Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION: Artificial Neural Networks for the Prediction of Solvation Energies Based on Experimental and Computational Data

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ANN Architecture for Experimental Data

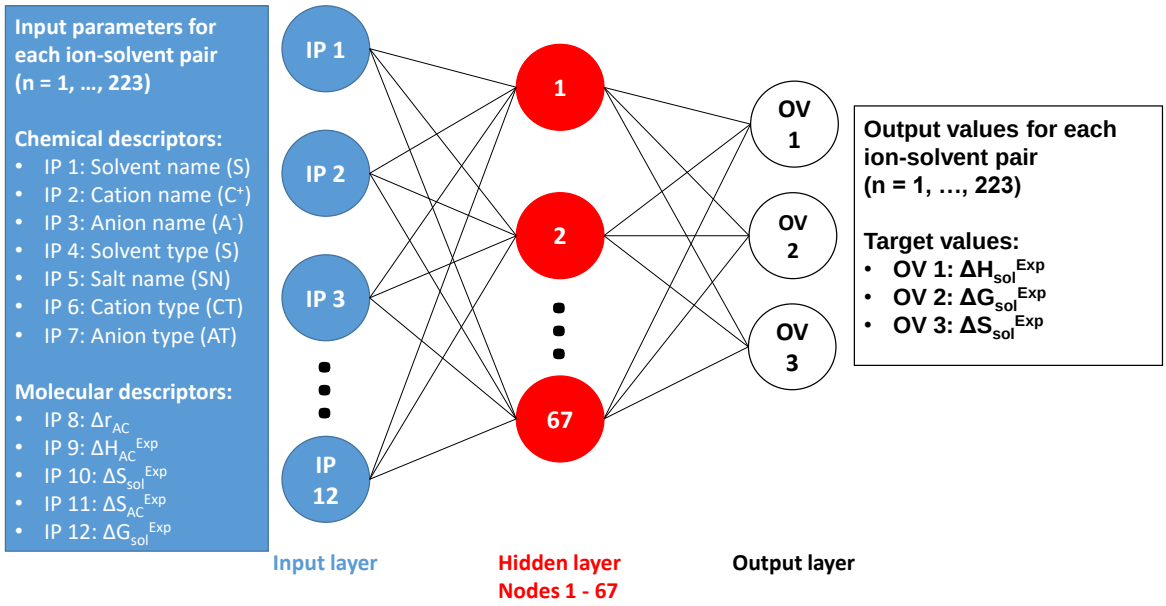

Figure 1: Schematic visualization of the ANN architecture based on experimental data. The corresponding chemical, molecular and conceptual DFT descriptors for the ANNs are listed on the left side. All target parameters are listed on the right side. Straight lines represent the connections between the nodes with the corresponding weights and activation functions.

ANN Architecture for Conceptual DFT Data

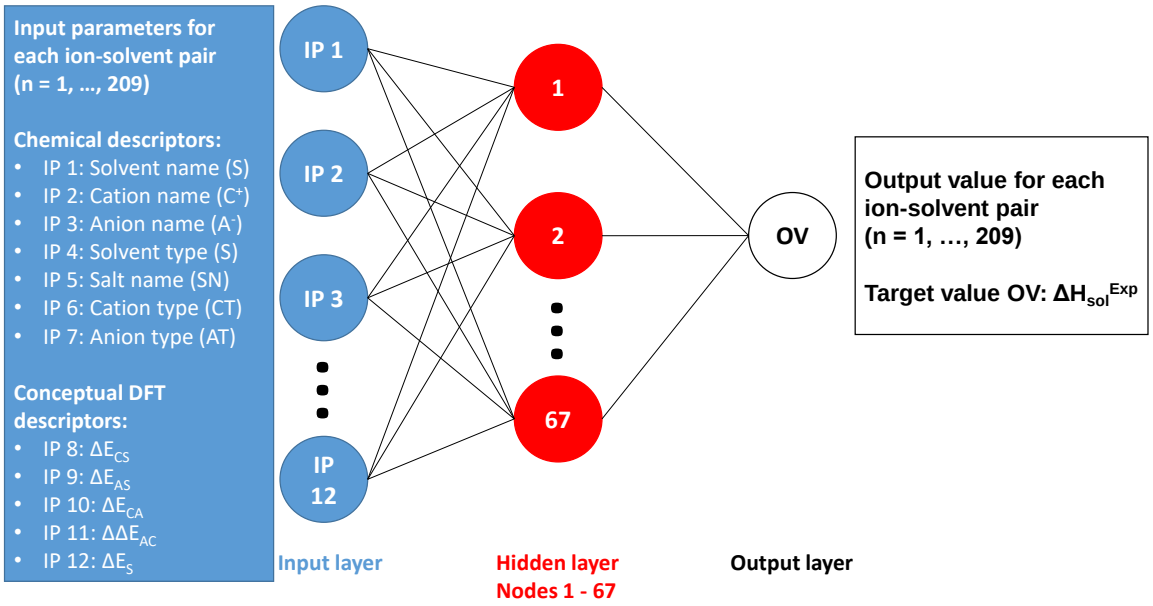

Figure 2: Schematic visualization of the ANN architecture based on conceptual DFT data. The corresponding chemical, molecular and conceptual DFT descriptors for the ANNs are listed on the left side. All target parameters are listed on the right side. Straight lines represent the connections between the nodes with the corresponding weights and activation functions.

Entropic and Enthalpic Contributions to the Solvation Enthalpy

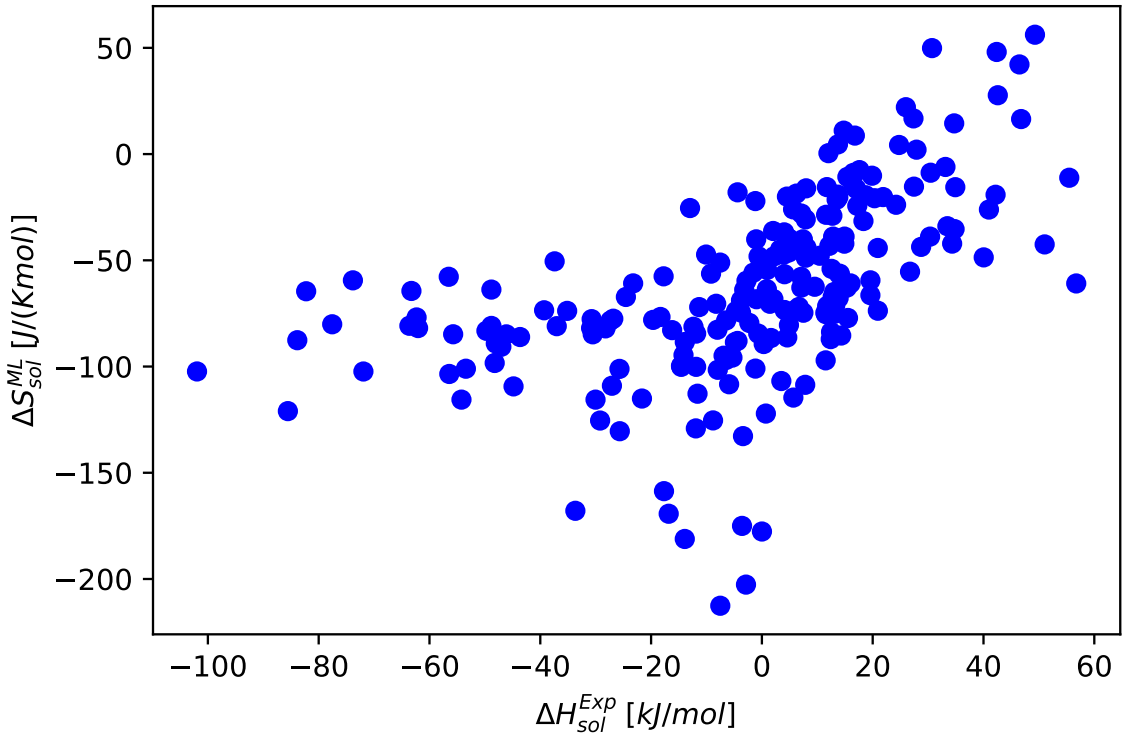

Figure 3: Experimental target values for the solvation enthalpies $\Delta H_{\mathrm{sol}}^{\mathrm{Exp}}$ and predicted values for the solvation entropies $\Delta S_{\mathrm{sol}}^{\mathrm{ML}}$ for identical ion pairs and solvent combinations.

