

Supporting information

Katharina Bica^(a), Maggel Deetlefs^(b), Christian Schröder^{*(c)} and Kenneth R. Seddon^(b)

- (a) Institute of Applied Synthetic Chemistry
Vienna University of Technology
Getreidemarkt 9/163, A-1010 Vienna, Austria
- (b) QUILL Research Centre
David Keir Building, Stranmillis Road,
Belfast, Northern Ireland
- (c) Department of Computational Biological Chemistry
University of Vienna
Währingerstrasse 17, A-1090 Vienna, Austria
University of Vienna
christian.schroeder@univie.ac.at

Densities and refractive indices of the learning set

ionic liquid	reference	ρ^{exp}	ρ^{DR}	n^{exp}	n^{DR}
1-butyl-2,3-dimethylimidazolium tetrafluoroborate	28	1.1912	1.163	1.433	1.425
1-ethyl-3-methylimidazolium tetrafluoroborate	23	1.28	1.256	1.4	1.412
1-ethyl-3-methylimidazolium tetrafluoroborate	87	1.27973	1.256	1.411	1.412
1-butyl-3-methylimidazolium tetrafluoroborate	24	1.2014	1.189	1.4219	1.421
1-butyl-3-methylimidazolium tetrafluoroborate	25	1.20141	1.189	1.4219	1.421
1-butyl-3-methylimidazolium tetrafluoroborate	26	1.2141	1.189	1.4197	1.421
1-butyl-3-methylimidazolium tetrafluoroborate	27	1.2	1.189	1.422	1.421
1-butyl-3-methylimidazolium tetrafluoroborate	28	1.2003	1.189	1.422	1.421
1-butyl-3-methylimidazolium tetrafluoroborate	29	1.201	1.189	1.4218	1.421
1-butyl-3-methylimidazolium tetrafluoroborate	30	1.12	1.189	1.429	1.421
1-butyl-3-methylimidazolium tetrafluoroborate	87	1.20257	1.189	1.4206	1.421
1-hexyl-3-methylimidazolium tetrafluoroborate	87	1.14603	1.141	1.4276	1.428
1-hexyl-3-methylimidazolium tetrafluoroborate	62	1.1439	1.141	1.42371	1.428
1-methyl-3-octylimidazolium tetrafluoroborate	68	1.10442	1.105	1.43329	1.433
1-methyl-3-octylimidazolium tetrafluoroborate	61	1.1144	1.105	1.4322	1.433
1-methyl-3-octylimidazolium tetrafluoroborate	26	1.103	1.105	1.4319	1.433
1-methyl-3-octylimidazolium tetrafluoroborate	42	1.10108	1.105	1.4319	1.433

1-methyl-3-octylimidazolium tetrafluoroborate	80	1.095	1.105	1.4322	1.433
1-methyl-3-octylimidazolium tetrafluoroborate	87	1.10422	1.105	1.4321	1.433
1-methyl-3-decylimidazolium tetrafluoroborate	80	1.064	1.078	1.4367	1.436
3-butyloxymethyl-1-methylimidazolium tetrafluoroborate	80	1.189	1.199	1.4239	1.423
3-pentyloxymethyl-1-methylimidazolium tetrafluoroborate	80	1.155	1.175	1.4257	1.426
3-hexyloxymethyl-1-methylimidazolium tetrafluoroborate	80	1.141	1.154	1.4293	1.429
3-heptyloxymethyl-1-methylimidazolium tetrafluoroborate	80	1.133	1.136	1.4313	1.431
3-octyloxymethyl-1-methylimidazolium tetrafluoroborate	80	1.113	1.12	1.4338	1.433
1-butyl-3-methylimidazolium hexafluorophosphate	60	1.35	1.359	1.409	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	79	1.38	1.359	1.40925	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	52	1.3673	1.359	1.40937	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	56	1.3673	1.359	1.40937	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	58	1.3673	1.359	1.40937	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	57	1.3673	1.359	1.40937	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	53	1.3673	1.359	1.40937	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	55	1.3673	1.359	1.40937	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	47	1.36607	1.359	1.4095	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	26	1.3679	1.359	1.4089	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	33	1.36788	1.359	1.4089	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	27	1.38	1.359	1.41	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	29	1.3639	1.359	1.4095	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	44	1.36788	1.359	1.4089	1.410
1-butyl-3-methylimidazolium hexafluorophosphate	87	1.36811	1.359	1.4075	1.410
1-hexyl-3-methylimidazolium hexafluorophosphate	78	1.2937	1.292	1.41787	1.417
1-hexyl-3-methylimidazolium hexafluorophosphate	52	1.2937	1.292	1.41787	1.417
1-hexyl-3-methylimidazolium hexafluorophosphate	58	1.2937	1.292	1.41787	1.417
1-hexyl-3-methylimidazolium hexafluorophosphate	56	1.29366	1.292	1.41787	1.417
1-hexyl-3-methylimidazolium hexafluorophosphate	57	1.2937	1.292	1.41787	1.417
1-hexyl-3-methylimidazolium hexafluorophosphate	55	1.2937	1.292	1.41787	1.417
1-hexyl-3-methylimidazolium hexafluorophosphate	59	1.2937	1.292	1.41787	1.417
1-hexyl-3-methylimidazolium hexafluorophosphate	87	1.29353	1.292	1.417	1.417

