SUPPORTING INFORMATION

CP-ART-12-2010-002958

Supporting information for the manuscript titled "**A critical theoretical study on the two-photon absorption properties of some selective triaryl borane-1-naphthylphenyl amine based charge transfer molecules**"

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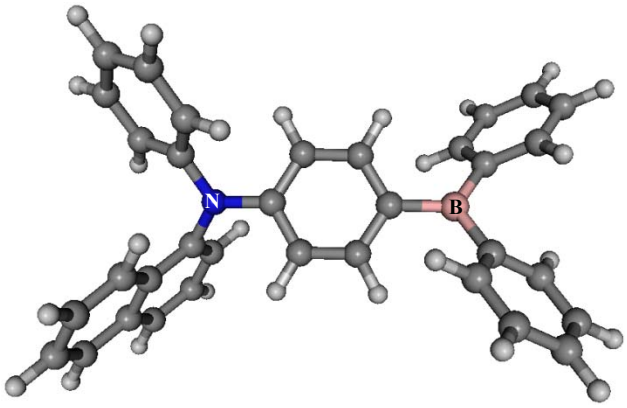
Contents:

1. **Gas phase optimized co-ordinates of the target molecules a) BN1, b) BN2 and c) BN3 and d) benchmark molecule; Optimization has been done at DFT level of theory using B3LYP functional and 6-311G (d, p) basis set**

a) Optimized co-ordinates of BN1 molecule



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C	-5.765809	1.221328	-0.100234
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H	6.417537	-3.185841	1.660675
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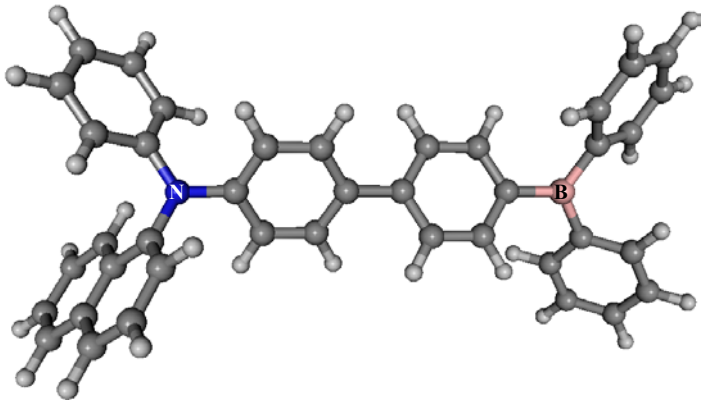
b) Optimized co-ordinates of BN2 molecule



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C	7.115885	3.296705	1.320063
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H	5.380038	2.077554	1.606126
H	8.330841	0.556861	-1.120035
H	6.781849	4.059304	2.015358
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H	8.943130	4.323749	0.826027
H	-6.441381	1.533825	1.342004
H	-3.696244	2.193526	-1.892386
H	-7.676347	3.566972	0.706240
H	-4.914032	4.243149	-2.506236
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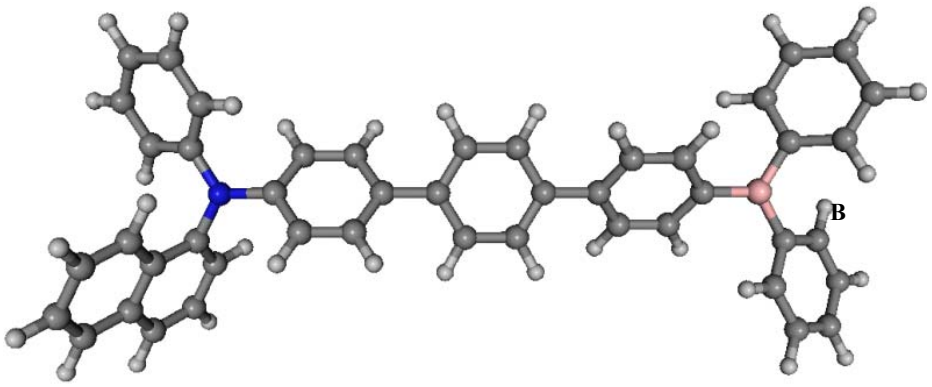
c) Optimized co-ordinates of BN3 molecule



