Supplement information

Article

Nitrated Graphene Oxide Derived from Graphite Oxide: A Promising Energetic Two-Dimensional Material

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Table S1. Bond length and angles of the stable configuration when the central epoxy and nitroxyl cation are at different distances

L(N··O_3)	∠$C_1O_3C_2$	L(C_1-O_3)	L(C_2-O_3)	L(C_1-C_2)	∠O_1NO_2	∠O_1NO_3	∠O_2NO_3	L(O_1-N)	L(O_2-N)	Coplanarity ($NO_1O_2O_3$)
3.43	68.70	1.43	1.43	1.62	133.08	72.69	66.44	1.21	1.21	272.21
2.86	68.23	1.43	1.44	1.61	133.34	85.94	85.57	1.21	1.21	304.85
2.47	68.10	1.44	1.44	1.61	133.16	98.66	102.76	1.21	1.21	334.58
2.29	67.69	1.44	1.44	1.60	132.84	104.96	102.54	1.21	1.21	340.34
1.93	63.73	1.48	1.48	1.57	131.66	107.47	109.15	1.21	1.22	348.28
1.84	44.40	2.18	1.47	1.53	134.74	107.64	117.58	1.19	1.20	359.96
1.65	28.30	2.73	3.04	1.44	132.25	114.57	113.19	1.21	1.21	360.00
1.46	10.63	5.78	4.71	1.44	127.25	115.30	117.45	1.22	1.23	359.99

*The unit of length is Ångstrom(Å) and the angle unit is degree(°). Coplanarity is the sum of angles with N as the vertex.

Table S2. Bond length and angles of the stable configuration when the marginal epoxy and nitroxyl cation are at different distances

L(N··O_4)	∠$C_3O_4C_4$	L(C_3-O_4)	L(C_4-O_4)	L(C_3-C_4)	∠O_1NO_2	∠O_1NO_4	∠O_2NO_4	L(O_1-N)	L(O_2-N)	Coplanarity ($NO_1O_2O_4$)
3.41	53.86	1.48	1.45	1.32	133.15	92.26	93.97	1.21	1.21	319.38
2.75	53.82	1.48	1.45	1.32	133.20	92.40	94.34	1.21	1.21	319.94
2.46	53.73	1.48	1.45	1.32	132.83	99.47	100.75	1.21	1.21	333.05
2.20	53.66	1.48	1.45	1.32	131.66	102.31	106.10	1.21	1.22	340.06
1.91	53.18	1.50	1.45	1.32	130.52	106.64	107.31	1.22	1.22	344.48
1.85	53.03	1.51	1.46	1.32	130.85	106.81	107.31	1.22	1.22	344.97
1.63	29.28	2.39	1.36	1.37	134.90	110.13	114.97	1.19	1.20	360.00
1.42	29.53	2.39	1.40	1.36	131.02	111.71	117.27	1.21	1.21	360.00

*The unit of length is Ångstrom(Å) and the angle unit is degree(°). Coplanarity is the sum of angles with N as the vertex.

Table S3. Bond length and angles of the stable configuration when the marginal hydroxyl and nitroxyl cation are at different distances

$L(N\cdot\cdot O_5)$	$\angle O_1NO_2$	$\angle O_1NO_5$	$\angle O_2NO_5$	$L(O_1\text{-}N)$	$L(O_2\text{-}N)$	$L(O_5\text{-}H_1)$	$L(O_5\text{-}C_5)$
3.42	133.13	84.52	88.97	1.19	1.21	0.960	1.35
2.89	133.34	84.20	87.70	1.21	1.21	0.978	1.36
2.42	133.13	97.86	102.97	1.21	1.21	0.979	1.36
2.16	132.23	100.14	104.86	1.21	1.21	0.980	1.36
1.92	131.13	103.40	106.43	1.22	1.22	0.982	1.37
1.86	131.58	104.30	107.33	1.22	1.22	0.983	1.38
$L(N\cdot\cdot C_5)$	$\angle O_1NC_5$	$\angle O_2NC_5$	Coplanarity ($NO_1O_2C_5$)			Coplanarity ($NO_1O_2O_5$)	
4.56	94.48	85.07	312.68			306.63	
4.00	96.04	83.54	312.92			305.24	
3.58	104.14	89.84	327.12			333.96	
3.29	116.40	90.45	339.08			337.24	
2.85	128.05	86.81	345.99			340.96	
2.83	128.63	85.91	346.11			343.21	

*The unit of length is Ångstrom(Å) and the angle unit is degree(°). Coplanarity is the sum of angles with N as the vertex.

Table S4. Bond length and angles of the stable configuration when the central hydroxyl and nitroxyl cation are at different distances

$L(N\cdot\cdot O_6)$	$\angle O_1NO_2$	$\angle O_1NO_6$	$\angle O_2NO_6$	$L(O_1\text{-}N)$	$L(O_2\text{-}N)$	$L(O_6\text{-}H2)$	$L(O_6\text{-}C_6)$
3.29	132.43	95.04	106.60	1.21	1.21	0.976	1.48
2.88	132.34	96.13	110.12	1.21	1.21	0.977	1.48
2.47	131.08	94.86	109.98	1.21	1.21	0.976	1.47
2.16	130.80	99.64	106.16	1.21	1.21	0.978	1.47
1.99	127.59	105.09	106.53	1.23	1.22	0.980	1.51
1.57	126.19	110.73	109.12	1.25	1.23	0.978	2.59
$L(N\cdot\cdot C_6)$	$\angle O_1NC_6$	$\angle O_2NC_6$	Coplanarity ($NO_1O_2C_6$)			Coplanarity ($NO_1O_2O_6$)	
4.01	106.73	107.69	346.86			334.08	
3.66	108.06	111.03	351.43			338.58	
2.91	106.61	116.15	353.83			335.92	
2.74	110.54	113.71	355.05			336.60	
2.13	115.52	116.17	359.28			339.22	
1.86	104.81	103.96	334.96			346.04	

*The unit of length is Ångstrom(Å) and the angle unit is degree(°). Coplanarity is the sum of angles with N as the vertex.