CLEANED UP VERSION OF THE REACTION LIST USED IN CRE's MODELING STUDY OF STRATOSPHERIC NO_x/NO_y AND NO_X/HNO_3 RATIOS

This is a cleaned up version of the list of reaction used in that study. It is cleaned up in the sense that several reactions that were used in the course of the study but were only on a trial and error basis have been removed.

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**Number of active species followed by total number of species

32 61

**Names of all species, starting with the 32 active species

co         hcl        hbr        ch2o       o3p        hoono      h          oh
ho2        h2o2       cl         cl2        clo        oclo       hocl       clono2
clno2      cl2o2      hono       no         no2        no3        hno3       n2o5
ho2no2     br         bro        hobr       brono2     brcl       ch3o2      ch3ooh
o3         o2         n2o        ch4        h2o        co2        h2         cfc10
cfc11      cfc12      cfc113     cfc114     cfc115     hcfc22     ch3ccl3    ch3cl
ha1211     ha1301     hf         ch3br      chbr3      n2         cox        o1d
o2b        o3*        o2(delt)   n

**Total number of photodissociation and chemical reactions

185

**The 47 photodissociation processes.
**           Note that in many cases there is no mass balance. What is happening
**           in those cases is that an effective reaction has been shown. The
**           rationale is explained in SOCRATES manual that can be found at NCAR's
**           Website (URL: http://acd.ucar.edu/models/SOCRATES/ ).

   1 o2                          o3p        o3p
   2 o2                          o1d        o3p
   3 o3                          o3p        o2
   4 h2o                         oh         h
   5 n2o                         n2         o1d
   6 hono                        oh         no
   7 ch4                         h2
   8 no2                         no         o3p
   9 hno3                        oh         no2
  10 cfc12                       cl         cl
  11 cfc11                       cl         cl         cl
  12 cfc10                       cl         cl         cl         cl
  13 hocl                        oh         cl
  14 ch3ccl3                     cl         cl         cl
  15 ho2no2                      ho2        no2
  16 ho2no2                      oh         no3
  17 ch3cl                       ch3o2      cl
  18 clono2                      clo        no2
  19 n2o5                        no2        no3
  20 o3                          o1d        o2
  21 cfc113                      cl         cl         cl         hf         hf         hf
  22 hcfc22                      cl         hf         hf
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23	ha1211	br	cl	hf	hf		
24	ha1301	br	hf	hf	hf		
25	h2o2	oh	oh				
26	ch2o	co	ho2	h			
27	ch2o	co	h2				
28	brono2	bro	no2				
29	hobr	oh	br				
30	ch3br	ch3o2	br				
31	oclo	o3p	clo				
32	cl2o2	cl	cl	o2			
33	cl2	cl	cl				
34	cfc114	cl	cl	hf	hf	hf	hf
35	cfc115	cl	hf	hf	hf	hf	hf
36	hcl	h	cl				
37	clno2	cl	no2				
38	no3	no2	o3p				
39	no	n	o3p				
40	brcl	br	cl				
41	bro	br	o3p				
42	clono2	cl	no3				
43	no3	no	o2				
44	chbr3	br	br	br			
45	ch3ooh	ch2o	oh	ho2			
46	ho2	oh	o3p				
47	brono2	br	no3				

**The 138 bimolecular and trimolecular reactions and collisional dissociation processes
** Note that the third body is not shown in trimolecular reactions or
** in collisional dissociation. These reactions are identified in the
** table of rate coefficients (that follws after this list) as negatve number
** that is used in a subroutine that calculates the rate coefficients using
** JPL-003 as explained in the NOx/NOy and NOx/HNO3 paper

1	h	o2	ho2		
2	o1d	h2o	oh	oh	
3	o1d	h2	oh	h	
4	h	o3	oh	o2	
5	o3p	oh	o2	h	
6	oh	o3	ho2	o2	
7	ho2	o3	oh	o2	o2
8	o3p	ho2	oh	o2	
9	oh	ho2	h2o	o2	
10	oh	h2	h2o	h	
11	h	ho2	oh	oh	
12	h	ho2	h2	o2	
13	h	ho2	h2o	o3p	
14	h2	o3p	oh	h	
15	no	ho2	no2	oh	
16	ho2	ho2	h2o2	o2	
17	oh	h2o2	h2o	ho2	
18	oh	co	co2	h	
19	o3p	h2o2	oh	ho2	
20	oh	oh	h2o	o3p	
21	oh	oh	h2o2		
22	o3p	no2	no	o2	
23	o3	no	no2	o2	
24	n	no	n2	o3p	

