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Modelling absorption and emission of a meso-aniline-BODIPY based dye with molecular mechanics†

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1 Supporting Information

1.1 Basis set dependence

Table 1 Gas phase excitation energies (in eV) to the locally excited (LE) state and the charge transfer (CT) state for N,N-dimethylaniline-BODIPY and the locally excited (LE) state for the BODIPY core calculated with CC2.

	BODIPY core	Aniline-BODIPY	
	LE	LE	CT
cc-pVTZ	2.90	2.79	3.14
aug-cc-pVTZ	2.87	2.78	3.11

Table 2 Absorption energies using the ωB97X-D functional with continuum solvation models for ethanol (in eV) to the locally excited (LE) and charge transfer (CT) state for N,N-dimethylaniline-BODIPY.

	LE/def2-SVP	LE/cc-pVTZ	CT/def2-SVP	CT/cc-pVTZ
LR-PCM	2.94	2.92	3.19	3.22
cLR-PCM	3.06	3.04	2.89	2.92
SS-PCM	3.09	3.06	2.12	2.17

1.2 PCM results

1.3 Calculation of the shift term

The MM forcefields for the ground, LE and CT states return absolute values of the potential energies for given structures that are not meaningful. In order to obtain spectra, energy differences for a given structure must be corrected by adding a constant shift term: $\Delta E = V_{\text{excited}}(R) - V_{\text{ground}}(R) + \lambda$. As described in the text, λ was obtained both by fitting to the experimental spectrum, and by comparison to EOM-CCSD gas-phase calculations.

1.4 Force field parametrization

For the BODIPY molecule, the boron was modeled loosely on a quaternary carbon (84/13), but with a new class and type so as to get correct bond lengths and angles. The fluorine atoms were modeled as Alkyl Fluoride (786/1) and the two rings as pyrroles with alkane groups attached. The carbon in the mesoposition and the aniline carbon bonded with this atom are based on a Biphenyl C1 (460/86). The rest of the aromatic ring are Aromatic C atoms (90/48), except for the carbon connected with the nitrogen, N-DiMe Aniline C-NR2 (748/48). The nitrogen is modeled on Amine R3N (732/44) and the methyl groups are again alkanes. We adjusted those types and classes in order to be able to adjust the bond length parameter for differing bonds separately.

Table 3 Absorption energies using ωB97X-D/def2-SVP with continuum solvation models for ethanol, THF and toluene (in eV) to the locally excited (LE) and charge transfer (CT) state for N,N-dimethylaniline-BODIPY. cLE and cCT represent corrected energies for LE and CT respectively.

	LE	cLE	CT	cCT
ethanol				
LR-PCM	2.94	2.79	3.19	3.37
cLR-PCM	3.06	2.91	2.89	3.07
SS-PCM	3.09	2.94	2.12	2.30
THF				
LR-PCM	2.93	2.78	3.25	3.43
cLR-PCM	3.06	2.91	2.94	3.12
SS-PCM	3.08	2.93	2.18	2.36
toluene				
LR-PCM	2.90	2.75	3.40	3.58
cLR-PCM	3.06	2.91	3.11	3.29
SS-PCM	3.06	2.91	2.38	2.56

1.5 Example of input files

Gaussian input file for the calculation of charges

%mem=50GB
%chk=LE.chk
#n int=ultrafine TD=(root=2) b3lyp/6-31+G(d,p) scrf(solvent=ethanol,smd) pop=(ESP) iop(6/42=100) density=current geom(check) guess(read)

title

0 1

Molpro input file for EOM-CCSD calculations

memory,5000,m
basis=cc-pVDZ
geometry=bodipy.xyz
hf

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gprint,orbital
put,molden,bodipy.molden
ccsd
eom,1.3,1.4

Molpro input file for LCC2 calculations
memory,5000,m
gdirect
symmetry,nosym;orient,noorient
basis={default,cc-pVTZ
set,jkfit
default,cc-pVTZ/JKFIT
set,mp2fit
default,cc-pVTZ/MP2FIT
}
geometry=bodipy.xyz
hf
{lt-df-lcc2
eom,-5.1
eomprint,popul=-1,loceom=-1}

