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An Expanded Listing of Revised Q and e Values

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ABSTRACT

Recalculation of reactivity ratios has led to improved Q and e values for a variety of monomers.

The original table of vinyl monomer Q and e values [1] was based on the reactivity ratio compilation of Young [2]. This has now been supplemented with Young's expanded listing [3] and the references found in Chemical Abstracts through 1977. As before, reactivity ratios with at least three comonomers must be known before the Q and e values for the monomer in question were calculated.

In an effort to further refine the Q and e values, all of the available references were consulted for all the copolymerizations of the qualifying monomers. For those 900 copolymerizations where the experimental data were reported, the reactivity ratios were recalculated [4] by the methods of Kelen and Tüdös for copolymerizations with unspecified conversions [5] and with conversion data [6]. The inclusion of these recalculated r values in the Q and e determinations resulted in a 5% increase in the correlation coefficient average for the complete tabulation (Table 1).

The Q and e values of telogens [7] were also recalculated by using these improved monomer values. They are presented in Table 2.

TABLE 1. Q and e Values Based on a Least-Squares Evaluation

Monomer	Gp[a]	Q	e	No.[b]	Corr. coeff. r
Acenaphthalene	IV	0.72	-1.88	5	0.98
Acetic acid, 2-chloropenyl ester	IV	0.20	-0.85	5	0.61
–, 2-methylpropenyl ester	V	0.040	-2.08		0.97
–, propenyl ester	III	0.024	-1.07	8	0.85
–, 2-propenyl ester	IV	0.023	-0.94	4	0.98
Acetylene, phenyl-	IV	0.68	+0.70	6	0.85
Aconitic acid, trimethyl ester	III	0.24	+2.27	5	0.63
Acrolein	IV	0.80	+1.31	16	0.97
–, 2-methyl-	IV	1.83	+0.71	5	0.98
Acrylamide	IV	0.23	+0.54	17	0.64
–, 1-deoxy-D-glucitol	V	0.22	+0.61		0.68
–, N-methylol-	IV	0.52	+1.15	6	0.91
–, N-octadecyl-	IV	0.66	+1.64	4	0.93
Acrylic acid	I	0.83 ± 0.47	+0.88 ± 0.23		
–, 2-acetoxyethyl ester	V	0.52	+0.77		0.99
–, benzyl ester	IV	0.33	+1.13	5	0.92
–, butyl ester	II	0.38	+0.85	20	0.94

–, 2-chloro-, methyl ester	IV	2.43	+0.35	4	0.38
–, 2-cyano-, methyl ester	IV	4.91	+0.91	4	0.99
–, 1,1-dihydroperfluorobutyl ester	V	0.96	+1.34		0.81
–, 2,3-epoxypropyl ester	IV	0.48	+1.28	4	0.87
–, ethyl ester	III	0.41	+0.55	12	0.91
–, 2-ethylhexyl ester	IV	0.37	+0.24	4	0.37
–, ferrocenylmethyl ester	IV	0.15	+0.51	4	0.65
–, methyl ester	I	0.45 ± 0.10	+0.64 ± 0.13		
–, 2-nitrobutyl ester	V	0.69	+1.09		0.98
–, octadecyl ester	IV	0.33	+1.26	7	0.97
–, octyl ester	V	0.63	+2.01		0.99
–, 2-phenyl-, methyl ester	IV	5.19	+0.96	8	0.90
–, propenyl ester	V	0.32	-0.99		0.96
–, trifluoro-, methyl ester	V	0.048	+1.20		0.55
Acrylic anhydride	V	1.46	+0.31		0.37
Acrylonitrile	I	0.48 ± 0.07	+1.23 ± 0.08		
Acrylyl chloride	IV	1.82	+1.92	6	0.90
Aniline, N,N-divinyl-	III	0.26	-0.68	5	0.78
Anthracene, 9-vinyl	IV	0.14	+0.82	5	0.90
Bicyclo [2.2.1] -2,5-heptadiene	III	0.051	-1.48	7	0.90

(continued)

TABLE 1.(continued)

