

Organoboron Complexes as Thermally Activated Delayed Fluorescence (TADF) Materials for Organic Light-Emitting Diodes (OLEDs): A computational Study.

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Table of Contents

Abstract	1
Table S1: The dihedral angles of the substrates in degrees.....	2
Table S2: Spin-orbit coupling SOC	2
Table S3: The reorganization energies of the S ₁ and T ₁ states	2
Table S4: IFCT of the second excited triplet state T ₂	3
Table S5: IFCT of the third excited triplet state T ₃	3
Table S6: XYZ coordinates of the Ac-B-X complexes	4
Figure S1: UV-Vis. spectra of Ac-B-X complexes.....	30
Figure S2: NTO of the second excited triplet state T ₂	32
Figure S2: NTO of the third excited triplet state T ₃	33
References.....	34

Abstract: We report on organoboron complexes characterized by very small energy gaps (ΔE_{ST}) between their singlet and triplet excited states, which allow for highly efficient harvesting of triplet excitons into singlet states for working as thermally activated delayed fluorescence (TADF) devices. Energy gaps ranging between 0.01 and 0.06 eV with dihedral angles of *ca.* 90° were registered. The spin-orbit couplings between the lowest excited S₁ and T₁ states yielded reversed intersystem crossing rate constants (K_{RISC}) of an average of 10⁵ s⁻¹. This setup accomplished radiative decay rates of *ca.* 10⁶ s⁻¹, indicating highly potent electroluminescent devices, and hence, being suitable for application as organic light-emitting diodes.

Keywords: organoboron; TADF; RISC; NTO; radiative decay rate; DFT

Table S1. The dihedral angles of the substrates in degrees.

Compound	Angle°
Ac-B	79.63
Ac-B-F	81.28
Ac-B-CN	81.16
Ac-B-NO ₂	70.52

Table S2. Spin-orbit coupling SOC $|\langle S_1 | \hat{H}_{\text{SOC}} | T_1 \rangle|$.

Compound	$ \langle S_1 \hat{H}_{\text{SOC}} T_1 \rangle $ cm ⁻¹
Ac-B	0.38
Ac-B-F	0.66
Ac-B-CN	0.14
Ac-B-NO ₂	1.41

Reorganization energies λ :

The reorganization energy is an average of $\lambda(S_1-T_1)$ and $\lambda(T_1-S_1)$.

$\lambda(S_1-T_1)$ = S_1 energy based on optimized T_1 geometry – optimized S_1 energy;

$\lambda(T_1-S_1)$ = T_1 energy based on optimized S_1 geometry – optimized T_1 energy.

Table S3. The reorganization energies associated with S_1 and T_1 excited states.

Compound	λ eV
Ac-B	5.0×10^{-1}
Ac-B-F	1.4×10^{-1}
Ac-B-CN	5.7×10^{-4}
Ac-B-NO ₂	3.0×10^{-3}

Table S4. IFCT of the second excited triplet (T_2) state.

Compound	CT%	LE%
Ac-B	94.55	05.45
Ac-B-F	20.00	80.00
Ac-B-CN	93.26	06.38
Ac-B-NO ₂	92.04	07.96

Table S5. IFCT of the third excited triplet (T_3) state.

Compound	CT%	LE%
Ac-B	47.15	52.85
Ac-B-F	44.06	55.94
Ac-B-CN	23.01	76.99
Ac-B-NO ₂	26.52	73.48

Table S6. XYZ Coordinates of the ground S_0 and vertical and adiabatic first excited S_1 and T_1 states of the studied complexes.**Ac-B****(S_0)**

```

C 3.84893500 -1.99047900 3.04563800
C 3.15314600 -1.32978100 2.03919500
C 3.84245400 -0.74863800 0.96597900
C 5.24378200 -0.87252300 0.87799100
C 5.91545200 -1.51558300 1.91848000
C 5.23667900 -2.07099500 3.00102800
C 5.24767000 0.87253100 -0.88070000
C 3.84644400 0.96477100 -0.75940200
C 3.16057000 2.03658100 -1.34707300
H 2.08171100 2.09421600 -1.27319800
C 3.85946400 3.03672600 -2.01394600
C 5.24711400 2.98735000 -2.09364700

```

C 5.92261300 1.90681900 -1.53033300
 H 3.29889800 -2.43080800 3.87100300
 H 2.07418000 -1.25519100 2.09387100
 H 6.99469600 -1.60696100 1.87989800
 H 5.78750100 -2.57227500 3.78953300
 H 3.31214000 3.86087900 -2.45990700
 H 5.80050000 3.77069300 -2.60017700
 H 7.00181300 1.86470000 -1.62070500
 N 3.15929200 -0.03420100 -0.03961400
 C 5.93399400 -0.40736600 -0.40411100
 C 5.70930000 -1.49846300 -1.48708800
 H 6.16033700 -2.44379200 -1.16903000
 H 4.64345900 -1.66862000 -1.65840800
 H 6.16342400 -1.18924300 -2.43385700
 C 7.44611600 -0.22290000 -0.21734900
 H 7.92009600 0.06531700 -1.15873200
 H 7.67286600 0.53727900 0.53564900
 H 7.91599800 -1.16267400 0.08269600
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 C -1.09001800 -0.01598900 -0.02348700
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 H -0.89958700 1.51978300 1.47712500
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 H -5.79174100 -2.40820900 -2.68040600
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 H -1.16351700 -3.01287600 0.88020700
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 H -2.49114600 3.47156500 -2.00999000

Vertical (S_I)

C 3.84894 -1.99048 3.04564
C 3.15315 -1.32978 2.03919
C 3.84245 -0.74864 0.96598
C 5.24378 -0.87252 0.87799
C 5.91545 -1.51558 1.91848
C 5.23668 -2.07099 3.00103
C 5.24767 0.87253 -0.8807
C 3.84644 0.96477 -0.7594
C 3.16057 2.03658 -1.34707
H 2.08171 2.09422 -1.2732
C 3.85946 3.03673 -2.01395
C 5.24711 2.98735 -2.09365
C 5.92261 1.90682 -1.53033
H 3.2989 -2.43081 3.871
H 2.07418 -1.25519 2.09387
H 6.9947 -1.60696 1.8799
H 5.7875 -2.57228 3.78953
H 3.31214 3.86088 -2.45991
H 5.8005 3.77069 -2.60018
H 7.00181 1.8647 -1.62071
N 3.15929 -0.0342 -0.03961
C 5.93399 -0.40737 -0.40411
C 5.7093 -1.49846 -1.48709
H 6.16034 -2.44379 -1.16903
H 4.64346 -1.66862 -1.65841
H 6.16342 -1.18924 -2.43386
C 7.44612 -0.2229 -0.21735
H 7.9201 0.06532 -1.15873
H 7.67287 0.53728 0.53565
H 7.916 -1.16267 0.0827
C 1.03086 -0.86533 -0.88279
C 1.72848 -0.01588 -0.02503
C 1.02955 0.83804 0.83432
C -0.36047 0.84251 0.82056
C -1.09002 -0.01599 -0.02349
C -0.36057 -0.87108 -0.8684
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H 1.58762 1.49219 1.49632
H -0.89959 1.51978 1.47713
H -0.89905 -1.54915 -1.52453
B -2.661 -0.02141 -0.02198
C -5.0529 -2.4568 -1.88347
C -4.39676 -1.28923 -1.49554
C -3.42068 -1.33197 -0.46765
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C -4.80036 -3.68448 -1.26722
H -5.79174 -2.40821 -2.68041
H -3.65578 -4.66107 0.26105
C -3.43442 1.28124 0.42298
C -4.41612 1.22752 1.44525
C -5.08812 2.3874 1.8289
C -4.84671 3.61782 1.21363
C -3.89581 3.66292 0.19711
C -3.18069 2.5275 -0.19558
H -5.83113 2.33027 2.62138
H -3.70459 4.60736 -0.30804
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H -5.18549 -0.79719 1.46709
H -3.86819 -0.52887 2.6012
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 H -2.00315 -1.81359 1.84732
 H -2.46217 -3.51388 1.96801
 C -5.58611 4.85819 1.65013
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 H -5.54419 5.63821 0.8857
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 H -1.19196 2.99569 -0.91202
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 H -2.49115 3.47157 -2.00999

Vertical (T_I)

C 3.84894 -1.99048 3.04564
 C 3.15315 -1.32978 2.03919
 C 3.84245 -0.74864 0.96598
 C 5.24378 -0.87252 0.87799
 C 5.91545 -1.51558 1.91848
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 C 5.24767 0.87253 -0.8807
 C 3.84644 0.96477 -0.7594
 C 3.16057 2.03658 -1.34707
 H 2.08171 2.09422 -1.2732
 C 3.85946 3.03673 -2.01395
 C 5.24711 2.98735 -2.09365
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 H 3.2989 -2.43081 3.871
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 H 6.9947 -1.60696 1.8799
 H 5.7875 -2.57228 3.78953
 H 3.31214 3.86088 -2.45991
 H 5.8005 3.77069 -2.60018
 H 7.00181 1.8647 -1.62071
 N 3.15929 -0.0342 -0.03961
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 H 6.16034 -2.44379 -1.16903
 H 4.64346 -1.66862 -1.65841
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 H 7.9201 0.06532 -1.15873
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 H 7.916 -1.16267 0.0827
 C 1.03086 -0.86533 -0.88279
 C 1.72848 -0.01588 -0.02503
 C 1.02955 0.83804 0.83432
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 C -0.36057 -0.87108 -0.8684
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 H -0.89905 -1.54915 -1.52453
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 C -4.39676 -1.28923 -1.49554
 C -3.42068 -1.33197 -0.46765
 C -3.15589 -2.57514 0.15242
 C -3.85524 -3.71872 -0.24482
 C -4.80036 -3.68448 -1.26722
 H -5.79174 -2.40821 -2.68041
 H -3.65578 -4.66107 0.26105
 C -3.43442 1.28124 0.42298
 C -4.41612 1.22752 1.44525
 C -5.08812 2.3874 1.8289

C -4.84671 3.61782 1.21363
 C -3.89581 3.66292 0.19711
 C -3.18069 2.5275 -0.19558
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 H -3.70459 4.60736 -0.30804
 C -4.74405 0.00016 -2.20803
 H -5.18234 0.72939 -1.52145
 H -3.86077 0.46972 -2.65283
 H -5.4594 -0.18134 -3.01402
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 H -3.86819 -0.52887 2.6012
 H -5.47248 0.10918 2.9603
 C -5.52182 -4.93347 -1.70923
 H -5.07702 -5.33825 -2.62532
 H -5.47328 -5.71435 -0.94604
 H -6.57572 -4.73077 -1.92105
 C -2.14627 -2.73097 1.27296
 H -1.16352 -3.01288 0.88021
 H -2.00315 -1.81359 1.84732
 H -2.46217 -3.51388 1.96801
 C -5.58611 4.85819 1.65013
 H -5.15038 5.27029 2.56733
 H -5.54419 5.63821 0.8857
 H -6.63825 4.64258 1.85787
 C -2.16709 2.69577 -1.3107
 H -1.19196 2.99569 -0.91202
 H -2.00496 1.7794 -1.8813
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Adiabatic S_I

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 C 3.64146100 1.93312600 -3.06027500
 C 5.03346300 1.93515200 -3.17082300
 C 5.81129300 1.30585100 -2.20098400
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 H -5.71274400 5.58719900 0.89612200
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 H -2.09191500 1.80135300 -1.85002000
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Adiabatic T_1

