Supporting Information

Surface Tensions of Ionic Liquids: Non-Regular Trend Along the Number of Cyano Groups

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Table S.I. 1. Electrostatic/misfit energy (E_{MF}), hydrogen bonding energy (E_{HB}), and van der Waals energy (E_{vdW}) of each cation-anion pair, obtained from COSMO-RS [1].

	E_{MF} / (kJ.mol^{-1})	E_{HB} / (kJ.mol^{-1})	E_{vdW} / (kJ.mol^{-1})
$[C_2C_1im][SCN]$	33.78	-17.17	-51.50
$[C_2C_1im][N(CN)_2]$	34.54	-22.88	-49.18
$[C_2C_1im][C(CN)_3]$	31.67	-16.99	-56.62
$[C_2C_1im][B(CN)_4]$	31.26	-12.76	-64.84
$[C_4C_1im][SCN]$	36.10	-16.64	-59.36
$[C_4C_1im][N(CN)_2]$	36.99	-22.12	-56.72
$[C_4C_1im][C(CN)_3]$	34.93	-16.30	-63.80
$[C_6C_1im][N(CN)_2]$	38.80	-21.81	-64.41
$[C_6C_1im][B(CN)_4]$	37.16	-11.82	-78.66

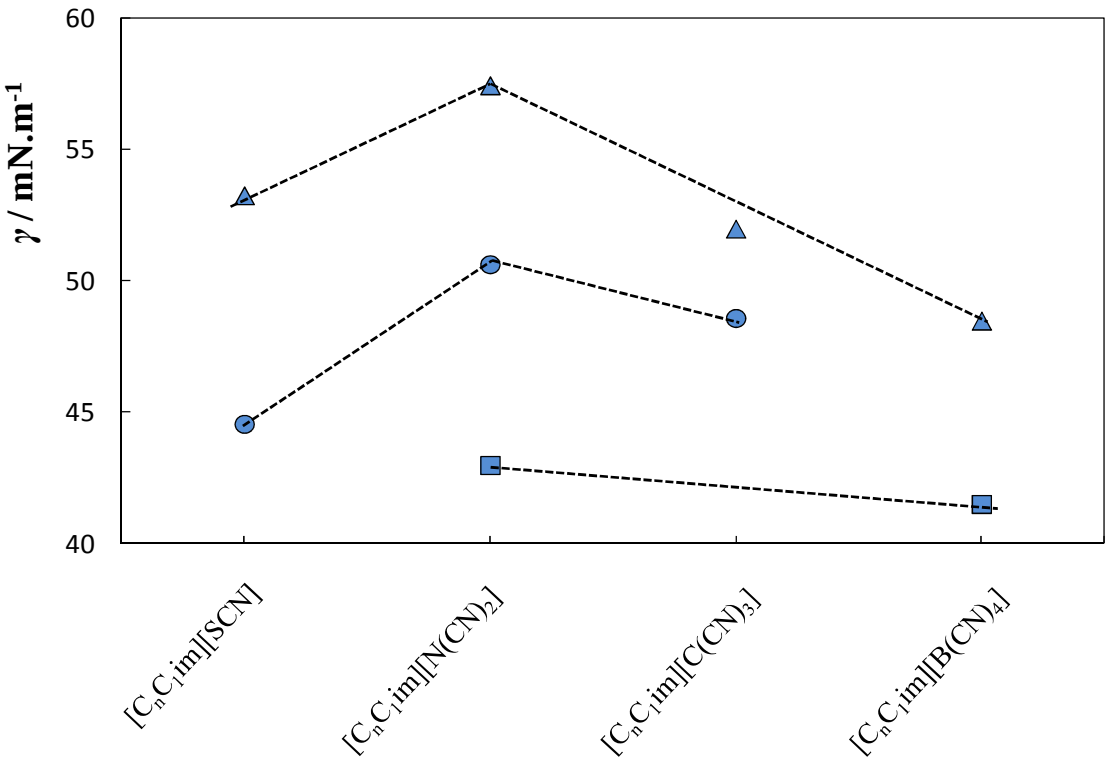

Figure S.I. 1. Surface tension at 298.15 K of cyano-functionalized anions combined with the cations: △, $[C_2C_1im]^+$; ○, $[C_4C_1im]^+$; □, $[C_6C_1im]^+$. Surface tension data of $[C_2C_1im][SCN]$ and $[C_2C_1im][N(CN)_2]$ were taken from a previous work [2]. The dashed lines have no physical meaning and are guides for the eyes.

