Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information for chemical communications

Li@Organic Superhalogens: Possible Electrolytes in Li-ion Batteries

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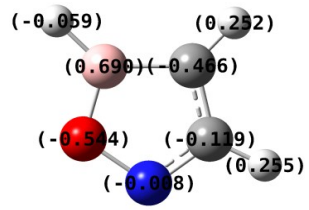
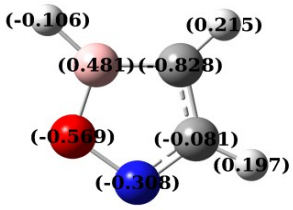
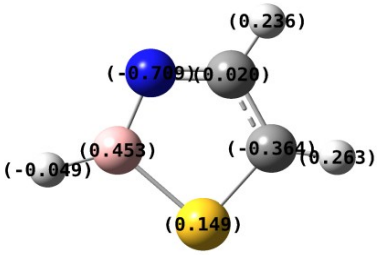
Figure S1. Natural Bond Orbital(NBO) Charges of neutral and anion of $[C_2H_3BNO]$, $[C_2H_3BNS]$, $[C_3H_4BN_2]$, $[C_3H_4BS]$, and $[C_4H_5BN]$.



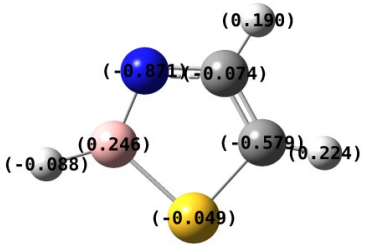
$[C_2H_3BNO]$



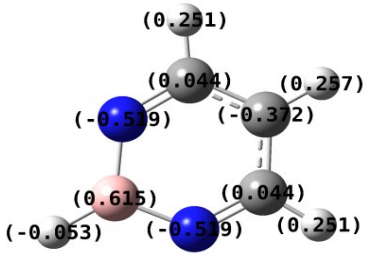
$[C_2H_3BNO]^-$



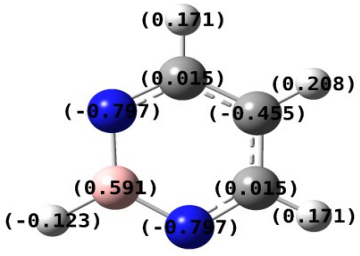
$[C_2H_3BNS]$



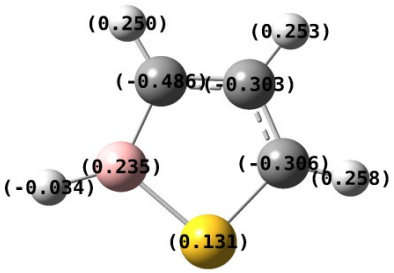
$[C_2H_3BNS]^-$



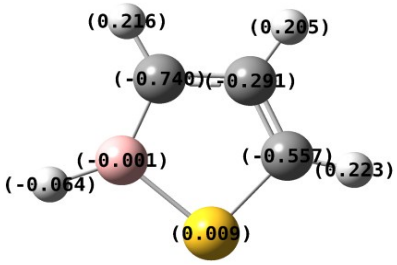
$[C_3H_4BN_2]$



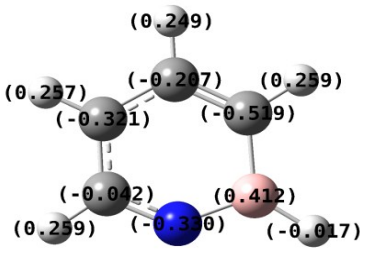
$[C_3H_4BN_2]^-$



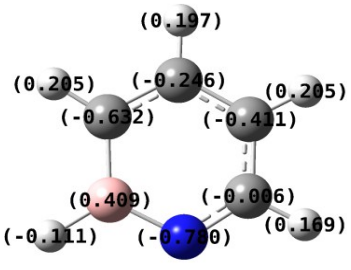
$[C_3H_4BS]$



$[C_3H_4BS]^-$

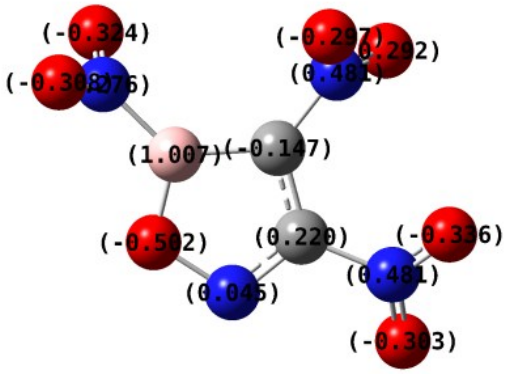


$[C_4H_5BN]$

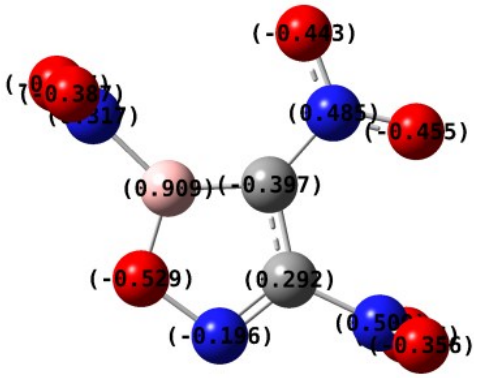


$[C_4H_5BN]^-$

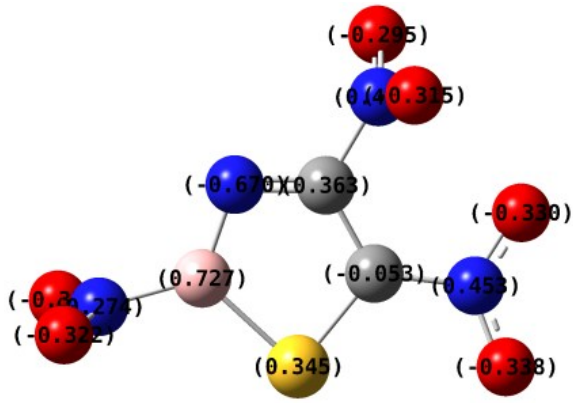
Figure S2. Natural Bond Orbital(NBO) Charges of neutral and anion of $[C_2BNO(NO_2)_3]$, $[C_2BNS(NO_2)_3]$, $[C_3BN_2(NO_2)_4]$, $[C_3BN_2(NO_2)_4]$, $[C_3BS(NO_2)_4]$, and $[C_4BN(NO_2)_5]$.



