

Supplementary information:

Flow tube studies of the C(³P) reactions with ethylene and propylene

Michael Capron,¹ Jérémy Bourgalais,¹ Ranjith Kumar Abhinavam Kailasanathan,² David L. Osborn,³ Sébastien D. Le Picard,^{1,} Fabien Goulay^{2,*}*

¹ Institut de Physique de Rennes, Département de Physique Moléculaire, Astrophysique de Laboratoire, UMR CNRS 6251, Université de Rennes 1, Campus de Beaulieu, 35042 Rennes Cedex, France

² Department of Chemistry, West Virginia University, Morgantown, West Virginia 26506, USA

³ Combustion Research Facility, Mail Stop 9055, Sandia National Laboratories, Livermore, California 94551, USA

*Electronic mail: sebastien.le-picard@univ-rennes1.fr, fabien.goulay@mail.wvu.edu

Table S1 Preponderant reactions expected to occur upon irradiation of a C₃O₂ + C₂H₄ mixture

Reactions	k (300K) / cm ³ s ⁻¹	Reference
1 C + C ₂ H ₄ → C ₃ H ₃ + H	2.1×10 ⁻¹⁰	1
2 C + C ₃ O ₂ → C ₂ + 2CO	2×10 ⁻¹⁰	2
3 C + C ₂ O → C ₂ + CO	4×10 ⁻¹¹	By comparison with C + O ₂ (triplet + triplet reaction)
4 C + C ₃ H ₃ → C ₄ H ₂ + H	1×10 ⁻¹⁰	OSU database ³
5 C + C ₂ H ₃ → C ₃ H ₂ + H	1×10 ⁻¹⁰	OSU database ³
6 C ₂ O + H → CH + CO	3×10 ⁻¹¹	4-6
7 C ₂ O + C ₃ O ₂ → C ₂ + 3CO	1×10 ⁻¹⁰	By comparison with ¹ C ₂ O + NH ₃ ⁷
8 C ₂ O + C ₂ H ₃ → C ₃ H ₃ + CO	4×10 ⁻¹¹	Considering no barrier (radical + radical reaction)
9 C ₂ O + C ₃ H ₃ → C ₄ H ₃ + CO	4×10 ⁻¹¹	Considering no barrier (radical + radical reaction)
10 C ₂ O + C ₂ H ₄ → C ₃ H ₄ + CO	1×10 ⁻¹⁰	By comparison with ¹ C ₂ O + NH ₃ ⁷
11 C ₂ O + C ₃ H ₄ → C ₄ H ₄ + CO	1×10 ⁻¹⁰	By comparison with ¹ C ₂ O + NH ₃
12 CH + C ₃ O ₂ → C ₂ H + 2CO	1×10 ⁻¹⁰	Sato et al. ⁸ propose 1.0e-11 inferred from a complex mechanism
13 CH + C ₂ H ₄ → C ₃ H ₄ + H	2.84×10 ⁻¹⁰	9
14 CH + C ₃ H ₄ → C ₄ H ₄ + H	4.6×10 ⁻¹⁰	10
15 C ₂ H + C ₂ H ₄ → C ₄ H ₄ + H	9.9×10 ⁻¹¹	11
16 C ₂ H + C ₃ O ₂ → HC ₄ O + CO	1.0×10 ⁻¹⁰	By comparison with C ₂ O + NH ₃ ⁷
17 C ₂ H + C ₂ O → C ₃ H + CO	4.0×10 ⁻¹⁰	Estimated by comparison with C ₂ H + NO

Table S2 Preponderant reactions expected to occur upon irradiation of a C₃O₂ + C₃H₆ mixture

