.59182400
H	-5.06702500	0.00000000	0.00000100
H	-3.81833700	2.06650000	0.59182500
H	-1.35684500	2.07101100	0.60927800
H	5.16507300	-0.89851600	0.24188300
H	5.16507300	0.89851600	-0.24188500
C	4.60471800	0.00000000	-0.00000100

$E_{\parallel}$ = 0.0115 a.u.

0 2

C	0.31394000	0.00050700	0.00104900

C	1.06390500	-1.17427900	0.28401200
C	2.44397300	-1.17968200	0.28555200
C	3.20694800	-0.00006200	-0.00023400
C	2.44433900	1.18004100	-0.28482500
C	1.06427200	1.17528700	-0.28133600
C	-1.15538800	0.00018600	0.00083500
C	-1.88575300	-1.17523600	-0.29122200
C	-3.27782900	-1.17337100	-0.29673600
C	-3.98290100	-0.00040200	-0.00144100
C	-3.27866000	1.17267600	0.29564100
C	-1.88655300	1.17525400	0.29224200
H	0.53369100	-2.08739600	0.53358300
H	2.97448500	-2.10002400	0.52244100
H	2.97508400	2.09989000	-0.52315900
H	0.53426200	2.08819600	-0.53189000
H	-1.36184900	-2.08919500	-0.55437300
H	-3.82061700	-2.08145300	-0.54000400
H	-5.06832300	-0.00057700	-0.00249700
H	-3.82216200	2.08084800	0.53687300
H	-1.36351400	2.08989900	0.55462000
H	5.17002400	-0.90544400	0.21799800
H	5.17031100	0.90366900	-0.22311900
C	4.60947500	-0.00065400	-0.00194800

$E_{\parallel}$ = 0.0130 a.u.

0 2

C	0.31394000	0.00050700	0.00104900
C	1.06390500	-1.17427900	0.28401200
C	2.44397300	-1.17968200	0.28555200
C	3.20694800	-0.00006200	-0.00023400
C	2.44433900	1.18004100	-0.28482500
C	1.06427200	1.17528700	-0.28133600
C	-1.15538800	0.00018600	0.00083500
C	-1.88575300	-1.17523600	-0.29122200
C	-3.27782900	-1.17337100	-0.29673600
C	-3.98290100	-0.00040200	-0.00144100
C	-3.27866000	1.17267600	0.29564100
C	-1.88655300	1.17525400	0.29224200
H	0.53369100	-2.08739600	0.53358300
H	2.97448500	-2.10002400	0.52244100
H	2.97508400	2.09989000	-0.52315900
H	0.53426200	2.08819600	-0.53189000
H	-1.36184900	-2.08919500	-0.55437300
H	-3.82061700	-2.08145300	-0.54000400
H	-5.06832300	-0.00057700	-0.00249700
H	-3.82216200	2.08084800	0.53687300
H	-1.36351400	2.08989900	0.55462000
H	5.17002400	-0.90544400	0.21799800
H	5.17031100	0.90366900	-0.22311900

C	4.60947500	-0.00065400	-0.00194800

$E_{\parallel}$ = 0.0145 a.u.

0 2

C	0.31394000	0.00050700	0.00104900
C	1.06390500	-1.17427900	0.28401200
C	2.44397300	-1.17968200	0.28555200
C	3.20694800	-0.00006200	-0.00023400
C	2.44433900	1.18004100	-0.28482500
C	1.06427200	1.17528700	-0.28133600
C	-1.15538800	0.00018600	0.00083500
C	-1.88575300	-1.17523600	-0.29122200
C	-3.27782900	-1.17337100	-0.29673600
C	-3.98290100	-0.00040200	-0.00144100
C	-3.27866000	1.17267600	0.29564100
C	-1.88655300	1.17525400	0.29224200
H	0.53369100	-2.08739600	0.53358300
H	2.97448500	-2.10002400	0.52244100
H	2.97508400	2.09989000	-0.52315900
H	0.53426200	2.08819600	-0.53189000
H	-1.36184900	-2.08919500	-0.55437300
H	-3.82061700	-2.08145300	-0.54000400
H	-5.06832300	-0.00057700	-0.00249700

H	-3.82216200	2.08084800	0.53687300
H	-1.36351400	2.08989900	0.55462000
H	5.17002400	-0.90544400	0.21799800
H	5.17031100	0.90366900	-0.22311900
C	4.60947500	-0.00065400	-0.00194800

$E_{\parallel}$ = 0.0160 a.u.

0 2

C	0.31394000	0.00050700	0.00104900
C	1.06390500	-1.17427900	0.28401200
C	2.44397300	-1.17968200	0.28555200
C	3.20694800	-0.00006200	-0.00023400
C	2.44433900	1.18004100	-0.28482500
C	1.06427200	1.17528700	-0.28133600
C	-1.15538800	0.00018600	0.00083500
C	-1.88575300	-1.17523600	-0.29122200
C	-3.27782900	-1.17337100	-0.29673600
C	-3.98290100	-0.00040200	-0.00144100
C	-3.27866000	1.17267600	0.29564100
C	-1.88655300	1.17525400	0.29224200
H	0.53369100	-2.08739600	0.53358300
H	2.97448500	-2.10002400	0.52244100
H	2.97508400	2.09989000	-0.52315900
H	0.53426200	2.08819600	-0.53189000

H	-1.36184900	-2.08919500	-0.55437300
H	-3.82061700	-2.08145300	-0.54000400
H	-5.06832300	-0.00057700	-0.00249700
H	-3.82216200	2.08084800	0.53687300
H	-1.36351400	2.08989900	0.55462000
H	5.17002400	-0.90544400	0.21799800
H	5.17031100	0.90366900	-0.22311900
C	4.60947500	-0.00065400	-0.00194800

$E^{\perp}$ = 0.0015 a.u.

0 2

C	-0.32591700	0.00004900	-0.00046400
C	-1.06035500	-1.15533600	-0.35683000
C	-2.44342500	-1.16130700	-0.35984300
C	-3.19511500	0.00006600	0.00001600
C	-2.44328900	1.16144900	0.35956300
C	-1.06022100	1.15545700	0.35611400
C	1.15398600	-0.00004600	-0.00036800
C	1.88091200	-1.14751700	0.37287300
C	3.27593900	-1.14767400	0.37291700
C	3.98189600	-0.00006200	0.00044600
C	3.27616700	1.14755400	-0.37244600
C	1.88113900	1.14740500	-0.37322500
H	-0.52723900	-2.05062900	-0.66274500

H	-2.97822600	-2.06140200	-0.65162500
H	-2.97796300	2.06138900	0.65203500
H	-0.52702300	2.05058900	0.66233700
H	1.34829700	-2.03795400	0.69301400
H	3.81238100	-2.04294200	0.67464600
H	5.06792400	0.00001300	0.00104700
H	3.81280700	2.04299200	-0.67333900
H	1.34868700	2.03800900	-0.69318800
H	-5.15945400	-0.88694000	-0.27433700
H	-5.15935200	0.88666000	0.27646800
C	-4.59852100	-0.00000200	0.00052600

$E^{\perp}$ = 0.0030 a.u.

