# Supporting Information

## Dicyanovinyl Substituted Triarylboranes- A Rational Approach to Distinguish Fluoride and Cyanide Ions

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**Table of Contents:**

1. NMR Plots **-S2**
2. Solvent dependent UV-Vis absorption spectra **-S4**
3. Excitation Spectra **-S4**
4. NMR plots in presence of Anions **-S5**
5. Binding Constant Fitting Data **-S7**
6. TD-DFT data **-S8**
7. Bond length & Bond angle parameters **-S10**
8. Coordinates of optimised geometries **-S19**
9. Reference **-S24**

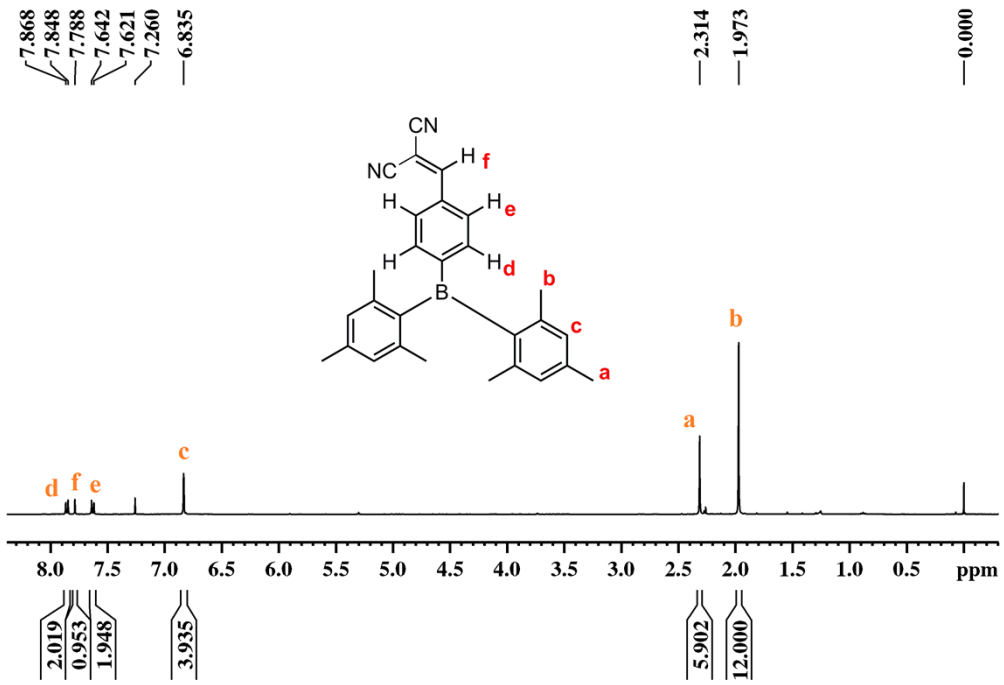



Figure S1: $^{1}$H NMR spectrum of **1**

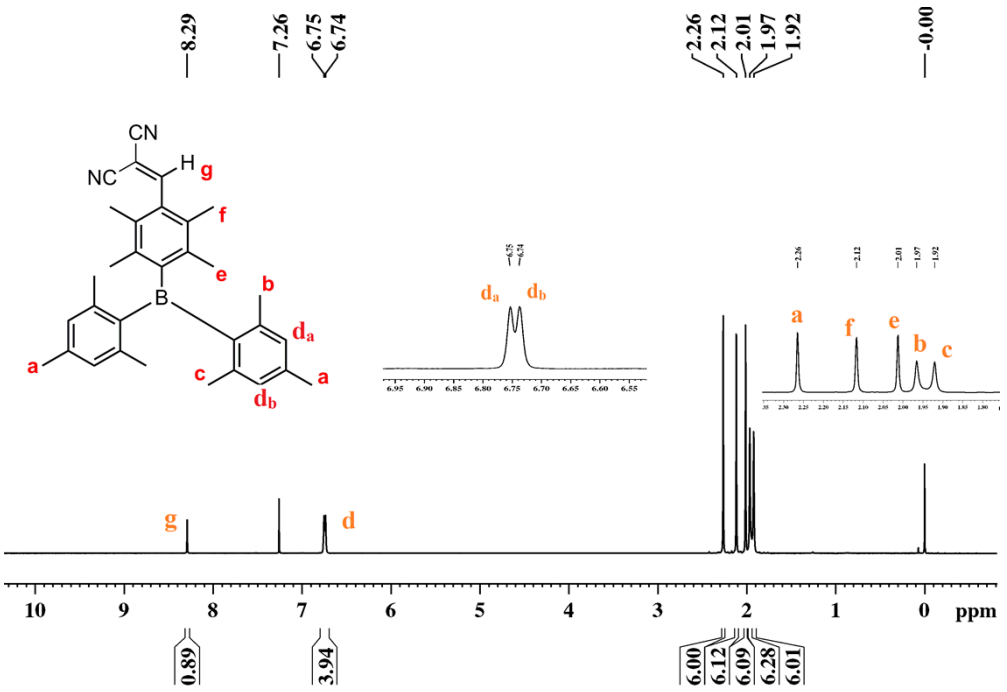



Figure S2: $^{1}$H NMR Spectrum of **2**