Monomer	Gp[a]	Q	e	No.[b]	Corr. coeff. r
1,3-Butadiene	II	1.70	-0.50	24	0.82
–, 2-chloro-	II	10.52	+1.20	10	0.98
–, 1,4-dicarboxylic acid diethyl ester	V	1.94	+1.39		0.99
–, 2,3-dichloro-	V	9.08	+0.14		0.93
–, 2,3-dimethyl-	V	1.42	-0.43		0.58
–, 2-fluoro-	III	1.88	+0.63	6	0.77
–, hexafluoro-	IV	0.82	+0.58	4	0.93
–, 2-methyl-	II	1.99	-0.55	11	0.86
1-Butene	IV	0.007	-0.06	5	0.08
2-Butene	IV	0.002	-0.29	6	0.44
3-Buten-2-one	II	0.66	+1.05	8	0.98
–, 1-chloro-	IV	16.00	+1.78	4	0.97
–, 3-methyl-	III	1.03	+0.64	6	0.78
Caprolactam, N-vinyl-	IV	0.14	-1.18	4	0.72
Carbamic acid					
–, diethyl-, vinyl ester	IV	0.028	-1.10	4	0.95
–, vinyl-, ethyl ester	V	0.037	-1.12		0.91

Carbazole, N-vinyl-	III	0.26	-1.29	12	0.99
Carbon monoxide	V	0.013	+1.68		0.70
Carbonic acid, vinylene ester	III	0.004	-0.49	9	0.73
Citraconimide, N-methyl-	IV	0.87	+1.59	4	0.94
Citric acid, tripropenyl ester	IV	0.054	-0.26	4	0.50
Crotonaldehyde	IV	0.023	+0.84	5	0.82
Crotonic acid	III	0.017	+0.89	6	0.98
Cyanamide, dipropenyl-	IV	0.14	+2.41	4	0.96
Cyanuric acid, tripropenyl-	V	0.036	-0.16		0.17
4-Cyclopentene-1,3-dione	IV	0.42	+2.43	4	0.96
Ethylene	III	0.016	+0.05	6	0.52
–, bromo-	IV	0.038	-0.23	10	0.94
–, chloro-	II	0.056	+0.16	38	0.37
–, chlorotrifluoro-	III	0.026	+1.56	5	0.99
–, 1,1-dichloro-	II	0.31	+0.34	40	0.68
–, 1,1-dicyano-	IV	14.22	+1.92	9	0.82
–, 1,1-diphenyl-	IV	0.17	-1.71	5	0.84
–, fluoro-	IV	0.008	+0.72	8	0.71
–, tetrachloro-	III	0.001	+1.24	7	0.99
–, tetrafluoro-	IV	0.032	+1.63	4	0.99
–, trichloro-	III	0.010	+1.29	11	0.94

(continued)

TABLE 1 (continued)

Monomer	Gp[a]	Q	e	No.[b]	Corr. coeff. r
Ferrocene, vinyl-	IV	0.31	-1.34	6	0.91
Fumaric acid, diethyl ester	IV	0.25	+2.26	10	0.91
Fumaronitrile	IV	0.29	+2.73	5	0.96
Glutaronitrile, 2-methylene-	IV	0.41	+1.25	6	0.83
1,3,5-Hexatriene, 2,3,4,5-tetrachloro-	IV	1.83	+0.94	6	0.98
1-Hexene	V	0.035	+0.92		0.69
1-Hexene-3,5-dione, 2-methyl-	V	5.48	-0.76		0.79
Hydroquinone, vinyl-	V	4.30	+2.26		0.87
—, vinyl-, dibenzoate	IV	1.73	+0.84	5	0.87
Imidazole					
—, 2-methyl-1-vinyl-	IV	0.14	-0.98	6	0.93
—, 1-vinyl-,	V	0.11	-0.68		0.98
Indene	IV	0.13	-0.71	8	0.45
Isocyanate					
—, 2-propenyl-	III	0.18	-1.05	8	0.94
—, vinyl-	III	0.14	-0.95	6	0.98
Isocyanuric acid, tripropenyl-	V	0.035	-0.23		0.35

