**Table: Summary of photodissociation review (reduced model).**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Photodissociation: |  |  | | | | |  | |  | | |  |  |  |
| CH3 → H + 1CH2 |  |  |  | | | |  | | | | | < 260 nm  100% | |  |
| CH4 + hν → 1CH2 + 1H2 q1= (λ-80)/8+46\*exp(1.0\*(λ-119))/(1+exp(1.0\*(λ-119)))  CH4 + hν → 3CH2 + 2H + 2H q2= 80\*exp(-1.0\*(λ-118.6))/(1+exp(-1.0\*(λ-118.6)))\*( λ/120)1.0  CH4 + hν → 2CH + 1H2 + 2H q3= 9.4e-2\*(136.85-λ)1.6  CH4 + hν → 2CH3 + 2H q4= 1-q1-q2-q3 | | | | | | | | | | | | | |  |
| C2H2 + hν → 1C2H + 2H 95\*exp(-0.22\*(λ-190))/(1+exp(-0.22\*(λ-190)))  C2H2 + hν → 1C2 + 1H2 5\*exp(-0.22\*(λ-180))/(1+exp(-0.22\*(λ-180))) | | | | | | | | | | | | | |  |
| C2H4 + hν → 1C2H2 + 2H + 2H 1.41\*(195-λ) (λ>150, sinon 64 pour λ<150)  C2H4 + hν → 1C2H2 + 1H2 85-0.98\*(200-λ) (λ>150, sinon 36 pour λ<150)  C2H4 + hν → 2C2H3 + 2H 15+0.98\*(200-λ)-1.41\*(195-λ) (λ>150, sinon 0 pour λ<150) | | | | | | | | | | | | | |  |
| 1C3 + hν → 1C2 + 3C |  |  |  | | | |  | | | | | <165 nm  100% | |  |
| 1C3H2 + hν → 2l-C3H + 2H  → 2c-C3H + 2H  → 1C3 + 1H2 (TS = 291 nm) | 448  435  333 |  | >291 nm  0  0  0 | | | | 291-274 nm  0  0  100% | | | | | <274 nm  30%  30%  40% | | There is a barrier for 1C3 + 1H2 channel (Mebel *et al.* 1998) |
| 2C3H3 + hν → 1C3H2 + 2H |  |  |  | | | |  | | | | | <330 nm  100% | |  |
| 1CH3CCH + hν → 2C3H3 + 2H  → 1C3H2 + 1H2  → 1CH2 + 1C2H2 |  |  |  | | | |  | | | | | <240 nm  85%  0%  15% | | (Seki & Okabe 1992, Ni *et al.* 1999, Sun *et al.* 1999) |
| 1H2CCCH2 + hν → 2C3H3 + 2H  → 1C3H2 + 1H2  → 1CH2 + 1C2H2 |  |  |  | | | |  | | | | | <240 nm  85%  10%  5% | | (Seki & Okabe 1992, Ni *et al.* 1999, Sun *et al.* 1999) |
| 1C3H6 + hν → 2C3H5 + 2H  → 2CH3CCH + 2H + 2H  → 2CH2CCH2 + 2H + 2H  → 2C3H3 + 2H + 1H2  → 2C2H3 + 2CH3  → 1C2H2 + 2H + 2CH3  → 1C2H4 + 1CH2  → 1C2H2 + 1CH4 |  |  |  | | | | 210-180nm  41%  1%  1%  7%  36%  14%  0%  0% | | | | | <180nm  2%  4%  3%  17%  4%  60%  6%  4% | | (Borrell *et al.* 1971, Lee *et al.* 2004, Lee *et al.* 2003) |
| 1C3H8 + hν → 2C3H7 + 2H  → 2C3H6 + 2H + 2H  → 2C2H5 + 2CH3  → 1C2H4 + 2H + 2CH3  → 1C2H6 + 1CH2  → 1C2H4 + 1CH4 |  |  |  | | | | 180-135nm  0%  65%  0%  20%  5%  10% | | | | | <135 nm  0%  30%  0%  45%  10%  15% | | (Obi *et al.* 1971, Wu *et al.* 2000) |
| C4H2 → C4H2\*\*  → C4H + H  → C2H + C2H  → C2H2 + C2 | >215  100  0  0  0 | 215-190  98%  2%  0%  0% | | | 190-150  91%  4%  1%  4% | | | <150  67%  20%  3%  10% | | | |  | | (Glicker & Okabe 1987, Silva *et al.* 2008, Zwier & Allen 1996) |