Volcano Plots

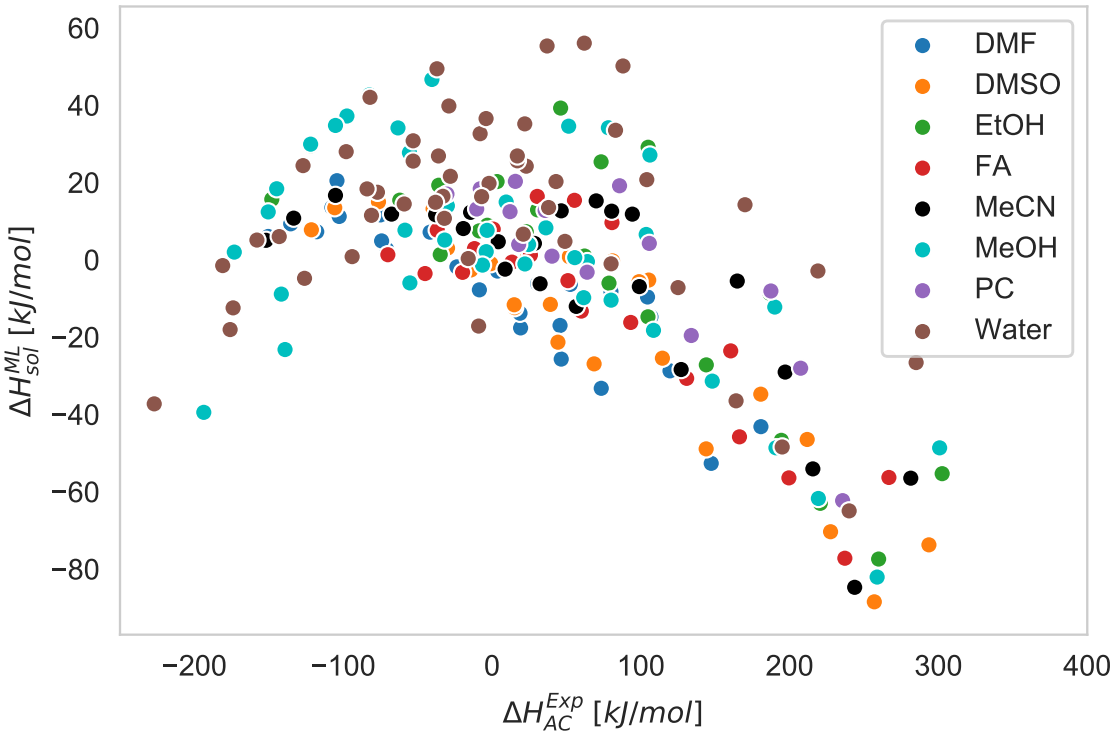

Figure 4: Volcano plots with predicted solvation enthalpies $\Delta H_{\mathrm{sol}}^{\mathrm{ML}}$ and experimental solvation enthalpy differences $\Delta H_{\mathrm{AC}}^{\mathrm{Exp}}$ for all ions in the respective solvents dimethylformamide (DMF), dimethyl sulfoxide (DMSO), ethanol (EtOH), formamide (FA), acetonitrile (MeCN), methanol (MeOH), propylene carbonate (PC) and water.

Data Set for Machine Learning Predictions with Conceptual DFT Calculations

Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
DMF	Cs	Br	A	-1.94	-1.25	9.42	6.23	0.68	-7.51
DMF	Cs	Cl	A	-1.94	-1.36	11.20	7.90	0.57	0.01
DMF	Cs	ClO[4]	A	-1.94	-0.65	2.79	0.20	1.29	-6.92
DMF	Cs	I	A	-1.94	-1.13	7.46	4.39	0.80	-17.67
DMF	Et4N	Br	A	-0.77	-1.25	5.99	3.97	-0.48	9.53
DMF	Et4N	Cl	A	-0.77	-1.36	7.12	4.99	-0.59	6.23
DMF	Et4N	ClO[4]	A	-0.77	-0.65	1.68	0.26	0.12	5.11
DMF	Et4N	I	A	-0.77	-1.13	4.74	2.84	-0.37	13.91
DMF	K	Br	A	-2.94	-1.25	11.64	7.45	1.69	-16.82
DMF	K	Cl	A	-2.94	-1.36	13.88	9.58	1.58	-3.58
DMF	K	ClO[4]	A	-2.94	-0.65	3.56	-0.03	2.30	-14.56
DMF	K	I	A	-2.94	-1.13	9.19	5.11	1.81	-33.67
DMF	Me4N	Br	A	-1.19	-1.25	7.38	4.94	-0.06	11.46
DMF	Me4N	Cl	A	-1.19	-1.36	8.77	6.22	-0.17	7.12
DMF	Me4N	ClO[4]	A	-1.19	-0.65	2.11	0.28	0.54	7.09
DMF	Me4N	I	A	-1.19	-1.13	5.85	3.53	0.05	11.78
DMF	Na	Br	A	-4.93	-1.25	15.89	9.71	3.68	-29.20
DMF	Na	Cl	A	-4.93	-1.36	18.99	12.70	3.57	-8.82

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
DMF	Na	ClO[4]	A	-4.93	-0.65	5.04	-0.54	4.28	-43.65
DMF	Na	I	A	-4.93	-1.13	12.50	6.44	3.79	-53.43
DMF	Rb	Br	A	-2.46	-1.25	10.64	6.93	1.21	-13.92
DMF	Rb	Cl	A	-2.46	-1.36	12.67	8.85	1.10	-2.87
DMF	Rb	ClO[4]	A	-2.46	-0.65	3.21	0.10	1.81	-7.96
DMF	Rb	I	A	-2.46	-1.13	8.42	4.82	1.33	-25.65
DMSO	Cs	Br	A	-2.06	-1.18	9.42	6.18	0.88	-3.41
DMSO	Cs	Cl	A	-2.06	-1.29	11.20	7.85	0.76	3.51
DMSO	Cs	ClO[4]	A	-2.06	-0.60	2.79	0.13	1.46	2.18
DMSO	Cs	I	A	-2.06	-1.07	7.46	4.34	0.99	-11.87
DMSO	K	Br	A	-3.08	-1.18	11.64	7.38	1.90	-11.92
DMSO	K	Cl	A	-3.08	-1.29	13.88	9.51	1.79	0.72
DMSO	K	ClO[4]	A	-3.08	-0.60	3.56	-0.11	2.48	-4.66
DMSO	K	I	A	-3.08	-1.07	9.19	5.04	2.01	-27.07
DMSO	Li	Br	A	-8.18	-1.18	22.07	12.72	6.99	-71.93
DMSO	Li	Cl	A	-8.18	-1.29	26.44	16.97	6.88	-44.83
DMSO	Li	ClO[4]	A	-8.18	-0.60	7.22	-1.56	7.58	-73.82
DMSO	Li	I	A	-8.18	-1.07	17.31	8.07	7.11	-101.96
DMSO	Me4N	Br	A	-1.29	-1.18	7.38	4.91	0.11	12.86
DMSO	Me4N	Cl	A	-1.29	-1.29	8.77	6.19	-0.00	7.92
DMSO	Me4N	ClO[4]	A	-1.29	-0.60	2.11	0.23	0.69	13.49