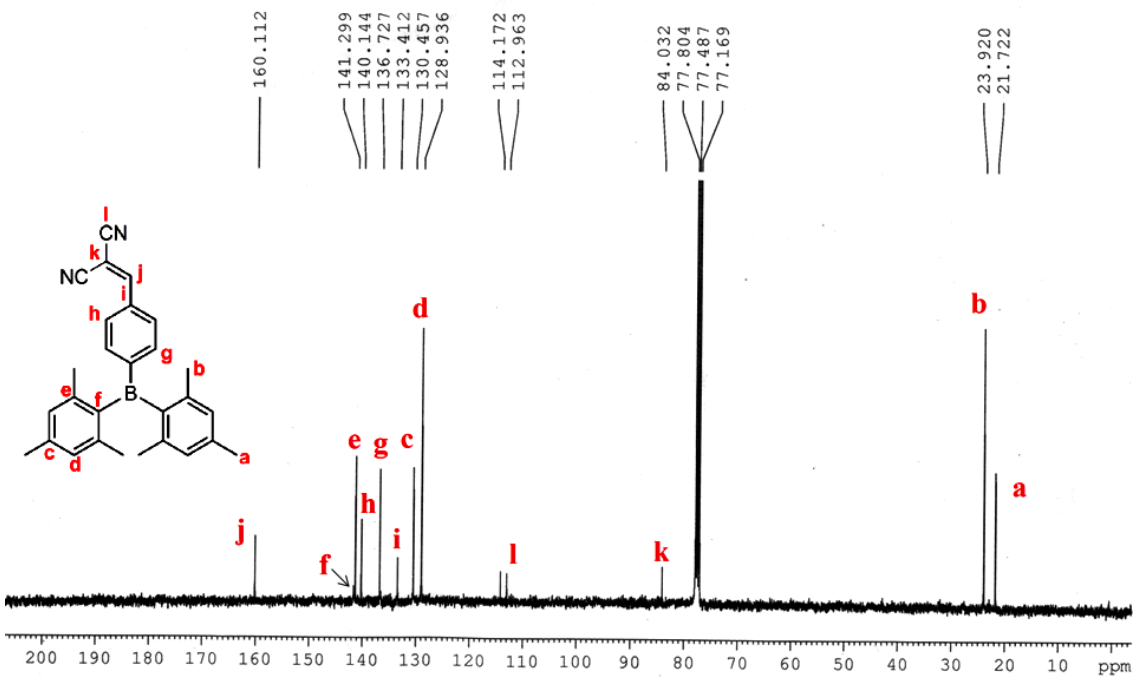



Figure S3: $^{13}$C NMR spectrum of **1**

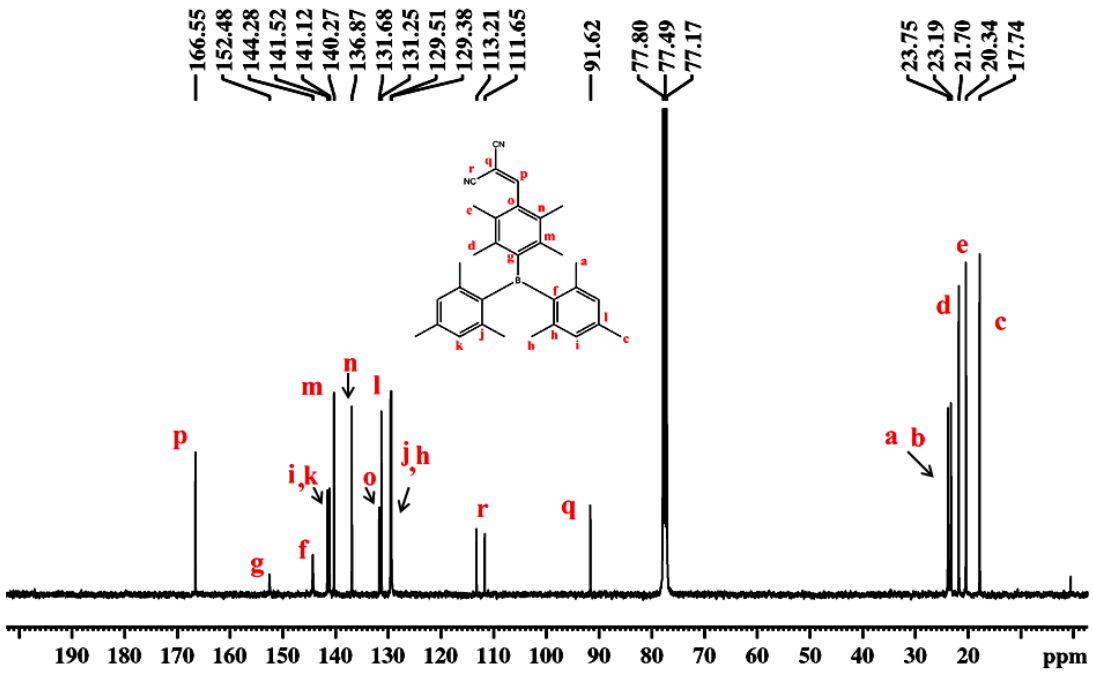



Figure S4: $^{13}$C NMR spectrum of **2**

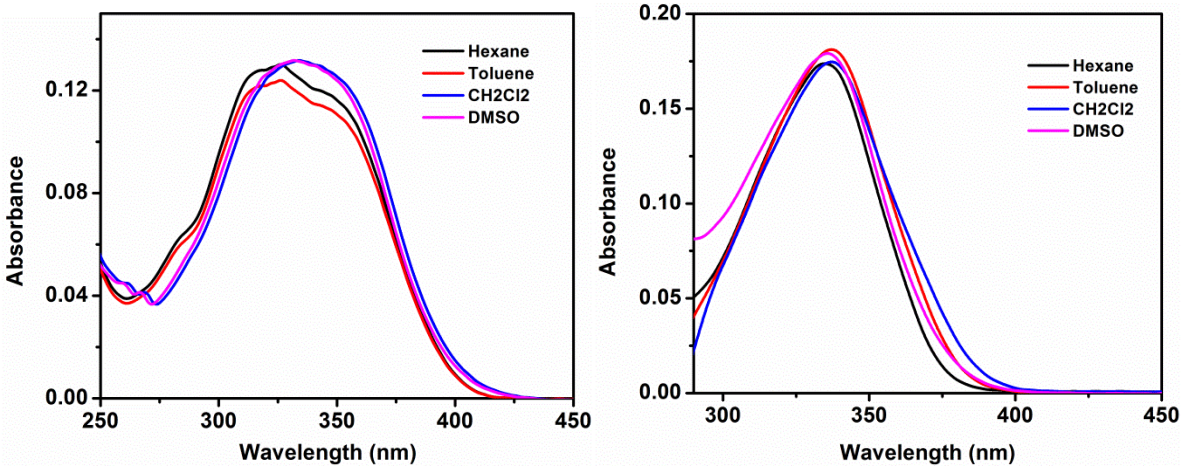



Figure **S5**: UV-Vis absorption spectrum of **1** and **2** in solvents of various polarity ($1\times10^{-5}$ M)

The changes in absorption spectrum of **1** and **2** with respect to solvent polarity are negligible.

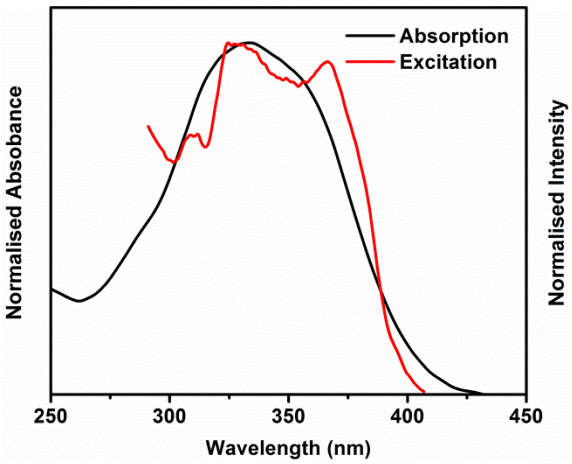



Figure **S6**: Absorption and Excitation spectrum of **1** ($\lambda_{em}$ = 509 nm).

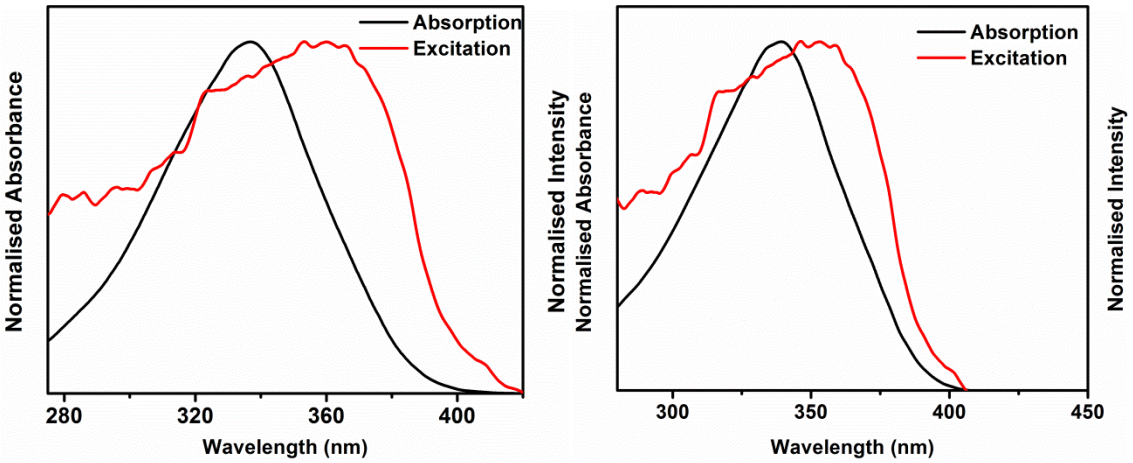



Figure **S7**: Absorption and Excitation spectra of **2** (left; $\lambda_{em}$ = 381 nm, right; $\lambda_{em}$ = 493 nm).