| CH3CN → CH3 + CN (235 nm)  → CH2CN + H (308 nm) | 508  389 | >308nm  0  0 | | | | 308-235nm  0  100% | | | | <235nm  20%  80% | | | | Absorption from (Eden *et al.* 2003) without including the UV (200-300nm). Qualitative branching ratio from (Schwell *et al.* 2008) |
| 1HC3N → 2H + 2C3N (220 nm)  → 2C2H + 2CN (185 nm)  → 1C2 + 1HCN (TS)  → HC3N\*\* (HC3N) | 545  647  619 | >220  0  0  0  0 | 220-185  30%  0%  0%  70% | | | | 185-160  30%  25%  0%  45% | | | | | <160nm  30%  25%  10%  35% | | (Clarke & Ferris 1995, Seki *et al.* 1996, Halpern *et al.* 1988, Luo *et al.* 2008, Silva *et al.* 2009) |
| 1C2H3CN → 1HC3N + 1H2 (TS)  → 1HCN + 1C2H2(TS≅240nm)  → 1HNC + 1C2H2 (TS)  → 2H2C3N + 2H (261nm)  → 2C2H3 + 2CN (213nm) | 191  181  236  458  561 | >261  0  0  0  0  0 | | | | 261-240  0  0  0  100%  0 | | | | <240  20%  60%  10%  10%  0% | | | | (Gandini & Hackett 1978): 50% of C2H2 + HCN and 31% of HC3N + H2 at 213.9 nm, (Fahr & Laufer 1992, North & Hall 1996, Blank et al. 1998): CN very low, (Derecskei-Kovacs & North 1999, Homayoon et al. 2011): RRKM calculations, (Wilhelm *et al.* 2009): HCN/HNC=3.34, HC3N low. |
| C2H5CN → C2H5 + CN (239 nm)  → CH3 + CH2CN (347 nm)  → C2H4CN + H (316 nm)  → C2H4 + HCN (TS=283nm)  → H2 + C2H3CN (TS=279nm) | 500  345  378  131  117 | >347 nm  0  0  0  0  0 | | | | 347-280  0  100  0  0  0 | | | | <280nm  0  20  0  40  40 | | | | Absorption = CH3CN  Qualitative branching ratio in the VUV. Absorption toward the second excited state around 8.8 eV supposed not correlated to products and then dissociation should occur trough ground.  TS calculated at M06-2X/cc-pVTZ level. |
| CH3NH2 → CH3NH + H (294 nm)  ~~→ CH~~~~2~~~~NH~~~~2~~ ~~+ H (316 nm)~~  → CH3 + NH2 (342 nm)  → CH2NH + H2 (TS=470nm) | 407  ~~378~~  350  146 | >342  0  0  0  0 | | | | | 342-294  100  0  0  0 | | | | | <294  70  0  20  10 | | Thermo : M06-2X/cc-pVTZ  Absorption: (Hubin-Franskin *et al.* 2002)  Branching ratio (no absorption above 250 nm): (Michael & Noyes 1963, Waschewsky *et al.* 1995)  TS value from (Xiang & Guillory 1986) but branching ratio small from measurement |
| CH3C3N → H + CH2C3N (322 nm)  → CH3 + C3N (237 nm)  → H2 + HC4N (TS)  → C3H3 + CN (isomerization) | 371  505  312  456 | >322  0  0  0  0 | | 322-237  100%  0  0  0 | | | 237-210  80%  20  0  0 | | | | <210  50%  50%  0  0 | | | Absorption = HC3N |
| C2N2 → CN + CN (213 nm) | 561 | >213 nm  0 | | | | | <213 nm  100% | | | | | | | Absorption = experiment |

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