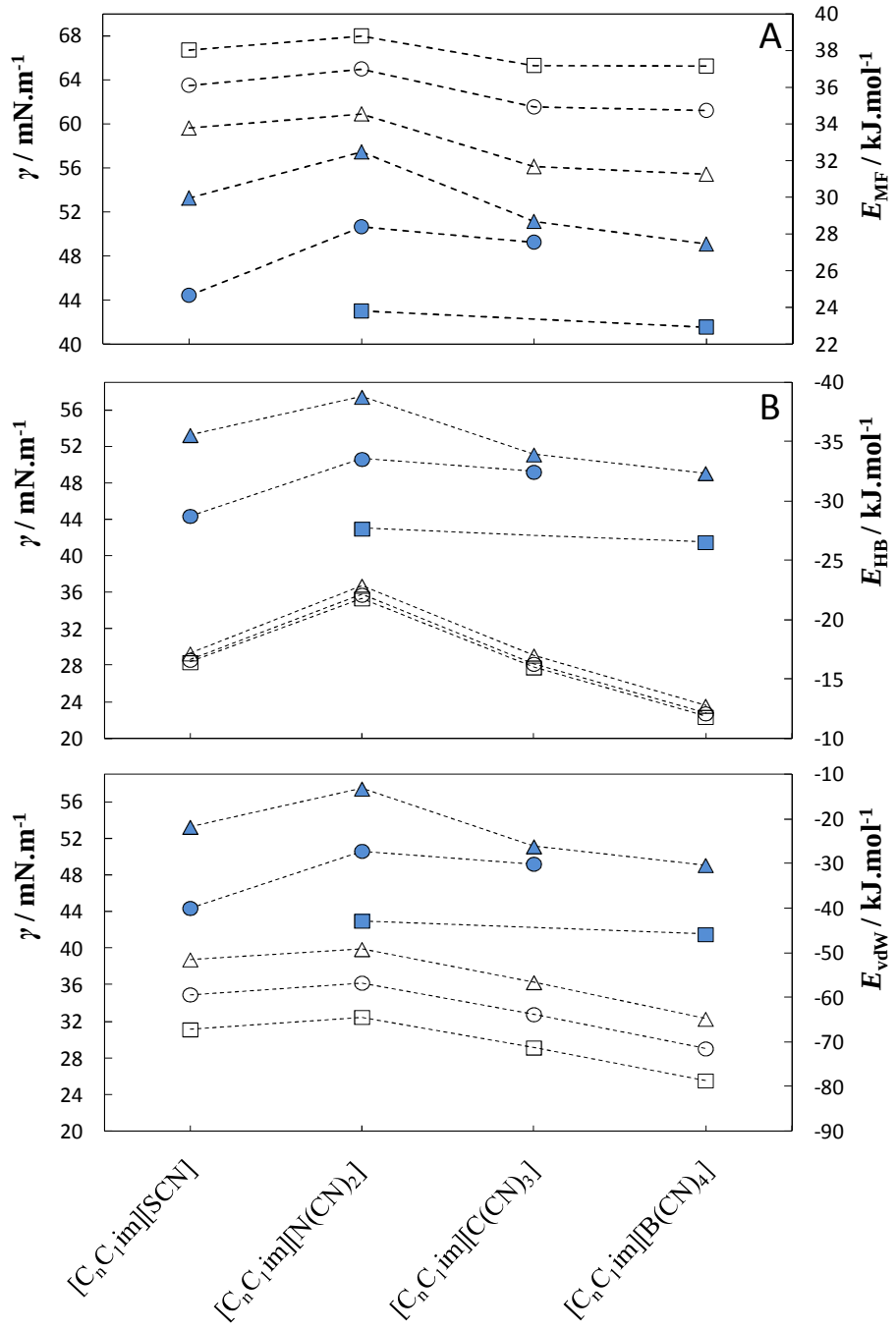

Figure S.I. 2. Surface tension at 298.15 K (blue symbols) and cation-anion interactions (white symbols), namely electrostatic/misfit, E_{MF} (A), hydrogen-bonding, E_{HB} (B), and van der Waals, E_{vdW} (C), energies, of cyano-functionalized anions combined with the cations: △, $[C_2C_1im]^+$; ○, $[C_4C_1im]^+$; □, $[C_6C_1im]^+$. Surface tension data of $[C_2C_1im][SCN]$ and $[C_2C_1im][N(CN)_2]$ were taken from a previous work [2]. The dashed lines have no physical meaning and are guides for the eyes.

