Subject: Re: Aromatic Amines

Posted by thomas on Tue, 12 May 2020 09:51:11 GMT

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Thank you for pointing this out. You are, of course, right that the number of aromatic amine atoms should be three.

I have checked the source code and atom 1 was not counted as amine, because it has a negative neighbour.

In this case one could even argue that the nitrogen has no basicity left, but finally it is an amine even if not basic.

I have changed the logic of the source code. It will be fixed in the next updates.