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Supporting Information: TABLES and FIGURES

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TITLE: Dynamics and resonances of the H(^2S) + CH^+($X^1\Sigma^+$) reaction in the electronic ground state: A detailed quantum wavepacket study

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Table S1: Vibrational energy levels of the CH_2^+ complex from the energetic minimum of the well in its ground 1 $^2A'$ PES. Eigenenergies and assignments of the well resolved bound states are presented.

Eigenvalues E_n (eV)	Assignments (ν_1, ν_2, ν_3)	Eigenvalues E_n (eV)	Assignments (ν_1, ν_2, ν_3)
-4.3791	(0,0,0)	-3.1056	(2,2,2)
-4.2816	(0,0,1)	-3.0737	(1,1,2)
-4.1701	(0,0,2)	-3.039	(1,1,2)
-4.0314	(0,0,3)	-3.0184	(2,2,5)
-4.0211	(1,1,0)	-2.9969	(1,1,5)
-3.9883	(1,1,0)	-2.9781	(3,3,0)
-3.9246	(1,1,1)	-2.9734	(2,2,3)
-3.8918	(-,-,1)	-2.965	(1,1,5)
-3.873	(0,0,4)	-2.9135	(1,1,3)
-3.8149	(1,1,2)	-2.9088	(3,3,0)
-3.785	(-,-,2)	-2.8825	(3,3,1)
-3.7016	(0,0,5)	-2.8703	(2,2,0)
-3.6688	(2,2,0)	-2.8497	(2,2,1)
-3.651	(-,-,3)	-2.8132	(3,3,1)
-3.6425	(1,1,0)	-2.7748	(2,2,1)
-3.6069	(2,2,0)	-2.7476	(2,2,2)
-3.5741	(2,2,1)	-2.7148	(3,3,2)
-3.5469	(1,1,1)	-2.6782	(2,2,2)
-3.5113	(1,1,1)	-2.608	(1,1,5)
-3.4645	(2,2,2)	-2.5939	(2,2,3)
-3.441	(1,1,2)	-2.5892	(3,3,3)
-3.4073	(1,1,2)	-2.5574	(2,2,3)
-3.3576	(1,1,5)	-2.5545	(2,2,0)
-3.3295	(-,-,5)	-2.5142	(2,3,0)
-3.3239	(3,3,0)	-2.4983	
-3.3202	(0,0,7)	-2.4655	
-3.3042	(2,2,0)	-2.459	
-3.278	(-,-,3)	-2.4505	
-3.2714	(2,2,0)	-2.4187	
-3.2349	(3,3,0)		
-3.2293	(3,3,1)		
-3.2096	(2,2,1)		
-3.1756	(1,1,1)		
-3.1618	(1,1,4)		
-3.1384	(1,1,1)		

Table S2: Eigenenergies (E_n in eV), assignments (ν_1, ν_2, ν_3), and decay lifetimes (τ_n in ps) of the quasibound state resonances of CH_2^+ complex in its electronic ground 1 $^2A'$ PES. The linewidth lifetimes for some of the resonances are given within the parentheses of decay lifetimes (in ps). Threshold energies (in eV) for different vibrational levels ($v = 0 - 6$) are also given within the parentheses of resonance energies.

