Thermophysical Properties of 1-Hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [C$_6$mim][(CF$_3$SO$_2$)$_2$N]—New Data, Reference Data, and Reference Correlations

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Thermophysical Properties of 1-Hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [C$_6$mim][(CF$_3$SO$_2$)$_2$N]—New Data, Reference Data, and Reference Correlations

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ABSTRACT

Published data on the thermophysical properties of ionic liquids are normally in disagreement if results from different laboratories, using different samples and different measurement protocols, are compared. This fact was recognized years ago at the level of the International Union of Pure and Applied Chemistry (IUPAC), which established IUPAC Project 2002-005-1-100 (Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems), with the main objective of recommending a reference ionic liquid, making reference-quality measurements on selected thermophysical properties of both the pure ionic liquid and its mixtures, establishing recommended values for the properties measured, and providing recommendations on measurement methods. The ionic liquid chosen was 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [C$_6$mim][(CF$_3$SO$_2$)$_2$N], because of its stability, low viscosity compared with that of most common ionic liquids, low water solubility, ease of preparation and purification, and commercial availability. Due to its hydrophobicity, it is capable of being obtained very pure, with water amounts as small as 20 ppm. This paper reports new results obtained with the sample of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] synthesized in the IUPAC project, namely on density, speed of sound, surface tension, and refractive index, as well as thermal conductivity of a commercial sample at $P = 0.1$ MPa, as a function of temperature, and proposes reference data and reference data correlations for the density, speed of sound, heat capacity, surface tension, viscosity, electrical conductivity, thermal conductivity, refractive index, ion self-diffusion coefficient, and melting temperature of this ionic liquid at 0.1 MPa, as a function of temperature, using these and other data reported up to July 2020. Rheological measurements demonstrated that this ionic liquid is Newtonian.

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1. Introduction

Published data on the thermophysical properties of ionic liquids are normally in disagreement to an extent that exceeds the mutual uncertainty of the data published and assigned by the authors from different laboratories, using different samples and different measurement protocols. This situation and its possible reasons were analyzed a decade ago by Nieto de Castro,[1] who found that the situation was very different from that found for molecular liquids, mostly due to improper sample characterization and handling, its purity, water and ion content, and improper use of available instrumentation and measurement protocols. It was then recommended that "all those that want to measure thermophysical properties of ionic liquids to measure them well, because the errors in their measurement can produce a tremendous effect on the upcoming design of heat and mass transfer equipment for chemical and energy plants, as demonstrated by the work of França *et al.*[2] This attitude will pave the way for the correct development of alternatives today in all important fields for economic development and sustainability. And ionic liquids can be key chemicals for the future."

This fact was recognized several years before at the level of the International Union of Pure and Applied Chemistry (IUPAC), which established IUPAC Project 2002-005-1-100 (Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems), with the main objective of recommending a reference ionic liquid, making reference-quality measurements on selected thermophysical properties of both the pure ionic liquid and its mixtures, establishing recommended values for the properties measured, and providing recommendations on measurement methods. The ionic liquid chosen was 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, $[C_6mim][(CF_3SO_2)_2N]$ (CAS RN 382150-50-7), because it is stable, has a low viscosity compared with that of most common ionic liquids, has a low water solubility, and is easily prepared and purified. In addition, due to its hydrophobicity, it is capable of being obtained very pure, with water amounts as small as 20 ppm.

The project started with the synthesis of the chosen ionic liquid, its chemical and physical characterization, purity determination

(namely, water content), and the establishment of a round robin test for the different thermophysical properties with samples sent by the National Institute of Standards and Technology (NIST), Boulder Laboratories, to all the project participants. Results were published in two reference papers, one dedicated to the experimental results obtained with the IUPAC samples by Marsh *et al.*[3] and the second dedicated to their critical evaluation and recommended property values by Chirico *et al.*[4] The properties measured of the pure ionic liquid included thermal properties (triple-point temperature, glass-transition temperature, enthalpy of fusion, and heat capacities of condensed states), volumetric properties, speeds of sound, viscosity, electrolytic conductivity, and relative permittivity, and recommended values with uncertainties were provided for the properties studied experimentally.

Two main reasons recommend the revision of the reference correlations recommended then. One is the fact that the work performed in a short period of time with the IUPAC samples was not complete and the other is that many papers were published between 2008 and 2020 with experimental data on the thermophysical properties of $[C_6mim][(CF_3SO_2)_2N]$, namely at atmospheric pressure, done with the IUPAC sample, synthesized in authors' laboratory (HS), and with commercial samples, all chemically and physically characterized and with water content determination.

It is the purpose of this paper to report new results obtained with the sample of $[C_6mim][(CF_3SO_2)_2N]$ synthesized in the IUPAC project, namely on density, speed of sound, surface tension, and refractive index, and thermal conductivity with a commercial sample, at $P = 0.1$ MPa, as a function of temperature, and to use these and other data reported up to mid-July 2020 to establish reference data and reference data correlations for the density, speed of sound, heat capacity at constant pressure, viscosity, surface tension, electrical conductivity, thermal conductivity, refractive index, and self-diffusion coefficient of this ionic liquid, at 0.1 MPa, as a function of temperature. Details of the rheological measurements performed in our laboratory demonstrate that this ionic liquid is a Newtonian fluid.

The metrological definitions of ISO for uncertainty (absolute and relative) and expanded global uncertainty (at a 95% confidence
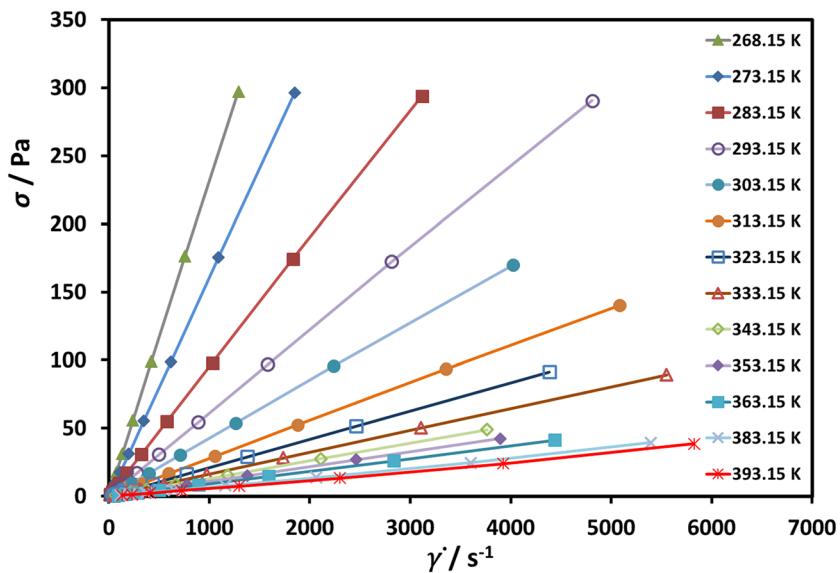
FIG. 1. Shear stress vs shear rate at different temperatures for [C$_6$mim][(CF$_3$SO$_2$)$_2$N].

level, $k = 2$) are used throughout this work. Deviations of experimental data from a correlation are defined as DEV (%) = $(X_{exp} - X_{corr})/X_{corr} \times 100$.

2. New Experimental Data

In this section, the new data obtained in our laboratory are presented. Comparison with other published data, when appropriate, is made in the framework of reference data and development of correlations (Sec. 4).

2.1. Material and sample handling

Due to our participation in the IUPAC Project,[3,4] we received from NIST a sample of the ionic liquid, part of a batch synthesized by Dr. Mark Muldoon in Professor Joan Brennecke's laboratories at the University of

Notre Dame and described by Widegren and Magee,[5] with a purity >99.5% (by NMR), a bromide content lower than 10 ppm, and a water content below 20 ppm. It was then used for measurements of viscosity and electrical conductivity described by Santos *et al.*[6] Special care was taken in the manipulation of the liquid and in the uncertainty budget of the measurements. As [C$_6$mim][(CF$_3$SO$_2$)$_2$N] is hygroscopic, the water content of samples collected from the measuring cells (viscometer and conductivity cell) before and after the measurements was determined by coulometric Karl Fisher titration. The rest of the sample was used to measure the density, speed of sound, surface tension, and refractive index, controlling the amount of water present when each property was measured. The amount was not enough for the measurement of thermal

TABLE 1. Density and speed of sound for [C$_6$mim][(CF$_3$SO$_2$)$_2$N] at P = 0.1 MPa[a]

T (K)	ρ (kg m^{-3})	c (m s^{-1})
283.15	1385.89	1262.22
288.15	1381.26	1250.08
293.15	1376.54	1238.27
298.15	1372.01	1226.52
303.15	1367.39	1215.06
308.15	1362.63	1203.76
313.15	1358.07	1192.64
318.15	1353.49	1181.67
323.15	1348.94	1170.90

[a]Standard uncertainties, u, are $u(T)$ = 0.01 K, $u(P)$ = 1 kPa, $u(\rho)$ = 0.07 kg m^{-3}, and $u(c)$ = 0.3 m s^{-1}. Expanded uncertainties are $U(\rho)$ = 0.14 kg m^{-3} and $U(c)$ = 0.6 m s^{-1} at a 95% confidence level (k = 2).

TABLE 2. Surface tension of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] at P = 0.1 MPa[a]

T (K)	γ (mN m^{-1})
289.00	32.16
292.20	31.93
292.27	31.90
293.67	31.86
298.32	31.64
303.25	31.44
306.10	31.32
306.80	31.33
311.79	31.05
311.80	31.06
320.53	30.70
328.50	30.28
336.20	29.99

[a]Standard uncertainties, u, are $u(T)$ = 0.1 K, $u(P)$ = 1 kPa, and $u(\gamma)$ = 0.04 mN m^{-1}. Expanded uncertainty is $U(\gamma)$ = 0.08 mN m^{-1} at a 95% confidence level (k = 2).

conductivity, and a commercial sample (IoLiTec, Germany, purity >99.90%) was bought, with a water content of 33 ppm and halide content less than 50 ppm. For each property measurement, the required amount of ionic liquid was carefully drawn from the transport/storage Schlenk tube using glass syringes (plastic in the case of the refractive index), stainless-steel needles, and Teflon tubing, always under a protective blanket of dry nitrogen, and introduced into the measuring cells.

2.2. Methods of property measurement

2.2.1. Density and speed of sound

Density, ρ, and speed of sound, c, were measured with an Anton Paar DSA-5000 in the temperature range between 283.15 K and 323.15 K. The densimeter was previously calibrated with high quality Millipore® water and tetrachloroethylene (H&D Fitzgerald, density certified, https://density.co.uk/products/liquid-standards/), with the calibration methodology.[7] Due to the high viscosity of the ionic liquid, the density values were corrected for extra damping, as recommended by the densimeter manufacturers. Calibration of the speed-of-sound cell was made at 293.15 K with Milli-Q water, according to the manufacturer recommendation. Uncertainty has been estimated by a complete uncertainty analysis, and details for ionic liquids are described in recent papers.[8,9] The temperature inside the densimeter cell was controlled with a PT100 to within 0.001 K and measured with an uncertainty of 0.02 K (k = 2). The water content of the samples was 0.003%, so its effect was negligible for both properties measured.[5,10]

The standard uncertainties of density and speed of sound measurements were found to be $u(\rho)$ = 0.07 kg m^{-3} and $u(c)$ = 0.3 m s^{-1}, respectively.[11] Expanded relative uncertainties at a 95% confidence level (k = 2) are, respectively, $U(\rho)$ = 0.14 kg m^{-3} and $U(c)$ = 0.6 m s^{-1}.

2.2.2. Surface tension

The surface tension, γ, of $[C_6mim][(CF_3SO_2)_2N]$ was measured with a K100MK2 tensiometer from Kruss GmbH, based on force measurements, with a 10 μg resolution precision balance using a platinum Wilhelmy plate. The measurements were made at atmospheric pressure for temperatures between 288 K and 343 K. Samples were transferred from the supplied glass storage (Schlenk tube) to lidded custom-made micro PTFE (polytetrafluoroethylene) sample vessels (~2 ml) under dry nitrogen atmosphere. PTFE was chosen to exclude the possibility of stainless-steel attack by ionic liquids with fluoride-containing anions.[12,13] The initial water content (weight fraction, in %) was checked by coulometric titration by the Karl Fisher method with a Metrohm 831 KF coulometer and found to have a value of 0.08%.

The sample vessels were thermostated inside an aluminum block placed in the tensiometer's double-jacketed stainless-steel thermostatic sleeve by means of a circulating water bath (HAAKE DC30/K10) controlled within 0.1 K. The sample temperature was monitored with an independent external Pt 100 thermometer placed in a hole drilled in the aluminum block close to the sample vessel and corrected for the temperature drop across the thermostatic media, resorting to a correlation between the temperatures registered by the Pt 100 sensor and a calibrated thermistor placed inside the sample vessel in the same position where the surface tension was measured. The tensiometer was calibrated with standard masses provided by the manufacturer, and before each measurement, at all temperatures, the calibration was further checked with grade 1 water from a Milli-Q apparatus.

TABLE 3. Refractive index of $[C_6mim][(CF_3SO_2)_2N]$ at P = 0.1 MPa[a]

T (K)	n_D
283.15	1.434 61
288.15	1.433 11
293.15	1.431 60
298.15	1.430 12
303.15	1.428 62
308.15	1.427 15
313.15	1.425 66
318.15	1.424 14
323.15	1.422 62
328.15	1.421 16
333.15	1.419 69
338.15	1.418 27
343.15	1.416 84

[a]Expanded relative uncertainty is $U(n)$ = 0.000 16 at a 95% confidence level (k = 2).

The curved roughened Wilhelmy platinum plate was rinsed with ethanol and water and finally flame cleaned in a Bunsen burner to eliminate any contamination before every measurement. Surface tension measurements were performed under dry nitrogen atmosphere on samples equilibrated in the lidded sample vessels for at least 2 h, the liquid surface being flushed with dry nitrogen before each measurement.

For each temperature, at least four independent sets of 10 immersion/detachment cycles were performed, values of which verified the temperature stabilization and allowed the determination of an average surface tension over at least 40 surface tension values. The estimated average uncertainty of the experimental measurements is $U_r(\gamma)$ = 1% (k = 2.02 for n = 40 at 95%). In order to evaluate the effect of the water content on the surface tension, measurements obtained on a heating cycle were checked on a cooling cycle and deviations smaller than 0.21% were obtained, which were slightly larger than those obtained in an independent evaluation of another fresh sample (0.16%) but well within measurement uncertainty.

2.2.3. Refractive index

The refractive index, n, of $[C_6mim][(CF_3SO_2)_2N]$ was measured with a digital refractometer (Anton Paar, Abbemat 500) calibrated at

TABLE 4. Thermal conductivity of $[C_6mim][(CF_3SO_2)_2N]$ at P = 0.1 MPa[a]

T (K)	λ (W m^{-1} K^{-1})
285.54	0.1242
295.26	0.1250
304.95	0.1249
305.14	0.1249
315.46	0.1264
325.63	0.1268
335.67	0.1276
345.89	0.1283
355.87	0.1280

[a]Expanded relative uncertainty is $U(\lambda)$ = 2% at a 95% confidence level (k = 2).

TABLE 5. Available data for the density of $[C_6mim][(CF_3SO_2)_2N]$, classified as primary and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class[c]	Observations
				Primary data					
Kumelan et al. (2006)[27]	VT	293.15–373.15	0.1	9	0.06	IUPAC	0.002	PDSA	Description in Sec. 2.1
Kandil et al. (2007)[28]	VT	298.15–423.15	0.1–40	28	0.30	IUPAC	0.041	PDSA	Description in Sec. 2.1
Widegren and Magee (2007a)[5]	VT(S)	278.15–373.15	0.1	19	0.01	IUPAC	0.001	PDSA	Description in Sec. 2.1
Widegren and Magee (2007b)[5]	VT	283.15–343.15	0.1	16	0.01	IUPAC	0.001	PDSA	Description in Sec. 2.1
Esperança et al. (2008)[29]	VT	293.15–338.15	0.1–65	163	0.05	IUPAC	0.002	PDSA	Description in Sec. 2.1
Lago et al. (2011)[30]	VT	298.15	0.1	1	0.02	HS	0.087	PDSA	Synthesized in authors' laboratory, dried by vacuum heating, and analysis by proton NMR spectroscopy
Shirota et al. (2011)[31]	VT	297	0.1	1	0.59	HS	0.0256	PDSA	Synthesized in authors' laboratory, dried under vacuum for 3 days at 35 °C to remove impurities, and analysis by proton NMR spectroscopy
Gomes et al. (2012)[32]	VT	288.15–328.15	0.1	5	0.10	HS	0.006	PDSA	Synthesized in authors' laboratory, dried by vacuum heating, and analysis by proton NMR spectroscopy
Gonzalez et al. (2012)[33]	VT	288.15–313.15	0.1	5	0.08	IoLiTec	0.007	D	Commercial source. Prior to its use, the compound was subjected to vacuum (0.2 Pa) at 60 °C until the density value remained constant
Oliveira et al. (2012)[34]	VT	298.15	0.1	1	0.08	IoLiTec	0.0307	PDSA	Synthesized in authors' laboratory, dried by vacuum heating, and analysis by proton NMR spectroscopy
Safarov et al. (2013)[35]	VT	273.13–413.17	0.1–50	266	0.2	Merck	0.03	D	Dried under vacuum for 48 h at 70 °C to remove impurities

TABLE 5. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class[c]	Observations
Diogo et al. (2013)[36]	VT	288.15–328.15	0.1	17	0.08	IoLiTec	0.005	D	Dried by vacuum heating (70 °C)
Iguchi et al. (2014)[37]	B-HB	312.6–452.3	0.1–90	168	0.13	Merck	0.002	MPNP	Used as received from the manufacturer
Harris and Kanakubo (2015)[38]	VT(S)	238.15–363.15	0.1	20	0.09	HS	0.0002	PDSA	Dried under vacuum at about 70 °C for 30 h to remove any excess water and purity determination by NMR analysis.
Kanakubo and Harris (2015)[39]	VT	273.15–363.15	0.1	39	0.06	HS	0.003	D	Dried by vacuum heating (60 °C)
Nazet et al. (2015)[40]	VT	278.15–363.15	0.1	18	0.21	IoLiTec	0.0014	MPNP	Used as received from the manufacturer
Fillion et al. (2016)[41]	VT	283.15–353.15	0.1	16	0.74	HS	0.007	PDSA	Synthesized in authors' laboratory, dried by vacuum heating, and analysis by proton NMR spectroscopy
Skowronek et al. (2016)[42]	ISOC-PV	288.15–363.15	0.1	9	0.02	HS	0.01	D	Dried with vacuum for 2 h and anhydrous phosphorous pentoxide
Xue et al. (2016)[43]	VT	283.15–313.15	0.1	7	0.07	HS	0.008	PDSA	Synthesized in authors' laboratory, dried by vacuum heating, and analysis by NMR spectroscopy.
Zorebski et al. (2016)[44]	VT	293.15–363.15	0.1	15	0.01	HS	0.0092	D	Synthesized by others; purification by spectroscopy, Karl Fischer titration, and fraction melting in an adiabatic calorimeter; and stored under argon.
Fillion and Brennecke (2017)[45]	VT	283.15–353.15	0.1	16	0.30	HS	0.002	PDSA	Synthesized in authors' laboratory, dried by vacuum heating, and analysis by proton NMR spectroscopy

