Electronic supplementary information for the PCCP paper

Capture and dissociation in the complex-forming $CH + H_2 \rightarrow CH_2 + H$, $CH + H_2$ reactions

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QCT capture rate coefficients (Table 1S and Figure 1S), QCT-C/PST1 and QCT-C/PST2 abstraction rate coefficients (Table 2S and Figure 2S), QCT-C2 and QCT-C2e abstraction rate coefficients (Table 3S and Figure 3S), and QCT-C/PST2, QCT-C2 and QCT-C2e exchange rate coefficients (Table 4S and Figure 4S). Here, the figures are plotted as a function of T, and in Figures 3S and 4S the rate coefficients obtained with all ZPE treatments examined are given.

Table 1S: QCT capture rate coefficients*

T /K	200	250	300	400	500	600	700	800
k_c^{QCT}	249.3	231.8	218.6	198.8	185.6	175.2	168.6	163.1

* 10^{-12} cm^3 molecule^{-1} mol^{-1}

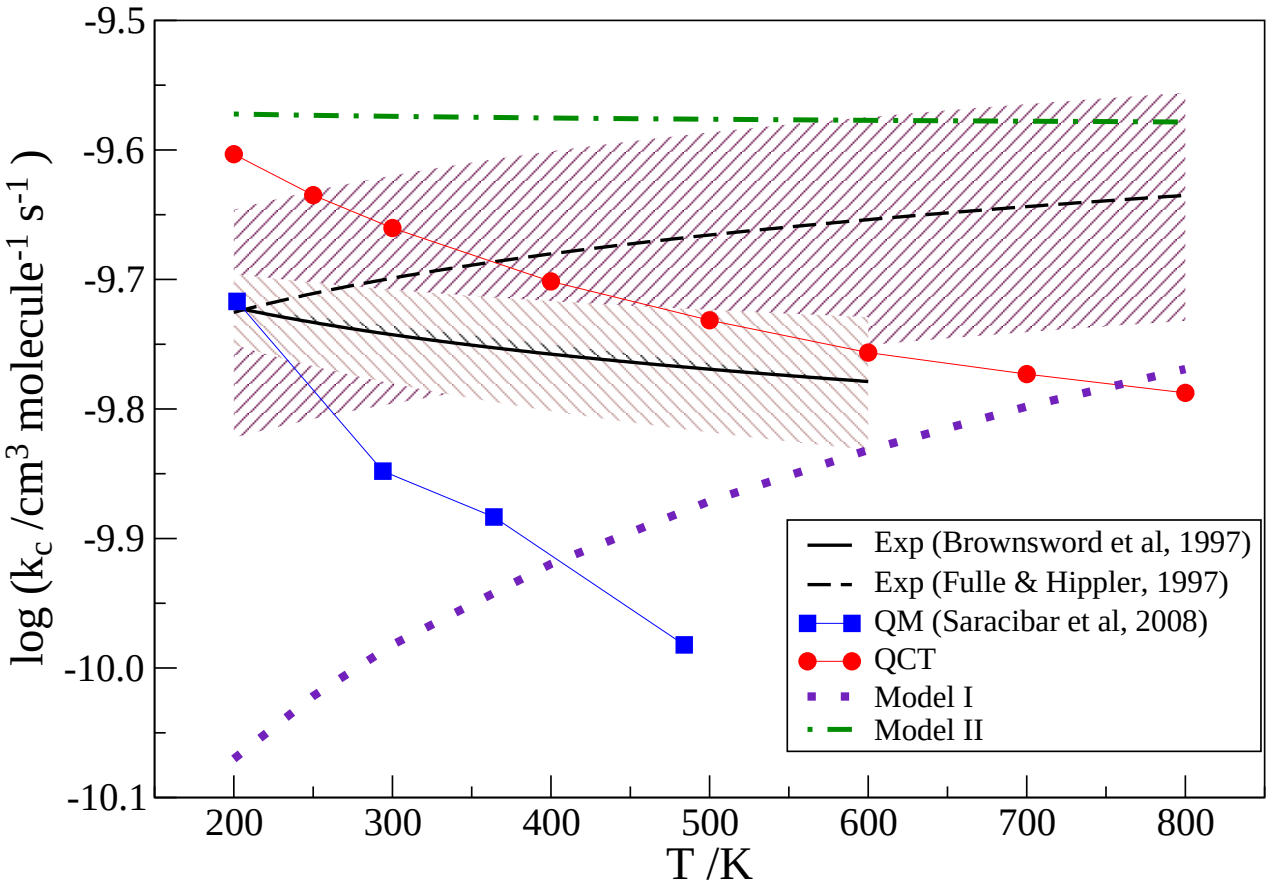

Figure 1S: QCT and QM [27] capture rate coefficients plotted as a function of temperature. Experimental values of refs. [16, 17] (with the corresponding error margins) are also plotted, together with the results of collision models I and II.

