Electronic Supplementary Information for PCCP article "An experimental and theoretical investigation of the C(^{1}D) + D_2 reaction"

Kevin M. Hickson and Yury V. Suleimanov

Table S1 Input parameters for the RPMDrate calculations of the C(^{1}D) + D_2 reaction. The explanation of the format of the input file can be found in the RPMDrate code manual (see http://rpmdrate.cyi.ac.cy).

Parameter	Potential Energy Surface		Explanation
	$^1A'$	$^1A''$	
Command line parameters			
Temp	300 127 75 50		Temperature (K)
N_{beads}	128 (50 and 75 K); 64 (127 K); 48(300 K)		Number of Beads
Dividing surface parameters			
R_∞	15 a_0	20 **Å**	Dividing surface parameter (distance)
N_{bond}	1	1	Number of forming and breaking bonds
$N_{channel}$	2	2	Number of equivalent product channels
X(^1D) H H	(1.635 a_0, 1.302 a_0, 0.000 a_0) (0.000 a_0, 0.000 a_0, 0.000 a_0) (3.270 a_0, 0.000 a_0, 0.000 a_0)	(-2.450 a_0, 0.000 a_0, 0.000 a_0) (0.000 a_0, 0.000 a_0, 0.000 a_0) (1.900 a_0, 0.000 a_0, 0.000 a_0)	Cartesian coordinates (x, y, z) of the intermediate geometry
Thermostat	'Andersen'	'Andersen'	Thermostat option
Biased sampling parameters			
$N_{windows}$	111	111	Number of Windows
$\xi 1$	-0.05	-0.05	Center of the first window
$d\xi$	0.01	0.01	Window spacing step
ξN	1.05	1.05	Center of the last window
dt	0.0001	0.0001	Time step (ps)
ki	2.72	2.72	Umbrella force constant ((T/K) eV)
$N_{trajectory}$	200	200	Number of trajectories
$t_{equilibration}$	20	20	Equilibration period (ps)
$t_{sampling}$	100	100	Sampling period in each trajectory (ps)
N_i	2×10^8	2×10^8	Total number of sampling points
Potential of mean force calculation			
ξ_0	0.00	0.00	Start of umbrella integration
$\xi_\ddagger$	0.604 (300 K)[a] 0.448 (127 K)[a] 0.398 (75 K)[a] 0.361 (50 K)[a]	0.915 (300 K)[a] 0.807 (128 K)[a] 0.765 (77 K)[a] 0.754 (50 K)[a]	End of umbrella integration
N_{bins}	5000	5000	Number of bins
Recrossing factor calculation			
dt	0.0001	0.0001	Time step (ps)
$t_{equilibration}$	20	20	Equilibration period (ps) in the constrained (parent) trajectory
$N_{totalchild}$	200000	200000	Total number of unconstrained (child) trajectories
$t_{childsampling}$	3	3	Sampling increment along the parent trajectory (ps)
N_{child}	100	100	Number of child trajectories per one initially constrained configuration
t_{child}	2	4	Length of child trajectories (ps)

[a]Detected automatically by RPMDrate.