0 2

C	0.32591700	0.00207200	0.01966600
C	1.05722500	1.15760600	-0.34278100
C	2.44025300	1.16403400	-0.35590400
C	3.19501600	0.00285000	-0.00183800
C	2.44636600	-1.15797200	0.36603000
C	1.06324100	-1.15249100	0.37253000
C	-1.15400900	-0.00199800	0.01616300
C	-1.88566400	1.14467500	0.38243200
C	-3.28064300	1.14466400	0.36507500
C	-3.98169600	-0.00262200	-0.01762900

C	-3.27118400	-1.14976600	-0.38286800
C	-1.87625300	-1.14948800	-0.36613400
H	0.52206100	2.04903900	-0.65594600
H	2.97201900	2.06041600	-0.66377500
H	2.98383200	-2.06093700	0.64420700
H	0.53189400	-2.05080000	0.67310500
H	-1.35634900	2.03838900	0.69937200
H	-3.82111600	2.04326900	0.64971600
H	-5.06742600	0.00059300	-0.04282100
H	-3.80344800	-2.04109100	-0.70268300
H	-1.34025000	-2.03607300	-0.69094400
H	5.15647500	0.88055100	-0.32348400
H	5.16106700	-0.89237400	0.22917400
C	4.59830500	-0.00006000	-0.02406400

$E^{\perp}$ = 0.0045 a.u.

0 2

C	0.32592300	0.00315700	0.02983400
C	1.05555100	1.15832900	-0.33718900
C	2.43856800	1.16495200	-0.35554800
C	3.19486600	0.00433700	-0.00282700
C	2.44790400	-1.15570900	0.37089300
C	1.06473300	-1.15052400	0.38234000
C	-1.15404400	-0.00304100	0.02450900

C	-1.88803600	1.14273400	0.38883600
C	-3.28294500	1.14260800	0.36276300
C	-3.98141400	-0.00399700	-0.02677100
C	-3.26849700	-1.15038900	-0.38978600
C	-1.87366700	-1.15007300	-0.36411700
H	0.51921500	2.04737000	-0.65499600
H	2.96868700	2.05901600	-0.67267500
H	2.98672100	-2.05977500	0.64310800
H	0.53422400	-2.05000700	0.68119900
H	-1.36027700	2.03763900	0.70532500
H	-3.82536400	2.04242600	0.64007500
H	-5.06676100	0.00088500	-0.06491800
H	-3.79838500	-2.03915200	-0.72029600
H	-1.33570200	-2.03415100	-0.69238400
H	5.15443000	0.87688800	-0.34945000
H	5.16144600	-0.89486300	0.20661700
C	4.59801800	-0.00009800	-0.03653700

$E^{\perp}$ = 0.0060 a.u.

0 2

C	0.32593100	0.00426500	0.03999600
C	1.05380500	1.15880700	-0.33249600
C	2.43681500	1.16560200	-0.35617400
C	3.19465300	0.00584700	-0.00384500

C	2.44944400	-1.15312700	0.37668400
C	1.06621500	-1.14826000	0.39303900
C	-1.15409200	-0.00410700	0.03285000
C	-1.89040900	1.14047500	0.39616100
C	-3.28521600	1.14021700	0.36141300
C	-3.98101400	-0.00539100	-0.03593300
C	-3.26567400	-1.15072100	-0.39769200
C	-1.87098600	-1.15038200	-0.36304300
H	0.51620000	2.04518900	-0.65546900
H	2.96520400	2.05707800	-0.68315800
H	2.98957500	-2.05804700	0.64372700
H	0.53650500	-2.04867000	0.69088400
H	-1.36416500	2.03630300	0.71291100
H	-3.82953100	2.04097100	0.63221100
H	-5.06582500	0.00117200	-0.08692100
H	-3.79306300	-2.03662500	-0.73950400
H	-1.33093600	-2.03166300	-0.69531600
H	5.15202500	0.87295300	-0.37594000
H	5.16152900	-0.89711600	0.18496900
C	4.59760800	-0.00014900	-0.04902600

$E^{\perp}$ = 0.0075 a.u.

0 2

C	0.32594200	0.00542500	0.05035200

C	1.05194600	1.15905800	-0.32858000
C	2.43495000	1.16600400	-0.35776700
C	3.19437200	0.00741100	-0.00492900
C	2.45103000	-1.15016600	0.38348700
C	1.06773300	-1.14564100	0.40481600
C	-1.15415700	-0.00521700	0.04134100
C	-1.89285800	1.13784300	0.40452100
C	-3.28752600	1.13743300	0.36096300
C	-3.98048700	-0.00684200	-0.04530600
C	-3.26263900	-1.15077600	-0.40671700
C	-1.86813600	-1.15042800	-0.36286300
H	0.51294800	2.04246500	-0.65729600
H	2.96148000	2.05457100	-0.69535400
H	2.99247500	-2.05571100	0.64604900
H	0.53880800	-2.04675400	0.70234500
H	-1.36813400	2.03435300	0.72226700
H	-3.83374700	2.03886600	0.62594600
H	-5.06460100	0.00145000	-0.10924900
H	-3.78733700	-2.03347200	-0.76060400
H	-1.32582900	-2.02856800	-0.69970900
H	5.14920300	0.86866400	-0.40340200
H	5.16132800	-0.89919200	0.16382800
C	4.59706300	-0.00021800	-0.06179000

$E_{\perp}$ = 0.0090 a.u.

0 2

C	0.32594200	0.00662900	0.06097500
C	1.06933700	-1.14260000	0.41786200
C	2.45270600	-1.14673400	0.39145700
C	3.19404200	0.00905900	-0.00611200
C	2.43292700	1.16612300	-0.36045600
C	1.04993700	1.15904100	-0.32549200
C	-1.15422900	-0.00640100	0.05005000
C	-1.86508800	-1.15017400	-0.36367700
C	-3.25935300	-1.15049900	-0.41705900
C	-3.97983800	-0.00835500	-0.05498000
C	-3.28991500	1.13417400	0.36151100
C	-1.89542300	1.13475100	0.41407600
H	0.54121300	-2.04417900	0.71588400
H	2.99548100	-2.05265600	0.65034100
H	2.95740500	2.05141900	-0.70951900
H	0.50940300	2.03911900	-0.66055500
H	-1.32034200	-2.02479800	-0.70570300
H	-3.78110600	-2.02958500	-0.78391200
H	-5.06308200	0.00173200	-0.13204200
H	-3.83805000	2.03601200	0.62149600
H	-1.37225000	2.03167600	0.73366900
H	5.16089200	-0.90103800	0.14317500
H	5.14593700	0.86395200	-0.43209000

C	4.59637100	-0.00028900	-0.07494700

$E^{\perp}$ = 0.0115 a.u.

