Prediction of aqueous solubility and octanol–water partition coefficient for pesticides based on their molecular structure

G.S. Patil

Chemical Engineering Division, Regional Research Laboratory,
Jorhat-785006, Assam (India)

Abstract

Correlations have been derived for the estimation of aqueous solubilities and octanol–water partition coefficients for pesticides, based solely on their molecular structure. The parameters used for obtaining these correlations are the zero order connectivity, zero order valence molecular connectivity, molecular polarizability, and carbon to hydrogen ratio. The results obtained are satisfactory for environmental applications. Such correlations may be used to predict the logarithm of aqueous solubilities (<0.1) and/or the logarithm of the octanol–water partition coefficients (> -0.4) for pesticides. However, these correlations cannot be used satisfactorily for pesticides having a carbon to hydrogen ratio $\geqslant 2$, or O-analogues.

1. Introduction

Pesticides are a class of compounds used for the control of pests including those directly hazardous to the health of man and animals. They are of immense agricultural and economic importance. However, after the application of pesticides, residue accumulation in soil and water are hazardous to aquatic organisms. Octanol–water partition coefficients (K_{ow}) and aqueous solubilities (S_w) are important because they can be used to predict soil/sediment adsorption coefficients and bioconcentration factors (BCF) for non-ionic pesticides from aqueous solutions [1]. Various models for estimating S_w [2–4] and K_{ow} [3] have been reported. Moreover, the modeling of the environmental fate of pollutants requires knowledge of certain properties, of which S_w and K_{ow} are most important. An excellent review covering the theoretical and experimental aspects of partition coefficients has been published [5]. This review also reports partition coefficients for a large number of compounds in different solvents and their uses. Data on S_w for a large number of pesticides have been compiled [6, 7], and data on K_{ow} [5, 7] have been reported and incorporated partly by Bowman and Sans [8]. However, data on S_w for a few,

and K_{ow} for a large number of pesticides are not available and it is desirable to have a simple predictive method to estimate these properties for pesticides for which data have not been reported or for newly synthesised pesticides.

During the past few years, Quantitative Structure–Activity Relationships (QSAR) have been used widely for developing models to predict various properties, viz. toxicity, bioconcentration factor, thermodynamic properties such as heat of formation, critical volume, etc. Reviews of the applications of QSAR for estimating the environmental distribution and toxicity of organic pollutants [9], and describing the detailed applications of QSAR have been published recently [10]. In an earlier communication [11] we reported correlations based on molecular structure for estimating S_w and K_{ow} for halogenated benzenes, polychlorinated biphenyls and polycyclic aromatic hydrocarbons. Similar correlations based on the molecular connectivity to estimate K_{ow} of polycyclic aromatic hydrocarbons and their alkyl derivatives have been proposed recently [12]. In this communication we have obtained correlations for estimating aqueous solubility and octanol–water partition coefficient for pesticides based on molecular structure. In addition, these correlations have been tested for 48 pesticides which were not included whilst deriving the correlations originally.

2. Methodology

A detailed description of molecular connectivity has been given elsewhere [13], and therefore only a brief description of molecular connectivities used is given here. The zero-order connectivity, ^0x, is calculated from the structure of the compound. Each non-hydrogen atom i is assigned a value, δ_i, which is equal to the number of bonds with which it is attached to neighbouring non-hydrogen atoms. ^0x can then be calculated by summing the reciprocal square roots of δ_i for each atom, and is given by the following expression,

$$^0x = \sum \delta_i^{-0.5} \tag{1}$$

The zero-order valence connectivity, $^0x^v$, is calculated by assigning a value, δ_v, for a non-hydrogen atom, which is equal to the number of outer-shell electrons (valence electrons) in the atom minus the number of hydrogen atoms bonded to that atom. $^0x^v$ can then be calculated by using the above expression. δ_v values used for the calculation of $^0x^v$ in fluorine, chlorine, bromine and iodine are -20, 0.69, 0.254 and 0.085, respectively, and are taken from Kier and Hall [14]. Finally, the empirical approach of Miller and Savchik [15] was used to calculate the average molecular polarizability values (P) of the compounds. Aqueous solubilities S_w and melting points (mp) are expressed in mol/L and °C, respectively.