TABLE 5. (*Continued.*)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class[c]	Observations
Andresová et al. (2017)[46]	VT	293.15–343.15	0.1	11	0.04	IoLiTec	0.036	PDSA	Decolorized by stirring with dichloromethane and active carbon powder for 24 h and by passing through a chromatography column, dried under vacuum for at least 16 h at 60 °C, and analysis by ion chromatography
Vranes et al. (2019)[47]	VT	283.15–323.15	0.1	9	0.36	Sigma-Aldrich	0.015	MPNP	Used as received from the manufacturer
Song et al. (2020)[48]	VT	283–333	0.1	7	0.20	IoLiTec	0.05	D	Commercial source, analysis by NMR (proton), and dried at 333 K under high vacuum for at least 48 h to remove any volatiles including water
Present work	VT	283.15–323.15	0.1	9	0.01	IUPAC	0.003	PDSA	Description in Sec. 2.1
					Secondary data				
Dzyuba and Bartsch (2002)[49]	VT	298.15	0.1	1	0.59	HS	NA	NA	Synthesized in authors' laboratory and no details of purity
Fitchett et al. (2004)[50]	PYC	295.1	0.1	1	0.11	HS	0.073	D	Synthesized in authors' laboratory and dried under vacuum for 4 h at 70 °C–80 °C to remove residual water
Aki et al. (2004)[51]	PYC	298.20–333.20	0.1	4	0.03	HS	0.016	PDSA	Synthesized in authors' laboratory, dried under vacuum for 48 h at 75 °C to remove residual water, and analysis by proton NMR spectroscopy
Azevedo et al. (2005)[52]	VT	298.15–333.15	0.1–59.5	156	0.07	HS	0.0075	D	Purified by vacuum evaporation and purity unknown
Kato and Gmehling (2005)[53]	VT	293.15–358.15	0.1	14	0.37	Merck	NA	D	Dried by vacuum heating

TABLE 5. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class[c]	Observations
Tokuda et al. (2005)[54]	VT	288.15–313.15	0.1	6	1	HS	0.001	PDSA	Synthesized in authors' laboratory, dried under vacuum for 48 h to remove residual water, and purity determination by NMR and MS analysis
Lachwa et al. (2006)[55]	VT	293–303	0.1	21	0.31	IUPAC	0.002	PDSA	Description in Sec. 2.1
Tokuda et al. (2006)[56]	VT	288.15–313.15	0.1	6	0.15	HS	0.004	PDSA	Synthesized in authors' laboratory, analysis by mass spectrometry, and dried by vacuum heating
Jacquemin et al. (2008)[57]	VT	293.15–363.15	0.1	8	0.36	HS	0.005	PDSA	Synthesized in authors' laboratory, ion chromatography, and dried by vacuum heating
McHale et al. (2008)[58]	VT	298.15	0.1	1	0.37	HS	0.089	PDSA	Synthesized in authors' laboratory, ion chromatography, and dried by vacuum heating
Muhammad et al. (2008)[59]	VT	298.15–358.15	0.1	7	0.19	Merck	0.0268	D	Dried by vacuum heating
Tariq et al. (2009)[60]	VT	293.15–333.15	0.1	4	0.16	HS	0.015	D	Synthesized in authors' laboratory and dried under vacuum for 48 h at 60 °C–80 °C to remove impurities
Ahosseini et al. (2010)[61]	VT	283.15–348.15	0.1	4	0.19	HS	0.035	PDSA	Synthesized in authors' laboratory, dried under vacuum for 48 h at 50 °C to remove impurities, and analysis by proton NMR spectroscopy
Fröba et al. (2010)[62]	VT	273.15–363.15	0.1	18	0.21	HS	0.0086	PDSA	Synthesized in authors' laboratory, dried under vacuum for 4 h at 60 °C to remove impurities, and analysis by proton NMR spectroscopy

TABLE 5. (*Continued.*)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class[c]	Observations
Kolbeck *et al.* (2010)[63]	VT	278.15–308.15	0.1	7	0.01	HS	0.0008	PDSA	Synthesized in authors' laboratory, dried after preparation in vacuum at 40 °C for 24 h, and analysis by NMR spectroscopy
Tariq *et al.* (2010)[64]	VT	293.15–473.15	0.1	19	0.41	HS	0.007	PDSA	Synthesized in authors' laboratory, dried under vacuum for 6 h at 60 °C to remove impurities, and analysis by proton NMR spectroscopy
Yunus *et al.* (2010)[65]	VT	298.15	0.1	1	0.13	HS	NA	PDSA	Synthesized in authors' laboratory, dried under vacuum for 3 days at 35 °C to remove impurities, and analysis by proton NMR spectroscopy
Akbar and Murugesan (2012)[66]	VT	303.15–323.15	0.1	5	0.11	Merck	0.023	PDSA	Analysis by HPLC and dried by vacuum heating
Seoane *et al.* (2012)[67]	VT	293.15–343.15	0.1	11	0.56	IoLiTec	0.007	D	Dried under vacuum for 70 h at 40 °C to remove impurities
Cade *et al.* (2014)[68]	VT	288.15–318.15	0.1	4	0.6	IoLiTec	0.015	PDSA	Dried under vacuum for 48 h at 40 °C to remove impurities and analysis by proton NMR spectroscopy
Gonzalez-Miquel *et al.* (2014)[69]	VT	298.15–323.15	0.1	3	0.81	IoLiTec	NA	MPNP	Used as received from the manufacturer
Matsuda *et al.* (2014)[70]	BV	298.15	0.1	1	0.96	Merck	0.01	MPNP	Used as received from the manufacturer
Souckova *et al.* (2014)[71]	VT	263.98–364.78	0.1	21	0.54	Solvent Innovation	0.001	PDSA	Analysis by NMR and dried by vacuum heating
Tenney *et al.* (2014)[72]	BHB	288.15–363.15	0.1	9	0.31	HS	0.0018	MPNP	Used as received from the manufacturer
Calado *et al.* (2015)[73]	VT	288.15–328.15	0.1	5	0.11	IoLiTec	0.0026	D	Dried by vacuum heating (80 °C)

TABLE 5. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class[c]	Observations
Gonzalez et al. (2015)[74]	VT	283.15	0.1	1	0.57	IoLiTec	0.06	D	Synthesized in authors' laboratory and dried under vacuum for 48 h to remove impurities
Montalban et al. (2015)[75]	VT	293.15–343.15	0.1	6	0.09	IoLiTec	0.0015	PDSA	Synthesized in authors' laboratory, dried under vacuum for 30 h at 70 °C to remove impurities, and analysis by proton NMR spectroscopy
Salinas et al. (2015)[76]	VT	278.15–338.15	0.1	4	0.19	IoLiTec	0.05	PDSA	Dried under vacuum for 1 week at 40 °C to remove impurities and analysis by proton NMR spectroscopy
Montalban et al. (2016)[77]	VT	303.15	0.1	1	1.1	IoLiTec	0.0089	PDSA	Dried under vacuum for 1 week at 40 °C to remove impurities and analysis by proton NMR spectroscopy
Papovic et al. (2016)[78]	VT	273.15–323.15	0.1	11	0.81	IoLiTec	0.0154	D	Dried with anhydrous phosphorous pentoxide
Polikhronidi et al. (2016)[79]	VT	325.26; 350.36	0.1	2	0.24	IoLiTec	0.007	D	Dried with anhydrous phosphorous pentoxide

[a]B-HB, Buoyancy-Hydrostatic Balance; ISOC-PV, Isochoric PV measurements; VT, Vibrating Tube; VT(S), Vibrating Tube, Staudinger model; and HS, synthesized in authors' laboratory.
[b]IUPAC sample, as described in text, and HS, synthesized in authors' laboratory.
[c]NA, Not Available.

293.15 K by the manufacturer with standards from PTB (Physikalisch-Technische Bundesanstalt, Germany) for the sodium D line (wavelength: 589.26 nm). The uncertainty in the temperature measurement is 0.03 K. Calibration was checked with water and n-hexadecane, as explained in Sec. 3.5 of Ref. 9. As reported there, the use of a refractometer single calibration point at 293.15 K, made by the manufacturer, is not enough for higher temperature measurements, requiring a correction to the measured values, which increases with temperature, and this was obtained from the water data reported by Marsh.[14] At the highest temperature (353 K), the correction is −0.0004, which is greater than the uncertainty of data. Since our last publication,[9] we have introduced a flow cell in the refractometer (Abbemat No. 101 380) to avoid contact of the liquid sample with the atmosphere, close to the measuring section, but just for filling. During the measurements, the liquid is stagnant. This accessory limits evaporation and gas dissolution, stabilizing the measurements. Calibration was checked by measuring the refractive index of water between 283.15 K and 343.15 K. Two sets of 13 points were measured in different days, and deviations between them and with the data used in the development of calibration correction[9] were never bigger than 0.000 05 RI units, the flow cell not altering significantly the data obtained. For our IUPAC sample, we studied three samples, one by increasing the temperature, the second by lowering the temperature to 283.15 K, and finally, in sample 3, increasing it again up to 343.15 K. For each temperature, a set of 7 measurements were taken. The agreement between the UP sets is better than 0.000 035 RI units, becoming slightly higher with the DOWN set (0.0004 RI units above 70 °C). Therefore, the data reported are based on sample 1 and sample 3 (average values at each temperature).
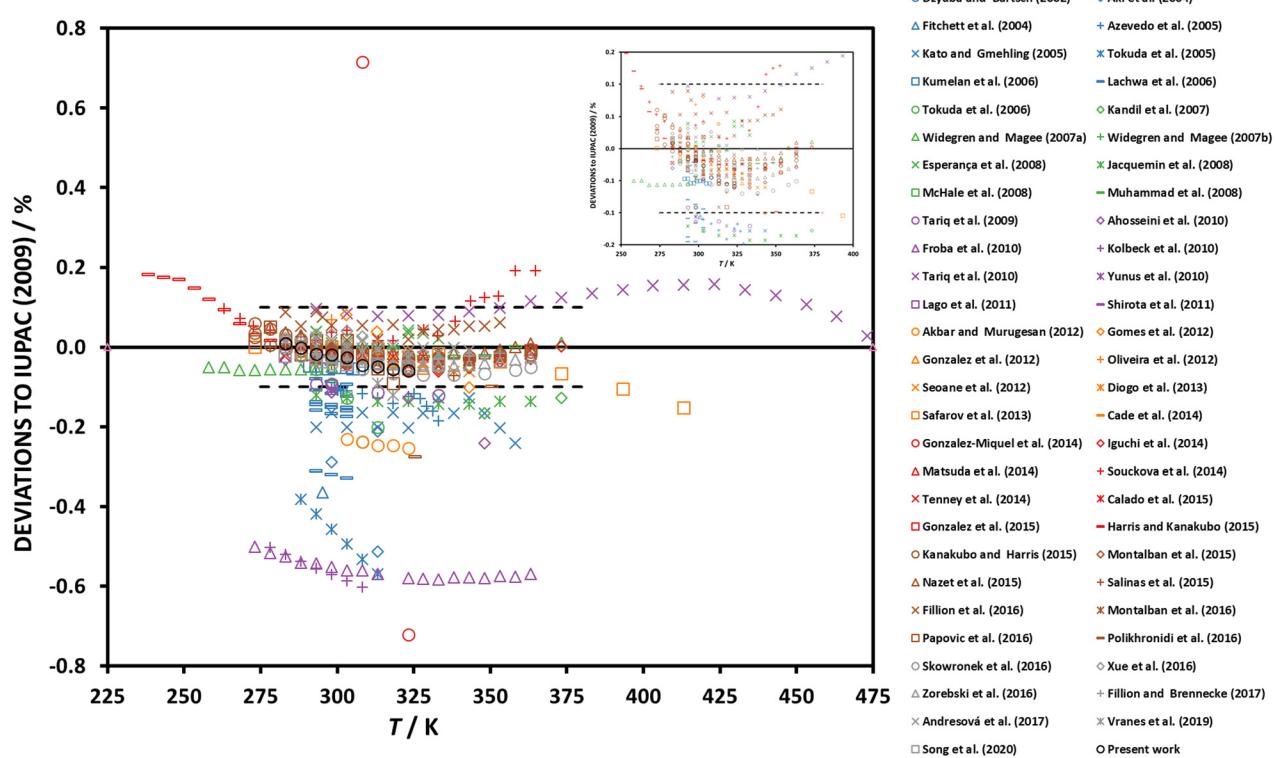
FIG. 2. Deviations from all the datasets for the density of [C$_6$mim][(CF$_3$SO$_2$)$_2$N], smaller than ±0.6%, as a function of temperature. The dashed lines represent the uncertainty boundaries of the IUPAC correlation at a 95% confidence level, 0.1%. The inset shows deviations up to 0.2% in the temperature range 250 K–400 K.
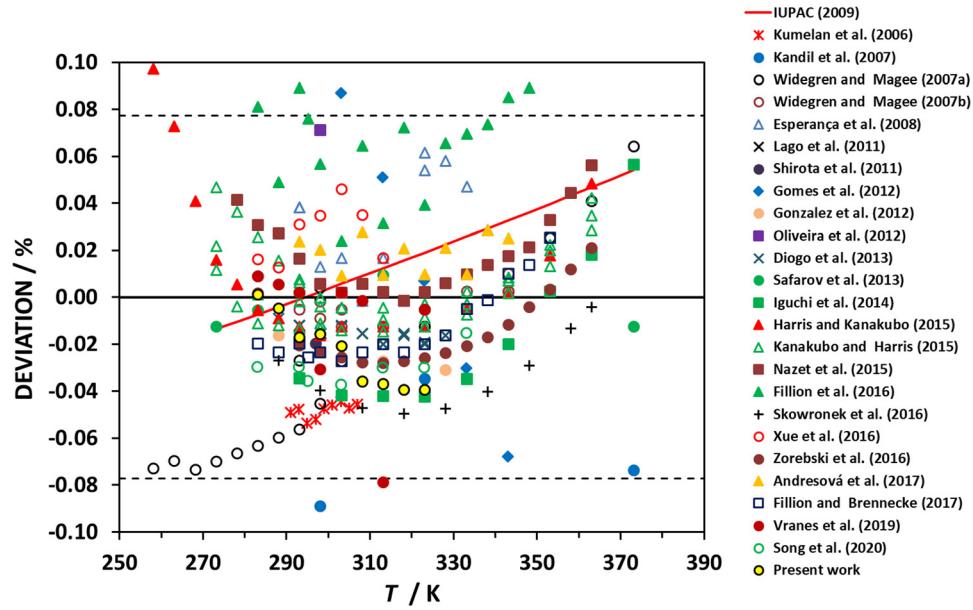
FIG. 3. Deviations between the primary data for the density of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature. Also shown are deviations from the previous correlation proposed by Chirico et al.[4] within the IUPAC project. The dashed line represents the uncertainty of the correlation of ±0.08%.
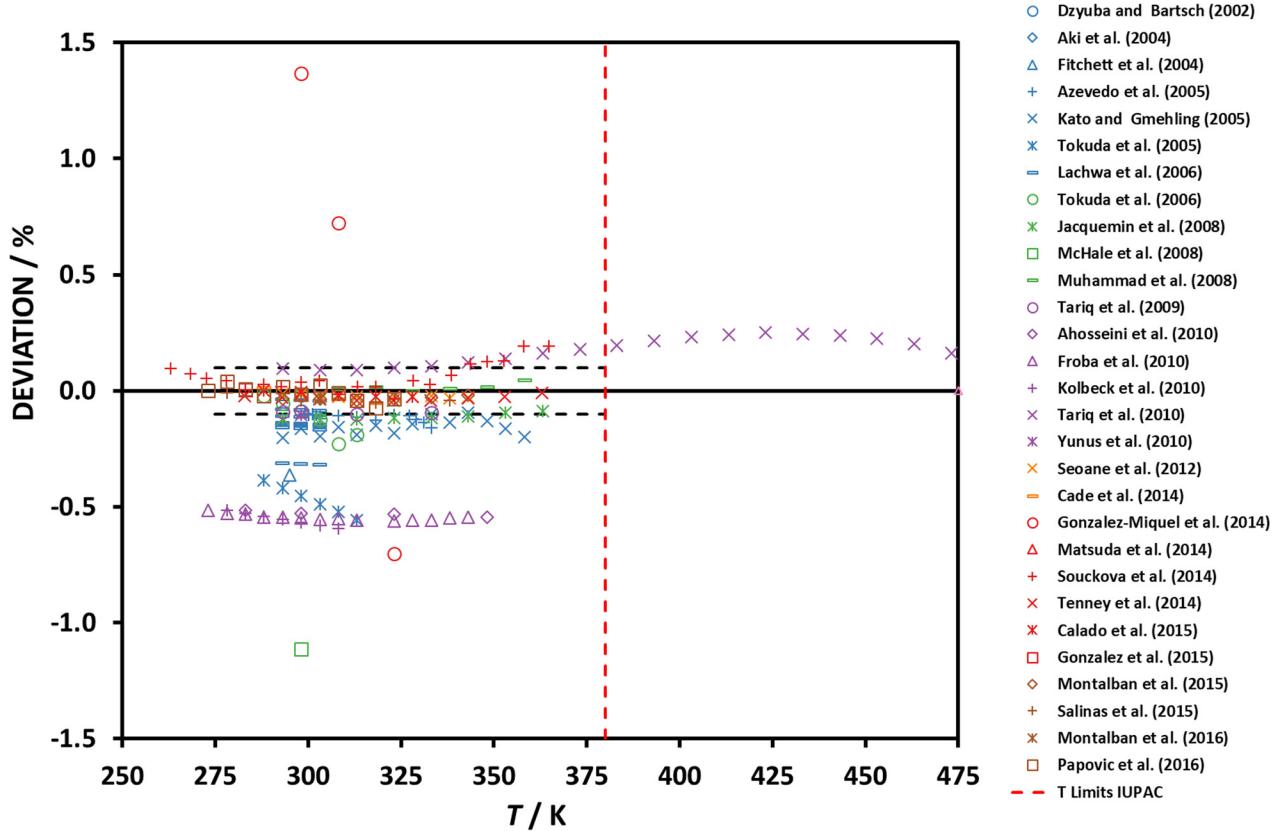
FIG. 4. Deviations between the secondary data for the density of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. The red dashed line marks the correlation high-temperature limit (380 K).
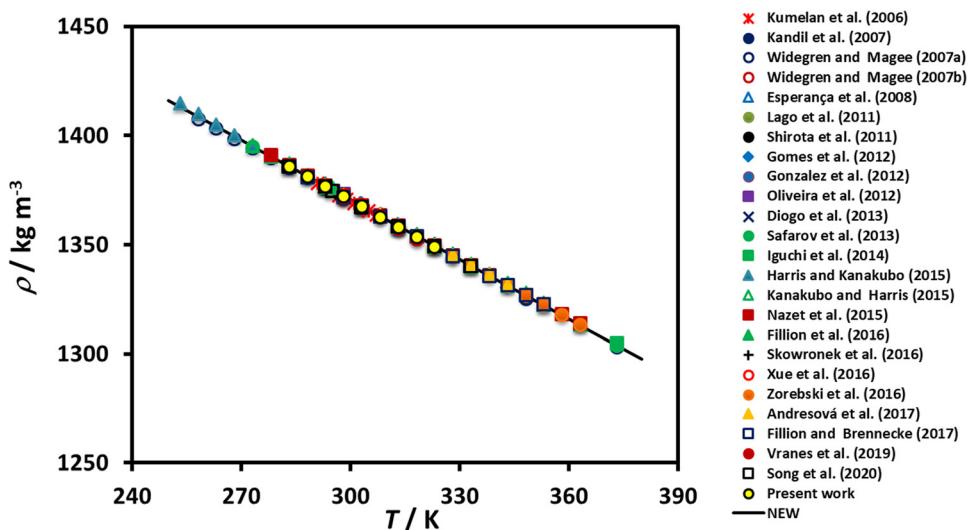
FIG. 5. Recommended variation of the density of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. Primary data and new correlation are shown.