0 2

C	0.32598000	0.00893800	0.07942200
C	1.07212400	-1.13643100	0.44250000
C	2.45565400	-1.13991700	0.40726600
C	3.19326300	0.01197700	-0.00833200
C	2.42920700	1.16573300	-0.36730600
C	1.04624500	1.15852200	-0.32213600
C	-1.15441200	-0.00847200	0.06506900
C	-1.85935300	-1.14906900	-0.36717300
C	-3.25308300	-1.14939600	-0.43719200
C	-3.97837300	-0.01115800	-0.07191900
C	-3.29418600	1.12756100	0.36452000
C	-1.90008800	1.12854800	0.43267400
H	0.54533200	-2.03821300	0.74315400
H	3.00073200	-2.04592300	0.66166800
H	2.94996200	2.04462600	-0.73732200
H	0.50279400	2.03215400	-0.66919700
H	-1.30992800	-2.01683800	-0.71911200
H	-3.76933400	-2.02149500	-0.82756900
H	-5.05977400	0.00205100	-0.17124200

H	-3.84576700	2.02939700	0.61782100
H	-1.37969800	2.02558000	0.75733400
H	5.15946900	-0.90388400	0.10975700
H	5.13936700	0.85500900	-0.48246100
C	4.59483000	-0.00057900	-0.09786500

$E^{\perp}$ = 0.0130 a.u.

0 2

C	0.32598800	0.01037800	0.09089200
C	1.07401700	-1.13211400	0.45893600
C	2.45764900	-1.13511400	0.41821000
C	3.19274400	0.01390000	-0.00981800
C	2.42668200	1.16511300	-0.37283700
C	1.04376600	1.15781400	-0.32114600
C	-1.15453900	-0.00991900	0.07445800
C	-1.85562200	-1.14801300	-0.37052100
C	-3.24893100	-1.14824100	-0.45099700
C	-3.97733300	-0.01291000	-0.08252500
C	-3.29691200	1.12289200	0.36755600
C	-1.90311300	1.12410600	0.44535000
H	0.54818000	-2.03373100	0.76234500
H	3.00419400	-2.04083300	0.67095700
H	2.94488700	2.03965900	-0.75642300
H	0.49834000	2.02707400	-0.67608500

H	-1.30315500	-2.01112000	-0.72918300
H	-3.76150100	-2.01553700	-0.85655700
H	-5.05737900	0.00233900	-0.19536900
H	-3.85060600	2.02439600	0.61786900
H	-1.38453000	2.02087900	0.77418100
H	5.15833700	-0.90527500	0.09031400
H	5.13471900	0.84908800	-0.51419500
C	4.59369000	-0.00071600	-0.11220000

$E^{\perp}$ = 0.0145 a.u.

0 2

C	0.32602300	0.01206000	0.10302700
C	1.07605600	-1.12681300	0.47782200
C	2.45981200	-1.12931100	0.43126800
C	3.19205900	0.01598100	-0.01153400
C	2.42383600	1.16398000	-0.38027100
C	1.04097800	1.15667300	-0.32154600
C	-1.15471000	-0.01145600	0.08430100
C	-1.85131900	-1.14634900	-0.37562100
C	-3.24411500	-1.14651000	-0.46723000
C	-3.97601700	-0.01490700	-0.09387100
C	-3.29995000	1.11716800	0.37226500
C	-1.90651300	1.11871000	0.46026200

H	0.55118400	-2.02780600	0.78542000
H	3.00795000	-2.03429600	0.68372000
H	2.93921600	2.03338300	-0.77900800
H	0.49327400	2.02081500	-0.68547800
H	-1.29530200	-2.00397700	-0.74198600
H	-3.75251100	-2.00819000	-0.88961000
H	-5.05448800	0.00249500	-0.22063900
H	-3.85604000	2.01778100	0.62098000
H	-1.38992600	2.01473600	0.79488300
H	5.15689400	-0.90646200	0.07150600
H	5.12934300	0.84216400	-0.54830700
C	4.59226100	-0.00100100	-0.12745100

$E^{\perp}$ = 0.0160 a.u.

0 2

C	0.32607200	0.01394600	0.11574200
C	1.07831600	-1.12054400	0.49893100
C	2.46221300	-1.12249300	0.44624100
C	3.19125600	0.01824600	-0.01346900
C	2.42064100	1.16232400	-0.38948800
C	1.03786800	1.15505900	-0.32325400
C	-1.15491900	-0.01315900	0.09458300
C	-1.84649900	-1.14408700	-0.38234900
C	-3.23867500	-1.14415500	-0.48569700
C	-3.97446900	-0.01710300	-0.10586400

C	-3.30331000	1.11039400	0.37852100
C	-1.91030300	1.11232100	0.47719500
H	0.55453300	-2.02049700	0.81213000
H	3.01208500	-2.02631100	0.69968200
H	2.93287700	2.02582700	-0.80473000
H	0.48760500	2.01336900	-0.69714100
H	-1.28650900	-1.99544700	-0.75733800
H	-3.74240200	-1.99940200	-0.92632300
H	-5.05114000	0.00260900	-0.24683200
H	-3.86203800	2.00960700	0.62694000
H	-1.39595500	2.00715300	0.81910800
H	5.15520300	-0.90739800	0.05340700
H	5.12322600	0.83430600	-0.58444800
C	4.59056000	-0.00138400	-0.14350200

Optimized Coordinate of Di-radical

$E_{\parallel}$ = 0.00 a.u.