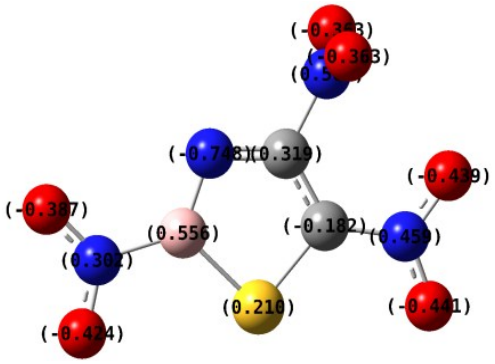
$[C_2BNO(NO_2)_3]$



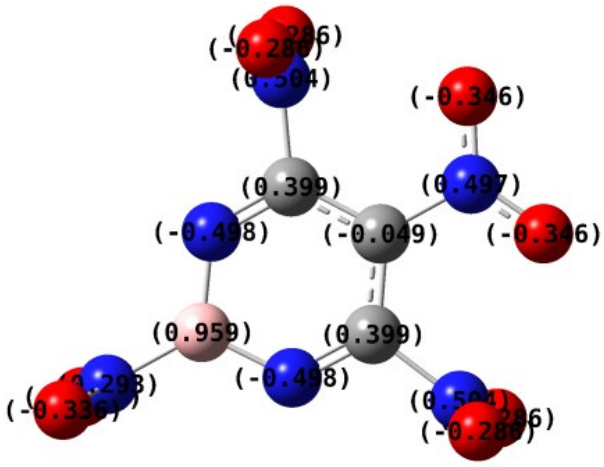
$[C_2BNO(NO_2)_3]^-$



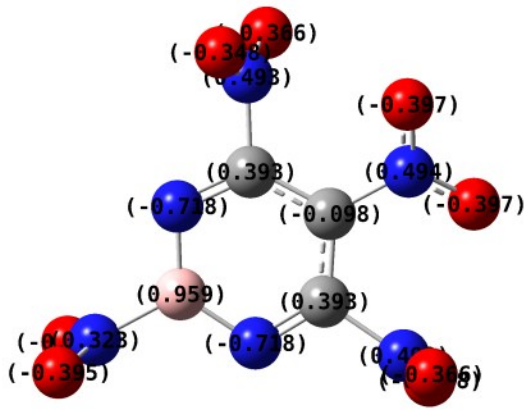
$[C_2BNS(NO_2)_3]$



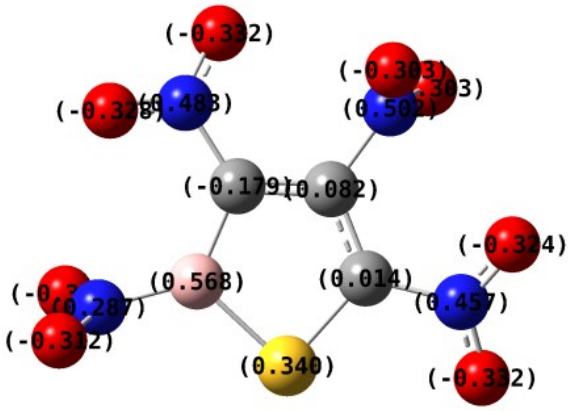
$[C_2BNS(NO_2)_3]^-$



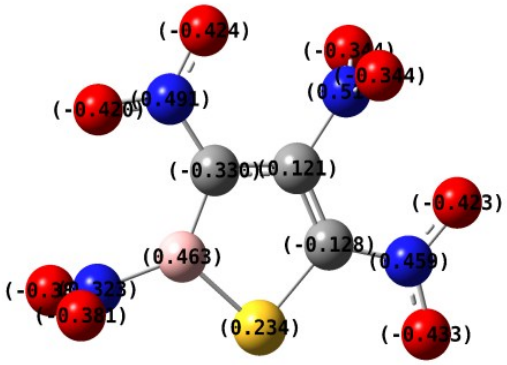
$[C_3BN_2(NO_2)_4]$



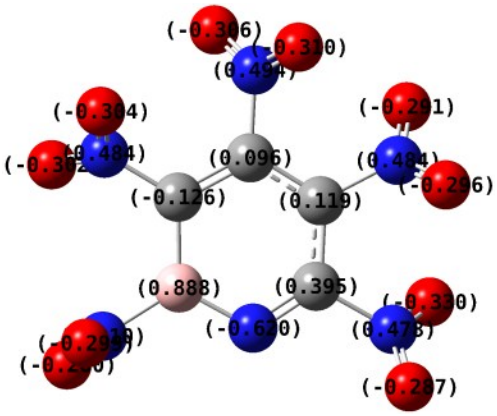
$[C_3BN_2(NO_2)_4]^-$



