Supporting Information:

Solvatochromic absorbance and fluorescence probes behaviour within ionic liquid + γ–Butyrolactone mixture

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Table S1. The extent of synergism (Δ) and whether synergism observed for equimolar mixture of [bmim][BF4]+GBL of solvatochromic parameter at 25 ^{0}C.

Parameter	**Extent of synergism (Δ)**	**Synergism observed**
E_T^N	0.5600	yes
π*	-0.5100	no
α	0.5800	yes
β	0.8500	yes
ANS	0.7200	yes
PRODAN	1.2500	yes
Py I_1/I_3	1.2500	yes

Table S2. Experimental values of densities, (ρ), viscosities, (η), of the IL [bmim][BF4] + GBL] mixture at the specified temperatures and 1 atm Pressure.

XIL	η			$(\ln\eta)^E$			Density(ρ)			V^E		
	25°C	30°C	35°C	25°C	30°C	35°C	25°C	30°C	35°C	25°C	30°C	35°
0	1.73	1.62	1.530	0	0	0	1.124	1.119	1.114	0	0	0
0.2	3.74	3.37	3.06	-0.048	-0.051	-0.054	1.158	1.154	1.149	-0.383	-0.394	-0.414
0.4	11.06	9.6	8.41	0.218	0.213	0.21	1.178	1.174	1.17	-0.571	-0.581	-0.606
0.6	20.76	17.82	15.05	0.028	0.048	0.044	1.186	1.182	1.178	-0.101	-0.099	-0.122
0.8	48.74	39.58	32.49	0.063	0.063	0.067	1.194	1.19	1.186	0.083	0.098	0.081
1.0	103.8	81.32	64.18	0	0	0	1.2013	1.1978	1.1941	0	0	0

Table S3. Mulliken charges of optimised BG5, BG6, [bmim][BF_4] and GBL.

Atom	Mulliken charge			
	BG5	**BG6**	**[bmim][BF_4]**	**GBL**
1 N	-0.240730	-0.242100	-0.231958	
2 C	0.241011	0.238234	0.232934	
3 C	0.021845	0.021236	0.027889	
4 C	0.004997	0.012862	0.014118	
5 N	-0.207947	-0.200512	-0.204185	
6 C	0.029615	0.038864	0.035399	
7 C	-0.098456	-0.098265	-0.097416	
8 C	-0.048816	-0.048665	-0.049116	
9 C	-0.092325	-0.091796	-0.091811	
10 C	-0.168496	-0.168273	-0.168311	
11 H	0.234352	0.226549	0.222484	
12 H	0.107220	0.102581	0.110650	
13 H	0.111265	0.094475	0.100245	
14 H	0.092298	0.093078	0.092858	
15 H	0.111042	0.110448	0.114130	
16 H	0.061523	0.063486	0.061321	
17 H	0.057978	0.059868	0.067162	
18 H	0.116554	0.112017	0.117440	
19 H	0.149958	0.155304	0.147954	
20 H	0.070780	0.071035	0.075276	
21 H	0.061792	0.057926	0.061722	
22 H	0.062643	0.062345	0.059864	
23 H	0.054738	0.054735	0.057697	
24 H	0.063529	0.063522	0.062832	
25 H	0.057313	0.058346	0.056877	

26 B	0.722846	0.735247	0.718477	
27 F	-0.435889	-0.431572	-0.437745	
28 F	-0.361666	-0.363030	-0.358830	
29 F	-0.373048	-0.380983	-0.379210	
30 F	-0.420926	-0.418100	-0.418748	
31 O	-0.284443	-0.295826		-0.287581
32 O	-0.266864	-0.258971		-0.287169
33 C	-0.116070	-0.116620		-0.115264
34 C	-0.155136	-0.152582		-0.153425
35 C	0.033987	0.034166		0.037225
36 C	0.343434	0.340754		0.350678
37 H	0.065071	0.064987		0.068568
38 H	0.075102	0.074690		0.068077
39 H	0.094236	0.096251		0.086405
40 H	0.076389	0.079804		0.084763
41 H	0.065713	0.065179		0.073305
42 H	0.083581	0.079303		0.074419

