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Ab initio MP2 study of the reaction mechanisms of C_2 with halogens and hydrohalides

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Table S1 Energy characteristics for the interaction of hydrohalides HX with dicarbene C_2.

System	E	E'	S	G
The level of calculation MP2/aug-cc-pVDZ				
C_2	-75.7063	-75.7021	45.598	-75.7204
HF	-100.2558045	-100.246503	41.497	-100.262915
TS1(C_2 + HF)	-175.9126088	-175.900968	60.793	-175.925169
HFC=C	-176.0441222	-176.026054	60.301	-176.050268
TS2'(HFC_2 … F C_2 H)	-176.0432387	-176.026772	58.556	-176.050522
TS2(HFC_2 … H C_2 F)	-175.9892229	-175.973310	60.236	-175.997576
HC=CF	-176.123916	-176.105712	46.597	-176.123120
HCl	-460.251823	-460.244936	44.609	-460.262826
TS1(C_2 + HCl)	-535.9474974	-535.935480	64.308	-535.960995
HClC=C	-536.0633528	-536.046492	63.946	-536.072169
TS2'($HClC_2$ … Cl C_2 H)	-536.0627169	-536.047165	61.114	-536.072031
TS2($HClC_2$ … H C_2 Cl)	-536.0445185	-536.028410	61.819	-536.053535
HC=CCl	-536.1462641	-536.128913	54.694	-536.150113
The level of calculation MP2/6-311+G*				
C_2	-75.7202534	-75.716000	45.562	-75.734342
HBr	-2573.0760586	-2573.070069	47.434	-2573.089301
TS1(C_2 + HBr)	-2648.7934073	-2648.782224	67.093	-2648.808957
HBrC=C	-2648.9202947	-2648.903481	65.718	-2648.930038
TS2'($HBrC_2$ … Br C_2 H)	-2648.914434	-2648.899840	63.776	-2648.925791
TS2($HBrC_2$ … H C_2 Br)	-2648.9116702	-2648.895507	64.105	-2648.921722
HC=CBr	-2649.00013	-2648.983014	63.035	-2649.007841

Comment:

E – Total (electronic) energies (a.u.)
E' – Sum of electronic and zero-point energies (a.u.)
S – Total entropy (CAL/MOL-KELVIN)
G – Sum of electronic and thermal free energies (a.u.)

Table S2 Energy characteristics for the interaction of halogens X_2 with dicarbene C_2.

System	E	E’	S	G
The level of calculation MP2/aug-cc-pVDZ				
C_2	-75.7063	-75.7021	45.598	-75.7204
F_2	-199.1269174	-199.124789	48.437	-199.144451
TS1(C_2 + F_2)	-274.7932243	-274.786239	64.079	-274.812298
F_2C=C	-275.0929457	-275.081069	64.564	-275.107082
TS2(F_2C_2 … F C_2 F)	-275.0366127	-275.026846	65.026	-275.053022
HC=CF	-275.1456901	-275.133630	54.054	-275.153953
Cl_2				
TS1(C_2 + Cl_2)	-994.9487137	-994.942733	75.795	-994.973349
Cl_2C=C	-995.1180178	-995.109170	71.693	-995.137762
TS2(Cl_2C_2 … Cl C_2 Cl)	-995.1063641	-995.098132	69.418	-995.126113
ClC=CCl	-995.1970054	-995.187596	62.844	-995.211411
The level of calculation MP2/6-311+G*				
C_2	-75.7202534	-75.716000	45.562	-75.734342
Br_2	-5144.9723659	-5144.971614	58.561	-5144.995750
TS1(C_2 + Br_2)	-5220.666972	-5220.658876	73.414	-5220.688661
Br_2C=C	-5220.8229002	-5220.8139632	74.960	-5220.8441832
TS2(Br_2C_2 … Br C_2 Br)	-5220.8224079	-5220.8144539	73.421	-5220.8442959
BrC=CBr	-5220.9034083	-5220.8928773	63.429	-5220.9176983

Comment:

E – Total (electronic) energies (a.u.)
E’ – Sum of electronic and zero-point energies (a.u.)
S – Total entropy (CAL/MOL-KELVIN)
G – Sum of electronic and thermal free energies (a.u.)