E_n/eV	(ν_1, ν_2, ν_3)	τ_n/ps	E_n/eV	(ν_1, ν_2, ν_3)	τ_n/ps	E_n/eV	(ν_1, ν_2, ν_3)	τ_n/ps
-1.7894	(8,0,0)		-0.6279	(12,0,2)		1.4806(1.447)	(9,9,1)	1.06(1.08)
-1.7318	(3,4,1)		-0.5838	(13,0,0)	1.04(1.12)	1.5631	(9,9,2)	0.60(0.63)
-1.6943	(7,8,1)		-0.4953	(13,0,1)	1.661(3.18)	1.6334	(9,10,0)	0.67(0.77)
-1.6830	(3,3,2)		-0.4437	(12,1,0)		1.7233(1.729)	(9,10,1)	0.66(0.69)
-1.6315	(-,-,0)		-0.4170	(13,0,2)		1.8049	(9,10,2)	0.45(0.48)
-1.5884	(-,-,0)		-0.3851	(13,0,0)		1.8695	(10,10,0)	0.18(0.32)
-1.5434	(3,4,0)		-0.3561	(12,1,1)		1.9577	(10,10,1)	0.20(0.26)
-1.5312	(3,4,3)		-0.2975	(13,0,1)	2.79(2.88)	2.0373(1.998)	(10,10,2)	0.39(0.45)
-1.5237	(0,9,0)		-0.2764	(12,1,2)	7.07			
-1.5233	(9,0,0)		-0.2343	(13,1,-)				
-1.4956	(4,4,0)		-0.2015	(14,0,0)	8.30			
-1.4394	(0,0,12)		-0.1471	(13,1,3)	7.66			
-1.4328	(0,0,0)		-0.1176	(14,0,1)	8.20			
-1.3054	(1,1,0)		0.0141	(13,1,3)	0.06			
-1.2913	(1,1,0)		0.0487	(6,7,0)	3.9(4.39)			
-1.2693	(10,0,0)		0.1064	(13,2,0)	0.67(0.59)			
-1.2492	(0,0,-)		0.1340	(6,6,4)	4.5			
-1.1793	(10,0,1)		0.1453(0.175)	(6,7,1)	4.4(4.6)			
-1.1686	(2,2,0)		0.2296	(6,7,2)	2.7			
-1.1554	(1,1,0)		0.3158	(6,7,3)	6.7			
-1.1086	(1,1,-)		0.3327	(7,7,0)	11.0			
-1.088	(2,2,12)	4.35(1.0)	0.4283	(7,7,1)	4.0			
-1.072	(4,5,1)		0.4320	(13,3,0)	(0.83)			
-1.066	(3,3,-)	1.16(1.06)	0.5117(0.514)	(7,7,2)	1.4(1.5)			
-1.0477	(2,2,0)	1.45(1.21)	0.6091	(7,8,0)	2.0(2.0)			
-1.0275	(11,0,0)	1.48(3.21)	0.7038	(7,8,1)	4.7(4.9)			
-1.0261	(2,1,0)	1.27(1.78)	0.7872	(7,8,2)	1.7(1.83)			
-0.9666	(3,0,0)		0.8668(0.839)	(7,8,3)	0.54(0.72)			
-0.9371	(11,0,1)		0.8771	(8,8,0)	1.5(1.6)			
-0.9104	(10,1,0)	2.95(3.03)	0.9708	(8,8,1)	1.5(1.5)			
-0.8921	(5,0,0)	1.72(2.22)	1.0542	(8,8,2)	0.4(0.41)			
-0.8532	(11,0,2)	0.41	1.1367(1.150)	(8,9,0)	1.2(1.26)			
-0.7984	(12,0,0)		1.2295	(8,9,1)	1.47(1.49)			
-0.7085	(12,0,1)	7.22	1.3129	(8,9,2)	1.04(1.08)			
-0.6700	(11,1,0)	8.29	1.3888	(9,9,0)	0.94(1.0)			

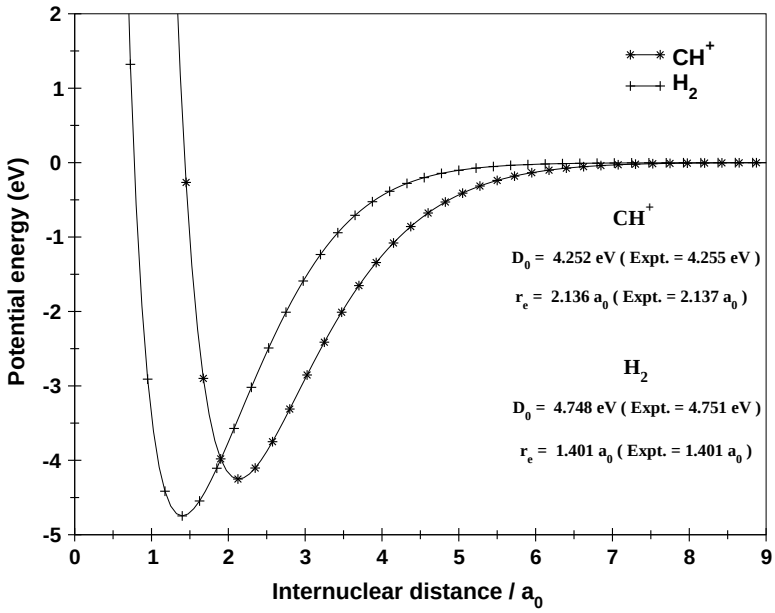

Fig. S1: Diatomic potential as a function of internuclear distance for the both reagent and product asymptotes of the title reaction in the electronic ground surface.