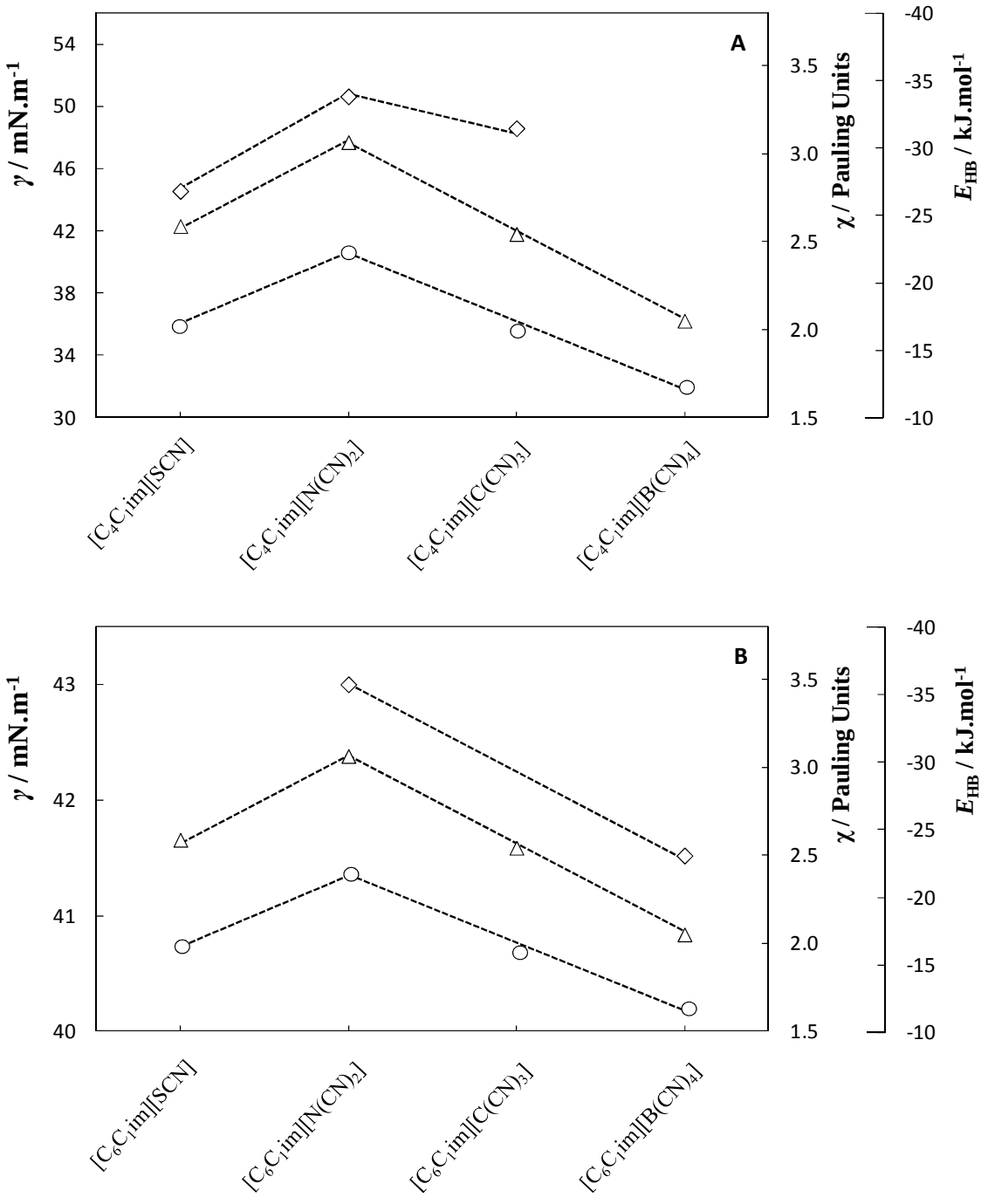

Figure S.I. 3. Surface tension at 298.15 K (◇), electronegativity of the central atom of the cyano-based anion (△) [3], and hydrogen-bonding energy, E_{HB} (○), of 1-butyl-3-methylimidazolium- (A) and 1-hexyl-3-methylimidazolium-based (B) ILs. The dashed lines have no physical meaning and are guides for the eyes.

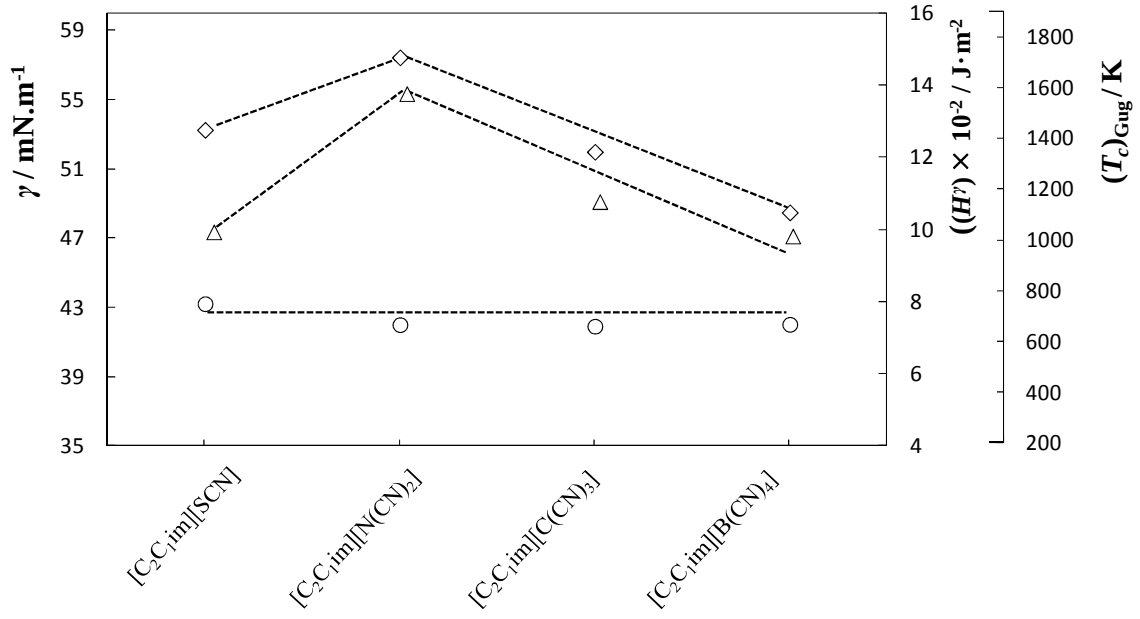

Figure S.I. 4. Surface tension at 298.15 K (◇), surface enthalpy, H', (○) and estimated critical temperature (T_c) using the equations of Guggenheim ($(T_c)_{Gug}$) [4] (△), of 1-ethyl-3-methylimidazolium–based ILs. Surface tension data of $[C_2C_1im][SCN]$ and $[C_2C_1im][N(CN)_2]$ were taken from a previous work [2]. The dashed lines have no physical meaning and are guides for the eyes.

