Subject: Name to structure - Triple bonds are not parsed
Posted by MaxPeters on Thu, 18 Feb 2016 11:38:53 GMT
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Entering the SMILES for HCN:
C#N
in the web form results in
CH4.
The same is true for organic nitriles, they either result in terminal groups or parsing errors.

Subject: Re: Name to structure - Triple bonds are not parsed
Posted by thomas on Sun, 21 Feb 2016 12:24:35 GMT
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Thank you for reporting this. I found and fixed the bug. The # sign was not properly encoded in the URL sent to the server causing the smiles to to be truncated at the #-position.