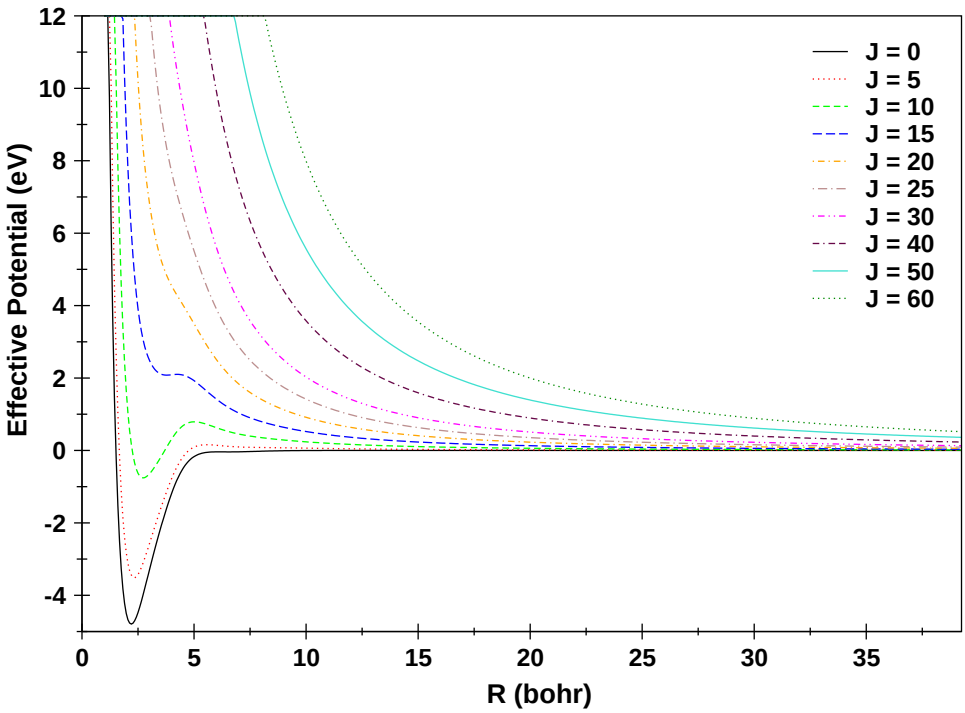

Fig. S2: A $1D$ cut of the effective potential along the Jacobi distance R for an increasing contributions of the partial waves J up to 60. The height of the barrier increases with increasing J, and for larger contributions of J (≥ 25), the potential energy curve attains highly repulsive nature and as a result the collision becomes more direct.

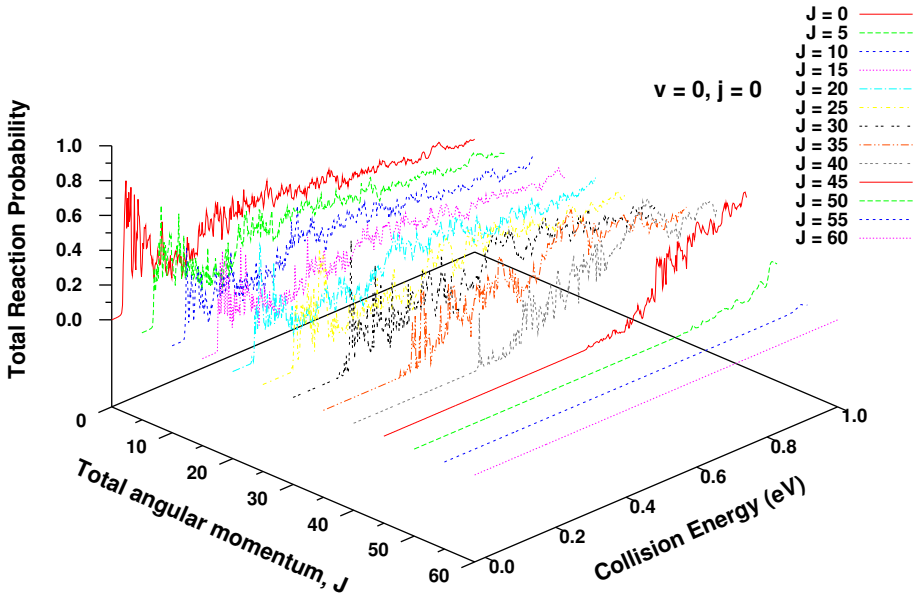

Fig. S3: A $3D$ representative plot of the J-dependent total (R1+R2) reaction probabilities for the title reaction.

