# On the heats of formation of methylketene, dimethylketene and related cations

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Abstract: Ab initio MO and DFT calculations up to the CCSD(T)/6-311++G(3df, 2p) level have been applied to the disagreement between theory and experiment concerning the standard enthalpies of formation of methylketene and dimethylketene. Our results confirm previous theoretical (G2) values, as well as the experimental proton affinities and ionization energies of both alkylketenes. A set of consistent values for $??H_{f,\ 298}^{o}$ are estimated as follow (kJ $mol^{-1}$): $CH_3CH=C=O$: -68; $CH_3CH=C=O^+$: 795; $CH_3CH_2CO^+$: 618; $(CH_3)_2C=C=O$: -92; $(CH_3)_2C=C=O^+$: 723 and $(CH_3)_2CHCO^+$: 583. The proton affinities (kJ $mol^{-1}$) are: PA(methylketene)=842 and PA(dimethylketene)=855. The persistent disagreement between the theoretical and experimental values appears to arise from an overestimation of the experimental heats of formation of $CH_3CH_2CO^+$, $CH_3CH=C=O^+$ and $(CH_3)_2C=C=O^+$.

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