## Screening and optimisation of Mo:Fe(2)/CAR catalysts in one-step synthesis of methylal via methanol oxidation

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## Abstract

In the one-step preparation of methylal from methanol, achieving high methylal yield is a huge challenge. To address this problem, in this study a new Mo:Fe(2)/CAR catalyst was designed, screened and optimised. The results showed that the optimised bifunctional catalyst had superior catalytic performance, and the yield of methylal could reach 81.33%, much higher than other research results of this process. Through the use of XPS, NH3-TPD and PY-FTIR it was found that the appearance of Mo5+ promoted the coordination of the two terminal oxygen with the Mo double bond in the Fe2(MoO4)3 octahedron, and that the increase in the weak acid strength of the catalyst and the coordination of suitable Brønsted acids (B acids) and Lewis acids (L acids) was the root cause of the catalytic activity. The apparent activation energy also further proved that Mo:Fe(2)/HZSM-5(80-80) was highly suitable for the one-step production of methylal from methanol.

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