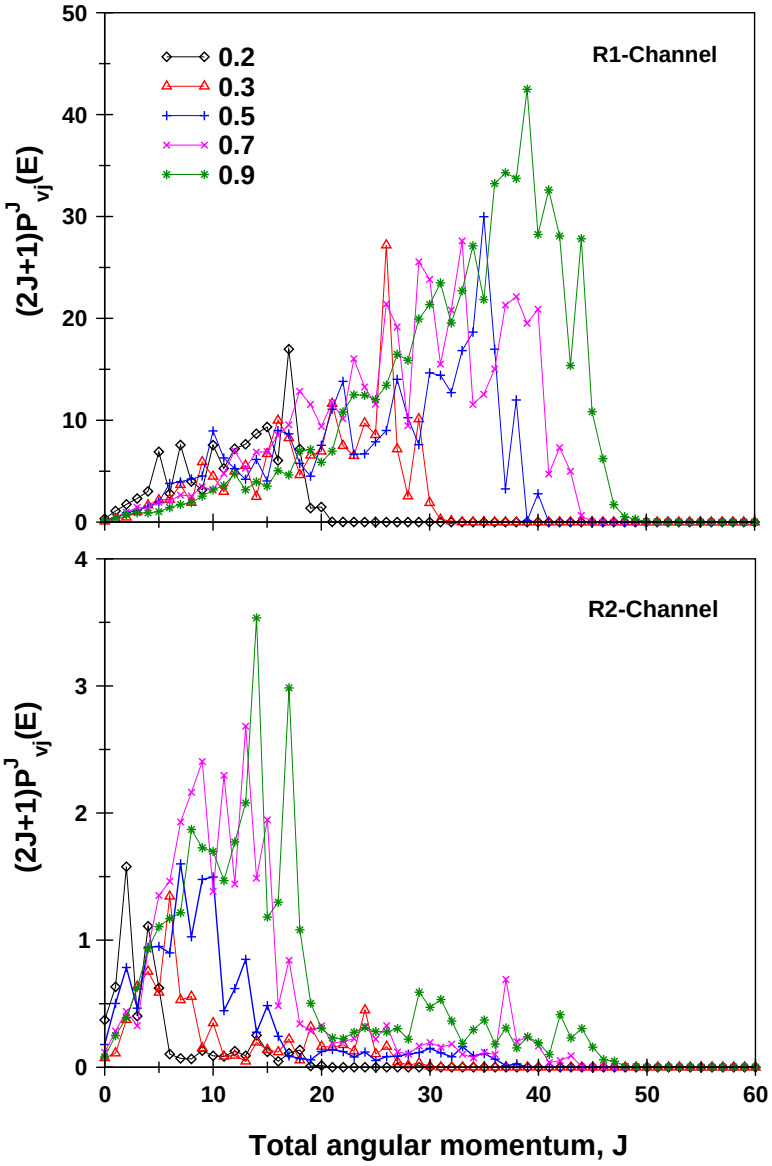

Fig. S4: $(2J + 1)$ weighted channel specific reaction probabilities as a function of total angular momentum J for few selected collision energies. It endorses the dominant characteristics of the H abstraction (R1) channel over the H exchange (R2) channel at given energies.

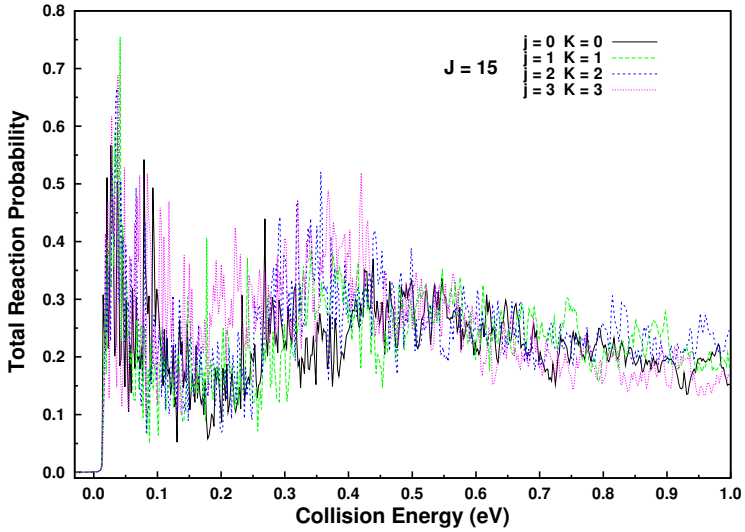

Fig. S5: $K \neq 0$ reaction probabilities as a function of collision energy for the title reaction for $J = 15$.

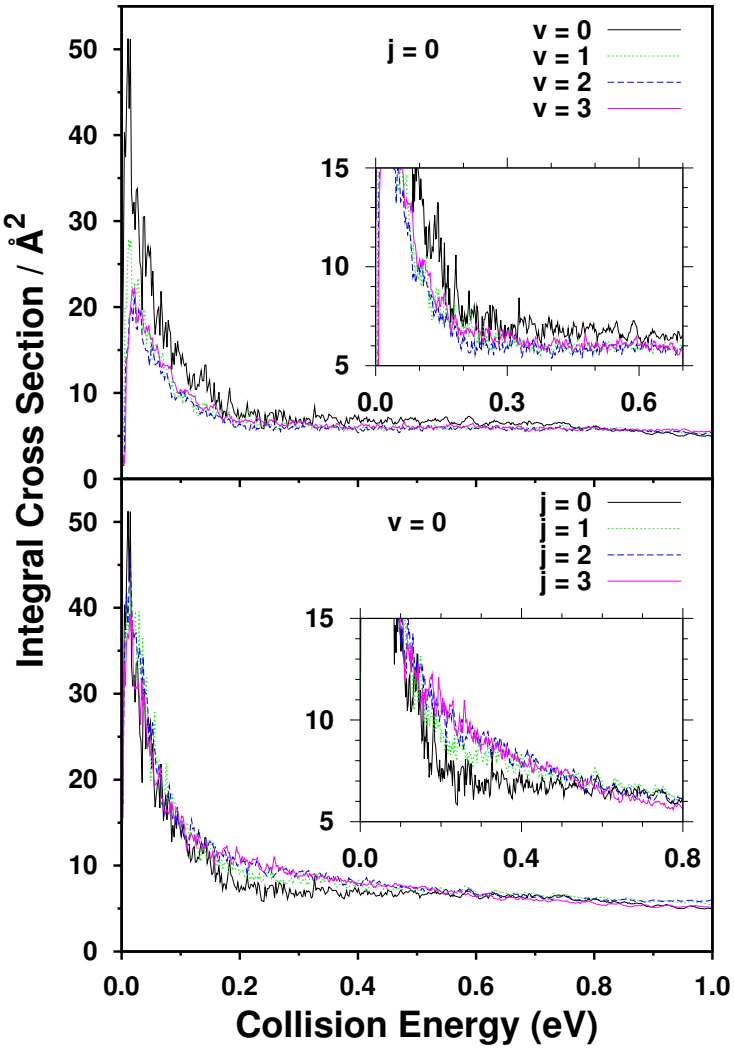

Fig. S6: Same as in Fig. 4, for the overall reaction (R1+R2).

