Subject: Re: Aromatic Amines
Posted by thomas on Tue, 12 May 2020 09:51:11 GMT
View Forum Message <> Reply to Message

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.