Isothiocyanic acid, vinyl ester	IV	0.59	+0.37	4	0.77
Itaconic acid	IV	0.78	+1.07	5	0.99
–, dibutyl ester	V	0.82	+0.56		0.88
–, diethyl ester	V	1.04	+0.88		0.98
–, dimethyl ester	III	0.73	+0.57	8	0.90
Maleic acid, diethyl ester	IV	0.053	+1.08	12	0.87
Maleic anhydride	IV	0.86	+3.69	25	0.98
Maleimide	V	0.94	+2.86		0.99
–, N-butyl-	V	0.88	+3.70		0.92
–, N-(2-hydroxyethyl)-	V	1.26	+1.07		0.68
–, N-phenyl-	IV	2.81	+3.24	4	0.99
Melamine, dipropenyl-	V	0.059	-1.57		0.99
Methacrylic acid	III	0.98	+0.62	23	0.73
–, benzyl ester	IV	0.88	+0.35	10	0.97
–, butyl ester	III	0.82	+0.28	10	0.68
–, 2-chloroethyl ester	IV	1.04	+0.31	7	0.79
–, 2-(N,N-dimethylcarbamoyloxy) ethyl ester	IV	1.14	+0.84	5	0.74
–, 2,3-epoxypropyl ester	III	0.96	+0.20	9	0.92
–, ethyl ester	III	0.76	+0.17	7	0.62

(continued)

TABLE 1 (continued)

Monomer	Gp[a]	Q	e	No.[b]	Corr. coeff. r
Methacrylic acid (continued)					
–, ferrocenylmethyl ester	IV	0.22	-0.65	7	0.85
–, 2-hydroxyethanesulfonic acid ester	IV	1.09	+0.25	4	0.52
–, 2-hydroxyethyl ester	IV	1.78	-0.39	7	0.67
–, isobutyl ester	III	0.82	+0.27	5	0.76
–, isopropyl ester	IV	0.97	+0.10	4	0.46
–, methyl ester	I	0.78 ± 0.06	+0.40 ± 0.08		
–, octyl ester	IV	0.88	+0.11	4	0.26
–, phenyl ester	IV	1.25	+0.79	7	0.91
–, sulfolanyl ester	V	1.19	+0.96		0.95
Methacrylic anhydride	IV	3.00	+0.56	5	0.93
Methacrylamide	IV	0.40	-0.05	8	0.29
–, 1-deoxy-1-D-glucitol	V	0.15	-0.16		0.19
–, N-phenyl-	V	0.40	+0.19		0.70
Methacrylonitrile	I	0.86 ± 0.10	+0.68 ± 0.11		
Methacryloyl chloride	V	2.04	+1.54		0.94
Octadecanamide, N-propenyl-	V	0.015	-0.36		0.74

Oxazolidone, N-vinyl-	III	0.087	-1.70	6	0.95
2-Oxazoline					
–, 4-acryloxymethyl-2,4-dimethyl-	IV	0.97	-0.51	4	0.71
–, 4-methacryloxy-2,4-dimethyl-	IV	0.44	-0.70	4	0.99
–, 2-isopropenyl-4,4-dimethyl-	IV	0.87	+0.34	4	0.65
Phosphonic acid					
–, vinyl-, bis(2-chloroethyl) ester	V	0.044	+1.64		0.89
–, vinyl-, diethyl ester	V	0.27	-0.40		0.54
–, vinyl-, dimethyl ester	V	0.24	-0.25		0.53
–, α-phenylvinyl-	IV	0.65	+0.52	5	0.76
Phthalic acid, dipropenyl ester	IV	0.031	-0.26	20	0.50
Propene	IV	0.009	-1.69	7	0.84
–, 2-chloro-	V	0.074	-0.16		0.98
–, 3-chloro-	III	0.026	-0.60	12	0.93
–, 2-chloro-3-hydroxy-	V	0.091	-0.95		0.99
–, 2,3-dichloro-	IV	0.12	-0.40	4	0.67
–, 3-hydroxy-	IV	0.005	-1.48	5	0.98
–, 2-methyl-	III	0.023	-1.20	7	0.99
–, 2-methyl-3-chloro	IV	0.17	-0.86	4	0.98
–, 3-phenyl-	IV	0.038	+0.40	4	0.60
–, 3,3,3-trichloro-	V	0.030	+1.00		0.99