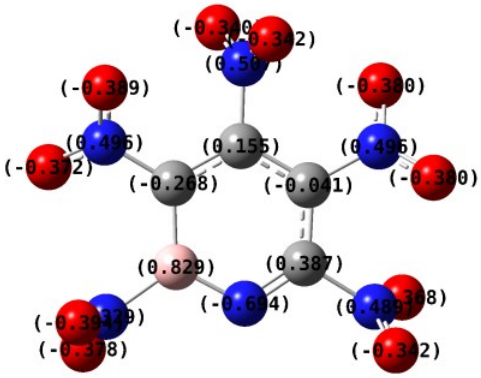
$[C_3BS(NO_2)_4]$



$[C_3BS(NO_2)_4]^-$

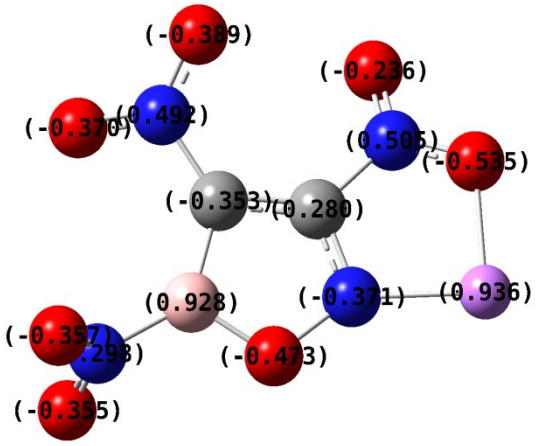


$[C_4BN(NO_2)_5]$

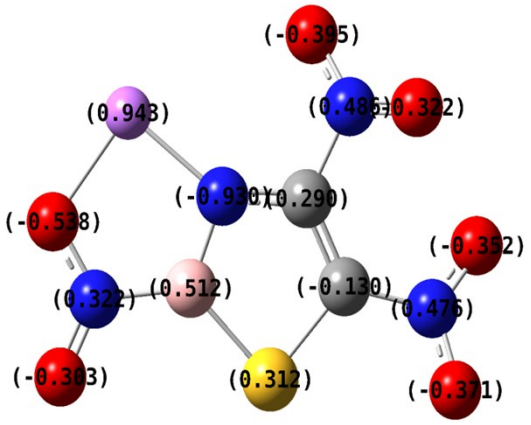


$[C_4BN(NO_2)_5]^-$

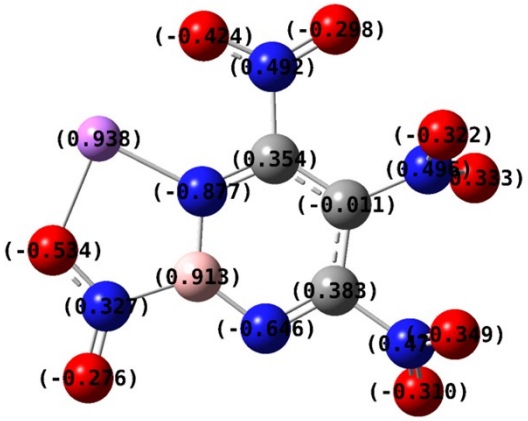
Figure S3. Natural Bond Orbital(NBO) Charges of $Li[C_2BNO(NO_2)_3]$, $Li[C_2BNS(NO_2)_3]$, $Li[C_3BN_2(NO_2)_4]$, $Li[C_3BS(NO_2)_4]$, and $Li[C_4BN(NO_2)_5]$.