TABLE 6. Available data for the speed of sound of [C$_6$mim][(CF$_3$SO$_2$)$_2$N], classified as primary and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)	Purity class	Observations
				Primary					
Widegren and Magee (2007)[5]	DSA 5000	283.15–343.15	0.1	16	0.083	IUPAC	0.001	PDSA	Description in Sec. 2.1
González et al. (2012)[33]	SAT-FPI	288.15–328.15	0.1	5	0.096	IoLiTec	0.007	D	Commercial source. Prior to its use, the compound was subjected to vacuum (0.2 Pa) at 60 °C until the density value remained constant
Seoane et al. (2012)[67]	SAT-FPI	293.15–343.15	0.1	11	0.17	IoLiTec	0.007	D	Commercial source; purification stated by the supplier, initial purity of 99 mass %, final purity of 0.007 water mass %, and 0.01 halide impurity mass %; and dried under vacuum for 48 h at 70 °C to remove impurities
Salinas et al. (2015)[76]	SAT-FPI	278.15–338.15	0.1	4	0.05	IoLiTec	0.05	D	Commercial source; initial purification stated by the supplier, initial purity of 99.9 mass %; and final purification by Karl Fischer titration, final purity of 0.05 water mass % (molecular sieve treatment)
Skowronek et al. (2016)[42]	PE	323.37	0.1–100	1	0.08	HS	0.0101	PDSA	Synthesized by the authors; initial purification stated by the supplier, initial purity of 99.95 mass %; and final purification by Karl Fischer titration, final purity of 0.0101 water mass %

TABLE 6. (*Continued.*)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)	Purity class	Observations
Zorebski *et al.* (2016)[44]	PE	293.09–318.36	0.1	6	0.097	HS	0.0092	PDSA	Synthesized by others; purification by spectroscopy, Karl Fischer titration, and fraction melting in an adiabatic calorimeter; and purity of 99.5% (basis not specified)
Andresova *et al.* (2017)[46]	DSA5000	288.15–343.15	0.1	12	0.080	IUPAC	0.017	PDSA	Commercial source, NMR analysis, and dried before every experiment for at least 16 h under vacuum (8–10 mbar) at ~60 °C
Secondary									
Frez *et al.* (2006)[80]	TGT	293.15	0.1	1	0.89	HS	NA	PDSA	Synthesized by the authors, purity analysis (NMR) by chemical reagent treatment, and dried by vacuum heating (60 °C)

[a]TGT, Transient Grating Technique; SAT-FPI, Sing-Around Technique in a Fixed-Path Interferometer; PE, Pulse-Echo method; and DSA 5000/M, Density and Speed of Sound Analyzer.
[b]Note that the IUPAC sample is as described in text and HS means synthesized in authors' laboratory.

The water weight fraction of sample 1 varied between 0.051% and 0.057%, while that of sample 3 varied between 0.036% in the beginning of experiments and 0.091% in the end. An average value of the water content of the reported data was assumed to be 0.06% (see Sec. 4.8 and the supplementary material).

Data were corrected by using the calibration function developed in Ref. 9. The estimated expanded uncertainty (*k* = 2) is *U*(*n*) = 0.000 162.

2.2.4. Thermal conductivity

The thermal conductivity, λ, of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] was measured using commercial equipment from Hukseflux Thermal Sensors TPSYS02 and a Non-Steady-State Probe (NSSP) TP08 with an accuracy of ± 0.02 W m^{-1} K^{-1} and a temperature accuracy of ± 0.02 K, as described in Ref. 8. The correct operation of this instrument was assessed by measurements with water, an IUPAC standard reference liquid. The data obtained for a sample of Milli-Q water between 283.6 K and 344.8 K deviated by less than 0.8% from the IUPAC SRD correlation,[15] a very

good sign of excellent operation. The expanded global relative uncertainty of the data was found to be $U_r(\lambda) = 2\%$ (*k* = 2). The tests for [C$_6$mim][(CF$_3$SO$_2$)$_2$N] were performed between 285.54 K and 355.87 K at atmospheric pressure. For temperatures above 323.15 K, the probe had to be removed and cleaned and the sample had to be equilibrated for longer times to reduce convection currents. In order to detect a possible onset of convection, in a recent paper,[16] detailed measurements with water around room temperature were performed, with three different power inputs in the THW probe (LOW, MEDIUM, and HIGH), giving temperature rises between 0.25 K and 0.70 K. No curvature in the straight-line fits, ΔT_{rise} vs ln *t*, was found, and no power dependence existed. These results also support that there is no convection in these measurements and that the working model for the transient hot-wire is valid, capable of producing results at room temperature within 0.55% standard deviation, confirming our previous statements[15] of $U_r(\lambda) = 2\%$ at a 95% confidence level (*k* = 2). As the viscosity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] at room temperature is 60 times greater than that of water, it is expected that no convection exists on the measurements reported here.
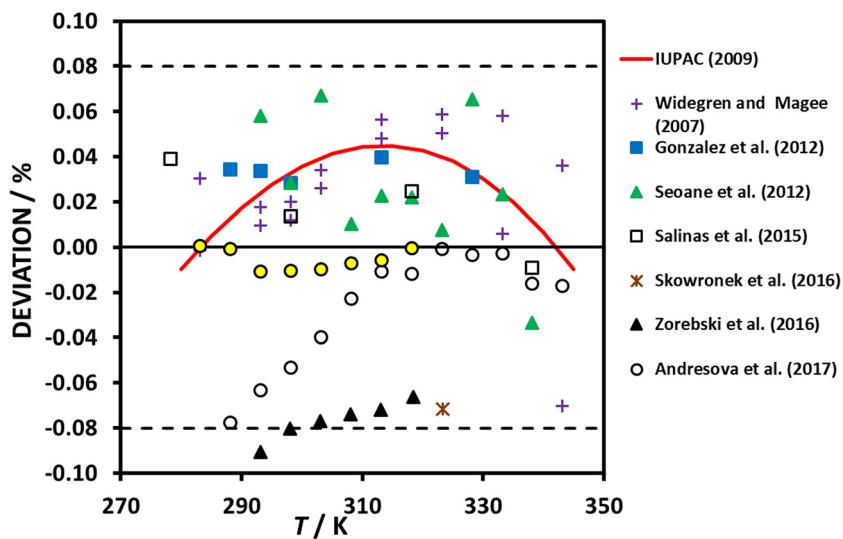
FIG. 6. Deviations between the primary data for the speed of sound of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. Also shown are deviations from the previous correlation proposed by Chirico et al.[4] within the IUPAC project. The dashed line represents the uncertainty of the correlation of $\pm0.08\%$.

The water weight fraction of the sample was measured before (0.0033%) and after the experiments (0.015%). As the experiments were performed in a week, a mean value of 0.009% was assigned to the water content.

2.2.5. Rheology

The results of viscosity reported before[6] require a proof that our ionic liquid is Newtonian in order to develop the reference correlation. To our knowledge, none of the works published before on viscosity have demonstrated this fact. Measurements of shear stress vs shear rate were done in an AR1500EX Rheometer with a 40 mm parallel plate of stainless steel using a shear rate from $0.000\,01\ \text{s}^{-1}$ to $7000\ \text{s}^{-1}$. It is a controlled stress, strain, and rate rheometer that comes standard with a wide shear stress range [0.008 Pa–12 000 Pa], ultra-high resolution [0.04 μrad], and high angular velocity [300 rad/s]. A

FIG. 7. Recommended variation of the speed of sound of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. Primary data and new correlation are shown.

Peltier plate allowed the test between 273.15 K and 393.15 K, with an accuracy of 0.1 K, at atmospheric pressure under a stream of dry nitrogen. Figure 1 displays the results obtained, where a proportionality between the shear stress, σ, and the shear rate can be seen, whose constant is the viscosity of the liquid. Slopes are constant to within 1%. This is the behavior of Newtonian liquids.[17] These results validate all the viscosity results obtained with Newtonian liquid instrumentation reported in Secs. 2.3 and 4.

2.3. Results

2.3.1. Density and speed of sound

The results obtained for the density and speed of sound are displayed in Table 1. The dependence on temperature of density is linear and can be expressed as follows:

$$\rho\,(\text{kg m}^{-3}) = a_1 + a_2 T\,(\text{K}), \tag{1}$$

whose coefficients are $a_1 = (1647.73 \pm 0.48)$ kg m^{-3} and $a_2 = (-924.9 \pm 1.6) \times 10^{-3}$ kg m^{-3} K^{-1}, with a standard deviation of 0.12 kg m^{-3} at a 95% confidence level ($k = 2$). No data depart from the fit by more than ±0.1 kg m^{-3}. For the case of speed of sound, the temperature dependence was found to be quadratic and can be expressed by Eq. (2), whose coefficients are $b_1 = (2250.41 \pm 6.88)$ m s^{-1}, $b_2 = (-4.549 \pm 0.045)$ m K^{-1} s^{-1}, and $b_3 = (3.74 \pm 0.08) \times 10^{-3}$ m K^{-2} s^{-1}, with a standard deviation of 0.07 m s^{-1}, also at a 95% confidence level ($k = 2$), and no point deviating by more than 0.05 m s^{-1},

$$c\,(\text{m s}^{-1}) = b_1 + b_2 T\,(\text{K}) + b_3 T\,(\text{K})^2. \tag{2}$$

2.3.2. Surface tension

The results obtained for the surface tension are displayed in Table 2. The dependence on temperature was found to be linear and can be expressed as follows:

TABLE 7. Available data for the heat capacity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N], classified as primary and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class	Observations
				Primary					
Blokhin et al. (2006a)[81]	AC (SS)	188.06–368.29	0.1	112	0.4–1.0	IUPAC	0.0005	PDSA	Description in Sec. 2.1
Blokhin et al. (2006b)[81]	AC (SS)	194.39–367.68	0.1	65	0.4–1.0	IUPAC	0.0005	PDSA	Description in Sec. 2.1
Blokhin et al. (2006)[81]	AC (SS)	272.03–370	0.1	12	0.4–1.0	IUPAC	0.0005	PDSA	Description in Sec. 2.1
Blokhin et al. (2006d)[81]	AC (SS)	190–272.03	0.1	10	0.4–1.1	IUPAC	0.0005	PDSA	Description in Sec. 2.1
Shimizu et al. (2006)[82]	VAC	272.1–310	0.1	6	1.3	IUPAC	0.0002	PDSA	Description in Sec. 2.1
Bochmann and Hefter (2010)[83]	TCmDSC	325.02–555.24	0.1	18	0.6	IUPAC	0.011	PDSA	Description in Sec. 2.1
Rocha et al. (2012)[84]	DC	298.15	0.1	1	0.95	IoLiTec	0.01	PDSA	Dried by vacuum heating
Zorebski et al. (2016)[44]	TCmDSC	293.15–323.15	0.1	13	3.8	HS	0.0005	PDSA	Source synthesized by others; purification by spectroscopy, Karl Fischer titration, and fraction melting in an adiabatic calorimeter; and purity of 99.5%
Andresova et al. (2017)[46]	TCmDSC	294.15–398.15	0.1	55	3.8	IoLiTec	0.017	PDSA	Commercial source; final purification by NMR analysis, final purity of 99.964 mass %; and dried before every experiment for at least 16 h under vacuum (8–10 mbar) at 60 °C
				Secondary					
Crosthwaite et al. (2005)[85]	DSC (LS)	298–323	0.1	2	10	HS	0.0031	D	No information on purity. Dried by vacuum heating
Archer (2006)[86]	DSC (SS)	196–370	0.1	164	2	IUPAC	0.002	PDSA	IUPAC sample, but data highly complex and scattered, especially at low temperatures
Diedrichs and Gmehling (2006a)[87]	DSC (SS)	320.15–425.15	0.1	22	5	Merck	NA	DGF	No information on the purity. Degassed
Diedrichs and Gmehling (2006b)[87]	DSC (LS)	318.17–418.13	0.1	21	5	Merck	NA	DGF	No information on the purity. Degassed

TABLE 7. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class	Observations
Diedrichs and Gmehling (2006)[87]	MDSC	323.15–413.15	0.1	19	6	Merck	NA	DGF	No information on the purity. Degassed
Ge et al. (2008)[88]	DSC (SS)	293–358	0.1	14	5.2	HS	0.0023	D	No information on purity. Samples dried overnight at 343 K under high vacuum
Hughes et al. (2011)[89]	DSC (LS)	302.86–372.64	0.1	15	3.3	HS	0.01	D	No information on purity. Samples heated in an oven to 343 K in vacuum for 48 h
Gomez et al. (2013)[90]	DSC (SS)	293.15–333.15	0.1	41	10	IoLiTec	0.005	MPFP	Manufacturers stated purity. Samples heated in an oven to 343 K in vacuum for 48 h
Polikhronidi et al. (2014)[91]	AC-LV	329.07–479.69	0.1	422	6.9	IoLiTec	0.007	MPNP	Manufacturers stated purity. No further purification

[a]DSC (LS), Large Sample (1 g) Scanning Calorimetry; DSC (SS), Small Sample (50 mg) Scanning Calorimetry; AC (SS), Small Sample (<1 g) Adiabatic Calorimetry; MDSC, Modulated-Temperature Differential Scanning Calorimetry; VAC, Vacuum Adiabatic Calorimetry; TCmDSC, Tian–Calvet Differential Microcalorimeter; and DC, High-Precision Drop Calorimetry.
[b]Note that the IUPAC sample is as described in text and HS means synthesized in authors' laboratory.
[c]NA, Not Available.
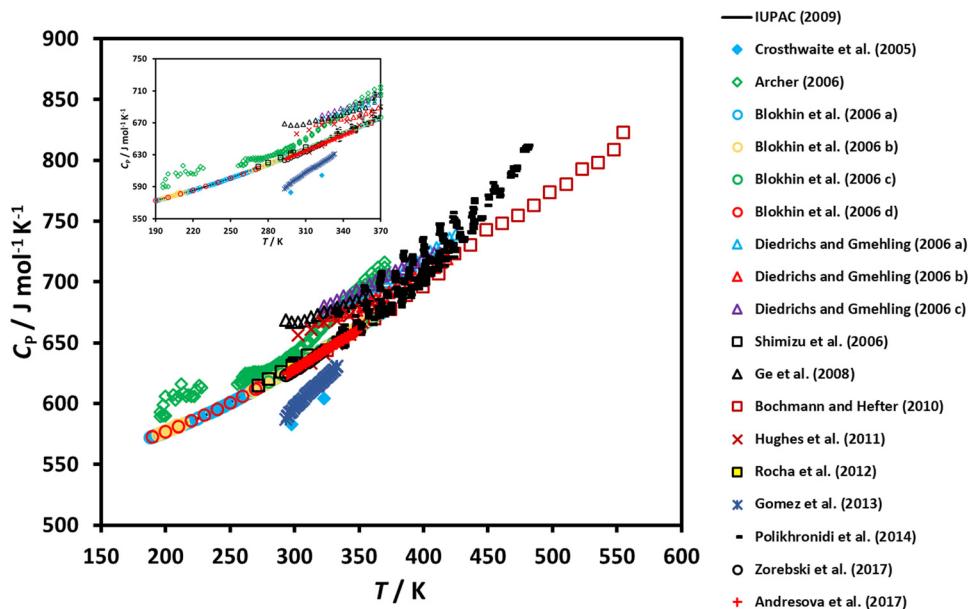
FIG. 8. The heat capacity at constant pressure of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature for all sets of data available. Also shown is the IUPAC correlation, valid for 190 < T/K < 370 (clearer in the inset, it follows Blokhin data[81] which were used for its development).
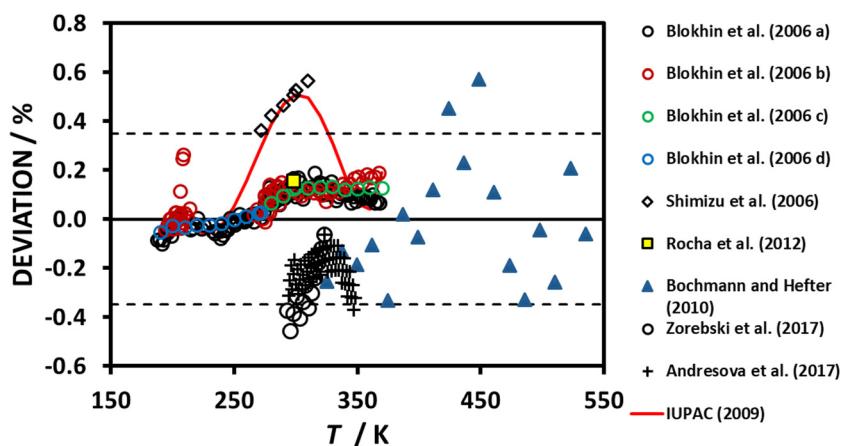
FIG. 9. Deviations between the primary data for the heat capacity of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. Also shown are deviations from the previous correlation proposed by Chirico et al.[4] within the IUPAC project. The dashed line represents the uncertainty of the correlation of $\pm 0.35\%$.
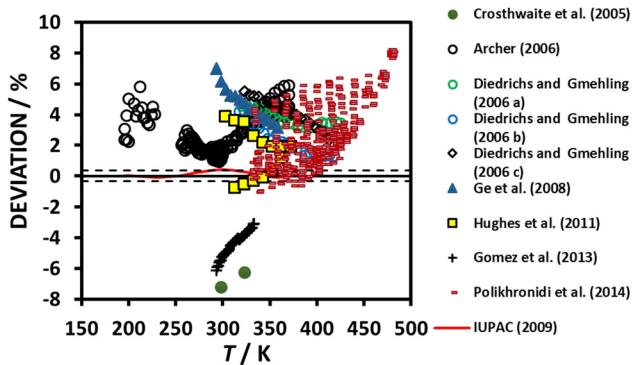
FIG. 10. Deviations between the secondary data for the heat capacity of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. Also shown are deviations from the previous correlation proposed by Chirico et al.[4] within the IUPAC project. The dashed line represents the uncertainty of the correlation of $\pm 0.35\%$.

$$\gamma\left(mN\ m^{-1}\right) = c_1 + c_2 T\,(K), \tag{3}$$

whose coefficients are $c_1 = (45.039 \pm 0.206)\ mN\ m^{-1}$ and $c_2 = (-0.4482 \pm 0.0007)\ mN\ m^{-1}\ K^{-1}$, with a standard deviation of $0.034\ mN\ m^{-1}$ and no point deviating by more than $0.07\ mN\ m^{-1}$.

2.3.3. Refractive index

The refractive index of $[C_6mim][(CF_3SO_2)_2N]$ was measured between 283.15 K and 343.15 K. The results obtained are displayed in Table 3. The dependence on temperature was found to be linear and can be expressed as follows:

$$n_D = d_1 + d_2 T\,(K), \tag{4}$$

with coefficients $d_1 = (1.518\,709 \pm 0.000\,204)$ and $d_2 = (-2.971\,39 \pm 0.006\,50) \times 10^{-4}\ K^{-1}$, with a standard deviation of 0.877×10^{-4} refractive index units, at a 95% confidence level ($k = 2$). No point deviates from the line by more than $0.000\,01$.
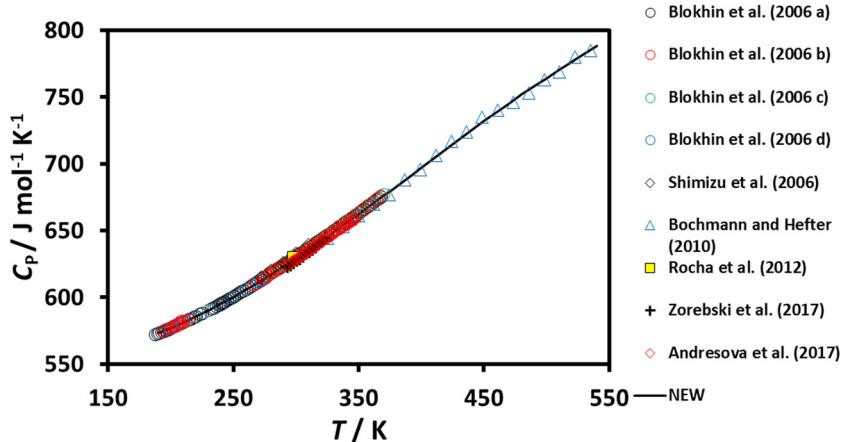
FIG. 11. Recommended variation of the heat capacity of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. Primary data and new correlation are shown.

