Complementary materials

Possibility of magnetic [BN Fullerene: B_6 cluster]$^-$ nanocomposite as vehicle for the delivery of Dapsone

[1]J. Cano Ordaz, [1,*]E. Chigo Anota, [2]M. Salazar Villanueva, [3]M. Castro

[1]Benemérita Universidad Autónoma de Puebla, Facultad de Ingeniería Química, Ciudad Universitaria, San Manuel, Puebla, Código Postal 72570, México.

[2]Benemérita Universidad Autónoma de Puebla, Facultad de Ingeniería, Apdo. Postal J-39, Puebla, Pue., 72570, México.

[3]Universidad Nacional Autónoma de México-Departamento de Física y Química Teórica, DEPg-Facultad de Química, México D.F., C.P. 04510, México.

[*] Corresponding author: [1]*ernesto.chigo@correo.buap.mx

Complementary Materials

Table S1. Total energy for three geometries for the BN fullerene —B_6^- cluster. Total energy (a. u.) and global charge. At the level HCTH/DNP.

Geometry	**Total energy** / Global charge
C1− Perpendicular al hexágono 5N1B	-2717.5678544
C2− Perpendicular al átomo de Boro	-2717.5680335
C3− Perpendicular al átomo de Nitrógeno	-2717.6363697; Q=0
C3− Perpendicular al átomo de Nitrógeno	-2717.7574748; Q= −1
	-2717.4077556; Q= +1
C3− Refinado con GAUSSIAN 6-311g(d)	-2715.89535270; Q= 0, M=1
	-2715.86481980; Q= 0, M=3; Octahedral structure
C3− Refinado con GAUSSIAN 6-311g(d,p)	-2716.12640691; Q= −1, M=2 Pyramidal structure of minimum energy ΔE(M2VsM4)= 2.51 eV
	-2716.03411350; Q= −1, M=4
	-2715.98542100; Q= −1, M=6; Triangular structure
	-2715.77636749 ; Q= +1, M=2

Table S2. The total energy obtained at the level HSEh1PBE/6-31g(d) and 6-311g(d,p) for the BNF^{-}—Dapsone systems and $[BNF:B_6]^{-}$Dapsone (six geometries).

Geometry	**Total energy** (a. u) /Q=0, M=1	**Total energy** (a. u)
C1— Perpendicular 5N1B—SO_2	-3688.36632680	
C2— Perpendicular N—NH_2	-3688.36561584	
C3— Perpendicular B— SO_2	-3688.36641837	
C4— Perpendicular N— SO_2	-3688.36541082	
C5— Perpendicular B—NH_2	6-31g(d) -3688.36764086; Q=0; M=1 -3688.27459250; Q=0; M=3 -3688.39619322; Q= -1; M=2 -3688.28162903; Q= -1; M=4 **ΔE** (M2 Vs M4) = **2.53 eV**	6-311g(d,p) -3689.11966922; Q= -1; M= 2 -3689.00602133; Q= -1; M= 4 **ΔE** (M2 Vs M4) = **2.48 eV**
C6— Perpendicular 5N1B—NH_2	-3688.36662692	
P1—Perpendicular B (Cluster)—SO_2		-3838.04609103; Q= -1, M=2
P2— Perpendicular B (Cluster)—NH_2		-3838.04261035
P3— Lateral B (Cluster)—NH_2		-3838.04825259; Q= -1, M= 2 The most stable -3837.99298685; Q= -1, M= 4 **ΔE** (M2 Vs M4) = **1.50 eV**
P4— Lateral B (Cluster)—SO_2		-3838.04105137