Table 2S: QCT-C/PST1 and QCT-C/PST2 abstraction rate coefficients*

T /K	200	250	300	400	500	600	700	800
$k_a^{\mathrm{QCT-C/PST1}}$	0.0392	0.209	0.572	2.12	4.64	7.72	11.2	14.7
$k_a^{\mathrm{QCT-C/PST2}}$	0.101	0.484	1.22	3.92	7.75	12.0	16.3	20.4

* 10^{-12} cm^3 molecule^{-1} mol^{-1}

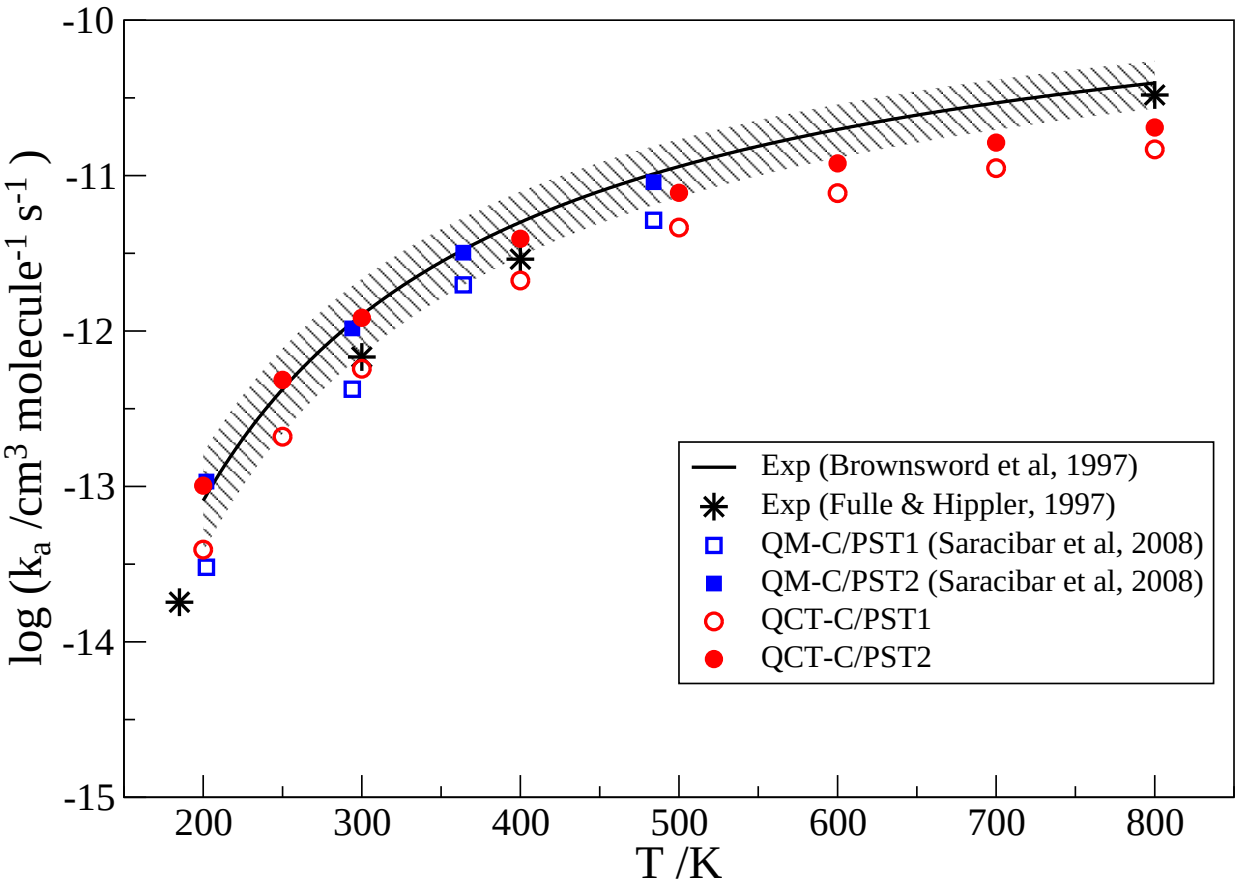

Figure 2S: QCT-C/PST and QM-C/PST [27] abstraction rate coefficients plotted as a function of temperature. Experimental values [16, 17] (with the corresponding error margins) are also plotted.