Atom	bminBF4	bmim	BG5	BG5	[bmim][BF4]
C(2)-H	8.15	8.27	8.16	8.16	1.0000000000
C(4)-H	7.40	7.5	7.41	7.41	1.0000000000
C(5)-H	7.40	7.5	7.41	7.41	1.0000000000
C(6)-H	2.91	3.15	2.94	2.94	1.0000000000
C(7)-H	3.17	3.38	3.21	3.21	1.0000000000
C(8)-H	0.84	1.13	0.85	0.54	1.0000000000
C(9)-H	0.51	0.77	0.54	0.52	1.0000000000
C(10)-H	0.19	0.34	0.2	0.2	1.0000000000

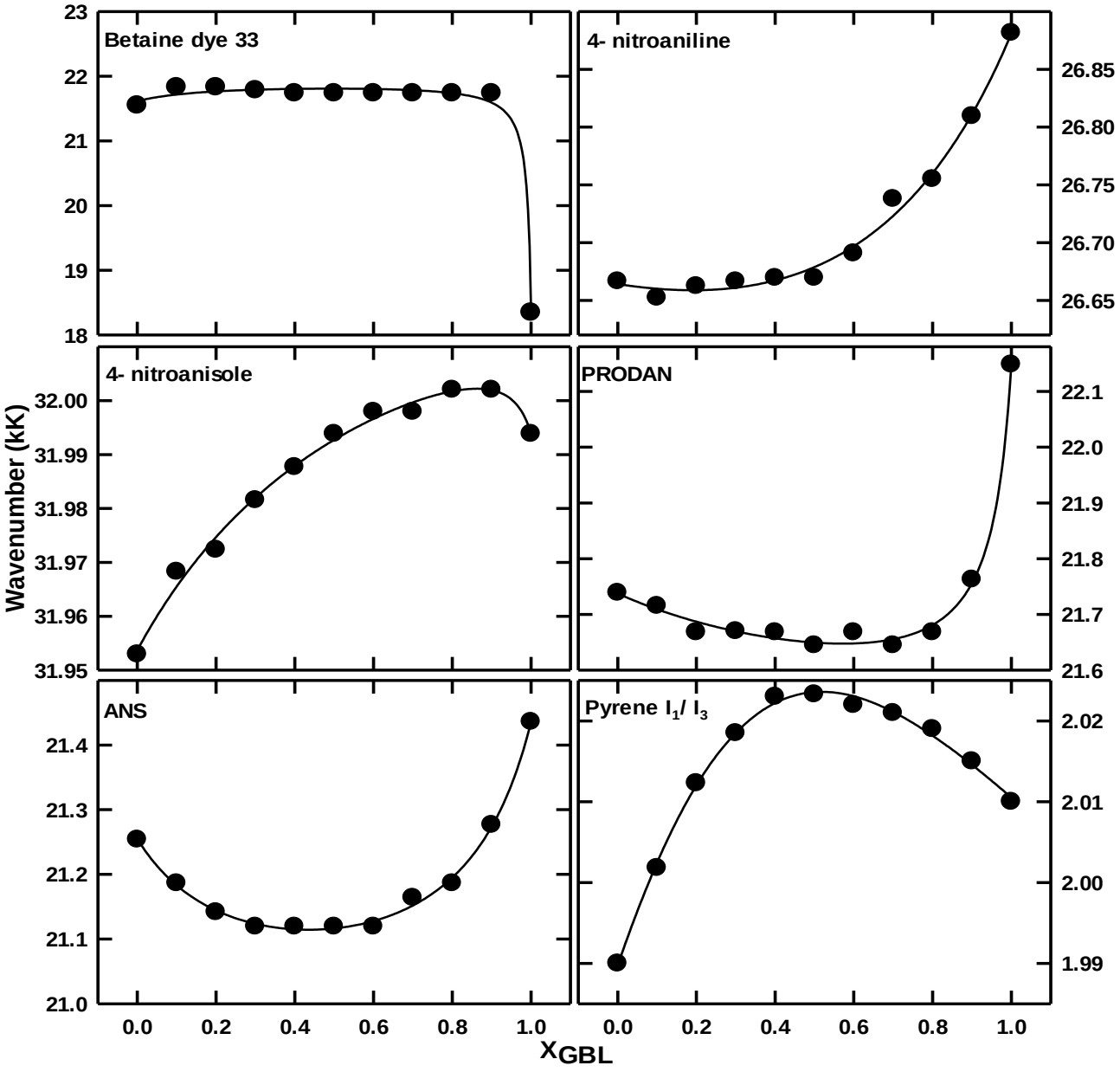

Figure S1. Maximum wave number of various indicators (i.e., betaine dye 33, 4–nitroaniline, 4–nitroanisole, PRODAN, ANS, and