(continued)

TABLE 1 (continued)

Monomer	Gp[a]	Q	e	No.[b]	Corr. coeff. r
Pyridazinone					
–, 3-(2-vinyl)-6-methyl-	V	0.57	+0.24		0.58
–, 3-(2-vinyl)-6-methyl-4,5-dihydro-	V	0.18	-0.32		0.35
Pyridine					
–, 5-ethyl-2-vinyl-	IV	1.29	-0.91	4	0.94
–, 2-methyl-5-vinyl-	III	1.32	-0.66	9	0.95
–, 2-vinyl-	II	1.41	-0.42	12	0.97
–, 4-vinyl-	III	2.47	+0.84	7	0.86
Pyrrolidinone, N-vinyl-	II	0.088	-1.62	12	0.95
Quinoline, 2-vinyl-	IV	1.04	-0.09	4	0.46
Silane					
–, trimethoxy vinyl	V	0.032	+0.54		0.66
–, tris-(trimethoxysiloxy)vinyl)	IV	0.022	-0.12	5	0.75
Styrene	I	1.00	-0.80		
–, m-bromo-	IV	1.25	-0.27	4	0.98
–, p-bromo-	IV	1.30	-0.68	7	0.99
–, p-carboxy-	V	5.17	+1.08		0.95

—, m-chloro-	IV	2.46	-0.90	4	0.87
—, o-chloro-	IV	2.66	+1.57	7	0.85
—, p-chloro-	III	1.33	-0.64	12	0.92
—, p-cyano-	IV	2.93	-0.38	5	0.75
—, 2,5-dichloro-	II	1.50	+0.94	12	0.96
—, p-1-(2-hydroxybutyl)-	V	.70	-0.97		0.65
—, p-1-(2-hydroxypropyl)-	IV	1.08	-0.35	4	0.51
—, p-2-(2-hydroxypropyl)-	IV	1.15	-0.49	4	0.91
—, p-methoxy-	III	1.53	-1.40	6	0.99
—, m-methyl-	V	1.57	-0.03		0.06
—, p-methyl-	III	1.10	-0.63	5	0.98
—, α-methyl-	III	0.97	-0.81	15	0.98
—, m-nitro-	V	2.19	+0.20		0.36
—, pentachloro-	V	0.20	+0.79		0.87
—, 2,4,6-trimethyl-	IV	0.15	-0.58	4	0.41
Succinimide, N-vinyl-	III	0.19	-1.42	8	0.96
Sulfonic acid, butyl-, vinyl ester	IV	0.16	+1.06	4	0.97
Sulfoxide, ethyl vinyl	IV	0.065	+0.05	4	0.21
Tetrazole					
—, 2-methyl-5-(4'-vinyl)phenyl-	V	0.86	+0.51		0.49

(continued)

TABLE 1 (continued)

Monomer	Gp[a]	Q	e	No.[b]	Corr. coeff. r
Tetrazole (continued)					
–, 2-phenyl-5-(4'-vinyl)phenyl-	V	0.84	-0.52		0.97
–, 5-phenyl-2-(4'-vinyl)phenyl-	V	1.11	+0.53		0.53
Urea, N-ethyl-N'-vinyl-	V	0.17	-1.88		0.98
Vinyl cyclopentadienyl manganese tricarbonyl	IV	0.39	-0.57	4	0.88
Vinyl ester of					
acetic acid	II	0.026	-0.88	49	0.87
benzoic acid	III	0.030	-0.70	9	0.95
butanoic acid	IV	0.024	-0.89	8	0.91
chloroacetic acid	IV	0.039	-1.61	5	0.98
cinnamic acid	IV	0.18	+0.76	4	0.99
dichloroacetic acid	V	0.059	-1.38		0.95
dodecanoic acid	V	0.011	-0.54		0.81
formic acid	III	0.043	-1.19	5	0.99
hendecanoic acid	III	0.056	-0.84	5	0.82
12-ketostearic acid	III	0.056	+0.30	3	0.84
monoethyl oxalic acid	IV	0.056	-0.65	4	0.53

