Reference Material for Review Only

Supporting Information for "Calculating the Enthalpy of Vaporization for Ionic Liquid Clusters"

Manish S. Kelkar[†] and Edward J. Maginn[†1]

[†]Department of Chemical and Biomolecular Engineering, University of Notre Dame, 182 Fitzpatrick Hall, Notre Dame, IN 46556-5637, USA.

Table 1: Effect of temperature on the enthalpy of vaporization of $[bmim][PF_6]$.[1]

T (K)	c (J/cm^3)	v (cm^3/mol)	Δu_{vap} (kJ/mol)	RT (kJ/mol)	Δh_{vap} (kJ/mol)
298	761	207.80	158	2.48	161
323	738	210.60	155	2.69	158
343	727	212.90	155	2.85	158

Table 2: Effect of temperature on the enthalpy of vaporization of $[bmim][NO_3]$.[2]

T (K)	c (J/cm^3)	v (cm^3/mol)	Δu_{vap} (kJ/mol)	RT (kJ/mol)	Δh_{vap} (kJ/mol)
298	892	175.60	157	2.48	159
323	866	178.30	154	2.69	157
363	824	182.40	150	3.02	153
423	756	190.80	144	3.52	148

[1]To whom correspondence should be addressed. Phone: (574) 631-5687. Fax: (574) 631-8366. E-mail: ed@nd.edu

Table 3: Effect of temperature, alkyl chain length and the alkyl substituents on the pyridinium ring on the enthalpy of vaporization for various pyridinium cations paired with the $[Tf_2N]$ anion.[3]

$System$	T (K)	c (J/cm^3)	v (cm^3/mol)	Δu_{vap} (kJ/mol)	RT (kJ/mol)	Δh_{vap} (kJ/mol)
$[hmpy][Tf_2N]$	298	549	325.36	179	2.48	181
	308	533	326.77	174	2.56	177
	318	542	329.34	179	2.64	181
	328	538	330.00	178	2.73	180
	338	532	332.83	177	2.81	180
	348	541	333.65	181	2.89	183
$[ompy][Tf_2N]$	298	513	362.30	186	2.48	188
	308	504	363.62	183	2.56	186
	318	505	364.84	184	2.64	187
	328	507	366.82	186	2.73	189
	338	481	368.63	177	2.81	180
	348	483	371.60	179	2.89	182
$[hdmpy][Tf_2N]$	298	503	346.75	174	2.48	177
	308	491	348.45	171	2.56	174
	318	483	351.78	170	2.64	173
	328	492	350.43	172	2.73	175
	338	490	351.89	172	2.81	175
	348	489	354.83	174	2.89	176

Table 4: Effect of temperature on the enthalpy of vaporization of triazolium nitrate species.[2]

$System$	T (K)	c (J/cm^3)	v (cm^3/mol)	Δu_{vap} (kJ/mol)	RT (kJ/mol)	Δh_{vap} (kJ/mol)
$[124tr][NO_3]$	373	2731	81.80	223	3.10	227
	398	2676	82.50	221	3.31	224
	423	2622	83.30	218	3.52	222
	448	2575	84.20	217	3.72	221
	473	2513	85.10	214	3.93	218
$[123tr][NO_3]$	373	2679	82.10	220	3.10	223
	398	2625	82.80	217	3.31	221
	423	2587	83.60	216	3.52	220
	448	2541	84.60	215	3.72	219
	473	2475	85.50	212	3.93	216
$[4am124tr][NO_3]$	373	2287	92.70	212	3.10	215
	398	2246	93.30	210	3.31	213
	423	2199	94.20	207	3.52	211
	448	2154	95.20	205	3.72	209
	473	2098	96.20	202	3.93	206

Table 5: Effect of temperature on the enthalpy of vaporization of triazolium based cation with perchlorate anion.[2]

$System$	T (K)	c (J/cm^3)	v (cm^3/mol)	Δu_{vap} (kJ/mol)	RT (kJ/mol)	Δh_{vap} (kJ/mol)
$[124tr][ClO_4]$	373	2422	97.00	235	3.10	238
	398	2384	97.80	233	3.31	236
	423	2353	98.60	232	3.52	236
	448	2313	99.30	230	3.72	233
	473	2261	100.60	227	3.93	231
$[123tr][ClO_4]$	373	2388	97.50	233	3.10	236
	398	2359	98.30	232	3.31	235
	423	2314	99.20	230	3.52	233
	448	2286	100.10	229	3.72	233
	473	2246	101.10	227	3.93	231
$[4am124tr][ClO_4]$	373	2078	107.90	224	3.10	227
	398	2039	108.90	222	3.31	225
	423	2011	109.80	221	3.52	224
	448	1961	111.10	218	3.72	222
	473	1910	112.20	214	3.93	218
$[1m4am124tr][ClO4]$	373	1322	129.00	171	3.10	174
	398	1289	130.40	168	3.31	171
	423	1261	131.80	166	3.52	170
	448	1223	133.50	163	3.72	167
	473	1196	135.00	161	3.93	165

References and Notes

1. Morrow, T. I.; Maginn, E. J. *J. Phys. Chem. B* **2002,** *106,* 12807–12813.

2. Cadena, C.; Maginn, E. J. *J. Phys. Chem. B* **2006,** *110,* 18026.

3. Cadena, C.; Zhao, Q.; Snurr, R. Q.; Maginn, E. J. *J. Phys. Chem. B* **2006,** *110,* 2821.