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 C 2.99293500 -1.12292600 2.15298100
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 C 5.74662100 -1.43983600 2.13298000
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 C 3.85732200 0.82956200 -0.84614800
 C 3.23657400 1.86290500 -1.56190300
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 C 3.99751300 2.75662200 -2.30729400
 C 5.38312100 2.64019100 -2.34022400
 C 5.99405400 1.59566700 -1.64947900
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 H 1.91741700 -0.99684200 2.16557700
 H 6.82140600 -1.57998900 2.13684500
 H 5.52384400 -2.28456900 4.10056900
 H 3.49941000 3.55277100 -2.85145400
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 H 7.07206200 1.49701000 -1.70329400
 N 3.10777500 -0.05594400 -0.04699500

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 C 0.98780500 0.99422800 0.64192100
 C -0.40026100 1.03314600 0.60070000
 C -1.15213900 0.09591400 -0.14103900
 C -0.42457700 -0.88285900 -0.84797300
 H 1.51328600 -1.67673700 -1.38329400
 H 1.55126600 1.71234100 1.22929600
 H -0.92042900 1.80290100 1.16559800
 H -0.96860300 -1.63133500 -1.41695000
 B -2.72258500 0.06815000 -0.11814100
 C -4.88629900 -2.70788000 -1.80456800
 C -4.27786300 -1.47808300 -1.54908900
 C -3.44085500 -1.31836300 -0.42097500
 C -3.24022800 -2.43142200 0.42514200
 C -3.87292700 -3.64683200 0.14623700
 C -4.69723700 -3.80853700 -0.96573400
 H -5.52613000 -2.81202000 -2.67867400
 H -3.72239500 -4.48660100 0.82156600
 C -3.54142100 1.35441000 0.15422600
 C -4.76638900 1.40122600 0.96460000
 C -5.06752500 2.57209500 1.59375500
 C -4.33194600 3.80541000 1.37535600
 C -3.37253500 3.82540700 0.35116100
 C -3.05647900 2.68265400 -0.35344000
 H -5.89495600 2.59782900 2.29931000
 H -2.93694800 4.77698800 0.05397400
 C -4.51402100 -0.33348500 -2.50971600
 H -4.89534000 0.55588100 -1.99505000
 H -3.58372600 -0.04081600 -3.00976200
 H -5.23547300 -0.60648500 -3.28412700
 C -5.57765900 0.16613800 1.24265000
 H -5.95852100 -0.28347600 0.32157600
 H -4.97162200 -0.60442900 1.72877300
 H -6.42506500 0.40302000 1.89082700
 C -5.36358600 -5.12860500 -1.26781800
 H -4.93638900 -5.58812300 -2.16597700
 H -5.24366000 -5.83693300 -0.44414800
 H -6.43543700 -4.99947900 -1.44875700
 C -2.36484700 -2.33690800 1.65606900
 H -1.30379000 -2.40105400 1.39237000
 H -2.50105500 -1.38515800 2.17948200
 H -2.58558800 -3.14465400 2.35905000
 C -4.70520200 5.02599900 2.15461500
 H -4.51956100 4.87729600 3.22648200
 H -4.13999600 5.90333600 1.83261400
 H -5.77519000 5.24829600 2.05302900
 C -2.21521500 2.74857100 -1.59070800
 H -1.16415200 2.51188300 -1.38148400
 H -2.54946500 2.01091100 -2.32816100
 H -2.25628500 3.74406100 -2.04035800

Ac-B-F

S₀

C 3.76000800 -1.81613400 3.16009500
 C 3.06269800 -1.16132800 2.15102100
 C 3.74263700 -0.65695700 1.03642600
 C 5.13199400 -0.84505100 0.90774900

C 5.80879600 -1.47809100 1.95137900
 C 5.14066800 -1.96123400 3.07434500
 C 5.15467500 0.83367800 -0.91653900
 C 3.76572300 0.99605900 -0.75449600
 C 3.10706500 2.07807400 -1.34982700
 H 2.03527400 2.18936900 -1.23872100
 C 3.82450800 3.02158400 -2.07664200
 C 5.20463200 2.90325500 -2.20308900
 C 5.85192700 1.81352000 -1.62455100
 H 3.21895200 -2.19842200 4.01941500
 H 1.99026200 -1.03634700 2.23767100
 H 6.88105200 -1.61954600 1.88321600
 H 5.69383200 -2.45727300 3.86448300
 H 3.30010000 3.85628300 -2.53010500
 H 5.77432000 3.64144800 -2.75702000
 H 6.92410800 1.71923800 -1.75017100
 N 3.06225500 0.05345400 0.02464700
 C 5.79582700 -0.46021500 -0.41471900
 C 5.47738500 -1.57810500 -1.44596600
 H 5.89279200 -2.53174500 -1.10458700
 H 4.40005900 -1.69984500 -1.57643700
 H 5.91606000 -1.32944800 -2.41760200
 C 7.32060300 -0.34201200 -0.28725400
 H 7.77227700 -0.10779200 -1.25423200
 H 7.61077100 0.43015600 0.43096500
 H 7.75690200 -1.29311100 0.02729800
 C 0.93967200 -0.80868500 -0.82250500
 C 1.64792900 0.05986400 0.01266100
 C 0.88817200 0.91317100 0.82193900
 C -0.49688800 0.91371900 0.80457700
 C -1.18733600 0.01766800 -0.02864900
 C -0.44552800 -0.85069000 -0.84478000
 H -1.03474200 1.60952800 1.43932100
 H -0.94195800 -1.56463100 -1.49288500
 B -2.76473100 -0.02243300 -0.03704300
 C -5.07271800 -2.63820900 -1.74083100
 C -4.46159300 -1.42736000 -1.41875500
 C -3.47994300 -1.37923600 -0.39568700
 C -3.16597600 -2.57630800 0.28935100
 C -3.82055100 -3.76542300 -0.04506300
 C -4.76885500 -3.82163200 -1.06348900
 H -5.81510500 -2.66025200 -2.53546400
 H -3.58236400 -4.67155200 0.50787200
 C -3.55919100 1.28977700 0.32038400
 C -4.55515600 1.27550500 1.33105500
 C -5.23513600 2.44877300 1.65470600
 C -4.98865600 3.65248700 0.99031300
 C -4.02733800 3.65652700 -0.01749800
 C -3.30420000 2.50799100 -0.35202800
 H -5.98696900 2.42417000 2.44026800
 H -3.83307600 4.57888200 -0.56059900
 C -4.86403500 -0.19176900 -2.19581300
 H -5.35156800 0.54421900 -1.55069700
 H -4.00136300 0.30368800 -2.65240200
 H -5.55693900 -0.44971900 -3.00040300
 C -4.90236400 0.01404200 2.09283400
 H -5.33980300 -0.74124300 1.43446100
 H -4.02154200 -0.43943100 2.55794000
 H -5.61980600 0.22783100 2.88880000
 C -5.44243100 -5.11801000 -1.43890200
 H -5.00082900 -5.53694700 -2.35001000
 H -5.34174600 -5.86628600 -0.64875700
 H -6.50866700 -4.96919700 -1.63275300
 C -2.15552200 -2.63406600 1.41838300
 H -1.16383500 -2.91113100 1.04507800
 H -2.04243300 -1.68123400 1.93960600
 H -2.45112400 -3.38374100 2.15730200
 C -5.73432200 4.90805300 1.36818600
 H -5.31618200 5.34889900 2.28005400
 H -5.67489800 5.66241200 0.57967600

H -6.79079200 4.70082600 1.56169900
 C -2.28257300 2.63018300 -1.46579000
 H -1.31124700 2.95052800 -1.07389000
 H -2.11629900 1.69122800 -1.99762900
 H -2.60368400 3.37480700 -2.19918200
 F 1.54163700 1.75700600 1.63031100
 F 1.63396700 -1.63557400 -1.61409800

Vertical S_L :

C 3.76001 -1.81613 3.1601
 C 3.0627 -1.16133 2.15102
 C 3.74264 -0.65696 1.03643
 C 5.13199 -0.84505 0.90775
 C 5.8088 -1.47809 1.95138
 C 5.14067 -1.96123 3.07435
 C 5.15468 0.83368 -0.91654
 C 3.76572 0.99606 -0.7545
 C 3.10706 2.07807 -1.34983
 H 2.03527 2.18937 -1.23872
 C 3.82451 3.02158 -2.07664
 C 5.20463 2.90326 -2.20309
 C 5.85193 1.81352 -1.62455
 H 3.21895 -2.19842 4.01942
 H 1.99026 -1.03635 2.23767
 H 6.88105 -1.61955 1.88322
 H 5.69383 -2.45727 3.86448
 H 3.3001 3.85628 -2.53011
 H 5.77432 3.64145 -2.75702
 H 6.92411 1.71924 -1.75017
 N 3.06225 0.05345 0.02465
 C 5.79583 -0.46022 -0.41472
 C 5.47738 -1.57811 -1.44597
 H 5.89279 -2.53175 -1.10459
 H 4.40006 -1.69985 -1.57644
 H 5.91606 -1.32945 -2.4176
 C 7.3206 -0.34201 -0.28725
 H 7.77228 -0.10779 -1.25423
 H 7.61077 0.43016 0.43097
 H 7.7569 -1.29311 0.0273
 C 0.93967 -0.80869 -0.82251
 C 1.64793 0.05986 0.01266
 C 0.88817 0.91317 0.82194
 C -0.49689 0.91372 0.80458
 C -1.18734 0.01767 -0.02865
 C -0.44553 -0.85069 -0.84478
 H -1.03474 1.60953 1.43932
 H -0.94196 -1.56463 -1.49289
 B -2.76473 -0.02243 -0.03704
 C -5.07272 -2.63821 -1.74083
 C -4.46159 -1.42736 -1.41876
 C -3.47994 -1.37924 -0.39569
 C -3.16598 -2.57631 0.28935
 C -3.82055 -3.76542 -0.04506
 C -4.76886 -3.82163 -1.06349
 H -5.81511 -2.66025 -2.53546
 H -3.58236 -4.67155 0.50787
 C -3.55919 1.28978 0.32038
 C -4.55516 1.27551 1.33106
 C -5.23514 2.44877 1.65471
 C -4.98866 3.65249 0.99031
 C -4.02734 3.65653 -0.0175
 C -3.3042 2.50799 -0.35203
 H -5.98697 2.42417 2.44027
 H -3.83308 4.57888 -0.5606
 C -4.86404 -0.19177 -2.19581
 H -5.35157 0.54422 -1.5507
 H -4.00136 0.30369 -2.6524

H -5.55694 -0.44972 -3.0004
 C -4.90236 0.01404 2.09283
 H -5.3398 -0.74124 1.43446
 H -4.02154 -0.43943 2.55794
 H -5.61981 0.22783 2.8888
 C -5.44243 -5.11801 -1.4389
 H -5.00083 -5.53695 -2.35001
 H -5.34175 -5.86629 -0.64876
 H -6.50867 -4.9692 -1.63275
 C -2.15552 -2.63407 1.41838
 H -1.16384 -2.91113 1.04508
 H -2.04243 -1.68123 1.93961
 H -2.45112 -3.38374 2.1573
 C -5.73432 4.90805 1.36819
 H -5.31618 5.3489 2.28005
 H -5.6749 5.66241 0.57968
 H -6.79079 4.70083 1.5617
 C -2.28257 2.63018 -1.46579
 H -1.31125 2.95053 -1.07389
 H -2.1163 1.69123 -1.99763
 H -2.60368 3.37481 -2.19918
 F 1.54164 1.75701 1.63031
 F 1.63397 -1.63557 -1.6141