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
DMSO	Me4N	I	A	-1.29	-1.07	5.85	3.50	0.22	14.88
DMSO	Na	Br	A	-5.08	-1.18	15.89	9.63	3.89	-25.70
DMSO	Na	Cl	A	-5.08	-1.29	18.99	12.62	3.78	-5.92
DMSO	Na	ClO[4]	A	-5.08	-0.60	5.04	-0.63	4.48	-35.15
DMSO	Na	I	A	-5.08	-1.07	12.50	6.36	4.01	-48.23
DMSO	Rb	Br	A	-2.59	-1.18	10.64	6.87	1.41	-11.62
DMSO	Rb	Cl	A	-2.59	-1.29	12.67	8.79	1.30	-1.17
DMSO	Rb	ClO[4]	A	-2.59	-0.60	3.21	0.02	2.00	-0.66
DMSO	Rb	I	A	-2.59	-1.07	8.42	4.76	1.53	-21.65
EtOH	Cs	Br	P	-1.74	-1.30	9.42	6.38	0.44	19.59
EtOH	Cs	Cl	P	-1.74	-1.41	11.20	8.05	0.33	16.01
EtOH	Cs	ClO[4]	P	-1.74	-0.70	2.79	0.35	1.03	40.98
EtOH	Cs	I	P	-1.74	-1.18	7.46	4.54	0.55	20.93
EtOH	K	Br	P	-2.72	-1.30	11.64	7.63	1.42	5.68
EtOH	K	Cl	P	-2.72	-1.41	13.88	9.76	1.31	7.82
EtOH	K	ClO[4]	P	-2.72	-0.70	3.56	0.14	2.02	28.74
EtOH	K	I	P	-2.72	-1.18	9.19	5.29	1.54	0.33
EtOH	Li	Br	P	-7.77	-1.30	22.07	13.00	6.47	-63.63
EtOH	Li	Cl	P	-7.77	-1.41	26.44	17.26	6.36	-47.03
EtOH	Li	ClO[4]	P	-7.77	-0.70	7.22	-1.25	7.07	-49.72
EtOH	Li	I	P	-7.77	-1.18	17.31	8.36	6.59	-83.86

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
EtOH	Me4N	Br	P	-1.03	-1.30	7.38	5.05	-0.27	30.36
EtOH	Me4N	Cl	P	-1.03	-1.41	8.77	6.33	-0.38	14.92
EtOH	Me4N	ClO[4]	P	-1.03	-0.70	2.11	0.38	0.33	46.79
EtOH	Me4N	I	P	-1.03	-1.18	5.85	3.64	-0.15	42.18
EtOH	Na	Br	P	-4.67	-1.30	15.89	9.92	3.37	-14.60
EtOH	Na	Cl	P	-4.67	-1.41	18.99	12.91	3.26	-5.32
EtOH	Na	ClO[4]	P	-4.67	-0.70	5.04	-0.33	3.97	-8.25
EtOH	Na	I	P	-4.67	-1.18	12.50	6.65	3.49	-27.33
EtOH	Rb	Br	P	-2.24	-1.30	10.64	7.10	0.95	13.28
EtOH	Rb	Cl	P	-2.24	-1.41	12.67	9.02	0.84	13.23
EtOH	Rb	ClO[4]	P	-2.24	-0.70	3.21	0.26	1.54	40.04
EtOH	Rb	I	P	-2.24	-1.18	8.42	4.99	1.06	13.05
FA	Cs	Br	P	-1.78	-1.30	9.42	6.33	0.47	7.39
FA	Cs	Cl	P	-1.78	-1.42	11.20	8.00	0.36	-3.19
FA	Cs	ClO[4]	P	-1.78	-0.70	2.79	0.31	1.08	14.08
FA	Cs	I	P	-1.78	-1.19	7.46	4.49	0.59	7.13
FA	K	Br	P	-2.77	-1.30	11.64	7.57	1.46	2.08
FA	K	Cl	P	-2.77	-1.42	13.88	9.70	1.35	-2.78
FA	K	ClO[4]	P	-2.77	-0.70	3.56	0.09	2.07	10.44
FA	K	I	P	-2.77	-1.19	9.19	5.23	1.58	-4.87
FA	Li	Br	P	-7.83	-1.30	22.07	12.94	6.53	-55.73

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
FA	Li	Cl	P	-7.83	-1.42	26.44	17.19	6.42	-46.13
FA	Li	ClO[4]	P	-7.83	-0.70	7.22	-1.31	7.13	-56.52
FA	Li	I	P	-7.83	-1.19	17.31	8.29	6.64	-77.56
FA	Na	Br	P	-4.73	-1.30	15.89	9.86	3.43	-16.20
FA	Na	Cl	P	-4.73	-1.42	18.99	12.84	3.31	-13.92
FA	Na	ClO[4]	P	-4.73	-0.70	5.04	-0.39	4.03	-24.55
FA	Na	I	P	-4.73	-1.19	12.50	6.58	3.54	-30.53
FA	Rb	Br	P	-2.29	-1.30	10.64	7.04	0.99	3.28
FA	Rb	Cl	P	-2.29	-1.42	12.67	8.96	0.88	-3.77
FA	Rb	ClO[4]	P	-2.29	-0.70	3.21	0.21	1.59	15.34
FA	Rb	I	P	-2.29	-1.19	8.42	4.94	1.10	1.45
MeCN	Cs	Br	A	-1.31	-1.57	9.42	6.54	-0.26	7.49
MeCN	Cs	Cl	A	-1.31	-1.68	11.20	8.21	-0.37	11.51
MeCN	Cs	ClO[4]	A	-1.31	-0.92	2.79	0.55	0.39	12.78
MeCN	Cs	I	A	-1.31	-1.45	7.46	4.70	-0.14	-2.27
MeCN	Et4N	Br	A	-0.39	-1.57	5.99	4.03	-1.18	11.73
MeCN	Et4N	Cl	A	-0.39	-1.68	7.12	5.05	-1.29	4.93
MeCN	Et4N	ClO[4]	A	-0.39	-0.92	1.68	0.36	-0.53	12.01
MeCN	Et4N	I	A	-0.39	-1.45	4.74	2.90	-1.06	16.51
MeCN	K	Br	A	-2.22	-1.57	11.64	7.85	0.65	4.58
MeCN	K	Cl	A	-2.22	-1.68	13.88	9.98	0.54	14.32