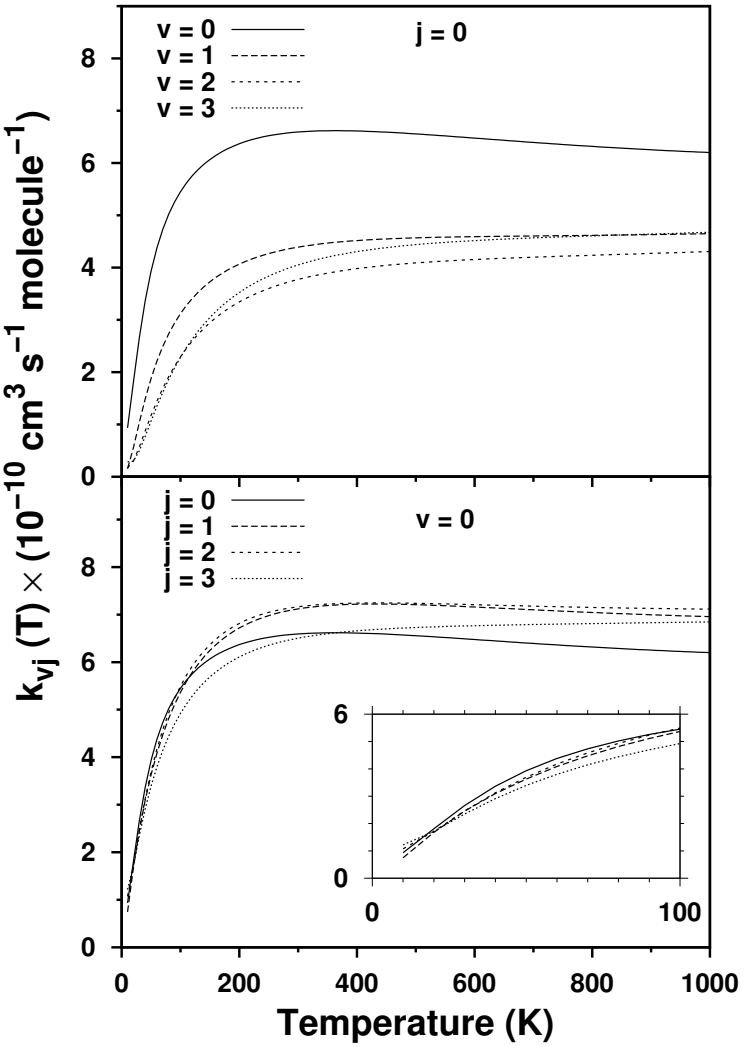

Fig. S7: Same as in Fig. 5, for the overall reaction (R1+R2).