Table 3S: QCT-C2 and QCT-C2e abstraction rate coefficients*

T /K	200	250	300	400	500	600	700	800
k_a^{QCT-C2}		0.0617	0.3421	2.296	6.788	17.03	29.39	42.33
$k_a^{QCT-C2e}$	0.1050	0.6420	2.146	9.228	19.55	40.55	59.81	77.33

* 10^{-12} cm^3 molecule^{-1} mol^{-1}

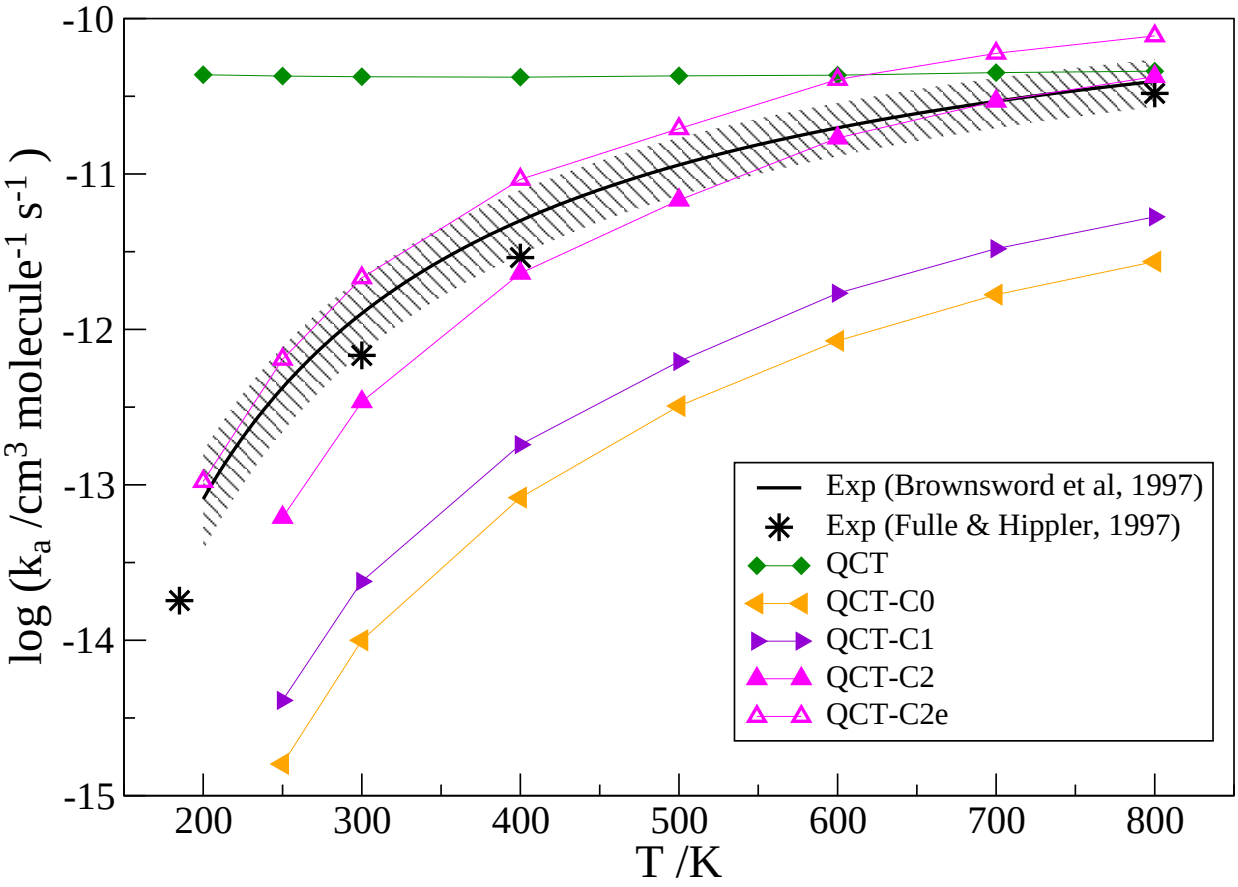

Figure 3S: QCT abstraction rate coefficients plotted as a function of temperature. Several treatments of the ZPE violation problem are taken into account. Experimental values (with the related error margins) [16, 17] are also plotted. QCT errors are smaller than the size of the symbols.

The C0 criterion to treat the ZPE problem consists in just to discard the abstraction trajectories leading to CH_2 molecules with vibrational energy below its ZPE, i.e., only those trajectories that satisfy $E_{vib}(CH_2) > E_{zpe}(CH_2)$ are taken into account to calculate N_r.