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
MeCN	K	ClO[4]	A	-2.22	-0.92	3.56	0.42	1.30	11.54
MeCN	K	I	A	-2.22	-1.45	9.19	5.52	0.77	-11.87
MeCN	Li	Br	A	-7.18	-1.57	22.07	13.33	5.61	-54.23
MeCN	Li	Cl	A	-7.18	-1.68	26.44	17.58	5.49	-30.03
MeCN	Li	ClO[4]	A	-7.18	-0.92	7.22	-0.88	6.25	-56.42
MeCN	Li	I	A	-7.18	-1.45	17.31	8.69	5.72	-85.56
MeCN	Na	Br	A	-4.10	-1.57	15.89	10.23	2.53	-4.40
MeCN	Na	Cl	A	-4.10	-1.68	18.99	13.21	2.42	12.48
MeCN	Na	ClO[4]	A	-4.10	-0.92	5.04	0.02	3.17	-14.15
MeCN	Na	I	A	-4.10	-1.45	12.50	6.95	2.65	-28.23
MeCN	Rb	Br	A	-1.77	-1.57	10.64	7.30	0.21	4.88
MeCN	Rb	Cl	A	-1.77	-1.68	12.67	9.22	0.09	12.43
MeCN	Rb	ClO[4]	A	-1.77	-0.92	3.21	0.51	0.85	15.54
MeCN	Rb	I	A	-1.77	-1.45	8.42	5.19	0.32	-6.45
MeOH	Cs	Br	P	-1.70	-1.31	9.42	6.40	0.39	13.79
MeOH	Cs	Cl	P	-1.70	-1.42	11.20	8.07	0.28	7.91
MeOH	Cs	ClO[4]	P	-1.70	-0.71	2.79	0.37	0.99	34.78
MeOH	Cs	F	P	-1.70	-2.03	19.22	15.49	-0.32	-39.31
MeOH	Cs	I	P	-1.70	-1.20	7.46	4.56	0.51	15.43
MeOH	Et4N	Br	P	-0.63	-1.31	5.99	4.05	-0.69	18.73
MeOH	Et4N	Cl	P	-0.63	-1.42	7.12	5.07	-0.80	2.03

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
MeOH	Et4N	ClO[4]	P	-0.63	-0.71	1.68	0.34	-0.09	34.71
MeOH	Et4N	I	P	-0.63	-1.20	4.74	2.92	-0.57	34.91
MeOH	K	Br	P	-2.68	-1.31	11.64	7.65	1.37	4.08
MeOH	K	Cl	P	-2.68	-1.42	13.88	9.78	1.26	3.92
MeOH	K	ClO[4]	P	-2.68	-0.71	3.56	0.17	1.97	26.74
MeOH	K	F	P	-2.68	-2.03	23.78	19.07	0.66	-23.24
MeOH	K	I	P	-2.68	-1.20	9.19	5.31	1.49	-0.97
MeOH	Li	Br	P	-7.73	-1.31	22.07	13.03	6.42	-62.33
MeOH	Li	Cl	P	-7.73	-1.42	26.44	17.28	6.31	-48.03
MeOH	Li	ClO[4]	P	-7.73	-0.71	7.22	-1.23	7.02	-48.82
MeOH	Li	F	P	-7.73	-2.03	44.96	35.21	5.70	1.65
MeOH	Li	I	P	-7.73	-1.20	17.31	8.39	6.53	-82.26
MeOH	Me4N	Br	P	-1.01	-1.31	7.38	5.06	-0.31	30.46
MeOH	Me4N	Cl	P	-1.01	-1.42	8.77	6.34	-0.42	12.72
MeOH	Me4N	ClO[4]	P	-1.01	-0.71	2.11	0.40	0.29	46.49
MeOH	Me4N	I	P	-1.01	-1.20	5.85	3.65	-0.19	42.58
MeOH	Na	Br	P	-4.63	-1.31	15.89	9.95	3.32	-18.30
MeOH	Na	Cl	P	-4.63	-1.42	18.99	12.94	3.21	-11.32
MeOH	Na	ClO[4]	P	-4.63	-0.71	5.04	-0.31	3.92	-12.35
MeOH	Na	F	P	-4.63	-2.03	32.40	25.75	2.61	-6.50
MeOH	Na	I	P	-4.63	-1.20	12.50	6.67	3.44	-30.73

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
MeOH	NH4	Br	P	-2.36	-1.31	11.38	7.71	1.05	-1.52
MeOH	NH4	Cl	P	-2.36	-1.42	13.53	9.74	0.94	-1.03
MeOH	NH4	ClO[4]	P	-2.36	-0.71	3.42	0.35	1.65	6.68
MeOH	NH4	F	P	-2.36	-2.03	23.08	18.69	0.34	-9.18
MeOH	NH4	I	P	-2.36	-1.20	9.03	5.47	1.16	-10.07
MeOH	Rb	Br	P	-2.21	-1.31	10.64	7.12	0.90	7.98
MeOH	Rb	Cl	P	-2.21	-1.42	12.67	9.04	0.79	5.63
MeOH	Rb	ClO[4]	P	-2.21	-0.71	3.21	0.28	1.50	34.34
MeOH	Rb	I	P	-2.21	-1.20	8.42	5.01	1.01	8.05
PC	Cs	Br	A	-1.53	-1.46	9.42	6.43	0.07	13.69
PC	Cs	Cl	A	-1.53	-1.57	11.20	8.10	-0.04	16.31
PC	Cs	I	A	-1.53	-1.34	7.46	4.59	0.19	4.03
PC	K	Br	A	-2.48	-1.46	11.64	7.71	1.03	12.58
PC	K	Cl	A	-2.48	-1.57	13.88	9.83	0.91	20.92
PC	K	I	A	-2.48	-1.34	9.19	5.37	1.14	-3.77
PC	Li	Br	A	-7.50	-1.46	22.07	13.12	6.04	-30.83
PC	Li	Cl	A	-7.50	-1.57	26.44	17.37	5.93	-8.03
PC	Li	I	A	-7.50	-1.34	17.31	8.48	6.16	-62.06
PC	Na	Br	A	-4.40	-1.46	15.89	10.03	2.95	4.10
PC	Na	Cl	A	-4.40	-1.57	18.99	13.02	2.84	19.58
PC	Na	I	A	-4.40	-1.34	12.50	6.76	3.07	-19.63

Continued on next page

Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
PC	Rb	Br	A	-2.02	-1.46	10.64	7.17	0.56	12.18
PC	Rb	Cl	A	-2.02	-1.57	12.67	9.08	0.45	18.33
PC	Rb	I	A	-2.02	-1.34	8.42	5.06	0.68	0.95
H_2O	Cs	Br	P	-1.41	-1.51	9.42	6.49	-0.10	25.99
H_2O	Cs	Cl	P	-1.41	-1.63	11.20	8.16	-0.22	17.61
H_2O	Cs	ClO[4]	P	-1.41	-0.88	2.79	0.50	0.53	55.48
H_2O	Cs	F	P	-1.41	-2.24	19.22	15.57	-0.83	-37.41
H_2O	Cs	I	P	-1.41	-1.40	7.46	4.65	0.01	33.13
H_2O	Et4N	Br	P	-0.45	-1.51	5.99	4.02	-1.07	6.23
H_2O	Et4N	Cl	P	-0.45	-1.63	7.12	5.05	-1.18	-12.97
H_2O	Et4N	ClO[4]	P	-0.45	-0.88	1.68	0.35	-0.43	30.71
H_2O	Et4N	I	P	-0.45	-1.40	4.74	2.90	-0.95	27.91
H_2O	K	Br	P	-2.34	-1.51	11.64	7.79	0.83	19.88
H_2O	K	Cl	P	-2.34	-1.63	13.88	9.91	0.71	17.22
H_2O	K	ClO[4]	P	-2.34	-0.88	3.56	0.34	1.47	51.04
H_2O	K	F	P	-2.34	-2.24	23.78	19.20	0.10	-17.74
H_2O	K	I	P	-2.34	-1.40	9.19	5.45	0.94	20.33
H_2O	K	SCN	P	-2.34	-1.30	7.70	4.06	1.04	24.22
H_2O	Li	Br	P	-7.33	-1.51	22.07	13.23	5.81	-48.83
H_2O	Li	Cl	P	-7.33	-1.63	26.44	17.48	5.70	-37.03
H_2O	Li	ClO[4]	P	-7.33	-0.88	7.22	-0.98	6.45	-26.82

