
Subject: Aromatic Amines

Posted by [sansun](#) on Sun, 10 May 2020 03:55:33 GMT

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I was wondering how DW calculates 'Aromatic Amines' property.
In the attached file, top structures shows 4 Aromatic amines, that I understand.
However, the bottom structure mentions only 2. I thought it should be 3.

File Attachments

1) [Aromatic amines.png](#), downloaded 546 times

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.

Subject: Re: Aromatic Amines

Posted by [sansun](#) on Wed, 13 May 2020 13:03:06 GMT

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Great! thanks for the clarification.
