

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PCI17

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This data sheet updated: 15<sup>th</sup> December 2000.

### CCl<sub>4</sub> + hν → products

#### Primary photochemical processes

| Reaction                                      |     | $\Delta H^\circ/\text{kJ}\cdot\text{mol}^{-1}$ | $\lambda_{\text{threshold}}/\text{nm}$ |
|---|-----|--|--|
| CCl <sub>4</sub> + hν → CCl <sub>3</sub> + Cl | (1) | 288  | 415                                    |
| → CCl <sub>2</sub> + 2Cl                      | (2) | 577  | 207                                    |

#### Preferred Values

#### Absorption cross-sections for CCl<sub>4</sub> at 295 K and 210 K

| $\lambda/\text{nm}$ | $10^{20} \sigma/\text{cm}^2$ |                    | $\lambda/\text{nm}$ | $10^{20} \sigma/\text{cm}^2$ |       |
|---------------------|------------------------------|--------------------|---------------------|------------------------------|-------|
|                     | 295K                         | 210 K <sup>a</sup> |                     | 295 K                        | 210 K |
| 174                 | 990                          | -                  | 220                 | 17.5                         | 12.5  |
| 6                   | 1010                         | -                  | 2                   | 13.6                         | 9.0   |
| 8                   | 975                          | -                  | 4                   | 10.2                         | 6.4   |
| 180                 | 720                          | -                  | 6                   | 7.6                          | 4.4   |
| 2                   | 590                          | -                  | 8                   | 5.6                          | 3.16  |
| 4                   | 440                          | -                  | 230                 | 4.28                         | 2.27  |
| 6                   | 310                          | -                  | 2                   | 3.04                         | 1.52  |
| 8                   | 198                          | -                  | 4                   | 2.20                         | 1.05  |
| 190                 | 147                          | -                  | 6                   | 1.60                         | 0.72  |
| 2                   | 99.2                         | -                  | 8                   | 1.16                         | 0.50  |
| 4                   | 76.7                         | -                  | 240                 | 0.830                        | 0.342 |
| 6                   | 69.5                         | -                  | 2                   | 0.590                        | 0.234 |
| 8                   | 68.0                         | -                  | 4                   | 0.413                        | 0.158 |
| 200                 | 66.0                         | -                  | 6                   | 0.290                        | 0.108 |
| 2                   | 63.8                         | -                  | 8                   | 0.210                        | 0.076 |
| 4                   | 61.0                         | 60.1               | 250                 | 0.148                        | 0.053 |
| 6                   | 57.0                         | 54.4               | 255                 | 0.066                        |       |
| 8                   | 52.5                         | 48.3               | 260                 | 0.025                        |       |
| 210                 | 46.9                         | 41.5               | 265                 | 0.013                        |       |

|   |      |      |     |       |
|---|------|------|-----|-------|
| 2 | 41.0 | 34.8 | 270 | 0.006 |
| 4 | 34.5 | 27.9 | 275 | 0.002 |
| 6 | 27.8 | 21.7 |     |       |
| 8 | 22.1 | 16.3 |     |       |

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<sup>a</sup>No significant temperature dependence observed at  $\lambda < 204$  nm.

### Quantum yields for CCl<sub>4</sub> photolysis at 298 K

$\Phi(1) = 1$  over wavelength range 174-275 nm.

#### *Comments on Preferred Values*

The preferred values of the absorption cross-sections for 174-230 nm at 295 K and 210 K are the values reported by Simon *et al.*<sup>1</sup> This recent publication reports the results of the most comprehensive study of the temperature dependence.<sup>1</sup> For  $\lambda > 230$  nm, the absorption cross-section values are those reported by Hubrich and Stuhl.<sup>2</sup> The values at room temperature are in good agreement with those recommended in our previous evaluation, CODATA, 1982,<sup>3</sup> where a detailed discussion of earlier work can be found. Photodissociation via C-Cl bond fission expected to occur with unit quantum yield. The earlier results of Rebbert and Ausloos<sup>4</sup> which indicated an increasing contribution from  $\Phi(2)$  at  $\lambda < 220$  nm is now considered dubious in the light of results for CF<sub>2</sub>Cl<sub>2</sub> and CFCl<sub>3</sub>.

#### References

- <sup>1</sup> P. C. Simon, D. Gillotay, N. Vanlaethem-Meuree, and J. Wisemberg, *J. Atmos. Chem.* **7**, 107 (1988).
- <sup>2</sup> C. Hubrich and F. Stuhl, *J. Photochem.* **12**, 93 (1980).
- <sup>3</sup> CODATA, Supplement I, 1982 (see references in Introduction).
- <sup>4</sup> R. E. Rebbert and P. J. Ausloos, *J. Photochem.* **6**, 265 (1976/77).