pyrene) in [bmim][BF_4] + GBL. Solid line represents fitting using preferential solvation model (eq 14).

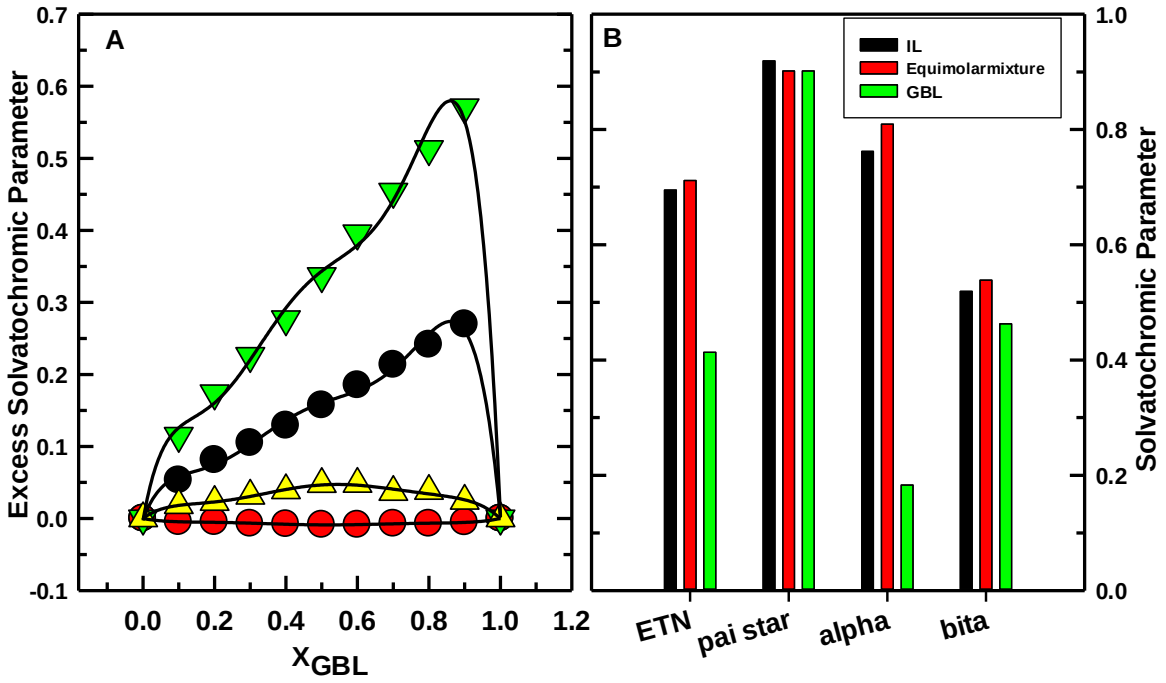

Figure S2. Variation in excess solvatochromic properties (ΔE_T^N •, $\Delta\pi^*$ • , $\Delta\alpha$ ▼ , and $\Delta\beta$ ▲) with X_{GBL} in IL + GBL (co solvent) mixture at ambient conditions and fits the curves according to the Redlich–Kister eq 15 in panel (A), whereas corresponding solvatochromic parameters represents in panel (B) by bar plots, respectively.