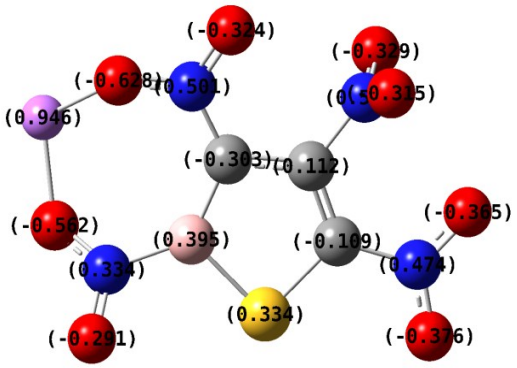
$Li[C_2BNO(NO_2)_3]$



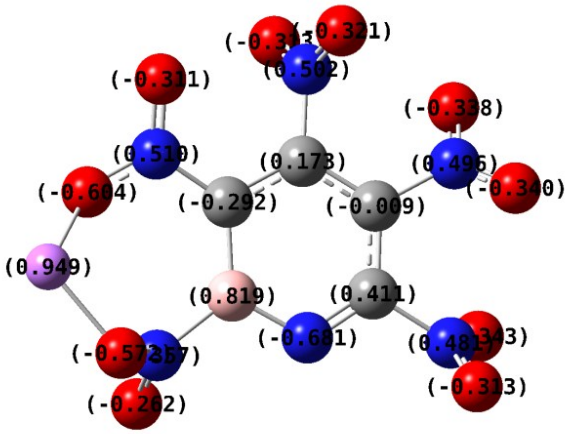
$Li[C_2BNS(NO_2)_3]$



$Li[C_3BN_2(NO_2)_4]$

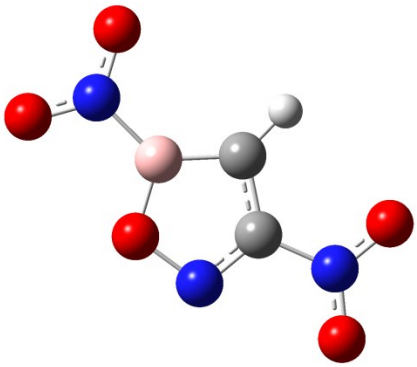


$Li[C_3BS(NO_2)_4]$

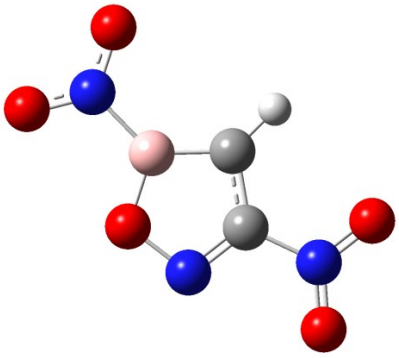


$Li[C_4BN(NO_2)_5]$

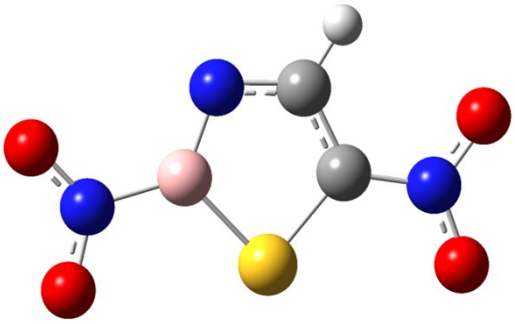
Figure S4. Optimized geometries of neutral and anions of $[C_2HBNS(NO_2)_2]$, $[C_2HBNS(NO_2)_2]$, $[C_3H_2BN_2(NO_2)_2]$, $[C_3H_2BS(NO_2)_2]$, and $[C_4H_2BN(NO_2)_2]$ in wB97XD/6-311+G(d) level.