25	n	o2	no	o3p		
26	o3	no2	no3	o2		
27	no2	no3	n2o5			
28	oh	no2	hno3			
29	ho2	no2	ho2no2			
30	ho2no2		ho2	no2		
31	oh	no2	hoono			
32	hoono		oh	no2		
33	hno3	oh	h2o	no3		
34	oh	ho2no2	h2o	no2	o2	
35	n2o5		no2	no3		
36	o1d	n2o	n2	o2		
37	o1d	n2o	no	no		
38	no3	o3p	no2	o2		
39	no3	oh	no2	ho2		
40	no3	ho2	oh	no2	o2	
41	no3	ho2	hno3	o2		
42	o3p	no2	no3			
43	no	o3p	no2			
44	no	no3	no2	no2		
45	ch4	o1d	ch3o2	oh		
46	ch4	o1d	ch2o	h2		
47	ch4	o1d	ch2o	h	ho2	
48	ch4	oh	ch3o2	h2o		
49	ch3o2	no	ho2	ch2o	no2	
50	ch3o2	ho2	ch3ooh	o2		
51	ch2o	oh	co	ho2	h2o	
52	ch2o	o3p	co	ho2	oh	
53	ch2o	no3	co	ho2	hno3	
54	ch3ooh	oh	ch3o2	h2o		
55	ch3ooh	oh	ch2o	h2o	oh	
56	oh	ch3cl	cl	ho2	h2o	
57	cl	ch3cl	hcl	hcl	co	ho2
58	cl	o3	clo	o2		
59	clo	o3p	cl	o2		
60	clo	no	no2	cl		
61	cl	ch4	hcl	ch3o2		
62	cl	h2	hcl	h		
63	cl	ho2	hcl	o2		
64	clo	oh	cl	ho2		
65	clo	oh	hcl	o2		
66	cl	ch2o	hcl	co	ho2	
67	oh	hcl	h2o	cl		
68	clo	no2	clono2			
69	o3p	clono2	no3	clo		
70	clo	ho2	hocl	o2		
71	clo	ho2	hcl	o3		
72	oh	hocl	h2o	clo		
73	o3p	hocl	oh	clo		
74	cl	no2	clno2			
75	cl	hocl	oh	cl2		
76	clo	clo	cl	oclo		
77	clo	clo	cl2	o2		
78	clo	clo	cl	cl	o2	
79	ch3ccl3	oh	cl	cl	cl	h2o
80	hcfc22	oh	cl	h2o		
81	clo	clo	cl2o2			

82	cl2o2		clo	clo				
83	oclo	oh	hocl	o2				
84	cl	oclo	clo	clo				
85	oclo	o3p	clo	o2				
86	oclo	no	no2	clo				
87	o1d	cl2	clo	cl				
88	cl2o2	cl	cl2	cl	o2			
89	no3	cl	no2	clo				
90	no3	clo	no2	cl	o2			
91	o1d	hcl	oh	cl				
92	oh	cl2	hocl	cl				
93	cl	clono2	cl2	no3				
94	ho2	cl	oh	clo				
95	cl	h2o2	hcl	ho2				
96	o3p	hcl	cl	oh				
97	clono2	oh	hocl	no3				
98	cfc10	o1d	cl	cl	cl	cl		
99	cfc11	o1d	cl	cl	cl	hf		
100	cfc12	o1d	cl	cl	hf	hf		
101	cfc113	o1d	cl	cl	cl	hf	hf	hf
102	cfc114	o1d	cl	cl	hf	hf	hf	hf
103	cfc115	o1d	cl	hf	hf	hf	hf	hf
104	hcfc22	o1d	cl	hf	hf			
105	ch3br	oh	ho2	br	h2o			
106	chbr3	oh	h2o	br	br	br		
107	br	o3	bro	o2				
108	bro	o3p	br	o2				
109	bro	no	no2	br				
110	bro	clo	oclo	br				
111	bro	clo	br	cl	o2			
112	bro	clo	brcl	o2				
113	bro	bro	br	br	o2			
114	br	ho2	hbr	o2				
115	br	oclo	bro	clo				
116	br	ch2o	hbr	co	ho2			
117	oh	hbr	h2o	br				
118	bro	no2	brono2					
119	bro	ho2	hobr	o2				
120	o1d	hbr	oh	br				
121	bro	oh	ho2	br				
122	o3p	hbr	br	oh				
123	ha1301	o1d	br	hf	hf	hf		
124	ha1211	o1d	br	cl	hf	hf		
125	ch3br	o1d	br					
126	o3p	o3p	o2					
127	o3p	o2	o3					
128	o3p	o3	o2	o2				
129	o1d	n2	o3p	n2				
130	o1d	o2	o3p	o2				
131	o1d	o3	o2	o2				
132	o1d	n2	n2o					

