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Understanding the formation of aromatic compounds in the interstellar space

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Understanding the formation of PoliAromatic Hydrocarbons (PAHs) can shed light on the origin of the prebiotic Earth and even on the origin of life.[1] Unfortunately, to date, the formation of organic compounds in space is a scarcely understood area.

In this arena, automated protocols for the identification of reaction mechanisms show great potential to aid in the learning of how PAHs are formed in space. Taking advantage of the AutoMeKin [2,3] program, we have found thousands of potential paths that account for the formation of the simplest PAH: benzene. We have not only uncovered several direct paths, for which reactants have been detected in space, but also some more indirect paths in which well-known intermediates such as benzyne or the very acetyl radical play a crucial role.

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