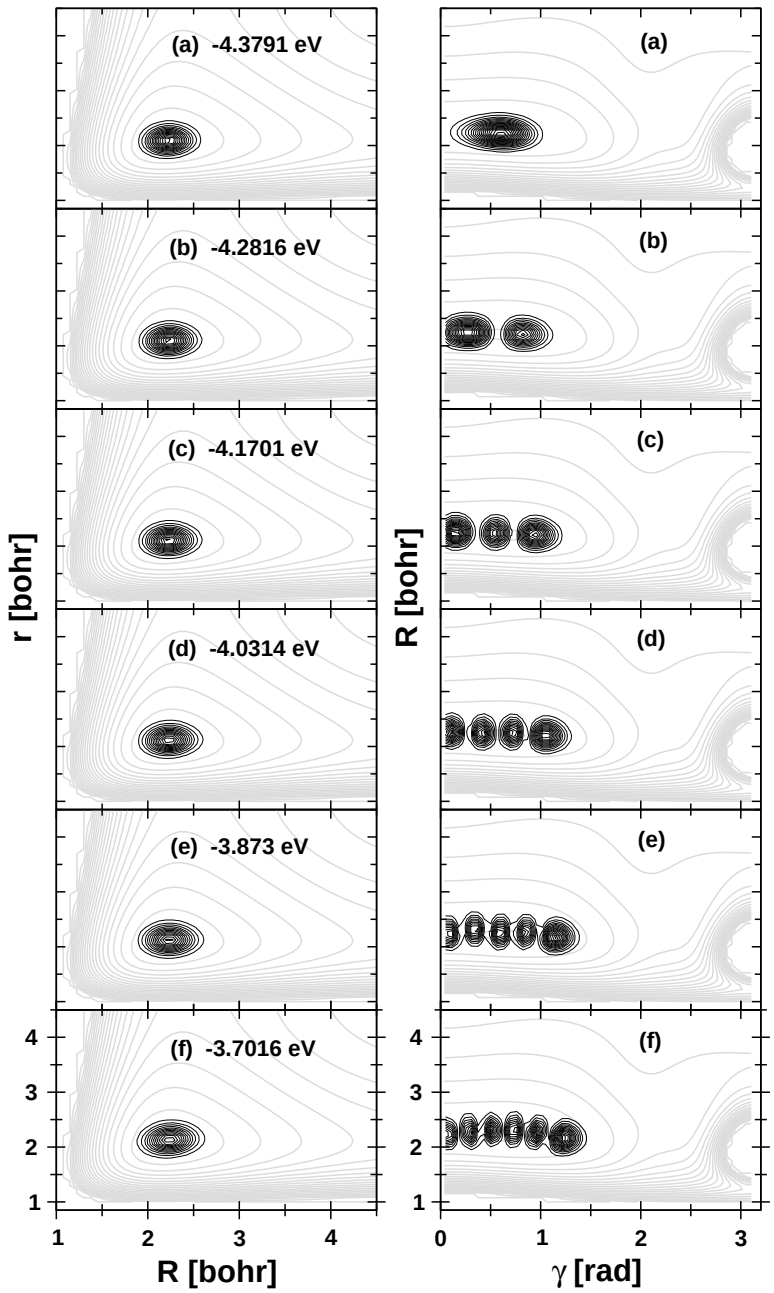

Fig. S8: Probability density contours of the six bound vibrational levels of CH_2^+ (belong to Type I, as stated in the text), plotted in the (R, r) plane (left column) and (γ, R) plane (right column). The ground vibrational level of CH_2^+ corresponds to (0,0,0) state with energy -4.3791 eV.

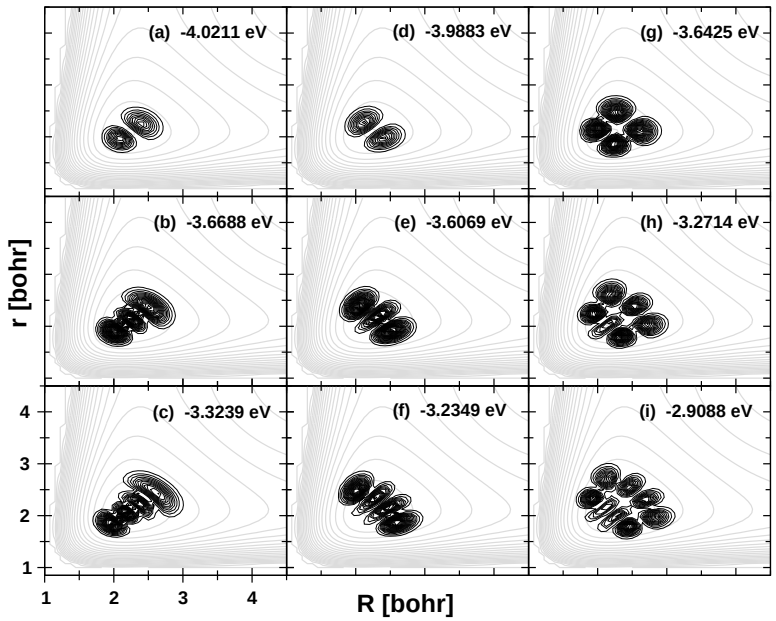

Fig. S9: Probability density contours of few low-lying vibrational levels of CH_2^+ (belong to Type II), plotted in the (R, r) plane.

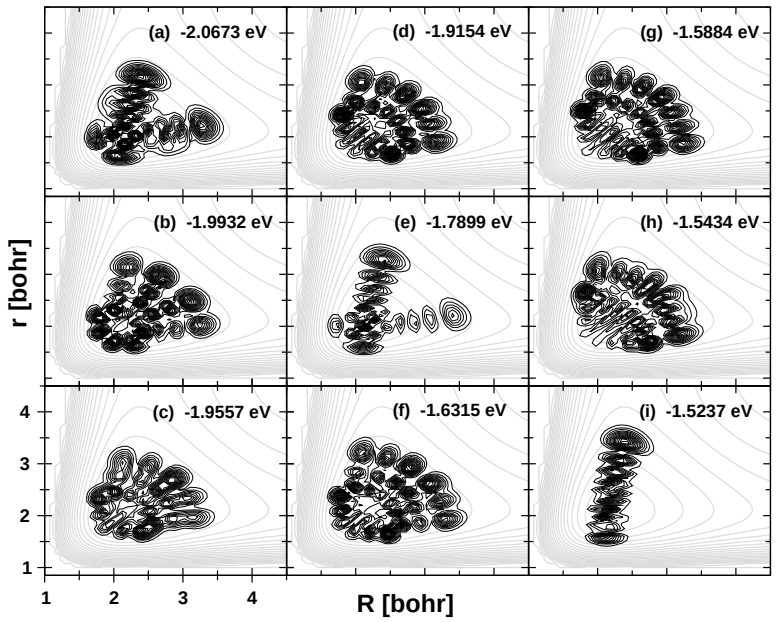

Fig. S9 (*Continued.*)