0 3

C	-0.64219400	0.11921100	-0.02910500
C	-1.26726900	-1.07686400	-0.45726500
C	-2.64117700	-1.22374600	-0.43481000
C	-3.49731900	-0.17444300	0.02617300
C	-2.85587000	1.02920800	0.45749800
C	-1.48086600	1.16520200	0.42602200
C	0.82762000	0.27151400	-0.05569700
C	1.67061300	-0.82026000	0.17844100
C	3.09131800	-0.70387900	0.15710800
C	3.64398800	0.58500500	-0.11350900
C	2.81399000	1.67225400	-0.34392600
C	1.42080500	1.52988400	-0.31832600
H	-0.65594600	-1.88758900	-0.84198100
H	-3.09055600	-2.14919700	-0.78531500
H	-3.47048800	1.84593900	0.82684300
H	-1.03335700	2.08613200	0.78764700
H	1.24110500	-1.78939900	0.41521700
H	4.72378800	0.70278200	-0.13613400
H	3.24673600	2.64569100	-0.55754000
H	0.79170000	2.38739500	-0.53337300

C	-4.89099000	-0.31766000	0.05223900
C	3.91650100	-1.81730700	0.40385200
H	3.49360600	-2.79370100	0.61462800
H	4.99733200	-1.72698200	0.39326800
H	-5.36754700	-1.23379300	-0.27994300
H	-5.53127100	0.48400700	0.40450700

$E_{\parallel}$ = 0.0015 a.u.

0 3

C	-0.64300700	0.11869900	-0.02809300
C	-1.26733100	-1.07836800	-0.45431800
C	-2.64132600	-1.22493500	-0.43281200
C	-3.49733300	-0.17447800	0.02579700
C	-2.85644400	1.02994900	0.45574400
C	-1.48140100	1.16585900	0.42463200
C	0.82667800	0.27097800	-0.05447100
C	1.67140900	-0.81990500	0.17928600
C	3.09202900	-0.70320400	0.15642700
C	3.64486100	0.58566200	-0.11392300
C	2.81382900	1.67248400	-0.34323100
C	1.42074000	1.52915400	-0.31741000
H	-0.65642500	-1.89013200	-0.83785800
H	-3.09085700	-2.15052900	-0.78236600
H	-3.47134700	1.84716900	0.82306900

H	-1.03489200	2.08779200	0.78523300
H	1.24203300	-1.78905200	0.41602500
H	4.72491600	0.70358400	-0.13724900
H	3.24512200	2.64680600	-0.55667500
H	0.79108100	2.38634200	-0.53179600
C	-4.89091700	-0.31723000	0.05069800
C	3.91753400	-1.81694000	0.40194600
H	3.49467400	-2.79386500	0.61081300
H	4.99863200	-1.72591800	0.38885800
H	-5.36745800	-1.23367900	-0.28054400
H	-5.53140300	0.48513300	0.40086000

$E_{\parallel}$ = 0.0030 a.u.

0 3

C	-0.64361500	0.11773000	-0.02634100
C	-1.26744400	-1.08202200	-0.44638900
C	-2.64138500	-1.22811500	-0.42634800
C	-3.49777300	-0.17462900	0.02512200
C	-2.85744900	1.03225000	0.44955500
C	-1.48250100	1.16781500	0.41929600
C	0.82550000	0.27008500	-0.05255200
C	1.67276900	-0.82011200	0.17843100
C	3.09323100	-0.70250000	0.15383800
C	3.64588600	0.58711900	-0.11384400

C	2.81325000	1.67360300	-0.33963000
C	1.42037200	1.52886000	-0.31346300
H	-0.65694900	-1.89631700	-0.82543000
H	-3.09106400	-2.15503600	-0.77176000
H	-3.47302600	1.85124600	0.81128700
H	-1.03740000	2.09207000	0.77585700
H	1.24446900	-1.78999400	0.41371400
H	4.72615500	0.70534900	-0.13787000
H	3.24255900	2.64938000	-0.55127300
H	0.79017000	2.38606700	-0.52569500
C	-4.89106500	-0.31658800	0.04817000
C	3.91966800	-1.81649200	0.39606500
H	3.49792000	-2.79412200	0.60360900
H	5.00087900	-1.72406300	0.38282600
H	-5.36798400	-1.23419500	-0.27891300
H	-5.53239300	0.48758100	0.39220000

$E_{\parallel}$ = 0.0045 a.u.

0 3

C	-0.64409700	0.11657700	-0.02409300
C	-1.26746400	-1.08719500	-0.43461100
C	-2.64127600	-1.23271700	-0.41644700
C	-3.49849800	-0.17490000	0.02415100

C	-2.85882800	1.03565600	0.43993700
C	-1.48405900	1.17081800	0.41093300
C	0.82410100	0.26909900	-0.04999200
C	1.67445800	-0.82065200	0.17650600
C	3.09471600	-0.70180200	0.15010800
C	3.64703000	0.58907100	-0.11323100
C	2.81244100	1.67535200	-0.33385900
C	1.41984500	1.52896900	-0.30724600
H	-0.65733100	-1.90523800	-0.80637800
H	-3.09082400	-2.16201100	-0.75524500
H	-3.47522200	1.85745800	0.79342200
H	-1.04078800	2.09844900	0.76114800
H	1.24755200	-1.79171900	0.40905800
H	4.72754500	0.70789900	-0.13806400
H	3.23957900	2.65295200	-0.54249800
H	0.78909900	2.38646900	-0.51616400
C	-4.89142100	-0.31593700	0.04478700
C	3.92249200	-1.81615100	0.38731900
H	3.50213600	-2.79502700	0.59185300
H	5.00387900	-1.72190100	0.37344200
H	-5.36852000	-1.23565500	-0.27589800
H	-5.53374200	0.49119300	0.37976000

$E_{\parallel}$ = 0.0060 a.u.

0 3

C	-0.64445400	0.11535300	-0.02128000
C	-1.26741400	-1.09384800	-0.41847600
C	-2.64099800	-1.23878900	-0.40270200
C	-3.49955800	-0.17530600	0.02276500
C	-2.86070200	1.04022100	0.42642700
C	-1.48620700	1.17497400	0.39915000
C	0.82240500	0.26806900	-0.04666300
C	1.67652600	-0.82151200	0.17331700
C	3.09645500	-0.70111500	0.14510800
C	3.64843200	0.59145800	-0.11197800
C	2.81152600	1.67771500	-0.32554200
C	1.41932600	1.52953000	-0.29838100
H	-0.65760500	-1.91690300	-0.77981000
H	-3.09014600	-2.17156800	-0.73203700
H	-3.47815800	1.86583700	0.76866900
H	-1.04534600	2.10708500	0.74050600
H	1.25140300	-1.79428800	0.40163400
H	4.72921100	0.71102700	-0.13776400
H	3.23620200	2.65754700	-0.52984400
H	0.78818600	2.38771900	-0.50272400
C	-4.89200000	-0.31535200	0.04035900
C	3.92599800	-1.81601100	0.37531700

H	3.50730400	-2.79674200	0.57451800
H	5.00757400	-1.71946600	0.36002500
H	-5.36908700	-1.23829100	-0.27104600
H	-5.53554600	0.49572200	0.36334300

$E_{\parallel}$ = 0.0075 a.u.