Vertical T₁

C 3.76001 -1.81613 3.1601
 C 3.0627 -1.16133 2.15102
 C 3.74264 -0.65696 1.03643
 C 5.13199 -0.84505 0.90775
 C 5.8088 -1.47809 1.95138
 C 5.14067 -1.96123 3.07435
 C 5.15468 0.83368 -0.91654
 C 3.76572 0.99606 -0.7545
 C 3.10706 2.07807 -1.34983
 H 2.03527 2.18937 -1.23872
 C 3.82451 3.02158 -2.07664
 C 5.20463 2.90326 -2.20309
 C 5.85193 1.81352 -1.62455
 H 3.21895 -2.19842 4.01942
 H 1.99026 -1.03635 2.23767
 H 6.88105 -1.61955 1.88322
 H 5.69383 -2.45727 3.86448
 H 3.3001 3.85628 -2.53011
 H 5.77432 3.64145 -2.75702
 H 6.92411 1.71924 -1.75017
 N 3.06225 0.05345 0.02465
 C 5.79583 -0.46022 -0.41472
 C 5.47738 -1.57811 -1.44597
 H 5.89279 -2.53175 -1.10459
 H 4.40006 -1.69985 -1.57644
 H 5.91606 -1.32945 -2.4176
 C 7.3206 -0.34201 -0.28725
 H 7.77228 -0.10779 -1.25423
 H 7.61077 0.43016 0.43097
 H 7.7569 -1.29311 0.0273
 C 0.93967 -0.80869 -0.82251
 C 1.64793 0.05986 0.01266
 C 0.88817 0.91317 0.82194
 C -0.49689 0.91372 0.80458
 C -1.18734 0.01767 -0.02865
 C -0.44553 -0.85069 -0.84478
 H -1.03474 1.60953 1.43932
 H -0.94196 -1.56463 -1.49289
 B -2.76473 -0.02243 -0.03704
 C -5.07272 -2.63821 -1.74083
 C -4.46159 -1.42736 -1.41876
 C -3.47994 -1.37924 -0.39569
 C -3.16598 -2.57631 0.28935
 C -3.82055 -3.76542 -0.04506

C -4.76886 -3.82163 -1.06349
 H -5.81511 -2.66025 -2.53546
 H -3.58236 -4.67155 0.50787
 C -3.55919 1.28978 0.32038
 C -4.55516 1.27551 1.33106
 C -5.23514 2.44877 1.65471
 C -4.98866 3.65249 0.99031
 C -4.02734 3.65653 -0.0175
 C -3.3042 2.50799 -0.35203
 H -5.98697 2.42417 2.44027
 H -3.83308 4.57888 -0.5606
 C -4.86404 -0.19177 -2.19581
 H -5.35157 0.54422 -1.5507
 H -4.00136 0.30369 -2.6524
 H -5.55694 -0.44972 -3.0004
 C -4.90236 0.01404 2.09283
 H -5.3398 -0.74124 1.43446
 H -4.02154 -0.43943 2.55794
 H -5.61981 0.22783 2.8888
 C -5.44243 -5.11801 -1.4389
 H -5.00083 -5.53695 -2.35001
 H -5.34175 -5.86629 -0.64876
 H -6.50867 -4.9692 -1.63275
 C -2.15552 -2.63407 1.41838
 H -1.16384 -2.91113 1.04508
 H -2.04243 -1.68123 1.93961
 H -2.45112 -3.38374 2.1573
 C -5.73432 4.90805 1.36819
 H -5.31618 5.3489 2.28005
 H -5.6749 5.66241 0.57968
 H -6.79079 4.70083 1.5617
 C -2.28257 2.63018 -1.46579
 H -1.31125 2.95053 -1.07389
 H -2.1163 1.69123 -1.99763
 H -2.60368 3.37481 -2.19918
 F 1.54164 1.75701 1.63031
 F 1.63397 -1.63557 -1.6141

Adiabatic S₁

C 4.36800800 -1.71398800 3.20043200
 C 3.49182700 -1.23031500 2.24982700
 C 3.98374700 -0.61086300 1.07745200
 C 5.37745200 -0.48201000 0.86422000
 C 6.22956900 -0.98045000 1.84688500
 C 5.74488500 -1.58849000 3.00243700
 C 4.85615800 0.64104600 -1.32529600
 C 3.47965300 0.47071000 -1.03209500
 C 2.49228200 0.92135100 -1.94287500
 H 1.44789300 0.78187400 -1.70748700
 C 2.86454400 1.53294900 -3.12300400
 C 4.21772100 1.70936400 -3.41842800
 C 5.18941700 1.26495800 -2.52422100
 H 3.98123000 -2.18688900 4.09502800
 H 2.42277900 -1.31522300 2.37841800
 H 7.30212000 -0.89356400 1.71439500
 H 6.44168700 -1.96237800 3.74405700
 H 2.10182200 1.87296400 -3.81269900
 H 4.51824300 2.19109000 -4.34189000
 H 6.23394600 1.41409400 -2.77431800
 N 3.07210100 -0.13451400 0.14728600
 C 5.95221700 0.17354500 -0.38093200
 C 6.84386700 -0.85785000 -1.12243500
 H 7.65882000 -1.19864800 -0.47959500
 H 6.25747800 -1.72833000 -1.42592200
 H 7.28885700 -0.41367400 -2.01570900
 C 6.80035900 1.40179400 0.04533400
 H 7.24974700 1.88264300 -0.82655800

H 6.18103200 2.13692500 0.56440000
 H 7.60984200 1.10009700 0.71395000
 C 0.91002200 -1.29477600 -0.18309100
 C 1.66917300 -0.25833200 0.42107600
 C 0.94185200 0.86103000 0.90397400
 C -0.41497400 0.93371400 0.83440100
 C -1.19290300 -0.11828400 0.22728800
 C -0.44821800 -1.25077600 -0.26357700
 H -0.91445100 1.79360400 1.26768700
 H -0.97084500 -2.08434300 -0.72044000
 B -2.70559100 -0.03649300 0.11086000
 C -5.10985700 -2.44214000 -1.83138500
 C -4.36858100 -1.31684800 -1.47319600
 C -3.54478700 -1.32791200 -0.31768300
 C -3.51398900 -2.51904800 0.44447100
 C -4.27955700 -3.62897000 0.06263800
 C -5.08208900 -3.61518700 -1.07275800
 H -5.72882600 -2.40503700 -2.72632800
 H -4.24645800 -4.52708400 0.67752400
 C -3.45158300 1.34442900 0.41643900
 C -4.45641800 1.43394000 1.41384900
 C -5.09962900 2.64470300 1.67060000
 C -4.79638100 3.80729400 0.95868400
 C -3.82175000 3.72133100 -0.02982500
 C -3.14909500 2.52376300 -0.30511200
 H -5.86265600 2.68333500 2.44594700
 H -3.57576200 4.60916800 -0.61038500
 C -4.43974100 -0.09854900 -2.36617200
 H -4.75049100 0.79087900 -1.81169700
 H -3.46117900 0.12374400 -2.80587200
 H -5.14444200 -0.25276300 -3.18825200
 C -4.84729400 0.22900600 2.24009300
 H -5.24459200 -0.57419000 1.61333000
 H -3.98497900 -0.18228900 2.77454100
 H -5.60507500 0.49122500 2.98353400
 C -5.89004300 -4.82239600 -1.48407400
 H -5.49459200 -5.26892700 -2.40357900
 H -5.87715200 -5.59375700 -0.70934400
 H -6.93480900 -4.55742200 -1.67696900
 C -2.67707000 -2.66340900 1.69936800
 H -1.73219700 -3.17644100 1.48455600
 H -2.41481700 -1.69879400 2.13590800
 H -3.20782500 -3.25427000 2.45270600
 C -5.49437700 5.10923500 1.26949400
 H -5.09274700 5.56400700 2.18258900
 H -5.37139800 5.83386900 0.45972100
 H -6.56675900 4.95839800 1.42789500
 C -2.11014900 2.55872700 -1.40781600
 H -1.13980300 2.89464700 -1.02300900
 H -1.94935100 1.57299800 -1.84795400
 H -2.41060900 3.25185100 -2.19982600
 F 1.67896400 1.85798200 1.45856300
 F 1.61703300 -2.33832600 -0.68785000

Adiabatic T₁

C 4.63974600 1.49348100 3.25747500
 C 3.67355100 1.07644100 2.35743500
 C 4.05509300 0.51613000 1.12690600
 C 5.41616400 0.27165000 0.83550800
 C 6.36204900 0.70195700 1.76431700
 C 5.98944600 1.32613700 2.95377300
 C 4.76994400 -0.40636100 -1.47131300
 C 3.43246700 -0.09043800 -1.13784600
 C 2.44868600 0.03098200 -2.14178900
 H 1.44381300 0.32842200 -1.87525800
 C 2.77986500 -0.19618500 -3.46682300
 C 4.09210600 -0.51836300 -3.80659300
 C 5.06951400 -0.61375000 -2.81376400

H 4.33776000 1.94404100 4.19574400
H 2.62577100 1.18955000 2.59163200
H 7.41489000 0.53459600 1.57562200
H 6.75233800 1.65364500 3.65120400
H 2.01906100 -0.10039200 -4.23243200
H 4.36256900 -0.68586400 -4.84315800
H 6.08290400 -0.85827700 -3.10646700
N 3.07387700 0.16140200 0.19010700
C 5.78375600 -0.60954600 -0.35547200
C 5.64962200 -2.08869200 0.12028200
H 6.33001600 -2.27646500 0.95568200
H 4.62946600 -2.30626000 0.44442200
H 5.90049800 -2.76661400 -0.70073300
C 7.22446300 -0.37146200 -0.83489000
H 7.48138800 -1.05560400 -1.64587100
H 7.37034400 0.65473300 -1.18194900
H 7.93974500 -0.57680100 -0.03622300
C 0.98154900 -1.11662200 0.26669500
C 1.70694300 0.09499300 0.54348600
C 0.89503300 1.27396300 0.66629800
C -0.45689800 1.24835100 0.55698800
C -1.17731700 0.01744700 0.31009300
C -0.37100100 -1.17602900 0.19838500
H -1.00427300 2.17850500 0.66469700
H -0.84984700 -2.13661900 0.04327100
B -2.69696300 -0.01270500 0.15554200
C -4.95551500 -3.04318900 -0.84645600
C -4.27628900 -1.82680300 -0.89600500
C -3.46930100 -1.40663900 0.19301600
C -3.39369900 -2.26143200 1.31784800
C -4.10134500 -3.46998400 1.34014900
C -4.88569900 -3.88298300 0.26814900
H -5.56220300 -3.34519200 -1.69831600
H -4.03839800 -4.10011100 2.22551900
C -3.48610100 1.35698600 -0.05116700
C -4.52338200 1.75395500 0.83186000
C -5.19879600 2.95862700 0.63602500
C -4.89852500 3.80916800 -0.43021500
C -3.89242000 3.41535400 -1.30679600
C -3.18517400 2.21977000 -1.13258200
H -5.98394800 3.24291100 1.33411700
H -3.64894900 4.05268900 -2.15512000
C -4.40117500 -0.98757700 -2.14782900
H -4.81433000 0.00102000 -1.93065000
H -3.42522800 -0.83086000 -2.61937200
H -5.04808400 -1.47354500 -2.88332900
C -4.90338500 0.90835800 2.02677400
H -5.15613000 -0.11378400 1.73400000
H -4.07698400 0.84175300 2.74294600
H -5.76059100 1.33671000 2.55308500
C -5.64242100 -5.18866100 0.29822700
H -5.28455400 -5.87288100 -0.47901400
H -5.53141100 -5.69227700 1.26215500
H -6.71179700 -5.03111300 0.12261600
C -2.56888600 -1.91872200 2.54152300
H -1.56528900 -2.35483000 2.47438500
H -2.43508500 -0.84251200 2.66396700
H -3.03742900 -2.31283200 3.44834000
C -5.63399400 5.11509500 -0.60784500
H -5.29673100 5.85894300 0.12308700
H -5.47236900 5.53452700 -1.60444400
H -6.71149700 4.98694900 -0.46504400
C -2.10962100 1.90556100 -2.15295300
H -1.15399100 2.36263800 -1.86994300
H -1.93035100 0.83317100 -2.24952300
H -2.38319600 2.29856500 -3.13687900
F 1.54610300 2.44601900 0.85007900
F 1.73450300 -2.23409100 0.14253600