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy ΔH_{sol}^{exp}. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{ca}$	ΔE_{sol}	ΔE_{AC}	ΔH_{sol}^{exp}
H_2O	Li	F	P	-7.33	-2.24	44.96	35.40	5.08	4.85
H_2O	Li	I	P	-7.33	-1.40	17.31	8.59	5.93	-63.26
H_2O	Me4N	Br	P	-0.78	-1.51	7.38	5.09	-0.74	24.76
H_2O	Me4N	Cl	P	-0.78	-1.63	8.77	6.36	-0.85	4.52
H_2O	Me4N	ClO[4]	P	-0.78	-0.88	2.11	0.46	-0.10	49.29
H_2O	Me4N	I	P	-0.78	-1.40	5.85	3.68	-0.62	42.38
H_2O	Na	Br	P	-4.24	-1.51	15.89	10.14	2.73	-0.60
H_2O	Na	Cl	P	-4.24	-1.63	18.99	13.13	2.61	3.88
H_2O	Na	ClO[4]	P	-4.24	-0.88	5.04	-0.08	3.36	13.85
H_2O	Na	F	P	-4.24	-2.24	32.40	25.92	2.00	0.90
H_2O	Na	I	P	-4.24	-1.40	12.50	6.87	2.84	-7.53
H_2O	NH4	Br	P	-2.01	-1.51	11.38	7.86	0.50	16.78
H_2O	NH4	Cl	P	-2.01	-1.63	13.53	9.89	0.39	14.77
H_2O	NH4	ClO[4]	P	-2.01	-0.88	3.42	0.53	1.14	33.48
H_2O	NH4	F	P	-2.01	-2.24	23.08	18.83	-0.23	-1.18
H_2O	NH4	I	P	-2.01	-1.40	9.03	5.62	0.62	13.73
H_2O	Pr4N	Br	P	-0.35	-1.51	5.59	3.72	-1.16	-4.39
H_2O	Pr4N	ClO[4]	P	-0.35	-0.88	1.55	0.32	-0.53	27.36
H_2O	Pr4N	I	P	-0.35	-1.40	4.43	2.68	-1.05	11.59
H_2O	Rb	Br	P	-1.89	-1.51	10.64	7.24	0.37	21.88
H_2O	Rb	Cl	P	-1.89	-1.63	12.67	9.16	0.26	17.03

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Table 1: Data set for machine learning on conceptual DFT calculations with solvent (S), cation (C^+), anion (A^-), solvent type (either protic (P) or aprotic (A)), cation-solvent reaction energy E_{cs}, anion-solvent reaction energy E_{as}, cation-anion reaction energy E_{ac}, full reaction energy E_{sol}, difference between anion-solvent and cation-solvent reaction energy ΔE_{ac} and experimental value for the solvation enthalpy $\Delta H_{\mathrm{sol}}^{\mathrm{exp}}$. All energy values have units of eV except the solvation enthalpy which has units of kcal/mol.

S	C^+	A^-	ST	E_{cs}	E_{as}	$-E_{\mathrm{ca}}$	ΔE_{sol}	ΔE_{AC}	$\Delta H_{\mathrm{sol}}^{\mathrm{exp}}$
H_2O	Rb	ClO[4]	P	-1.89	-0.88	3.21	0.44	1.01	56.74
H_2O	Rb	I	P	-1.89	-1.40	8.42	5.13	0.49	27.45

Data Set for Machine Learning Predictions: Experimental Values

Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
DMF	Bu[4]*N	ClO[4]	A	-173	96.2	-107.0	-70.8	2.50	-1.65	21.90
DMF	Bu[4]*N	I	A	-193	98.1	-141.6	-104.2	20.84	7.38	50.20
DMF	Cs	Br	A	26	-15.2	-3.9	-8.5	-7.51	19.74	-94.53
DMF	Cs	Cl	A	11	-25.1	-17.8	-23.6	0.01	27.69	-101.72
DMF	Cs	ClO[4]	A	70	-7.2	52.9	52.6	-6.92	5.82	-50.94
DMF	Cs	I	A	50	-5.3	18.3	19.2	-17.67	5.49	-88.79
DMF	Et[4]*N	Br	A	-141	12.2	-146.8	-135.3	9.53	17.78	-5.20
DMF	Et[4]*N	Cl	A	-156	2.3	-160.7	-150.4	6.23	25.53	-48.00
DMF	Et[4]*N	ClO[4]	A	-97	20.2	-90.0	-74.2	5.11	6.04	14.30
DMF	Et[4]*N	I	A	-117	22.1	-124.6	-107.6	13.91	17.21	3.50
DMF	K	Br	A	58	20.5	39.3	45.7	-16.82	20.53	-128.29
DMF	K	Cl	A	43	10.6	25.4	30.6	-3.58	33.85	-134.31
DMF	K	ClO[4]	A	102	28.5	96.1	106.8	-14.56	6.20	-77.71
DMF	K	I	A	82	30.4	61.5	73.4	-33.67	1.34	-128.41
DMF	Me[4]*N	Br	A	-84	-1.7	-110.5	-102.7	11.46	27.59	-53.10
DMF	Me[4]*N	Cl	A	-99	-11.6	-124.4	-117.8	7.12	26.05	-46.00
DMF	Me[4]*N	ClO[4]	A	-40	6.3	-53.7	-41.6	7.09	13.13	-2.10

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
DMF	Me[4]*N	I	A	-60	8.2	-88.3	-75.0	11.78	24.85	-29.30
DMF	Na	Br	A	94	25.4	111.8	119.6	-29.20	8.73	-130.45
DMF	Na	Cl	A	79	15.5	97.9	104.5	-8.82	28.70	-134.81
DMF	Na	ClO[4]	A	138	33.4	168.6	180.7	-43.65	-22.16	-80.36
DMF	Na	I	A	118	35.3	134.0	147.3	-53.43	-17.61	-131.32
DMF	Rb	Br	A	47	1.3	17.4	18.8	-13.92	19.85	-112.99
DMF	Rb	Cl	A	32	-8.6	3.5	3.7	-2.87	30.70	-118.06
DMF	Rb	ClO[4]	A	91	9.3	74.2	79.9	-7.96	8.19	-58.96
DMF	Rb	I	A	71	11.2	39.6	46.5	-25.65	3.50	-105.46
DMSO	Cs	Br	A	26	0.8	-14.8	-14.2	-3.41	6.84	-38.53
DMSO	Cs	Cl	A	11	19.9	-26.2	-29.9	3.51	17.29	-16.72
DMSO	Cs	ClO[4]	A	70	3.8	48.9	51.9	2.18	-0.18	0.06
DMSO	Cs	I	A	50	14.7	13.0	15.2	-11.87	-1.81	-28.79
DMSO	K	Br	A	58	27.5	30.5	39.2	-11.92	5.53	-63.29
DMSO	K	Cl	A	43	46.6	19.1	23.5	0.72	21.35	-40.31
DMSO	K	ClO[4]	A	102	30.5	94.2	105.3	-4.66	-1.90	-17.71
DMSO	K	I	A	82	41.4	58.3	68.6	-27.07	-8.06	-59.41
DMSO	Li	Br	A	127	48.0	212.6	227.5	-71.93	-48.27	-83.39
DMSO	Li	Cl	A	112	67.1	201.2	211.8	-44.83	-18.61	-58.33
DMSO	Li	ClO[4]	A	171	51.0	276.3	293.6	-73.82	-66.39	-32.67