0 3

C	-0.64467900	0.11387500	-0.01811900
C	-1.26755500	-1.10167900	-0.39894200
C	-2.64080400	-1.24591900	-0.38582200
C	-3.50094800	-0.17575200	0.02117600
C	-2.86282500	1.04566000	0.40972900
C	-1.48871500	1.17984000	0.38445800
C	0.82050700	0.26678600	-0.04293900
C	1.67896600	-0.82284600	0.16875800
C	3.09852000	-0.70046900	0.13883200
C	3.65002100	0.59434700	-0.11011800
C	2.81038700	1.68064000	-0.31491900
C	1.41866400	1.53038600	-0.28719900
H	-0.65813600	-1.93067900	-0.74731400
H	-3.08952100	-2.18289000	-0.70334200
H	-3.48143300	1.87583700	0.73827300
H	-1.05050000	2.11720100	0.71470400

H	1.25614300	-1.79781700	0.39146400
H	4.73107000	0.71489300	-0.13678300
H	3.23237800	2.66306100	-0.51352200
H	0.78718300	2.38955200	-0.48564600
C	-4.89274000	-0.31465500	0.03538700
C	3.93029200	-1.81580100	0.36048500
H	3.51390700	-2.79875000	0.55362800
H	5.01204000	-1.71649000	0.34451700
H	-5.36998000	-1.24138400	-0.26441300
H	-5.53769700	0.50099600	0.34384000

$E_{\parallel}$ = 0.0090 a.u.

0 3

C	-0.64475300	0.11217700	-0.01498500
C	-1.26804500	-1.11030600	-0.37680900
C	-2.64085800	-1.25370100	-0.36632100
C	-3.50270100	-0.17617400	0.01952300
C	-2.86507600	1.05172200	0.39023600
C	-1.49144000	1.18513100	0.36707200
C	0.81846900	0.26523700	-0.03919600
C	1.68175100	-0.82466400	0.16274100
C	3.10087300	-0.69986000	0.13161900
C	3.65184200	0.59763200	-0.10747100
C	2.80911700	1.68399400	-0.30208900

C	1.41794000	1.53145800	-0.27394600
H	-0.65925200	-1.94603000	-0.71004700
H	-3.08912700	-2.19541000	-0.66991300
H	-3.48471300	1.88706800	0.70311600
H	-1.05604300	2.12831100	0.68420700
H	1.26171800	-1.80228200	0.37843000
H	4.73316800	0.71945700	-0.13479100
H	3.22827700	2.66931100	-0.49361600
H	0.78629800	2.39196000	-0.46520800
C	-4.89370200	-0.31383000	0.03039300
C	3.93527700	-1.81553600	0.34340100
H	3.52158700	-2.80109900	0.52912400
H	5.01720200	-1.71305900	0.32705500
H	-5.37123100	-1.24481900	-0.25567900
H	-5.54004400	0.50691000	0.32231200

$E_{\|}$ = 0.0115 a.u.

0 3

C	-0.64472800	0.10884900	-0.00918500
C	-1.26957000	-1.12180600	-0.34842200
C	-2.64172200	-1.26323700	-0.34282300
C	-3.50550900	-0.17661000	0.01704600
C	-2.86792600	1.05862900	0.36720000
C	-1.49510800	1.19064400	0.34713800

C	0.81455900	0.26193500	-0.03314100
C	1.68656400	-0.82764000	0.15683700
C	3.10482800	-0.69842100	0.12218400
C	3.65477500	0.60290700	-0.10589400
C	2.80616800	1.68840600	-0.28753900
C	1.41607900	1.53182800	-0.25731200
H	-0.66198000	-1.96578200	-0.66291100
H	-3.09010200	-2.20962500	-0.63096200
H	-3.48875200	1.89999100	0.66068600
H	-1.06340000	2.14088800	0.64779800
H	1.27112800	-1.80892500	0.36395500
H	4.73663300	0.72691700	-0.13552700
H	3.22018000	2.67780300	-0.47169000
H	0.78354200	2.39357600	-0.43896600
C	-4.89527000	-0.31173700	0.02213200
C	3.94468500	-1.81308000	0.32165300
H	3.53648600	-2.80247900	0.49945000
H	5.02691800	-1.70442900	0.30374900
H	-5.37422600	-1.24683300	-0.24854300
H	-5.54338300	0.51491000	0.29372600

$E_{\parallel}$ = 0.0130 a.u.

0 3

C	-0.64467400	0.10814000	-0.00547600

C	-1.27029100	-1.13569300	-0.30097000
C	-2.64157800	-1.27727400	-0.29852900
C	-3.50901900	-0.17769400	0.01382100
C	-2.87305200	1.07054600	0.32143200
C	-1.50103800	1.20203400	0.30539700
C	0.81178500	0.26100500	-0.02679400
C	1.69058400	-0.83117800	0.13910000
C	3.10804600	-0.69894500	0.10610700
C	3.65893400	0.60737000	-0.09576600
C	2.80639600	1.69454400	-0.25466000
C	1.41726000	1.53575100	-0.22570400
H	-0.66346200	-1.99283900	-0.57879000
H	-3.08827600	-2.23436100	-0.55176600
H	-3.49610300	1.92191600	0.57912300
H	-1.07544400	2.16394200	0.57508100
H	1.27947200	-1.81817400	0.32576600
H	4.74118400	0.73267100	-0.12461900
H	3.21717800	2.68902700	-0.41957400
H	0.78690900	2.40220100	-0.39005200
C	-4.89743200	-0.31261400	0.01487300
C	3.95121400	-1.81566200	0.28240500
H	3.54647300	-2.80995000	0.44029300
H	5.03364300	-1.70271000	0.26625700
H	-5.37601800	-1.25708200	-0.22294800
H	-5.54837200	0.52337900	0.24980700

$E_{\parallel}$ = 0.0145 a.u.