## NMR Spectra in presence of anions

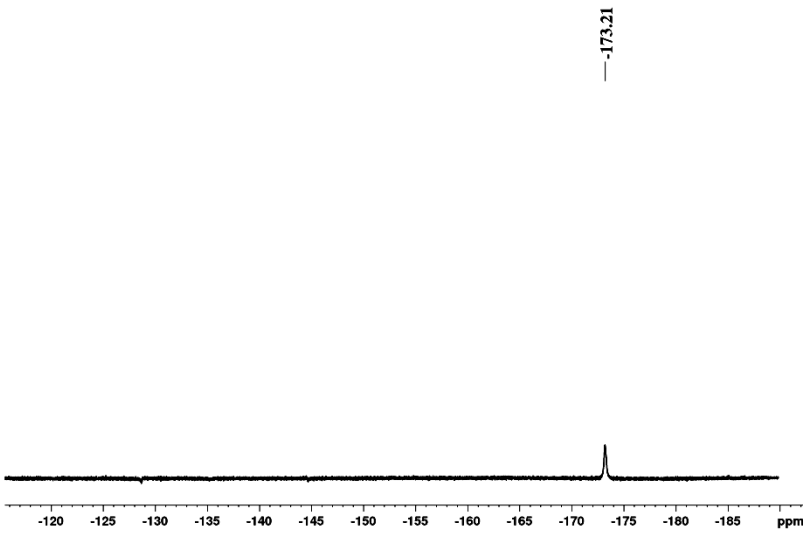



Figure **S8**: $^{19}F$ NMR spectrum of **1** in presense of 1 eq of TBAF. The signal at -173.2 ppm assigned to ($-C_6H_4$) ($Mes_2$)B·F moiety (Mes = Mesityl group).

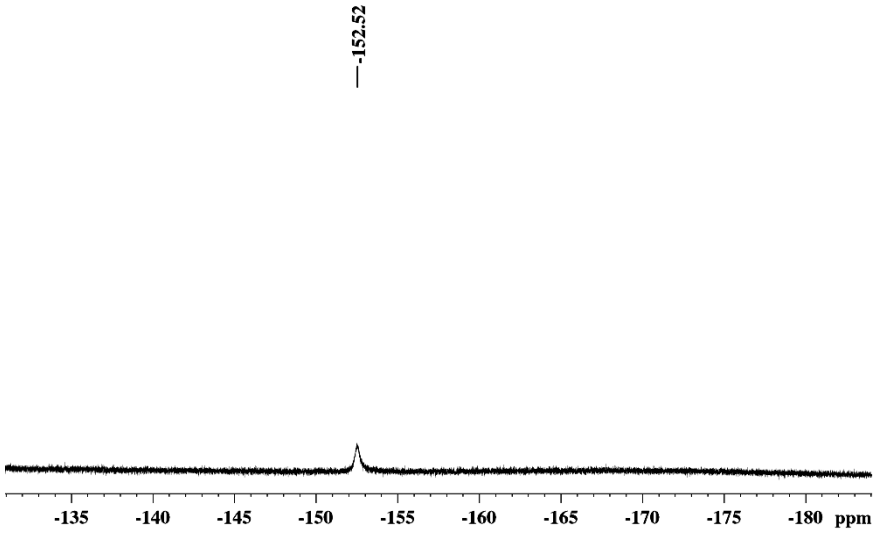



**Figure S9**: $^{19}F$ NMR spectrum of **2** in presence of 1 eq of TBAF. The signal at -152.5 ppm assigned to ($-C_6(CH_3)_4$) ($Mes_2$)B·F moiety (Mes = Mesityl group).

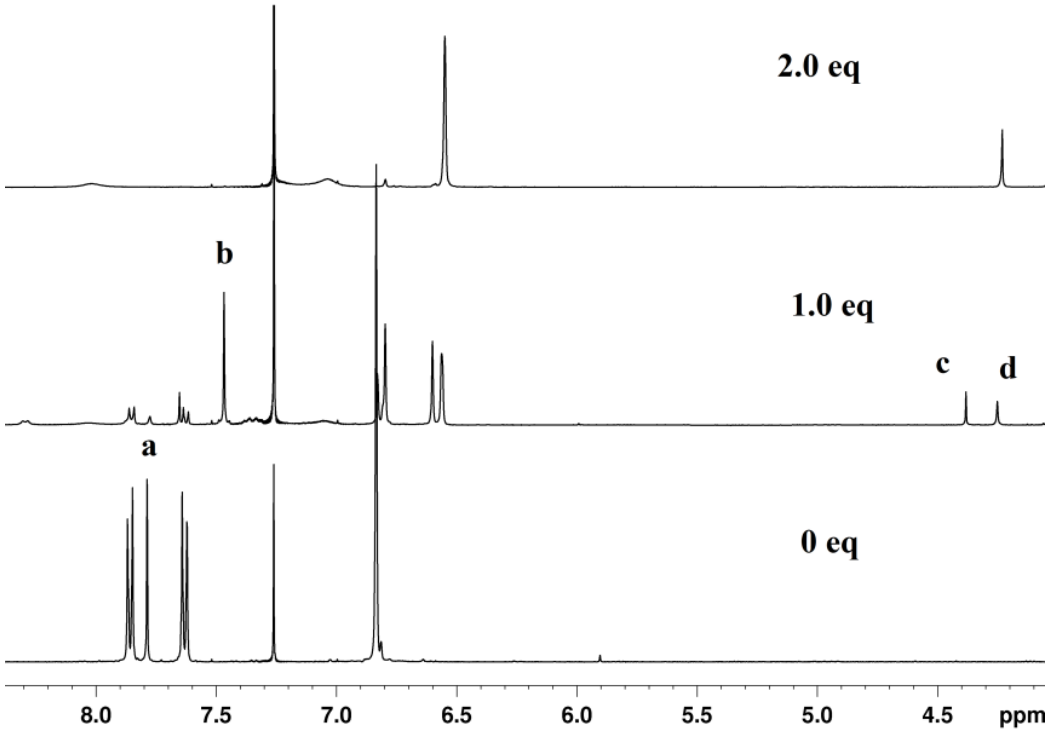



**Figure S10**: $^{1}$H NMR titration of **1** against TBAF in $CDCl_3$ (2 μL = 0.1 eq)

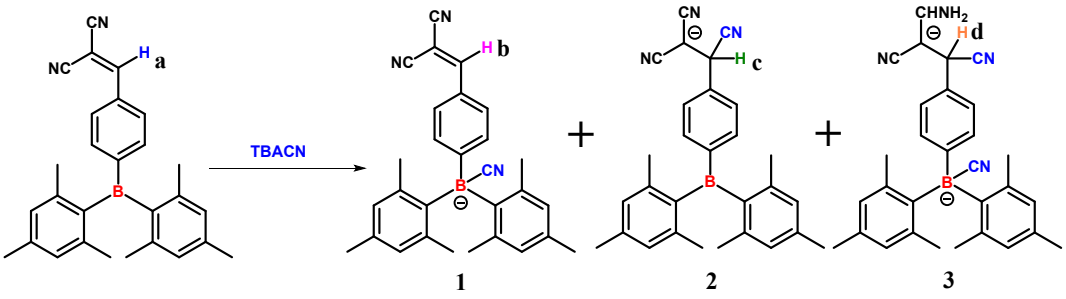



Figure **S11**: Predicted binding modes of **2** with cyanide**.**

## Binding Constant Fitting Plots[1]

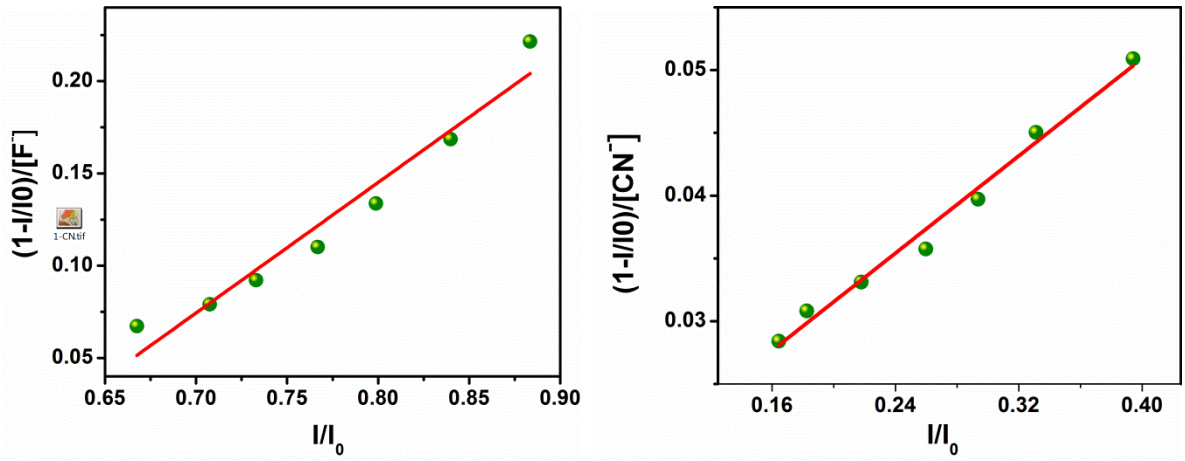



Figure **S12**: : Fitting of UV-Vis absorption titration of **1** with fluoride (left, at $\lambda_{ab}$ = 334 nm) and cyanide (right, at $\lambda_{ab}$ = 334 nm)