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
DMSO	Li	I	A	151	61.9	240.4	256.9	-101.96	-77.71	-76.27
DMSO	Me[4]*N	Br	A	-84	39.3	-125.7	-105.7	12.86	18.99	-22.10
DMSO	Me[4]*N	Cl	A	-99	58.4	-137.1	-121.4	7.92	19.95	14.00
DMSO	Me[4]*N	ClO[4]	A	-40	42.3	-62.0	-39.6	13.49	11.43	23.90
DMSO	Me[4]*N	I	A	-60	53.2	-97.9	-76.3	14.88	21.85	5.70
DMSO	Na	Br	A	94	39.4	102.0	114.5	-25.70	-5.27	-72.45
DMSO	Na	Cl	A	79	58.5	90.6	98.8	-5.92	17.20	-47.81
DMSO	Na	ClO[4]	A	138	42.4	165.7	180.6	-35.15	-29.26	-27.36
DMSO	Na	I	A	118	53.3	129.8	143.9	-48.23	-26.01	-69.32
DMSO	Rb	Br	A	47	30.3	5.5	14.9	-11.62	7.95	-69.99
DMSO	Rb	Cl	A	32	49.4	-5.9	-0.8	-1.17	21.30	-46.06
DMSO	Rb	ClO[4]	A	91	33.3	69.2	81.0	-0.66	3.19	-20.96
DMSO	Rb	I	A	71	44.2	33.3	44.3	-21.65	-2.80	-58.46
EtOH	Cs	Br	P	26	48.8	-49.1	-35.8	19.59	30.54	-32.53
EtOH	Cs	Cl	P	11	41.9	-73.8	-62.0	16.01	27.69	-36.72
EtOH	Cs	ClO[4]	P	70	47.8	30.9	46.1	40.98	39.82	2.06
EtOH	Cs	I	P	50	68.7	-16.1	3.4	20.93	27.09	-16.79
EtOH	K	Br	P	58	85.5	-2.4	23.0	5.68	27.83	-67.29
EtOH	K	Cl	P	43	78.6	-27.1	-3.2	7.82	30.35	-70.31
EtOH	K	ClO[4]	P	102	84.5	77.6	104.9	28.74	36.70	-25.71

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
EtOH	K	I	P	82	105.4	30.6	62.2	0.33	19.44	-57.41
EtOH	Li	Br	P	127	141.0	179.7	220.6	-63.63	-25.97	-122.39
EtOH	Li	Cl	P	112	134.1	155.0	194.4	-47.03	-9.61	-123.33
EtOH	Li	ClO[4]	P	171	140.0	259.7	302.5	-49.72	-27.79	-75.67
EtOH	Li	I	P	151	160.9	212.7	259.8	-83.86	-50.21	-109.27
EtOH	Me[4]*N	Br	P	-84	78.3	-148.6	-121.8	30.36	31.29	-7.10
EtOH	Me[4]*N	Cl	P	-99	71.4	-173.3	-148.0	14.92	18.95	3.00
EtOH	Me[4]*N	ClO[4]	P	-40	77.3	-68.6	-39.9	46.79	40.03	34.90
EtOH	Me[4]*N	I	P	-60	98.2	-115.6	-82.6	42.18	39.35	26.70
EtOH	Na	Br	P	94	117.4	69.1	104.8	-14.60	17.03	-96.45
EtOH	Na	Cl	P	79	110.5	44.4	78.6	-5.32	26.20	-97.81
EtOH	Na	ClO[4]	P	138	116.4	149.1	186.7	-8.25	9.34	-55.36
EtOH	Na	I	P	118	137.3	102.1	144.0	-27.33	1.49	-87.32
EtOH	Rb	Br	P	47	66.3	-26.6	-8.6	13.28	29.45	-51.99
EtOH	Rb	Cl	P	32	59.4	-51.3	-34.8	13.23	29.50	-54.06
EtOH	Rb	ClO[4]	P	91	65.3	53.4	73.3	40.04	40.99	-6.96
EtOH	Rb	I	P	71	86.2	6.4	30.6	13.05	23.90	-34.46
FA	Cs	Br	P	26	-1.2	-35.3	-36.8	7.39	0.14	25.47
FA	Cs	Cl	P	11	-11.1	-58.3	-70.0	-3.19	-1.01	18.28
FA	Cs	ClO[4]	P	70	-0.2	31.0	30.4	14.08	-4.28	62.06

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
FA	Cs	I	P	50	13.7	-0.7	0.8	7.13	-1.71	36.21
FA	K	Br	P	58	4.5	9.0	13.4	2.08	-0.17	21.71
FA	K	Cl	P	43	-5.4	-14.0	-19.8	-2.78	4.05	15.69
FA	K	ClO[4]	P	102	5.5	75.3	80.6	10.44	-5.00	65.29
FA	K	I	P	82	19.4	43.6	51.0	-4.87	-6.96	26.59
FA	Li	Br	P	127	31.0	191.7	199.5	-55.73	-54.57	-4.39
FA	Li	Cl	P	112	21.1	168.7	166.3	-46.13	-36.51	-8.33
FA	Li	ClO[4]	P	171	32.0	258.0	266.7	-56.52	-70.09	44.33
FA	Li	I	P	151	45.9	226.3	237.1	-77.56	-77.21	3.73
FA	Na	Br	P	94	34.4	83.7	93.2	-16.20	-14.17	-5.45
FA	Na	Cl	P	79	24.5	60.7	60.0	-13.92	-3.30	-9.81
FA	Na	ClO[4]	P	138	35.4	150.0	160.4	-24.55	-35.56	37.64
FA	Na	I	P	118	49.3	118.3	130.8	-30.53	-28.11	-1.32
FA	Rb	Br	P	47	-0.7	-13.3	-11.8	3.28	-0.45	23.01
FA	Rb	Cl	P	32	-10.6	-36.3	-45.0	-3.77	1.30	17.94
FA	Rb	ClO[4]	P	91	0.3	53.0	55.4	15.34	-2.61	70.04
FA	Rb	I	P	71	14.2	21.3	25.8	1.45	-4.40	35.54
MeCN	Cs	Br	A	26	6.8	-25.2	-19.3	7.49	31.24	-82.53
MeCN	Cs	Cl	A	11	-8.1	-40.4	-37.9	11.51	37.89	-94.72
MeCN	Cs	ClO[4]	A	70	25.8	34.5	46.5	12.78	20.22	-27.94