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C	5.834129	0.912879	0.782766
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C	-4.277238	-0.619148	0.486469
C	-4.936628	0.389556	-0.230836
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C	-6.647807	2.758049	0.400565
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C	-7.050635	-0.810793	-0.499511
C	-8.041605	-1.262797	0.429939
C	-6.752104	-1.568390	-1.613173
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H	11.018775	4.521695	0.579351
H	7.380306	-2.615110	1.019479
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H	8.559550	-4.769222	0.839006
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H	10.709964	-4.912675	-0.389935
H	6.374066	1.628232	1.393203
H	6.300799	-1.714895	-1.300788
H	3.929517	1.684880	1.386945
H	3.859937	-1.594076	-1.381724
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H	1.940461	-2.026099	-0.081755
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H	-5.993912	-1.214722	-2.301851
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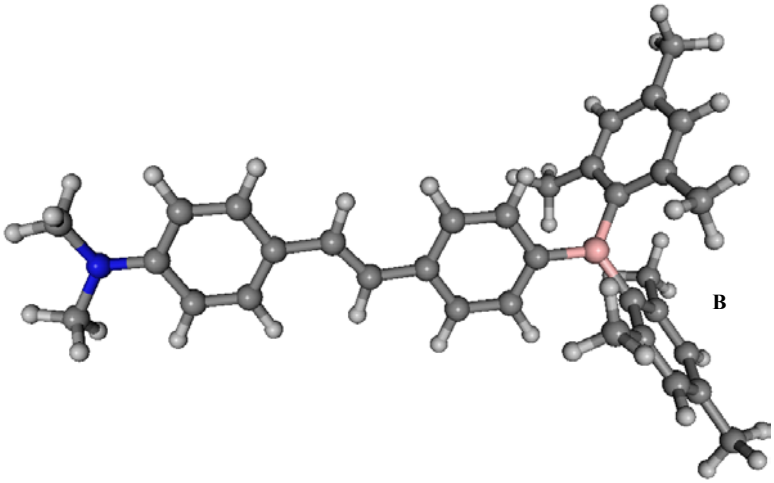
H	-9.536840	-0.490916	3.397492
H	-10.239847	-3.868586	0.845051
H	-8.916879	-4.162020	-1.203896
H	-10.765001	-2.594250	2.892154

d) Optimized co-ordinates of the benchmark molecule



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C	-6.206348	1.181033	0.619651
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C	-8.235534	-0.008038	-0.006516
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H	-5.443482	-1.743010	-0.898955
H	-5.749001	2.051701	1.079487
H	-8.166534	1.905511	1.015077
C	-3.930221	0.329119	0.167360
C	-2.987990	-0.521825	-0.288604
H	-3.605764	1.244888	0.655489
H	-3.304315	-1.441275	-0.774297
C	-1.540461	-0.353762	-0.202400
C	-0.705945	-1.374217	-0.697665
C	-0.912503	0.780663	0.350901
C	0.675720	-1.277073	-0.626560
H	-1.161434	-2.257482	-1.134915
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C	3.249304	2.388084	-0.976716
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C	3.842603	3.652556	-0.919361
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C	3.548371	-2.341238	0.964592
C	5.501634	-2.742898	-0.975205
C	4.339309	-3.493381	0.966236
C	5.315182	-3.722392	-0.000383
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H	4.186880	-4.231000	1.749694
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C	5.041862	-0.566198	-2.096940
C	6.129321	-4.993328	-0.006359
C	4.759079	0.848957	2.202480
C	2.341951	2.106136	-2.159557
C	5.287002	5.410190	0.188714

H	2.834796	-2.768669	2.953786
H	2.337075	-1.180930	2.367653
H	1.548214	-2.620517	1.756229
H	5.321268	0.410299	-1.696827
H	5.857227	-0.918266	-2.732169
H	4.171105	-0.412808	-2.741490
H	7.132577	-4.822421	-0.404477
H	6.228838	-5.408444	0.999334
H	5.656857	-5.759649	-0.631261
H	5.224957	-0.065387	1.830014
H	5.452733	1.323073	2.899845
H	3.876170	0.549618	2.775347
H	2.627667	2.725575	-3.013294
H	2.371689	1.064054	-2.478644
H	1.298047	2.332124	-1.922799
H	5.298183	5.888418	-0.793291
H	4.711318	6.055268	0.861950
H	6.312861	5.382953	0.565501
C	-10.430468	0.884961	0.624165
C	-10.242354	-1.329653	-0.507841
H	-10.285256	0.856380	1.713775
H	-11.480698	0.686913	0.414442
H	-10.212177	1.900209	0.279843
H	-9.923487	-1.604358	-1.517742
H	-11.322136	-1.189585	-0.533152
H	-10.020793	-2.173833	0.160854

Table: S1

1. **Table for TPA tensor elements and two photon transition probability (in a.u) of BN1 molecule using cc-pVDZ, aug-cc-pVDZ and cc-pVTZ basis sets and CAMB3LYP functional (Gas Phase results)**