TABLE 8. Available data for the surface tension of [C$_6$mim][(CF$_3$SO$_2$)$_2$N], classified as primary and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class	Observations
				Primary					
Carvalho et al. (2008)[92]	RT	293.15–343.15	0.1	6	2.0	IoLiTec	0.002	PDSA	Commercial sample; initial purification: initial purity of 99 mass %; final purification: dried by vacuum heating, stirring, and moderate temperature (80 °C) for at least 48 h; and analysis by NMR spectroscopy
Osada et al. (2009)[93]	DLS	303.15	0.1	1	3.3	Kanto Chemical	NA	D	Commercial sample, purity of 99.3%, and dried at 60 °C under vacuum for about 12 h to eliminate adsorbed water
Klomfar et al. (2010)[94]	WP	283.17–351.11	0.1	15	1.1	Solvent Innovation	0.0045	D	Commercial sample; initial purification: initial purity of 99.9 mass %; and final purification: dried by evaporation under vacuum at temperature 70 °C for 7 h
Oliveira et al. (2012)[34]	PDS	298.15	0.1	1	1.2	IoLiTec	0.0307	PDSA	Commercial sample, initial purity of 99 mass %, analysis by NMR spectroscopy, and dried by vacuum heating for a minimum period of 48 h under constant stirring
Present work	WP	289.0–336.2	0.1	13	1.0	IUPAC	0.008	PDSA	Description in Sec. 2.1

TABLE 8. (*Continued.*)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class	Observations
				Secondary					
Kilaru et al. (2007)[95]	RT	297.22–346.42	0.1	13	17.0	Covalent Assoc.	0.011	MPFP	Commercial source, purification stated by the supplier, and purity of 99%
Muhammad et al. (2008)[59]	DW	298.15–338.15	0.1	5	4.7	Merck	0.0268	D	Commercial sample, initial purification: initial purity of 99%, and final purification: dried in a vacuum drier at 313 K for 3 days
Tariq et al. (2010)[64]	PDS	313–532	0.1	12	3.3	HS	0.007	D	Commercial sample, purification: purity of 99 mol. %, and dried for at least 24 h under vacuum (0.1 Pa) and moderate temperature (6 h period up to 60 °C)
Ahosseini et al. (2010)[61]	SPVT	283.1–348.15	0.1	4	3.0	HS	NA	PDSA	Synthesized in the authors' laboratory, purification: purity of 99%, dried under vacuum at 80 °C, and chemical and NMR spectroscopy analysis
Kolbeck et al. (2010)[63]	PDS	298.15	0.1	2	1.0	HS	0.0008	PDSA	Synthesized in the authors' laboratory, initial purity of 99%, dried after preparation in vacuum at 40 °C for 24 h, and analysis by NMR spectroscopy

TABLE 8. (*Continued.*)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	w_{water} (%)[c]	Purity class	Observations
Shirota *et al.* (2011)[31]	RG	297	0.1	1	2.3	HS	0.0003	PDSA	Synthesized in the authors' laboratory, initial purity of 98%, analysis by NMR spectroscopy, and dried under vacuum at 35 °C for 3 days

[a]RG, Ring Tensiometer; DW, Drop Weight; DLS, Dynamic Light Scattering; WP, Wilhelmy Plate method; PDS, Pendant Drop Shape; and SPVT, Spinning Drop Video Tensiometer.
[b]Note that the IUPAC sample is as described in text.
[c]NA, Not Available.

2.3.4. Thermal conductivity

The results obtained for the thermal conductivity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] are displayed in Table 4. Data were fitted as a function of temperature to a linear equation

$$\lambda\left(\text{W m}^{-1}\text{ K}^{-1}\right) = e_1 + e_2 T\,(\text{K}), \tag{5}$$

with coefficients $e_1 = (0.1062 \pm 0.0019)$ W m^{-1} K^{-1} and $e_2 = (6.286 \pm 0.609) \times 10^{-5}$ W m^{-1} K^{-2}, and a standard deviation of 8.2×10^{-4} W m^{-1} K^{-1}. No point deviates from the line by more than 0.0004 W m^{-1} K^{-1}.

3. The Establishment of Reference Data Correlations

3.1. Experimental techniques and data selection

The experimental techniques for the measurement of thermophysical properties of liquids are widely published and will not be described here. However, their applications to ionic liquids are still a matter of discussion as researchers used a wide range of instruments, from state-of-the-art to user-friendly. This also produces a large variation in the uncertainties of the measured data, which restricts the selection of data used to base the reference correlations. A careful analysis, assessing their quality, shows that there are discrepancies between data from different laboratories and sometimes from samples of different synthesis batches,[1] and this is necessary to be aware about the use and misuse of traditional equipment.

The reports produced by IUPAC[3,4] did not select the data used in the reference correlations by method accuracy but essentially by results obtained with samples originated in the project and in the instrumentation available in the different groups that were project partners, fortunately and in many cases, some of the best groups existing in the world.

This was not the approach followed by the earlier work of the Subcommittee on Transport Properties of the Physical Chemistry Division of IUPAC, expressed in several publications in this journal as
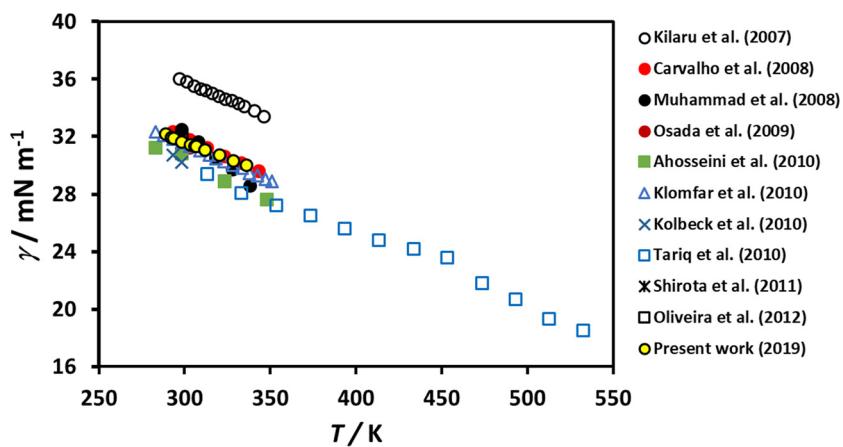

FIG. 12. The surface tension at constant pressure of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature for all sets of data available.

for thermal conductivity and viscosity, where the group has been involved,[15,18–20] and continued by other colleagues also in this journal, namely for a wide range of temperatures and pressures in fluids, as, for example, in Refs. 21–23. Then, the approach was mostly developed for a single fluid and a single property, and it was possible to select the most accurate instruments used and very low data uncertainty. The data were then classified into primary and secondary data, whereby primary data were defined as results carried out with a high-precision instrument for which a working equation existed with a detailed set of corrections, distinguishing the ideal mathematical model from the real instrument,[18] and therefore used in the reference correlations developed. These data are, whenever possible, absolute data, not needing calibration of the main physical variables of the apparatus. Secondary data were the results of inferior accuracy due to extreme conditions, incomplete characterization of the instrument, or deficient characterization of the samples measured. These data were not used in primary correlations and were used to develop secondary correlations, namely if temperature range extension was recommended.

In this work, we tried to use the same definition of primary data, but in some cases, it was necessary to use relative instrument data of high accuracy (in the case of density, for instance, whereby 90% of the data available for ionic liquids are produced with vibrating tube densimeters, usually calibrated with water and certified liquids, as described in Sec. 2.2.1).

3.2. The concept of primary and secondary data for ionic liquids

In the sections dedicated to each property (Secs. 4.1-4.9), we discuss the available data and the criteria used to select the "primary" data to develop the reference correlations. However, it is necessary to report here that, in view of the well-recognized effect of impurity water on some thermophysical properties, such as viscosity,[1,5,6,8] only data whose samples were well characterized and with water contents commensurate with its effect on the quality of the data were chosen. In addition, instruments not well described or without mention of calibration procedures were also not used. Finally, data that departed from the average of the best published data by more than a percentage depending on the property and described below were not considered in the primary set.

As $[C_6mim][(CF_3SO_2)_2N]$ is a weak water absorber, capable of being obtained in a very pure form, it was not necessary to have data on the mixture IL + water, as applied, for instance, for $[C_2mim][(OAc)]$.[9] However, the results obtained for lower water contents by Widegren and Magee[5,10] for the effect on density and speed of sound (negligible effect) and viscosity and electrical conductivity (significant) were used. In the case of surface tension, thermal conductivity, and self-diffusion coefficient, the effect of the sample water content is well below the uncertainty of the data, while for the refractive index, the sample water content was very small, having a negligible contribution.

3.3. Correlation procedures

The reference correlations developed used only data at $P = 0.1$ MPa. The data selected as "primary" were fitted using the method of least squares as a function of temperature to polynomials of the type

$$X = \sum_{i=0}^{n} a_i T^i, \qquad (6)$$

where T is the absolute temperature in K and the coefficients a_i have units defined by the respective property in the supplementary material. No weight was given to the data points as the uncertainty of the primary data was very similar. The degree of the polynomial was chosen by minimizing the mean square deviation of the fit, commensurate with the average uncertainty of the data used.

For the viscosity, electrical conductivity, and ion self-diffusion coefficients, a correlation equation different from the polynomial in Eq. (6) was applied, based on previous work on the standard reference data of toluene and water.[15,20] The IAPS (International Association for the Properties of Steam) formulation for the transport properties of water developed by Sengers et al.[24] and Kestin et al.[25] for viscosity takes the form

$$\ln \eta^* = \sum_{i=0}^{3} A_i \left(T^*\right)^{-i}, \qquad (7)$$

where η^* and T^* are the dimensionless variables defined as

$$\begin{aligned} T^* &= T\,(\mathrm{K}) \big/ 298.15\ \mathrm{K} \\ \eta^* &= \eta(T) \big/ \eta(298.15\ \mathrm{K}). \end{aligned} \qquad (8)$$

The procedure used to obtain the value of the property at 298.15 K is explained in Secs. 4.5, 4.6, and 4.9. In the case of self-diffusion coefficients, it was necessary to use a reference temperature of 303.15 K.

4. Results and Discussion

The main source for bibliographic information was the NIST Database ILThermo,[26] although several other papers were found by normal bibliographic search. All temperature data refer to ITS-90.

The tables have the following information: Literature source, technique, temperature range/K, pressure range/MPa, number of data points, assigned uncertainty [in the presented tables, the assigned uncertainty is that claimed by the authors, corrected, when applicable, to expanded global uncertainty (relative or absolute) ($k = 2$)], sample origin, purity class, primary/secondary data, and observations. In the case of origin, IUPAC means the IUPAC sample, as described in Sec. 2.1, and HS means synthesized in authors' laboratory; otherwise, the manufacturer company is mentioned. Purity class: the acronyms
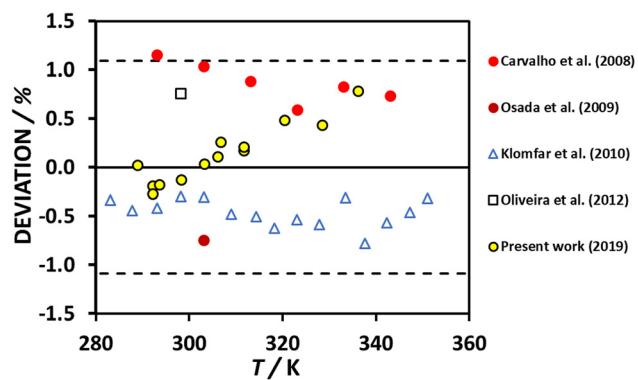
FIG. 13. Deviations between the primary data for the surface tension of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. The dashed line represents the uncertainty of the correlation of $\pm 1.09\%$.
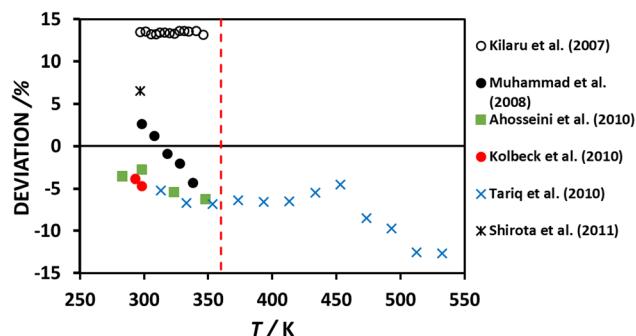
FIG. 14. Deviations between the secondary data for the surface tension of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature.

FIG. 15. Recommended variation of the surface tension of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature.

are the following: MPNP—manufacturers stated purity, no further purification; MPFP—manufacturers stated purity, further purification; D—dried with molecular sieves, with silica gel, with phosphorous pentoxide, or in vacuum; DF—dried and filtered sample; DGF—degassed and filtered sample; and PDSA—purified and dried samples with chemical analysis, GC, GC–MS, NMR, etc., and/or Karl Fisher (water content) analysis.

4.1. Density

All the density data available are summarized in Table 5. A total of 1168 data points were found from 55 sets of data, 49 of them using vibrating-tube densimetry, for 238 < T/K < 473. Only data at 0.1 MPa were used. Figure 2 shows the deviations of all data with deviations

smaller than ±0.8% from the IUPAC correlation for density.[3] As is easily seen, some sets of data, namely, those of Fitchett et al.[50] and Aki et al.[51] using pycnometry and those of Tokuda et al.,[54] Lachwa et al.,[55] McHale et al.,[58] Fröba et al.,[62] Kolbeck et al.,[63] and Gonzalez-Miquel et al.[69] using vibrating-tube densimetry, have deviations from the IUPAC correlation greater than 0.3%, three times the uncertainty of the IUPAC correlation. This is possibly due to deficient equipment calibration. Many other sets were also not considered as primary data, either for lack of purity analysis after synthesis at the authors' laboratory, large water content, or quoted uncertainties greater than 0.2%. The primary data selected are shown in Table 5, 25 datasets
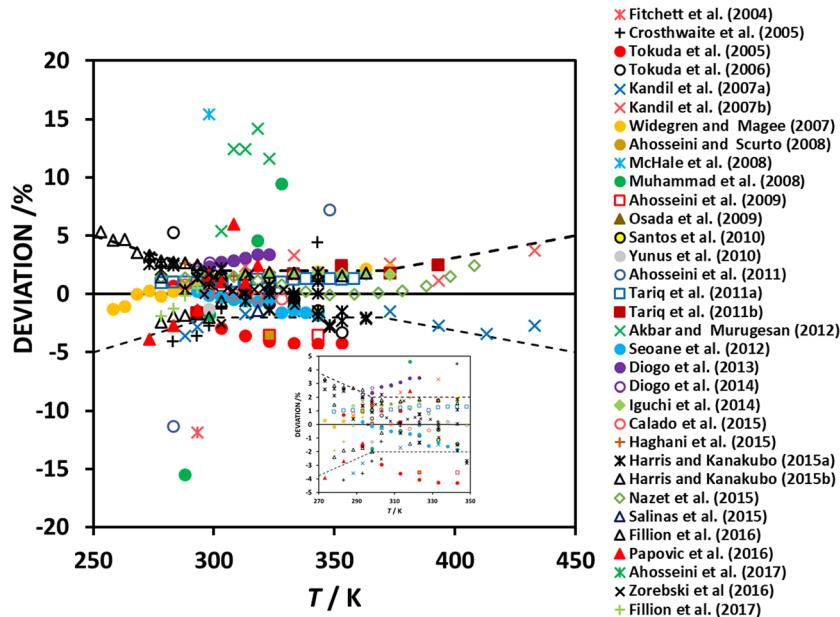
FIG. 16. Deviations from all the datasets for the viscosity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature. The dashed lines represent the uncertainty boundaries of the IUPAC correlation[4] at a 95% confidence level, as described in the text. The inset shows the detail for temperatures between 280 K and 360 K, with ±3% deviations, for clarity.

TABLE 9. Available data for the viscosity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N], classified as primary and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
				Primary					
Kandil et al. (2007a)[28]	VW	288.15–433.15	0.1–40	42	2	IUPAC	PDSA	0.041	Description in Sec. 2.1
Kandil et al. (2007b)[28]	VW	293.15–433.15	0.1–40	31	2.2	IUPAC	PDSA	0.0117	Description in Sec. 2.1
Widegren and Magee (2007)[5]	SV	258.15–373.15	0.1	19	2	IUPAC	PDSA	0.001	Description in Sec. 2.1
Santos et al. (2010)[6]	CT	298.15–343.15	0.1	6	2.8	IUPAC	PDSA	0.0158[d]	Description in Sec. 2.1
Tariq et al. (2011a)[97]	CCV	278–358	0.1	17	2	HS	PDSA	0.007	Synthesized in authors' laboratory, dried under vacuum for 6 h at 60 °C to remove impurities, and analysis by proton NMR spectroscopy
Tariq et al. (2011b)[97]	FB/RS V	293–393	0.1	6	2	HS	PDSA	0.007	Synthesized in authors' laboratory, dried under vacuum for 6 h at 60 °C to remove impurities, and analysis by proton NMR spectroscopy
Seoane et al. (2012)[67]	CT	293.15–343.15	0.1	11	1.5	IoLiTec	D	0.007	Dried under vacuum for 70 h at 40 °C to remove impurities
Diogo et al. (2013)[36]	VW	293.14–323.1	0.1	8	2	IoLiTec	D	0.0158	Dried by vacuum heating (70 °C)
Iguchi et al. (2014)[37]	CCV	293.15–373.15	0.1	9	1.9	Merck	MPNP	0.002	Used as received from the manufacturer
Diogo et al. (2014)[98]	CT	293.25–298.19	0.1	2	2	IoLiTec	D	0.0221	Dried under vacuum for about 48 h at around 323 K and left under vacuum for several days at room temperature
Calado et al. (2015)[73]	CT	288.19–328.08	0.1	5	1	IoLiTec	D	0.0026	Dried by vacuum heating (80 °C)
Haghani et al. (2015)[99]	FB/RS V	288.2–318.2	0.1	4	2	IoLiTec	MPNP	0.0158	Used as received from the manufacturer

TABLE 9. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
Harris and Kanakubo (2015a)[38]	FB/RS V	273.15–363.15	0.1	37	2	HS	PDSA	0.002	Dried under vacuum at about 70 °C for 30 h to remove any excess water and purity determined by NMR analysis
Harris and Kanakubo (2015b)[38]	SV	248.15–363.15	0.1	18	2	HS	PDSA	0.002	Dried under vacuum at about 70 °C for 30 h to remove any excess water and purity determined by NMR analysis
Nazet et al. (2015)[40]	FB/RS V	278.15–408.15	0.1	14	2	IoLiTec	D	0.014	Dried for one week at 60 °C with a high-vacuum line
Salinas et al. (2015)[76]	FB/RS V	278.15–318.15	0.1	3	2	IoLiTec	PDSA	0.05	Dried under vacuum for 1 week at 40 °C to remove impurities and analysis by proton NMR spectroscopy
Fillion et al. (2016)[41]	C&PV	278.15–303.15	0.1	6	6.9	HS	MPNP	0.013	Used as received from the manufacturer
Zorebski et al. (2016)[44]	CT	292.87–333.42	0.1	14	2	HS	D	0.0092	Synthesized by others; purification by spectroscopy, Karl Fischer titration, and fraction melting in an adiabatic calorimeter; and stored under argon
Fillion et al. (2017)[100]	C&PV	278.15–293.15	0.1	4	6	HS	PDSA	0.0005	Synthesized in authors' laboratory, dried under vacuum, and analysis by proton NMR spectroscopy

