

## Supplementary Information to:

### Reaction of HO with Hydroxyacetone (HOCH<sub>2</sub>C(O)CH<sub>3</sub>): Rate Coefficients (233 - 363 K) and Mechanism

Terry J. Dillon, Abraham Horowitz,<sup>#</sup> Dirk Hölscher and John N. Crowley\*  
Max-Planck-Institut für Chemie, Division of Atmospheric Chemistry  
55020 Mainz, Germany

Luc Vereecken and Jozef Peeters  
Katholieke Universiteit Leuven, Division of Quantum Chemistry and Physical Chemistry  
Celestijnenlaan 200 F, 3001 Heverlee-Leuven, Belgium

## Summary of rate coefficients and conditions.

T / K	OH source / bath gas	n <sup>a</sup>	[HOCH <sub>2</sub> C(O)CH <sub>3</sub> ] <sub>b</sub>	k <sub>1</sub> <sup>c</sup>	±
233	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	7	2 – 12	803	74
233	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	8	2 – 17	762	84
233	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	9	3 – 25	747	43
233	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	8	3 – 25	902	81
237	351 nm HONO / N <sub>2</sub>	7	2 – 14	773	95
237	351 nm HONO / N <sub>2</sub>	8	2 – 22	824	36
237	351 nm HONO / N <sub>2</sub>	8	2 – 18	869	86
238	351 nm HONO / N <sub>2</sub>	7	2 – 22	717	63
238	351 nm HONO / N <sub>2</sub>	8	4 – 24	752	77
238	351 nm HONO / air	5	3 - 22	747	99
243	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	8	2 – 13	838	81
243	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	9	6 – 61	760	18
243	351 nm HONO / N <sub>2</sub>	7	4 - 28	747	49
252	351 nm HONO / N <sub>2</sub>	7	2 – 25	752	46
253	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	7	5 – 60	673	33
260	351 nm HONO / N <sub>2</sub>	8	6 - 65	670	43
263	351 nm HONO / N <sub>2</sub>	8	4 - 42	716	23
268	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	8	4 – 41	652	26
273	351 nm HONO / N <sub>2</sub>	7	6 - 35	627	53
273	351 nm HONO / N <sub>2</sub>	7	4 – 36	687	23

283	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	7	5 – 70	587	26
288	351 nm HONO / N <sub>2</sub> / O <sub>2</sub>	7	5 – 49	637	21
298	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	6	6 – 49	614	28
298	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	11	7 – 71	574	38
298	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	11	5 – 102	561	23
298	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	8	8 – 82	584	36
298	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	6	8 – 48	586	13
298	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	5	7 – 60 N-valve	584	20
298	248 nm D <sub>2</sub> O <sub>2</sub> / N <sub>2</sub>	7	5 - 43	647	8
298	351 nm HONO / N <sub>2</sub>	6	4 - 35	622	41
298	351 nm HONO / N <sub>2</sub>	6	4 - 40	589	46
298	351 nm HONO / N <sub>2</sub>	7	6 – 40	608	30
298	351 nm HONO / N <sub>2</sub>	6	9 - 51	599	23
298	351 nm HONO / N <sub>2</sub>	8	4 – 48	615	23
298	351 nm HONO / N <sub>2</sub>	7	4 – 52	592	28
298	351 nm HONO / N <sub>2</sub>	8	9 – 37	606	26
298	351 nm HONO / N <sub>2</sub>	7	9 – 51	579	25
298	351 nm HONO / N <sub>2</sub> / O <sub>2</sub>	8	9 - 58	589	20
318	351 nm HONO / N <sub>2</sub>	7	9 – 69	584	16
326	351 nm HONO / N <sub>2</sub>	6	8 - 58	618	56
328	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	7	6 – 65	566	30
338	351 nm HONO / N <sub>2</sub>	7	8 – 67	536	13
343	351 nm HONO / N <sub>2</sub>	8	8 - 46	532	31
358	351 nm HONO / N <sub>2</sub>	6	7 - 49	543	46
358	351 nm HONO / N <sub>2</sub>	6	8 - 60	510	20
363	248 nm O <sub>3</sub> + CH <sub>4</sub> / He	8	7 – 70	444	30

Notes: <sup>a</sup> n is the number of  $k'$  (or  $k'_{init}$ ) values collected, <sup>b</sup> units are  $10^{13}$  molecule  $\text{cm}^{-3}$ , <sup>c</sup> units are  $10^{-14}$   $\text{cm}^3$  molecule<sup>-1</sup> s<sup>-1</sup>, errors are 2  $\sigma$  statistical only, incorporating scatter in both  $k'$  and  $[\text{HOCH}_2\text{C}(\text{O})\text{CH}_3]$ . N-valve : Teflon needle valve used in place of flow controller.