** Six reactions occurring on aerosols **

133	clono2	hocl	hno3	
134	n2o5	hno3	hno3	
135	clono2	hocl	hno3	

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 136 hocl                          cl2       h2o
 137 brono2                        hobr      hno3
 138 hobr                          brcl      h2o

** Rate coefficients are expressed as k=A(T**alfa)exp(beta/T) where T is the temperature
**    In the tabulation below the first integer (in i4 format) is the reaction number.
**    The next three real numbers in 3e10.3 format are A, alfa and beta.
**    The photo rates are exceptions. Hence for then A, alfa and beta are shown as zeros.
**    The three body reactions and the heterogeneous reactions are other exeptions. In
**    their cases the first real number after the reaction number (integer) is simply an
**    identification mark that tells the appropriate subroutine about where to go
**    (in that subroutine) to calculate the rate constant.


   1 0.000E+00 0.000E+00 0.000E+00
   2 0.000E+00 0.000E+00 0.000E+00
   3 0.000E+00 0.000E+00 0.000E+00
   4 0.000E+00 0.000E+00 0.000E+00
   5 0.000E+00 0.000E+00 0.000E+00
   6 0.000E+00 0.000E+00 0.000E+00
   7 0.000E+00 0.000E+00 0.000E+00
   8 0.000E+00 0.000E+00 0.000E+00
   9 0.000E+00 0.000E+00 0.000E+00
  10 0.000E+00 0.000E+00 0.000E+00
  11 0.000E+00 0.000E+00 0.000E+00
  12 0.000E+00 0.000E+00 0.000E+00
  13 0.000E+00 0.000E+00 0.000E+00
  14 0.000E+00 0.000E+00 0.000E+00
  15 0.000E+00 0.000E+00 0.000E+00
  16 0.000E+00 0.000E+00 0.000E+00
  17 0.000E+00 0.000E+00 0.000E+00
  18 0.000E+00 0.000E+00 0.000E+00
  19 0.000E+00 0.000E+00 0.000E+00
  20 0.000E+00 0.000E+00 0.000E+00
  21 0.000E+00 0.000E+00 0.000E+00
  22 0.000E+00 0.000E+00 0.000E+00
  23 0.000E+00 0.000E+00 0.000E+00
  24 0.000E+00 0.000E+00 0.000E+00
  25 0.000E+00 0.000E+00 0.000E+00
  26 0.000E+00 0.000E+00 0.000E+00
  27 0.000E+00 0.000E+00 0.000E+00
  28 0.000E+00 0.000E+00 0.000E+00
  29 0.000E+00 0.000E+00 0.000E+00
  30 0.000E+00 0.000E+00 0.000E+00
  31 0.000E+00 0.000E+00 0.000E+00
  32 0.000E+00 0.000E+00 0.000E+00
  33 0.000E+00 0.000E+00 0.000E+00
  34 0.000E+00 0.000E+00 0.000E+00
  35 0.000E+00 0.000E+00 0.000E+00
  36 0.000E+00 0.000E+00 0.000E+00
  37 0.000E+00 0.000E+00 0.000E+00
  38 0.000E+00 0.000E+00 0.000E+00
  39 0.000E+00 0.000E+00 0.000E+00
  40 0.000E+00 0.000E+00 0.000E+00
  41 0.000E+00 0.000E+00 0.000E+00
  42 0.000E+00 0.000E+00 0.000E+00
  43 0.000E+00 0.000E+00 0.000E+00
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  44 0.000E+00 0.000E+00 0.000E+00
  45 0.000E+00 0.000E+00 0.000E+00
  46 0.000E+00 0.000E+00 0.000E+00
  47 0.000E+00 0.000E+00 0.000E+00
**
** Now the other 138 reactions gas phase bimolecular and termolecular & the reactions
** aerosol surface