Ac-B-CN

S₀

C 3.59312100 -1.83032700 3.15019400
C 2.92771700 -1.22018500 2.09294800
C 3.64803300 -0.68992900 1.01547900
C 5.04959900 -0.80410600 0.97097200
C 5.68902100 -1.39767100 2.06088200
C 4.98096300 -1.90668000 3.14712800
C 5.08800400 0.81670400 -0.91770800
C 3.68546600 0.90509500 -0.84572200
C 3.00078800 1.89956900 -1.55484800
H 1.91924600 1.95157800 -1.52141300
C 3.70240700 2.83894100 -2.30194900
C 5.09124600 2.79965400 -2.34055900
C 5.76398400 1.79111600 -1.65440400
H 3.01984800 -2.23209600 3.97883100
H 1.84694400 -1.15143000 2.11828800
H 6.76876000 -1.48524100 2.06123800
H 5.51062300 -2.36805800 3.97319500
H 3.15606700 3.60533900 -2.84134200
H 5.65005400 3.53449200 -2.90938600
H 6.84499800 1.75746600 -1.71523800
N 2.98455900 -0.03120300 -0.04803000
C 5.78894100 -0.39698300 -0.30474100
C 5.66856100 -1.57105300 -1.31540500
H 6.13670000 -2.47046600 -0.90315500
H 4.62418400 -1.80215200 -1.53634600
H 6.16697200 -1.31172500 -2.25471600
C 7.27938100 -0.13035600 -0.04390600
H 7.79821400 0.11332200 -0.97367900
H 7.42699500 0.68814400 0.66618600
H 7.76900100 -1.02513900 0.34696600
C 0.84961800 -0.92418000 -0.81150500
C 1.56812100 0.00228100 -0.04135200
C 0.84689700 0.93459700 0.72764800
C -0.55258000 0.93608000 0.70816800
C -1.27631600 -0.00025700 -0.04375800
C -0.55063300 -0.93142000 -0.79741500
H -1.08522400 1.67833300 1.29442200
H -1.07953800 -1.67768700 -1.38170900
B -2.85964100 -0.01469400 -0.03200100
C -5.18424000 -2.73279100 -1.53048400
C -4.57799100 -1.50108200 -1.28921700
C -3.58507700 -1.38727700 -0.28102500
C -3.26110800 -2.53815300 0.47582800
C -3.91071400 -3.74907600 0.22017000
C -4.86595300 -3.87209200 -0.78617000
H -5.93294200 -2.80736600 -2.31576000
H -3.66302800 -4.61802900 0.82570900
C -3.61595000 1.33773700 0.23069100
C -4.61094500 1.41950400 1.24065300
C -5.24385100 2.63500800 1.49509500
C -4.95183800 3.78872000 0.76254900
C -3.99652500 3.69674400 -0.24693100
C -3.32059800 2.50329900 -0.51595700
H -5.99336900 2.68496500 2.28144900
H -3.77002200 4.57691700 -0.84446700
C -4.99869700 -0.31543800 -2.13201000
H -5.50413400 0.44306100 -1.52797500
H -4.14484500 0.17359600 -2.61093700
H -5.68322800 -0.62821200 -2.92397800
C -5.00646000 0.21798900 2.07312300
H -5.47914300 -0.55341700 1.45920000
H -4.14436800 -0.24667100 2.56141600
H -5.71057900 0.50670400 2.85689600
C -5.53252600 -5.19278900 -1.07978600
H -5.11207100 -5.64606600 -1.98421900

H -5.39771500 -5.90294100 -0.26045000
 H -6.60580600 -5.06590600 -1.24840700
 C -2.24821300 -2.51921100 1.60440300
 H -1.26157700 -2.84587000 1.25778500
 H -2.12158100 -1.52993100 2.04924100
 H -2.55424100 -3.20203300 2.40147500
 C -5.64635400 5.09129300 1.07151500
 H -5.23047200 5.54608300 1.97729800
 H -5.53271000 5.81134900 0.25761800
 H -6.71543900 4.93894400 1.24547900
 C -2.31158800 2.51962300 -1.64818400
 H -1.33098000 2.86267200 -1.30011200
 H -2.16573200 1.53918000 -2.10619400
 H -2.63451100 3.20644300 -2.43504200
 C 1.54507700 1.89629700 1.53321400
 N 2.07365700 2.68901100 2.19689000
 C 1.55985200 -1.88605700 -1.60625200
 N 2.09049900 -2.68259500 -2.26405900

Vertical S₁

C 3.59312 -1.83033 3.15019
 C 2.92772 -1.22019 2.09295
 C 3.64803 -0.68993 1.01548
 C 5.0496 -0.80411 0.97097
 C 5.68902 -1.39767 2.06088
 C 4.98096 -1.90668 3.14713
 C 5.088 0.8167 -0.91771
 C 3.68547 0.9051 -0.84572
 C 3.00079 1.89957 -1.55485
 H 1.91925 1.95158 -1.52141
 C 3.70241 2.83894 -2.30195
 C 5.09125 2.79965 -2.34056
 C 5.76398 1.79112 -1.6544
 H 3.01985 -2.2321 3.97883
 H 1.84694 -1.15143 2.11829
 H 6.76876 -1.48524 2.06124
 H 5.51062 -2.36806 3.9732
 H 3.15607 3.60534 -2.84134
 H 5.65005 3.53449 -2.90939
 H 6.845 1.75747 -1.71524
 N 2.98456 -0.0312 -0.04803
 C 5.78894 -0.39698 -0.30474
 C 5.66856 -1.57105 -1.31541
 H 6.1367 -2.47047 -0.90316
 H 4.62418 -1.80215 -1.53635
 H 6.16697 -1.31173 -2.25472
 C 7.27938 -0.13036 -0.04391
 H 7.79821 0.11332 -0.97368
 H 7.42699 0.68814 0.66619
 H 7.769 -1.02514 0.34697
 C 0.84962 -0.92418 -0.81151
 C 1.56812 0.00228 -0.04135
 C 0.8469 0.9346 0.72765
 C -0.55258 0.93608 0.70817
 C -1.27632 -0.00026 -0.04376
 C -0.55063 -0.93142 -0.79742
 H -1.08522 1.67833 1.29442
 H -1.07954 -1.67769 -1.38171
 B -2.85964 -0.01469 -0.032
 C -5.18424 -2.73279 -1.53048
 C -4.57799 -1.50108 -1.28922
 C -3.58508 -1.38728 -0.28103
 C -3.26111 -2.53815 0.47583
 C -3.91071 -3.74908 0.22017
 C -4.86595 -3.87209 -0.78617
 H -5.93294 -2.80737 -2.31576
 H -3.66303 -4.61803 0.82571
 C -3.61595 1.33774 0.23069

C -4.61095 1.4195 1.24065
 C -5.24385 2.63501 1.4951
 C -4.95184 3.78872 0.76255
 C -3.99653 3.69674 -0.24693
 C -3.3206 2.5033 -0.51596
 H -5.99337 2.68497 2.28145
 H -3.77002 4.57692 -0.84447
 C -4.9987 -0.31544 -2.13201
 H -5.50413 0.44306 -1.52798
 H -4.14485 0.1736 -2.61094
 H -5.68323 -0.62821 -2.92398
 C -5.00646 0.21799 2.07312
 H -5.47914 -0.55342 1.4592
 H -4.14437 -0.24667 2.56142
 H -5.71058 0.5067 2.8569
 C -5.53253 -5.19279 -1.07979
 H -5.11207 -5.64607 -1.98422
 H -5.39771 -5.90294 -0.26045
 H -6.60581 -5.06591 -1.24841
 C -2.24821 -2.51921 1.6044
 H -1.26158 -2.84587 1.25779
 H -2.12158 -1.52993 2.04924
 H -2.55424 -3.20203 2.40148
 C -5.64635 5.09129 1.07151
 H -5.23047 5.54608 1.9773
 H -5.53271 5.81135 0.25762
 H -6.71544 4.93894 1.24548
 C -2.31159 2.51962 -1.64818
 H -1.33098 2.86267 -1.30011
 H -2.16573 1.53918 -2.10619
 H -2.63451 3.20644 -2.43504
 C 1.54508 1.8963 1.53321
 N 2.07366 2.68901 2.19689
 C 1.55985 -1.88606 -1.60625
 N 2.0905 -2.6826 -2.26406

Vertical T₁

C 3.59312 -1.83033 3.15019
 C 2.92772 -1.22019 2.09295
 C 3.64803 -0.68993 1.01548
 C 5.0496 -0.80411 0.97097
 C 5.68902 -1.39767 2.06088
 C 4.98096 -1.90668 3.14713
 C 5.088 0.8167 -0.91771
 C 3.68547 0.9051 -0.84572
 C 3.00079 1.89957 -1.55485
 H 1.91925 1.95158 -1.52141
 C 3.70241 2.83894 -2.30195
 C 5.09125 2.79965 -2.34056
 C 5.76398 1.79112 -1.6544
 H 3.01985 -2.2321 3.97883
 H 1.84694 -1.15143 2.11829
 H 6.76876 -1.48524 2.06124
 H 5.51062 -2.36806 3.9732
 H 3.15607 3.60534 -2.84134
 H 5.65005 3.53449 -2.90939
 H 6.845 1.75747 -1.71524
 N 2.98456 -0.0312 -0.04803
 C 5.78894 -0.39698 -0.30474
 C 5.66856 -1.57105 -1.31541
 H 6.1367 -2.47047 -0.90316
 H 4.62418 -1.80215 -1.53635
 H 6.16697 -1.31173 -2.25472
 C 7.27938 -0.13036 -0.04391
 H 7.79821 0.11332 -0.97368
 H 7.42699 0.68814 0.66619
 H 7.769 -1.02514 0.34697
 C 0.84962 -0.92418 -0.81151
 C 1.56812 0.00228 -0.04135