Gaussian input file for LR-PCM and SS-PCM
%chk=01-bodipy.chk
%mem=30GB
wb97xd/cc-pVTZ Opt SCRF=(Solvent=Ethanol)

ground state

0 1

–link1–
%oldchk=01-bodipy.chk
%chk=02-bodipy.chk
%mem=30GB
wb97xd/cc-pVTZ TD=NStates=6 SCRF=(Solvent=Ethanol) Geom=Check Guess=Read

linear response vertical excited states

0 1

–link1–
%oldchk=01-bodipy.chk
%chk=03-bodipy.chk
%mem=30GB
wb97xd/cc-pVTZ SCRF=(Solvent=Ethanol,Read) Geom=Check Guess=Read

prepare for state-specific non-eq solvation by saving the solvent reaction field from the ground state

0 1

NonEq=write

–link1–
%chk=03-bodipy.chk
%mem=30GB
wb97xd/cc-pVTZ TD(NStates=6,Root=1) Geom=Check Guess=Read SCRF=(Solvent=Ethanol,ExternalIteration,Read)

read non-eq solvation from ground state and compute energy of the first excited with the state-specific method

0 1

NonEq=read

Gaussian input file for cLR-PCM
%oldchk=01-bodipy.chk
%chk=021-bodipy.chk
%mem=30GB
wb97xd/cc-pVTZ TD=(NStates=6,Root=1,noneq) SCRF=(pisalr,Solvent=Ethanol) IOP(10/74=10) Geom=Check Guess=Read

linear response vertical excited states

0 1

Parameters in ethanol
Ground state (GS)

atom 907 120 B "Bodipy Boron atom" 5 10.811 4
atom 908 1 F "Bodipy Fluoride B-F" 9 18.998 1
atom 909 57 N "BODIPY N" 7 14.007 3
atom 910 84 C "Bodipy C2" 6 12.011 3
atom 911 87 C "Bodipy C3" 6 12.011 3
atom 912 87 C "Bodipy C4" 6 12.011 3
atom 913 121 C "Bodipy C5" 6 12.011 3
atom 914 86 C "Bodipy C6" 6 12.011 3
atom 915 86 C "AnilineB C" 6 12.011 3
atom 916 49 H "Bodipy HC" 1 1.008 1
atom 917 48 CA "Aromatic C under" 6 12.011 3
atom 919 44 NT "Amine R3N" 7 14.007 3
atom 920 13 CT "Amine CH3-NR2" 6 12.011 4
atom 921 48 CA "Aromatic C up" 6 12.011 3
atom 922 49 HA "Aromatic H-C up" 1 1.008 1
atom 923 49 HA "Aromatic H-C under" 1 1.008 1
atom 924 46 HC "Alkane H-C-N1" 1 1.008 1
atom 925 46 HC "Alkane H-C Bod up1" 1 1.008 1
atom 926 46 HC "Alkane H-C Bod under" 1 1.008 1
atom 927 46 HC "Alkane H-C-N2" 1 1.008 1
atom 928 46 HC "Alkane H-C Bod up2" 1 1.008 1
atom 929 13 CT "Alkane CH3-" 6 12.011 4
atom 930 13 CT "Alkane CH3-" 6 12.011 4

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charge 914 0.076
charge 915 0.043
charge 916 0.230
charge 917 0.012
charge 919 0.008
charge 920 -0.249
charge 921 -0.369
charge 922 0.181
charge 923 0.091
charge 924 0.102
charge 925 0.070
charge 926 0.154
charge 929 -0.218
charge 930 -0.499
charge 748 0.199

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bond 57 120 300. 1.5572
bond 86 86 385. 1.4936
bond 121 86 385. 1.4052
bond 121 57 385. 1.4002
bond 121 87 546. 1.4351
bond 84 87 546. 1.4096
bond 87 87 469. 1.3904
bond 57 84 427. 1.3469
bond 84 13 317. 1.4942
bond 87 13 317. 1.5007

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angle 1 120 57 80. 110.
angle 57 120 57 80. 106.
angle 84 57 120 30. 125.
angle 87 84 87 0. 106.
angle 87 87 13 63. 125.
angle 86 121 87 70. 132.
angle 87 121 57 70. 108.
angle 121 57 120 30. 126.
angle 121 86 121 63. 121.
angle 121 86 86 63. 120.
angle 57 121 86 70. 120.
angle 121 57 84 70. 109.
angle 121 87 87 70. 106.
angle 13 87 121 70. 130.