   1 -1.800E+01 0.000E+00 0.000E+00
   2  2.200E-10 0.000E+00 0.000E+00
   3  1.000E-10 0.000E+00 0.000E+00
   4  1.400E-10 0.000E+00-4.700E+02
   5  2.200E-11 0.000E+00 1.200E+02
   6  1.500E-12 0.000E+00-8.800E+02
   7  2.000E-14 0.000E+00-6.800E+02
   8  3.000E-11 0.000E+00 2.000E+02
   9  4.800E-11 0.000E+00 2.500E+02
  10  5.500E-12 0.000E+00-2.000E+03
  11  7.290E-11 0.000E+00 0.000E+00
  12  6.480E-12 0.000E+00 0.000E+00
  13  1.622E-12 0.000E+00 0.000E+00
  14  8.800E-12 0.000E+00-4.200E+03
  15  3.500E-12 0.000E+00 2.500E+02
  16  1.500E-12 0.000E+00 1.900E+01
  17  2.900E-12 0.000E+00-1.600E+02
  18 -1.700E+01 0.000E+00 0.000E+00
  19  1.400E-12 0.000E+00-2.000E+03
  20  4.200E-12 0.000E+00-2.400E+02
  21 -1.900E+01 0.000E+00 0.000E+00
  22  5.600E-12 0.000E+00 1.800E+02
  23  3.000E-12 0.000E+00-1.500E+03
  24  2.100E-11 0.000E+00 1.000E+02
  25  1.500E-11 0.000E+00-3.600E+03
  26  1.200E-13 0.000E+00-2.450E+03
  27 -4.000E+00 0.000E+00 0.000E+00
  28 -1.300E+01 0.000E+00 0.000E+00
  29 -1.400E+01 0.000E+00 0.000E+00
  30 -1.500E+01 0.000E+00 0.000E+00
  31 -2.800E+01 0.000E+00 0.000E+00
  32 -2.900E+01 0.000E+00 0.000E+00
  33 -1.600E+01 0.000E+00 0.000E+00
  34  1.300E-12 0.000E+00 3.800E+02
  35 -5.000E+00 0.000E+00 0.000E+00
  36  0.000E-11 0.000E+00 0.000E+00
  37  0.000E-11 0.000E+00 0.000E+00
  38  1.000E-11 0.000E+00 0.000E+00
  39  2.200E-11 0.000E+00 0.000E+00
  40  3.500E-12 0.000E+00 0.000E+00
  41  0.000E-13 0.000E+00 0.000E+00
  42 -6.000E+00 0.000E+00 0.000E+00
  43 -7.000E+00 0.000E+00 0.000E+00
  44  1.500E-11 0.000E+00 1.700E+02
  45  1.500E-10 0.000E+00 0.000E+00
  46  1.500E-11 0.000E+00 0.000E+00
  47 -2.000E+01 0.000E+00 0.000E+00
  48  2.450E-12 0.000E+00-1.770E+03
  49  3.000E-12 0.000E+00 2.800E+02
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50	3.800E-13	0.000E+00	8.000E+02
51	1.000E-11	0.000E+00	0.000E+00
52	3.400E-11	0.000E+00	-1.600E+03
53	6.300E-13	0.000E+00	-2.058E+03
54	2.204E-12	0.000E+00	2.000E+02
55	1.596E-12	0.000E+00	2.000E+02
56	4.100E-12	0.000E+00	-1.400E+03
57	3.200E-11	0.000E+00	-1.250E+03
58	2.300E-11	0.000E+00	-2.000E+02
59	3.000E-11	0.000E+00	7.000E+01
60	6.400E-12	0.000E+00	2.900E+02
61	9.600E-12	0.000E+00	-1.360E+03
62	3.700E-11	0.000E+00	-2.300E+03
63	1.800E-11	0.000E+00	1.700E+02
64	7.400E-12	0.000E+00	2.700E+02
65	3.200E-13	0.000E+00	3.200E+02
66	8.100E-11	0.000E+00	-3.000E+01
67	2.600E-12	0.000E+00	-3.500E+02
68	-8.000E+00	0.000E+00	0.000E+00
69	2.900E-12	0.000E+00	-8.000E+02
70	4.800E-13	0.000E+00	7.000E+02
71	-2.100E+01	0.000E+00	0.000E+00
72	3.000E-12	0.000E+00	-5.000E+02
73	1.700E-13	0.000E+00	0.000E+00
74	-9.000E+00	0.000E+00	0.000E+00
75	2.500E-12	0.000E+00	-1.300E+02
76	3.500E-13	0.000E+00	-1.370E+03
77	1.000E-12	0.000E+00	-1.590E+03
78	3.000E-11	0.000E+00	-2.450E+03
79	1.800E-12	0.000E+00	-1.550E+03
80	1.000E-12	0.000E+00	-1.600E+03
81	-1.000E+01	0.000E+00	0.000E+00
82	-1.100E+01	0.000E+00	0.000E+00
83	4.500E-13	0.000E+00	8.000E+02
84	3.400E-11	0.000E+00	1.600E+02
85	2.400E-12	0.000E+00	-9.600E+02
86	2.500E-12	0.000E+00	-6.000E+02
87	2.800E-10	0.000E+00	0.000E+00
88	1.000E-10	0.000E+00	0.000E+00
89	2.400E-11	0.000E+00	0.000E+00
90	4.700E-13	0.000E+00	0.000E+00
91	1.500E-10	0.000E+00	0.000E+00
92	1.400E-12	0.000E+00	-9.000E+02
93	6.500E-12	0.000E+00	1.350E+02
94	4.100E-11	0.000E+00	-4.500E+02
95	1.100E-11	0.000E+00	-9.800E+02
96	1.000E-11	0.000E+00	-3.300E+03
97	1.200E-12	0.000E+00	-3.300E+02
98	3.300E-10	0.000E+00	0.000E+00
99	2.300E-10	0.000E+00	0.000E+00
100	1.400E-10	0.000E+00	0.000E+00
101	2.000E-10	0.000E+00	0.000E+00
102	1.300E-10	0.000E+00	0.000E+00
103	5.000E-11	0.000E+00	0.000E+00
104	1.000E-10	0.000E+00	0.000E+00
105	4.000E-12	0.000E+00	-1.470E+03
106	1.600E-13	0.000E+00	-7.100E+02