0 3

C	-0.64468200	0.10624700	-0.00196000
C	-1.27217600	-1.14488300	-0.27055000
C	-2.64287700	-1.28546400	-0.27120600
C	-3.51191400	-0.17799400	0.01139200
C	-2.87600100	1.07702300	0.29368500
C	-1.50458000	1.20747100	0.28054900
C	0.80913400	0.25880500	-0.02219800
C	1.69456200	-0.83417600	0.12889300
C	3.11103700	-0.69862300	0.09573200
C	3.66231400	0.61142100	-0.09042400
C	2.80532300	1.69863500	-0.23477700
C	1.41714400	1.53706400	-0.20566900
H	-0.66663500	-2.01006500	-0.52497100
H	-3.08937500	-2.24789100	-0.50359600
H	-3.49987400	1.93413900	0.52939700
H	-1.08247600	2.17603300	0.53059100
H	1.28740600	-1.82499000	0.30278700
H	4.74493200	0.73798300	-0.12023400
H	3.21251400	2.69673900	-0.38846700
H	0.78721300	2.40575100	-0.35846900
C	-4.89939000	-0.31151700	0.00868300
C	3.95841700	-1.81513200	0.25714400

H	3.55833800	-2.81321800	0.40309100
H	5.04099500	-1.69682400	0.24146300
H	-5.37911600	-1.26052700	-0.20905800
H	-5.55178300	0.52959700	0.22170700

$E_{\parallel}$ = 0.0160 a.u.

0 3

C	-0.68989000	-0.10505000	0.07135900
C	-1.41105100	-1.24357800	-0.36553500
C	-2.81459300	-1.25538000	-0.39471600
C	-3.57902400	-0.12465100	0.02992800
C	-2.85389000	1.00068900	0.52289200
C	-1.45848200	0.99832200	0.53946900
C	0.83313700	0.04967300	0.01500200
C	1.85627100	-0.92169600	0.20884500
C	3.27404700	-0.60381000	0.13684900
C	3.61176600	0.74128600	-0.21916100
C	2.62948500	1.68688800	-0.44575800
C	1.27347500	1.35309300	-0.34219000
H	-0.88694600	-2.11789200	-0.73981200
H	-3.34039000	-2.13264700	-0.76561200
H	-3.39881400	1.87202200	0.88129600
H	-0.96422800	1.87394200	0.94792900
H	1.56650000	-1.93716800	0.47160800

H	4.67157100	0.99429500	-0.29639300
H	2.89665400	2.70358600	-0.72919500
H	0.53259600	2.10923000	-0.57230900
C	-5.00350500	-0.08133600	-0.08801100
C	4.40022300	-1.44201700	0.36014300
H	4.28158600	-2.48843100	0.63819100
H	5.41793600	-1.08017500	0.27006600
H	-5.59700400	-0.90985700	-0.49439000
H	-5.58728000	0.79849400	0.21391700

$E^{\perp}$ = 0.0015 a.u.

0 3

C	-0.64215100	0.11732800	-0.01932200
C	-1.26562200	-1.07910500	-0.44880300
C	-2.63965100	-1.22578300	-0.43154000
C	-3.49752500	-0.17581300	0.02462800
C	-2.85760000	1.02771100	0.45846800
C	-1.48241600	1.16359200	0.43209700
C	0.82745200	0.27169400	-0.04684000
C	1.67231700	-0.81864200	0.18725700
C	3.09278600	-0.70161900	0.15782000
C	3.64329100	0.58680800	-0.11911100
C	2.81149100	1.67280300	-0.34907400
C	1.41854800	1.52969100	-0.31585300

H	-0.65352800	-1.88828000	-0.83536600
H	-3.08767700	-2.14940100	-0.78838500
H	-3.47395900	1.84688100	0.81971500
H	-1.03615600	2.08667500	0.78997300
H	1.24431100	-1.78854200	0.42391700
H	4.72283300	0.70408500	-0.15373300
H	3.24243600	2.64448100	-0.57379800
H	0.78809500	2.38485400	-0.53618900
C	-4.89164600	-0.31682900	0.03958300
C	3.91994500	-1.81513600	0.39800400
H	3.49822600	-2.79353900	0.60242300
H	5.00069900	-1.72640700	0.36994500
H	-5.36717100	-1.22980700	-0.30275800
H	-5.53343400	0.48879600	0.38037000

$E_{\perp}$ = 0.0030 a.u.

0 3

C	-0.64208000	0.11546100	-0.00972200
C	-1.26403600	-1.08096200	-0.44144800
C	-2.63816100	-1.22743000	-0.42928300
C	-3.49762900	-0.17715400	0.02322900
C	-2.85914800	1.02590900	0.46049700
C	-1.48381600	1.16166400	0.43903600

C	0.82729200	0.27183600	-0.03822400
C	1.67394000	-0.81703900	0.19607300
C	3.09417900	-0.69940100	0.15857800
C	3.64250800	0.58853100	-0.12494900
C	2.80892700	1.67321100	-0.35475100
C	1.41623500	1.52941800	-0.31390200
H	-0.65116200	-1.88824700	-0.83058100
H	-3.08499900	-2.14880400	-0.79314600
H	-3.47721500	1.84710300	0.81442000
H	-1.03861900	2.08656100	0.79379800
H	1.24745600	-1.78765800	0.43280900
H	4.72166900	0.70512400	-0.17145800
H	3.23799800	2.64298000	-0.59078200
H	0.78436600	2.38210000	-0.53965800
C	-4.89209500	-0.31598300	0.02728200
C	3.92322700	-1.81284100	0.39285200
H	3.50288100	-2.79281500	0.59280000
H	5.00359700	-1.72562100	0.34913400
H	-5.36671700	-1.22521700	-0.32596500
H	-5.53532100	0.49317200	0.35701800

$E^{\perp}$ = 0.0045 a.u.

0 3

C	-0.64203200	0.11370300	-0.00039800
C	-1.26248800	-1.08190400	-0.43644500
C	-2.63677100	-1.22806400	-0.42950300
C	-3.49758700	-0.17844500	0.02194200
C	-2.86046500	1.02310300	0.46530100
C	-1.48496400	1.15877600	0.44856300
C	0.82718200	0.27200200	-0.03008400
C	1.67546400	-0.81521400	0.20559900
C	3.09544600	-0.69703800	0.16027700
C	3.64161500	0.58993300	-0.13160100
C	2.80634100	1.67319500	-0.36218000
C	1.41390400	1.52894400	-0.31336600
H	-0.64878100	-1.88645300	-0.82984000
H	-3.08253700	-2.14627000	-0.80243300
H	-3.48004700	1.84557500	0.81382300
H	-1.04049700	2.08463500	0.80205100
H	1.25016600	-1.78625900	0.44310000
H	4.72026300	0.70561100	-0.19047600
H	3.23355400	2.64065800	-0.61054800
H	0.78050800	2.37887100	-0.54514800
C	-4.89241000	-0.31499100	0.01508000
C	3.92627700	-1.81026800	0.38995200

H	3.50701600	-2.79153600	0.58604400
H	5.00601900	-1.72470300	0.33016500
H	-5.36599000	-1.21954100	-0.35123100
H	-5.53674100	0.49702200	0.33567500

$E^{\perp}$ = 0.0060 a.u.

