TYPE	E (eV)	r_1	r_2	R	θ_1	θ_2	P_{r_1}	P_{r_2}	P_R	P_{θ_1}	P_{θ_2}	T (t.u.)	STABILITY
SS	-16.5950	1.66250	1.66250	1.20517	.00000	3.14159	.88279	.88279	-1.32621	.00000	.00000	.9488	SSSS
SS1A	-13.6985	1.66250	1.66250	1.21137	.00000	3.14159	1.66179	1.66179	-3.42566	.00000	.00000	3.1514	USSS
AS	-16.5950	1.75389	1.66250	1.20208	.00000	3.14159	-.79830	.95948	-.07983	.00000	.00000	1.0072	USSS
AS1A	-16.6450	1.76776	1.66250	1.19872	.00000	3.14159	-1.02452	.53937	.42830	.00000	.00000	1.0175	SSSS
AS1B	-16.6441	1.70983	1.66250	1.20619	.00000	3.14159	-.45388	1.18885	-.55117	.00000	.00000	1.0176	SSSS
CC	-16.5950	1.66250	1.66250	1.16219	.00000	3.14159	.45342	.45342	2.79136	.00000	.00000	1.6493	SSSS
CC1A	-13.9250	1.62648	1.66250	1.09059	.00000	3.14159	1.04594	1.28082	4.33775	.00000	.00000	3.4886	SSSS
CIS	-16.5950	1.66250	1.66250	1.20741	-.19456	3.33615	.06944	.06944	-.57385	1.37769	-1.37769	4.4103	SSSS
CIS1A	-13.1851	1.66890	1.66250	1.08027	.14259	2.96674	.10622	.14173	-2.67028	-2.72379	2.70366	4.3324	SSSS
CIS1B	-13.1851	1.6543	1.66250	1.10629	.22740	2.94613	.15774	.12716	-3.28113	-2.63453	2.66041	4.3324	SSSS
TR	-16.5950	1.66250	1.66250	1.21743	.24657	3.38816	.13254	.13254	-.05348	-1.13436	-1.13436	4.3203	SSSS
TR1A	-16.5085	1.66250	1.66250	1.21143	-.22432	2.91727	.77249	.77249	-1.08613	.56261	.56261	4.7258	SSSS
TR1A1A	-16.1515	1.64722	1.66250	1.21366	-.26351	2.96008	.96191	.94699	-1.35626	.33878	.66513	4.8089	SSSS
TR1A2A	-15.4050	1.65996	1.66250	1.18220	-.26943	2.97960	1.14679	1.17273	-2.22542	.66443	.26856	4.9576	USSS
TR1A2A1A	-14.8425	1.65236	1.66250	1.18596	-.40971	3.03389	1.18798	1.26422	-2.42686	1.07243	-.11027	5.1014	USSS
TR2A	-16.5050	1.67346	1.66250	1.21109	-.19343	3.07260	.57549	.64864	-.87407	1.41543	.168773	4.7095	SSSS
TR3A	-14.6450	1.66250	1.66250	1.18218	-.43284	2.70875	.65014	.65012	2.63641	1.39376	1.39376	5.1317	SSSS
TR3B	-14.6442	1.66250	1.66250	1.18198	-.43284	2.70875	.65076	.65076	2.63802	1.39274	1.39274	5.1318	SSSS

TABLE I Initial conditions for periodic orbits of acetylene. The coordinate system is that shown in Fig. A1 in the Appendix. The time units are 1 t.u. = 1.018×10^{-14} sec, and the absolute minimum is at -17.552 eV.

TYPE	E (eV)	r_1	r_2	R	θ_1	θ_2	P_{r_1}	P_{r_2}	P_R	P_{θ_1}	P_{θ_2}	T (t.u.)	STABILITY
VSS	-14.10501	1.55449	1.55449	1.30804	.64449	5.63869	1.20633	1.20633	-.48289	.65347	-.65347	1.07346	ΔSS
VAS	-14.05372	1.70842	1.55449	1.316644	.67244	5.65233	-.91359	1.23416	-.10251	-.45737	-.58017	1.0797	USSS
VCC	-14.10345	1.55449	1.55449	1.23006	.59262	5.69056	.15607	.15607	2.45826	-1.38488	1.38488	3.53039	ΔSS
SCIS	-14.07444	1.55449	.155449	1.34816	.82951	5.45367	.23253	.23253	-.74194	-1.07842	1.07842	1.53736	SSSS
ROCK	-14.10751	1.55653	1.55449	1.30741	.74113	5.74732	.88457	1.18819	-.28375	1.34106	-0.02446	12.00995	UUUS

TABLE IIa Initial conditions for periodic orbits of vinylidene.