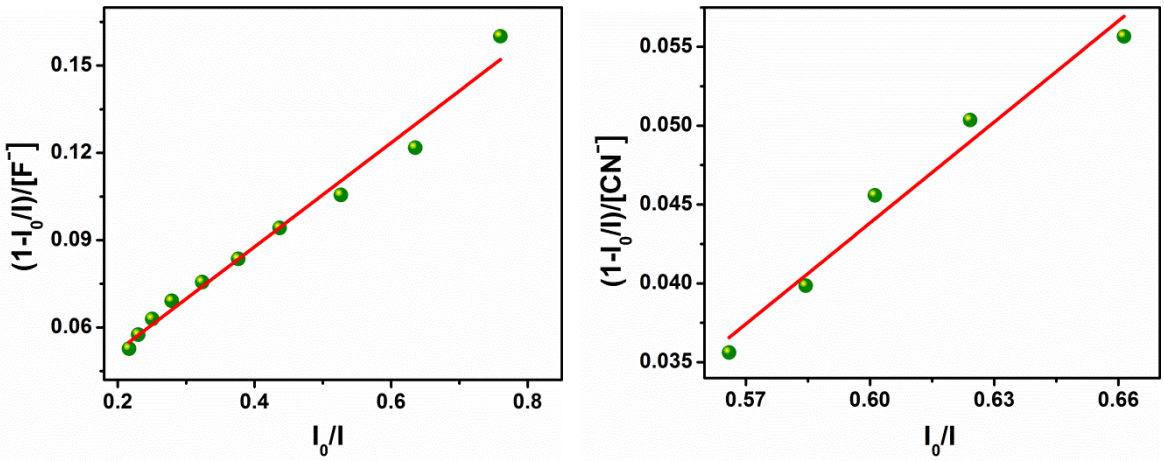
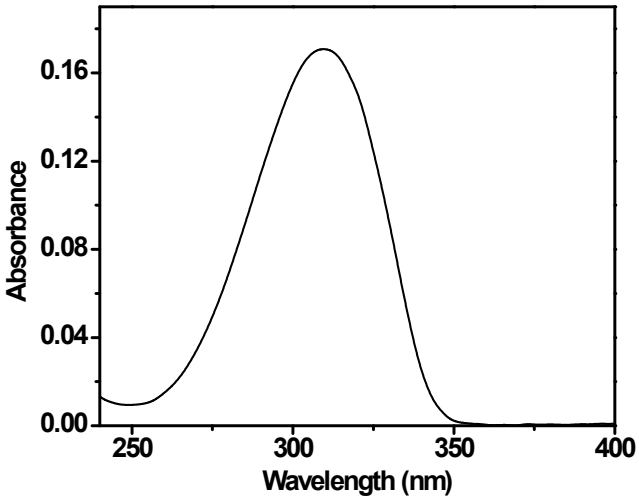
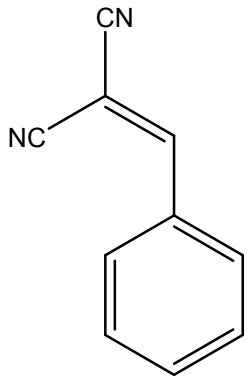



Figure **S13**: Fitting of UV-Vis absorption titration of **1** with fluoride (left, at $\lambda_{ab}$ = 340 nm) and cyanide (right, at $\lambda_{ab}$ = 340 nm).




M1

Figure S14: UV-Vis absorption spectrum of **M1**

**TD-DFT data**

Excitation energies and oscillator strengths: (for **1**)

Excited State 1: Singlet-A 2.7214 eV 455.59 nm f=0.0295
HOMO to LUMO 0.70013
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.8725 eV 431.62 nm f=0.0481
HOMO-1 to LUMO 0.70031

Excited State 3: Singlet-A 2.9545 eV 419.64 nm f=0.0637
HOMO-3 to LUMO -0.15657
HOMO-2 to LUMO 0.68321

Excited State 4: Singlet-A 2.9812 eV 415.89 nm f=0.0127
HOMO-3 to LUMO 0.68424

HOMO-2 to LUMO 0.15561

Excited State 5: Singlet-A 3.7727 eV 328.63 nm f=0.7562
HOMO-5 to LUMO -0.18304
HOMO-4 to LUMO 0.65624
HOMO-1 to LUMO -0.13379

Excited State 6: Singlet-A 3.8758 eV 319.89 nm f=0.0910
HOMO-5 to LUMO 0.66175
HOMO-4 to LUMO 0.16990
HOMO-4 to LUMO+2 0.13616

Excitation energies and oscillator strengths: (for **2**)

Excited State 1: Singlet-A 3.2320 eV 383.62 nm f=0.0246
HOMO-2 to LUMO -0.39240
HOMO-1 to LUMO 0.13234
HOMO to LUMO 0.55190
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2866 eV 377.24 nm f=0.0082
HOMO-3 to LUMO 0.52546
HOMO-2 to LUMO -0.10195
HOMO-1 to LUMO -0.15684
HOMO to LUMO 0.40995
HOMO to LUMO+1 -0.12650

Excited State 3: Singlet-A 3.3978 eV 364.90 nm f=0.2222
HOMO-5 to LUMO 0.18405
HOMO-3 to LUMO 0.15406
HOMO-2 to LUMO -0.17060
HOMO-1 to LUMO 0.62282
HOMO-1 to LUMO+1 -0.12805

Excited State 4: Singlet-A 3.5036 eV 353.88 nm f=0.0068

HOMO-3 to LUMO 0.18565

HOMO-2 to LUMO 0.64913

HOMO-2 to LUMO+1 -0.13347

HOMO-1 to LUMO 0.14206

Excited State 5: Singlet-A 3.6003 eV 344.37 nm f=0.0287

HOMO-5 to LUMO -0.17754

HOMO -4 to LUMO 0.66091

HOMO-4 to LUMO+1 -0.14008

Excited State 6: Singlet-A 3.6562 eV 339.11 nm f=0.1073

HOMO-5 to LUMO 0.64768

HOMO-4 to LUMO 0.19588

HOMO-1 to LUMO -0.15103

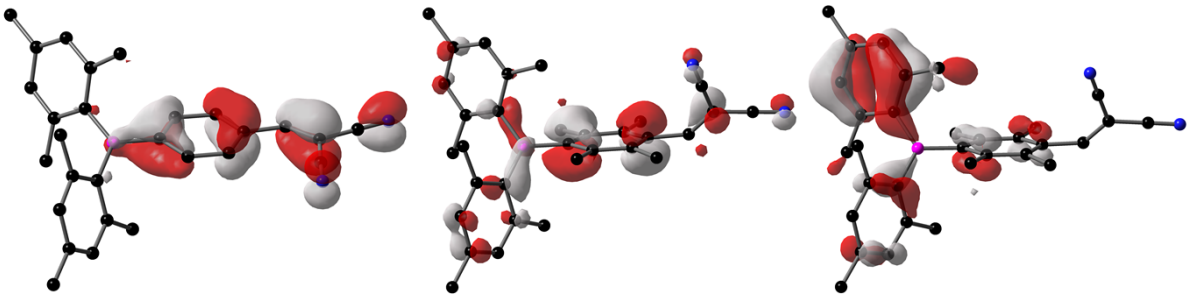


Figure **S14**: Selected MO's (i) HOMO-4 of **1** (left) (ii) HOMO-5 of **2** (middle) ( iii) HOMO-1 of **2** (right).