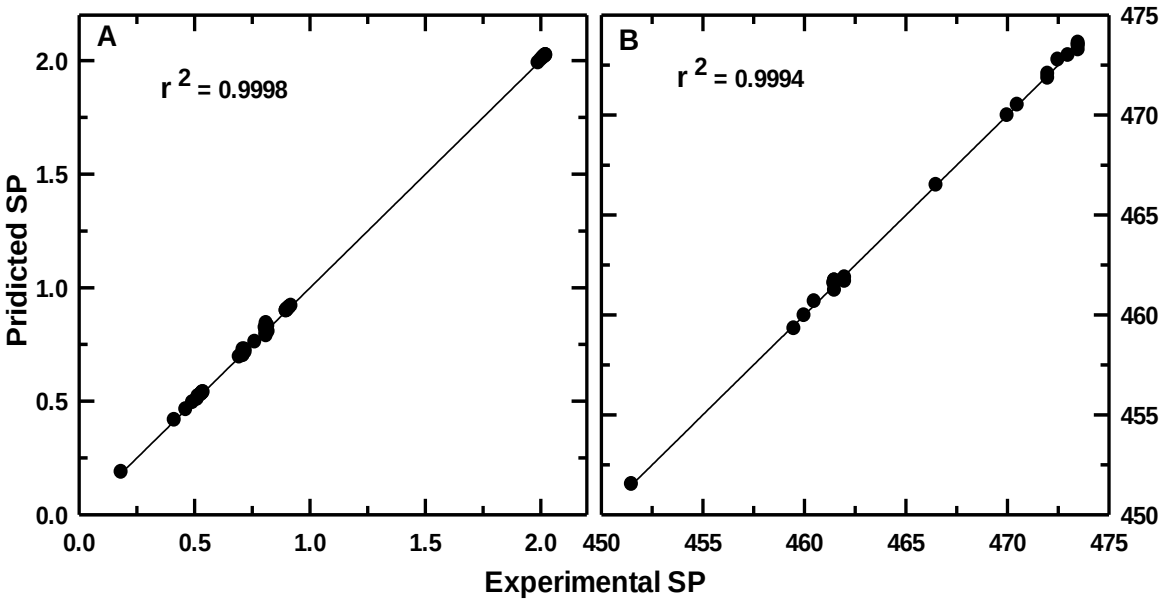

Figure S3. Predicted values of solvatochromic parameters from the correlation equation *versus* its experimental values (E_T^N, α, β, and π* and Py I_1/I_3 (Panel A)) and (emission maxima of ANS and PRODAN (Panel B)) for binary mixtures of [bmim][BF_4]+GBL.