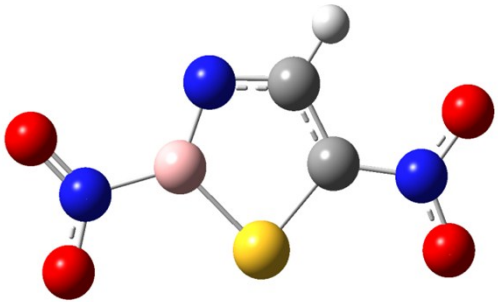
$[C_2HBNO(NO_2)_2]$



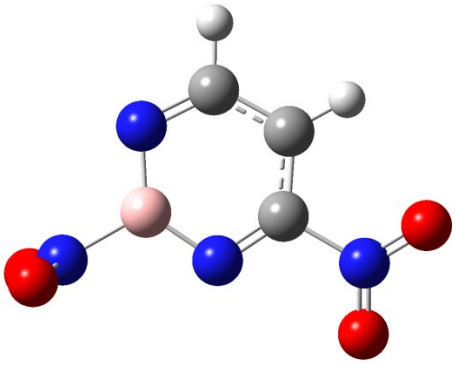
$[C_2HBNO(NO_2)_2]^-$



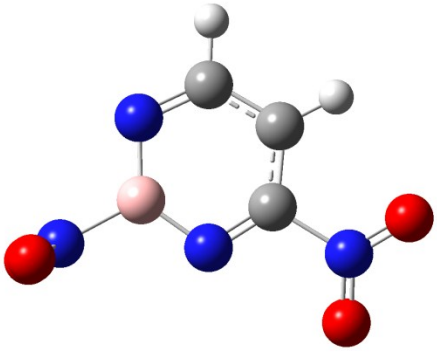
$[C_2HBNS(NO_2)_2]$



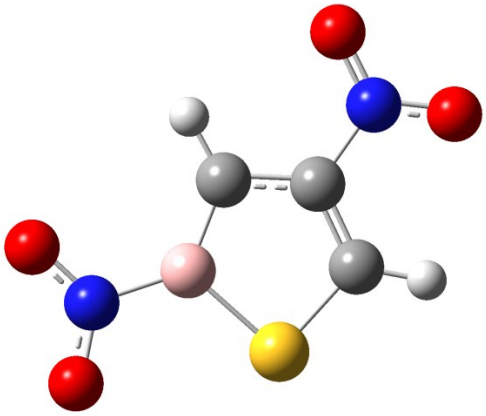
$[C_2HBNS(NO_2)_2]^-$



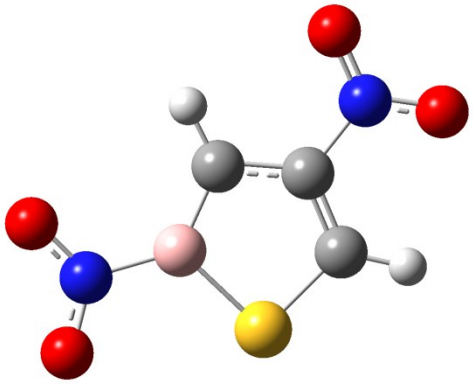
$[C_3H_2BN_2(NO_2)_2]$



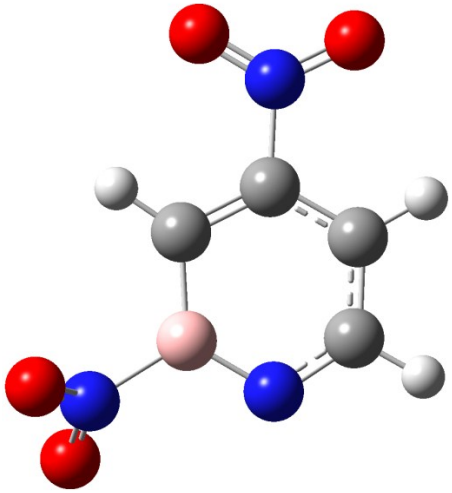
$[C_3H_2BN_2(NO_2)_2]^-$



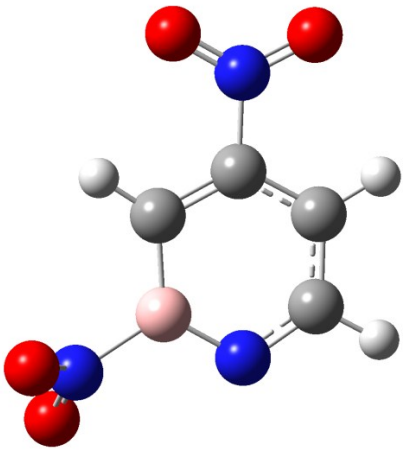
$[C_3H_2BS(NO_2)_2]$



$[C_3H_2BS(NO_2)_2]$

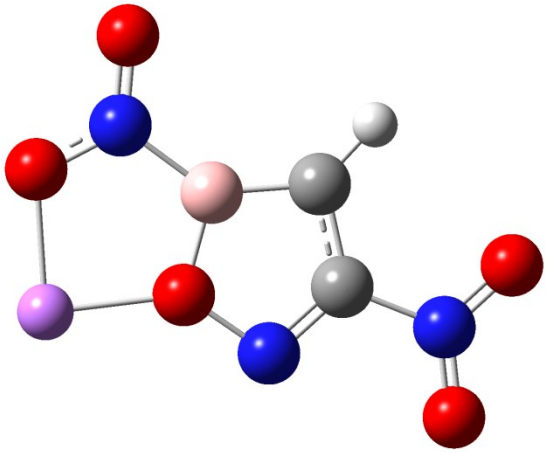


$[C_4H_2BN(NO_2)_2]$

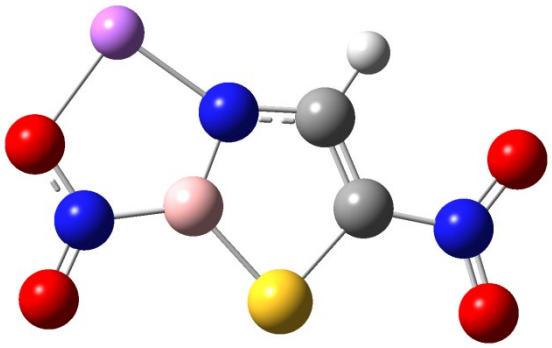


$[C_4H_2BN(NO_2)_2]^-$

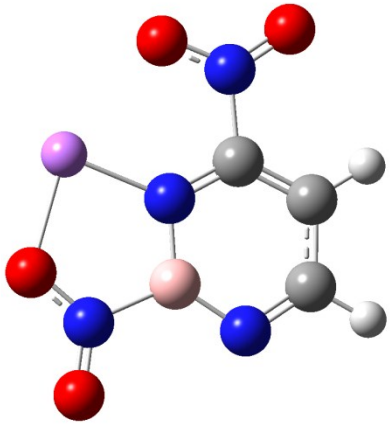