TABLE 9. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
					Secondary				
Fitchett et al. (2004)[50]	CT	293.15	0.1	1	7.7	HS	D	1.79	Synthesized in the authors' laboratory and dried under vacuum for 4 h at 70 °C–80 °C to remove residual water
Crosthwaite et al. (2005)[85]	C&PV	283–343	0.1	8	6.7	HS	D	0.003	Synthesized in the authors' laboratory and dried under vacuum for at least 48 h at 40 °C–80 °C to remove organic solvents and water
Tokuda et al. (2005)[54]	C&PV	283.15–353.15	0.1	8	3.9	HS	PDSA	0.001	Synthesized in the authors' laboratory, dried under vacuum for 48 h to remove residual water, and purity determined by NMR and MS analysis
Tokuda et al. (2006)[56]	C&PV	283.15–353.15	0.1	9	10	HS	PDSA	0.004	Synthesized in the authors' laboratory, analysis by mass spectrometry, and dried by vacuum heating
Ahosseini and Scurto (2008)[96]	MP	298.15–343.15	0.1–124	33	3	HS	PDSA	0.0125	Synthesized in the authors' laboratory, analysis by NMR, and dried under vacuum for 48 h at 40 °C to remove impurities
Muhammad et al. (2008)[59]	C&PV	288.2–328.2	0.1	5	???	Merck	D	0.0268	Dried by vacuum heating
McHale et al. (2008)[58]	MP	298.15	0.1	1	3.1	HS	PDSA	0.013	Synthesized in the authors' laboratory, ion chromatography, and dried by vacuum heating

TABLE 9. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
Ahosseini et al. (2009)[101]	C&PV	323.15	0.1	1	2.4	HS	PDSA	0.01	Synthesized in the authors' laboratory, analysis by NMR, and dried under vacuum for 48 h at 40 °C to remove impurities
Osada et al. (2009)[93]	DLS	303.15	Vacuum	1	NA	Kanto Chemical Co., Inc.	D	<1	Dried at 60 °C under vacuum for about 12 h to eliminate adsorbed water
Yunus et al. (2010)[65]	CCV	298.15	0.1	1	2.3	HS	PDSA	NA	Synthesized in the authors' laboratory, dried under vacuum for 3 days at 35 °C to remove impurities, and analysis by proton NMR spectroscopy
Ahosseini et al. (2011)[102]	C&PV	283.15–348.15	0.1	4	2	HS	PDSA	0.005	Synthesized in the authors' laboratory, dried under vacuum for 48 h at 50 °C to remove impurities, and analysis by proton NMR spectroscopy
Akbar and Murugesan (2012)[66]	C&PV	303.15–323.15	0.1	5	2.3	Merck	PDSA	0.003	Analysis by HPLC and dried by vacuum heating
Papovic et al. (2016)[78]	CT	273.15–323.15	0.1	9	4.6	IoLiTec	D	0.0154	Dried with anhydrous phosphorous pentoxide
Ahosseini et al. (2017)[103]	OP	343.15	0.1	1	2.8	HS	PDSA	0.0125	Synthesized in the authors' laboratory, dried under vacuum, and analysis by proton NMR spectroscopy

[a]CT, Capillary Tube (Ostwald and Ubbelohde) method; C&PV, Cone and Plate Viscometry; VW, Vibrating Wire viscometry; SV, Stabinger Viscometer; MP, Moving Piston method; CCV, Concentric Cylinder Viscometry; FB/RS V, Falling Body or Rolling Sphere Viscometer OP, Oscillating Piston.
[b]Note that the IUPAC sample is as described in text and HS means synthesized in authors' laboratory.
[c]NA, Not Available.
[d]Samples varied between 119.3 and 196.4 ppm.
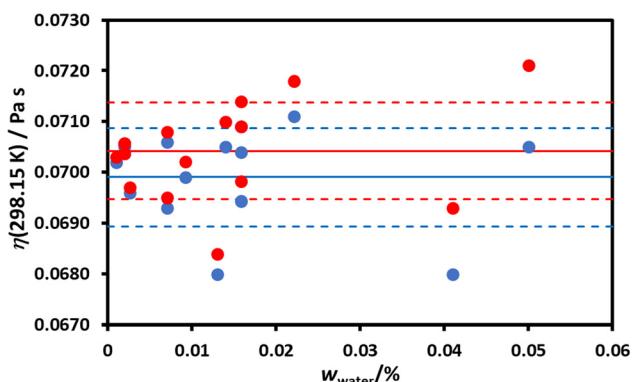
FIG. 17. The viscosity of [C₆mim][(CF₃SO₂)₂N] at 298.15 K obtained from different sets of water-free primary data as a function of the water content of the measured samples (in red). Also shown, for comparison, is the result that we would have obtained if the raw data were used (in blue).

(including the present work) with a total of 284 data points. The remaining data, 31 datasets considered secondary, are also displayed in Table 5.

The variation of the selected data with temperature was found to be linear [$n = 1$, Eq. (6)], with $a_0 = 1643.582 \pm 0.383$ kg m^{-3}, $a_1 = -0.910\,14 \pm 0.001\,22$ kg m^{-3} K^{-1}, and an uncertainty of 0.08% at a 95% confidence level, for the temperature interval $250 < T/K < 380$. The value predicted for the density $\rho(298.15\ \text{K})$ is (1372.2 ± 1.1) kg m^{-3}.

Figure 3 shows the deviations of the primary datasets from the reference correlation, not amounting to more than ±0.1%. The proposed reference correlation has a slightly different slope from that of IUPAC (2009) but a better uncertainty. The deviation is negligible around room

temperature and below but increases to 0.05% at 373 K, well within the mutual uncertainty of both correlations. One interesting point is that this correlation is very robust and can be extended in temperature range up to 473.15 K, as shown in Fig. 4, where the deviations of all secondary data, 32 datasets, with 210 points, some extending up to 473.15 K,[64] are presented, extrapolating very well to within 0.3%. In addition, most of the secondary data do not deviate by more than ±0.5%.

The correlation obtained, as well as the supporting primary data, is plotted in Fig. 5.

4.2. Speed of sound

All the data available are summarized in Table 6. There are 9 sets of data published, one of which, by Frez *et al.*,[80] has a much higher uncertainty than the other sets and no water analysis is described, although the authors claim good sample handling and characterization. It must be said that the water content, within the values shown by the other sets of data (0.001%–0.05%), does not affect the values of the speed of sound within their mutual uncertainties. All the other sets were considered as primary data, two using the IUPAC sample, those of Widegren and Magee[5] and the present work, and the others, either synthesized in authors' laboratory or commercial samples, were classified as PDSA quality. These data are presented in Table 6, involving a total of nine datasets and 64 data points between 278.15 K and 343.15 K.

The variation of the primary data with temperature was found to be quadratic ($n = 2$, Eq. (6)), with $a_0 = (2199.49 \pm 20.08)$ m s^{-1}, $a_1 = (-4.2162 \pm 0.1287)$ m K^{-1} s^{-1}, and $a_2 = (3.20 \pm 0.21) \times 10^{-3}$ m K^{-2} s^{-1} and with an uncertainty of 0.08% at a 95% confidence level. The value predicted for the speed of sound $c(298.15\ \text{K})$ is (1226.7 ± 1.0) m s^{-1} at a 95% confidence level ($k = 2$). Figure 6 shows the deviations of the primary datasets from the reference correlation for the temperature range $280 < T/K < 360$, not amounting to more than ±0.08% except for one point by Zorebski *et al.*[44] at −0.09%. Also shown is the deviation of the
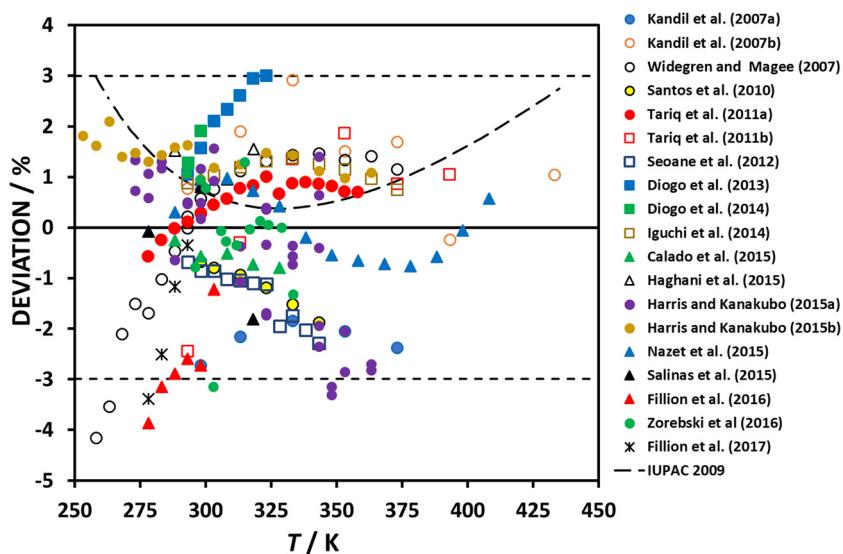
FIG. 18. Deviations between the primary data for the viscosity of [C₆mim][(CF₃SO₂)₂N] as a function of temperature. The dashed line represents the uncertainty of the correlation of ±3.0%.
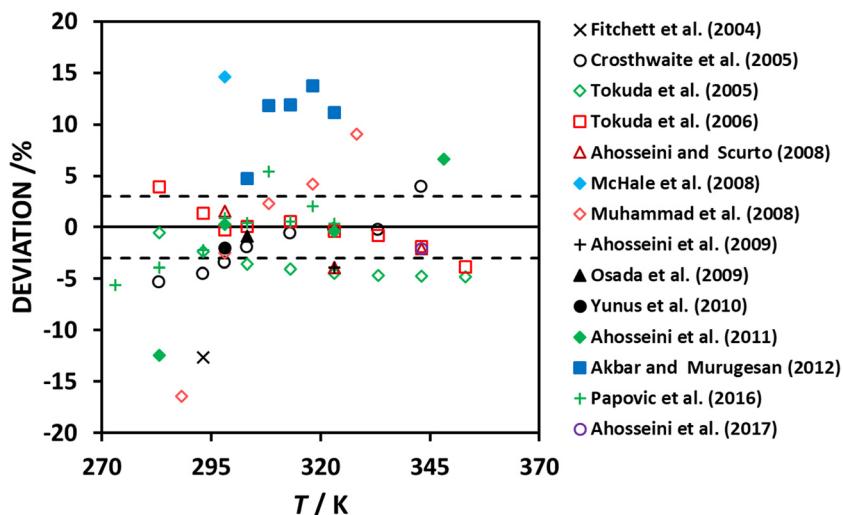
FIG. 19. Deviations between the secondary data for the viscosity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature.

IUPAC (2009) equation,[4] which has a slightly different curvature but well within the mutual uncertainty of both correlations, smaller in this new equation. The secondary data of Frez *et al.*[80] deviate by −0.5%. The correlation obtained, as well as the supporting primary data, are plotted in Fig. 7.

4.3. Heat capacity at constant pressure

In the case of heat capacity at constant pressure, there are 18 sets of data with 957 points. All the available data are summarized in

Table 7. Figure 8 illustrates the temperature dependence of the heat capacity obtained by all the authors. It is clear that the scatter of data is high (assigned uncertainties between 0.4% and 10%).

From these, several sets of data were published after the IUPAC correlation,[4] which was based on only three sets of data: those of Archer[86] obtained with a small sample (50 mg) by scanning calorimetry and those of Blokhin *et al.*[81] and Shimizu *et al.*[82] obtained with adiabatic calorimeters. From the other data, those of Bochmann and Hefter[83] obtained with a Tian–Calvet differential microcalorimeter
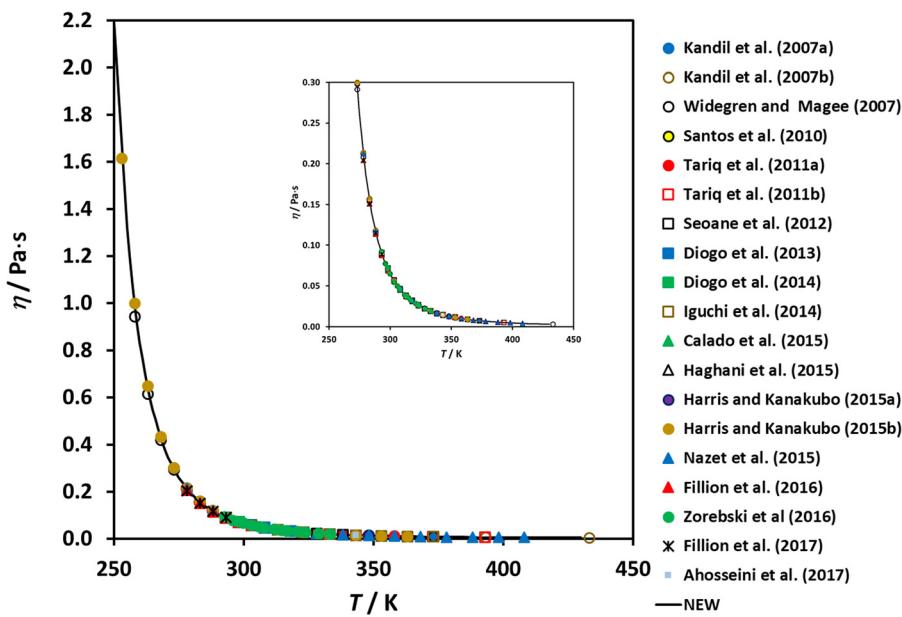
FIG. 20. Recommended variation of the viscosity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature.

TABLE 10. Available data for the electrical conductivity of [C₆mim][(CF₃SO₂)₂N], classified as primary and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	Purity class	w_{water} (%)	Observations
				Primary					
Tokuda et al. (2005)[54]	AC	263–373	0.1	12	3.9	HS	D	0.001	Dried under vacuum for 48 h to remove residual water and purity determined by NMR and MS analysis
Widegren et al. (2005)[105]	AC	295.1	0.1	5	2	IUPAC	PDSA	0.001	Description in Sec. 2.1
Tokuda et al. (2006)[56]	AC	263–373	0.1	10	10	HS	D	0.004	Dried under vacuum and purity determined by NMR analysis
Kandil et al. (2007)[28]	DC	278.15–323.15	0.1	9	2	IUPAC	PDSA	0.041	Description in Sec. 2.1
Widegren and Magee (2007)[5]	AC	288.15–323.15	0.1	5	2	IUPAC	PDSA	0.001	Description in Sec. 2.1
Santos et al. (2010)[6]	AC	278.15–333.15	0.1	11	2	IUPAC	PDSA	0.0004	Description in Sec. 2.1
Calado et al. (2013)[73]	AC	288–333	0.1	9	2	IoLiTec	PDSA	0.0106	Dried under vacuum for several days at 60 °C and purity determined by NMR analysis
Harris and Kanakubo (2015)[38]	AC	243.48–353.15	0.1	17	2	HS	PDSA	0.0002	Purity determined by NMR analysis and dried under vacuum at about 70 °C for 30 h to remove any excess water
Nazet et al. (2015)[40]	AC	278.15–468.15	0.1	20	2	IoLiTec	D	0.0014	Dried for 1 week at 40 °C with a high-vacuum line and no further purification steps
Papovic et al. (2016)[78]	AC	293.15–323.15	0.1	7	3	IoLiTec	D	0.0154	Dried under vacuum for 2 h to remove residual water, NMR analysis, and kept in a desiccator with P_2O_5 for 24 h prior to measurement

TABLE 10. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)	Sample origin[b]	Purity class	w_{water} (%)	Observations
				Secondary					
Fitchett et al. (2004)[50]	AC	295.1	0.1	1	8	HS	D	0.0732	Dried under vacuum for 4 h at 70 °C–80 °C to remove residual water and identity of the ionic liquid was confirmed by EMS
Leys et al. (2008)[106]	DM	288.15–308.15	0.1	4	3	HS	D	0.0066	Dried by vacuum heating

[a]AC, alternating current cell with electrodes and DC, direct current cell with electrodes.
[b]Note that the IUPAC sample is as described in text and HS means synthesized in authors' laboratory.

with the IUPAC sample, Rocha et al.[84] obtained with a high-precision drop calorimeter, Zorebski et al.[44] and Andresova et al.[46] obtained with a Tian–Calvet micro-DSC have the quality to be considered as primary. It must be said that the water content, within the values shown by all these sets of data (<0.02%), does not affect the values of the heat capacity within their mutual uncertainties. These data are presented in Table 7, involving a total of nine datasets and 292 data points, between 190 K and 370 K. The variation of the primary data with temperature was found to be cubic [$n = 3$, Eq. (6)], with $a_0 = (577.01 \pm 4.17)$ J mol^{-1} K^{-1}, $a_1 = (-0.4999 \pm 0.0400)$ J mol^{-1} K^{-2}, $a_2 = (3.001 \pm 0.123) \times 10^{-3}$ J mol^{-1} K^{-3}, and $a_3 = (-2.50 \pm 0.12) \times 10^{-6}$ J mol^{-1} K^{-4}, with an uncertainty of 0.35% at a 95% confidence level, for $190 < T/K < 540$. The value calculated for the heat capacity $C_P(298.15$ K) is (629.1 ± 2.2) J mol^{-1} K^{-1}.

Figure 9 shows the deviations of the primary datasets from the reference correlation for the temperature range 150 K–550 K, not amounting to more than ±0.6%. This new correlation extends considerably the range in temperature with respect to the IUPAC correlation,[4] without significant loss of uncertainty. Figure 10 shows the deviations of the secondary data from the proposed reference correlation. Deviations of up to ±7% are found. The correlation obtained, as well as the supporting primary data, is plotted in Fig. 11.

4.4. Surface tension

Surface tension was not a property considered in the IUPAC project.[3,4] There are 11 sets of data with 85 data points. All the available data are summarized in Table 8. Figure 12 illustrates the
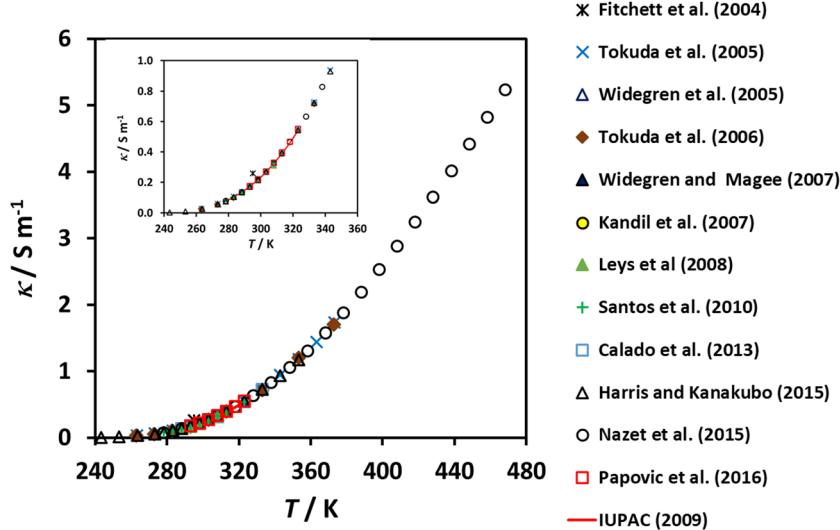
FIG. 21. The electrical conductivity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature for all sets of data available. Also shown is the IUPAC correlation, valid for $278 < T/K < 373$, better viewed on the inset.
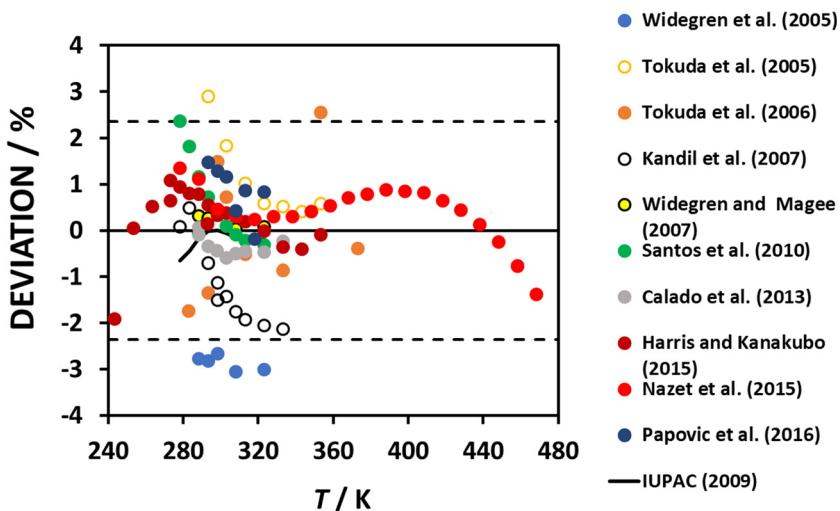
FIG. 22. Deviations of the primary data for the electrical conductivity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] from the proposed reference correlation as a function of temperature. The dashed line represents the uncertainty of the correlation at a 95% confidence level (2.4%). Also shown is the IUPAC (2009) correlation.[4]

temperature dependence of the surface tension obtained by all the authors. It is clear that the scatter of data is high, namely, for temperatures below 350 K (assigned uncertainties between 1% and 17%). The data of Kilaru et al.,[95] using a sample directly from a commercial source, have a very high uncertainty and cannot be considered as primary. Only our measurements have used the IUPAC sample. However, there are data from other authors that can be used in the development of the reference correlation and considered primary as all the measuring methods are well established and are absolute. This is the case for Carvalho et al.,[92] Osada et al.,[93] Klomfar et al.,[94] and Oliveira et al.,[34] as well as the present work. The water content, within the values shown by all these sets of data (<0.03%), does not affect the values of the surface tension within their mutual uncertainties, as explained in Sec. 2.2.2.