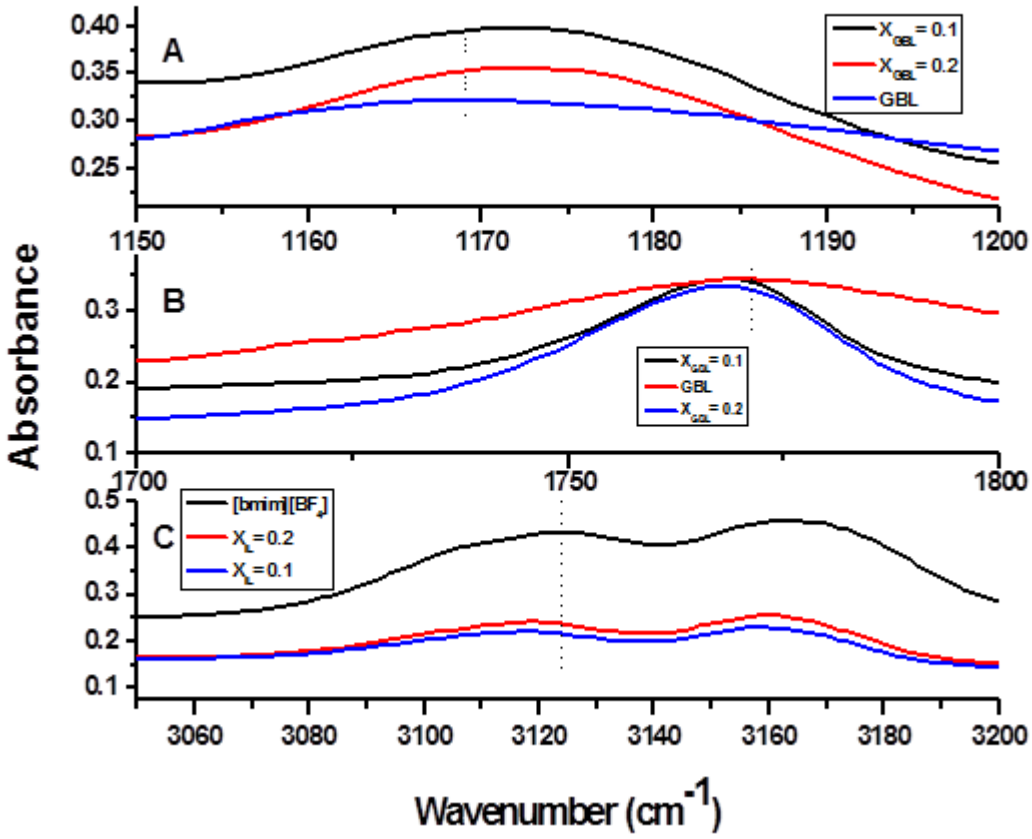

Figure S4. FTIR spectra of representative [bmim][BF_4] + GBL mixtures in the (A)1150–1200 cm^{-1}, (B) 1700–1800 cm^{-1} , and (C) 3050–3200 cm^{-1} windows.