1-methyl-3-octylimidazolium hexafluorophosphate	60	1.237	1.241	1.423	1.423
1-methyl-3-octylimidazolium hexafluorophosphate	52	1.2357	1.241	1.42302	1.423
1-methyl-3-octylimidazolium hexafluorophosphate	56	1.23572	1.241	1.42302	1.423
1-methyl-3-octylimidazolium hexafluorophosphate	58	1.2357	1.241	1.42302	1.423
1-methyl-3-octylimidazolium hexafluorophosphate	57	1.2357	1.241	1.42302	1.423
1-methyl-3-octylimidazolium hexafluorophosphate	55	1.2357	1.241	1.42302	1.423
1-methyl-3-octylimidazolium hexafluorophosphate	59	1.2357	1.241	1.42302	1.423
1-methyl-3-octylimidazolium hexafluorophosphate	87	1.23617	1.241	1.4227	1.423
1-ethyl-3-methylimidazolium trifluoroacetate	81	1.285	1.295	1.4405	1.437
1-butyl-3-methylimidazolium trifluoroacetate	60	1.21	1.226	1.449	1.442
1-butyl-3-methylimidazolium trifluoroacetate	81	1.209	1.226	1.4487	1.442
1-butyl-3-methylimidazolium trifluoroacetate	81	1.183	1.226	1.4441	1.442
1,3-diethylimidazolium trifluoroacetate	81	1.25	1.258	1.4431	1.440
1-ethyl-3-methylimidazolium acetate	Sigma-Aldrich	1.027	1.109	1.502	1.484
1-ethyl-3-methylimidazolium dicyanamide	46	1.10891	1.162	1.5102	1.537
1-butyl-3-methylimidazolium perchlorate	61	1.2527	1.242	1.4725	1.499
1-ethyl-3-methylimidazolium methylphosphonate	41	1.1885	1.306	1.4928	1.508
1-hexyl-3-methylimidazolium chloride	60	1.03	1.034	1.515	1.513
1-hexyl-3-methylimidazolium chloride	76	1.03967	1.034	1.5172	1.513
1-hexyl-3-methylimidazolium chloride	36	1.0404	1.034	1.52182	1.513
1-methyl-3-octylimidazolium chloride	60	1.	1.01	1.505	1.506
1-methyl-3-octylimidazolium chloride	50	1.0104	1.01	1.507	1.506
1-methyl-3-octylimidazolium chloride	63	1.007	1.01	1.5058	1.506
1-methyl-3-octylimidazolium chloride	76	1.00882	1.01	1.50987	1.506
1-methyl-3-octylimidazolium chloride	34	1.00882	1.01	1.51051	1.506
1-methyl-3-octylimidazolium chloride	38	1.00882	1.01	1.51051	1.506
1-methyl-3-octylimidazolium chloride	43	1.0096	1.01	1.5062	1.506
1-vinyl-3-hexylimidazolium bis(trifluoromethylsulfonyl)imide	32	1.36	1.515	1.443	1.474
1-vinyl-3-nonylimidazolium bis(trifluoromethylsulfonyl)imide	32	1.28	1.316	1.445	1.445
1-vinyl-3-dodecylimidazolium bis(trifluoromethylsulfonyl)imide	32	1.23	1.264	1.448	1.448
1,9-di(3-vinylimidazolium)nonane bis(trifluoromethylsulfonyl)imide	32	1.47	1.441	1.457	1.444