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
MeCN	Cs	I	A	50	30.7	-1.7	8.8	-2.27	18.29	-62.79
MeCN	Et[4]*N	Br	A	-141	35.2	-152.7	-133.3	11.73	13.88	5.80
MeCN	Et[4]*N	Cl	A	-156	20.3	-167.9	-151.9	4.93	20.33	-42.00
MeCN	Et[4]*N	ClO[4]	A	-97	54.2	-93.0	-67.5	12.01	5.04	36.30
MeCN	Et[4]*N	I	A	-117	59.1	-129.2	-105.2	16.51	14.61	28.50
MeCN	K	Br	A	58	15.5	18.8	28.5	4.58	31.23	-89.29
MeCN	K	Cl	A	43	0.6	3.6	9.9	14.32	43.25	-100.31
MeCN	K	ClO[4]	A	102	34.5	78.5	94.3	11.54	19.80	-27.71
MeCN	K	I	A	82	39.4	42.3	56.6	-11.87	13.34	-75.41
MeCN	Li	Br	A	127	93.0	173.8	215.6	-54.23	4.53	-166.39
MeCN	Li	Cl	A	112	78.1	158.6	197.0	-30.03	30.39	-175.33
MeCN	Li	ClO[4]	A	171	112.0	233.5	281.4	-56.42	-17.59	-99.67
MeCN	Li	I	A	151	116.9	197.3	243.7	-85.56	-29.21	-149.27
MeCN	Na	Br	A	94	41.4	84.4	99.0	-4.40	26.33	-112.45
MeCN	Na	Cl	A	79	26.5	69.2	80.4	12.48	45.00	-121.81
MeCN	Na	ClO[4]	A	138	60.4	144.1	164.8	-14.15	-1.66	-51.36
MeCN	Na	I	A	118	65.3	107.9	127.1	-28.23	1.29	-99.32
MeCN	Rb	Br	A	47	17.3	-3.1	4.2	4.88	30.55	-94.99
MeCN	Rb	Cl	A	32	2.4	-18.3	-14.4	12.43	40.10	-105.06
MeCN	Rb	ClO[4]	A	91	36.3	56.6	70.0	15.54	21.79	-29.96

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
MeCN	Rb	I	A	71	41.2	20.4	32.3	-6.45	15.50	-73.46
MeOH	Bu[4]*N	ClO[4]	P	-173	189.2	-110.4	-55.5	27.80	6.75	76.90
MeOH	Bu[4]*N	I	P	-193	209.1	-160.6	-97.5	37.54	0.18	123.20
MeOH	Cs	Br	P	26	60.8	-49.6	-30.0	13.79	15.24	-14.53
MeOH	Cs	Cl	P	11	44.9	-73.5	-58.5	7.91	13.19	-27.72
MeOH	Cs	ClO[4]	P	70	64.8	34.8	51.5	34.78	28.92	25.06
MeOH	Cs	F	P	-37	-9.6	-191.6	-193.7	-39.31	-16.51	-82.50
MeOH	Cs	I	P	50	84.7	-15.4	9.5	15.43	12.99	5.21
MeOH	Et[4]*N	Br	P	-141	166.2	-180.9	-144.7	18.73	1.68	-3.20
MeOH	Et[4]*N	Cl	P	-156	150.3	-204.8	-173.2	2.03	-0.57	-52.00
MeOH	Et[4]*N	ClO[4]	P	-97	170.2	-96.5	-63.2	34.71	17.54	12.30
MeOH	Et[4]*N	I	P	-117	190.1	-146.7	-105.2	34.91	13.11	19.50
MeOH	K	Br	P	58	83.5	-3.3	24.6	4.08	12.93	-35.29
MeOH	K	Cl	P	43	67.6	-27.2	-3.9	3.92	16.25	-47.31
MeOH	K	ClO[4]	P	102	87.5	81.1	106.1	26.74	26.20	11.29
MeOH	K	F	P	-5	13.1	-145.3	-139.1	-23.24	4.19	-93.96
MeOH	K	I	P	82	107.4	30.9	64.1	-0.97	5.74	-21.41
MeOH	Li	Br	P	127	128.0	179.1	219.3	-62.33	-41.17	-79.39
MeOH	Li	Cl	P	112	112.1	155.2	190.8	-48.03	-24.01	-89.33
MeOH	Li	ClO[4]	P	171	132.0	263.5	300.8	-48.82	-38.59	-27.67

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
MeOH	Li	F	P	64	57.6	37.1	55.6	1.65	38.91	-129.76
MeOH	Li	I	P	151	151.9	213.3	258.8	-82.26	-64.21	-62.27
MeOH	Me[4]*N	Br	P	-84	75.3	-147.9	-121.9	30.46	14.79	25.90
MeOH	Me[4]*N	Cl	P	-99	59.4	-171.8	-150.4	12.72	3.25	27.00
MeOH	Me[4]*N	ClO[4]	P	-40	79.3	-63.5	-40.4	46.49	27.93	72.90
MeOH	Me[4]*N	I	P	-60	99.2	-113.7	-82.4	42.58	24.05	63.70
MeOH	Na	Br	P	94	125.4	69.1	108.5	-18.30	1.23	-74.45
MeOH	Na	Cl	P	79	109.5	45.2	80.0	-11.32	11.20	-84.81
MeOH	Na	ClO[4]	P	138	129.4	153.5	190.0	-12.35	-2.06	-28.36
MeOH	Na	F	P	31	55.0	-72.9	-55.2	-6.50	29.91	-127.43
MeOH	Na	I	P	118	149.3	103.3	148.0	-30.73	-13.11	-61.32
MeOH	NH[4]*	Br	P	48	124.8	-17.2	22.1	-1.52	14.34	-44.69
MeOH	NH[4]*	Cl	P	33	108.9	-41.1	-6.4	-1.03	16.85	-51.80
MeOH	NH[4]*	ClO[4]	P	92	128.8	67.2	103.6	6.68	18.72	-16.79
MeOH	NH[4]*	F	P	-15	54.4	-159.2	-141.6	-9.18	21.99	-92.40
MeOH	NH[4]*	I	P	72	148.7	17.0	61.6	-10.07	0.22	-19.30
MeOH	Rb	Br	P	47	81.3	-27.5	-3.3	7.98	14.55	-36.99
MeOH	Rb	Cl	P	32	65.4	-51.4	-31.8	5.63	15.40	-48.06
MeOH	Rb	ClO[4]	P	91	85.3	56.9	78.2	34.34	30.49	13.04
MeOH	Rb	I	P	71	105.2	6.7	36.2	8.05	10.20	-15.46

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
PC	Cs	Br	A	26	14.8	-15.0	-10.3	13.69	18.44	-14.53
PC	Cs	Cl	A	11	5.9	-31.2	-30.3	16.31	24.09	-20.72
PC	Cs	I	A	50	24.7	6.7	17.9	4.03	3.69	-8.79
PC	K	Br	A	58	53.5	18.7	35.7	12.58	28.73	-51.29
PC	K	Cl	A	43	44.6	2.5	15.7	20.92	39.75	-56.31
PC	K	I	A	82	63.4	40.4	63.9	-3.77	9.04	-51.41
PC	Li	Br	A	127	97.0	177.2	207.4	-30.83	-1.47	-94.39
PC	Li	Cl	A	112	88.1	161.0	187.4	-8.03	23.39	-97.33
PC	Li	I	A	151	106.9	198.9	235.6	-62.06	-37.01	-91.27
PC	Na	Br	A	94	76.4	80.4	105.7	4.10	27.73	-71.45
PC	Na	Cl	A	79	67.5	64.2	85.7	19.58	45.40	-74.81
PC	Na	I	A	118	86.3	102.1	133.9	-19.63	0.89	-72.32
PC	Rb	Br	A	47	32.3	2.0	12.1	12.18	22.85	-33.99
PC	Rb	Cl	A	32	23.4	-14.2	-7.9	18.33	31.40	-38.06
PC	Rb	I	A	71	42.2	23.7	40.3	0.95	6.00	-26.46
H_2O	Bu[4]*N	ClO[4]	P	-173	361.2	-140.0	-32.0	10.50	23.35	-43.10
H_2O	Bu[4]*N	I	P	-193	382.1	-191.0	-77.0	17.24	15.98	4.20
H_2O	Cs	Br	P	26	-0.2	-52.0	-53.0	25.99	-4.56	102.47
H_2O	Cs	Cl	P	11	-17.1	-78.0	-84.0	17.61	-8.71	88.28
H_2O	Cs	ClO[4]	P	70	1.8	37.0	37.0	55.48	13.72	140.06