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torsion 84 87 87 49 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 49 87 87 13 0.000 0.0 1 0.000 0.0 1 0.000 0.0 3
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torsion 121 87 87 84 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 57 121 86 86 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
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torsion 87 121 86 121 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
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torsion 86 121 87 87 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 86 121 87 13 0.000 0.0 1 0.000 0.0 1 0.000 0.0 3
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torsion 57 121 87 13 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 121 57 120 1 0.000 0.0 1 1.970 90.0 4 0.000 0.0 3
torsion 121 86 86 48 0.000 0.0 1 1.970 90.0 4 0.000 0.0 3
torsion 57 120 57 121 0.000 0.0 1 0 000 0.0 1 0.000 0.0 3
torsion 120 57 121 87 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 120 57 121 86 0.000 0.0 1 0.000 0.0 1 0.000 0.0 3
torsion 49 87 87 121 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 86 121 57 84 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3

Locally excited state (LE)

atom 907 120 B "Bodipy Boron atom" 5 10.811 4
atom 908 1 F "Bodipy Fluoride B-F" 9 18.998 1
atom 909 57 N "BODIPY N" 7 14.007 3
atom 910 84 C "Bodipy C2" 6 12.011 3
atom 911 87 C "Bodipy C3" 6 12.011 3
atom 912 87 C "Bodipy C4" 6 12.011 3
atom 913 121 C "Bodipy C5" 6 12.011 3
atom 914 86 C "Bodipy C6" 6 12.011 3
atom 915 86 C "AnilineB C" 6 12.011 3
atom 916 49 H "Bodipy HC" 1 1.008 1
atom 917 48 CA "Aromatic C under" 6 12.011 3
atom 919 44 NT "Amine R3N" 7 14.007 3
atom 920 13 CT "Amine CH3-NR2" 6 12.011 4
atom 921 48 CA "Aromatic C up" 6 12.011 3
atom 922 49 HA "Aromatic H-C up" 1 1.008 1
atom 923 49 HA "Aromatic H-C under" 1 1.008 1
atom 924 46 HC "Alkane H-C-N1" 1 1.008 1

atom 925 46 HC "Alkane H-C Bod up1" 1 1.008 1
atom 926 46 HC "Alkane H-C Bod under" 1 1.008 1
atom 927 46 HC "Alkane H-C-N2" 1 1.008 1
atom 928 46 HC "Alkane H-C Bod up2" 1 1.008 1
atom 929 13 CT "Alkane CH3-" 6 12.011 4
atom 930 13 CT "Alkane CH3-" 6 12.011 4

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charge 915 0.127
charge 916 0.233
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charge 922 0.183
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bond 121 86 385. 1.4224
bond 86 86 385. 1.4892
bond 57 84 427. 1.3501
bond 84 87 546. 1.4180
bond 87 87 469. 1.3963
bond 121 57 385. 1.4171
bond 121 87 546. 1.4349

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angle 1 120 57 80. 110.
angle 57 120 57 80. 106.
angle 84 57 120 30. 124.
angle 87 87 13 63. 125.
angle 86 121 87 70. 131.
angle 87 121 57 70. 108.
angle 121 57 120 30. 127.
angle 121 86 121 63. 119.
angle 121 86 86 63. 121.
angle 57 121 86 70. 121.
angle 121 57 84 70. 109.
angle 121 87 87 70. 106.
angle 13 87 121 70. 129.

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torsion 84 87 87 49 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
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torsion 49 87 87 121 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 86 121 57 84 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3

