
Subject: Unable to display zwitterion structure correctly in both + and - separately

Posted by [SallyS](#) on Fri, 02 Jun 2023 07:35:52 GMT

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Hi,

I was writing this message to report a display issue for zwitterion structures.

For instance,

O=C([O-])c1cc(NS(=O)(=O)c2ccccc2Cl)cnc1N1CCC[C@H](C[NH+]2CCCC2)C1

This structure contains both N⁺ and O⁻, and the net charge is 0.

However this structure was displayed as attachment 'strcuturedisplay.jpg',

unlike what it could be correctly in attachment 'strcuturedisplay.jpg'

I am not sure its a bug or I could set any function to show the structure correctly.

Thank you for your time and I am looking forward to hearing from you soon.

Best regards,

Sally

File Attachments

- 1) [strcuture_correct.jpg](#), downloaded 617 times
 - 2) [strcuturedisplay.jpg](#), downloaded 540 times
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