

Supplementary material of

**A theoretical study about the effect of C₆₀ particle on the growth of
coronene radical based on the HACA pathway**

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● **Rate coefficients in modified Arrhenius expression.**

Table S1. Modified Arrhenius parameters of high-pressure limit rate coefficients for C₂H₂ addition to R1 and R2. $k = A T^n \exp(-E/RT)$. The units of E are cal/mol. Units of rate constants for bimolecular and unimolecular reactions are cm³molecule⁻¹s⁻¹ and s⁻¹, respectively. The bath gas is Ar.

Reactions	A	n	E
R1+C ₂ H ₂ →INT1'	8.08E-21	2.62E+00	1.40E+03
R2+C ₂ H ₂ →INT1	1.20E-20	2.60E+00	5.32E+02
INT1→INT2	1.36E+11	3.13E-01	1.69E+04
INT1→INT2-2	1.12E+11	2.98E-01	1.39E+04
INT1→INT3	6.87E+07	1.35E+00	7.24E+03
INT2→PC2	4.96E+07	1.48E+00	6.23E+03
INT2-2→PC1	1.59E+10	1.11E+00	2.76E+04
INT3→INT4	1.34E+11	2.90E-01	1.24E+04
INT4→PC1	5.13E+10	1.01E+00	4.79E+04
INT4→PC2	2.99E+10	9.84E-01	4.55E+04
INT1'→INT2'	3.24E+11	2.50E-01	1.84E+04
INT1'→INT3'	1.77E+08	1.21E+00	8.94E+03
INT3'→INT4'	1.24E+11	2.96E-01	1.26E+04
INT2'→PC1'	8.61E+09	1.13E+00	2.58E+04
INT4'→PC1'	9.69E+10	1.02E+00	4.77E+04

Table S2. Modified Arrhenius parameters of high-pressure limit rate coefficients for C₂H₂ addition to R3 and R4. $k = A T^n \exp(-E/RT)$. The units of E are cal/mol. Units of rate constants for bimolecular and unimolecular reactions are cm³molecule⁻¹s⁻¹ and s⁻¹, respectively. The bath gas is Ar.

Reactions	A	n	E
R3+C ₂ H ₂ →INT9	7.22E-24	3.08E+00	2.30E+04
R4+C ₂ H ₂ →INT15	1.83E-22	2.60E+00	1.10E+04
INT9→INT10	5.99E+11	2.17E-01	5.21E+03
INT10→INT11	2.84E+12	1.77E-01	2.56E+03
INT11→INT12	8.02E+07	1.53E+00	5.73E+04
INT12→INT13	6.44E+01	3.24E+00	1.74E+04
INT12→INT14	2.02E+11	2.91E-01	1.78E+04
INT13→PC3	3.12E+11	5.58E-01	1.06E+04
INT14→PC4	8.48E+11	5.12E-01	1.33E+04
INT15→INT16	5.66E+11	2.11E-01	3.52E+03
INT16→INT17	8.38E+12	1.06E-01	5.95E+03
INT17→INT18	2.74E+07	1.38E+00	3.87E+04
INT18→INT19	1.11E+02	3.22E+00	1.75E+04
INT18→INT20	1.20E+11	2.98E-01	1.60E+04
INT19→PC3	1.97E+12	3.22E-01	2.01E+04
INT20→PC4	1.32E+13	2.42E-01	2.08E+04