**Bond length parameters of 1 (Å)**

| Number | Atom1 | Atom2 | Length |
|---|---|---|---|
| 1 | N2 | C2 | 1.150(3) |
| 2 | N1 | C1 | 1.146(3) |
| 3 | C2 | C3 | 1.438(3) |
| 4 | C3 | C4 | 1.352(3) |
| 5 | C3 | C1 | 1.442(3) |

| | | | |
|---|---|---|---|
| 6 | C4 | H4 | 0.931 |
| 7 | C4 | C5 | 1.454(2) |
| 8 | C5 | C6 | 1.404(3) |
| 9 | C5 | C10 | 1.405(3) |
| 10 | C6 | H6 | 0.929 |
| 11 | C6 | C7 | 1.387(3) |
| 12 | C7 | H7 | 0.93 |
| 13 | C7 | C8 | 1.407(3) |
| 14 | C8 | C9 | 1.402(3) |
| 15 | C8 | B1 | 1.578(3) |
| 16 | C17 | C22 | 1.417(2) |
| 17 | C17 | C18 | 1.415(2) |
| 18 | C17 | B1 | 1.575(3) |
| 19 | C22 | C21 | 1.398(3) |
| 20 | C22 | C28 | 1.512(3) |
| 21 | C21 | H21 | 0.93 |
| 22 | C21 | C20 | 1.385(3) |
| 23 | C20 | C27 | 1.505(3) |
| 24 | C20 | C19 | 1.395(3) |
| 25 | C27 | H27A | 0.96 |
| 26 | C27 | H27B | 0.96 |
| 27 | C27 | H27C | 0.96 |
| 28 | C19 | H19 | 0.93 |
| 29 | C19 | C18 | 1.398(3) |
| 30 | C18 | C26 | 1.507(2) |
| 31 | C26 | H26A | 0.959 |
| 32 | C26 | H26B | 0.96 |
| 33 | C26 | H26C | 0.961 |
| 34 | C28 | H28A | 0.959 |
| 35 | C28 | H28B | 0.961 |
| 36 | C28 | H28C | 0.96 |
| 37 | C11 | C16 | 1.418(3) |
| 38 | C11 | C12 | 1.416(2) |
| 39 | C11 | B1 | 1.575(3) |
| 40 | C16 | C15 | 1.397(3) |
| 41 | C16 | C25 | 1.504(2) |
| 42 | C15 | H15 | 0.93 |
| 43 | C15 | C14 | 1.390(3) |
| 44 | C14 | C13 | 1.389(3) |
| 45 | C14 | C24 | 1.515(3) |
| 46 | C13 | H13 | 0.93 |
| 47 | C13 | C12 | 1.393(3) |
| 48 | C12 | C23 | 1.515(3) |
| 49 | C23 | H23A | 0.96 |
| 50 | C23 | H23B | 0.96 |
| 51 | C23 | H23C | 0.961 |

| | | | |
|---|---|---|---|
| 52 | C24 | H24A | 0.959 |
| 53 | C24 | H24B | 0.959 |
| 54 | C24 | H24C | 0.961 |
| 55 | C25 | H25A | 0.96 |
| 56 | C25 | H25B | 0.96 |
| 57 | C25 | H25C | 0.96 |
| 58 | C9 | H9 | 0.93 |
| 59 | C9 | C10 | 1.384(3) |
| 60 | C10 | H10 | 0.93 |

**Bond angle parameters of 1 (deg)**

| Number | Atom1 | Atom2 | Atom3 | Angle |
|---|---|---|---|---|
| 1 | N2 | C2 | C3 | 176.8(2) |
| 2 | C2 | C3 | C4 | 125.8(2) |
| 3 | C2 | C3 | C1 | 114.0(2) |
| 4 | C4 | C3 | C1 | 120.1(2) |
| 5 | C3 | C4 | H4 | 115 |
| 6 | C3 | C4 | C5 | 130.0(2) |
| 7 | H4 | C4 | C5 | 115 |
| 8 | C4 | C5 | C6 | 124.4(2) |
| 9 | C4 | C5 | C10 | 117.0(2) |
| 10 | C6 | C5 | C10 | 118.5(2) |
| 11 | C5 | C6 | H6 | 119.7 |
| 12 | C5 | C6 | C7 | 120.5(2) |
| 13 | H6 | C6 | C7 | 119.8 |
| 14 | C6 | C7 | H7 | 119.3 |
| 15 | C6 | C7 | C8 | 121.4(2) |
| 16 | H7 | C7 | C8 | 119.3 |
| 17 | C7 | C8 | C9 | 117.4(2) |
| 18 | C7 | C8 | B1 | 120.9(2) |
| 19 | C9 | C8 | B1 | 121.7(2) |
| 20 | C22 | C17 | C18 | 118.2(2) |
| 21 | C22 | C17 | B1 | 121.4(2) |
| 22 | C18 | C17 | B1 | 120.3(2) |
| 23 | C17 | C22 | C21 | 119.7(2) |
| 24 | C17 | C22 | C28 | 121.7(2) |
| 25 | C21 | C22 | C28 | 118.4(2) |
| 26 | C22 | C21 | H21 | 119 |
| 27 | C22 | C21 | C20 | 122.1(2) |
| 28 | H21 | C21 | C20 | 118.9 |
| 29 | C21 | C20 | C27 | 121.1(2) |
| 30 | C21 | C20 | C19 | 118.2(2) |
| 31 | C27 | C20 | C19 | 120.6(2) |
| 32 | C20 | C27 | H27A | 109.4 |
| 33 | C20 | C27 | H27B | 109.4 |

| | | | | |
|---|---|---|---|---|
| 34 | C20 | C27 | H27C | 109.5 |
| 35 | H27A | C27 | H27B | 109.5 |
| 36 | H27A | C27 | H27C | 109.5 |
| 37 | H27B | C27 | H27C | 109.5 |
| 38 | N1 | C1 | C3 | 179.4(2) |
| 39 | C20 | C19 | H19 | 119.2 |
| 40 | C20 | C19 | C18 | 121.5(2) |
| 41 | H19 | C19 | C18 | 119.3 |
| 42 | C17 | C18 | C19 | 120.2(2) |
| 43 | C17 | C18 | C26 | 121.7(2) |
| 44 | C19 | C18 | C26 | 118.0(2) |
| 45 | C18 | C26 | H26A | 109.5 |
| 46 | C18 | C26 | H26B | 109.4 |
| 47 | C18 | C26 | H26C | 109.4 |
| 48 | H26A | C26 | H26B | 109.4 |
| 49 | H26A | C26 | H26C | 109.5 |
| 50 | H26B | C26 | H26C | 109.5 |
| 51 | C22 | C28 | H28A | 109.5 |
| 52 | C22 | C28 | H28B | 109.5 |
| 53 | C22 | C28 | H28C | 109.5 |
| 54 | H28A | C28 | H28B | 109.5 |
| 55 | H28A | C28 | H28C | 109.5 |
| 56 | H28B | C28 | H28C | 109.4 |
| 57 | C16 | C11 | C12 | 118.0(2) |
| 58 | C16 | C11 | B1 | 122.1(2) |
| 59 | C12 | C11 | B1 | 119.9(2) |
| 60 | C11 | C16 | C15 | 119.8(2) |
| 61 | C11 | C16 | C25 | 121.8(2) |
| 62 | C15 | C16 | C25 | 118.4(2) |
| 63 | C16 | C15 | H15 | 118.9 |
| 64 | C16 | C15 | C14 | 122.2(2) |
| 65 | H15 | C15 | C14 | 118.9 |
| 66 | C15 | C14 | C13 | 117.8(2) |
| 67 | C15 | C14 | C24 | 121.2(2) |
| 68 | C13 | C14 | C24 | 121.0(2) |
| 69 | C14 | C13 | H13 | 119 |
| 70 | C14 | C13 | C12 | 122.0(2) |
| 71 | H13 | C13 | C12 | 119 |
| 72 | C11 | C12 | C13 | 120.2(2) |
| 73 | C11 | C12 | C23 | 121.9(2) |
| 74 | C13 | C12 | C23 | 117.8(2) |
| 75 | C12 | C23 | H23A | 109.5 |
| 76 | C12 | C23 | H23B | 109.4 |
| 77 | C12 | C23 | H23C | 109.5 |
| 78 | H23A | C23 | H23B | 109.5 |
| 79 | H23A | C23 | H23C | 109.5 |