The C1 criterion discards, in addition to the abstraction trajectories not satisfying the CH_2 ZPE condition, the inelastic and exchange trajectories that do not satisfy the condition $E_{vib}(CH) + E_{vib}(H_2) > E_{zpe}(CH) + E_{zpe}(H_2)$.

Table 4S: QCT-C/PST2, QCT-C2 and QCT-C2e exchange rate coefficients*

T /K	200	250	300	400	500	600	700	800
$k_e^{QCT-C/PST2}$	1.58	5.73	11.5	26.4	40.0	50.0	57.0	61.1
k_e^{QCT-C2}	3.998	5.157	6.367	8.838	10.68	13.60	15.43	18.10
$k_e^{QCT-C2e}$	3.357	4.706	6.483	9.792	12.03	16.70	18.68	21.19

* 10^{-12} cm^3 molecule^{-1} mol^{-1}

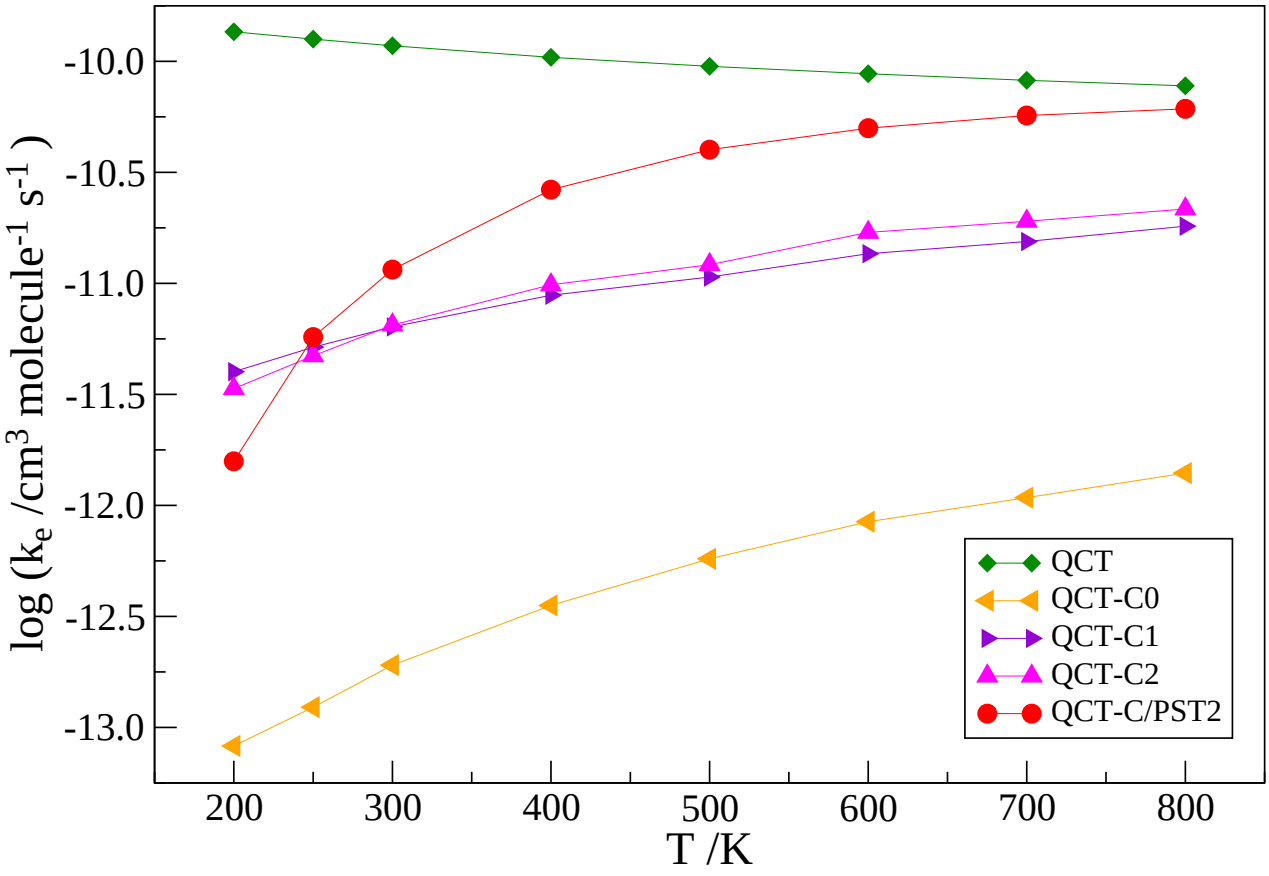

Figure 4S: QCT and QCT-C/PST exchange rate coefficients plotted as a function of temperature. Several treatments of the ZPE violation problem are taken into account. QCT errors are smaller than the size of the symbols.