Experimental data on K_{ow} and the compiled data on S_w for pesticides have been taken from Bowman and Sans [8] which are given in Table 1 (Set A). These data have been used for deriving correlations. Table 1 also contains data on ^0x,

$^{\circ}x^{v}$, mp, P, carbon to hydrogen ratio (C/H) for ready reference. For liquid solutes, $0\,^{\circ}$C was used while for solids average values of melting points were taken. Since the pesticides analysed included both solids and liquids, a correction term for fusion was also applied for solids involving mp as stressed by Yalkowsky and Mishra [16].

The data on $^{\circ}x$, $^{\circ}x^{v}$, mp, P, C/H, observed S_{w} and K_{ow} values for the pesticides used to test the correlations are given in Table 2 (Set B).

Multiple linear regression analysis was performed for data given in Table 1 using standard statistical procedures.

3. Results and discussion

Data on S_{w} and K_{ow} for 54 and 56 pesticides, respectively (Table 1), were used in the regression to obtain the correlations for these properties. The O-analogues were excluded from the regression as they gave much larger deviations from their observed values. The relationships obtained by the regression for S_{w} and K_{ow} are given by eqs. (2) and (3), respectively.

$$\log S_{w} = 0.403\,^{\circ}x - 15.294\log P - 3.616\,C/H - 0.286\,^{\circ}x^{v} + 19.905$$

$$n = 52, \quad r = 0.90, \quad SE = 0.72 \tag{2}$$

$$\log K_{ow} = 0.170\,P + 1.771\,C/H - 0.500\,^{\circ}x + 0.557\,^{\circ}x^{v} - 2.616$$

$$n = 55, \quad r = 0.85, \quad SE = 0.76 \tag{3}$$

The relationships obtained after introducing the correction term mp for solids are given by eqs. (4) and (5), respectively.

$$\log S_{w} = 0.372\,^{\circ}x + 0.01\,mp - 13.520\log P - 4.589\,C/H - 0.237\,^{\circ}x^{v} + 16.714$$

$$n = 52, \quad r = 0.92, \quad SE = 0.65 \tag{4}$$

$$\log K_{ow} = 0.137\,P + 3.210\,C/H - 0.0144\,mp - 0.469\,^{\circ}x + 0.486\,^{\circ}x^{v} - 1.830$$

$$n = 55, \quad r = 0.91, \quad SE = 0.61 \tag{5}$$

Comparison of eqs. (2) and (4) for S_{w}, and (3) and (5) for K_{ow}, indicates that eqs. (4) and (5) yield marginally better results as evidenced by their lower standard errors (SE). This suggests that the correction term for fusion does not play a significant role in the estimation of S_{w}. These results also confirm the findings of Isnard and Lambert [17] and Patil [11]. However, it is always preferable to use the correction term especially for the estimation of K_{ow} if mp is available but in its absence eqs. (2) and (3) can still be used. In the subsequent discussion, only the values calculated using eqs. (4) and (5) will be considered. Table 1 indicates the validity of the correlations derived.

The differences of about 1 and 0.6 in the experimentally determined values of $\log S_{w}$ and $\log K_{ow}$ can be noted from the results on different stationary phases (nucleosil 5CN, nucleosil 5C 18, sepralyte diphenyl) and eluents (methanol,

TABLE 1

Water solubility, octanol–water partition coefficients, molecular connectivity values (^0x and $^0x^v$), molecular polarizabilities, melting points and carbon/hydrogen ratios for insecticides of set A[a,b]