0 3

C	-0.64208500	0.11307500	0.00259700
C	-1.26218500	-1.08084000	-0.43849800
C	-2.63658800	-1.22681400	-0.43307800
C	-3.49746100	-0.17880600	0.02195300
C	-2.86062500	1.02103500	0.47018200
C	-1.48504200	1.15677000	0.45450200
C	0.82720600	0.27195800	-0.02751600
C	1.67592500	-0.81456400	0.20951400
C	3.09582600	-0.69616200	0.16180500
C	3.64123300	0.59010200	-0.13460700
C	2.80545000	1.67259900	-0.36713900
C	1.41306900	1.52827300	-0.31528600
H	-0.64842600	-1.88333500	-0.83597500
H	-3.08216700	-2.14287600	-0.81142100
H	-3.48059900	1.84282500	0.81976500
H	-1.04039200	2.08194800	0.80967300

H	1.25090100	-1.78546600	0.44821800
H	4.71969600	0.70544800	-0.19756000
H	3.23205300	2.63888100	-0.62102100
H	0.77905600	2.37693300	-0.55005600
C	-4.89248100	-0.31466600	0.01197500
C	3.92733100	-1.80884200	0.39209200
H	3.50834900	-2.79019500	0.58850700
H	5.00681900	-1.72368700	0.32736100
H	-5.36586700	-1.21655800	-0.36100900
H	-5.53685700	0.49738200	0.33254700

$E^{\perp}$ = 0.0075 a.u.

0 3

C	-0.64200800	0.11131900	0.01062000
C	-1.26097600	-1.07996600	-0.43881300
C	-2.63558600	-1.22554500	-0.43777300
C	-3.49724400	-0.17980500	0.02102000
C	-2.86131900	1.01701700	0.47852500
C	-1.48551200	1.15266700	0.46656200
C	0.82709900	0.27196700	-0.02076800
C	1.67716900	-0.81281800	0.21885000
C	3.09681700	-0.69391500	0.16428900
C	3.64023700	0.59108000	-0.14129200

C	2.80290000	1.67195200	-0.37633700
C	1.41075700	1.52722800	-0.31718600
H	-0.64659000	-1.87863100	-0.84301300
H	-3.08035400	-2.13737000	-0.82698500
H	-3.48232500	1.83860700	0.82705200
H	-1.04108100	2.07738800	0.82361800
H	1.25313500	-1.78376700	0.45959000
H	4.71813200	0.70556800	-0.21468600
H	3.22767200	2.63576800	-0.64221700
H	0.77508900	2.37304000	-0.55790000
C	-4.89257600	-0.31364200	0.00213000
C	3.92996000	-1.80588700	0.39306700
H	3.51193400	-2.78795600	0.58828300
H	5.00869100	-1.72214700	0.31489900
H	-5.36514300	-1.21002400	-0.38482300
H	-5.53747400	0.49961300	0.31881600

$E^{\perp}$ = 0.0090 a.u.

0 3

C	-0.64200800	0.11011900	0.01580600
C	-1.26027900	-1.07820200	-0.44217200
C	-2.63504000	-1.22337800	-0.44410500
C	-3.49699300	-0.18048800	0.02060400

C	-2.86156100	1.01292700	0.48768100
C	-1.48561200	1.14861800	0.47784400
C	0.82711100	0.27196900	-0.01649900
C	1.67795400	-0.81141500	0.22606600
C	3.09747500	-0.69223000	0.16700100
C	3.63941800	0.59147200	-0.14673800
C	2.80111000	1.67091200	-0.38497100
C	1.40912100	1.52620700	-0.32034600
H	-0.64543500	-1.87296800	-0.85337300
H	-3.07956100	-2.13106800	-0.84311600
H	-3.48319500	1.83339900	0.83799000
H	-1.04092300	2.07197200	0.83847000
H	1.25428400	-1.78204100	0.46916300
H	4.71685500	0.70516400	-0.22769200
H	3.22470700	2.63251700	-0.66049400
H	0.77220500	2.36960600	-0.56625800
C	-4.89257500	-0.31270000	-0.00421700
C	3.93175400	-1.80328700	0.39661100
H	3.51432300	-2.78564900	0.59195400
H	5.00986600	-1.72067400	0.30900900
H	-5.36473500	-1.20398200	-0.40325000
H	-5.53764300	0.50058800	0.31221500

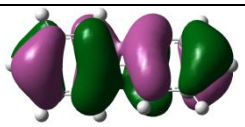
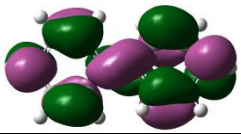
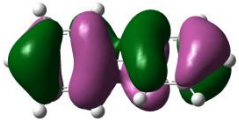
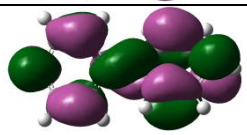
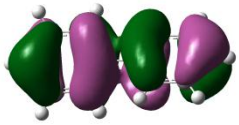
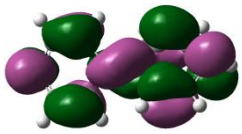
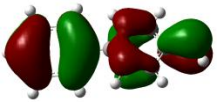
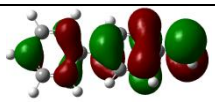
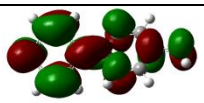
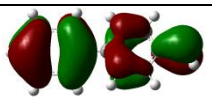
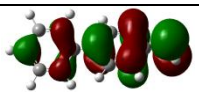
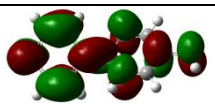
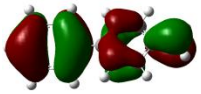
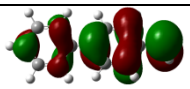
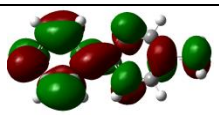
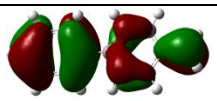
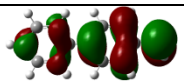
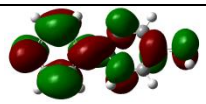
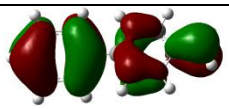
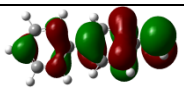
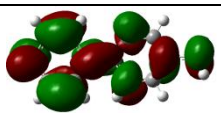
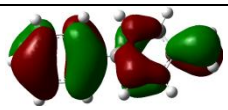
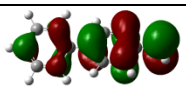
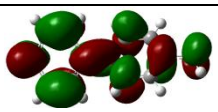
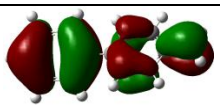
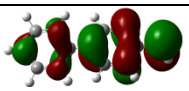
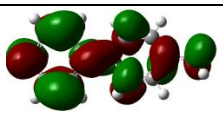
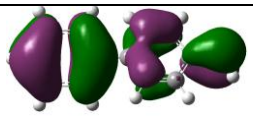
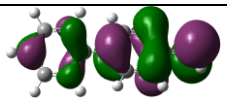
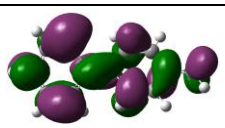
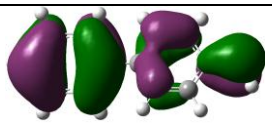
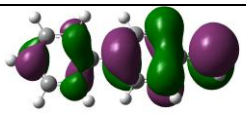
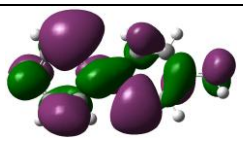
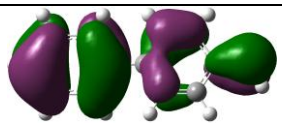
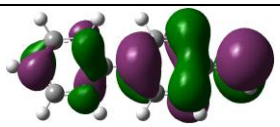
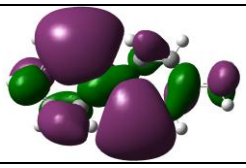
Field(a.u)	Molecular Orbital	
	HOMO	LUMO
0.00		
0.0015		
0.0030		

