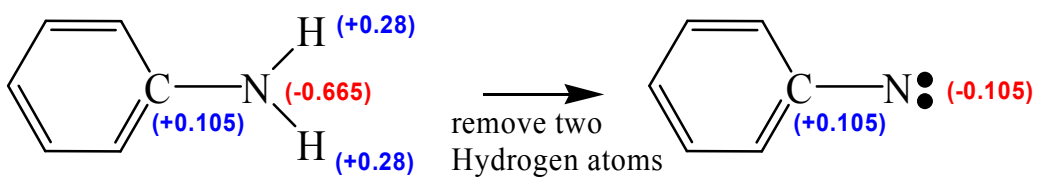
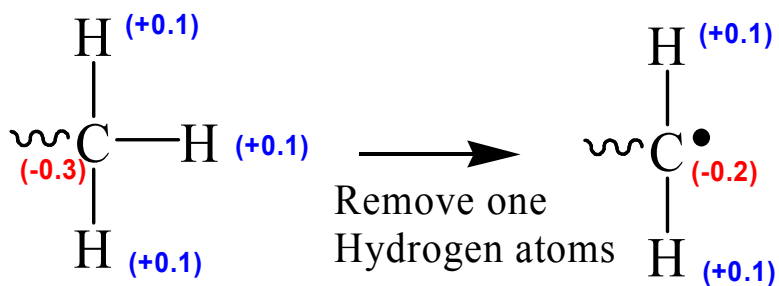


## Charge updation before the start of the cross-linking procedure

### Charge updation at amine end terminals

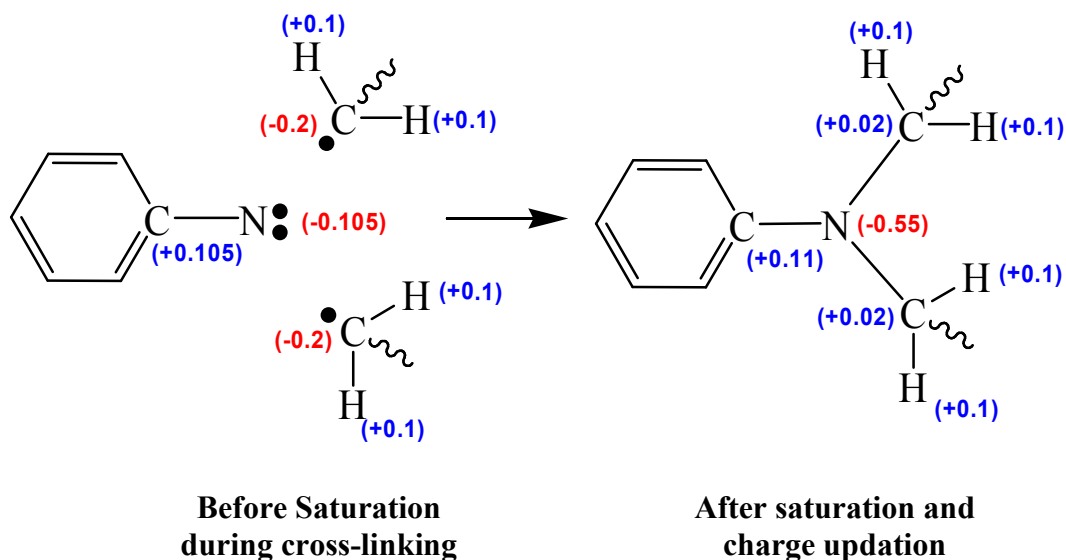


### Charge updation at epoxy end terminals.



## Charge updation after the cross-linking procedure

**Case 1: When the nitrogen is crosslinked to two epoxy molecules at the end of the cross-linking procedure.**



The atoms at which charges were modified are listed below. The modified charges are shown in Table 1.

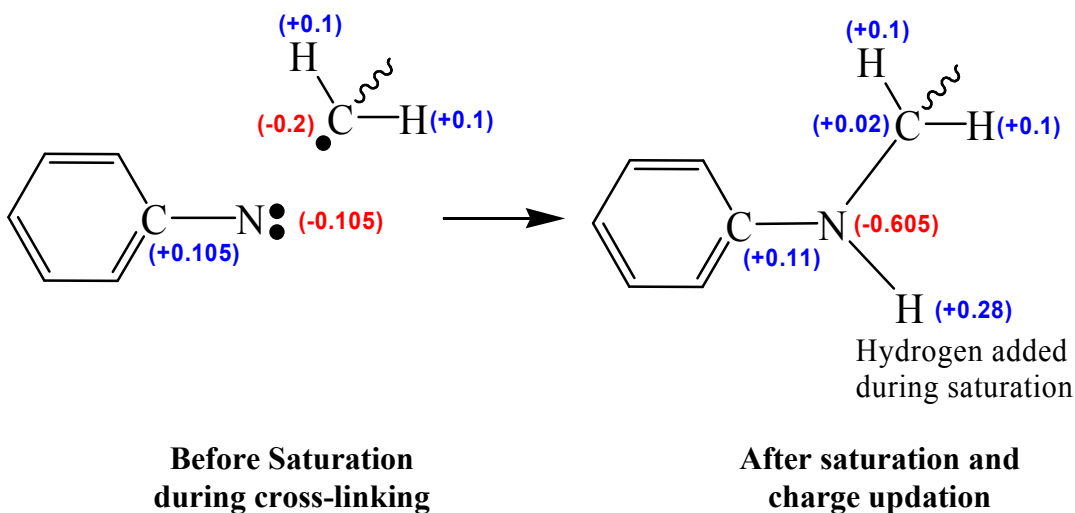
**Caro:** The phenyl carbon atom which is attached to nitrogen.  
**Nterm:** The amine nitrogen atom of the crosslinker  
**Cterm:** The terminal carbon atom of the epoxy molecule.