Charge transfer state (CT)

atom 907 120 B "Bodipy Boron atom" 5 10.811 4
atom 908 1 F "Bodipy Fluoride B-F" 9 18.998 1
atom 909 57 N "BODIPY N" 7 14.007 3
atom 910 84 C "Bodipy C2" 6 12.011 3
atom 911 87 C "Bodipy C3" 6 12.011 3
atom 912 87 C "Bodipy C4" 6 12.011 3

atom 913 121 C "Bodipy C5" 6 12.011 3
atom 914 86 C "Bodipy C6" 6 12.011 3
atom 915 86 C "AnilineB C" 6 12.011 3
atom 916 49 H "Bodipy HC" 1 1.008 1
atom 917 48 CA "Aromatic C under" 6 12.011 3
atom 919 44 NT "Amine R3N" 7 14.007 3
atom 920 13 CT "Amine CH3-NR2" 6 12.011 4
atom 921 48 CA "Aromatic C up" 6 12.011 3
atom 922 49 HA "Aromatic H-C up" 1 1.008 1
atom 923 49 HA "Aromatic H-C under" 1 1.008 1
atom 924 46 HC "Alkane H-C-N" 1 1.008 1
atom 925 46 HC "Alkane H-C Bod up1" 1 1.008 1
atom 926 46 HC "Alkane H-C Bod under" 1 1.008 1
atom 927 46 HC "Alkane H-C-N2" 1 1.008 1
atom 928 46 HC "Alkane H-C Bod up2" 1 1.008 1
atom 929 13 CT "Alkane CH3-" 6 12.011 4
atom 930 13 CT "Alkane CH3-" 6 12.011 4
atom 931 49 H "Link H Aniline" 1 1.008 1
atom 932 49 H "Link H Bodipy" 1 1.008 1
atom 748 122 CA "N-DiMe Aniline C-NR2" 6 12.011 3

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charge 915 0.146
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charge 917 -0.141
charge 919 0.144
charge 920 -0.276
charge 921 -0.161
charge 922 0.180
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charge 925 0.053
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charge 929 -0.179
charge 930 -0.428
charge 748 0.247

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bond 87 87 469. 1.4162
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bond 13 44 382. 1.4725

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angle 13 44 122 50. 116.

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torsion 13 44 122 48 -7.582 0.0 1 3.431 180.0 2 3.198 0.0 3
torsion 46 13 44 122 0.000 0.0 1 0.000 180.0 2 0.560 0.0 3
torsion 48 48 122 49 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3
torsion 48 48 122 44 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3
torsion 48 122 48 49 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3

Additional parameters in THF and toluene
Ground state (GS)

atom 907 120 B "Bodipy Boron atom" 5 10.811 4
atom 908 1 F "Bodipy Fluoride B-F" 9 18.998 1
atom 909 57 N "BODIPY N" 7 14.007 3
atom 910 84 C "Bodipy C2" 6 12.011 3
atom 911 87 C "Bodipy C3" 6 12.011 3
atom 912 87 C "Bodipy C4" 6 12.011 3
atom 913 121 C "Bodipy C5" 6 12.011 3
atom 914 86 C "Bodipy C6" 6 12.011 3
atom 915 86 C "AnilineB C" 6 12.011 3
atom 916 49 H "Bodipy HC" 1 1.008 1
atom 917 48 CA "Aromatic C under" 6 12.011 3
atom 919 44 NT "Amine R3N" 7 14.007 3
atom 920 13 CT "Amine CH3-NR2" 6 12.011 4
atom 921 48 CA "Aromatic C up" 6 12.011 3
atom 922 49 HA "Aromatic H-C up" 1 1.008 1
atom 923 49 HA "Aromatic H-C under" 1 1.008 1
atom 924 46 HC "Alkane H-C-N1" 1 1.008 1
atom 925 46 HC "Alkane H-C Bod up1" 1 1.008 1
atom 926 46 HC "Alkane H-C Bod under" 1 1.008 1
atom 927 46 HC "Alkane H-C-N2" 1 1.008 1
atom 928 46 HC "Alkane H-C Bod up2" 1 1.008 1
atom 929 13 CT "Alkane CH3-" 6 12.011 4
atom 930 13 CT "Alkane CH3-" 6 12.011 4

vdw 907 3.5000 0.0660
vdw 908 2.9400 0.0610
vdw 909 3.2500 0.1700
vdw 910 3.5500 0.0700
vdw 911 3.5500 0.0700
vdw 912 3.5500 0.0700
vdw 913 3.5500 0.0700
vdw 914 3.5500 0.0700
vdw 915 3.5500 0.0700
vdw 916 2.4200 0.0300
vdw 917 3.5500 0.0700
vdw 919 3.3000 0.1700
vdw 920 3.5000 0.0660
vdw 921 3.5500 0.0700
vdw 922 2.4200 0.0300
vdw 923 2.4200 0.0300
vdw 924 2.5000 0.0300
vdw 925 2.5000 0.0300
vdw 926 2.5000 0.0300
vdw 929 3.5000 0.0660
vdw 930 3.5000 0.0660