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107  1.700E-11 0.000E+00-8.000E+02
108  1.900E-11 0.000E+00 2.300E+02
109  8.800E-12 0.000E+00 2.600E+02
110  9.500E-13 0.000E+00 5.500E+02
111  2.300E-12 0.000E+00 2.600E+02
112  4.100E-13 0.000E+00 2.900E+02
113  1.500E-12 0.000E+00 2.300E+02
114  1.500E-11 0.000E+00-6.000E+02
115  2.600E-11 0.000E+00-1.300E+03
116  1.700E-11 0.000E+00-8.000E+02
117  1.100E-11 0.000E+00 0.000E+00
118 -1.200E+01 0.000E+00 0.000E+00
119  3.400E-12 0.000E+00 5.400E+02
120  1.500E-10 0.000E+00 0.000E+00
121  7.500E-11 0.000E+00 0.000E+00
122  5.800E-12 0.000E+00-1.500E+03
123  1.000E-10 0.000E+00 0.000E+00
124  1.500E-10 0.000E+00 0.000E+00
125  1.800E-10 0.000E+00 0.000E+00
126 -1.000E+00 0.000E+00 0.000E+00
127 -2.000E+00 0.000E+00 0.000E+00
128  8.000E-12 0.000E+00-2.060E+03
129  1.800E-11 0.000E+00 1.100E+02
130  3.200E-11 0.000E+00 7.000E+01
131  1.200E-10 0.000E+00 0.000E+00
132 -3.000E+00 0.000E+00 0.000E+00
133 -2.200E+01 0.000E+00 0.000E+00
134 -2.300E+01 0.000E+00 0.000E+00
135 -2.400E+01 0.000E+00 0.000E+00
136 -2.500E+01 0.000E+00 0.000E+00
137 -2.600E+01 0.000E+00 0.000E+00
138 -2.700E+01 0.000E+00 0.000E+00
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