| 80 | H23B | C23 | H23C | 109.5 |
|---|---|---|---|---|
| 81 | C14 | C24 | H24A | 109.4 |
| 82 | C14 | C24 | H24B | 109.5 |
| 83 | C14 | C24 | H24C | 109.4 |
| 84 | H24A | C24 | H24B | 109.5 |
| 85 | H24A | C24 | H24C | 109.5 |
| 86 | H24B | C24 | H24C | 109.5 |
| 87 | C16 | C25 | H25A | 109.5 |
| 88 | C16 | C25 | H25B | 109.4 |
| 89 | C16 | C25 | H25C | 109.4 |
| 90 | H25A | C25 | H25B | 109.4 |
| 91 | H25A | C25 | H25C | 109.5 |
| 92 | H25B | C25 | H25C | 109.5 |
| 93 | C8 | C9 | H9 | 119.1 |
| 94 | C8 | C9 | C10 | 121.8(2) |
| 95 | H9 | C9 | C10 | 119.1 |
| 96 | C5 | C10 | C9 | 120.3(2) |
| 97 | C5 | C10 | H10 | 119.8 |
| 98 | C9 | C10 | H10 | 119.9 |
| 99 | C8 | B1 | C17 | 119.0(2) |
| 100 | C8 | B1 | C11 | 117.8(2) |
| 101 | C17 | B1 | C11 | 123.2(2) |

**Bond length parameters of 2 (Å)**

| Number | Atom1 | Atom2 | Length |
|---|---|---|---|
| 1 | B1 | C8 | 1.5936(1) |
| 2 | B1 | C17 | 1.5774(1) |
| 3 | B1 | C11 | 1.5750(1) |
| 4 | N1 | C1 | 1.1349(1) |
| 5 | N2 | C2 | 1.1269(1) |
| 6 | C8 | C9 | 1.4135(1) |
| 7 | C8 | C7 | 1.4009(1) |
| 8 | C10 | C9 | 1.3880(1) |
| 9 | C10 | C5 | 1.4121(1) |
| 10 | C10 | C26 | 1.5065(1) |
| 11 | C17 | C22 | 1.4107(1) |
| 12 | C17 | C18 | 1.4111(1) |
| 13 | C9 | C25 | 1.5137(1) |
| 14 | C11 | C16 | 1.4195(1) |
| 15 | C11 | C12 | 1.4131(1) |
| 16 | C22 | C21 | 1.3946(1) |
| 17 | C22 | C32 | 1.5081(1) |
| 18 | C16 | C15 | 1.3864(1) |
| 19 | C16 | C29 | 1.5117(1) |

| | | | |
|---|---|---|---|
| 20 | C5 | C6 | 1.3905(1) |
| 21 | C5 | C4 | 1.4750(1) |
| 22 | C18 | C19 | 1.3791(1) |
| 23 | C18 | C30 | 1.5219(1) |
| 24 | C6 | C7 | 1.4060(1) |
| 25 | C6 | C23 | 1.5135(1) |
| 26 | C12 | C13 | 1.3866(1) |
| 27 | C12 | C27 | 1.5086(1) |
| 28 | C7 | C24 | 1.5108(1) |
| 29 | C13 | H13 | 0.9300(1) |
| 30 | C13 | C14 | 1.3821(1) |
| 31 | C19 | H19 | 0.9300(1) |
| 32 | C19 | C20 | 1.3849(1) |
| 33 | C21 | H21 | 0.9300(1) |
| 34 | C21 | C20 | 1.3744(1) |
| 35 | C4 | H4 | 0.9300(1) |
| 36 | C4 | C3 | 1.3259(1) |
| 37 | C15 | H15 | 0.9300(1) |
| 38 | C15 | C14 | 1.3790(1) |
| 39 | C20 | C31 | 1.5041(1) |
| 40 | C32 | H32A | 0.9600(1) |
| 41 | C32 | H32B | 0.9600(1) |
| 42 | C32 | H32C | 0.9600(1) |
| 43 | C26 | H26A | 0.9600(1) |
| 44 | C26 | H26B | 0.9600(1) |
| 45 | C26 | H26C | 0.9600(1) |
| 46 | C24 | H24A | 0.9600(1) |
| 47 | C24 | H24B | 0.9600(1) |
| 48 | C24 | H24C | 0.9600(1) |
| 49 | C29 | H29A | 0.9600(1) |
| 50 | C29 | H29B | 0.9600(1) |
| 51 | C29 | H29C | 0.9600(1) |
| 52 | C25 | H25A | 0.9600(1) |
| 53 | C25 | H25B | 0.9600(1) |
| 54 | C25 | H25C | 0.9600(1) |
| 55 | C3 | C1 | 1.4423(1) |
| 56 | C3 | C2 | 1.4247(1) |
| 57 | C27 | H27A | 0.9600(1) |
| 58 | C27 | H27B | 0.9600(1) |
| 59 | C27 | H27C | 0.9600(1) |
| 60 | C14 | C28 | 1.4943(1) |
| 61 | C30 | H30A | 0.9600(1) |
| 62 | C30 | H30B | 0.9600(1) |
| 63 | C30 | H30C | 0.9600(1) |

| | | | |
|---|---|---|---|
| 64 | C23 | H23A | 0.9600(1) |
| 65 | C23 | H23B | 0.9600(1) |
| 66 | C23 | H23C | 0.9600(1) |
| 67 | C28 | H28A | 0.9600(1) |
| 68 | C28 | H28B | 0.9600(1) |
| 69 | C28 | H28C | 0.9600(1) |
| 70 | C31 | H31A | 0.9600(1) |
| 71 | C31 | H31B | 0.9600(1) |
| 72 | C31 | H31C | 0.9600(1) |