1,11-di(3-vinylimidazolium)undecane bis(trifluoromethylsulfonyl)imide	32	1.44	1.411	1.457	1.445
1-nonyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	32	1.3	1.311	1.434	1.438
1,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.559	1.551	1.422	1.423
1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.52	1.508	1.4231	1.426
1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	46	1.51845	1.508	1.4229	1.426
1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	87	1.519	1.508	1.421	1.426
1-ethyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	31	1.51	1.47	1.43	1.428
1-ethyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.495	1.47	1.4305	1.428
1-ethyl-3,5-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.47	1.47	1.4275	1.428
1,3-diethylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.452	1.47	1.426	1.428
1,3-diethyl-5-methylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.432	1.436	1.43	1.430
1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	75	1.436	1.436	1.42692	1.430
1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	60	1.43	1.436	1.4271	1.430
1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.429	1.436	1.4271	1.430
1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	87	1.43663	1.436	1.4258	1.430
1-isobutyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.428	1.436	1.4289	1.430
1-MeOEt-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.496	1.489	1.4293	1.427
1-CF3CH2-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.656	1.595	1.409	1.402
1-butyl-3-ethylimidazolium bis(trifluoromethylsulfonyl)imide	81	1.404	1.405	1.4285	1.432
1,3-dibutylimidazolium bis(trifluoromethylsulfonyl)imide	41	1.33551	1.354	1.4324	1.435
1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	87	1.37191	1.378	1.43	1.434
1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	68	1.32076	1.331	1.43331	1.437
1-vinyl-3-hexylimidazolium bis(trifluoromethylsulfonyl)imide	72	1.36	1.515	1.443	1.474
1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	71	1.31978	1.331	1.4327	1.437
1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	69	1.32076	1.331	1.43331	1.437
1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	73	1.32059	1.331	1.43298	1.437
1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	74	1.32059	1.331	1.43298	1.437
1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	87	1.32035	1.331	1.4325	1.437
1-methyl-3-nonylimidazolium bis(trifluoromethylsulfonyl)imide	32	1.3	1.311	1.434	1.438
3-butyloxymethyl-1-methylimidazolium bis(trifluoromethylsulfonyl)imide	80	1.422	1.424	1.4309	1.431
3-pentyloxymethyl-1-methylimidazolium bis(trifluoromethylsulfonyl)imide	80	1.391	1.397	1.432	1.432