C 0.8469 0.9346 0.72765
 C -0.55258 0.93608 0.70817
 C -1.27632 -0.00026 -0.04376
 C -0.55063 -0.93142 -0.79742
 H -1.08522 1.67833 1.29442
 H -1.07954 -1.67769 -1.38171
 B -2.85964 -0.01469 -0.032
 C -5.18424 -2.73279 -1.53048
 C -4.57799 -1.50108 -1.28922
 C -3.58508 -1.38728 -0.28103
 C -3.26111 -2.53815 0.47583
 C -3.91071 -3.74908 0.22017
 C -4.86595 -3.87209 -0.78617
 H -5.93294 -2.80737 -2.31576
 H -3.66303 -4.61803 0.82571
 C -3.61595 1.33774 0.23069
 C -4.61095 1.4195 1.24065
 C -5.24385 2.63501 1.4951
 C -4.95184 3.78872 0.76255
 C -3.99653 3.69674 -0.24693
 C -3.3206 2.5033 -0.51596
 H -5.99337 2.68497 2.28145
 H -3.77002 4.57692 -0.84447
 C -4.9987 -0.31544 -2.13201
 H -5.50413 0.44306 -1.52798
 H -4.14485 0.1736 -2.61094
 H -5.68323 -0.62821 -2.92398
 C -5.00646 0.21799 2.07312
 H -5.47914 -0.55342 1.4592
 H -4.14437 -0.24667 2.56142
 H -5.71058 0.5067 2.8569
 C -5.53253 -5.19279 -1.07979
 H -5.11207 -5.64607 -1.98422
 H -5.39771 -5.90294 -0.26045
 H -6.60581 -5.06591 -1.24841
 C -2.24821 -2.51921 1.6044
 H -1.26158 -2.84587 1.25779
 H -2.12158 -1.52993 2.04924
 H -2.55424 -3.20203 2.40148
 C -5.64635 5.09129 1.07151
 H -5.23047 5.54608 1.9773
 H -5.53271 5.81135 0.25762
 H -6.71544 4.93894 1.24548
 C -2.31159 2.51962 -1.64818
 H -1.33098 2.86267 -1.30011
 H -2.16573 1.53918 -2.10619
 H -2.63451 3.20644 -2.43504
 C 1.54508 1.8963 1.53321
 N 2.07366 2.68901 2.19689
 C 1.55985 -1.88606 -1.60625
 N 2.0905 -2.6826 -2.26406

Adiabatic S₁

C 3.15937400 -1.35996500 3.31367400
 C 2.65840900 -0.82950800 2.14250000
 C 3.53968600 -0.41230900 1.11619000
 C 4.94127800 -0.53501700 1.27816000
 C 5.40696200 -1.07988800 2.47232900
 C 4.53989700 -1.48914200 3.48244500
 C 5.21567600 0.48402900 -1.00586400
 C 3.80503700 0.56898400 -1.08758300
 C 3.17995000 1.11813900 -2.23146400
 H 2.10062700 1.16255500 -2.25758700
 C 3.94276200 1.58092100 -3.28358400
 C 5.33623800 1.49955200 -3.21587100
 C 5.95100600 0.95563900 -2.09050800
 H 2.47695900 -1.67523300 4.09343900
 H 1.59318100 -0.72710100 2.00144500
 H 6.47387200 -1.19706400 2.62416300

H 4.94252300 -1.90926500 4.39701300
 H 3.45833200 2.00249500 -4.15576300
 H 5.94499900 1.85656200 -4.03872800
 H 7.03329300 0.89653300 -2.06567800
 N 3.00240200 0.11352300 -0.05178900
 C 5.92412700 -0.11913500 0.19550400
 C 6.70002600 -1.38094100 -0.27375700
 H 7.23602500 -1.83524900 0.56292300
 H 6.01364800 -2.12235400 -0.68917200
 H 7.43298800 -1.11768500 -1.03986700
 C 6.90665000 0.92985000 0.78067700
 H 7.64419900 1.22893700 0.03297700
 H 6.36853900 1.82099800 1.11163000
 H 7.45050500 0.51794000 1.63338400
 C 0.87515900 -0.98995800 -0.68870800
 C 1.57865600 0.16324600 -0.20478700
 C 0.82600400 1.27153400 0.30943500
 C -0.55570000 1.21294400 0.31186000
 C -1.28556600 0.07801900 -0.15612400
 C -0.50607600 -1.00692600 -0.66346400
 H -1.10567700 2.06217100 0.70531300
 H -1.01789400 -1.88159300 -1.05261600
 B -2.81624600 0.01189000 -0.08534300
 C -5.15099600 -2.78170300 -1.50681600
 C -4.52366000 -1.55036600 -1.32086300
 C -3.54761400 -1.38673900 -0.30433400
 C -3.25752000 -2.50571600 0.51161100
 C -3.91763100 -3.72353000 0.30568800
 C -4.86201600 -3.88708000 -0.70260300
 H -5.89091800 -2.88274200 -2.29836500
 H -3.68448400 -4.56414500 0.95652400
 C -3.64808100 1.33445600 0.22378700
 C -4.51012600 1.40659500 1.34886300
 C -5.23030300 2.57049700 1.61321400
 C -5.14883000 3.69398900 0.78633800
 C -4.31410200 3.62017800 -0.32367800
 C -3.56303700 2.47292600 -0.61058800
 H -5.87872100 2.60373800 2.48656800
 H -4.24174500 4.47608000 -0.99209200
 C -4.89688400 -0.40977400 -2.24176200
 H -5.31306600 0.43501000 -1.68644500
 H -4.02526400 -0.03547700 -2.78838800
 H -5.63580000 -0.72926300 -2.98120100
 C -4.65013900 0.24587000 2.30860800
 H -4.97541100 -0.66317800 1.79628300
 H -3.69650100 0.01722600 2.79655200
 H -5.37451800 0.47276600 3.09518800
 C -5.54458200 -5.21252400 -0.93799500
 H -5.14719400 -5.70385000 -1.83327800
 H -5.40025600 -5.89388900 -0.09549000
 H -6.62072800 -5.08384500 -1.08961800
 C -2.25108000 -2.45587900 1.64466600
 H -1.27612600 -2.84076200 1.32241300
 H -2.08615300 -1.44242000 2.01331500
 H -2.58544500 -3.07458500 2.48283900
 C -5.93508400 4.94262300 1.10410300
 H -5.55351900 5.42611100 2.01020600
 H -5.87816700 5.67070200 0.29076100
 H -6.99139600 4.71472300 1.27922200
 C -2.68332000 2.51838500 -1.84460200
 H -1.73326000 3.02291900 -1.63245000
 H -2.43530500 1.52488600 -2.22069900
 H -3.17491500 3.07445100 -2.64863600
 C 1.51474000 2.41358700 0.81612100
 N 2.12334800 3.32053500 1.22277900
 C 1.61793600 -2.10161900 -1.18792400
 N 2.27577200 -2.98434400 -1.57052300

Adiabatic T₁

C 3.00262500 -1.36763400 3.27628700

C 2.55715700 -0.82162800 2.08991900
C 3.48499000 -0.41116300 1.10297200
C 4.87642100 -0.55771600 1.31891500
C 5.28629500 -1.11689600 2.52701700
C 4.37337700 -1.51890700 3.49877600
C 5.25427900 0.46890600 -0.94644900
C 3.84937900 0.58306700 -1.08122600
C 3.28208600 1.15587300 -2.24384700
H 2.20724600 1.23073200 -2.31781800
C 4.09573800 1.60917600 -3.26179300
C 5.48311800 1.49540800 -3.14268300
C 6.04127200 0.93132900 -1.99829400
H 2.28539400 -1.67768900 4.02623900
H 1.50067000 -0.70017700 1.90309800
H 6.34476400 -1.25095400 2.71943600
H 4.73288700 -1.95079700 4.42576000
H 3.65382900 2.04842100 -4.14774900
H 6.13119900 1.84406700 -3.93864400
H 7.12005700 0.84840800 -1.93055300
N 3.00023300 0.13185000 -0.08111600
C 5.90622800 -0.15202200 0.27767100
C 6.68071400 -1.42334600 -0.16765600
H 7.18060900 -1.88690000 0.68614400
H 5.99908800 -2.15407100 -0.60901200
H 7.44367800 -1.16919700 -0.90713300
C 6.88100500 0.87931600 0.90562400
H 7.65191500 1.16966700 0.18872100
H 6.34401900 1.77759100 1.21873100
H 7.38391300 0.45548800 1.77743100
C 0.87977900 -0.95715600 -0.75866600
C 1.58332800 0.20174100 -0.28550300
C 0.82723500 1.30282900 0.24245500
C -0.55392200 1.23510100 0.26003700
C -1.28133400 0.09617600 -0.20027700
C -0.50072800 -0.98312800 -0.71775100
H -1.10510500 2.08065700 0.65979900
H -1.01132900 -1.86047800 -1.10242600
B -2.81045200 0.01808600 -0.10619300
C -5.14056400 -2.79053900 -1.50450200
C -4.51863900 -1.55561300 -1.32507500
C -3.53478200 -1.38558700 -0.31704800
C -3.23071500 -2.50218200 0.49657200
C -3.88593500 -3.72390400 0.29780800
C -4.83844300 -3.89354500 -0.70167100
H -5.88653000 -2.89654200 -2.28967800
H -3.64199100 -4.56252700 0.94730500
C -3.64780500 1.33341200 0.21849900
C -4.49193700 1.39680900 1.35756200
C -5.21745400 2.55429000 1.63535600
C -5.15933700 3.67914600 0.80839900
C -4.34193400 3.61382600 -0.31502200
C -3.58528700 2.47369200 -0.61537900
H -5.85098100 2.58120900 2.51979800
H -4.28752400 4.47121000 -0.98321800
C -4.90533900 -0.41806200 -2.24400900
H -5.31702000 0.42708600 -1.68591000
H -4.04090900 -0.04345400 -2.80174900
H -5.65189200 -0.74075800 -2.97432500
C -4.60707400 0.23340000 2.31738800
H -4.94074900 -0.67548400 1.81022900
H -3.64266900 0.00643900 2.78440600
H -5.31527900 0.45610600 3.11978100
C -5.51549400 -5.22313400 -0.92954900
H -5.11807100 -5.71653100 -1.82367700
H -5.36568100 -5.90005600 -0.08441100
H -6.59258500 -5.10007600 -1.07887800
C -2.21490200 -2.44661400 1.62108600
H -1.25136100 -2.86084900 1.30123600
H -2.02670300 -1.42878800 1.96517400
H -2.55613500 -3.03811000 2.47614500

C -5.95228800 4.92012500 1.13927400
 H -5.56949300 5.39971200 2.04688700
 H -5.90444200 5.65416700 0.33076100
 H -7.00619800 4.68383200 1.31792200
 C -2.72376100 2.52902900 -1.86171700
 H -1.77157600 3.03374600 -1.66005000
 H -2.47933400 1.53883500 -2.24859500
 H -3.22792300 3.08981400 -2.65458200
 C 1.51371200 2.44691700 0.74747700
 N 2.12026600 3.35489800 1.15498000
 C 1.62397400 -2.06585800 -1.26261900
 N 2.28296500 -2.94728700 -1.64611800