charge 907 0.970
charge 908 -0.486
charge 909 -0.377
charge 910 0.463
charge 911 -0.544
charge 912 0.193
charge 913 -0.054
charge 914 0.076
charge 915 0.043
charge 916 0.230
charge 917 0.012
charge 919 0.008
charge 920 -0.249
charge 921 -0.369
charge 922 0.181
charge 923 0.091
charge 924 0.102
charge 925 0.070
charge 926 0.154
charge 929 -0.218
charge 930 -0.499
charge 748 0.199

bond 1 120 400. 1.3944
bond 57 120 300. 1.5572
bond 86 86 385. 1.4936
bond 121 86 385. 1.4052
bond 121 57 385. 1.4002

bond 121 87 546. 1.4351
bond 84 87 546. 1.4096
bond 87 87 469. 1.3904
bond 57 84 427. 1.3469
bond 84 13 317. 1.4942
bond 87 13 317. 1.5007

angle 1 120 1 80. 110.
angle 1 120 57 80. 110.
angle 57 120 57 80. 106.
angle 84 57 120 30. 125.
angle 87 84 87 0. 106.
angle 87 87 13 63. 125.
angle 86 121 87 70. 132.
angle 87 121 57 70. 108.
angle 121 57 120 30. 126.
angle 121 86 121 63. 121.
angle 121 86 86 63. 120.
angle 57 121 86 70. 120.
angle 121 57 84 70. 109.
angle 121 87 87 70. 106.
angle 13 87 121 70. 130.

restrain-torsion 121 86 86 48 1.0 87 93

torsion 1 120 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 120 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 84 87 87 49 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 49 87 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 84 87 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 87 87 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 86 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 86 121 87 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 57 121 86 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 86 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 57 120 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 87 121 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 87 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 87 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 57 120 1 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 86 86 48 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 57 120 57 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 120 57 121 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 120 57 121 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 49 87 87 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3

Locally excited state (LE)

atom 907 120 B "Bodipy Boron atom" 5 10.811 4
atom 908 1 F "Bodipy Fluoride B-F" 9 18.998 1
atom 909 57 N "BODIPY N" 7 14.007 3
atom 910 84 C "Bodipy C2" 6 12.011 3
atom 911 87 C "Bodipy C3" 6 12.011 3
atom 912 87 C "Bodipy C4" 6 12.011 3
atom 913 121 C "Bodipy C5" 6 12.011 3
atom 914 86 C "Bodipy C6" 6 12.011 3
atom 915 86 C "AnilineB C" 6 12.011 3
atom 916 49 H "Bodipy HC" 1 1.008 1
atom 917 48 CA "Aromatic C under" 6 12.011 3
atom 919 44 NT "Amine R3N" 7 14.007 3
atom 920 13 CT "Amine CH3-NR2" 6 12.011 4
atom 921 48 CA "Aromatic C up" 6 12.011 3
atom 922 49 HA "Aromatic H-C up" 1 1.008 1
atom 923 49 HA "Aromatic H-C under" 1 1.008 1
atom 924 46 HC "Alkane H-C-N1" 1 1.008 1
atom 925 46 HC "Alkane H-C Bod up1" 1 1.008 1
atom 926 46 HC "Alkane H-C Bod under" 1 1.008 1
atom 927 46 HC "Alkane H-C-N2" 1 1.008 1
atom 928 46 HC "Alkane H-C Bod up2" 1 1.008 1
atom 929 13 CT "Alkane CH3-" 6 12.011 4
atom 930 13 CT "Alkane CH3-" 6 12.011 4

