Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Material

Inter-Moieties Reactivity Correlations: An approach to estimate reactivity endpoints of major atmospheric reactants towards organic chemicals.

Shikha Gupta[1], Nikita Basant[2], Dinesh Mohan[3], Kunwar P. Singh*[1]

[1]Environmental Chemistry Division,
CSIR-Indian Institute of Toxicology Research,
Post Box 80, Mahatma Gandhi Marg, Lucknow-226 001, India

[2]ETRC, Gomtinagar, Lucknow-226010, India

[3]School of Environmental Sciences, Jawaharlal Nehru University,
New Mehrauli Road, New Delhi 110067, India

***Author for all correspondance :** kpsingh_52@yahoo.com; kunwarpsingh@gmail.com

Table S1: Data set used in IMRC QRRR modeling

S.no.	Chemical name	log$k_{O3\ (Exp.)}$	log$k_{OH\ (Exp)}$
1	ethene	-17.76	-11.07
2	propene	-16.90	-10.58
3	2-methyl-2-propene	-16.94	-10.29
4	cis-2-butene	-15.90	-10.25
5	trans-2-butene	-15.59	-10.19
6	1-pentene	-16.97	-10.50
7	cis-2-pentene	-15.68	-10.19
8	trans-2-pentene	-15.50	-10.17
9	2-methyl-2-butene	-15.40	-10.06
10	1-hexene	-16.96	-10.43
11	2-methyl-1-pentene	-16.77	-10.20
12	cis-3-methyl-2-pentene	-15.34	-10.05
13	2,3-dimethyl-2-butene	-14.98	-9.96
14	1-heptene	-16.76	-10.39
15	1,3-butadiene	-17.17	-10.18
16	3-methylene-7-methyl-1,6-octadiene	-14.90	-9.67
17	cis-3,7-dimethyl-1,3,6-octatriene	-14.70	-9.98

18	cis-2,trans-4-hexadiene	-15.50	-9.87
19	trans-2,trans-4-hexadiene	-15.43	-9.87
20	cyclohexene	-15.80	-10.17
21	cycloheptene	-15.50	-10.13
22	1,3-cyclohexadiene	-14.71	-9.79
23	1,4-cyclohexadiene	-16.19	-10.00
24	bicyclo[2.2.1]-2-heptene	-14.67	-10.31
25	bicyclo[2.2.2]-2-octene	-16.14	-10.39
26	bicyclo[2.2.1]-2,5-heptadiene	-14.33	-9.92
27	1,3-cycloheptadiene	-15.81	-9.86
28	1,3,5-cycloheptatriene	-16.27	-10.01
29	alpha-pinene	-16.08	-10.27
30	beta-pinene	-16.68	-10.10
31	beta-phellandrene	-15.75	-9.77
32	carvomenthene	-15.28	-9.90
33	alpha-phellandrene	-13.92	-9.50
34	vinyl fluoride	-18.16	-11.25
35	1,1-difluoroethene	-18.72	-11.68
36	trifluoroethene	-18.85	-12.09
37	vinyl chloride	-18.61	-11.16
38	1,1-dichloroethene	-20.43	-10.96
39	cis-1,2-dichloroethene	-19.21	-11.58
40	trans-1,2-dichloroethene	-18.75	-11.63
41	cis-1,3-dichloropropene	-18.82	-11.08
42	trans-1,3-dichloropropene	-18.17	-10.85
43	acetylene	-19.07	-12.09
44	propyne	-17.89	-11.23
45	1-butyne	-17.75	-11.10
46	diacetylene	-19.22	-10.72
47	toluene	-19.92	-11.22
48	o-xylene	-21.16	-10.86
49	p-xylene	-21.40	-10.86
50	1,2,4-trimethylbenzene	-20.89	-10.45
51	1,3,5-trimethylbenzene	-20.66	-10.26
52	styrene	-16.67	-10.24
53	o-cresol	-18.59	-10.38
54	m-cresol	-18.71	-10.19
55	p-cresol	-18.33	-10.33
56	acrolein	-18.55	-10.70
57	crotonaldehyde	-18.05	-10.44
58	methacrolein	-17.95	-10.47