**Bond angle parameters of 2 (deg)**

| Number | Atom1 | Atom2 | Atom3 | Angle |
|---|---|---|---|---|
| 1 | C8 | B1 | C17 | 120.38 |
| 2 | C8 | B1 | C11 | 118.05 |
| 3 | C17 | B1 | C11 | 121.57 |
| 4 | B1 | C8 | C9 | 120.29 |
| 5 | B1 | C8 | C7 | 120.51 |
| 6 | C9 | C8 | C7 | 119.13 |
| 7 | C9 | C10 | C5 | 118.98 |
| 8 | C9 | C10 | C26 | 121.34 |
| 9 | C5 | C10 | C26 | 119.61 |
| 10 | B1 | C17 | C22 | 121.41 |
| 11 | B1 | C17 | C18 | 121.06 |
| 12 | C22 | C17 | C18 | 117.47 |
| 13 | C8 | C9 | C10 | 120.71 |
| 14 | C8 | C9 | C25 | 120.58 |
| 15 | C10 | C9 | C25 | 118.58 |
| 16 | B1 | C11 | C16 | 120.44 |
| 17 | B1 | C11 | C12 | 122.44 |
| 18 | C16 | C11 | C12 | 117.08 |
| 19 | C17 | C22 | C21 | 119.76 |
| 20 | C17 | C22 | C32 | 121.97 |
| 21 | C21 | C22 | C32 | 118.09 |
| 22 | C11 | C16 | C15 | 119.71 |
| 23 | C11 | C16 | C29 | 122.72 |
| 24 | C15 | C16 | C29 | 117.55 |
| 25 | C10 | C5 | C6 | 121.28 |
| 26 | C10 | C5 | C4 | 116.66 |
| 27 | C6 | C5 | C4 | 122.06 |
| 28 | C17 | C18 | C19 | 120.49 |
| 29 | C17 | C18 | C30 | 122.65 |
| 30 | C19 | C18 | C30 | 116.85 |
| 31 | C5 | C6 | C7 | 118.98 |

| | | | | |
|---|---|---|---|---|
| 32 | C5 | C6 | C23 | 122.02 |
| 33 | C7 | C6 | C23 | 118.98 |
| 34 | C11 | C12 | C13 | 120.54 |
| 35 | C11 | C12 | C27 | 121.89 |
| 36 | C13 | C12 | C27 | 117.54 |
| 37 | C8 | C7 | C6 | 120.68 |
| 38 | C8 | C7 | C24 | 120.74 |
| 39 | C6 | C7 | C24 | 118.53 |
| 40 | C12 | C13 | H13 | 118.78 |
| 41 | C12 | C13 | C14 | 122.45 |
| 42 | H13 | C13 | C14 | 118.78 |
| 43 | C18 | C19 | H19 | 118.85 |
| 44 | C18 | C19 | C20 | 122.3 |
| 45 | H19 | C19 | C20 | 118.85 |
| 46 | C22 | C21 | H21 | 118.71 |
| 47 | C22 | C21 | C20 | 122.58 |
| 48 | H21 | C21 | C20 | 118.71 |
| 49 | C5 | C4 | H4 | 116.89 |
| 50 | C5 | C4 | C3 | 126.23 |
| 51 | H4 | C4 | C3 | 116.89 |
| 52 | C16 | C15 | H15 | 118.38 |
| 53 | C16 | C15 | C14 | 123.24 |
| 54 | H15 | C15 | C14 | 118.38 |
| 55 | C19 | C20 | C21 | 117.36 |
| 56 | C19 | C20 | C31 | 121.5 |
| 57 | C21 | C20 | C31 | 121.13 |
| 58 | C22 | C32 | H32A | 109.47 |
| 59 | C22 | C32 | H32B | 109.47 |
| 60 | C22 | C32 | H32C | 109.47 |
| 61 | H32A | C32 | H32B | 109.47 |
| 62 | H32A | C32 | H32C | 109.47 |
| 63 | H32B | C32 | H32C | 109.47 |
| 64 | C10 | C26 | H26A | 109.47 |
| 65 | C10 | C26 | H26B | 109.47 |
| 66 | C10 | C26 | H26C | 109.47 |
| 67 | H26A | C26 | H26B | 109.47 |
| 68 | H26A | C26 | H26C | 109.47 |
| 69 | H26B | C26 | H26C | 109.47 |
| 70 | C7 | C24 | H24A | 109.47 |
| 71 | C7 | C24 | H24B | 109.47 |
| 72 | C7 | C24 | H24C | 109.47 |
| 73 | H24A | C24 | H24B | 109.47 |
| 74 | H24A | C24 | H24C | 109.47 |
| 75 | H24B | C24 | H24C | 109.47 |

| | | | | |
|---|---|---|---|---|
| 76 | C16 | C29 | H29A | 109.47 |
| 77 | C16 | C29 | H29B | 109.47 |
| 78 | C16 | C29 | H29C | 109.47 |
| 79 | H29A | C29 | H29B | 109.47 |
| 80 | H29A | C29 | H29C | 109.47 |
| 81 | H29B | C29 | H29C | 109.47 |
| 82 | C9 | C25 | H25A | 109.47 |
| 83 | C9 | C25 | H25B | 109.47 |
| 84 | C9 | C25 | H25C | 109.47 |
| 85 | H25A | C25 | H25B | 109.47 |
| 86 | H25A | C25 | H25C | 109.47 |
| 87 | H25B | C25 | H25C | 109.47 |
| 88 | C4 | C3 | C1 | 121.55 |
| 89 | C4 | C3 | C2 | 123.83 |
| 90 | C1 | C3 | C2 | 114.49 |
| 91 | C12 | C27 | H27A | 109.47 |
| 92 | C12 | C27 | H27B | 109.47 |
| 93 | C12 | C27 | H27C | 109.47 |
| 94 | H27A | C27 | H27B | 109.47 |
| 95 | H27A | C27 | H27C | 109.47 |
| 96 | H27B | C27 | H27C | 109.47 |
| 97 | C13 | C14 | C15 | 116.87 |
| 98 | C13 | C14 | C28 | 121.67 |
| 99 | C15 | C14 | C28 | 121.46 |
| 100 | C18 | C30 | H30A | 109.47 |
| 101 | C18 | C30 | H30B | 109.47 |
| 102 | C18 | C30 | H30C | 109.47 |
| 103 | H30A | C30 | H30B | 109.47 |
| 104 | H30A | C30 | H30C | 109.47 |
| 105 | H30B | C30 | H30C | 109.47 |
| 106 | C6 | C23 | H23A | 109.47 |
| 107 | C6 | C23 | H23B | 109.47 |
| 108 | C6 | C23 | H23C | 109.47 |
| 109 | H23A | C23 | H23B | 109.47 |
| 110 | H23A | C23 | H23C | 109.47 |
| 111 | H23B | C23 | H23C | 109.47 |
| 112 | N1 | C1 | C3 | 177.64 |
| 113 | C14 | C28 | H28A | 109.47 |
| 114 | C14 | C28 | H28B | 109.47 |
| 115 | C14 | C28 | H28C | 109.47 |
| 116 | H28A | C28 | H28B | 109.47 |
| 117 | H28A | C28 | H28C | 109.47 |
| 118 | H28B | C28 | H28C | 109.47 |
| 119 | C20 | C31 | H31A | 109.47 |

| | | | | |
|---|---|---|---|---|
| 120 | C20 | C31 | H31B | 109.47 |
| 121 | C20 | C31 | H31C | 109.47 |
| 122 | H31A | C31 | H31B | 109.47 |
| 123 | H31A | C31 | H31C | 109.47 |
| 124 | H31B | C31 | H31C | 109.47 |
| 125 | N2 | C2 | C3 | 177.45 |

## Coordinates of Optimised geometries

Coordinates of **1**

| | | | |
|---|---|---|---|
| C | -5.882337000 | -0.355366000 | 0.016916000 |
| C | -4.757730000 | -1.028077000 | -0.374248000 |
| C | -3.348084000 | -0.703871000 | -0.248181000 |
| C | -2.831648000 | 0.465931000 | 0.352117000 |
| C | -2.431712000 | -1.643167000 | -0.771024000 |
| C | -1.460065000 | 0.676139000 | 0.404074000 |
| C | -1.062169000 | -1.431186000 | -0.687819000 |
| C | -0.533695000 | -0.260659000 | -0.105508000 |
| B | 1.027766000 | -0.012923000 | -0.023123000 |
| C | 1.556236000 | 1.474527000 | 0.008575000 |
| C | 1.980821000 | -1.273772000 | 0.000800000 |
| C | 2.423611000 | 1.916822000 | 1.047232000 |
| C | 1.170483000 | 2.419520000 | -0.979662000 |
| C | 1.853903000 | -2.290583000 | 0.981886000 |
| C | 2.973594000 | -1.446839000 | -1.008299000 |
| C | 2.848793000 | 3.246723000 | 1.086828000 |
| C | 2.887608000 | 0.995493000 | 2.158397000 |
| C | 1.646441000 | 3.734030000 | -0.920232000 |
| C | 0.265171000 | 2.068672000 | -2.147637000 |