Sl. No.	Compound	^0x	$^0x^v$	mp (°C)	P	C/H	$\log S_w$ Obs.	Calc.	Error	$\log K_{ow}$ Obs.	Calc.	Error
1	Aldicarb	9.49	7.75	99.0	20.71	0.50	-1.50	-0.69	-0.81	1.13	0.50	0.63
2	Aminocarb	10.72	9.50	93.5	24.21	0.69	-2.36	-2.48	0.12	1.73	1.93	-0.20
3	Azinphos-ethyl	14.54	11.76	53.0	35.93	0.75	-4.52	-4.60	0.08	3.40	3.69	-0.20
4	Azinphos-methyl	13.13	10.35	73.5	32.12	0.83	-4.18	-4.31	0.13	2.69	3.18	-0.49
5	Bromophos	11.28	11.63	53.5	30.54	1.00	-6.09	-5.98	-0.11	4.88	5.16	-0.28
6	Bromophos-ethyl	13.19	13.04	–	34.35	0.83	-5.95	-6.06	0.11	5.68	5.68	0.00
7	Carbaryl	9.75	8.36	142.0	23.00	1.09	-3.29	-3.65	0.36	2.31	2.27	0.04
8	Carbofuran	11.35	8.96	151.0	23.61	0.80	-2.84	-1.91	-0.93	1.63	0.83	0.80
9	Carbophenothion	12.76	11.12	–	36.46	0.69	-5.74	-5.45	-0.29	5.12	4.80	0.32
10	Carbophenothion-methyl	11.34	9.71	–	32.65	0.75	-5.29	-5.28	-0.01	4.82	4.32	0.50
11	Chlordimeform	9.09	8.91	32.0	22.14	0.77	-2.86	-3.41	0.55	2.89	3.54	-0.45
12	Chlorfenvinphos	13.84	13.41	–	27.89	0.86	-3.46	-4.80	1.34	3.81	4.53	-0.72
13	Chlorpyrifos	13.32	12.13	42.7	33.64	0.82	-5.68	-5.18	-0.50	4.96	4.50	0.46
14	Chlorpyrifos-methyl	11.90	9.72	46.0	29.83	1.00	-5.00	-5.23	0.23	4.30	3.94	0.36
15	Diazinon	13.05	11.63	–	33.3	0.57	-3.65	-4.38	0.73	3.81	4.16	-0.35
16	Dicapthon	12.43	10.96	51.5	27.91	0.89	-4.31	-4.37	0.06	3.62	3.60	0.02
17	Dichlorvos	8.31	6.62	–	17.96	0.57	-1.34	-1.34	0.00	1.47	1.78	-0.31
18	Dimethoate	9.53	7.19	51.5	23.53	0.42	-0.96	-1.39	0.43	0.77	1.02	-0.25
19	Disulfoton	10.86	9.02	–	30.53	0.42	-4.23	-3.39	-0.84	4.02	3.00	1.02
20	Disulfoton-sulfone	12.86	9.84	–	32.20	0.42	-2.54	-3.15	0.61	1.87	2.68	-0.81
21	Disulfoton-sulfoxide	11.86	9.43	–	31.31	0.42	–	-3.26	–	1.73	2.83	-1.10
22	Ethion	14.78	11.70	–	40.83	0.59	-5.54	-5.05	-0.49	5.07	4.42	0.65
23	Fenamiphos	13.84	12.10	49.2	33.68	0.59	-2.96	-3.87	0.91	3.23	3.36	-0.13
24	Fenitrothion	12.43	9.58	–	27.98	0.75	-4.04	-3.94	-0.10	3.40	3.24	0.16
25	Fensulfothion	12.92	10.62	–	33.07	0.65	-2.19	-4.47	2.28	2.23	3.89	-1.66
26	Fensulfothion-sulfide	12.05	10.21	–	32.32	0.65	-4.90	-4.59	-0.31	4.16	3.99	0.17
27	Fensulfothion-sulfoxide	14.05	11.03	44.0	33.98	0.65	-3.58	-8.90	0.32	2.59	3.04	-0.45