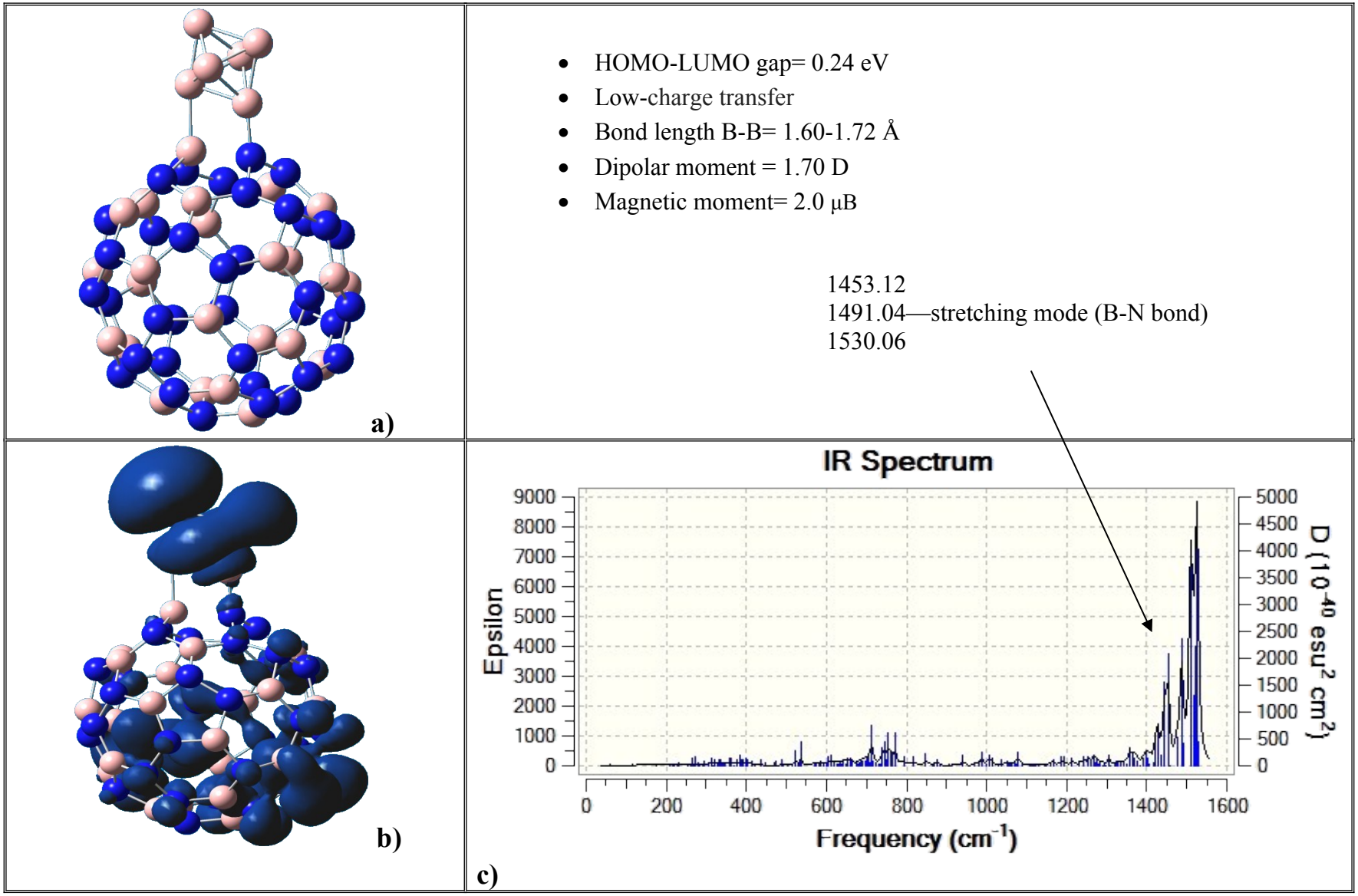
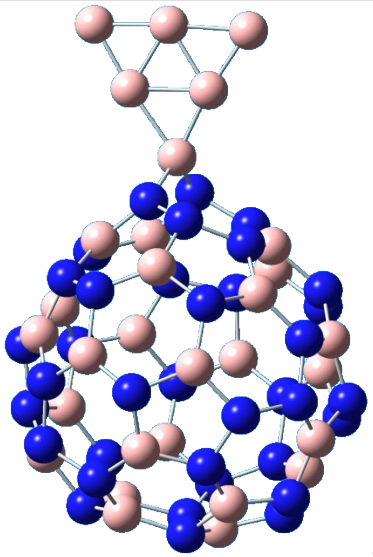


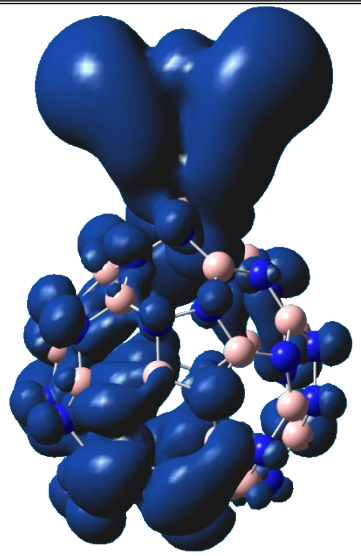
Figure S1. a) BN fullerene functionalized with B_6^-clsuter where it is observed that the octahedral structure is maintained for Q= −1 and M= 3, **b**) spin density surface located on the B_6 cluster and BN fullerene, **c**) IR spectrum.



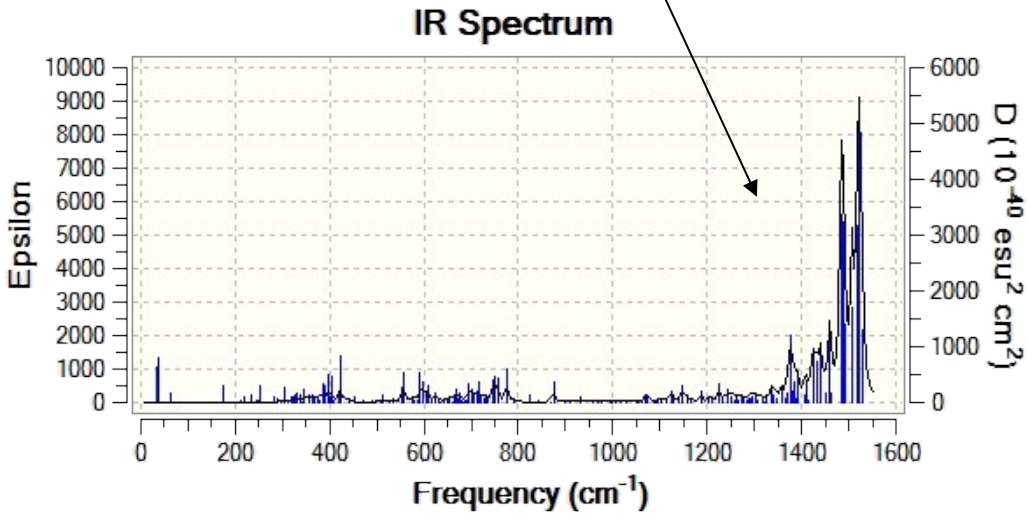
a)

- HOMO-LUMO gap= 1.23 eV
- High charge transfer
- Bond length B-B= 1.60-1.79 Å
- Dipolar moment = 19.40 D
- Magnetic moment= 5.0 μB

1487.11
1523.21—stretching for the B-N bond



b)



c
)

Figure S2. a) BN fullerene functionalized with B_6^- cluster where it is observed that the triangular structure is remained for Q= −1 and M= 6, **b**) spin density surface located on the B_6 cluster and BN fullerene, **c**) IR spectrum.