Ac-B-NO₂

S₀

C -3.76552900 0.24966700 3.63806100
 C -3.01800300 0.18296000 2.46820500
 C -3.65291700 0.14137000 1.22098000
 C -5.05445200 0.23563800 1.13471100
 C -5.77631900 0.27921800 2.32934500
 C -5.15337200 0.27667000 3.57454100
 C -4.91623900 -0.30709800 -1.29959200
 C -3.52244800 -0.42549100 -1.16463400
 C -2.75550000 -0.98689800 -2.19309500
 H -1.68373500 -1.09328600 -2.07957400
 C -3.36164500 -1.43593100 -3.35908900
 C -4.74171200 -1.34704200 -3.50203100
 C -5.49772600 -0.79022400 -2.47445200
 H -3.25432400 0.27248700 4.59439000
 H -1.93717200 0.16396000 2.53973900
 H -6.85740100 0.33656200 2.29384400
 H -5.74815600 0.31492800 4.48044800
 H -2.75047900 -1.86621000 -4.14526300
 H -5.22847700 -1.70208300 -4.40362100
 H -6.57038400 -0.71574800 -2.60554000
 N -2.90502500 0.01682700 0.02940800
 C -5.71923400 0.43429900 -0.22970100
 C -5.66819700 1.95004600 -0.56409600
 H -6.21563100 2.52129200 0.19251100
 H -4.63972200 2.31684300 -0.58900800
 H -6.12323000 2.13338600 -1.54284700
 C -7.19161400 -0.01059300 -0.21552300
 H -7.66495700 0.17888800 -1.18120200
 H -7.29154200 -1.07381300 0.01930900
 H -7.76551800 0.56569400 0.51335900
 C -0.75781500 1.07367300 -0.43721500
 C -1.49481800 0.00412200 0.08412200
 C -0.73273400 -1.05418500 0.60450100
 C 0.65571500 -1.03999500 0.61069100
 C 1.36990600 0.02748800 0.05045900
 C 0.62841000 1.08905900 -0.48387000
 H 1.18291500 -1.88492400 1.04018800
 H 1.13279400 1.94309600 -0.92339000
 B 2.95258800 0.03496000 0.01809200
 C 5.25014900 2.94148700 -1.12021100
 C 4.63865000 1.69131300 -1.05276200
 C 3.68566900 1.42454000 -0.03424100
 C 3.41004200 2.44008000 0.91068900
 C 4.06582800 3.67182800 0.82506900
 C 4.97938700 3.94827400 -0.18895900
 H 5.96642500 3.13706900 -1.91485400
 H 3.85612500 4.43261200 1.57360700
 C 3.70345200 -1.34577800 0.03456300
 C 4.70293800 -1.60131300 1.00995100
 C 5.33822900 -2.84107800 1.04363600
 C 5.04574000 -3.84695100 0.11836600

C 4.08368600 -3.58162500 -0.85314700
 C 3.40285900 -2.36175700 -0.90223100
 H 6.09085400 -3.02837100 1.80600100
 H 3.85510300 -4.34207600 -1.59642600
 C 5.00617700 0.65440200 -2.09254500
 H 5.50573600 -0.20546400 -1.63818600
 H 4.12691100 0.27136700 -2.61960800
 H 5.67754000 1.07867600 -2.84286400
 C 5.09764400 -0.56263500 2.03789800
 H 5.57012300 0.30384700 1.56726800
 H 4.23437500 -0.19091300 2.59851100
 H 5.80134800 -0.98062700 2.76170300
 C 5.65194800 5.29413000 -0.29498100
 H 5.21917900 5.88086700 -1.11254400
 H 5.53858300 5.87153800 0.62563800
 H 6.72099600 5.18706100 -0.50089700
 C 2.44471600 2.24774000 2.06455600
 H 1.47112000 2.70174400 1.84927000
 H 2.26514000 1.19772400 2.30288900
 H 2.83200200 2.72723000 2.96783000
 C 5.74624300 -5.18101500 0.18452700
 H 5.33299700 -5.79743400 0.99036700
 H 5.63513700 -5.73733300 -0.74936500
 H 6.81480300 -5.05787900 0.38316900
 C 2.38213200 -2.18060800 -2.00935800
 H 1.42187100 -2.63546200 -1.74188500
 H 2.18817000 -1.13272200 -2.24646900
 H 2.72514200 -2.66660600 -2.92686200
 N -1.38327300 -2.25129900 1.16496100
 O -2.33228200 -2.72191000 0.55978000
 O -0.89282800 -2.70530400 2.19132700
 N -1.45742800 2.25835400 -0.95644500
 O -2.25082600 2.81195400 -0.21046600
 O -1.15318800 2.62593300 -2.08243700

Vertical S₁

C -3.76553 0.24967 3.63806
 C -3.018 0.18296 2.46821
 C -3.65292 0.14137 1.22098
 C -5.05445 0.23564 1.13471
 C -5.77632 0.27922 2.32934
 C -5.15337 0.27667 3.57454
 C -4.91624 -0.3071 -1.29959
 C -3.52245 -0.42549 -1.16463
 C -2.7555 -0.9869 -2.1931
 H -1.68374 -1.09329 -2.07957
 C -3.36165 -1.43593 -3.35909
 C -4.74171 -1.34704 -3.50203
 C -5.49773 -0.79022 -2.47445
 H -3.25432 0.27249 4.59439
 H -1.93717 0.16396 2.53974
 H -6.8574 0.33656 2.29384
 H -5.74816 0.31493 4.48045
 H -2.75048 -1.86621 -4.14526
 H -5.22848 -1.70208 -4.40362
 H -6.57038 -0.71575 -2.60554
 N -2.90503 0.01683 0.02941
 C -5.71923 0.4343 -0.2297
 C -5.6682 1.95005 -0.5641
 H -6.21563 2.52129 0.19251
 H -4.63972 2.31684 -0.58901
 H -6.12323 2.13339 -1.54285
 C -7.19161 -0.01059 -0.21552
 H -7.66496 0.17889 -1.1812
 H -7.29154 -1.07381 0.01931
 H -7.76552 0.56569 0.51336
 C -0.75782 1.07367 -0.43722

C -1.49482 0.00412 0.08412
 C -0.73273 -1.05418 0.6045
 C 0.65572 -1.04 0.61069
 C 1.36991 0.02749 0.05046
 C 0.62841 1.08906 -0.48387
 H 1.18292 -1.88492 1.04019
 H 1.13279 1.9431 -0.92339
 B 2.95259 0.03496 0.01809
 C 5.25015 2.94149 -1.12021
 C 4.63865 1.69131 -1.05276
 C 3.68567 1.42454 -0.03424
 C 3.41004 2.44008 0.91069
 C 4.06583 3.67183 0.82507
 C 4.97939 3.94827 -0.18896
 H 5.96643 3.13707 -1.91485
 H 3.85613 4.43261 1.57361
 C 3.70345 -1.34578 0.03456
 C 4.70294 -1.60131 1.00995
 C 5.33823 -2.84108 1.04364
 C 5.04574 -3.84695 0.11837
 C 4.08369 -3.58163 -0.85315
 C 3.40286 -2.36176 -0.90223
 H 6.09085 -3.02837 1.806
 H 3.8551 -4.34208 -1.59643
 C 5.00618 0.6544 -2.09254
 H 5.50574 -0.20546 -1.63819
 H 4.12691 0.27137 -2.61961
 H 5.67754 1.07868 -2.84286
 C 5.09764 -0.56264 2.0379
 H 5.57012 0.30385 1.56727
 H 4.23438 -0.19091 2.59851
 H 5.80135 -0.98063 2.7617
 C 5.65195 5.29413 -0.29498
 H 5.21918 5.88087 -1.11254
 H 5.53858 5.87154 0.62564
 H 6.721 5.18706 -0.5009
 C 2.44472 2.24774 2.06456
 H 1.47112 2.70174 1.84927
 H 2.26514 1.19772 2.30289
 H 2.832 2.72723 2.96783
 C 5.74624 -5.18102 0.18453
 H 5.333 -5.79743 0.99037
 H 5.63514 -5.73733 -0.74937
 H 6.8148 -5.05788 0.38317
 C 2.38213 -2.18061 -2.00936
 H 1.42187 -2.63546 -1.74189
 H 2.18817 -1.13272 -2.24647
 H 2.72514 -2.66661 -2.92686
 N -1.38327 -2.2513 1.16496
 O -2.33228 -2.72191 0.55978
 O -0.89283 -2.7053 2.19133
 N -1.45743 2.25835 -0.95645
 O -2.25083 2.81195 -0.21047
 O -1.15319 2.62593 -2.08244

Vertical T_1

C -3.76553 0.24967 3.63806
 C -3.018 0.18296 2.46821
 C -3.65292 0.14137 1.22098
 C -5.05445 0.23564 1.13471
 C -5.77632 0.27922 2.32934
 C -5.15337 0.27667 3.57454
 C -4.91624 -0.3071 -1.29959
 C -3.52245 -0.42549 -1.16463
 C -2.7555 -0.9869 -2.1931
 H -1.68374 -1.09329 -2.07957
 C -3.36165 -1.43593 -3.35909

C -4.74171 -1.34704 -3.50203
 C -5.49773 -0.79022 -2.47445
 H -3.25432 0.27249 4.59439
 H -1.93717 0.16396 2.53974
 H -6.8574 0.33656 2.29384
 H -5.74816 0.31493 4.48045
 H -2.75048 -1.86621 -4.14526
 H -5.22848 -1.70208 -4.40362
 H -6.57038 -0.71575 -2.60554
 N -2.90503 0.01683 0.02941
 C -5.71923 0.4343 -0.2297
 C -5.6682 1.95005 -0.5641
 H -6.21563 2.52129 0.19251
 H -4.63972 2.31684 -0.58901
 H -6.12323 2.13339 -1.54285
 C -7.19161 -0.01059 -0.21552
 H -7.66496 0.17889 -1.1812
 H -7.29154 -1.07381 0.01931
 H -7.76552 0.56569 0.51336
 C -0.75782 1.07367 -0.43722
 C -1.49482 0.00412 0.08412
 C -0.73273 -1.05418 0.6045
 C 0.65572 -1.04 0.61069
 C 1.36991 0.02749 0.05046
 C 0.62841 1.08906 -0.48387
 H 1.18292 -1.88492 1.04019
 H 1.13279 1.9431 -0.92339
 B 2.95259 0.03496 0.01809
 C 5.25015 2.94149 -1.12021
 C 4.63865 1.69131 -1.05276
 C 3.68567 1.42454 -0.03424
 C 3.41004 2.44008 0.91069
 C 4.06583 3.67183 0.82507
 C 4.97939 3.94827 -0.18896
 H 5.96643 3.13707 -1.91485
 H 3.85613 4.43261 1.57361
 C 3.70345 -1.34578 0.03456
 C 4.70294 -1.60131 1.00995
 C 5.33823 -2.84108 1.04364
 C 5.04574 -3.84695 0.11837
 C 4.08369 -3.58163 -0.85315
 C 3.40286 -2.36176 -0.90223
 H 6.09085 -3.02837 1.806
 H 3.8551 -4.34208 -1.59643
 C 5.00618 0.6544 -2.09254
 H 5.50574 -0.20546 -1.63819
 H 4.12691 0.27137 -2.61961
 H 5.67754 1.07868 -2.84286
 C 5.09764 -0.56264 2.0379
 H 5.57012 0.30385 1.56727
 H 4.23438 -0.19091 2.59851
 H 5.80135 -0.98063 2.7617
 C 5.65195 5.29413 -0.29498
 H 5.21918 5.88087 -1.11254
 H 5.53858 5.87154 0.62564
 H 6.721 5.18706 -0.5009
 C 2.44472 2.24774 2.06456
 H 1.47112 2.70174 1.84927
 H 2.26514 1.19772 2.30289
 H 2.832 2.72723 2.96783
 C 5.74624 -5.18102 0.18453
 H 5.333 -5.79743 0.99037
 H 5.63514 -5.73733 -0.74937
 H 6.8148 -5.05788 0.38317
 C 2.38213 -2.18061 -2.00936
 H 1.42187 -2.63546 -1.74189
 H 2.18817 -1.13272 -2.24647
 H 2.72514 -2.66661 -2.92686
 N -1.38327 -2.2513 1.16496
 O -2.33228 -2.72191 0.55978