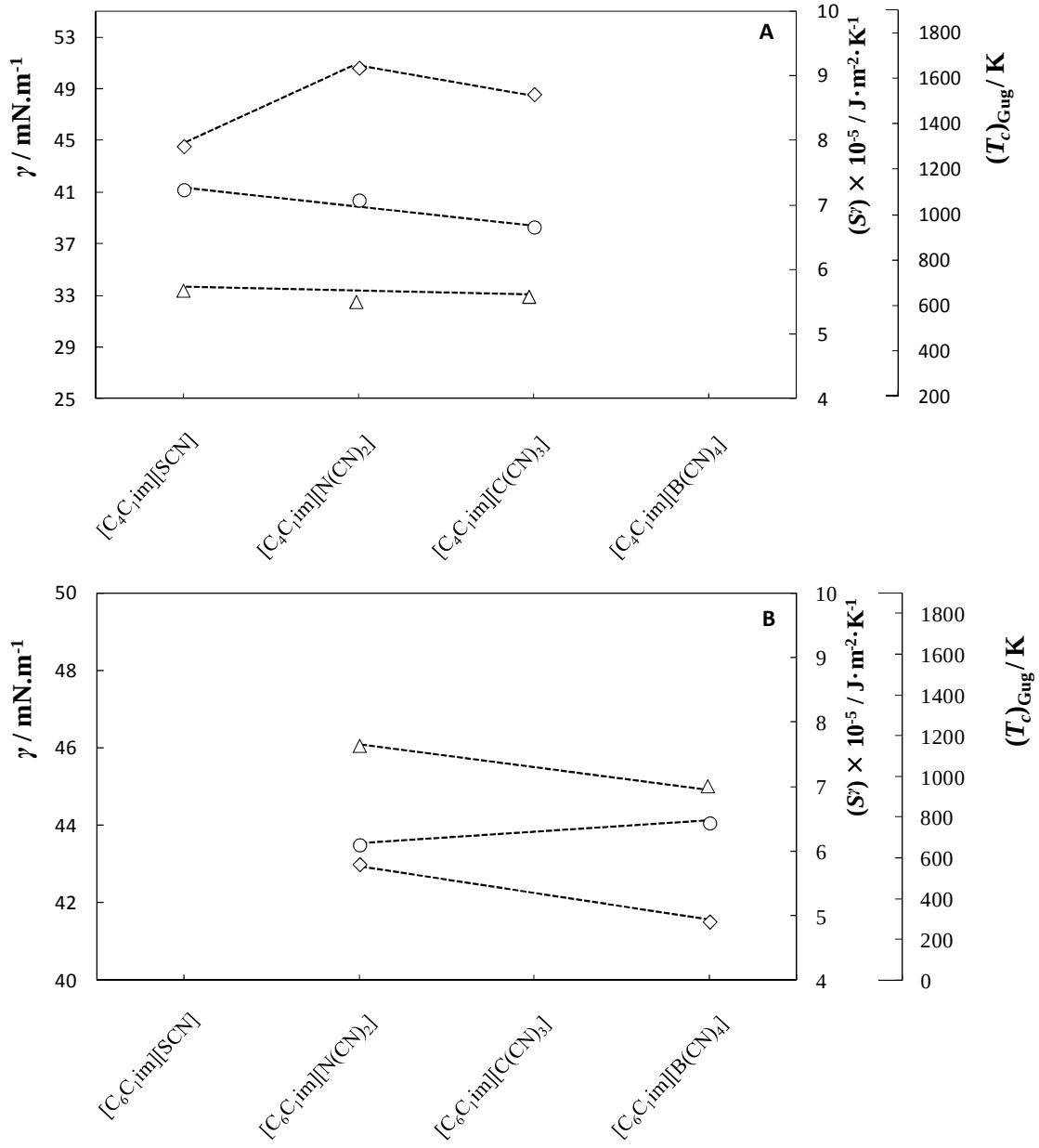

Figure S.I. 5. Surface tension at 298.15 K (◇), surface entropy, S^{γ}, (○) and estimated critical temperatures (T_c) using the equations of Guggenheim ($(T_c)_{Gug}$) [4] (△), of 1-butyl-3-methylimidazolium- (A) and 1-hexyl-3-methylimidazolium-based (B) ILs. The dashed lines have no physical meaning and are guides for the eyes.