nonanoic acid	III	0.046	-1.22	4	0.80
propanoic acid	IV	0.027	-0.68	7	0.82
octadecanoic acid	III	0.043	-0.97	7	0.85
thiolacetic acid	IV	0.27	-0.52	5	0.85
Vinyl ether					
–, butyl	IV	0.038	-1.50	10	0.87
–, 2-chloroethyl	IV	0.017	-1.58	7	0.98
–, dodecyl	IV	0.041	-1.69	6	0.83
–, ethyl	III	0.018	-1.80	8	0.90
–, isobutyl	IV	0.030	-1.27	7	0.98
–, octadecyl	IV	0.024	-1.93	4	0.87
–, octyl	IV	0.020	-1.57	4	0.98
–, phenyl	IV	0.046	-2.16	9	0.95
–, 1-phenyl-, methyl	IV	0.39	-1.02	5	0.77
Vinyl ether, di-	IV	0.029	-1.16	4	0.80
Vinyl sulfide					
–, tert-butyl	IV	0.046	-2.20	4	0.72
–, ethyl	IV	0.27	-1.31	6	0.96
–, isobutyl	IV	0.49	-0.95	7	0.99
–, methyl	IV	0.42	-1.66	5	0.99

(continued)

TABLE 1 (continued)

Monomer	Gp[a]	Q	e	No.[b]	Corr. coeff. r
Vinyl sulfide (continued)					
—, phenyl	IV	0.33	-0.99	5	0.96

[a]Gp = group; I: Based on reactivity ratios with styrene only; II, initial values based on group 1; III, initial values based on groups I and II (six iterations were required to stabilize the values of groups II and III); IV, values based on groups I, II, and III; V, only three citations available for groups I, II, and III.

[b]No. = number of reactivity ratio citations employed in the evaluation.

TABLE 2. Q and e Values of Telogens Based on a Least Squares Evaluation

Telogen	Temp. (°C)	$Q \times 10^4$	e	No.[a]	Corr. coeff. r
Acetone	60	0.11	+0.35	5	0.80
	80	0.32	+0.45	5	0.68
Benzene	60	0.05	-1.21	16	0.94
	80	0.07	-0.61	9	0.72
—, chloro-	60	0.07	+0.08	7	0.30
	80	0.13	-0.06	5	0.31
—, ethyl-	60	0.95	-1.02	8	0.84
	80	0.91	-0.61	7	0.86
—, methyl-	60	0.16	-0.95	12	0.93
	80	0.34	-0.87	11	0.94
Benzoyl peroxide	60	36.	-1.89	4	0.93
Butanol	60	0.53	-0.57	6	0.63
Butanone	60	0.82	+0.53	4	0.60
	80	1.40	+1.00	7	0.80
Cyclohexane	60	0.11	-0.64	6	0.86
	80	0.14	-1.41	7	0.77
1,2-Dichloroethane	60	0.62	+1.34	3	0.96
	80	1.1	+2.07	6	0.96

(continued)

TABLE 2 (continued)

Telogen	Temp. (°C)	$Q \times 10^4$	e	No.[a]	Corr. coeff. r
Ethyl acetate	60	0.07	-0.87	11	0.97
Mercaptan, alkyl	60	14,500.	+2.44	11	0.99
Mercaptoacetate, alkyl	60	15,100.	+3.27	4	0.99
Methane					
–, dichloro-	60	0.10	-0.68	4	0.82
–, nitro-	60	3.26	-1.50	4	0.92
–, tetrabromo-	60	7,300.	+2.90	8	0.99
–, tetrachloro-	60	3.64	+3.21	13	0.99
	80	5.15	+3.41	9	0.99
–, trichloro-	60	1.18	+0.47	8	0.95
	80	1.24	+0.70	10	0.82
Methanol	60	0.18	-0.93	5	0.76
Triethylamine	60	28.8	-2.39	7	0.99

[a]No. = number of chain transfer constant citations employed in the evaluation.

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