Room Temperature and Shock Tube Study of the Reaction HCO + O_2 using the Photolysis of Glyoxal as an Efficient HCO Source

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Supporting Information

TABLE IS: Room temperature experiments for the determination of the rate constant of reaction (4), H + $(CHO)_2$, and the H atom yield in terms of the initial ratio $f = [H]_0/[HCO]_0^{total}$.

T/ K	p/ mbar	ρ/ (10^{-6} mol cm^{-3})	$x((CHO)_2)$/ %	x(HCO)/ ppm	x(HCO*)/ ppm	x(H)/ ppm	f	k_4/ (10^{10} cm^{3}mol^{-1}s^{-1})
295	20.4	0.832	1.00	17	17	60	1.76	4.0
	20.0	0.815	1.69	58	58	170	1.47	3.5
	20.0	0.815	1.69	110	110	360	1.64	4.0
	20.0	0.815	2.04	18	18	55	1.53	2.6
	20.0	0.815	2.04	31	31	105	1.69	3.5
	22.0	0.938	2.80	78	78	250	1.60	4.0
	20.0	0.815	2.80	105	105	300	1.43	4.0
	23.0	0.938	2.80	180	180	610	1.69	4.0
	20.0	0.815	2.80	185	185	650	1.76	4.0
	39.0	1.59	0.50	7	7	30	2.14	3.8
	40.0	1.63	1.02	10	10	41	2.05	3.5
	40.0	1.63	1.69	69	69	220	1.59	4.5
	40.0	1.63	1.69	112	112	422	1.88	3.5
	40.0	1.63	2.80	100	100	300	1.50	5.0
	40.0	1.63	2.80	205	205	760	1.86	5.0
	60.0	2.45	1.69	59	59	220	1.86	4.0
	60.0	2.45	1.69	113	113	445	1.97	4.0
	60.0	2.45	2.80	96	96	360	1.88	5.0
	60.0	2.45	2.80	200	200	780	1.95	4.5
	79.1	3.23	0.25	3.4	3.4	13.4	1.97	3.0
	80.0	3.26	1.69	66	66	240	1.82	3.8
	80.0	3.26	1.69	116	116	468	2.02	3.5
	81.0	3.30	2.80	98	98	370	1.89	4.0
	81.0	3.30	2.80	190	190	780	2.05	4.0
	200	8.13	0.10	1.36	1.36	6.20	2.28	3.2
	200	8.13	0.20	1.85	1.85	8.50	2.30	3.0
	201	8.20	0.20	2.52	2.52	12.0	2.38	3.0
	495	20.2	2.00	29	29	160	2.76	3.0
	495	20.2	2.00	37	37	190	2.57	3.0
	522	21.3	0.04	0.42	0.42	2.60	3.10	3.4
	524	21.4	0.08	0.79	0.79	5.00	3.16	2.8
	524	21.4	0.08	0.52	0.52	3.40	3.27	3.0

TABLE IIS: Shock tube experiments for the determination of the rate constant of reaction (4), $H + (CHO)_2$.

T/ K	p/ mbar	ρ/ (10^{-5} mol cm^{-3})	$x((CHO)_2)$/ %	$x(HCO)$/ ppm	$x(H)$/ ppm	k_4/ (10^{12} cm^{3}mol^{-1}s^{-1})
815	911	1.34	0.50	80	228	3.9
820	912	1.34	0.49	85	242	4.4
884	1041	1.42	0.50	100	289	4.8
897	1039	1.39	0.49	85	245	5.8
1085	1771	1.96	0.39	80	245	9.7
1091	1836	2.02	0.75	150	459	5.9
1107	1840	2.00	0.39	72	220	7.6
769	820	1.28	1.00	135	378	3.6
790	948	1.44	1.17	170	490	3.9
801	900	1.35	1.05	130	370	3.5
823	940	1.37	1.00	130	372	2.9
824	978	1.43	1.17	160	462	4.8
880	1110	1.52	1.17	180	529	3.9
901	1163	1.55	1.17	190	561	4.2
941	1175	1.50	1.00	150	441	5.8
953	1255	1.58	1.00	140	416	3.9
1038	1498	1.74	1.20	175	530	6.1

TABLE IIIS: Room temperature experiments for the determination of the rate constant of reaction (1), HCO + O_2.

T/ K	p/ mbar	ρ/ (10^{-6} mol cm^{-3})	$x((CHO)_2)$/ %	$x(O_2)$/ ppm	$x(HCO)$/ ppm	$x(HCO^*)$/ ppm	$x(H)$/ ppm	k_1/ (10^{12} cm^{3}mol^{-1}s^{-1})
295	49.4	2.01	0.72	1005	4.2	4.2	15.5	3.40
	49.5	2.02	0.72	1005	3.8	3.8	14.1	3.60
	50.7	2.07	0.72	1995	4.0	4.0	14.8	3.60
	49.5	2.02	1.14	995	7.5	7.5	29.3	3.50
	51.0	2.08	1.14	995	8.7	8.7	33.9	3.65
	50.1	2.04	1.14	2005	7.5	7.5	29.3	3.50
	51.8	2.11	1.14	2005	8.4	8.4	32.8	3.60
	51.0	2.08	1.14	3985	8.4	8.4	32.8	3.60
	199	8.09	0.28	245	1.5	1.5	8.0	3.50
	199	8.10	0.28	245	1.5	1.5	7.7	3.50
	204	8.30	0.28	515	1.4	1.4	7.5	3.65

TABLE IVS: Shock tube experiments for the determination of the rate constant of reaction (1), $HCO + O_2$.

T/ K	p/ mbar	ρ/ (10^{-5} mol cm^{-3})	$x((CHO)_2)$/ %	$x(O_2)$/ ppm	$x(HCO)$/ ppm	$x(H)$/ ppm	k_1/ (10^{12} cm^{3}mol^{-1}s^{-1})
829	942	1.37	0.53	1560	50	143	4.1
838	966	1.39	0.53	1560	55	158	6.2
839	964	1.38	0.53	1560	55	158	7.8
960	1241	1.55	0.53	1560	75	222	5.0
1029	1405	1.64	0.53	1560	60	180	7.2
1061	1483	1.68	0.53	1560	75	226	9.2
771	819	1.28	0.60	3115	60	168	4.5
787	859	1.31	0.60	3115	80	226	5.4
836	960	1.38	0.60	3115	50	143	5.7
848	988	1.40	0.60	3115	80	230	5.0
895	1095	1.47	0.60	3115	60	175	7.5
776	854	1.32	1.20	1560	145	410	5.0
783	856	1.31	1.00	1560	82	231	5.0
934	1213	1.56	1.05	1560	102	302	9.0
936	1216	1.56	1.05	1560	130	385	7.0
1108	1669	1.81	1.20	1560	140	427	9.5
739	768	1.25	1.05	3115	112	311	5.3
742	802	1.30	2.00	1560	130	364	4.0
746	813	1.31	2.00	1560	125	351	3.7
793	920	1.40	2.00	1560	155	444	4.5
828	1014	1.47	2.00	1560	115	335	6.0
883	1137	1.55	2.00	1560	170	502	8.0
753	837	1.34	2.00	3115	210	593	5.0
816	979	1.44	2.00	3115	150	434	6.0
857	1081	1.52	2.00	3115	160	469	5.6
862	1090	1.52	2.00	3115	210	617	5.0
956	1356	1.71	2.00	3115	160	482	6.3