The primary data in Table 8 involve a total of five datasets and 41 data points between 280 K and 360 K. The variation of the primary

data with temperature was found to be linear [$n = 1$, Eq. (6)], with $a_0 = (46.822 \pm 0.487)$ mN m^{-1} and $a_1 = (-0.050\,75 \pm 0.001\,55)$ mN m^{-1} K^{-1}, with an uncertainty of 1.09% at a 95% confidence level. The value predicted for the surface tension $\gamma(298.15\ \text{K})$ is (31.69 ± 0.35) mN m^{-1}. Figure 13 shows the deviations of the primary datasets from the reference correlation for the temperature range $280 < T/\text{K} < 360$, not amounting to more than ±1%.

Figure 14 shows the deviations of the secondary data, also presented in Table 8, from the proposed reference correlation. Deviations from +14% to −7% are found for the temperature range of the
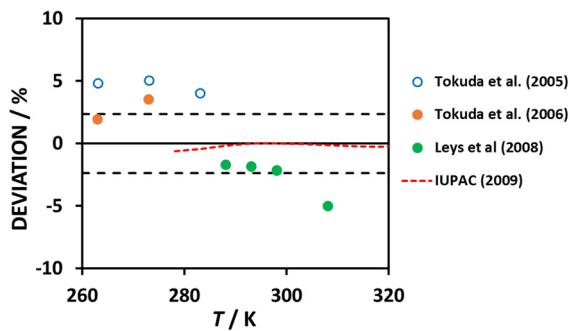
FIG. 23. Deviations of the secondary data for the electrical conductivity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] from the proposed reference correlation as a function of temperature. The dashed line represents the uncertainty of the correlation at a 95% confidence level (2.4%). Also shown is the IUPAC (2009) correlation.[4]
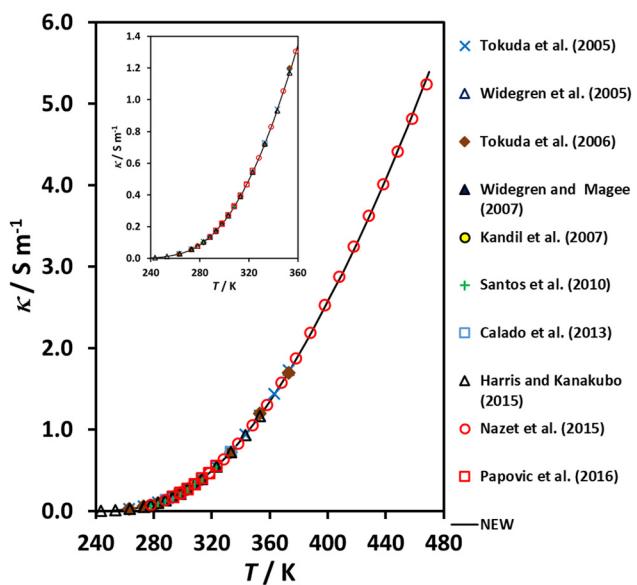
FIG. 24. Recommended variation of the electrical conductivity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature.
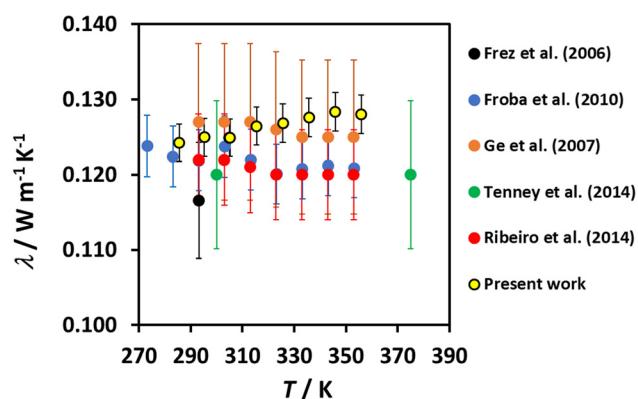
FIG. 25. The thermal conductivity of [C_6mim][($CF_3SO_2)_2$N] as a function of temperature for all sets of data available.

correlation. Above 360 K, namely, with the data of Tariq et al.,[64] deviations can be as big as −15%. The correlation, as well as the supporting primary data, is plotted in Fig. 15.

4.5. Viscosity

Viscosity was considered in the IUPAC project,[3,4] where the data of Kandil et al.,[28] Widegren and Magee,[5] and Santos et al.[6] were obtained with the IUPAC samples. Also used were the data of

Crosthwaite et al.,[85] Tokuda et al.,[56] Ahosseini and Scurto,[96] and Muhammad et al.,[59] with the temperature ranging from 258 K to 433 K and an uncertainty of 2% for $298 < T/K < 370$, increasing linearly to 5% at the limits of the validity range. However, since then, there were many publications with viscosity data of this ionic liquid that can be used to improve the correlation. Figure 16 shows deviations of all existing data from the IUPAC correlation for viscosities varying between 2.75 Pa s and 0.0031 Pa s, a factor greater than 880, in the temperature range covered. There are, at the pressure of 0.1 MPa, 33 datasets with 343 points. These data are summarized in Table 9.

The data mentioned above were all analyzed according to the criteria explained above for the definition of primary data. All data with deviations greater than 3% from the IUPAC correlation were not considered as primary data. In addition, the balance of uncertainty of the instruments used should have been explained by the authors as many different methods were used for the viscosity measurement. In addition, the methodology described in the paper by Nieto de Castro et al.[104] to access the quality of state-of-the-art instruments/viscometers was used in analyzing the instrumentation used. Finally, as mentioned in several works,[3,5,6,8,9] among others, the viscosity of an ionic liquid is very sensitive to its water content. Fortunately, as said above, [C_6mim][($CF_3SO_2)_2$N] is not a strong absorbent of water, although care has to be taken in handling the samples and measuring the water content of the sample before and after the measurements. So, after selecting the primary data, a correction is necessary to obtain water-free viscosity data.

The primary data are summarized in Table 9, involving a total of 19 datasets and 195 data points, between $248 < T/K < 435$. All the data

TABLE 11. Available data for the thermal conductivity of [C_6mim][($CF_3SO_2)_2$N], classified as reference and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. data points	Assigned uncertainty (%)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
					Reference				
Ge et al. (2007)[107]	THW Probe	293–353	0.1	7	8.2	HS	PDSA	0.08	Synthesized in authors' laboratory, dried under vacuum at 70 °C to remove residual water, analysis by proton and ^{13}C NMR spectroscopy, and chemical analysis
Fröba et al. (2010)[62]	GHP	273.15–353.15	0.1	9	3.3	Solvent Innovation	PDSA	0.0086	Commercial sample with purity >98%, dried under vacuum for 4 h at 60 °C to remove residual water, and analysis by proton NMR spectroscopy

TABLE 11. (*Continued.*)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. data points	Assigned uncertainty (%)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
Ribeiro *et al.* (2014)[108]	THW Probe	293–353	0.1	7	5.0	HS	PDSA	0.002	Synthesized in authors' laboratory, dried under vacuum at 70 °C to remove residual water, analysis by proton and ^{13}C NMR spectroscopy, and chemical analysis
Present work	THW Probe	293.15–343.15	0.1	9	2.0	IoLiTec	PDSA	0.0093	Commercial sample with purity >99.9% and used from the manufacturer bottle. Water content before measurements is 33 ppm and after measurements is 154 ppm
					Secondary				
Frez *et al.* (2006)[80]	TGT (calculated)	295	0.1	1	8.4	HS	D	NA	Synthesized in the authors' laboratory, dried under vacuum at 60 °C to remove residual water, and analysis by proton NMR spectroscopy
Tenney *et al.* (2014)[72]	GHFM	300–375	0.1	21	8.2	HS	D	0.0008	Synthesized in authors' laboratory and dried under vacuum for 48 h to remove residual water

[a]GHP, Guarded Hot Plate; GHFM, Guarded Heat Flow Meter; and THW, Transient Hot-Wire.
[b]HS, Home Synthesis.
[c]NA, Not Available.

were corrected for water content using the methodology developed by Widegren and Magee,[5] and also applied by Santos *et al.*,[6] using the water content present in Table 9. As mentioned, Eqs. (7) and (8) will be applied for viscosity. The best estimate of the value of η(298.15 K) was found with the following procedure in the absence of enough data on the viscosity of IL + water mixtures. All the primary datasets where the value of the viscosity at 298.15 K was available were corrected for water-free values using the equation developed by Widegren and Magee.[5] In Fig. 17, we represent all the data points for the primary datasets as a function of their water content (in red). No definitive

trend was found to extrapolate to pure ionic liquid, probably due to the uncertainty of each batch of experimental data. Therefore, all the values were averaged giving η_{wf}(298.15 K) = (0.0704 ± 0.0019) Pa s, with 2.7% uncertainty. Figure 17 also shows (in blue) the uncorrected values of the viscosities, which average to a value 0.75% less than the water-free value, smaller than the uncertainty of the experimental data.

The coefficients of Eq. (7) are $A_0 = -10.846\,18 \pm 0.546\,03$, $A_1 = 21.505\,21 \pm 1.742\,56$, $A_2 = -24.565\,56 \pm 1.841\,98$, and $A_3 = 13.899\,12 \pm 0.645\,03$, with an uncertainty of 3.0% at a 95% confidence level, for $250 < T/K < 435$.

Figure 18 shows the deviations between the primary data points and the new correlation for viscosity. It can be seen than no point deviates from the equation by more than 2 standard deviations (±3.0%). Also shown is the deviation from the IUPAC 2009 equation,[4] also within their mutual uncertainty. Figure 19 shows the deviations of the secondary data from the proposed reference correlation, amounting to ±15%. The correlation obtained, as well as the supporting primary data, is plotted in Fig. 20.

4.6. Electrical conductivity

Electrical (or electrolytic) conductivity was also considered in the IUPAC project,[3,4] with the data of Widegren et al.,[105] Kandil et al.,[28] and Widegren and Magee[5] performed with IUPAC samples. A correlation of electrical conductivity as a function of temperature was obtained for 278 < T/K < 323, with an estimated combined expanded uncertainty of 2% at the 95% confidence level. Performed with an IUPAC sample, Santos et al.[6] obtained measurements between 270 K and 350 K, with an uncertainty of 2%, which agreed with the IUPAC correlation within their mutual uncertainties. These data were corrected with the results of Widegren and Magee[5] to obtain water-free electrical conductivity.

Twelve datasets, with a total of 110 data points, were found in the literature, extending the temperature range down to 243.48 K[38] and up to 468.15 K.[40] Table 10 shows all the information about the available data, and Fig. 21 plots the variation of the electrical conductivity with temperature, including the IUPAC (2009) correlation.[4] It can be seen that the data of Fitchett et al.[50] and 5 data points of Tokuda et al.[54,56] at the lower temperatures have deviations that do not recommend their use as primary data. In addition to Fitchett et al.[50] data, those of Leys et al.[106] do not provide any information for the purity of the home-prepared samples, so they were not considered as primary.

The measuring methods used by the authors can be classified into strong and weak techniques. By strong, we mean those where both the capacitance and resistance are balanced and the measurements are corrected to infinite frequency, and by weak, we mean the others often suffering from polarization effects, for example, those of Fitchett et al.[50] and Leys et al.[106] Only strong techniques were used in the primary data choice. The data considered as primary are summarized in Table 10. Some of the data of Tokuda et al.[54] (3 points) and Tokuda et al.[56] (2 points) at the lower temperatures (263 K–283 K) were not used, as explained above.

The same type of equation used for viscosity was used [Eqs. (7) and (8)]. The best estimate of the value of κ(298.15 K) was found with the same procedure used for viscosity. All the primary datasets where the value of the electrical conductivity at 298.15 K was available were corrected to water-free values using the equation developed by Widegren and Magee.[5] A value of κ_{wf}(298.15 K) = (0.217 ± 0.006) S m^{-1} (2.6% uncertainty at a 95% confidence level) was found. The coefficients of Eq. (7) are A_0 = 10.399 91 ± 0.304 73, A_1 = −22.1253 ± 1.0183, A_2 = 26.2132 ± 1.1169, and A_3 = −14.4874 ± 0.4031, with an uncertainty of 2.4% at a 95% confidence level, for 240 < T/K < 470.

Figure 22 shows the deviations between the primary data points and the new correlation for electrical conductivity. It can be seen than most of the data fall between the uncertainty of the data. Also shown are the deviations from the IUPAC 2009 equation[4] in the temperature

range 278 < T/K < 323, less than ±1%. This new equation has a wider temperature range than the IUPAC equation.[4] Figure 23 shows the deviations of the secondary data from the proposed correlation. The data of Fitchett et al.[50] are +38% and are not shown. The two data points of Tokuda et al.[56] mentioned before are outside the equation range.

The correlation obtained, as well as the supporting primary data, are plotted in Fig. 24.

4.7. Thermal conductivity

Thermal conductivity was not an object of analysis in the IUPAC project[3,4] as only one set of data was available at the time, namely, those of Ge et al.[107] Since then, few datasets have become available, probably due to the known difficulty of performing good measurements with electrically conducting liquids. There are 6 sets of data available with a total of 35 points, including the present data. Unfortunately, the uncertainty of the data varies between 2% and 8.2%, three of them taken with transient hot-wire probes, one with a steady-state guarded plate, one with a guarded heat flow meter, and one calculated from thermal diffusivity, density, and heat capacity using
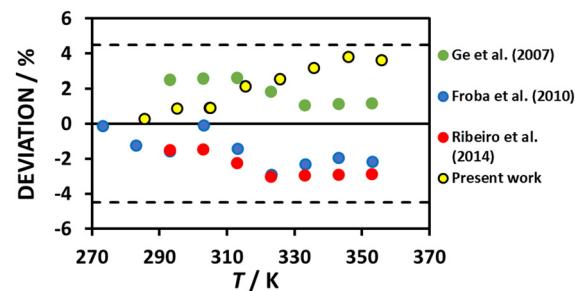
FIG. 26. Deviations between the selected data for the thermal conductivity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature. The dashed line represents the uncertainty of the correlation at a 95% confidence level (4.5%).
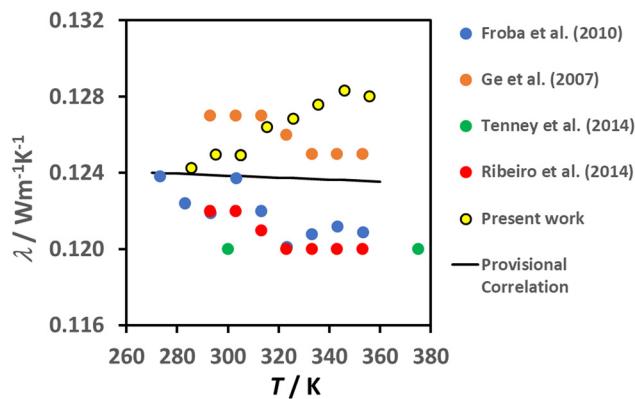
FIG. 27. Recommended variation of the thermal conductivity of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature.

TABLE 12. Available data for the refractive index of $[C_6mim][(CF_3SO_2)_2N]$, classified as primary and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (RI units)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
				Primary					
Tariq et al. (2009)[60]	SAR	293.15–333.15	0.1	4	0.0008	HS	D	0.015	Synthesized in authors' laboratory and dried under vacuum for 48 h at 60 °C–80 °C to remove impurities
Fröba et al. (2010)[62]	SAR	283.15–313.15	0.1	4	0.0006	HS	PDSA	0.086	Synthesized in authors' laboratory, dried under vacuum for 4 h at 60 °C to remove impurities, and analysis by proton NMR spectroscopy
Lago et al. (2011)[30]	SAR	298.15	0.1	1	0.000 33	HS	PDSA	0.087	Synthesized in authors' laboratory, dried by vacuum heating for 48 h at 70 °C, and analysis by proton NMR spectroscopy
González et al. (2012)[33]	SAR	298.15	0.1	1	0.000 08	IoLiTec	D	0.007	Commercial source. Prior to its use, the compound was subjected to vacuum (0.2 Pa) at 60 °C until the density value remained constant
Seoane et al. (2012)[67]	SAR	293.15–343.15	0.1	11	0.000 48	IoLiTec	D	0.007	Dried under vacuum for 70 h at 40 °C to remove impurities

TABLE 12. (*Continued.*)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (RI units)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
Montalban et al. (2015)[75]	SAR	293.15–343.15	0.1	6	0.0016	IoLiTec	PDSA	0.0089	Synthesized in authors' laboratory, dried under vacuum for 30 h at 70 °C to remove impurities, and analysis by proton NMR spectroscopy
Branco et al. (2015)[109]	SAR	298.15	0.1	1	0.0014	IoLiTec	MPFP	0.026	Dried under vacuum for 48 h at 40 °C to remove impurities
Montalban et al. (2016)[77]	SAR	298.15	0.1	1	0.0011	IoLiTec	PDSA	0.089	Synthesized in authors' laboratory, dried under vacuum for 30 h at 70 °C to remove impurities, and analysis by proton NMR spectroscopy
Andresova et al. (2017)[46]	SAR	298.15	0.1	1	0.0007	IoLiTec		0.017	Commercial source, NMR analysis, and dried for at least 16 h under vacuum (8–10 mbar) at ~60 °C
Saien et al. (2018)[110]	SAR	293.2–308.2	0.09	3	0.0014	HS	PDSA	0.065	Synthesized in authors' laboratory, dried under vacuum for 6 h at 70 °C to remove impurities, and analysis by proton NMR spectroscopy
Present work	SAR	283.15–343.15	0.1	13	0.000 16	IUPAC	PDSA	0.060	Description in Sec. 2.1
Secondary									
Muhammad et al. (2008)[59]	SAR	302.95–332.95	0.1	7	0.0013	Merck	D	0.0268	Dried by vacuum heating

TABLE 12. (Continued.)