O -0.89283 -2.7053 2.19133
 N -1.45743 2.25835 -0.95645
 O -2.25083 2.81195 -0.21047
 O -1.15319 2.62593 -2.08244

Adiabatic S_1

C -3.44721000 1.81065700 3.16347100
 C -2.81541100 1.26151800 2.06785300
 C -3.57025400 0.64260500 1.04666100
 C -4.97883300 0.58169700 1.13152100
 C -5.58182300 1.13897200 2.25749700
 C -4.83940800 1.74710500 3.26481700
 C -4.98703000 -0.56921100 -1.10430300
 C -3.57697600 -0.48369700 -1.10472500
 C -2.82832200 -0.98353700 -2.19397000
 H -1.74985800 -0.92792200 -2.16848200
 C -3.46834000 -1.55051300 -3.27656500
 C -4.86252300 -1.63801500 -3.28925200
 C -5.59804300 -1.15518200 -2.21147000
 H -2.86003700 2.28230300 3.94217700
 H -1.73964700 1.30049100 1.98595000
 H -6.65982100 1.09122800 2.36196600
 H -5.34436800 2.16810100 4.12677000
 H -2.88511000 -1.93014500 -4.10679600
 H -5.37430000 -2.08711200 -4.13278400
 H -6.67773800 -1.24991100 -2.23408400
 N -2.91086400 0.09152900 -0.03677000
 C -5.82603200 -0.10119300 0.07196300
 C -6.90706300 0.88829700 -0.43302800
 H -7.54762300 1.21852600 0.38748000
 H -6.44395200 1.76826300 -0.88556300
 H -7.55208700 0.41544600 -1.17668200
 C -6.48838900 -1.35126700 0.71637700
 H -7.11940400 -1.86753900 -0.01170100
 H -5.72405800 -2.04428400 1.07250100
 H -7.11735600 -1.05679600 1.56047900
 C -0.72031200 1.06335400 -0.67134900
 C -1.47225900 0.06311400 -0.02506600
 C -0.78493800 -1.00814200 0.61177900
 C 0.62581700 -0.98901000 0.58870100
 C 1.36252600 0.00851400 -0.03576900
 C 0.65934500 1.05174000 -0.69153200
 H 1.11705100 -1.81852600 1.08402000
 H 1.18842000 1.84520100 -1.20350800
 B 2.93522800 -0.01740000 0.00022900
 C 5.35675700 2.73880600 -1.28200500
 C 4.70396900 1.51450600 -1.14213400
 C 3.70875300 1.35149000 -0.14525100
 C 3.42754500 2.44626500 0.70447100
 C 4.12260300 3.64956700 0.55134500
 C 5.08211700 3.82183600 -0.44341100
 H 6.10765500 2.85055500 -2.06122800
 H 3.90587000 4.47290800 1.22867500
 C 3.67506000 -1.39808100 0.17246300
 C 4.65513800 -1.57154400 1.18440800
 C 5.28045200 -2.80658000 1.34560400
 C 4.99355500 -3.89325100 0.51549300
 C 4.05405800 -3.71098900 -0.49541300
 C 3.38668300 -2.49534500 -0.67257700
 H 6.01688900 -2.92627000 2.13726700
 H 3.82778300 -4.53741600 -1.16557700
 C 5.08128500 0.38743200 -2.07982500
 H 5.56400800 -0.43293400 -1.54144500
 H 4.20818700 -0.03504000 -2.58639200
 H 5.77072000 0.73934800 -2.85132700
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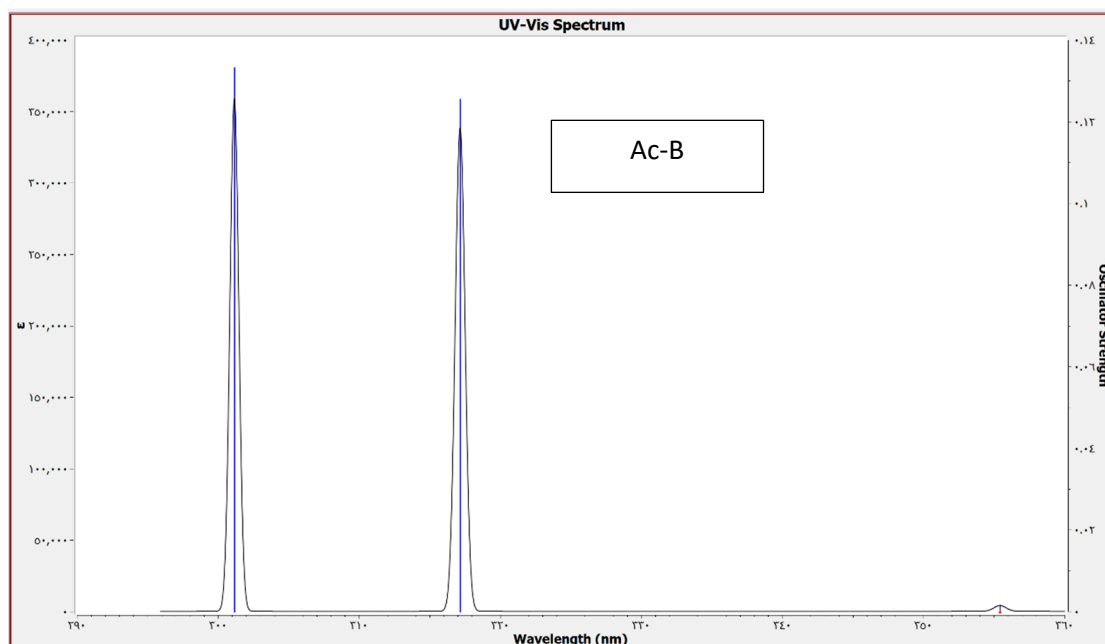
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 H 5.38558300 5.68393600 -1.48720300
 H 5.68773900 5.77945700 0.25089200
 H 6.86152000 4.99124600 -0.81486300
 C 2.40049000 2.37164800 1.81704900
 H 1.42026500 2.71508200 1.46770200
 H 2.26349500 1.36008300 2.20495600
 H 2.69432800 3.01205400 2.65339800
 C 5.67194600 -5.22375400 0.72747000
 H 5.24771500 -5.73968300 1.59580800
 H 5.55116900 -5.87876400 -0.13890900
 H 6.74281800 -5.09833100 0.91376900
 C 2.38632200 -2.41970300 -1.80977900
 H 1.40557100 -2.78879100 -1.49115200
 H 2.24159700 -1.40520600 -2.18657300
 H 2.71584200 -3.04178500 -2.64699800
 N -1.42965500 -2.08542300 1.23776300
 O -2.69714800 -2.17703800 1.14513800
 O -0.72177000 -2.93251600 1.85442900
 N -1.38070500 2.18222500 -1.36032600
 O -2.46137700 2.57644700 -0.92888400
 O -0.80505400 2.67063600 -2.32319100

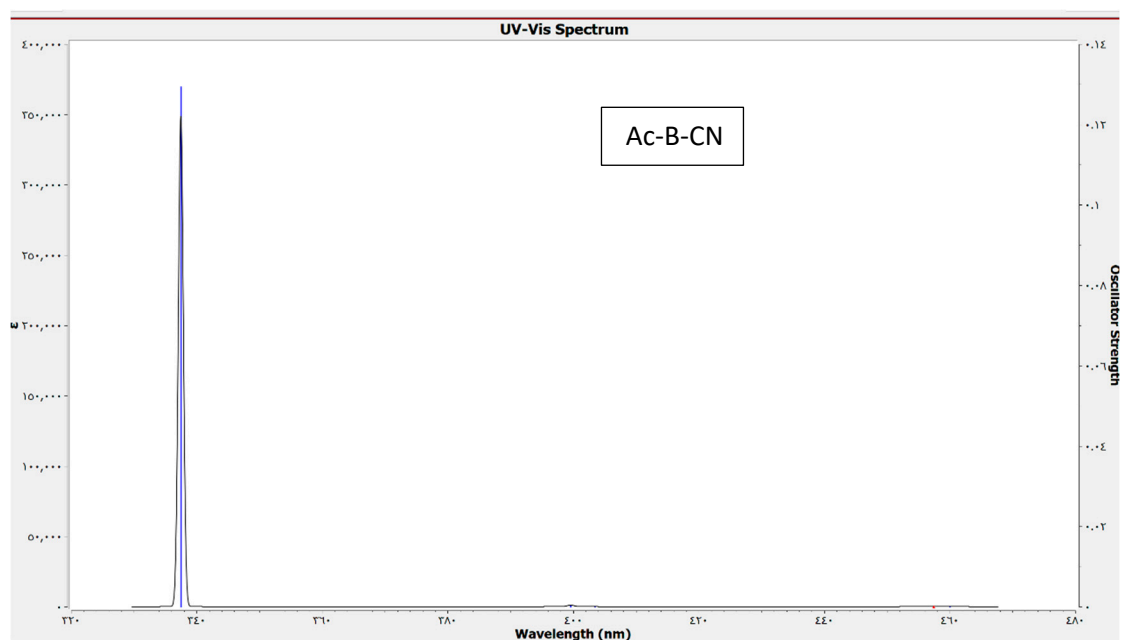
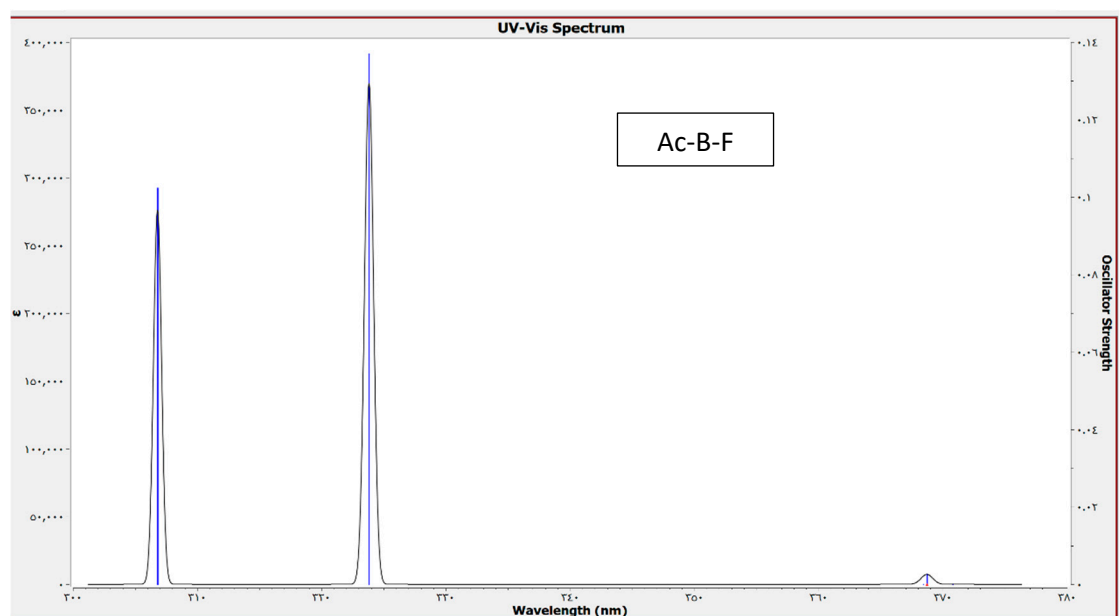
Adiabatic T_1

