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SUPPLEMENTARY MATERIAL TO

Aqueous nicotine solutions: pH-measurements and salting-out effects – Analysis of the effective Gibbs energies of hydration and ionic strengths of the solutions

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CALCULATION OF THE MCGOWAN VOLUMES AND THE PAULING IONIC RADIUS

McGowan volumes, V_x , in Å³ per molecule, were calculated applying the following equation:¹

$$V = \frac{1}{0.602} \left[\sum_i (AC)_i - \sum 6.56B \right] \quad (\text{S-1})$$

in which $(AC)_i$ are the related atom contributions (McGowan volumes of atoms, listed in the literature³³) and B signifies the number (sum) of the existing bonds, whether being single-, double- or triple-. This number is approximated by the equation:²

$$B = N - 1 + R_g \quad (\text{S-2})$$

In Eq. (S-2), N and R_g are the numbers of all atoms and ring structures, respectively; ($R_g = 0$ in the present case).

The McGowan radius per mol, R_x , was obtained from Eq. (S-1) using the volume–radius relation for a sphere.

Finally, Pauling (ionic radius) R_p is calculated using the relation² between R_x and R_p :

$$R_x = 1.115R_p + 0.0623 \quad (\text{S-3})$$

REFERENCES

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