Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Quasi-classical trajectory study of the OH^- + CH_3I reaction: Theory meets experiment

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Table S1. Integral cross sections (bohr^2) of the possible pathways for the OH^- + CH_3I reaction at different collision energies.

Reaction channels[a]	E_{coll} **(kcal/mol)**			
	11.5	**23.1**	**34.6**	**46.1**
S_N2	78.97	23.33	13.10	10.36
ABS	169.84	59.31	32.81	22.20
ABS soft	100.04	40.06	23.69	16.46
ABS hard	23.94	14.81	10.45	8.02
Iodine ABS	0.04	0.03	0.02	0.02
S_N2 retention	0.07	0.02	0.02	0.07
ABS proton exch.	0.77	0.10	0.03	0.01
S_N2 proton exch.	1.19	0.14	0.02	0.01
Proton exch.	0.36	0.07	0.02	0.00
ABS dissociation[b]	0.00	0.29	1.25	2.26
$CH_2 + I^- + H_2O$	0.00	0.12	0.67	1.45
$H_2O + [I\cdots CH_2]^-$	0.00	0.08	0.31	0.52
$CH_2 + [I\cdots H_2O]^-$	0.00	0.06	0.21	0.24
$I^- + [CH_2\cdots H_2O]$	0.00	0.04	0.06	0.04

[a] $ICS_{total} = ICS_{S_N2} + ICS_{Proton\ abs.} + ICS_{Iodine\ abs.} + ICS_{Proton\ abs.\ diss.} + ICS_{Proton\ exch.}$

[b] $ICS_{Proton\ abs.\ diss.} = ICS(CH_2 + I^- + H_2O) + ICS(H_2O + [I\cdots CH_2]^-) + ICS(CH_2 + [I\cdots H_2O]^-) + ICS(I^- + [CH_2\cdots H_2O])$