28	Fenthion	11.56	9.73	–	31.54	0.67	–4.57	–4.62	0.05	4.09	3.94	0.15
29	Fenofos	9.71	8.47	–	28.58	0.67	–4.20	–4.47	0.27	3.89	3.79	0.10
30	Iodofos	11.78	13.07	76.0	31.58	1.00	–6.62	–6.10	–0.52	5.16	5.44	–0.28
31	Isofenphos	16.29	13.66	–	32.51	0.62	–4.19	–3.77	–0.42	4.12	3.63	0.49
32	Leptophos	13.45	13.60	70.4	32.93	1.30	–7.21	–7.28	0.07	5.88	6.14	–0.26
33	Malathion	15.32	11.41	–	33.34	0.53	–3.36	–3.30	–0.06	2.84	2.79	0.05
34	Methidathion	12.03	8.91	39.5	29.29	0.54	–3.21	–2.86	–0.35	2.42	2.05	0.37
35	Methomyl	7.54	5.67	78.5	16.57	0.50	0.55	0.18	0.37	0.13	0.19	–0.06
36	Paraoxon	12.92	10.07	–	26.62	0.71	–1.88	–3.41	1.53	1.98	2.94	–0.96
37	Parathion	12.92	10.07	–	28.93	0.71	–4.37	–3.89	–0.48	3.76	3.26	0.50
38	Parathion-amino	10.58	7.83	–	21.59	0.80	–2.79	–2.91	0.12	2.60	2.54	0.06
39	Parathion-methyl	11.41	8.65	35.5	26.00	0.80	–3.84	–3.54	–0.30	2.94	2.64	0.30
40	Phorate	10.16	8.32	–	28.58	0.42	–4.16	–3.08	–1.08	3.83	2.70	1.13
41	Phorate-sulfoxide	11.16	7.31	–	29.41	0.41	–	–2.60	–	1.77	1.84	–0.07
42	Phorate sulfone	12.16	9.13	–	30.24	0.41	–2.53	–2.84	0.31	1.98	2.37	–0.39
43	Phosalone	14.89	12.40	48.0	34.72	0.80	–5.15	–4.71	–0.44	4.38	3.85	–0.53
44	Phosmet	13.21	10.36	71.9	32.67	0.92	–4.11	–4.79	0.68	2.78	3.39	–0.61
45	Phoxim	12.58	10.37	–	23.07	0.80	–4.86	–3.12	–1.74	4.39	3.03	1.36
46	Pyrimiphos-ethyl	15.52	13.33	–	36.78	0.54	–4.92	–4.33	–0.59	4.85	4.27	0.58
47	Pyrimiphos-methyl	14.10	11.91	–	32.97	0.55	–4.13	–3.91	–0.22	4.20	3.63	0.57
48	Propoxur	10.51	9.11	85.5	23.47	0.73	–2.05	–2.58	0.53	1.55	2.01	–0.46
49	Ronnel	11.78	10.85	41.0	27.06	1.00	–5.73	–5.02	–0.71	4.81	4.25	0.56
50	Temephos	18.57	15.19	30.0	49.38	0.80	–6.24	–6.25	0.01	5.95	5.75	0.20
51	Terbufos	11.95	10.11	–	32.44	0.43	–4.72	–3.63	–1.09	4.48	3.30	1.18
52	Terbufos sulfone	13.95	10.93	–	34.10	0.43	–2.89	–3.38	0.49	2.48	2.99	–0.51
53	Terbufos-sulfoxide	12.95	10.52	–	33.27	0.43	–2.44	–3.50	1.06	2.21	3.14	–0.87
54	Triazophos	13.49	10.70	–	34.74	0.75	–4.10	–5.08	0.98	3.55	4.34	–0.79
55	Trichlorfon	9.99	8.75	83.5	20.17	0.50	–0.22	–0.75	0.53	0.43	0.90	–0.47
56	Trichloronat	12.48	11.85	–	31.04	0.83	–5.75	–5.45	–0.30	5.22	5.00	0.22

[a] The data on water solubility, octanol–water partition coefficients and melting points are reproduced from Reference [8]. Other values were calculated.
[b] Solubility is expressed in mol/L.

TABLE 2

Water solubility, octanol–water partition coefficients, molecular connectivity values (^0x and $^0x^v$), molecular polarizabilities, melting points and carbon/hydrogen ratios for insecticides of set B