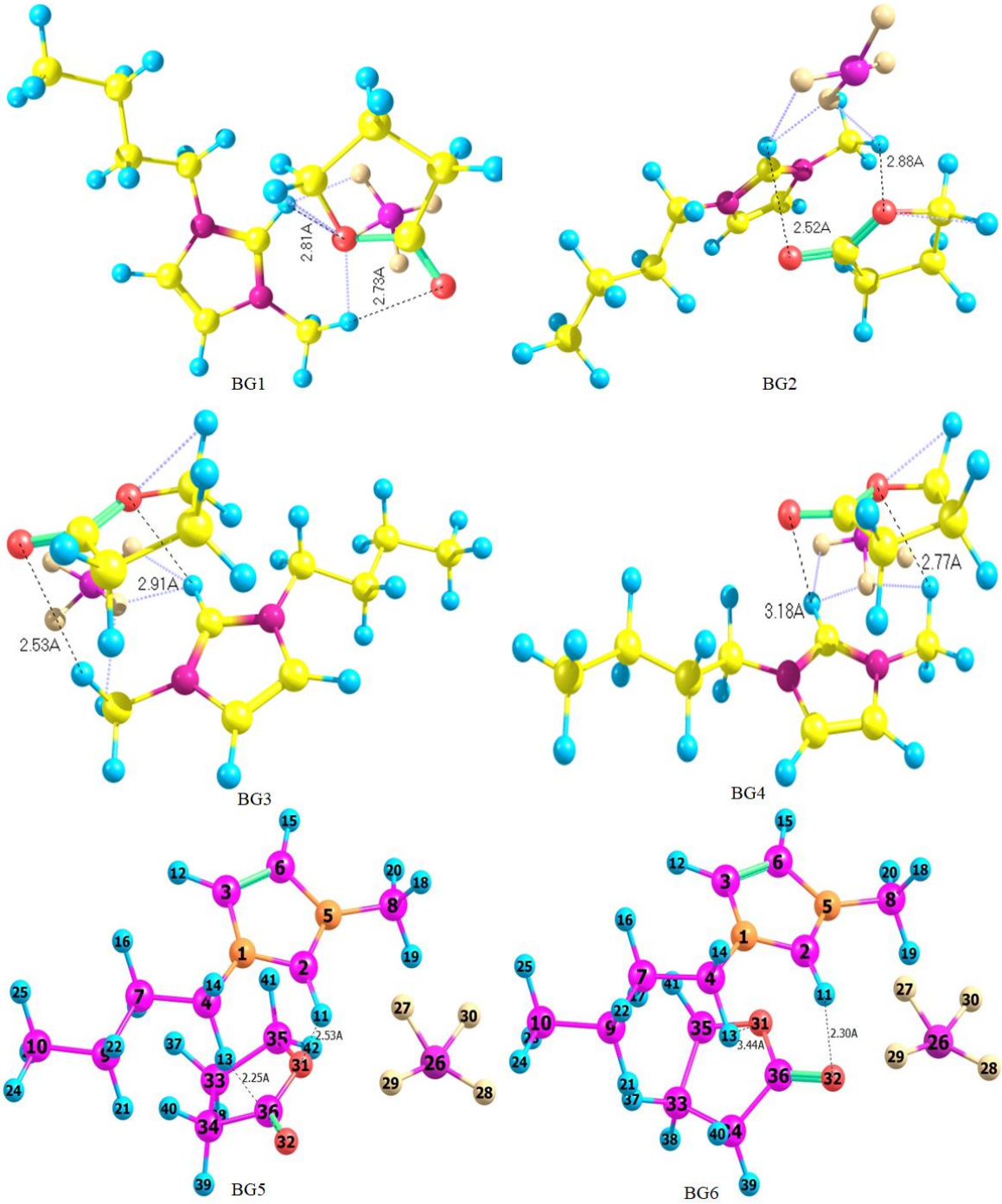

Figure S5. The optimised geometries for exploring interactions between [bmim][BF_4] and GBL in six state BG1, BG2, BG3, BG4, BG5 and BG6.

Calculation of individual HOMO, LUMO, and gap between them for BG 5 as follows:

ENERGY COMPONENTS

WAVEFUNCTION NORMALIZATION	=	1.0000000000
ONE ELECTRON ENERGY	=	-5632.8127803805
TWO ELECTRON ENERGY	=	2460.3222844494
NUCLEAR REPULSION ENERGY	=	2040.4585841232
TOTAL ENERGY	=	-1132.0319118078

ELECTRON-ELECTRON POTENTIAL ENERGY	=	2460.3222844494
NUCLEUS-ELECTRON POTENTIAL ENERGY	=	-6760.6321013991
NUCLEUS-NUCLEUS POTENTIAL ENERGY	=	2040.4585841232
TOTAL POTENTIAL ENERGY	=	-2259.8512328264
TOTAL KINETIC ENERGY	=	1127.8193210186
VIRIAL RATIO (V/T)	=	2.0037351646

ELECTROSTATIC MOMENTS

POINT 1	X	Y	Z (BOHR)	CHARGE
	4.603696	-5.421985	-1.724263	-0.00 (A.U.)
	DX	DY	DZ	/D/ (DEBYE)
	-15.632855	-1.983945	-3.685793	16.183549

HOMO = -1.653363 eV

LUMO = -0.441928 eV

Gap = 1.2114508 eV

Calculation of individual HOMO, LUMO, and gap between them for BG 6 as follows:

ENERGY COMPONENTS

WAVEFUNCTION NORMALIZATION	=	1.0000000000
ONE ELECTRON ENERGY	=	-5640.8517168914
TWO ELECTRON ENERGY	=	2464.4904562146
NUCLEAR REPULSION ENERGY	=	2044.3315662750
TOTAL ENERGY	=	-1132.0296944017

ELECTRON-ELECTRON POTENTIAL ENERGY	=	2464.4904562146
NUCLEUS-ELECTRON POTENTIAL ENERGY	=	-6768.6553114435
NUCLEUS-NUCLEUS POTENTIAL ENERGY	=	2044.3315662750
TOTAL POTENTIAL ENERGY	=	-2259.8332889538
TOTAL KINETIC ENERGY	=	1127.8035945521
VIRIAL RATIO (V/T)	=	2.0037471949

ELECTROSTATIC MOMENTS

POINT 1	X	Y	Z (BOHR)	CHARGE
	4.345900	-5.266719	-1.771932	-0.00 (A.U.)
	DX	DY	DZ	/D/ (DEBYE)
	-15.374041	-4.327245	-3.409390	16.331262

HOMO = -1.440026 eV

LUMO = -0.303951 eV

Gap = 1.136075 eV