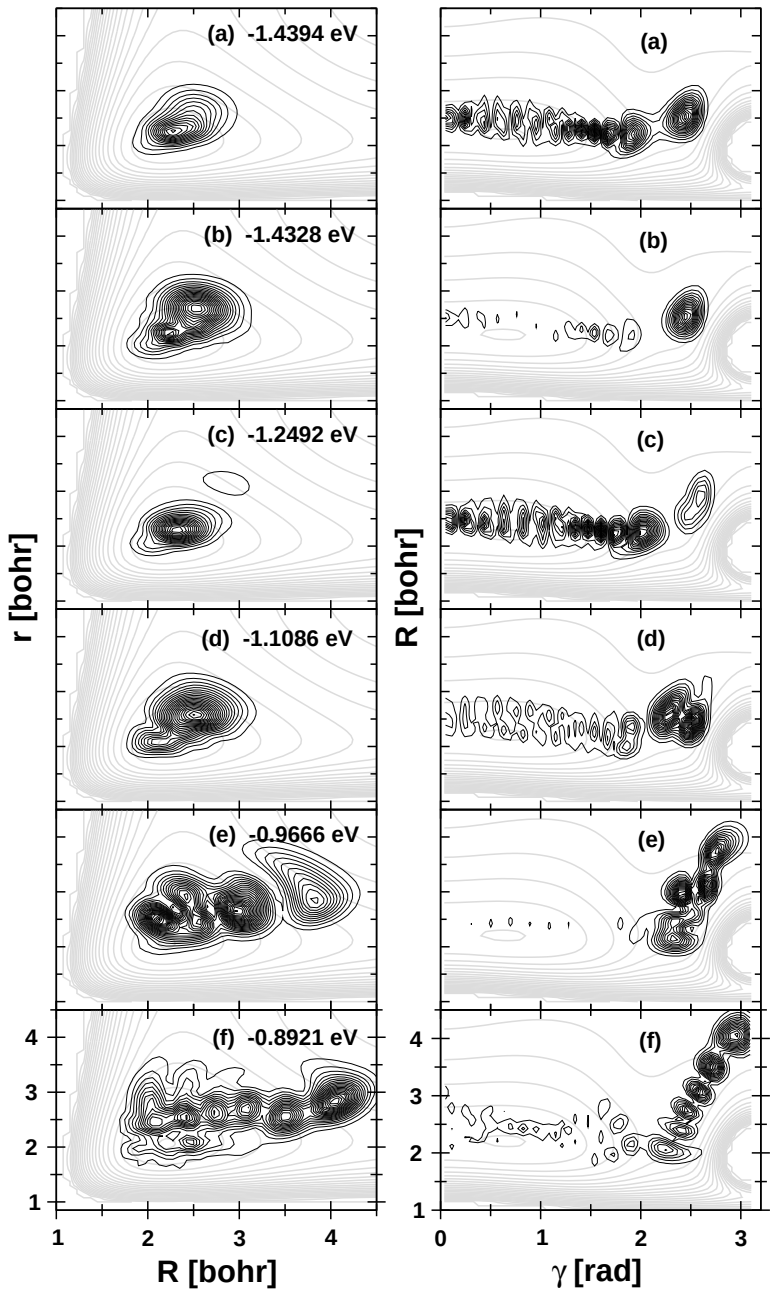

Fig. S10: Quasibound eigenfunctions belong to Type I, same as in Fig. S8.