Sl. No.	Compound	^0x	$^0x^v$	mp (°C)	P	C/H	log S_w			log K_{ow}		
							Obs.	Calc.	Error	Obs.	Calc.	Error
1	Acifluorfen[a]	16.75	10.80	151.0	30.46	2.00	−3.48	−7.46	3.98	–	3.98	–
2	Aldrin[b]	15.33	16.55	104.3	30.62	1.50	−6.26	−7.54	1.28	5.52	6.53	−1.01
3	Anthraquinone[a]	9.62	8.43	285.0	23.66	1.75	−5.54	−5.46	−0.08	–	2.51	–
4	Antu[a]	8.75	7.93	198.0	24.31	1.10	−2.93	−3.72	−0.79	–	1.93	–
5	Azobenzene[b]	8.19	7.67	69.0	22.08	1.20	−2.78	−5.05	−2.27	3.82	3.96	0.14
6	X-BHC[c]	9.00	10.22	112.0	22.89	1.00	−4.60	−4.22	−0.38	3.72	3.65	0.07
7	Bromacil[c]	10.57	10.03	158.5	23.53	0.69	−2.51	−1.87	−0.64	2.02	0.29	1.73
8	4-Bromophenol[b]	5.31	5.70	64.0	14.51	1.20	–	−3.24	–	2.59	3.37	−0.78
9	Captafol[b]	13.08	12.29	160.5	30.52	0.90	−5.39	−4.15	−1.24	3.83	2.77	1.06
10	Captan[b]	11.29	10.50	178.0	31.90	1.12	−5.78	−5.32	−0.46	2.54	3.40	−0.86
11	Chlorpropham[c]	9.88	8.98	41.4	22.69	0.83	−3.30	−3.46	0.16	3.06	3.09	−0.03
12	Chlorbromuron[b]	10.72	10.75	96.0	25.48	0.90	−3.92	−4.03	0.11	3.09	3.26	−0.27
13	Chlortoluron[b]	12.82	9.36	147.5	23.39	0.77	−3.48	−1.30	−2.18	2.41	0.26	2.15
14	Cynazine[c]	11.74	10.20	166.6	24.44	0.69	−3.15	−1.60	−1.55	2.24	0.79	1.45
15	p,p'-DDT[c]	12.70	13.71	108.5	33.62	1.05	−8.05	−8.43	0.38	6.19	6.82	−0.63
16	Dieldrin[d]	14.38	15.08	175.5	32.33	1.62	−7.24	−7.61	0.37	5.16	5.88	−0.72
17	Diphenylamine[b]	6.48	7.27	53.5	21.83	1.09	−2.74	−4.80	2.06	3.42	3.92	−0.50
18	Diuron[c]	10.09	9.57	158.5	23.48	0.90	−3.75	−2.88	−0.87	1.97	1.95	0.02
19	Fenoprop[d]	10.94	10.07	180.0	20.64	1.29	−3.28	−4.35	1.07	3.86	2.75	1.11
20	Fenuron[c]	8.17	6.09	133.5	19.66	0.75	−1.63	−1.29	−0.34	1.00	0.48	0.52
21	Fluometuron[c]	11.59	6.99	163.8	21.75	0.91	−3.42	−1.24	−2.18	1.34	0.33	1.01
22	Folpet[d]	11.22	10.09	117.0	26.20	2.25	−5.47	−9.83	4.36	3.63	6.94	−3.31
23	Heptachlor[d]	12.39	13.80	95.5	30.20	2.00	−6.82	−10.18	3.36	5.44	8.25	−2.81
24	Linuron[c]	11.01	9.09	93.5	23.48	0.90	−3.53	−3.08	−0.45	2.19	2.19	0.00
25	Methiocarb[b]	10.77	9.38	117.5	25.69	0.73	−3.87	−2.75	−1.12	2.92	1.86	1.06
26	3-Methylaniline[b]	4.59	4.39	–	13.98	0.78	−1.22	−2.67	0.45	1.40	2.56	−1.16
27	4-Methylaniline[b]	4.59	4.39	–	13.98	0.78	−1.22	−1.67	0.45	1.40	2.56	−1.16