Figure S5. Optimized geometries of $Li[C_2HBNO(NO_2)_2]$, $Li[C_2HBNS(NO_2)_2]$, $Li[C_3H_2BN_2(NO_2)_2]$, $Li[C_3H_2BS(NO_2)_2]$, and $Li[C_4H_3BN(NO_2)_2]$ in wB97XD/6-311+G(d) level.



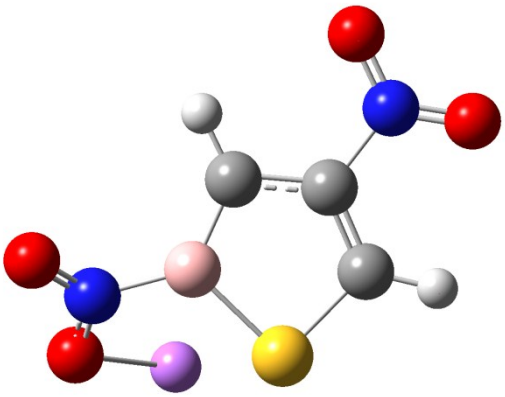
$Li[C_2HBNO(NO_2)_2]$



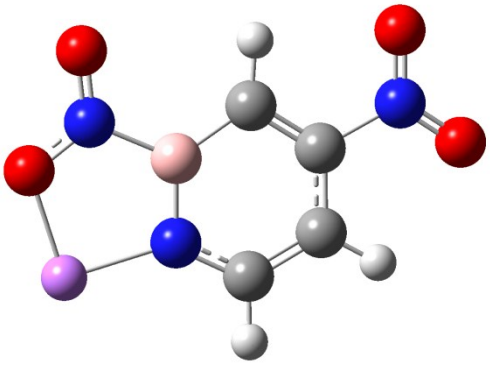
$Li[C_2HBNS(NO_2)_2]$



$Li[C_3H_2BN_2(NO_2)_2]$



$Li[C_3H_2BS(NO_2)_2]$



$Li[C_4H_3BN(NO_2)_2]$

Table 1. Calculated VDE of two NO_2-substituted electrolytes in gas phase and in solvent(ethylenecarbonate) phase at wB97XD level of theory using 6-311+G(d) basis set.

Anions	VDE (in eV) (in gas phase)	VDE (in eV) (in solvent phase)	Anions	VDE* (in eV) (In gas phase)
$C_3H_2BN_2(NO_2)_2$	4.66	6.11	ClO_4	5.83
$C_2HBNO(NO_2)_2$	4.91	6.36	$N(SO_2CF_3)_2$	7.01
$C_2HBNS(NO_2)_2$	5.41	6.93	BF_4	7.66
$C_4H_3BN(NO_2)_2$	3.93	6.09	PF_6	8.55
$C_3H_2BS(NO_2)_2$	4.58	5.45	$CB_{11}H_{12}$	5.99

*Values taken from reference 28.

Table 2. Calculated BE's of Li-heterocycles in gas phase and solvent(ethylene carbonate) phase at wB97XD level of theory using 6-311+G(d) basis set.

Li-Salts	Binding energy(BE) $BE= E_{Salt}-(E_{Li^+} + E_{Anion})$ (in eV)		Li-Salts	BE* (in eV) (In gas phase)
	(in gas phase)	(in solvent phase)		
$Li[C_3H_2BN_2(NO_2)_2]$	5.60	5.11	$LiClO_4$	5.96
$Li[C_2HBNO(NO_2)_2]$	6.05	5.37	$LiN(SO_2CF_3)_2$	6.01
$Li[C_2HBNS(NO_2)_2]$	6.43	5.42	$LiBF_4$	6.08
$Li[C_4H_3BN(NO_2)_2]$	5.23	5.52	$LiPF_6$	5.73
$Li[C_3H_2BS(NO_2)_2]$	6.34	4.97	$LiCB_{11}H_{12}$	5.08

*Values taken from reference 28.