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (RI units)	Sample origin[b]	Purity class	w_{water} (%)[c]	Observations
Yunus et al. (2010)[65]	SAR	298.15	0.1	1	0.000 51	HS	PDSA	NA	Synthesized in the authors' laboratory, dried under vacuum for 3 days at 35 °C to remove impurities, and analysis by proton NMR spectroscopy
Akbar and Murugesan (2012)[66]	SAR	303.15–323.15	0.1	5	0.000 83	Merck	PDSA	0.023	Analysis by HPLC and dried by vacuum heating at 80 °C for 48 h before use
Corderi et al. (2013)[111]	SAR	298.15–313.15	0.1	2	0.000 37	IoLiTec	MPFP	0.007	Dried under vacuum at 343 K to remove impurities
Tao et al. (2016)[112]	MDA	282.99–293.39	0.1	11	0.000 3	Cheng Jie Chemical Co. Ltd.	MPFP	0.041	Dried under vacuum for 48 h at 40 °C to remove impurities and kept in the vacuum desiccator with P_2O_5 before use

[a]SAR, Standard Abbé Refractometry; MDA, Minimum Deviation Angle.
[b]Note that the IUPAC sample is as described in text and HS means synthesized in authors' laboratory.
[c]NA, Not Available.

a thermal grating technique, which limits the establishment of primary data.

Figure 25 shows all the available data present in Table 11 in the temperature range of 273 K–375 K, including the error bars of each set of measurements. Data scatter is high with very low temperature dependencies, ranging from negative (Ge et al.,[107] Fröba et al.,[62] and Ribeiro et al.[108]), null (Frez et al.[80] and Tenney et al.[72]), to slightly positive (this work). One set of data has an uncertainty of 8.2%—the data of Tenney et al.[72] (one single value of thermal conductivity valid in the temperature range of 330 K–375 K).

As described above, particular care, affording a better uncertainty, was taken in the evaluation of the new data presented in this work, which show a minor increase with temperature (3.3% in 70 K). This positive coefficient is known for associated liquids such as water and alcohols; several ionic liquids, namely, measured in our laboratory;[8,9] and molten salts. However, we do not have enough data to produce primary correlations and decided that the existing data can support a provisional reference correlation, using all the data available except the datum of

Frez et al.,[80] which was a calculated value obtained from the direct measurement of thermal diffusivity and density and heat capacity data of others with an estimated uncertainty of 6.6%, and those of Tenney et al.,[72] which were obtained with a guarded heat flow meter, an average data point in a temperature interval.

All data are summarized in Table 11, involving a total of four reference datasets and 32 data points between 273 < T/K < 353. The variation of the reference data with temperature was found to be linear [$n = 1$, Eq. (6)], with $a_0 = 0.1254 \pm 0.0069$ W m^{-1} K^{-1} and $a_1 = (-5.087 \pm 2.15) \times 10^{-5}$ W m^{-1} K^{-2}, with an uncertainty of 4.5% at a 95% confidence level. The value predicted for the thermal conductivity λ(298.15 K) was found to be (0.124 ± 0.006) W m^{-1} K^{-1}. Deviations of reference data from the correlation are shown in Fig. 26, no point amounting to more than the uncertainty of data. In fact, all the points fall within the ±2σ band, a possible sign of the data basis heterogeneous uncertainty. Secondary data of Frez et al.[80] (2006) deviate by −5.8% and those of Tenney et al.[72] deviate by a maximum of −3.1% from the present correlation. The obtained temperature variation
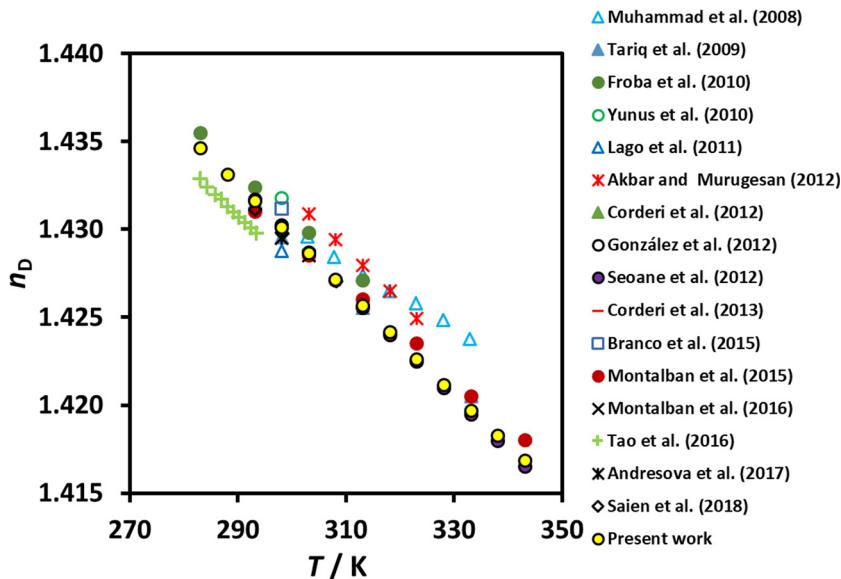
FIG. 28. The refractive index (sodium D line) of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature for all sets of data available.

slope is very small and negative. New data on this property are necessary in the near future to improve the quality of the present recommendation.

The correlation obtained, as well as the supporting reference data, is plotted in Fig. 27.

4.8. Refractive index

Refractive index was also not an object of the IUPAC project due to the small number of datasets available at that time. Today, there are

16 datasets with 72 data points, the uncertainty of the data varying between 0.0008 and 0.0016 RI units and the water content (in mass %) varying between 0.0008 and 0.0268. Table 12 summarizes all the available data, also shown in Fig. 28, in the temperature range 283 < T/K < 343. There is a large scatter, probably due to deficient calibration of Abbé refractometers, for some datasets. A careful analysis of Table 12 shows that the data of Muhammad et al.,[59] Yunus et al.,[65] Akbar and Murugesan,[66] Corderi et al.,[111] and Tao et al.[112] cannot be selected as primary data, either for deficient sample purity and water content analysis or by incorrect use of instrumentation. Therefore, 11 datasets, including the present work, were considered as primary. As
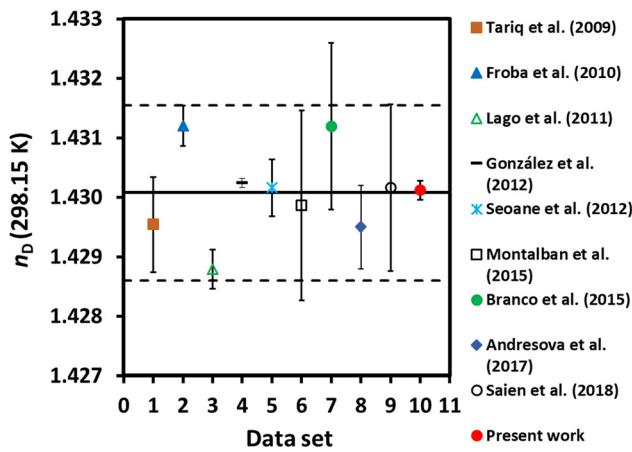
FIG. 29. Deviations of the refractive index of $[C_6mim][(CF_3SO_2)_2N]$ at 298.15 K from their average (line). The dashed lines represent the uncertainty at a 95% confidence level. Error bars of individual datasets are also shown. The black line represents the average value of the primary datasets at 298.15 K.
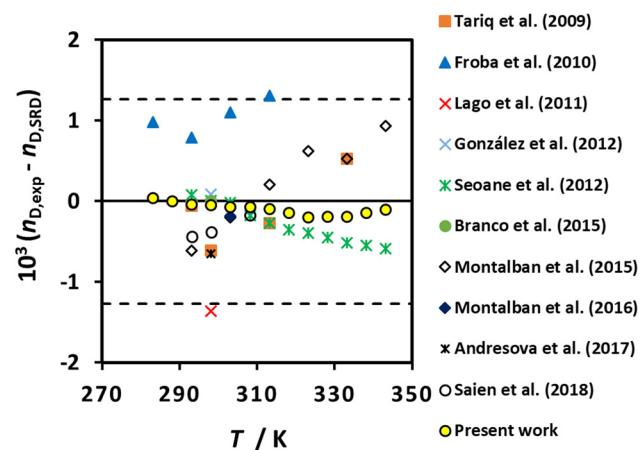
FIG. 30. Deviations between the primary data for the refractive index of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. The dashed line represents the uncertainty of the correlation at a 95% confidence level (0.001 29 RI units).
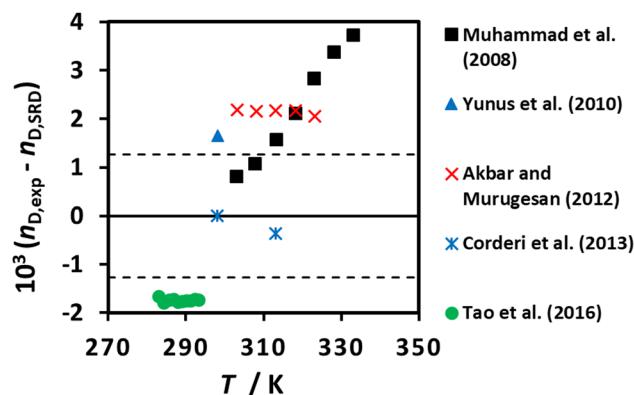
FIG. 31. Deviations between the secondary data for the refractive index of [C$_6$mim] [(CF$_3$SO$_2$)$_2$N] as a function of temperature. The dashed line represents the uncertainty of the correlation at a 95% confidence level (0.001 29 RI units).

there are no data for the refractive index dependence on the water content, we follow the procedure used in the viscosity and electrical conductivity to define the value of n(298.15 K) by averaging the value of the primary datasets, n(298.15 K) = 1.430 08 ± 0.001 47, at a 95% confidence level. Figure 29 shows the deviations from the average value of all data used in its derivation, no data deviating by more than 2 standard deviations from the average and within their mutual uncertainty.

The primary datasets are presented in Table 12. A regression line [$n = 1$, Eq. (6)] was fitted to the dependence of the refractive index on temperature in the temperature range 280 < T/K < 350, with a_0 = 1.516 89 ± 0.002 12 and a_1 = (−29.092 ± 0.668) × 10^{-6} K^{-1}, with an uncertainty of 0.001 27 RI units at a 95% confidence level. Deviations from the primary data to this line are shown in Fig. 30, not amounting to more than the uncertainty of the correlation.

Figure 31 shows the deviations of the secondary data from the reference correlation, most of it outside the correlation uncertainty, with different temperature coefficients. It includes 25 points in five datasets. The correlation obtained, as well as the supporting reference data, is plotted in Fig. 32.

4.9. Ion self-diffusion coefficient

Self-diffusion is also a very important transport property in theoretical work and electrochemical applications. In an ionic liquid, there are two types of diffusion coefficients, the cation self-diffusion coefficients, D_+, and the anion self-diffusion coefficients, D_-, which characterize the mass transfer of the ion movement.[113] An ionic liquid could be considered as a completely dissociated electrolyte (without solvent) or having the possibility of ion-pairs and other ion aggregates, causing ion association, and making the diffusion process more complex.

The diffusion of a completely dissociated electrolyte (in a solvent) can be obtained from the work of Bartel et al.,[114] and D^∞, the infinite dilution mutual (or inter-diffusion coefficient), can be related to D_+ and D_- by Eq. (9), the Nernst–Hartley limiting expression

$$D = \frac{D_+ D_- (q_+^2 + q_-^2)}{q_+^2 D_+ + q_-^2 D_-} = \frac{2 D_+ D_-}{D_+ + D_-} = D_{NH}^\infty, \qquad (9)$$

where q_+ and q_- are, respectively, the charges of the cation and the anion, ±1 in the case of [C$_6$mim][(CF$_3$SO$_2$)$_2$N]. In the case of an electrolyte forming ion-pairs, Eq. (9) is transformed to

$$D = \frac{D_{NH}^\infty}{1 + 2 K_A c_f} + \frac{D_{IP}^\infty}{1 + \dfrac{1}{2 K_A c_f}}, \qquad (10)$$

where $c_f = c_+^{eq} = c_-^{eq}$ is the average concentration of the free ions, K_A is the association constant of the ions, and D_{IP}^∞ is the diffusion coefficient of the ion-pair. These quantities are very difficult to obtain and are not known for our system. However, our system is not strictly
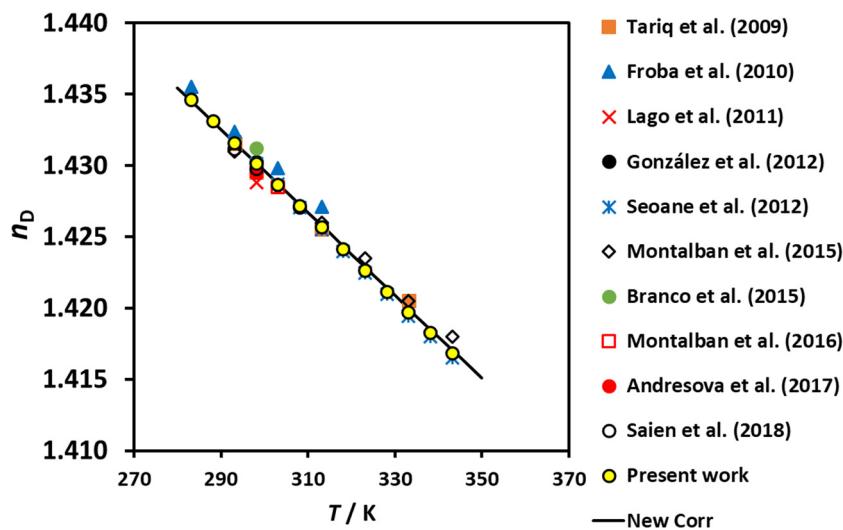

FIG. 32. Recommended variation of the refractive index of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature.

TABLE 13. Available data for the self-diffusion of $[C_6mim][(CF_3SO_2)_2N]$, classified as reference and secondary. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified

Literature source	Technique[a]	Temperature range (K)	Pressure range (MPa)	No. of data points	Assigned uncertainty (%)[b]	Sample origin[c]	Purity class	w_{water} (%)[d]	Observations
				Reference					
Tokuda et al. (2006)[56]	SE	263–353	0.1	8	5	HS	PDSA	0.001	Synthesized in the authors' laboratory, analysis by mass spectrometry, and dried by vacuum heating
Martinelli et al. (2013)[118]	SE	303	0.1	1	NA	IoLiTec	MPNP	NA	Commercial source, transferred directly to a glove box and sealed in NMR vials
Harris and Kanakubo (2015a)[38]	SE	293.3–364	0.1	37	3	HS	PDSA	0.002	Dried under vacuum at about 70 °C for 30 h to remove any excess water and purity determined by NMR analysis
				Secondary					
Tokuda et al. (2005)[54]	SE	263.15–353.15	0.1	10	NA	HS	PDSA	0.001	Synthesized in the authors' laboratory, dried under vacuum for 48 h to remove residual water, and purity determined by NMR and MS analysis
Ahosseini et al. (2017)[103]	SE	298.15–343.15	0.1	3	10	HS	PDSA	0.0125	Synthesized in the authors' laboratory, dried under vacuum, and analysis by proton NMR spectroscopy

[a]SE, NMR Spin-Echo technique.
[b]NA, Not Available.
[c]HS, synthesized in authors' laboratory.
[d]NA, Not Available.

an electrolyte but a salt. Therefore, we can have non-bonded cations (or free cations), non-bonded anions (or free anions), ion-pairs (cation–anion), and ionic aggregates of different complexity. D'Agostino et al.[115] studied the effect of aggregation in the self-diffusion coefficients of the system $[C_2mim][(CF_3SO_2)_2N]$ and found that there was a weak interaction between cations and anions. This result was also found for this compound and for $[C_4mim]$ $[(CF_3SO_2)_2N]$ by Feng et al.[116] using molecular dynamics

simulations, whereby they proved that the electrical conductivity of the electrolyte could be described by a modified Nernst–Einstein equation based exclusively on free ions but where $c_+^{eq} \approx c_-^{eq} \approx 0.2$ between 300 K and 600 K.

This complementary analysis suggests that we can assume that ion-pairing (if neutral, the ion-pairs' movement in the liquid will not transport charge and therefore not contribute to the electrical conductivity) is present in $[C_6mim][(CF_3SO_2)_2N]$. We cannot consider this ionic
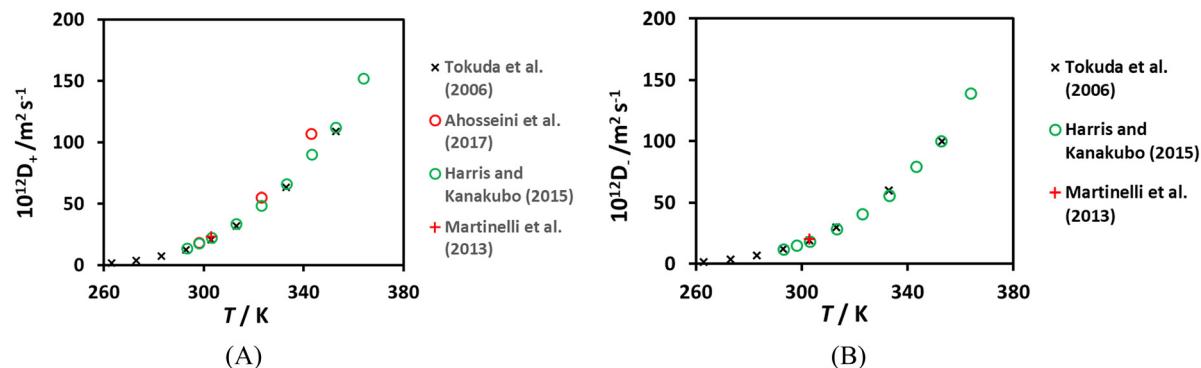
FIG. 33. Available data for the self-diffusion coefficients of $[C_6mim][(CF_3SO_2)_2N]$. (a) $[C_6mim]^+$ self-diffusion coefficient and (b) $[(CF_3SO_2)_2N]^-$ self-diffusion coefficient.

liquid as a completely dissociated electrolyte, and then, Eq. (9) is not applicable. This fact was also discussed by Harris and Kanakubo[38,117] when analyzing the Nernst–Einstein equation, which includes a factor Δ, the Nernst–Einstein deviation parameter, different from zero (~0.42) to correct the electrical conductivity in an ionic medium from the free ion expression [correction is $(1 - \Delta)$]. For these reasons, we restrict here our analysis to the ion self-diffusion coefficients, the only experimentally measurable diffusion coefficients in a pure salt.

There are only five datasets on the self-diffusion coefficients, all summarized in Table 13: One set with diffusion by Tokuda et al.[54] (registered in ILThermo[26]) and four sets with ionic self-diffusion coefficients by Tokuda et al.,[56] Martinelli et al.,[118] Harris and Kanakubo,[38] and Ahosseini et al.,[103] the last one being only for the cation, all obtained with the NMR spin-echo technique (pulsed gradient field) and a total of 59 data points. The data of Tokuda et al.[54] registered in ILThermo were wrongly calculated from ionic species data and therefore will not be used in the foregoing analysis. We report in Fig. 33 the available data for the two ion self-diffusion coefficients as a function of temperature.

The data of Ahosseini et al.[103] for the self-diffusion coefficient of the cation have a claimed uncertainty of 10% and deviate very much from the data of the other authors, namely, for temperatures above 300 K [see Fig. 33(a)]. As we only have three sets of data,[38,56,118] we used these sets to define a provisional correlation, as we did for thermal conductivity. The data of Harris and Kanakubo[38] were averaged for the same nominal temperatures (9 points) in order to calculate the chemical diffusion coefficients and not overweight the correlation. A total of 18 data points were used. Reference data for the ion self-diffusion coefficient correlation are summarized in Table 13.

