

Supplementary Materials

Table S1. Continue of Table 1. $B_2N^{(-,0,+)}$ in ground and exited states, Electric Potential (EP) and Isotropic Fermi Contact Couplings (MHz) (IFCC) for isolated and non- isolated positions of BNB.

State (*N _e)	$E_e +$ (-104(Hartree) Isolated BNB	Configuration (Energy of $ \alpha\rangle$ * (Homo - Lumo)**	β electron Configuration Total Energy of $ \beta\rangle$ * Beta virtual**	$r_e(B_1N)$ $r_e(NB_2)$ (*)in BNNT	A_1 (2,1,3,-2,-1) A_2 (2,1,3,-1,-2)	$B^{EP_1} - N^{EP_2} - B^{EP_3}$ *Dipole **IFCC(N,B ₁ ,B ₂) isolated	$B^{EP_1} - N^{EP_2} - B^{EP_3}$ *Dipole **IFCC(N,B ₁ ,B ₂)in BNNT(non-isolated)
$\tilde{A}^2\Sigma_g^+$ (*17e)	-0.1047579 ^k -0.0781729 ^{k'}	$[A']\pi_u^4, 4\sigma_g^1, 3\sigma_u^2 \alpha\rangle$ = -0.44640 ^u * (-34.8739) ^u ** (-0.48630) ^u	$[A']\pi_u^4, 4\sigma_u^1 = -0.26129$ * (-34.15399) ** (-0.17670)	1.3149 ^k 1.3149 ^k	$A_1 = 180.0^k$ $A_2 = 180.0^k$		
$\tilde{X}^2\Sigma^+$ (C _{ov}) (*17e)	-0.0781960 ^a -0.0820329 ^{a'} -0.0754909 ^{a''}	$[A], \pi^4, \sigma^2, \sigma^1 \alpha\rangle = -0.44639^a$ * $E(\alpha\rangle) = -34.87079)^a$ ** (-0.48609) ^a	$[B]\sigma^1 \beta\rangle = -0.26179^a$ * (-34.15050) ^a ** (-0.17700) ^a				
$\tilde{X}^1\Sigma_g^+$ (*18e)	-0.1145479 ^c -0.1162879 ^{c'} -0.112569 ^{c''}	$[A']\pi_u^4, \sigma_g^2, \sigma_u^2 = -0.13449^c$		1.3460 ^c 1.3460 ^c	$A_1 = 179.897^c$ $A_2 = 179.911^c$		
$\tilde{X}^1\Sigma_g^+$ (*18e)	-0.1965675 ^b	* $E(\alpha\rangle) = -32.48644^b$		1.3291 ^b 1.3291	$A_1 = 180.0^b$ $A_2 = 180.0$		
$\tilde{X}^1\Sigma_g^+$ (*16e)	-1.7454370 ^d -1.8054929 ^{a'} -1.7545011 ^{a''}	$[D](1\pi_u^4), (4\sigma_g^2 = -0.57791^a)$ * $E(\alpha\rangle) = -36.52420^a$ ** -0.17930 ^a		1.2941 ^v 1.2941 ^v	$A_1 = 180.0^v$ $A_2 = 180.0^v$	$EP_1 = EP_3 = -11.50^v$ $EP_2 = -18.39^v$ * 0.000	$EP_1 = EP_3 = -11.03^v$ $EP_2 = -18.04^v$ * 0.007
$\tilde{X}^1\Sigma_g^+$ (*16e)	-1.6023119 ^m -1.3012049 ^g -1.8377399 ^f -1.7903299 ^h	$[D](1\pi_u^4), (4\sigma_g^2 = -0.57799^g)$ * $E(\alpha\rangle) = -36.51990^g$ ** -0.17939 ^g		1.3150 ^m 1.3150 ^m 1.3013 ^h 1.3014 ^h	$A_1 = 179.979^m$ $A_2 = 179.979^m$		