| | | | |
|---|---|---|---|
| C | 2.676295000 | -3.424724000 | 0.935453000 |
| C | 0.918309000 | -2.176567000 | 2.169694000 |
| C | 3.760328000 | -2.598726000 | -1.026473000 |
| C | 3.188495000 | -0.428233000 | -2.110433000 |
| C | 2.480089000 | 4.174057000 | 0.108036000 |
| H | 3.493856000 | 3.567552000 | 1.902836000 |
| H | 3.464121000 | 0.149932000 | 1.770326000 |
| H | 3.520433000 | 1.537295000 | 2.868218000 |
| H | 2.046999000 | 0.578129000 | 2.725713000 |
| H | 1.354941000 | 4.434195000 | -1.701382000 |
| H | -0.790805000 | 2.236328000 | -1.902930000 |
| H | 0.500220000 | 2.695648000 | -3.014355000 |
| H | 0.356182000 | 1.025348000 | -2.461130000 |
| C | 3.632063000 | -3.604505000 | -0.061050000 |
| H | 2.564569000 | -4.184933000 | 1.707084000 |
| H | 1.474334000 | -1.879057000 | 3.069033000 |
| H | 0.123913000 | -1.442608000 | 2.022884000 |
| H | 0.445998000 | -3.140047000 | 2.392891000 |
| H | 4.497259000 | -2.717297000 | -1.819184000 |
| H | 2.296047000 | -0.304276000 | -2.736540000 |
| H | 3.438017000 | 0.559378000 | -1.711110000 |
| H | 4.003532000 | -0.741316000 | -2.770490000 |
| C | 2.994402000 | 5.593201000 | 0.147876000 |
| C | 4.507129000 | -4.834528000 | -0.104245000 |
| H | 4.010334000 | 5.658421000 | -0.264389000 |
| H | 2.360226000 | 6.266319000 | -0.438162000 |
| H | 3.038733000 | 5.974734000 | 1.174001000 |

| | | | |
|---|---|---|---|
| H | 5.568088000 | -4.572902000 | -0.003856000 |
| H | 4.257484000 | -5.531845000 | 0.701528000 |
| H | 4.398969000 | -5.368717000 | -1.056381000 |
| C | -7.168724000 | -0.933939000 | -0.246069000 |
| C | -5.905204000 | 0.911181000 | 0.684310000 |
| N | -8.209040000 | -1.408229000 | -0.462163000 |
| N | -5.951302000 | 1.939862000 | 1.226773000 |
| H | -4.956226000 | -1.976645000 | -0.868411000 |
| H | -3.497671000 | 1.211103000 | 0.769325000 |
| H | -1.087284000 | 1.590663000 | 0.857137000 |
| H | -2.810933000 | -2.549736000 | -1.237024000 |
| H | -0.382192000 | -2.181818000 | -1.080165000 |

Coordinates of **2**

| | | | |
|---|---|---|---|
| B | 1.218532000 | -0.000091000 | 0.071402000 |
| C | -0.364540000 | -0.153280000 | 0.248498000 |
| C | -1.127469000 | -0.904982000 | -0.677445000 |
| C | -1.030771000 | 0.466225000 | 1.336754000 |
| C | -2.524689000 | -1.033086000 | -0.539682000 |
| C | -2.424437000 | 0.366835000 | 1.476336000 |
| C | -3.173117000 | -0.366821000 | 0.525579000 |
| C | 2.135771000 | -1.290291000 | 0.016877000 |
| C | 3.135913000 | -1.430812000 | -0.989996000 |
| C | 1.987149000 | -2.356414000 | 0.947707000 |
| C | 3.916632000 | -2.588500000 | -1.049881000 |
| C | 2.815176000 | -3.481445000 | 0.870323000 |
| C | 3.784683000 | -3.624439000 | -0.122375000 |

| | | | |
|---|---|---|---|
| H | 4.654828000 | -2.681569000 | -1.844627000 |
| H | 2.693200000 | -4.274433000 | 1.605879000 |
| C | 1.850344000 | 1.447821000 | -0.045919000 |
| C | 1.302337000 | 2.436875000 | -0.910780000 |
| C | 2.986835000 | 1.811218000 | 0.733686000 |
| C | 1.885806000 | 3.705625000 | -0.988719000 |
| C | 3.515001000 | 3.102904000 | 0.648836000 |
| C | 2.990230000 | 4.065826000 | -0.215560000 |
| H | 1.457991000 | 4.437703000 | -1.671230000 |
| H | 4.367112000 | 3.362767000 | 1.274635000 |
| C | 0.108437000 | 2.174982000 | -1.809691000 |
| H | 0.230051000 | 1.270376000 | -2.415523000 |
| H | -0.817133000 | 2.052842000 | -1.238630000 |
| H | -0.037758000 | 3.010229000 | -2.501669000 |
| C | 3.665115000 | 0.858427000 | 1.702832000 |
| H | 4.249276000 | 0.093422000 | 1.180691000 |
| H | 4.348576000 | 1.408314000 | 2.357994000 |
| H | 2.956093000 | 0.324678000 | 2.344424000 |
| C | 3.610484000 | 5.437779000 | -0.327267000 |
| H | 4.416866000 | 5.448190000 | -1.073111000 |
| H | 2.873967000 | 6.187114000 | -0.636158000 |
| H | 4.046710000 | 5.760047000 | 0.624383000 |
| C | 3.392974000 | -0.378641000 | -2.054718000 |
| H | 2.474884000 | -0.024471000 | -2.535436000 |
| H | 3.889810000 | 0.505452000 | -1.642393000 |
| H | 4.036485000 | -0.786343000 | -2.840976000 |
| C | 0.975246000 | -2.328492000 | 2.078081000 |

| | | | |
|---|---|---|---|
| H | 1.031411000 | -1.407382000 | 2.668244000 |
| H | -0.051978000 | -2.407769000 | 1.708488000 |
| H | 1.148036000 | -3.164266000 | 2.763558000 |
| C | 4.674291000 | -4.842766000 | -0.182638000 |
| H | 4.861274000 | -5.152119000 | -1.217000000 |
| H | 5.652400000 | -4.642482000 | 0.275162000 |
| H | 4.231381000 | -5.689911000 | 0.351153000 |
| C | -4.630505000 | -0.442132000 | 0.721005000 |
| H | -4.985047000 | -0.764953000 | 1.698280000 |
| C | -5.606842000 | -0.109870000 | -0.167117000 |
| C | -6.990874000 | -0.253929000 | 0.189100000 |
| C | -5.338795000 | 0.436404000 | -1.466631000 |
| N | -8.109321000 | -0.371452000 | 0.485968000 |
| N | -5.138340000 | 0.888155000 | -2.519360000 |
| C | -0.271718000 | 1.230553000 | 2.403935000 |
| H | -0.527781000 | 0.869609000 | 3.407727000 |
| H | 0.807611000 | 1.147117000 | 2.289229000 |
| H | -0.508532000 | 2.302468000 | 2.382884000 |
| C | -0.480195000 | -1.574485000 | -1.875112000 |
| H | 0.557634000 | -1.274165000 | -2.009008000 |
| H | -0.480461000 | -2.668378000 | -1.779650000 |
| H | -1.017798000 | -1.335855000 | -2.800098000 |
| C | -3.273564000 | -1.933328000 | -1.499605000 |
| H | -4.271310000 | -2.186800000 | -1.138358000 |
| H | -3.390607000 | -1.469693000 | -2.486898000 |
| H | -2.733583000 | -2.873942000 | -1.649034000 |
| C | -3.107954000 | 1.080677000 | 2.625640000 |

| | | | |
|---|---|---|---|
| H | -2.762440000 | 2.116849000 | 2.709686000 |
| H | -4.192991000 | 1.121371000 | 2.513393000 |
| H | -2.888935000 | 0.598893000 | 3.588404000 |

**Reference:**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