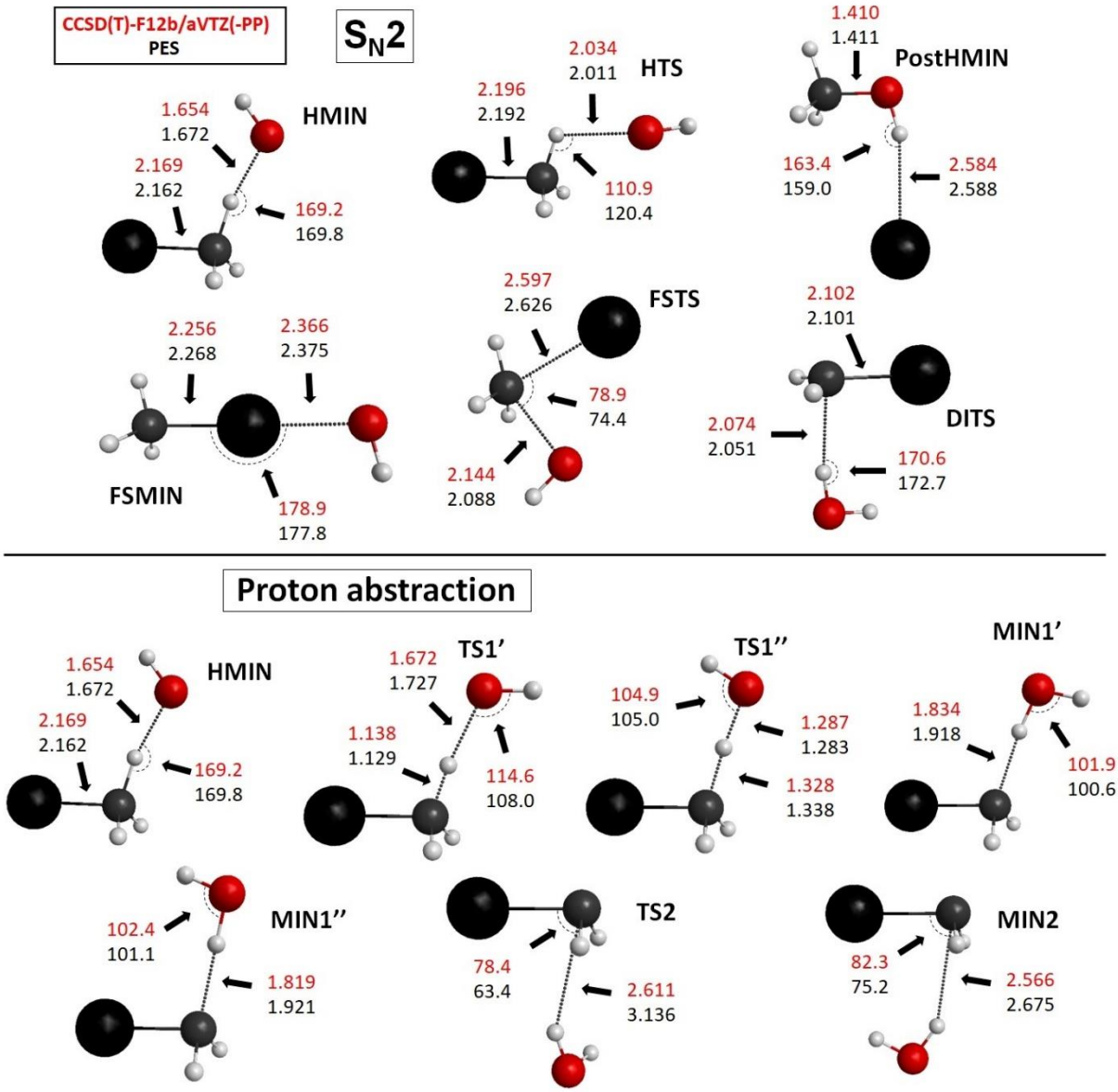

Figure S1. The structures of the stationary points for the S_N2 and proton-abstraction pathways of the $OH^- + CH_3I$ reaction showing the most important bond lengths (Å) and angles (deg) obtained on the PES compared to the CCSD(T)-F12b/aug-cc-pVTZ values. For the S_N2 channel, the *ab initio* data are adapted from ref. 1. Regarding the PES development, a detailed description is provided in ref 2.

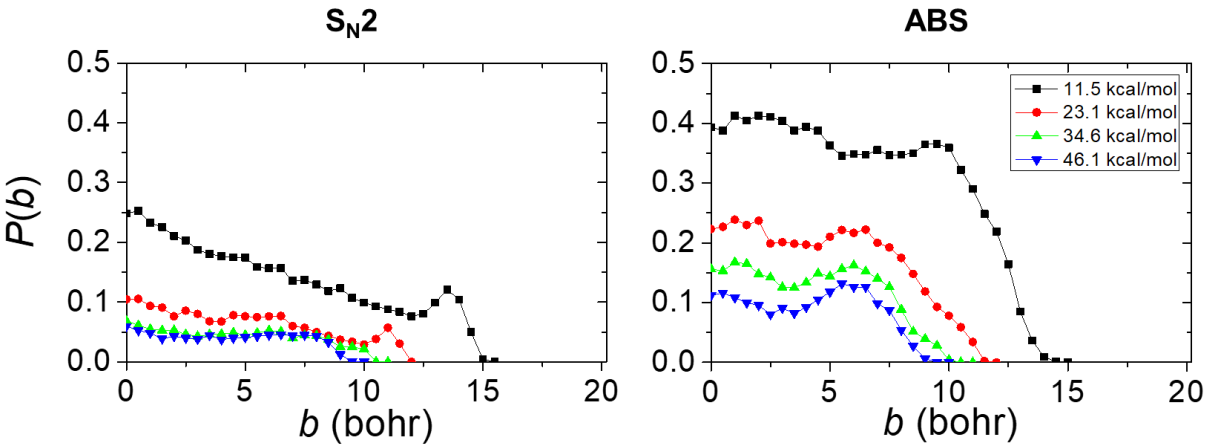

Figure S2. Opacity functions of the S_N2 and proton-abstraction pathways of the $OH^- + CH_3I$ reaction at different collision energies.

References

1. D. A. Tasi, Z. Fábián and G. Czakó, *J. Phys. Chem. A*, 2018, **122**, 5773.
2. D. A. Tasi, T. Győri and G. Czakó, *Phys. Chem. Chem. Phys.*, 2020, **22**, 3775.