3-hexyloxymethyl-1-methylimidazolium bis(trifluoromethylsulfonyl)imide	80	1.359	1.372	1.4337	1.434
3-heptyloxymethyl-1-methylimidazolium bis(trifluoromethylsulfonyl)imide	80	1.329	1.349	1.4346	1.435
3-octyloxymethyl-1-methylimidazolium bis(trifluoromethylsulfonyl)imide	80	1.316	1.328	1.4362	1.437
3-nonyloxymethyl-1-methylimidazolium bis(trifluoromethylsulfonyl)imide	80	1.29	1.309	1.4369	1.438
1-ethyl-3-methylimidazolium trifluoromethanesulfonate	48	1.38358	1.384	1.4332	1.440
1-ethyl-3-methylimidazolium trifluoromethanesulfonate	64	1.3851	1.384	1.43338	1.440
1-ethyl-3-methylimidazolium trifluoromethanesulfonate	81	1.39	1.384	1.4332	1.440
1-ethyl-3-methylimidazolium trifluoromethanesulfonate	23	1.384	1.384	1.4318	1.440
1-butyl-3-methylimidazolium trifluoromethanesulfonate	29	1.3038	1.307	1.4368	1.444
1-butyl-3-methylimidazolium trifluoromethanesulfonate	81	1.29	1.307	1.438	1.444
1-butyl-3-methylimidazolium trifluoromethanesulfonate	3	1.2968	1.307	1.433	1.444
1-MeOEt-3-methylimidazolium trifluoromethanesulfonate	81	1.364	1.373	1.4428	1.439
1,3-diethylimidazolium trifluoromethanesulfonate	81	1.33	1.343	1.4367	1.442
1-ethyl-3,5-dimethylimidazolium trifluoromethanesulfonate	81	1.334	1.343	1.44	1.442
1-hexyl-3-propanetrileimidazolium trifluoromethanesulfonate	49	1.2857	1.199	1.52975	1.513
1-butyl-3-methylimidazolium nonaflate	81	1.473	1.42	1.4052	1.401
1-butyl-3-ethylimidazolium nonaflate	81	1.427	1.392	1.4025	1.404
1-ethyl-3-methylimidazolium methylsulfonate	41	1.23815	1.225	1.4977	1.483
1-ethyl-3-methylimidazolium tosylate	27	1.21	1.219	1.538	1.524
1-hexyl-3-propanetrileimidazolium dioctylsulfosuccinate	49	1.089	1.078	1.4797	1.483
1-hexyl-3-propanetrileimidazolium benzenesulfonate	49	1.2227	1.177	1.527	1.525
1-hexyl-3-propanetrileimidazolium sulfobenzoate	49	1.2446	1.232	1.52295	1.525
1,3-dimethylimidazolium methylsulfate	77	1.32725	1.308	1.4827	1.479
1,3-dimethylimidazolium methylsulfate	58	1.3272	1.308	1.4827	1.479
1,3-dimethylimidazolium methylsulfate	57	1.3272	1.308	1.4827	1.479
1,3-dimethylimidazolium methylsulfate	53	1.3272	1.308	1.4827	1.479
1,3-dimethylimidazolium methylsulfate	55	1.3272	1.308	1.4827	1.479
1,3-dimethylimidazolium methylsulfate	39	1.32912	1.308	1.48296	1.479
1-ethyl-3-methylimidazolium methylsulfate	64	1.24373	1.266	1.495	1.478
1-butyl-3-methylimidazolium methylsulfate	54	1.21222	1.203	1.47942	1.476
1-butyl-3-methylimidazolium methylsulfate	58	1.2122	1.203	1.47942	1.476

1-butyl-3-methylimidazolium methylsulfate	25	1.20775	1.203	1.4794	1.476
1-butyl-3-methylimidazolium methylsulfate	40	1.21343	1.203	1.47792	1.476
1-butyl-3-methylimidazolium methylsulfate	29	1.2057	1.203	1.4792	1.476
1-butyl-3-methylimidazolium methylsulfate	43	1.2058	1.203	1.4782	1.476
1-ethyl-3-methylimidazolium ethylsulfate	35	1.23763	1.232	1.4794	1.477
1-ethyl-3-methylimidazolium ethylsulfate	65	1.23882	1.232	1.47889	1.477
1-ethyl-3-methylimidazolium ethylsulfate	37	1.2376	1.232	1.4794	1.477
1-ethyl-3-methylimidazolium ethylsulfate	66	1.23882	1.232	1.47889	1.477
1-ethyl-3-methylimidazolium ethylsulfate	70	1.23817	1.232	1.47903	1.477
1-ethyl-3-methylimidazolium ethylsulfate	46	1.2367	1.232	1.4788	1.477
1-ethyl-3-methylimidazolium octylsulfate	51	1.095	1.107	1.471	1.473
1-ethyl-3-methylimidazolium octylsulfate	41	1.0983	1.107	1.4737	1.473
1-butyl-3-methylimidazolium octylsulfate	45	1.06668	1.082	1.4654	1.473
1-butyl-3-methylimidazolium octylsulfate	43	1.0676	1.082	1.4699	1.473
1-butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethylsulfate	27	1.17	1.177	1.48	1.468
1-hexyl-3-propanetrileimidazolium dodecylsulfate	49	1.0978	1.053	1.48409	1.481

