

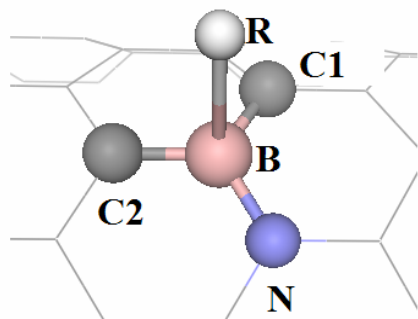


Figure 10 Position of R groups, B atom, N atom, C1 atom, C2 atom on side-wall (5,5) SWCNT

Table 2 Structural parameters of BN-doped SWCNT grafted with N-nucleophiles

	R-B	B-N	B-C1	B-C2	$\angle$ N-B-C1	$\angle$ N-B-C2	$\angle$ C1-B-C2	$\angle$ R-B-N	$\angle$ R-B-C1	$\angle$ R-B-C2
BN-SWCNT	-	1.46	1.53	1.51	118.0	118.6	114.7	-	-	-
m-nitroaniline	1.79	1.52	1.59	1.57	111.8	113.8	110.0	105.1	108.3	107.5
pyridine	1.67	1.54	1.60	1.58	109.9	112.0	108.3	105.7	112.1	108.9
chitosan	1.70	1.54	1.61	1.58	109.3	112.1	107.3	106.5	112.2	109.2
imidazole	1.64	1.55	1.60	1.59	109.7	111.9	108.0	106.6	111.0	109.7
ammonia	1.69	1.54	1.60	1.58	110.8	112.9	109.0	105.9	109.6	108.5
arginine	1.60	1.57	1.61	1.59	108.3	110.4	107.2	107.2	110.4	113.3
guanidine	1.61	1.57	1.61	1.59	108.2	110.5	107.0	108.2	109.6	113.2