vdw 907 3.5000 0.0660
vdw 908 2.9400 0.0610
vdw 909 3.2500 0.1700
vdw 910 3.5500 0.0700
vdw 911 3.5500 0.0700
vdw 912 3.5500 0.0700
vdw 913 3.5500 0.0700
vdw 914 3.5500 0.0700
vdw 915 3.5500 0.0700
vdw 916 2.4200 0.0300
vdw 917 3.5500 0.0700
vdw 919 3.3000 0.1700
vdw 920 3.5000 0.0660
vdw 921 3.5500 0.0700
vdw 922 2.4200 0.0300
vdw 923 2.4200 0.0300
vdw 924 2.5000 0.0300
vdw 925 2.5000 0.0300
vdw 926 2.5000 0.0300
vdw 927 2.5000 0.0300
vdw 928 2.5000 0.0300
vdw 929 3.5000 0.0660
vdw 930 3.5000 0.0660

charge 907 0.986
charge 908 -0.492
charge 909 -0.430
charge 910 0.452
charge 911 -0.512
charge 912 0.122
charge 913 0.138
charge 914 -0.162
charge 915 0.127
charge 916 0.233
charge 917 0.004
charge 919 0.016

charge 920 -0.253
charge 921 -0.383
charge 922 0.183
charge 923 0.086
charge 924 0.102
charge 925 0.065
charge 926 0.158
charge 929 -0.2085
charge 930 -0.497
charge 748 0.198

bond 1 120 400. 1.4001
bond 57 120 300. 1.5448
bond 121 86 385. 1.4224
bond 86 86 385. 1.4892
bond 57 84 427. 1.3501
bond 84 87 546. 1.4180
bond 87 87 469. 1.3963
bond 121 57 385. 1.4171
bond 121 87 546. 1.4349

angle 1 120 1 80. 110.
angle 1 120 57 80. 110.
angle 57 120 57 80. 106.
angle 84 57 120 30. 124.
angle 87 87 13 63. 125.
angle 86 121 87 70. 131.
angle 87 121 57 70. 108.
angle 121 57 120 30. 127.
angle 121 86 121 63. 119.
angle 121 86 86 63. 121.
angle 57 121 86 70. 121.
angle 121 57 84 70. 109.
angle 121 87 87 70. 106.
angle 13 87 121 70. 129.

restrain-torsion 121 86 86 48 1.0 87 93

torsion 1 120 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 120 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 84 87 87 49 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 49 87 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 84 87 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 87 87 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 86 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 86 121 87 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 57 121 86 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 86 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 57 120 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 87 121 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 87 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 87 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 57 120 1 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 86 86 48 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 57 120 57 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 120 57 121 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 120 57 121 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 49 87 87 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3

Charge transfer state (CT)

atom 907 120 B "Bodipy Boron atom" 5 10.811 4
atom 908 1 F "Bodipy Fluoride B-F" 9 18.998 1
atom 909 57 N "BODIPY N" 7 14.007 3
atom 910 84 C "Bodipy C2" 6 12.011 3
atom 911 87 C "Bodipy C3" 6 12.011 3
atom 912 87 C "Bodipy C4" 6 12.011 3
atom 913 121 C "Bodipy C5" 6 12.011 3
atom 914 86 C "Bodipy C6" 6 12.011 3
atom 915 86 C "AnilineB C" 6 12.011 3
atom 916 49 H "Bodipy HC" 1 1.008 1
atom 917 48 CA "Aromatic C under" 6 12.011 3
atom 919 44 NT "Amine R3N" 7 14.007 3
atom 920 13 CT "Amine CH3-NR2" 6 12.011 4
atom 921 48 CA "Aromatic C up" 6 12.011 3
atom 922 49 HA "Aromatic H-C up" 1 1.008 1
atom 923 49 HA "Aromatic H-C under" 1 1.008 1
atom 924 46 HC "Alkane H-C-N" 1 1.008 1
atom 925 46 HC "Alkane H-C Bod up1" 1 1.008 1
atom 926 46 HC "Alkane H-C Bod under" 1 1.008 1
atom 927 46 HC "Alkane H-C-N2" 1 1.008 1
atom 928 46 HC "Alkane H-C Bod up2" 1 1.008 1
atom 929 13 CT "Alkane CH3-" 6 12.011 4
atom 930 13 CT "Alkane CH3-" 6 12.011 4
atom 931 49 H "Link H Aniline" 1 1.008 1
atom 932 49 H "Link H Bodipy" 1 1.008 1
atom 748 122 CA "N-DiMe Aniline C-NR2" 6 12.011 3