Experimental data of the test set

1-Decyl-3-methyl-1H-imidazol-3-ium 1,4-bis(2-ethylhexyloxy)-1,4-dioxobutane-2-sulfonate [C₁₀mim][Doc] 1H-NMR (200 MHz, d₆-DMSO) δ (ppm) =5.29 (br s, 1H), 3.89 (m, 4H), 3.76 (m, 2H), 3.62 (dd, J1 = 11.42 Hz, J2 = 3.88 Hz, 1H), 2.85 (m, 2H), 2.42 (m, 2H), 2.22 (m, 6H), 1.57-1.19 (m, 14H), 0.91 (t, J = 7.01 Hz, 9H), 0.84 (m, 12H). 13C-NMR (50 MHz, d₆ -DMSO) δ (ppm) = 170.9, 168.3, 136.5, 123.5, 122.2, 66.1, 66.0, 61.4, 48.7, 38.1, 35.6, 34.0, 31.2, 29.7, 29.6, 29.5, 29.4, 28.9, 28.8, 28.6, 28.4, 28.3, 25.5, 23.1, 22.9, 22.4, 22.3, 22.1, 13.8. m/z (ES+) 223.0, m/z (ES-) 421.1.

compound	n^{exp}	n^{DR}
1-ethyl-3-methylimidazolium methylsulfate	1.4810	1.4781
1-ethyl-3-methylimidazolium dicyanamide	1.5134	1.5368
1-butyl-3-methylimidazolium dicyanamide	1.5080	1.5241
1-hexyl-3-methylimidazolium dicyanamide	1.5031	1.5153
1-methyl-3-octylimidazolium dicyanamide	1.4991	1.5088
1-decyl-3-methylimidazolium dicyanamide	1.4954	1.5038
1-ethyl-3-methylimidazolium dioctylsulfosuccinate	1.4747	1.4767
1-butyl-3-methylimidazolium dioctylsulfosuccinate	1.4740	1.4760
1-hexyl-3-methylimidazolium dioctylsulfosuccinate	1.4738	1.4754
1-methyl-3-octylimidazolium dioctylsulfosuccinate	1.4724	1.4749
1-decanyl-3-methylimidazolium dioctylsulfosuccinate	1.4724	1.4745
1-methyl-3-octylimidazolium hexafluorophosphate	1.4228	1.4228
1-decyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	1.4350	1.4392
1-dodecyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	1.4376	1.4413
1,12-di(3-vinylimidazolium)dodecane bis(trifluoromethylsulfonyl)imide	1.458	1.4577

Designed Regress analysis

If we assume that the atomic polarisabilities do not correlate with each other, the molar polarisability α_{mol} of an ionic liquid can be computed by the scalar product of a vector , containing the number or occurence of each atom type, and a polarisability vector α containing the polarisability of each atom type:

$$\alpha_{mol} = X \alpha$$

The last equation can be applied to a set of ionic liquids (1 ... m) with various molar polarisabilities α_{mol}^m and various compositions X^m . This point of view changes equation (5) to a matrix equation:

$$\begin{pmatrix} \alpha_{mol}^1 \\ \alpha_{mol}^2 \\ \vdots \\ \alpha_{mol}^m \end{pmatrix} = \begin{pmatrix} X_H^1 & X_B^1 & X_C^1 & X_N^1 & X_O^1 & X_F^1 & X_P^1 & X_S^1 & X_{Cl}^1 \\ X_H^2 & X_B^2 & X_C^2 & X_N^2 & X_O^2 & X_F^2 & X_P^2 & X_S^2 & X_{Cl}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ X_H^m & X_B^m & X_C^m & X_N^m & X_O^m & X_F^m & X_P^m & X_S^m & X_{Cl}^m \end{pmatrix} \begin{pmatrix} \alpha_H \\ \alpha_B \\ \alpha_C \\ \alpha_N \\ \alpha_O \\ \alpha_F \\ \alpha_P \\ \alpha_S \\ \alpha_{Cl} \end{pmatrix}$$

The rows of α_{mol} and of the design matrix X contain information of the corresponding ionic liquids m . The columns of X and the rows of α are related to the number and the atomic polarisability of a species. In principle, it is possible to include several molar polarisabilities α_{mol} from an ionic liquid, e.g. different measurements, to minimize the error from impurities. In this case, the rows of the design matrix become linearly dependent. Furthermore, the design matrix is usually not a square matrix unless the number of ionic liquids of investigation equals the number of atomic polarisabilities.