28	Methoxychlor[c]	14.11	14.12	77.0	36.00	1.07	−6.46	−6.55	0.09	5.08	5.67	−0.59
29	Metobromuron[b]	9.80	7.25	95.8	23.56	0.82	−2.89	−2.70	−0.19	2.38	1.57	−0.81
30	Metoxuron[b]	10.72	9.78	126.5	24.22	0.77	−2.52	−2.59	0.07	1.64	2.62	−0.98
31	Monolinuron[c]	10.09	8.77	81.5	22.41	0.82	−2.57	−2.81	0.24	1.60	2.21	−0.61
32	Monuron[c]	8.88	7.86	174.5	21.57	0.82	−2.94	−1.89	−1.05	1.46	0.89	0.57
33	Napthalene[c]	5.62	5.62	80.0	16.75	1.25	−3.65	−4.00	0.35	3.36	3.41	−0.05
34	Nitrapyrin[b]	7.94	8.49	62.5	19.23	2.00	−3.76	−8.16	4.40	3.02	6.73	−3.71
35	Oxadizone[d]	15.93	14.76	90.0	34.06	0.83	−5.69	−4.49	1.20	4.10	3.91	0.19
36	Oxamyl[b]	10.90	8.53	101.0	21.58	0.54	0.11	−0.75	0.86	−0.47	0.43	−0.90
37	Phenol[b]	4.39	3.79	40.8	11.35	1.00	−0.06	−0.82	0.76	1.46	2.14	−0.68
38	Propham[b]	8.88	7.78	87.3	21.74	0.77	–	–	–	2.60	1.98	0.62
39	Strychnine[a]	15.38	14.23	275.0	37.99	0.95	−3.37	−3.95	0.55	–	2.17	–
40	2,3,6-TBA[a]	8.65	8.12	93.0	17.97	2.33	−1.47	−8.77	7.30	–	6.66	–
41	Terbacil[c]	10.78	9.47	176.0	21.01	0.69	−2.49	−0.81	−1.68	1.89	0.29	1.60
42	1,2,3,4-Tetrachlorobenzene[d]	7.15	7.34	46.5	18.14	3.00	−4.44	−12.89	8.45	4.65	9.83	−5.18
43	4,5,6,7-Tetrachlorophthalide[a]	9.91	9.84	209.5	22.21	4.00	−5.04	−16.40	11.36	–	11.17	–
44	Tetrasul[a]	11.17	11.69	80.0	30.95	2.00	−4.03	−10.44	6.41	–	8.12	–
45	Thidizuron[a]	9.50	7.67	213.0	23.36	1.12	−4.04	−3.10	−0.94	–	1.17	–
46	1,2,3-Trichlorobenzene[d]	6.23	6.84	54.0	16.23	2.00	−4.18	0.41	−4.59	4.27	6.44	−2.17
47	Trietazine[c]	11.03	10.11	100.5	24.48	0.56	−3.11	−1.94	−1.17	3.35	1.65	1.20
48	Trifluralin[d]	11.51	10.89	48.7	29.62	0.81	−5.75	−4.70	−1.05	5.34	4.19	1.15

[a] Reference [6], [b] Reference [1], [c] Reference [7] and [d] Reference [17].

acetonitrile) in reverse phase liquid chromatography [18]. Moreover, deviations of 3.7 orders of magnitude in $\log S_w$ [19, 20] and of 2.7 orders of magnitude in $\log K_{ow}$ [8, 19, 20] are observed when the data of different workers are compared.

Equations (4) and (5) were obtained from the data for organophosphorus and carbamate insecticides only; their applicability has been tested for 48 different pesticides of mixed classes, with varied structures, and atoms which include C/H ratios and *mp* values as high as 4 and 304 °C, respectively. The observed and calculated values of $\log S_w$ and $\log K_{ow}$ for these pesticides are given in Table 2. The data in Table 2 show that eqs. (4) and (5) are not applicable for the estimation of S_w and K_{ow} for pesticides having C/H ratios $\geqslant 2$. In the further discussion, compounds in Table 2 having C/H ratios $\geqslant 2$ will not be considered since these compounds gave much larger deviations from observed values for both $\log S_w$ and $\log K_{ow}$. The maximum deviations of 2.27 and 1.73 were observed for $\log S_w$ and $\log K_{ow}$, respectively, for the compounds having C/H ratios less than 2 (Table 2). From the above discussion it can be inferred that eqs. (4) and (5) may be used to predict S_w and K_{ow} for pesticides, for $\log S_w < 0.1$ and $\log K_{ow} > -0.4$, satisfactorily for estimation of environmentally related parameters.

Shortcomings of these correlations are: (i) They give large errors > 4 in $\log S_w$ and > 3 in $\log K_{ow}$ for compounds with C/H ratios $\geqslant 2$; (ii) they fail for O-analogues; (iii) since calculation of "x^v" was based on the number of outer-shell electrons, it is not possible to distinguish between nitrogen and phosphorus or oxygen and sulfur. Nevertheless these correlations yield satisfactory results for compounds having one or more of these atoms. In short, these correlations cannot be used satisfactorily for O-analogues and compounds with C/H ratios $\geqslant 2$.

4. Conclusion

The correlations obtained can be used for the estimation of aqueous solubilities and octanol–water partition coefficients for pesticides of different classes, varying structures and over a large range of melting points. The results obtained are satisfactory for environmental applications except for O-analogues and for compounds having C/H ratios $\geqslant 2$.

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