vdw 907 3.5000 0.0660
vdw 908 2.9400 0.0610
vdw 909 3.2500 0.1700
vdw 910 3.5500 0.0700
vdw 911 3.5500 0.0700
vdw 912 3.5500 0.0700
vdw 913 3.5500 0.0700
vdw 914 3.5500 0.0700
vdw 915 3.5500 0.0700
vdw 916 2.4200 0.0300
vdw 917 3.5500 0.0700
vdw 919 3.3000 0.1700
vdw 920 3.5000 0.0660
vdw 921 3.5500 0.0700
vdw 922 2.4200 0.0300
vdw 923 2.4200 0.0300
vdw 924 2.5000 0.0300
vdw 925 2.5000 0.0300
vdw 926 2.5000 0.0300
vdw 927 2.5000 0.0300

vdw 928 2.5000 0.0300
vdw 929 3.5000 0.0660
vdw 930 3.5000 0.0660

charge 907 1.120
charge 908 -0.544
charge 909 -0.382
charge 910 0.262
charge 911 -0.552
charge 912 0.097
charge 913 0.038
charge 914 -0.231
charge 915 0.146
charge 916 0.217
charge 917 -0.141
charge 919 0.144
charge 920 -0.276
charge 921 -0.161
charge 922 0.180
charge 923 0.166
charge 924 0.1545
charge 925 0.053
charge 926 0.1225
charge 929 -0.179
charge 930 -0.428
charge 748 0.247

bond 1 120 400. 1.4134
bond 57 120 300. 1.5474
bond 86 86 385. 1.4936
bond 121 86 385. 1.4131
bond 121 57 385. 1.3930
bond 121 87 546. 1.4137
bond 84 87 546. 1.3899
bond 87 87 469. 1.4162
bond 57 84 427. 1.3746
bond 84 13 317. 1.4967
bond 87 13 317. 1.5003
bond 48 86 469. 1.4081
bond 48 48 469. 1.3787
bond 48 122 469. 1.4337
bond 44 122 481. 1.3591
bond 13 44 382. 1.4725

angle 1 120 1 80. 110.
angle 1 120 57 80. 110.
angle 57 120 57 80. 104.
angle 84 57 120 30. 121.
angle 87 84 87 0. 106.
angle 84 86 84 63. 117.
angle 84 86 86 63. 121.
angle 87 87 13 63. 122.
angle 86 121 87 70. 132.
angle 87 121 57 70. 108.
angle 121 57 120 30. 121.
angle 87 121 87 70. 106.
angle 121 86 121 63. 117.
angle 121 86 86 63. 121.
angle 57 121 86 70. 121.
angle 121 57 84 70. 109.
angle 121 87 87 70. 107.
angle 13 87 121 70. 125.
angle 48 86 49 35. 120.
angle 121 86 49 63. 121.
angle 122 48 48 63. 120.
angle 48 122 48 63. 120.
angle 122 48 49 35. 120.
angle 44 122 48 70. 120.
angle 13 44 122 50. 116.

restrain-torsion 121 86 86 48 1.0 87 93

torsion 1 120 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 120 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 84 87 87 49 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 49 87 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 84 87 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 87 87 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 86 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 86 121 87 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 57 121 86 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 86 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 121 57 120 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 87 87 121 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 87 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 87 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 57 121 87 13 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 57 120 1 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 121 86 86 48 0.000 0.0 1 2.170 180.0 2 0.000 0.0 3
torsion 57 120 57 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 120 57 121 87 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 120 57 121 86 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 49 87 87 121 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 86 121 57 84 0.000 0.0 1 7.170 180.0 2 0.000 0.0 3
torsion 49 48 86 49 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3
torsion 48 48 86 49 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3
torsion 48 48 122 48 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3
torsion 44 122 48 49 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3
torsion 13 44 122 48 -7.582 0.0 1 3.431 180.0 2 3.198 0.0 3
torsion 46 13 44 122 0.000 0.0 1 0.000 180.0 2 0.560 0.0 3
torsion 48 48 122 49 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3
torsion 48 48 122 44 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3
torsion 48 122 48 49 0.000 0.0 1 7.250 180.0 2 0.000 0.0 3