C -3.37785400 1.72364800 3.21396400
 C -2.77114300 1.21737400 2.08372100
 C -3.54671100 0.61754500 1.06733500
 C -4.95115100 0.53877000 1.18795100
 C -5.52811200 1.04925600 2.34951200
 C -4.76494400 1.63463900 3.35457300
 C -5.01245000 -0.50312100 -1.09941700
 C -3.60357800 -0.40978600 -1.13515200
 C -2.88546000 -0.84152300 -2.27225100
 H -1.80668300 -0.78906400 -2.28157700
 C -3.55550300 -1.34292200 -3.36981800
 C -4.94845500 -1.43791500 -3.34783400
 C -5.65322900 -1.02685000 -2.22128200
 H -2.77435300 2.18222000 3.98802400
 H -1.69930600 1.27995200 1.97113000
 H -6.60143400 0.98040200 2.48443800
 H -5.25033500 2.02020300 4.24394000
 H -2.99487300 -1.66770000 -4.23809800
 H -5.48285900 -1.83930900 -4.20131800
 H -6.73204100 -1.13157400 -2.21606400
 N -2.91042800 0.10096300 -0.04867600
 C -5.81757400 -0.12660500 0.13285400
 C -6.96494800 0.83260000 -0.27136200
 H -7.57607800 1.09820700 0.59359300
 H -6.56454200 1.75124100 -0.70671900
 H -7.62934100 0.36491400 -1.00076000
 C -6.39167500 -1.43701100 0.74296400
 H -7.03326900 -1.94543100 0.01835400
 H -5.58102000 -2.10958200 1.02909900
 H -6.99008400 -1.21169500 1.62978500
 C -0.71674600 1.06991200 -0.68534400
 C -1.47276000 0.06043000 -0.05929900
 C -0.78783200 -1.02502800 0.55284000
 C 0.62234300 -1.00894100 0.54006900
 C 1.36276200 0.00033100 -0.06101900
 C 0.66307600 1.05492700 -0.70219400
 H 1.10977800 -1.84805500 1.02299600
 H 1.19557700 1.85788200 -1.19569200
 B 2.93536600 -0.02478200 -0.01064000
 C 5.37120200 2.74288900 -1.23795600
 C 4.71365900 1.51874300 -1.11996000
 C 3.71082300 1.34516200 -0.13263700

C	3.42576200	2.42918500	0.72940700
C	4.12610100	3.63200200	0.59870200
C	5.09413300	3.81472600	-0.38599200
H	6.12808500	2.86313400	-2.01008400
H	3.90684900	4.44645800	1.28587200
C	3.67354400	-1.40708900	0.15456200
C	4.64157400	-1.59212300	1.17624400
C	5.26385600	-2.82929800	1.33163500
C	4.98601300	-3.90689100	0.48649700
C	4.05895700	-3.71299600	-0.53349200
C	3.39480800	-2.49473000	-0.70579900
H	5.99083600	-2.95816400	2.13057200
H	3.84016900	-4.53174000	-1.21546900
C	5.09415200	0.40345300	-2.07027100
H	5.57342300	-0.42425500	-1.54007200
H	4.22297300	-0.01152200	-2.58622200
H	5.78761400	0.76418700	-2.83406400
C	5.01646000	-0.47826900	2.13034100
H	5.51173200	0.34522100	1.60851600
H	4.14014800	-0.05755400	2.63273900
H	5.69377900	-0.84468000	2.90572800
C	5.81180400	5.13222400	-0.54589700
H	5.40303300	5.69774800	-1.39062300
H	5.71264700	5.75330100	0.34789000
H	6.87809100	4.98276100	-0.73965500
C	2.38833200	2.34225000	1.83144000
H	1.41302800	2.69545200	1.47797600
H	2.24346700	1.32535400	2.20219000
H	2.67695100	2.96823700	2.68046200
C	5.66145300	-5.23986600	0.69233900
H	5.23479700	-5.75980000	1.55706400
H	5.54116700	-5.88964800	-0.17799200
H	6.73223800	-5.11735200	0.88127400
C	2.40947200	-2.40630800	-1.85516000
H	1.43098500	-2.80107500	-1.56127400
H	2.25182300	-1.38498500	-2.20704400
H	2.76204100	-2.99988800	-2.70365900
N	-1.44289100	-2.11429000	1.14243600
O	-2.71223300	-2.18701000	1.03680800
O	-0.75091900	-2.98823400	1.73861100
N	-1.37370800	2.20833800	-1.34398100
O	-2.44069000	2.60888400	-0.88555800
O	-0.80786200	2.70489500	-2.30853600

Figure S1. UV-Vis. spectra of the studied complexes.





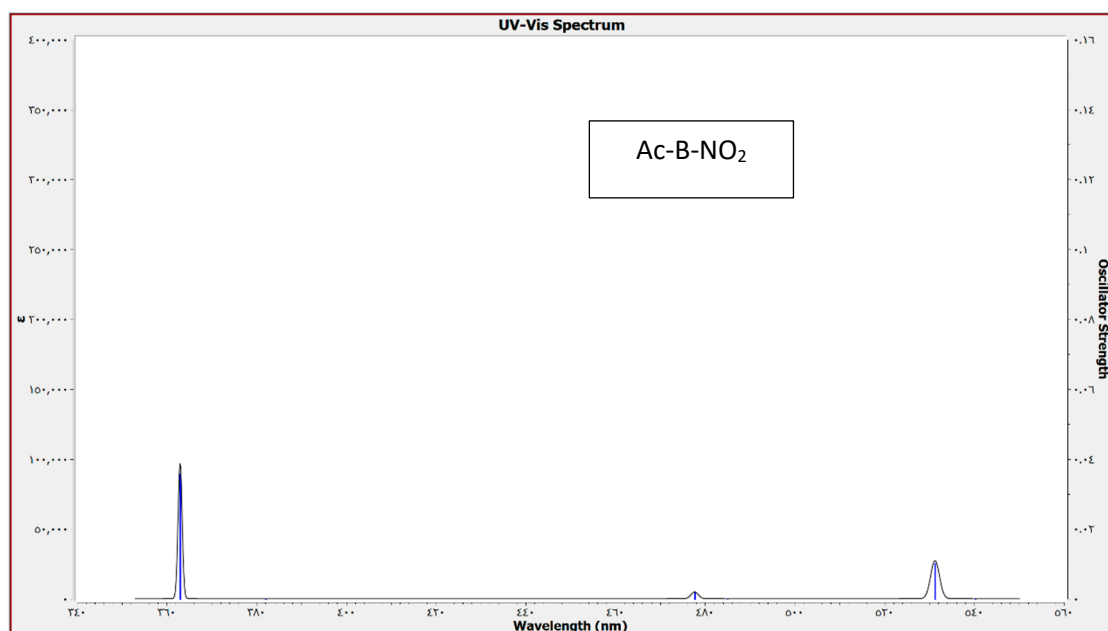
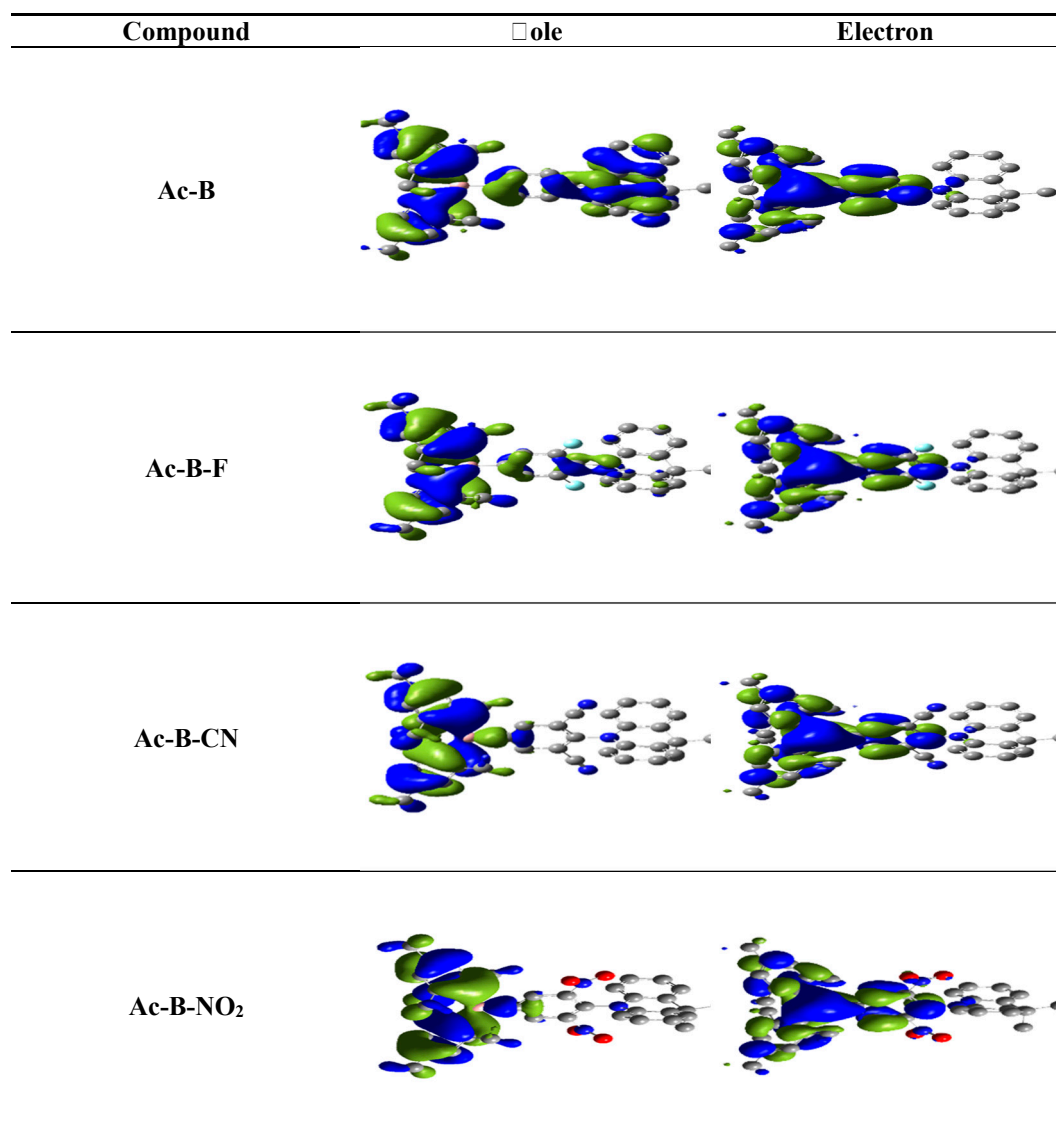


Figure S2. NTO of the second excited triplet state (T_2).

Compound	hole	Electron
Ac-B		
Ac-B-F		
Ac-B-CN		
Ac-B-NO ₂		

Figure S3. NTO of the third excited triplet state (T_3).



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