TYPE	E (eV)	r_1	r_2	R	θ_1	ϕ	θ_2	P_{r_1}	P_{r_2}	P_R	P_{θ_1}	P_ϕ	P_{θ_2}	T (t.u.)	STABILITY
VOUT	-14.21871	1.59075	1.58494	1.35511	2.41182	1.57080	.80112	.0	.0	.0	.0	1.50747	.0	2.35707	SSSS

TABLE IIb Initial conditions for the out of plane periodic orbit of vinylidene. The coordinate system is defined in the Fig. A3 of the Appendix.

TYPE	E (eV)	r_1	r_2	R	θ_1	θ_2	P_{r_1}	P_{r_2}	P_R	P_{θ_1}	P_{θ_2}	T(t.u.)	STABILITY
TSA	-14.82393	1.14797	1.66507	1.18470	4.5387	2.9664	.09812	1.08283	-.53032	.04658	-.15734	.98293	USSS
TSB	-14.82388	1.30864	1.66507	1.19360	4.65549	3.03488	-.76886	.07793	.26544	-.03433	-.17731	1.3252	ΔUS
TSC	-14.82391	1.17006	1.66507	1.25011	4.71625	2.94615	.06591	.89160	-.68662	-.15281	.33933	1.93426	ΔUU
TSD	-15.43135	1.12925	1.66507	1.18712	4.57401	2.97575	-.02612	.05238	.18360	0.02935	.34931	7.19700	UUUS

TABLE IIIa Initial conditions for periodic orbits of the transition state.

TYPE	E (eV)	r_1	r_2	R	θ_1	ϕ	θ_2	P_{r_1}	P_{r_2}	P_R	P_{θ_1}	P_ϕ	P_{θ_2}	T(t.u.)	STABILITY
TSOUT	-14.63367	1.09596	1.69033	1.19202	1.30824	1.57080	-1.28460	.0	.0	.0	.0	1.54271	.0	2.56117	ΔUS

TABLE IIIb Initial conditions for the out of plane periodic orbits of the transition state.

TYPE	E (eV)	r_1	r_2	R	θ_1	θ_2	P_{r_1}	P_{r_2}	P_R	P_{θ_1}	P_{θ_2}	T(t.u.)	STABILITY
R1A	-14.99971	1.26090	1.69805	1.37360	4.33369	2.97864	-.51943	.34832	-.38186	.780816	.53989	12.649	ΔSS
R1B	-14.99952	1.17257	1.71026	1.36458	4.3891	2.97864	-.00423	.40317	.48844	.91070	.39418	13.074	UUUS
R2A	-14.52924	1.26621	1.83816	1.34009	4.5848	2.97864	-.21199	-.28093	.43533	1.14418	.51890	11.220	USSS
R2B	-14.52918	1.16015	1.78837	1.35488	4.74434	2.97864	-.13772	-.21328	.60494	.96082	.95368	11.102	USSS
R2B1A	-14.50993	1.14999	1.80963	1.33993	4.60199	2.97864	-.31076	.11809	.60242	1.19070	.58031	10.956	USSS
R3A	-14.01194	1.77865	1.77865	1.33772	6.12024	2.97864	-.06398	-.06398	2.2059	2.01199	2.01199	10.591	UUSS
R3B	-14.01194	1.80359	1.80359	1.3390	6.12023	2.97864	.16832	.16832	1.74645	2.04063	2.04063	10.111	UUSS
R3B1A	-14.01192	1.79138	1.82089	1.34645	6.16459	2.97864	.20888	.04579	1.60613	2.03470	2.01974	10.160	ΔUS
R3B2A	-14.01105	1.80148	1.80555	1.33884	6.11914	2.97864	.15824	.18018	1.74969	2.04610	2.03594	10.111	UUSS
R4A	-14.01102	1.81681	1.81681	1.35261	6.12023	2.97864	.17128	.17128	2.27342	1.86325	1.86325	9.477	USSS
R4B	-14.01105	1.812448	1.812448	1.35283	6.12023	2.97864	.11056	.11056	2.44488	1.84239	1.84239	9.686	UUSS
R4A1A	-13.95000	1.81264	1.81264	1.34619	6.12023	2.97864	.31471	.31471	2.42296	1.86690	1.86690	9.225	ΔUS
R4A1A1A	-13.75675	1.87234	1.87234	1.37341	0.07310	3.21469	.22356	.22356	-.94779	1.97751	1.97751	9.010	USSS

TABLE IV Initial conditions for saddle-node periodic orbits and their bifurcations.

TYPE	E (eV)	T(t.u.)	STABILITY
R1A	-15.128860	12.8619	ΔUS
R1B			ΔUU
R2A	-14.597589	11.1055	USSS
R2B			SSSS
R3A	-14.076243	10.3668	UUSS
R3B			USSS
R4A	-14.017656	9.5959	USSS
R4B			UUSS

TABLE V Stability properties and period of the saddle-node bifurcating periodic orbits at the energy of generation.