Atomic polarisabilities [Å³]

	Estimate	SE	TStat	PValue
H	0.209845	0.0243196	8.62862	8.88178 × 10 ⁻¹⁵
B	1.18597	0.236394	5.01692	1.48502 × 10 ⁻⁶
C	1.3682	0.0454045	30.1336	0.
N	1.12326	0.088179	12.7384	0.
O	0.640965	0.0556726	11.5131	0.
F	0.402679	0.0324883	12.3946	0.
P	1.76805	0.271241	6.51838	1.05018 × 10 ⁻⁹
S	2.37593	0.157584	15.0772	0.
Cl	3.45106	0.222691	15.4971	0.

RSquared → 0.999724, AdjustedRSquared → 0.999707, EstimatedVariance → 0.230463,

	DF	SumOfSq	MeanSq	FRatio	PValue
Model	9	123390.	13710.	59489.	0.
Error	148	34.1085	0.230463		
U Total	157	123424.			

The Designed Regress analysis can also be applied to the molar volumes

$$V_{mol} = X V$$

of the ionic liquids yielding a vector $V = \{V_H, V_B, \dots, V_{Cl}\}$ of the atomic volumes.

Atomic volumes [$\text{\AA}^3$]

		Estimate	SE	TStat	PValue	
{ParameterTable→	H	7.15216	0.444022	16.1077	0.	
	B	5.53475	4.31603	1.28237	0.201718	
	C	12.7257	0.828985	15.3509	0.	
	N	14.5367	1.60995	9.02928	8.88178×10^{-16}	
	O	11.9171	1.01646	11.7241	0.	
	F	18.0223	0.593164	30.3833	0.	
	P	1.06074	4.95225	0.214194	0.830691	
	S	25.5293	2.87713	8.87317	2.22045×10^{-15}	
	Cl	33.308	4.06585	8.19214	1.11022×10^{-13}	
RSquared→0.999628, AdjustedRSquared→0.999605, EstimatedVariance→76.8242,						
ANOVATable→		DF	SumOfSq	MeanSq	FRatio	PValue
	Model	9	3.05574×10^7	3.39526×10^6	44195.2	0.
	Error	148	11370.	76.8242		
	U Total	157	3.05687×10^7			

Atomic masses / g mol^{-1}

		Estimate	SE	TStat	PValue
{ParameterTable→	H	1.0079	1.19277×10^{-14}	8.45006×10^{13}	$1.738625178919851 \times 10^{-1902}$
	B	10.81	1.15941×10^{-13}	9.32369×10^{13}	$8.249637542777374 \times 10^{-1909}$
	C	12.011	2.2269×10^{-14}	5.39361×10^{14}	$1.251114710745563 \times 10^{-2021}$
	N	14.0067	4.32481×10^{-14}	3.23869×10^{14}	$7.599663546538476 \times 10^{-1989}$
	O	15.9994	2.7305×10^{-14}	5.8595×10^{14}	$5.916183601808347 \times 10^{-2027}$
	F	18.9984	1.59341×10^{-14}	1.19231×10^{15}	$1.287721094558342 \times 10^{-2072}$
	P	30.9738	1.33032×10^{-13}	2.3283×10^{14}	$1.240926608022108 \times 10^{-1967}$
	S	32.06	7.72881×10^{-14}	4.14811×10^{14}	$9.40889743264829 \times 10^{-2005}$
	Cl	35.453	1.0922×10^{-13}	3.246×10^{14}	$5.442382686898555 \times 10^{-1989}$
RSquared→1., AdjustedRSquared→1., EstimatedVariance→ 5.54376×10^{-26} , ANOVA Table→					
Model					
Error					
U Total					

The last analysis checks the consistency of the Designed Regress learning set. All atomic masses are reproduced with highest possible accuracy.