Basis - Set	States	TPA tensor elements						δ_{TP} (in 10^5 order)
		S_{xx}	S_{yy}	S_{zz}	S_{xy}	S_{xz}	S_{yz}	
cc-pVDZ	1	20.5	18.2	-207.3	-15.7	18.9	6.5	2.369
	2	-15.2	-19.7	-170.2	22.3	53.5	-44.9	2.455
aug-cc-pVDZ	1	-21.1	-20.4	190.4	17.1	-15.8	-9.1	1.98
	2	-13.2	-17.2	-175.6	19.5	52.8	-45.5	2.52
cc-pVTZ	1	-20.3	-18.8	194.9	16.2	-16.9	-7.7	2.084
	2	13.6	17.8	170.6	-20.4	-52.0	43.7	2.403

Table: S2

2. **Table for One-photon absorption data – Excitation energy (in eV), Transition moment (in a.u), Lambda parameter, kappa values and Orbitals involved in the transition (H ≡ HOMO, L ≡ LUMO) for S_1 state of benchmark molecule in THF solvent**

State	Excitation Energy (eV)	Transition moment in a.u			Λ	κ	Orbitals involved
		X	Y	Z			
1	3.30	-0.1249	0.0401	-4.6139	0.5673	-0.6442 -0.1840 -0.1545	H – L H – L+1 H-1 – L

Table: S3

3. **TPA tensor elements and TP transition probability (in 10^5 a.u order) of the benchmark molecule using CAM-B3LYP/cc-pVDZ basis set level of theory in THF solvent**

States	S_{xx}	S_{yy}	S_{zz}	S_{xy}	S_{xz}	S_{yz}	δ_{TP} (in a.u)
1	12.5	2.2	-573.1	5.3	-8.3	4.2	19.39