	Reaction	k (300K) / cm ³ s ⁻¹	Reference
1	C + C ₃ H ₆ → C ₄ H ₅ + H → C ₃ H ₃ + CH ₃	1.3×10 ⁻¹⁰ 1.3×10 ⁻¹⁰	¹²
2	C + C ₃ O ₂ → C ₂ + 2CO	2×10 ⁻¹⁰	²
3	C + C ₂ O → C ₂ + CO	4×10 ⁻¹¹	By comparison with C + O ₂ (triplet + triplet reaction)
4	C + C ₃ H ₃ → C ₄ H ₂ + H	1×10 ⁻¹⁰	OSU database ³
5	C + C ₄ H ₅ → C ₅ H ₄ + H	1×10 ⁻¹⁰	Estimated based on C + C ₃ H ₃
6	C + C ₂ H ₃ → C ₃ H ₂ + H	1×10 ⁻¹⁰	OSU database ³
7	C + C ₃ H ₅ → C ₄ H ₄ + H	1×10 ⁻¹⁰	Estimated based on C + C ₃ H ₃
8	C + CH ₃ → C ₂ H ₂ + H	1×10 ⁻¹⁰	OSU database ³
9	C ₂ O + H → CH + CO	3×10 ⁻¹¹	^{5,6,13}
10	C ₂ O + C ₃ O ₂ → C ₂ + 3CO	1×10 ⁻¹⁰	By comparison with ¹ C ₂ O + NH ₃
11	C ₂ O + C ₃ H ₅ → C ₄ H ₅ + CO	4×10 ⁻¹¹	Considering no barrier (radical + radical reaction)
12	C ₂ O + CH ₃ → C ₂ H ₃ + CO	4×10 ⁻¹¹	Considering no barrier (radical + radical reaction)
13	C ₂ O + C ₂ H ₃ → C ₃ H ₃ + CO	4×10 ⁻¹¹	Considering no barrier (radical + radical reaction)
14	C ₂ O + C ₃ H ₃ → C ₄ H ₃ + CO	4×10 ⁻¹¹	Considering no barrier (radical + radical reaction)
15	C ₂ O + C ₃ H ₆ → C ₄ H ₆ + CO	1×10 ⁻¹⁰	By comparison with ¹ C ₂ O + NH ₃
16	C ₂ O + C ₄ H ₆ → C ₅ H ₆ + CO	1×10 ⁻¹⁰	By comparison with ¹ C ₂ O + NH ₃
17	CH + C ₃ O ₂ → C ₂ H + 2CO	1×10 ⁻¹⁰	Sato et al. ⁸ propose 1.0e-11 deduced from a complex mechanism
18	CH + C ₃ H ₆ → C ₄ H ₆ + H	3×10 ⁻¹⁰	Extrapolation to 300 K ¹⁴
19	CH + C ₄ H ₆ → C ₅ H ₆ + H	3×10 ⁻¹⁰	By comparison with CH + C ₃ H ₆
20	C ₂ H + C ₃ H ₆ → C ₄ H ₄ + CH ₃ → C ₅ H ₆ + H	5×10 ⁻¹⁰ 9×10 ⁻¹¹	¹⁵
21	C ₂ H + C ₃ O ₂ → HC ₄ O + CO	1.0×10 ⁻¹⁰	By comparison with C ₂ O + NH ₃
22	C ₂ H + C ₂ O → C ₃ H + CO	4.0×10 ⁻¹⁰	Estimated by comparison with C ₂ H + NO

References

1. A. Bergeat and J. C. Loison, *Phys. Chem. Chem. Phys.*, 2001, **3**, 2038-2042.
2. M. P. Deeyamulla and D. Husain, *J. Photochem. Photobiol. A Chem.*, 2006, **184**, 347-353.
3. S. S. Prasad and W. T. Huntress, *Astrophysical Journal Supplement Series*, 1980, **43**, 1-35.
4. W. Bauer, K. H. Becker and R. Meuser, *Ber. Bunsen-Ges. Phys. Chem. Chem. Phys.*, 1985, **89**, 340-341.
5. V. H. Schmidt, R. Meuser, O. Horie, W. Bauer and K. H. Becker, *Bull. Soc. Chim. Belg.*, 1983, **92**, 655-655.
6. O. Horie, W. Bauer, R. Meuser, V. H. Schmidt and K. H. Becker, *Chem. Phys. Lett.*, 1983, **100**, 251-254.
7. J. Bourgalais, C. M., R. K. Abhinavam Kailasanathan, D. L. Osborn, K. M. Hickson, J.-C. Loison, V. Wakelam, F. Goulay and S. D. Le Picard, Under review.
8. K. Sato, N. Ishida, T. Kurakata, A. Iwasaki and S. Tsnuashima, *Chem. Phys.*, 1998, **237**, 195-204.
9. H. Thiesemann, E. P. Clifford, C. A. Taatjes and S. J. Klippenstein, *J. Phys. Chem. A*, 2001, **105**, 5393-5401.
10. J. E. Butler, J. W. Fleming, L. P. Goss and M. C. Lin, *Chem. Phys.*, 1981, **56**, 355-365.
11. D. Chastaing, P. L. James, I. R. Sims and I. W. M. Smith, *J. Chem. Soc., Faraday Trans.*, 1998, **109**, 165-181.
12. J. C. Loison and A. Bergeat, *Phys. Chem. Chem. Phys.*, 2004, **6**, 5396-5401.
13. W. Bauer, K. H. Becker and R. Meuser, *Ber. Bunsenges. Phys. Chem.*, 1985, **89**, 340.
14. N. Daugey, P. Caubet, B. Retail, M. Costes, A. Bergeat and G. Dorthe, *Phys. Chem. Chem. Phys.*, 2005, **7**, 2921-2927.
15. J. Bouwman, F. Goulay, S. R. Leone and K. R. Wilson, *J. Phys. Chem. A*, 2012, **116**, 3907-3917.