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
H_2O	Cs	F	P	-37	-78.6	-203.0	-227.0	-37.41	-45.31	26.50
H_2O	Cs	I	P	50	22.7	-14.0	-8.0	33.13	-3.01	121.21
H_2O	Cs	NO[3]	P	30	-27.8	-20.0	-29.0	40.33	3.27	124.30
H_2O	Et[4]*N	Br	P	-141	163.2	-191.0	-143.0	6.23	-10.42	55.80
H_2O	Et[4]*N	Cl	P	-156	146.3	-217.0	-174.0	-12.97	-14.77	6.00
H_2O	Et[4]*N	ClO[4]	P	-97	165.2	-102.0	-53.0	30.71	10.04	69.30
H_2O	Et[4]*N	I	P	-117	186.1	-153.0	-98.0	27.91	4.81	77.50
H_2O	K	Br	P	58	15.5	-6.0	-2.0	19.88	-6.57	88.71
H_2O	K	Cl	P	43	-1.4	-32.0	-33.0	17.22	-5.35	75.69
H_2O	K	ClO[4]	P	102	17.5	83.0	88.0	51.04	11.30	133.29
H_2O	K	F	P	-5	-62.9	-157.0	-176.0	-17.74	-24.31	22.04
H_2O	K	I	P	82	38.4	32.0	43.0	20.33	-9.96	101.59
H_2O	K	NO[3]	P	62	-12.1	26.0	22.0	34.89	0.33	115.91
H_2O	K	SCN	P	75	8.3	21.0	23.0	24.22	-12.25	122.32
H_2O	Li	Br	P	127	83.0	171.0	195.0	-48.83	-55.27	21.61
H_2O	Li	Cl	P	112	66.1	145.0	164.0	-37.03	-40.21	10.67
H_2O	Li	ClO[4]	P	171	85.0	260.0	285.0	-26.82	-48.09	71.33
H_2O	Li	F	P	64	4.6	20.0	21.0	4.85	15.81	-36.76
H_2O	Li	I	P	151	105.9	209.0	240.0	-63.26	-74.51	37.73
H_2O	Li	NO[3]	P	131	55.4	203.0	219.0	-2.72	-23.40	69.36

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies ΔS_{sol}^{exp}, solvation enthalpies ΔH_{sol}^{exp} as well as the free energies of solvation ΔG_{sol}^{exp}. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	ΔS_{sol}^{exp}	ΔG_{sol}^{exp}	ΔH_{sol}^{exp}
H_2O	Me[4]*N	Br	P	-84	85.3	-152.0	-127.0	24.76	-3.31	71.90
H_2O	Me[4]*N	Cl	P	-99	68.4	-178.0	-158.0	4.52	-16.95	72.00
H_2O	Me[4]*N	ClO[4]	P	-40	87.3	-63.0	-37.0	49.29	14.43	116.90
H_2O	Me[4]*N	I	P	-60	108.2	-114.0	-82.0	42.38	9.75	108.70
H_2O	Na	Br	P	94	52.4	65.0	80.0	-0.60	-16.87	54.55
H_2O	Na	Cl	P	79	35.5	39.0	49.0	3.88	-8.99	43.19
H_2O	Na	ClO[4]	P	138	54.4	154.0	170.0	13.85	-15.56	98.64
H_2O	Na	F	P	31	-26.0	-86.0	-94.0	0.90	2.81	-6.43
H_2O	Na	Form	P	102	-12.8	-12.0	-16.0	0.83	-13.00	46.39
H_2O	Na	I	P	118	75.3	103.0	125.0	-7.53	-27.41	66.68
H_2O	Na	NO[3]	P	98	24.8	97.0	104.0	20.37	-6.15	88.95
H_2O	Na	OAc	P	130	-58.2	9.0	-9.0	-17.32	-24.02	22.47
H_2O	NH[4]*	Br	P	48	52.8	-17.0	-7.0	16.78	-8.06	83.31
H_2O	NH[4]*	Cl	P	33	35.9	-43.0	-38.0	14.77	-7.65	75.20
H_2O	NH[4]*	ClO[4]	P	92	54.8	72.0	83.0	33.48	0.92	109.21
H_2O	NH[4]*	F	P	-15	-25.6	-168.0	-181.0	-1.18	-9.41	27.60
H_2O	NH[4]*	I	P	72	75.7	21.0	38.0	13.73	-18.38	107.70
H_2O	NH[4]*	NO[3]	P	52	25.2	15.0	17.0	25.69	-6.69	108.60
H_2O	Pr[4]*N	Br	P	-183	268.2	-205.0	-126.0	-4.39	-6.69	7.70
H_2O	Pr[4]*N	ClO[4]	P	-139	270.2	-116.0	-36.0	27.36	20.33	23.60

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Table 2: Data set for machine learning on experimental data with solvent (S), cation (C^+), anion (A^-), solvent type (ST), meaning either protic (P) or aprotic (A), the difference in the cationic and anionic radii Δr_{AC}, the difference in the cation and anion solvation entropies ΔS_{AC}, solvation enthalpies ΔH_{AC} and free solvation energies ΔH_{AC}, respectively, and the full solvation entropies $\Delta S_{\mathrm{sol}}^{\mathrm{exp}}$, solvation enthalpies $\Delta H_{\mathrm{sol}}^{\mathrm{exp}}$ as well as the free energies of solvation $\Delta G_{\mathrm{sol}}^{\mathrm{exp}}$. All energy and enthalpy values have units of kcal/mol and all entropies have units of cal/Kmol. The values for Δr_{AC} are in pm.

S	C^+	A^-	ST	Δr_{AC}	ΔS_{AC}	ΔG_{AC}	ΔH_{AC}	$\Delta S_{\mathrm{sol}}^{\mathrm{exp}}$	$\Delta G_{\mathrm{sol}}^{\mathrm{exp}}$	$\Delta H_{\mathrm{sol}}^{\mathrm{exp}}$
H_2O	Pr[4]*N	I	P	-159	291.1	-167.0	-81.0	11.59	8.91	9.00
H_2O	Rb	Br	P	47	6.3	-29.0	-28.0	21.88	-6.15	94.01
H_2O	Rb	Cl	P	32	-10.6	-55.0	-59.0	17.03	-7.40	81.94
H_2O	Rb	ClO[4]	P	91	8.3	60.0	62.0	56.74	14.39	142.04
H_2O	Rb	I	P	71	29.2	9.0	17.0	27.45	-6.70	114.54
H_2O	Rb	NO[3]	P	51	-21.3	3.0	-4.0	36.53	0.54	120.71