

ERRATA

Correlation of the Melting Points of Potential Ionic Liquids (Imidazolium Bromides and Benzimidazolium Bromides) Using the CODESSA Program [*J. Chem. Inf. Comput. Sci.* 42, 225-231 (2002)] by Alan R. Katritzky, Ritu Jain, Andre Lomaka, Ruslan Petrukhin, Mati Karelson, Ann. E. Visser, and Robin D. Rogers. Centre for Heterocyclic Compounds, Department of Chemistry, University of Florida, P.O. Box 11720, Gainesville, Florida 32611-7200, Department of Chemistry, University of Tartu, Jakobi Street 2, Tartu 51014, Estonia, and Department of Chemistry and Center for Green Manufacturing, The University of Alabama, P.O. Box 870336, Alabama 35487-0336

Pages 227–229. In Tables 2–5 some of the substituent positions defined for structures are ambiguous or wrong. Corrections should be made as follows:

Table 2 to structures (ID: 1, 6, 14, 33, 35, 39, 41, 47, and 55)

Table 3 to structure (ID: 18)

Table 4 to structures (ID: 15, 16, and 18)

Table 5 to structures (ID: 41).

The corrections of Tables 2–5 are listed below.

Table 2. Corrections to Structures in Set A

ID	expt MP	calcd MP	1-substituent	3-substituent	other substituents
1	49.0	86.8	$-\text{CH}_2-(\text{CH}_2)_{10}-\text{CH}_3$	$-\text{CH}=\text{CH}_2$	
6	88.5	87.3	$-\text{CH}_2-\text{CH}=\text{CH}_2$	$-\text{CH}_2\text{CH}_2\text{CN}$	
14	116.5	140.5	$n-\text{C}_5\text{H}_{11}$	$-\text{CH}_2\text{Ph}$	2- $n\text{-C}_{11}\text{H}_{23}$
15	117.0	148.7	$-\text{CH}_3$	$-\text{CH}_2\text{COPh}$	
33	180.0	155.3	$-\text{CH}_3$	$-\text{CH}_2\text{COC}_6\text{H}_3$ [2,4- $(\text{CH}_3)_2$]	
35	185.0	196.4	$-\text{CH}_3$	$-\text{CH}_2\text{COPh}$	2- $\text{CH}=\text{CH}-\text{Ph}$
39	194.0	160.4	$-\text{CH}_3$	$-\text{CH}_2\text{Ph}$	2- $n\text{-C}_9\text{H}_{19}$
41	200.0	177.9	$-\text{CH}_3$	$-\text{CH}_2\text{COPh}$	2- $\text{CH}=\text{CH}-\text{C}(\text{CH}_3)_3$
47	220.5	237.5	$-\text{CH}_3$	$-\text{CH}_3$	2-SCN
55	260.5	231.8	$-\text{CH}_3$	$-\text{CH}=\text{CH}-\text{C}_6\text{H}_4-(p\text{-OH})$	

Table 3. Correction to Structure in Set B

ID	expt MP	calcd MP	1-substituent	3-substituent	other substituents
18	166.0	161.9	$-\text{O}-\text{CO}-\text{C}(\text{CH}_3)_3$	$-\text{CH}_2-\text{COC}_6\text{H}_4(p\text{-Cl})$	

Table 4. Corrections to Structures in Set A

ID	expt MP	calcd MP	1-substituent	3-substituent	other substituents
15	250.0	241.3	$-\text{CH}_2\text{C}_6\text{H}_4(p\text{-F})$	$-\text{CH}_2\text{C}_6\text{H}_4(p\text{-Cl})$	2- CH_3 , 4- CH_3
16	267.5	263.8	$-\text{Ph}$	$-\text{C}_6\text{H}_4(p\text{-CH}_3)$	2- Ph , 4- NH_2

Table 5. Correction to Structure in Set A

ID	expt MP	calcd MP	1-substituent	3-substituent	other substituents
41	270.0	250.6	H	$-\text{CH}_3$	2- $\text{C}_6\text{H}_4(o\text{-COOH})$

Page 228. The descriptor N_H in eq 2 is “number of hydrogen atoms” that has not been referred to in the text.

On the same page, the third descriptor in eq 3 is misprinted and should read as $E_{\min,e-n,C-N}$ instead of $E_{\min,C-N}$.

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Boiling Points of Halogenated Aliphatic Compounds: A Quantitative Structure–Property Relationship for Prediction and Validation [*J. Chem. Inf. Comput. Sci.* 44, 187–192 (2004)] by T. Öberg. Department of Biology and Environmental Science, University of Kalmar, SE-391 82 Kalmar, Sweden

Page 189. Rücker et al. [*J. Chem. Inf. Comput. Sci.* 44, 2070–2076 (2004)] have drawn attention to the occurrence of duplicate structures in the data by Horvath (ref 19). Nineteen duplicates occur in the calibration set and twelve in the external test set for the reported calibration model. Five duplicates were among the removed outliers. Removing the duplicates gives a slight change in the model performance parameters reported: SEC, 4.74 K; R_{cal}^2 , 0.990; SEP, 6.34 K; and Q_{ext}^2 , 0.979.

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