FIG. S1. Molecular orbital picture of the biphenyl; when, the electric field applied perpendicular to the molecular plane.

Field(a.u)	HOMO	SOMO	LUMO
0.00			
0.0015			
0.0030			
0.0045			
0.0060			
0.0075			
0.0090			
0.0115			
0.0130			
0.0145			

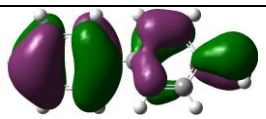
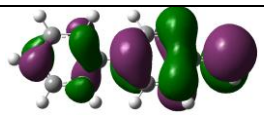
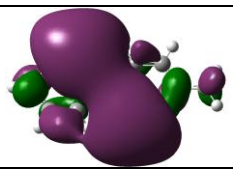
0.0160			

FIG. S2. Molecular orbital picture of the monoradical; when, the electric field applied perpendicular to the molecular plane.

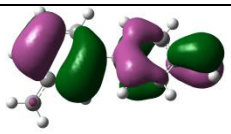
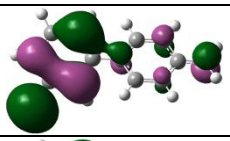
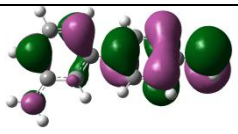
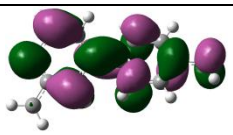
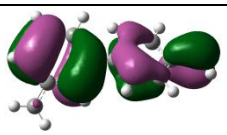
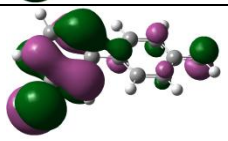
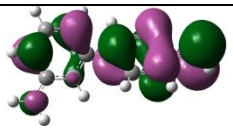
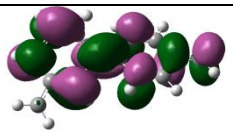
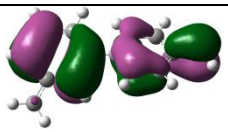
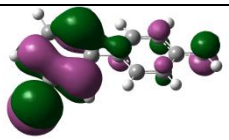
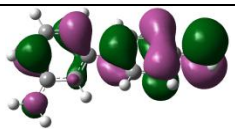
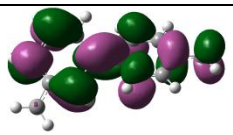
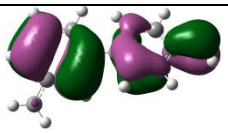
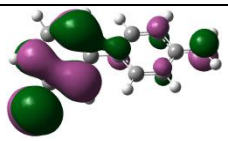
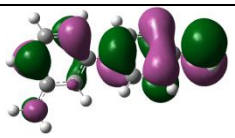
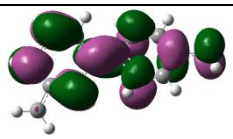
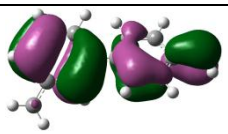
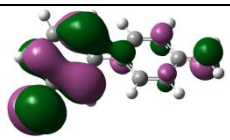
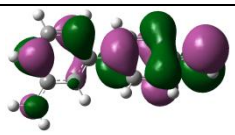
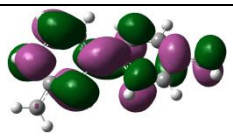
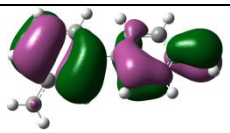
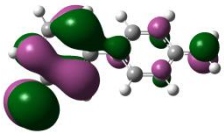
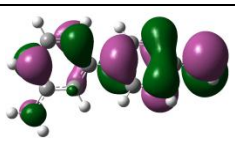
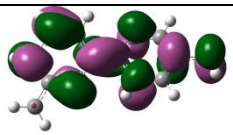
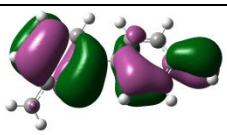
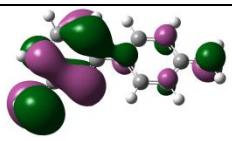
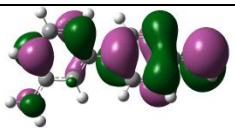
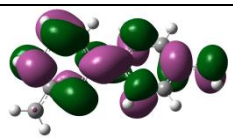
Field(a.u)	HOMO	SOMO1	SOMO2	LUMO
0.00				
0.0015				
0.0030				
0.0045				
0.0060				
0.0075				
0.0090				

FIG. S3. Molecular orbital picture of the diradical; when, the electric field applied perpendicular to the molecular plane.

TABLE S1. HOMO-LUMO Gap of the Molecules Under Different Electric Field ($E_{\perp}$).

Field×10^{-4} a.u. **($E_{\parallel}$)**	HOMO-LUMO Gap (eV)		
	Biphenyl	Monoradical	Diradical
0	5.27	4.43	4.17
15	5.27	3.09	4.17
30	5.29	4.16	4.17
45	----	4.16	4.17
60	----	4.16	4.17
75	----	4.16	4.17
90	----	4.15	4.16
115	----	4.12	----
130	----	4.10	----
145	----	4.05	----
160	----	3.98	----