The correlation equation used was Eq. (7). The value of the self-diffusion coefficients at 298.15 K could not be obtained accurately, so we decided to have a reference temperature of 303.15 K. The values chosen for the ion self-diffusion coefficients at 303.15 K were $10^{12}D_+(303.15 \text{ K}) = (22.5 \pm 0.6) \text{ m}^2 \text{ s}^{-1}$ and $10^{12}D_-(303.15 \text{ K}) = (19.0 \pm 0.9) \text{ m}^2 \text{ s}^{-1}$. The optimized parameters for the two different correlation equations are as follows: For the cation self-diffusion coefficient, $A_0 = 0.463\,46 \pm 0.719\,71$, $A_1 = 12.674 \pm 1.471$, and $A_2 = -13.158 \pm 0.747$, with an uncertainty of 5% at a 95% confidence level. For the anion self-diffusion coefficient, $A_0 = 0.351\,54 \pm 1.100\,80$, $A_1 = 13.102 \pm 2.249$, and $A_2 = -13.459 \pm 1.143$, with an uncertainty of

7.7% at a 95% confidence level. The correlations are valid for the temperature interval $260 < T/\text{K} < 370$.

The correlation obtained, as well as the supporting reference data, is plotted in Fig. 34, which shows the deviations of the experimental data from the correlated equations.

4.10. An inter-property consistency check

The properties of ionic liquids show several relations between them, some with theoretical basis and some others with mostly empirical confirmation. One of the proposed ways to understand the interionic/molecular forces in ionic liquid systems is the use of the Walden rule, proposed by Angell and co-workers[119–121] to classify the ionic power of the ionic liquid. The Walden rule relates limiting molar conductivity, Λ_m^0, of the ionic liquid system and the viscosity, η, of the pure liquid, in the form

$$\Lambda_m^0 \times \eta^\alpha = C', \qquad (11)$$

where α was originally proposed as 1 ("ideal" Walden rule) but found to be of the order of 0.8 ± 0.1 by several workers, well analyzed by Schreiner et al.,[122] and C' is a constant. By definition, for a pure ionic liquid,
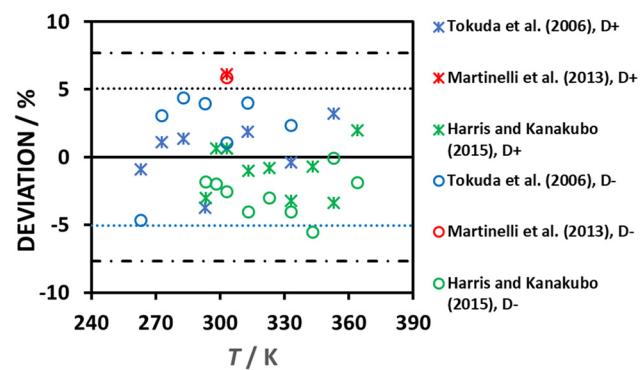
FIG. 34. Deviations between the reference data for the ionic self-diffusion coefficients of $[C_6mim][(CF_3SO_2)_2N]$ as a function of temperature. ✳, D_+ and o, D_-. Blue, Tokuda et al. (2006)[56]; green, Harris and Kanakubo (2015)[38]; and red, Martinelli et al. (2013).[118] Also represented is the uncertainty of the correlation at a 95% confidence level. Dotted lines, D_+, 5%, and dashed-dotted lines, D_-, 7.7%.
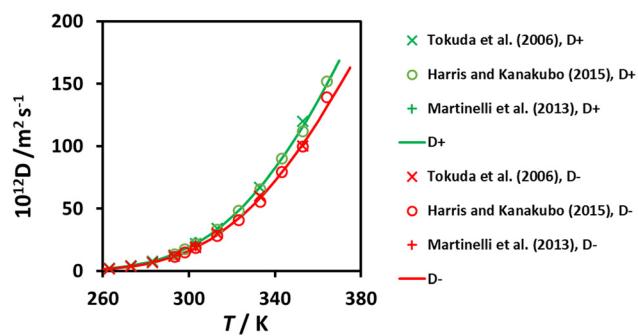
FIG. 35. Recommended variation of the ion self-diffusion coefficient of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature.
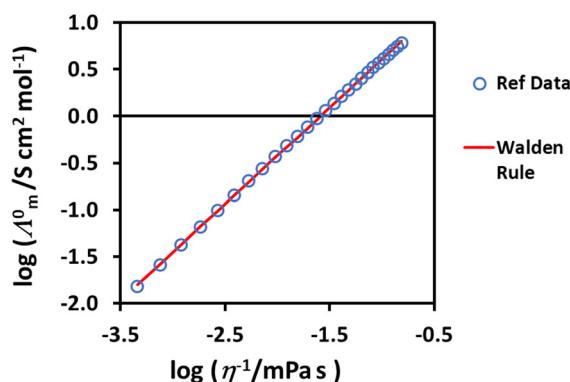
FIG. 36. Walden rule verification for [C$_6$mim][(CF$_3$SO$_2$)$_2$N].

$$\Lambda_m^0 = \kappa \left(\frac{M}{\rho} \right) \tag{12}$$

and

$$\log \Lambda_m^0 = \log C' + \alpha \log \left(\eta^{-1} \right). \tag{13}$$

In Fig. 36, we represent $\log \Lambda_m^0$ as a function of $\log \left(\eta^{-1} \right)$, using our reference data for density, electrical conductivity, and viscosity, as a function of temperature, between 250 K and 380 K. A straight line is obtained with an intercept of 1.634 20 ± 0.004 72 and a slope of 1.0277 ± 0.0025, giving $\alpha = 1.03$. This confirms that [C$_6$mim][(CF$_3$SO$_2$)$_2$N] obeys the "ideal" Walden rule, with a coefficient very close to one, a sign of inter-property consistency. Notably, there is a current discussion about the definition of Angell and co-workers of the ionicity concept, namely, about the use of deviations to an arbitrarily chosen 1 M KCl aqueous solution as a reference, not thermodynamically ideal (activity coefficients greater than unity), and the consideration of the "ideal" Walden rule.[122,123] However, this fact does not affect the inter-property consistency check performed.

No other effort was made in the present work to explain theoretically the variation of the different properties with temperature.

4.11. Some comments about the normal melting temperature

To define the temperature range of the tabulations, namely, in the lower temperature side, it is necessary to define the normal melting temperature based on published results. The ILThermo database[26] includes 9 datasets, 6 obtained with DSC/DTA experiments, 2 from heating/cooling curves, and 1 from visual observation. These results are presented in Table 14 and in Fig. 37, and it can be concluded that there are deviations between the published data greater than their mutual uncertainty. The works of Archer,[86] Shevelyova et al.,[124] Wachter et al.,[125] and Hughes et al.[89] agree within their mutual uncertainty [expanded uncertainty at a 0.95 level of confidence ($k = 2$)]. An average value of $T_{melt} = (271.72 \pm 0.45)$ K was taken as the best estimate of the normal melting temperature. From the thermophysical properties studied in this work, it is clear that

TABLE 14. Available publications for the normal melting temperature of [C$_6$mim][(CF$_3$SO$_2$)$_2$N], classified as reference and secondary. Methods of measurement, phase transition, sample purity, melting point temperature, quoted uncertainty, and water content are identified

Literature source	Phase transition	Technique[a]	Purity (wt. %)[b]	T_{melt} (K)	U (K)[c]	w_{water} (%)
		Reference				
Archer (2006)[86]	Crys–liquid	DSC	99.5[d]	272.11	0.29	0.002
Shevelyova et al. (2007)[124]	Crys–liquid	VO	99.76[d]	272.0	0.4	0.002
Wachter et al. (2010)[125]	Crys–liquid	HCC	99.5	271.3	0.8	0.005
Hughes et al. (2011)[89]	Crys–liquid	DSC	NA	271.45	0.61	0.01
		Secondary				
Tokuda et al. (2005)[54]	Crys–liquid	DSC	99	267.1	1	0.01
Archer (2006)[86]	MetCrys–liquid	DSC	99.5[d]	265.8	1	0.002
Tokuda et al. (2006)[56]	Crys–liquid	DSC	99	267.1	6	0.04
Gomez et al. (2013)[90]	Crys–liquid	HCC	99	269	3	0.005
Rodrigues et al. (2016)[126]	Crys–liquid	DSC	>98	262.6	1.1	NA
Xue et al. (2016)[43]	Crys–liquid	DSC	99.8	261.9	3.4	0.008

[a]DSC, Differential Scanning Calorimetry; HCC, Heating/Cooling Curves; and VO, Visual Observation.
[b]NA, Not Available.
[c]With expanded uncertainty at a 95% confidence level ($k = 2$).
[d]IUPAC sample as described in text.
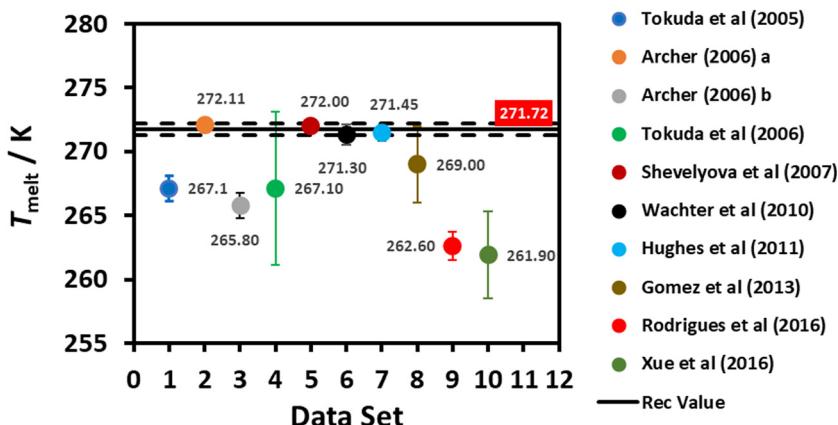
FIG. 37. The normal melting temperature of [C$_6$mim][(CF$_3$SO$_2$)$_2$N]. x-axis entries 1 (Ref. 54), 2 (Ref. 86), 3 (Ref. 86), 4 (Ref. 56), 5 (Ref. 124), 6 (Ref. 125), 7 (Ref. 89), 8 (Ref. 90), 9 (Ref. 126), and 10 (Ref. 43) correspond to the values in Table 14. The black line (and data point 11) shows the suggested normal melting temperature, $T_m = (271.72 \pm 0.45)$ K. The dashed lines represent the uncertainty at a 95% confidence level.

several literature data have been obtained with supercooled liquid samples, namely, for density, heat capacity, electrical conductivity, and viscosity, or with high scanning rates in the DSC measurements. Noteworthy, and given the recommended value of the triple point as $T_t = 272.13 \pm 0.05$ K,[4] the value of the upper limit of T_{melt}, 272.17 K, agrees very well with the triple-point temperature, to within 0.04 K.

5. Tabulations

The reference equations developed can now be used to tabulate recommended values of the thermophysical properties of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] within the range of temperatures for which they have been developed in the current work and at the pressure of 0.1 MPa. They refer only to the liquid state for temperatures above the recommended triple-point temperature, $T_t = (272.13 \pm 0.05)$ K.[4] Whenever the values for water-free data could be obtained, the correlations refer to these data (viscosity and electrical conductivity).

Table 15 presents the recommended reference data for all the properties studied, including their uncertainties and the value of each property at 298.15 K. The number of digits of each tabulated value is consistent with the proposed uncertainty of the correlations, at the 95% confidence level, shown in the last line of Table 15. For the different properties covered by the IUPAC project, comparison was made in the respective section with the IUPAC reference correlations (density, speed of sound, heat capacity, viscosity, and electrical conductivity), and it was demonstrated that both correlations agree within mutual uncertainties in the overlapping temperature interval. The dashed line represents the melting line, the separation between data on supercooled liquid and normal liquid.

6. Cautions in the Use of Tabulated Thermophysical Properties

As the pressure at the triple point is nearly zero, the results can also be considered at the saturation line of the ionic liquid, as the dependence of the studied properties on pressure is very weak, up to 10 MPa. However, the data on the heat capacity of the liquid

phase have a branch of metastable liquid, up to 190 K (glass transition temperature),[4] which has no discontinuity. Therefore, the values tabulated must be used with care[3,86] above the dashed line.

As mentioned in previous works,[15,18–21] the values presented in Table 15 serve two main purposes:

- They can act as a test of quality (and uncertainty) of absolute instruments, applied to measurements in ionic liquids, checking if the instruments are operating according to their design/specifications.
- They are a means for calibrating relative instruments, for which no full working equation is available. Nonetheless, calibration robustness relies on the use of at least two calibrants with very different density values in the case of vibrating-tube densimetry or on sensor wettability in surface tension measurements.

7. Conclusions

New experimental results for the density, speed of sound, surface tension, thermal conductivity, and refractive index of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] were obtained with low uncertainty, respectively, 0.12 kg m^{-3}, 0.07 m s^{-1}, 0.035 mN m^{-1}, 0.8 mW m^{-1} K^{-1}, and 0.000 09 RI units.

New standard reference data for the density, speed of sound, heat capacity, viscosity, electrical conductivity, thermal conductivity, refractive index, and ion self-diffusion coefficients of [C$_6$mim][(CF$_3$SO$_2$)$_2$N], based on ITS-90, are proposed, covering most of the normal liquid range at 0.1 MPa. This work complements and replaces previous IUPAC correlations, presented in 2009, with a better uncertainty and/or a more extensive temperature range. Calibration of secondary instruments is now possible in temperature ranges where ionic liquids are thermally and kinetically stable and also for other high-viscosity liquids for which there are not many accepted calibrants.

The proposed values of the properties at 298.15 K have uncertainties (95% confidence level) that are the best possible now.

TABLE 15. Recommended reference data for the thermophysical properties of [C$_6$mim][(CF$_3$SO$_2$)$_2$N] as a function of temperature at P = 0.1 MPa[a]

T (K)	ρ (kg m^{-3})	c (m s^{-1})	C_p (J mol^{-1} K^{-1})	γ (mN m^{-1})	η (mPa s)	κ (S m^{-1})	λ (mW m^{-1} K^{-1})	$10^{12}D_+$ (m^2 s^{-1})	$10^{12}D_-$ (m^2 s^{-1})	n
190			573.2							
200			577.1							
210			581.2							
220			585.6							
230			590.3							
240			595.3			0.0026				
250	1416.0		600.5		2191	0.0048				
255	1411.5		603.2		1321	0.0082				
260	1406.9		605.9		833	0.0133	1.59	1.32		
265	1402.4		608.7		546	0.0207	2.35	1.96		
270	1397.8		611.6		371	0.0310	0.1240	3.38	2.83	
275	1393.3	1281.8	614.5		260	0.0448	0.1240	4.74	4.00	
280	1388.7	1269.6	617.4	32.61	188	0.0628	0.1240	6.51	5.51	1.435 43
285	1384.2	1257.6	620.4	32.36	139	0.0855	0.1239	8.75	7.44	1.433 98
290	1379.6	1245.7	623.4	32.10	105	0.1136	0.1239	11.54	9.84	1.432 52
295	1375.1	1234.0	626.5	31.85	81.4	0.1476	0.1239	14.95	12.79	1.431 07
300	1370.5	1222.4	629.6	31.60	64.1	0.1879	0.1238	19.04	16.35	1.429 61
305	1366.0	1211.0	632.7	31.34	51.4	0.2348	0.1238	23.89	20.57	1.428 16
310	1361.4	1199.7	635.9	31.09	41.8	0.2887	0.1238	29.56	25.52	1.426 70
315	1356.9	1188.6	639.1	30.83	34.5	0.3497	0.1238	36.09	31.23	1.425 25
320	1352.3	1177.7	642.4	30.58	28.8	0.4179	0.1237	43.52	37.75	1.423 80
325	1347.8	1166.9	645.6	30.33	24.4	0.4933	0.1237	51.89	45.09	1.422 34
330	1343.2	1156.3	648.9	30.07	20.8	0.5760	0.1237	61.21	53.29	1.420 89
335	1338.7	1145.9	652.3	29.82	18.0	0.6658	0.1237	71.48	62.34	1.419 43
340	1334.1	1135.6	655.6	29.56	15.6	0.7625	0.1236	82.71	72.24	1.417 98
345	1329.6	1125.5	659.0	29.31	13.7	0.8661	0.1236	94.88	82.98	1.416 52
350	1325.0		662.4	29.06	12.1	0.976	0.1236	108.0	94.5	1.415 07
355	1320.5		665.8	28.80	10.8	1.093	0.1236	121.9	106.9	
360	1315.9		669.2	28.55	9.63	1.216	0.1235	136.7	119.9	
365	1311.4		672.7		8.66	1.345		152.2	133.7	
370	1306.8		676.1		7.84	1.479		168.4	148.1	
375	1302.3		679.6		7.12	1.619		185.3	163.0	
380	1297.7		683.1		6.50	1.765				
385			686.6		5.96	1.915				
390			690.1		5.48	2.071				
395			693.6		5.06	2.232				
400			697.1		4.69	2.397				
405			700.6		4.36	2.567				
410			704.1		4.06	2.741				
415			707.6		3.79	2.920				
420			711.1		3.55	3.102				
425			714.5		3.33	3.290				
430			718.0		3.13	3.481				
435			721.5		2.95	3.677				
440			724.9			3.877				
445			728.3			4.081				
450			731.7			4.289				
460			738.5			4.501				
470			745.2			4.717				
480			751.8							

TABLE 15. (*Continued.*)

T (K)	ρ (kg m^{-3})	c (m s^{-1})	C_p (J mol^{-1} K^{-1})	γ (mN m^{-1})	η (mPa s)	κ (S m^{-1})	λ (mW m^{-1} K^{-1})	$10^{12}D_+$ (m^2 s^{-1})	$10^{12}D_-$ (m^2 s^{-1})	n
490			758.2							
500			764.5							
510			770.7							
520			776.7							
530			782.5							
540			788.1							
298.15	1372.2	1226.7	629.1	31.69	70.4	0.217	0.124	22.5	19.0	1.430 08
	±1.1	±1.0	±2.2	±0.35	±1.9	±0.006	±0.006	±1.2	±1.8	±0.001 47
	0.08%	0.08%	0.35%	1.1%	2.7%	2.6%	4.5%	5.3%	7.7%	0.1%

[a]With expanded uncertainty at a 0.95 level of confidence ($k = 2$).

Whenever possible, water-free values were obtained. Details of the temperature range of each property reference equation and their uncertainty are conveniently displayed in the recommended reference data table (Table 15) and in the supplementary material.

As an inter-property consistency check for the ionic liquid, the Walden rule was found to be obeyed.

8. Supplementary Material

The supplementary material contains tables of all the available experimental data up to mid-July 2020 for the thermophysical properties of [C$_6$mim][(CF$_3$SO$_2$)$_2$N]. Methods of measurement, temperature and pressure ranges, quoted uncertainty, sample purity, and water content are identified. It also includes the numerical coefficients of the VFT (Vogel-Fulcher-Tammann) equation for the viscosity, electrical conductivity, and self-diffusion of [C$_6$mim][(CF$_3$SO$_2$)$_2$N], as well as Table S11 with all the recommended reference equations for the different properties.

9. Authors' Contributions

The new experimental measurements were performed by X.P. and M.J.V.L. (thermal conductivity), C.S.G.P.Q. (refractive index), Â.F.S. (density and speed of sound), and M.S.C.S.S. (surface tension), who also contributed to the respective section analysis. Viscosity, electrical conductivity, and rheology measurements were performed by F.J.V.S. X.P. was responsible for the collection and comparison of available literature data, in conjunction with Carlos Nieto de Castro. The establishment of the recommended reference correlations and data was performed by F.J.V.S., M.J.V.L., X.P., and C.A.N.C., who wrote the final version of this manuscript.

10. Data Availability

The data that support the findings of this study are available within the article and in the supplementary material. The authors are willing to provide any additional information for sensible requests (cacastro@ciencias.ulisboa.pt).

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