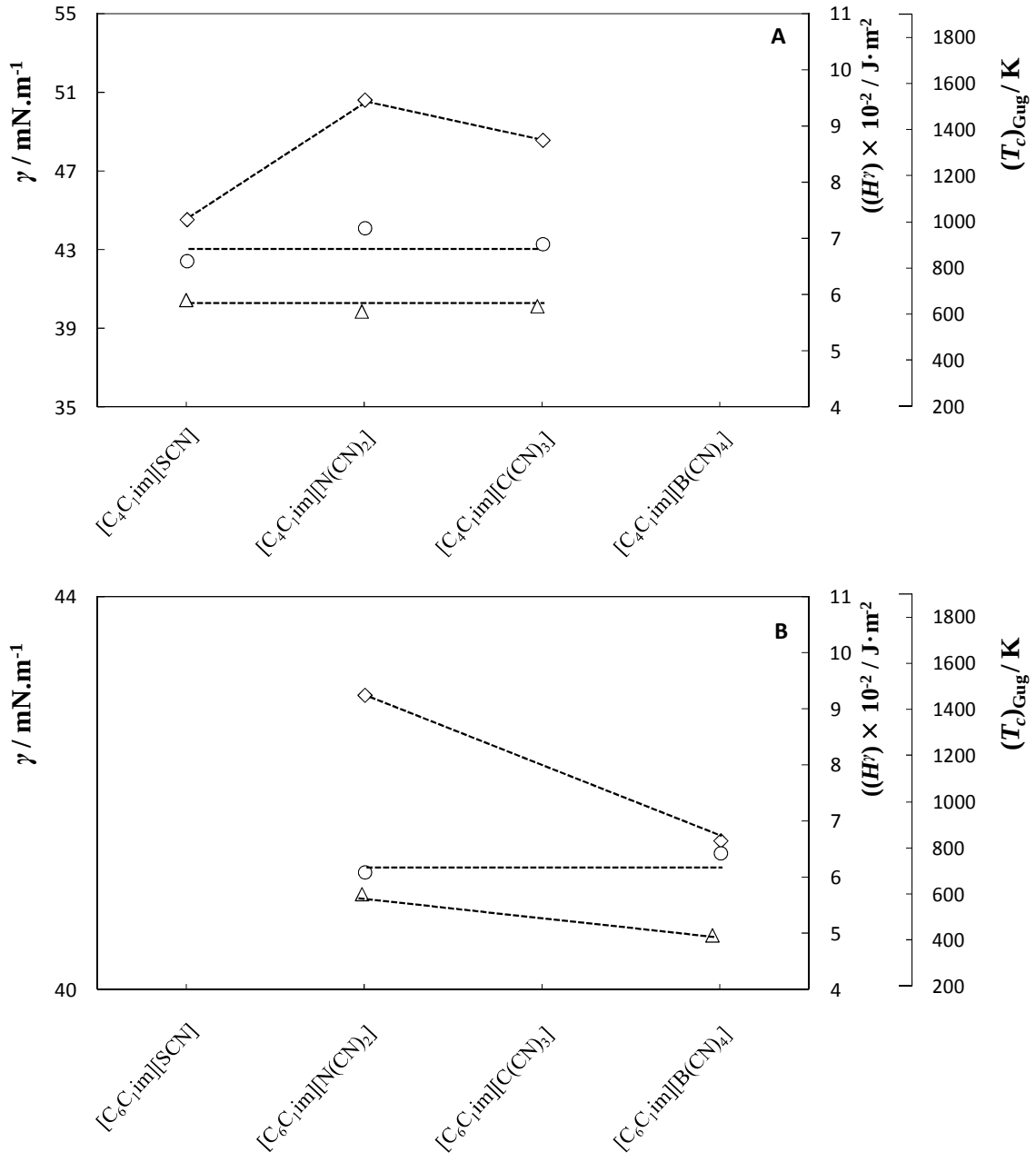

Figure S.I. 6. Surface tension at 298.15 K (◇), surface enthalpy, H^{γ}, (○) and estimated critical temperatures (T_c) using the equation of Guggenheim ($(T_c)_{Gug}$) [4] (△), of 1-butyl-3-methylimidazolium- (A) and 1-hexyl-3-methylimidazolium-based (B) ILs. The dashed lines have no physical meaning and are guides for the eyes.

References

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