a QCISD/EPR-III; **d** CASSCF(11,12)/UHF **zb3p86/6-31g***; **a'** MP4D/EPR-III//QCISD/EPR-III **m** CASSCF(10,12)/EPR-II **xb3lyp/6-31g***; **a''** MP4SDQ/EPR-III//QCISD/EPR-III **g** CASSCF(10,12)/ROHF **AUG-cc-pvqz ym062x/epr-ii**; **b** QCISD/EPR-III($\theta_{const} = 180.0$) **[A]**: $1\sigma^2, 2\sigma^2, 3\sigma^2, 4\sigma^2, 5\sigma^2$ **wb3lyp/6-31g***; **c** QCISD/EPR-II **[A']**: $1\sigma_g^2, 1\sigma_u^2, 2\sigma_g^2, 3\sigma_g^2, 2\sigma_u^2$ **v** CASSCF(11,12)/ **AUG-cc-pvqz**; **c'** MP4D/EPR-II//QCISD/EPR-II **[B]**: $\sigma^1, \sigma^1, \sigma^1, \sigma^1, \pi^2$ **nCBS40**; **c''** MP4SDQ/EPR-II//QCISD/EPR-II **[B']**: $1\sigma_g^1, 2\sigma_g^1, 1\sigma_u^1, 3\sigma_g^1, 2\sigma_u^1, 1\pi_u^2$ **uTD/EPR-II**; **f** CBS-lq; **h**QCISD(T)/EPR-III **[C]**: $1\sigma_g^2, 1\sigma_u^2, 2\sigma_g^2, 3\sigma_g^2, 2\sigma_u^2, 4\sigma_g^2$ **[C']**: $1\sigma_g, 1\sigma_u, 2\sigma_g, 3\sigma_g, 2\sigma_u$; **k**TD/EPR-III//QCISD (T)/EPR-III **K'** TD/EPR-III//QCISD /EPR-III **[D]**: $1\sigma_g^2, 2\sigma_g^2, 1\sigma_u^2, 3\sigma_g^2, 2\sigma_u^2$.

Table S2. Continue of table 2. Energies of $B_2N^{(-,0,+)}$ in ground and exited states inside the BNNT ring.

State E_e (Hartree) of BNB inside BNNT (+104)	All electron Configuration * (Homo - Lumo)	β electron $r_e(B_1N), r_e(NB_2)$ * (Homo - Lumo) in BNNT
Radical(*17e)		
$\tilde{X}^2\Sigma^+$ (C _{ov})	-0.3236680 ^a $[A], \pi^4, \sigma^2, \sigma^1 \alpha\rangle = -0.32764^a$ * (-0.11361) ^a	$[B]\sigma^1 \beta\rangle = -0.26180^a$ * (-0.10711) ^a 1.3005 ^a , -1.3111 ^a $\Delta = 0.04$
$\tilde{X}^2\Sigma^+$ (C _{ov})	-0.7363845 ^b $[A], \pi^4, \sigma^2, \sigma^1 \alpha\rangle = -0.29698^b$ * (-0.08395) ^b	$[B]\sigma^1 \beta\rangle = -0.27855^b$ * (-0.06184) ^b 1.3405 ^b , -1.2995 ^b $\Delta = 0.02$
$\tilde{B}^4\Pi_g$	-0.4168690 ^c $[A']\pi_u^4, \pi_g^2, \sigma_g^1 \alpha\rangle = -0.24531^c$	$[A']\pi_u^2 \beta\rangle = -0.28057^c$ 1.3164 ^c , -1.2994 ^c

$(D_{\infty h})$		$* (-0.05861)^c$	$* (-0.05587)^c$	$\Delta = 0.03$
Anion(*18e)				
$\tilde{X}^1\Sigma_g^+$ ($D_{\infty h}$)	-0.4992770^c	$[A']\pi_u^4, \sigma_g^2, \sigma_u^2 = -0.16695^c$ $* (-0.08082)^c$		$1.326^c, -1.348^c$ $\Delta = 0.00$
Cation (*16e)				
$\tilde{X}^1\Sigma_g^+$ ($D_{\infty h}$)	-0.2335070^c	$[D](1\pi_u^4), (4\sigma_g^2 = -0.46871^c)$ $* (-0.02983)^c$		$1.285^c, -1.286^c$ $\Delta = 0.02$
$\tilde{X}^1\Sigma_g^+$ ($C_{\infty v}$)	-0.234080^c	$[D](1\pi_u^4), (4\sigma_g^2 = -0.46856^c)$ $* (-0.02957)^c$		$1.313^c, -1.302^c$ $\Delta = 0.04$
aM062x/6-31g*dM062x/EPR-II; bB3p86/6-31g*eB3p86/EPR-II; cB3LYP/6-31g*; ; [A]: $1\sigma^2, 2\sigma^2, 3\sigma^2, 4\sigma^2, 5\sigma^2$ [A']: $1\sigma_g^2, 1\sigma_u^2, 2\sigma_g^2, 3\sigma_g^2, 2\sigma_u^2$ [B]: $\sigma^1, \sigma^1, \sigma^1, \sigma^1, \sigma^1, \pi^2$. [B']: $1\sigma_g^1, 2\sigma_g^1, 1\sigma_u^1, 3\sigma_g^1, 2\sigma_u^1, 1\pi_u^2$ [C]: $1\sigma_g^2, 1\sigma_u^2, 2\sigma_g^2, 3\sigma_g^2, 2\sigma_u^2, 4\sigma_g^2$ [C']: $1\sigma_g, 1\sigma_u, 2\sigma_g, 3\sigma_g, 2\sigma_u$ [D]: $1\sigma_g^2, 2\sigma_g^2, 1\sigma_u^2, 3\sigma_g^2, 2\sigma_u^2$				

Table S3. Continue of Table 3. Charges from ECP fitting for BNB in two position of isolated and external field of (5, 5) BNNT.