59	methyl vinyl ketone	-17.32	-10.73
60	3-penten-2-one	-16.67	-10.29
61	2-cyclohexen-1-one	-17.91	-10.24
62	trans-3-hexene-2,5-dione	-17.08	-10.33
63	furan	-17.62	-10.39
64	2,5-dihydrofuran	-16.79	-10.20
65	methyl nitrite	-19.89	-12.66
66	ethyl nitrite	-18.93	-12.15
67	ethylamine	-19.56	-10.56
68	dimethylamine	-17.58	-10.18
69	trimethylamine	-17.01	-10.22
70	2-methyl-3-buten-2-ol	-17.00	-10.19
71	2-vinyl pyridine	-16.84	-10.25
72	3-Buten-1-ol	-17.31	-10.50
73	6-methyl-5-hepten-2-one	-15.41	-9.80
74	allyl alcohol	-16.84	-10.59
75	1-buten-3-ol	-16.79	-10.48
76	camphene	-18.05	-10.27
77	cis-3-hexen-1-ol	-16.19	-9.96
78	E,E-2,4-hexadienedial	-17.00	-10.06
79	E,Z-2,4-hexadienedial	-17.00	-9.96
80	ethyl acrylate	-17.24	-10.80
81	ethyl vinyl ether	-15.81	-10.39
82	linalool	-15.37	-9.80
83	methyl acrylate	-17.98	-11.03
84	methylenecyclohexane	-16.98	-10.24
85	trans-2-hexenal	-17.70	-10.36
86	trans-4-octene	-15.88	-10.16
87	trans-cinnamaldehyde	-17.66	-10.32
88	vinyl acetate	-17.50	-10.60
89	vinylcyclohexane	-17.12	-10.44
90	trichloroethene	-19.97	-11.63
91	tetrachloroethene	-19.37	-12.78
92	(E)-1,3-pentadiene	-16.37	-9.98
93	(Z)-1,3-pentadiene	-16.56	-10.00
94	1,3-butadiene, 2,3-dimethyl	-16.58	-9.91
95	1,4-pentadiene	-16.84	-10.28
96	1,5-hexadiene, 2,5-dimethyl	-16.85	-9.92
97	1-butene, 2,3,3-trimethyl	-17.11	-10.28
98	1-butene, 3,3-dimethyl	-17.41	-12.65
99	1-butene, 3-methyl	-17.02	-10.50

100	1-decene	-17.10	-10.45
101	1-octene	-16.90	-10.44
102	2-pentene, 2,4,4-trimethyl	-15.86	-10.06
103	ethane	-17.77	-12.61
104	isoprene	-16.85	-10.00
105	methyl methacrylate	-17.12	-10.37
106	3-buten-2-ol	-16.79	-10.48
107	trans-3-methyl-2-pentene	-15.25	-10.05
108	2-methyl-1,3-butadiene	-16.92	-10.00
109	3,7-dimethyl-1,6-octadiene	-15.17	-9.74
110	cyclopentene	-15.56	-10.17
111	d-limonene	-15.19	-9.77
112	2-(chloromethyl)-3-chloro-1-propene	-18.41	-10.47
113	2-butyne	-19.48	-10.56
114	m-xylene	-21.22	-10.63
115	1,2,3-trimethylbenzene	-20.80	-10.52
116	acetaldehyde	-19.47	-10.80
117	methylglyoxal	-20.96	-10.76
118	cis-3-hexene-2,5-dione	-17.74	-10.18
119	methylamine	-19.67	-10.66
120	pyrrole	-16.80	-9.96
121	2-(5H)-furanone	-18.66	-10.91
122	3,7-dimethyl-1,3,6-octatriene	-14.70	-9.60
123	4-acetyl-1-methylcyclohexene	-15.82	-9.89
124	E,E-2-methyl-2,4-hexadienedial	-16.70	-9.93
125	trans-5-decene	-15.89	-10.19
126	1,4-pentadiene, 2-methyl	-16.88	-10.10
127	1-butene, 2-methyl	-16.88	-10.21