4. Orbital pictures of benchmark molecule

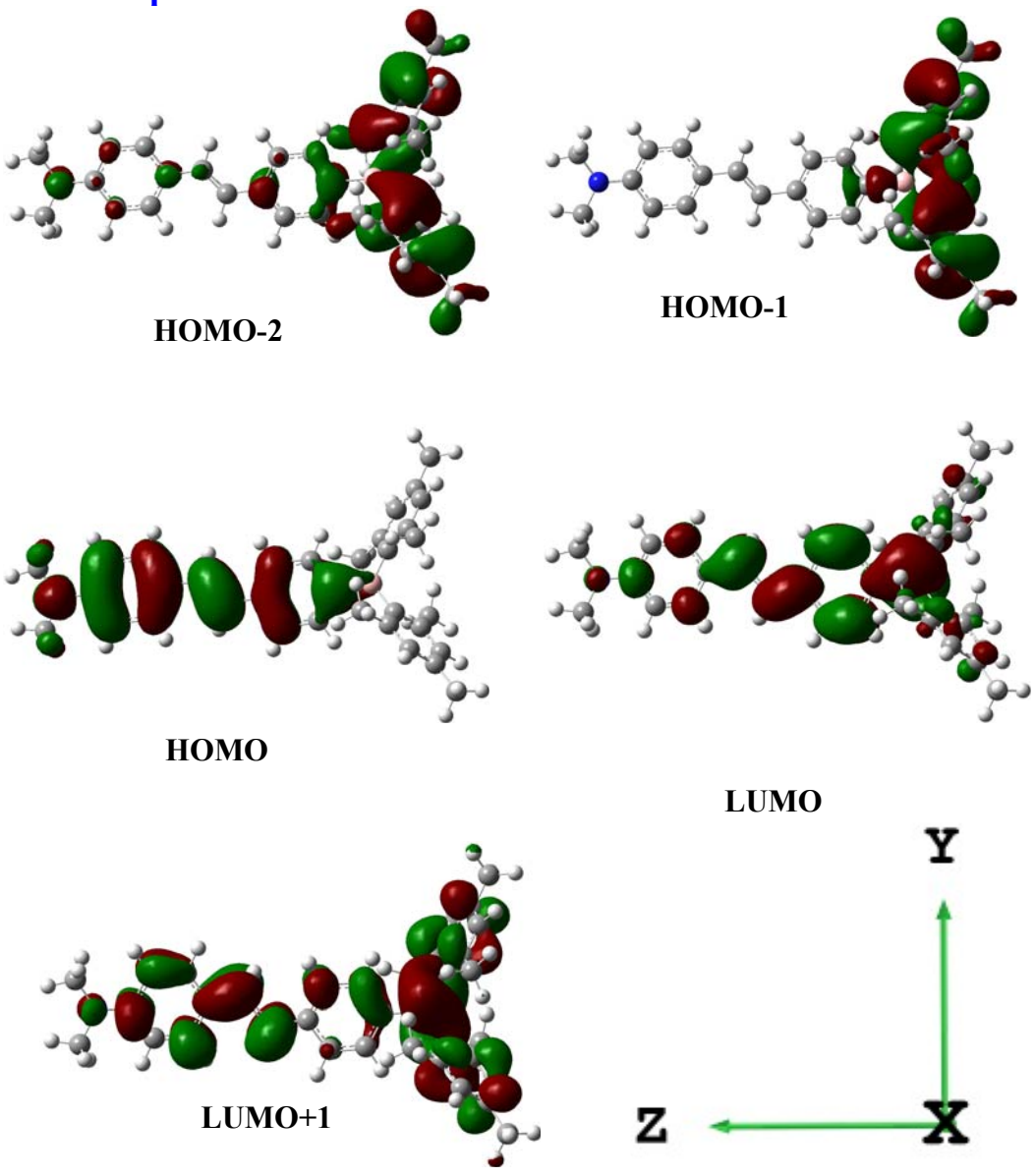

Fig: S1. Molecular orbital pictures of benchmark molecule in THF solvent.

Table: S4

a) **Table for Dipole moment difference between ground and 1st excited states (μ^{11})**

Molecule	μ^{11}		
	X	Y	Z
BN1	-0.260	0.493	-2.450
BN2	-1.206	-0.266	-1.758
BN3	-1.701	-0.662	0.144

b) **Table for Dipole moment difference between ground and 2nd excited states (μ^{22})**

Molecule	μ^{22}		
	X	Y	Z
BN1	-1.222	0.980	0.565
BN2	-0.973	-0.122	-1.408
BN3	-0.447	-0.193	-2.537

c) **Table for transition moment between 1st and 2nd excited states (μ^{21})**

Molecule	μ^{21}		
	X	Y	Z
BN1	1.310	-1.001	-2.821
BN2	-1.546	-0.133	4.110
BN3	1.158	0.543	-3.531

d) **Table for transition moment between 1st and 3rd excited states(μ^{31})**

Molecule	μ^{31}		
	X	Y	Z
BN1	0.243	-0.067	-0.685
BN2	-0.202	0.078	0.770
BN3	-0.061	-0.115	0.394

e) Table for transition moment between 2nd and 3rd excited states (μ^{32})

Molecule	μ^{32}		
	X	Y	Z
BN1	-0.165	0.105	-0.141
BN2	-0.076	-0.026	-0.632
BN3	0.050	-0.023	0.981

f) Table for excitation energy from ground to excited state

Molecule	Excited state	Excitation energy (in a.u)
BN1	1	0.1375
	2	0.1484
	3	0.1629
BN2	1	0.1388
	2	0.1475
	3	0.1607
BN3	1	0.1401
	2	0.1486
	3	0.1601

2. Formula used in Sum-over states calculation

TPA transition moment tensor elements (S_{ij}) are given by,

$$S_{ij} = \sum_{n} \left[\frac{\mu_i^{0n} \mu_j^{nf}}{\omega_n - \frac{\omega_f}{2}} + \frac{\mu_j^{0n} \mu_i^{nf}}{\omega_n - \frac{\omega_f}{2}} \right]$$ Where i, j are the Cartesian components x, y and z.

For $S_0 - S_f$ transition involving 'n' states the formula for S_{ij} becomes

$$S_{ij} = \frac{\mu_i^{00}\mu_j^{0f}}{\omega_0 - \frac{\omega_f}{2}} + \frac{\mu_j^{00}\mu_i^{0f}}{\omega_0 - \frac{\omega_f}{2}} + \frac{\mu_i^{01}\mu_j^{1f}}{\omega_1 - \frac{\omega_f}{2}} + \frac{\mu_j^{01}\mu_i^{1f}}{\omega_1 - \frac{\omega_f}{2}} + \frac{\mu_i^{02}\mu_j^{2f}}{\omega_2 - \frac{\omega_f}{2}} + \frac{\mu_j^{02}\mu_i^{2f}}{\omega_2 - \frac{\omega_f}{2}}$$
$$+ \frac{\mu_i^{03}\mu_j^{3f}}{\omega_3 - \frac{\omega_f}{2}} + \frac{\mu_j^{03}\mu_i^{3f}}{\omega_3 - \frac{\omega_f}{2}} + ... + \frac{\mu_i^{0n}\mu_j^{3f}}{\omega_n - \frac{\omega_f}{2}} + \frac{\mu_j^{0n}\mu_i^{3f}}{\omega_n - \frac{\omega_f}{2}}$$