State of BNB	$\gamma = \frac{V_B - V_N}{r_{BN}}$	$f_{\text{force}} = (\Sigma_x^2 + \Sigma_y^2 + \Sigma_z^2)^{\frac{1}{2}},$ $\theta = \text{angle of force vector},$ $\delta(q_B - q_N) \text{ from ECP}$	$*B^{\delta q_1} - N^{\delta q_2} - B^{\delta q_3} \&$ $\Delta = r_1(B_1N) - r_2(B_2N)$ Inside BNNT Charges from ESP fitting
$\tilde{X}^2\Sigma_u^+$ Radical	$\gamma = 4.7184^a$ $\gamma = 4.7168^a$ $\gamma = 4.7191^a$ $\gamma = 4.7186^a$	$0.89, -38.18^\circ, 0.806^a$ $0.86, -53.92^\circ, 0.804^a$ $0.88, -55.22^\circ, 0.807^a$ $0.93, -37.11^\circ, 0.806^a$	$\Delta^u = 0.2 \& \delta q_1 = \delta q_3 = 0.31, \delta q_2 = -0.42$ $\Delta^u = 0.1 \& \delta q_1 = 0.30, \delta q_3 = 0.20, \delta q_2 = -0.40$ $\Delta^k = 0.2 \& \delta q_1 = -0.16, \delta q_3 = -0.16, \delta q_2 = 0.52$ $\Delta^k = 0.1 \& \delta q_1 = 0.40, \delta q_3 = 0.40, \delta q_2 = -0.9$ $\Delta^k = 0.32 \& \delta q_1 = -0.15, \delta q_3 = -0.15, \delta q_2 = 0.62$ $\Delta^y = 0.13 \& \delta q_1 = \delta q_3 = -0.23, \delta q_2 = 0.59$ $\Delta^y = 0.22 \& \delta q_1 = -0.08, \delta q_3 = -0.06, \delta q_2 = 0.36$ $\Delta^y = 0.2 \& \delta q_1 = 0.12, \delta q_3 = 0.03, \delta q_2 = -0.35$
$\tilde{X}^1\Sigma_g^+$ Anion	$\gamma = 4.6644^a$ $\gamma = 4.6630^a$ $\gamma = 4.6651^a$ $\gamma = 4.6649^a$	$1.28, -88.21^\circ, 0.232$ $1.35, -3.39^\circ, 0.228$ $1.23, -2.79^\circ, 0.232$ $1.41, -89.59^\circ, 0.242$	$\Delta^z = -0.6 \& \delta q_1 = \delta q_3 = -0.60, \delta q_2 = 0.6$ $\Delta^z = -0.8 \& \delta q_1 = -0.60, \delta q_3 = -0.6, \delta q_2 = 0.4$ $\Delta^z = -0.8 \& \delta q_1 = -0.81, \delta q_3 = -0.69, \delta q_2 = 0.7$ $\Delta^z = -0.7 \& \delta q_1 = -0.71, \delta q_3 = -0.39, \delta q_2 = 0.4$ $\Delta^x = -0.8 \& \delta q_1 = \delta q_3 = -1.0, \delta q_2 = 1.2$ $\Delta^x = -0.9 \& \delta q_1 = -1.04, \delta q_3 = -1.04, \delta q_2 = 1.18$ $\Delta^x = -0.9 \& \delta q_1 = -1.01, \delta q_3 = -0.99, \delta q_2 = 1.1$ $\Delta^x = -0.9 \& \delta q_1 = -1.03, \delta q_3 = -1.06, \delta q_2 = 1.19$ $\Delta^x = -0.8 \& \delta q_1 = -0.79, \delta q_3 = -0.86, \delta q_2 = 0.85$
$\tilde{X}^1\Sigma_g^+$ Cation			$\Delta^x = +0.9 \& \delta q_1 = 0.30, \delta q_3 = 0.29, \delta q_2 = 0.31$ $\Delta^x = +0.9 \& \delta q_1 = 0.32, \delta q_3 = 0.38, \delta q_2 = 0.2$ $\Delta^x = +0.8 \& \delta q_1 = 0.20, \delta q_3 = 0.4, \delta q_2 = 0.2$ $\Delta^x = +0.9 \& \delta q_1 = 0.20, \delta q_3 = 0.55, \delta q_2 = 0.15$

^a QCISD/EPR-III; ^u m062x/6-31g*; ^b b3p86/6-31g*; ^y hf/epr-ii*hf/6-31g*; ^z m062x/epr-ii.