**Table 1**

Atom Type	Before Charge Updation	After Charge Updation	Net Change
Caro	+0.105	+0.11	+0.005
Nterm	-0.105	-0.55	-0.445
Cterm	$(-0.2) \times 2 = -0.4$	$(0.02) \times 2 = +0.04$	+0.44
Net change in system charge			0.0

The charges on the molecule after updation were calculated separately (as shown in Figure 4) and changes were made accordingly.

**Case 2: When the nitrogen is crosslinked to one epoxy molecule at the end of the cross-linking procedure**



The atoms at which charges were modified are listed below. The modified charges are shown in Table 2.

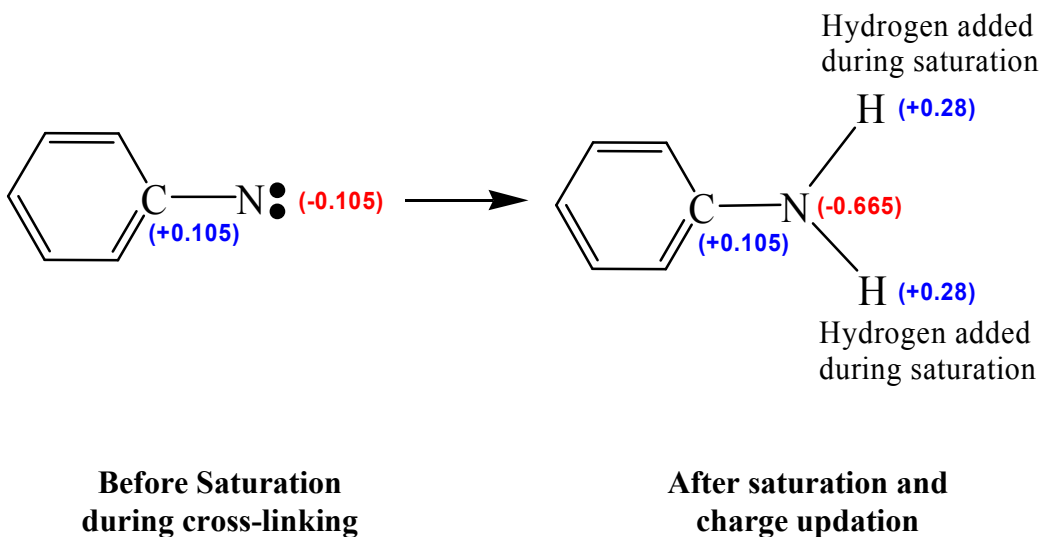
**Caro:** The phenyl carbon atom which is attached to nitrogen.  
**Nterm:** The amine nitrogen atom of the crosslinker  
**Cterm:** The terminal carbon atom of the epoxy molecule.

**Table 2**

Atom Type	Before Charge Updation	After Charge Updation	Net Change
Caro	+0.105	+0.11	+0.005
Nterm	-0.105	-0.61	-0.505
Cterm	-0.2	+0.02	+0.22
H	-	0.28	+0.28
Net change in system charge			0.0

An extra hydrogen atom was added to full-fill the sp<sup>2</sup> nature of the amine nitrogen and a charge of 0.28 was assigned to the hydrogen atom in accordance to the charges of H's in DETDA molecule where amine nitrogen is bonded to hydrogen atoms.

**Case 3: When the nitrogen was not at all reacted during cross-linking process.**



The atoms at which charges were modified are listed below. The modified charges are shown in Table 3.

**Caro:** The phenyl carbon atom which is attached to nitrogen.  
**Nterm:** The amine nitrogen atom of the crosslinker

**Table 3**

Atom Type	Before Charge Updation	After Charge Updation	Net Change
Caro	+0.105	+0.105	0
Nterm	-0.105	-0.665	-0.56
H	-	$0.28 \times 2 = 0.56$	+0.56
Net change in system charge			0.0

Two hydrogen atoms were added to full-fill the  $sp^2$  nature of the amine nitrogen and a charge of 0.28 was assigned to the hydrogen atoms in accordance to the charges of H's in DETDA molecule where amine nitrogen is bonded to hydrogen atoms.