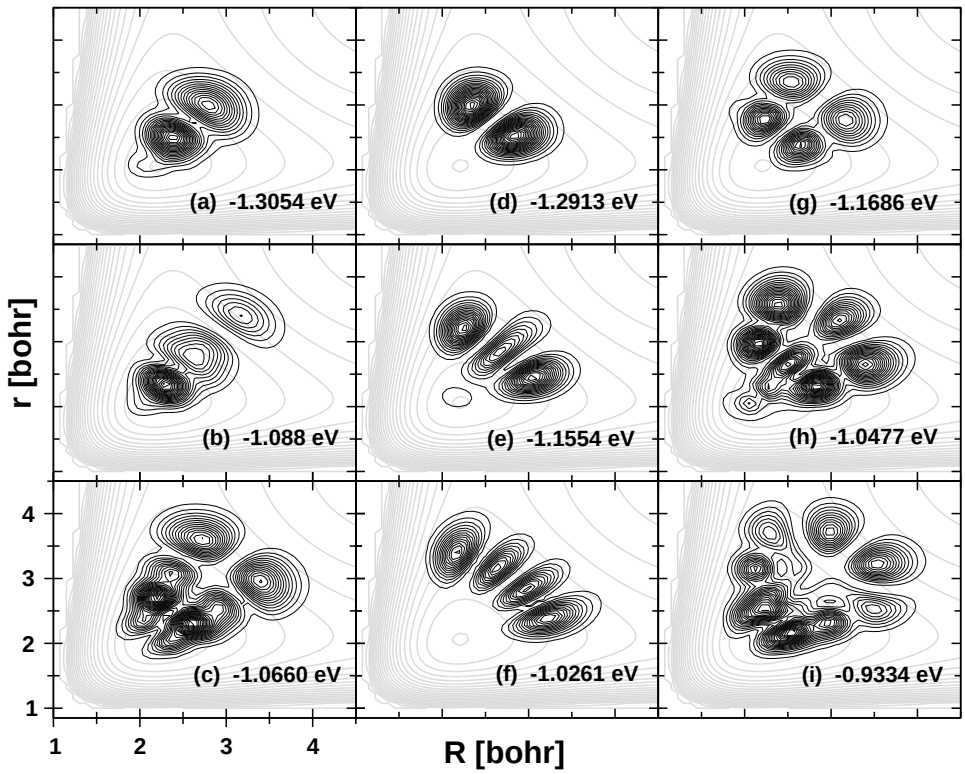

Fig. S11: Quasibound eigenfunctions belong to Type II, same as in Fig. S9.

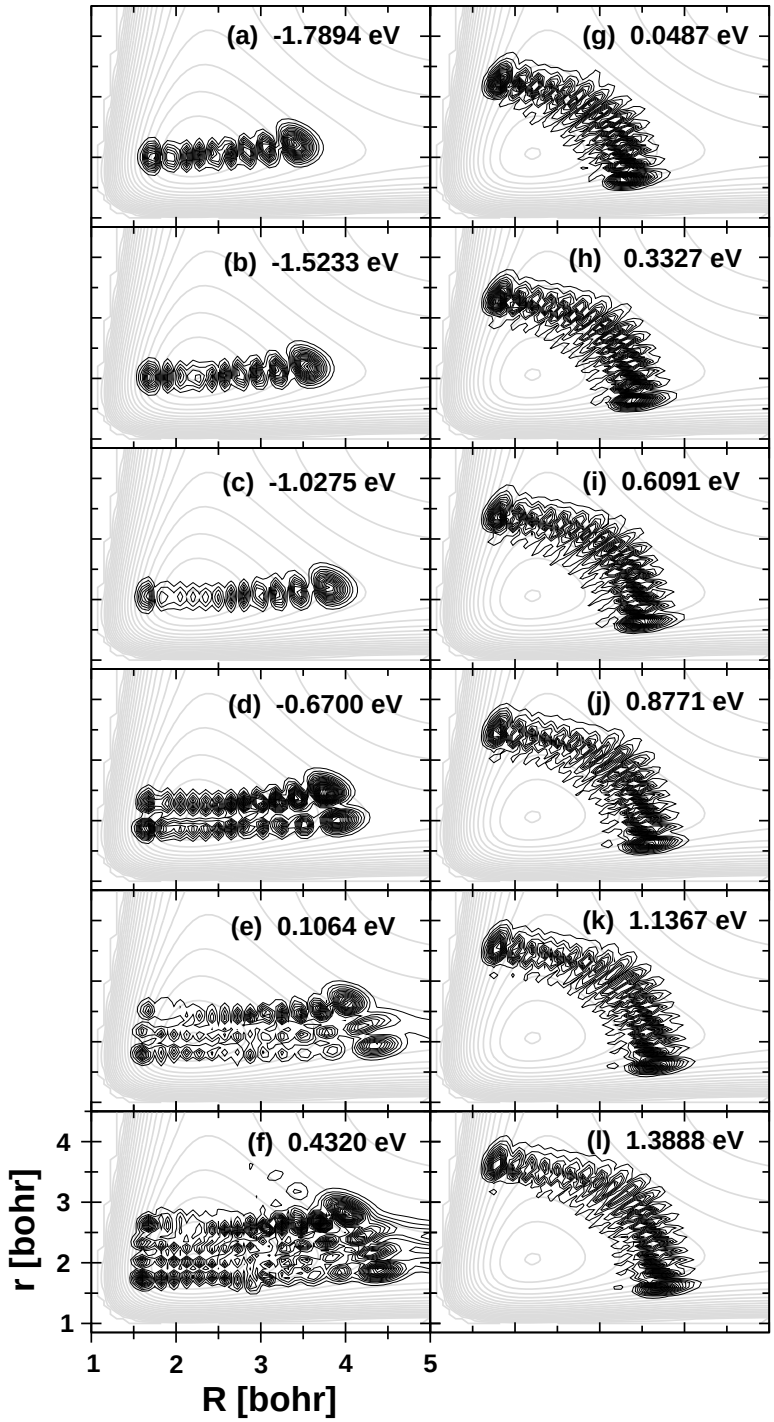

Fig. S12: Probability density contours of the decaying resonances belong to Type III and IV, plotted in the (R, r) plane.