A Study of the Hydration of the Alkali Metal Ions in Aqueous Solution

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Supplementary material

Appendix 1 - Considered structures

Table S1a. *Considered lithium-oxygen structures of different classes as described in appendix 2. Structures in which $d_{max}/d_{min} > 1.10$ has not been used in the calculations of the main report. Structures denoted letters have been found in the Cambridge Crystallographic Data Centre database while structures denoted by numbers have been found in the Inorganic Crystal Structure Database.*

Structure	N_c	Distance Å	Stdev Å	Stdev %	d_{max}/d_{min}	Classif.
FUHQEE	3	1.823	0.021	1.130	1.02	1121
KETMOL	3	1.948	0.022	1.104	1.02	1221
OGOPEF	3	1.891	0.011	0.589	1.01	1244
TOXMUO	3	1.847	0.051	2.765	1.06	1121
XARLOS	3	1.896	0.099	5.234	1.10	1211
YAPKIJ	3	1.895	0.049	2.564	1.05	1111
DOLJAP	5	2.083	0.075	3.611	1.09	1237
YESHIN	5	2.173	0.204	9.388	1.19	1111
UCIJOG	6	2.186	0.132	6.058	1.16	1214
XONQEW	6	2.180	0.090	4.119	1.11	1147
YEKYIW01	6	2.172	0.235	10.803	1.30	1234
AJUZEK	4	1.908	0.066	3.450	1.10	1213
AKACAQ	4	1.950	0.080	4.105	1.08	1123
BADTUV10	4	1.920	0.063	3.262	1.08	1111
CECZEQ	4	1.911	0.014	0.755	1.01	1121
CECZOA	4	1.936	0.055	2.865	1.08	1223
CELGUV	4	1.965	0.081	4.103	1.08	1113
CENJAH	4	1.963	0.008	0.386	1.01	1121
CENJEL	4	1.987	0.004	0.194	1.00	1121
CENJIP	4	1.973	0.006	0.307	1.01	1121
CENJOV	4	1.975	0.010	0.511	1.01	1121
CENJUB	4	1.968	0.013	0.681	1.02	1121
CENKAI	4	1.968	0.015	0.771	1.02	1121
CIPJOA	4	1.968	0.036	1.840	1.04	1213
COVBEU	4	1.945	0.029	1.476	1.03	1111
DEMSOE	4	1.889	0.004	0.231	1.00	1121
DEQCOS	4	1.949	0.072	3.709	1.11	1121
DOLJAP	4	1.955	0.092	4.683	1.11	1211
DOTJOM	4	1.901	0.027	1.439	1.05	1231
FALZEY	4	2.444	0.000	0.000	1.00	G
FALZIC	4	2.392	0.000	0.000	1.00	G
FEDHUR	4	1.928	0.031	1.617	1.03	1111
FILWEC	4	1.922	0.000	0.000	1.00	1121
FIYFUO	4	1.914	0.061	3.179	1.11	1124
GAQPOE	4	1.935	0.018	0.940	1.03	1211
GEFDEA	4	1.951	0.085	4.338	1.09	1113
GIVBUI	4	1.958	0.069	3.545	1.08	1223
GOJGIV	4	1.925	0.037	1.912	1.04	1213
HENNAQ	4	1.925	0.011	0.571	1.02	1121
HIDFIJ	4	1.911	0.020	1.020	1.02	1121
IDOZAC	4	1.933	0.035	1.794	1.04	1111
IGAZUL	4	1.946	0.039	2.019	1.05	1111
IXUFIQ	4	1.923	0.000	0.000	1.00	1121
JESRIJ	4	1.965	0.075	3.793	1.07	1121
KABDEW01	4	1.949	0.048	2.447	1.06	1221
KEZKAB	4	1.917	0.029	1.530	1.03	1213
KIJZUZ	4	1.936	0.000	0.000	1.00	1111
KUPFUW	4	1.946	0.076	3.901	1.10	1211
KUPFUW	4	1.958	0.075	3.828	1.09	1113
LAPNAR	4	1.928	0.022	1.125	1.02	1111

LIHMAL01	4	1.983	0.064	3.236	1.08	1213
LIMNOK	4	1.690	0.234	13.840	1.27	1111
MAKHEL	4	1.918	0.027	1.416	1.03	1121
NAKCUX	4	1.919	0.072	3.767	1.09	1123
NOXBIL	4	1.928	0.022	1.144	1.03	1111
OGIQIE	4	1.948	0.015	0.748	1.02	1121
PAJTUQ	4	1.922	0.000	0.000	1.00	1121
PAJVAY	4	1.924	0.041	2.123	1.08	1121
PAJVEC	4	1.916	0.048	2.493	1.10	1121
PUPCUY	4	1.957	0.000	0.000	1.00	1111
QECKOY	4	1.944	0.026	1.339	1.03	1121
REHBUC	4	1.937	0.060	3.084	1.07	1213
RIBDEM	4	1.946	0.000	0.000	1.00	1111
ROHLIJ	4	2.010	0.125	6.196	1.13	1114
SIRLOV	4	1.912	0.013	0.692	1.02	1141
SONDUV	4	1.934	0.045	2.325	1.05	1111
SONDUV	4	1.931	0.019	0.978	1.02	1211
SOXQAX	4	1.954	0.062	3.162	1.06	1124
TAGMEU	4	1.951	0.050	2.578	1.08	1212
TANKOI	4	1.970	0.042	2.114	1.04	1124
TARLIH	4	1.964	0.065	3.321	1.07	1124
TEFHOC	4	1.927	0.017	0.905	1.02	1121
TIPWOE	4	1.944	0.105	5.413	1.12	1111
TOQFIP	4	1.918	0.033	1.711	1.04	1111
VERDEC	4	1.940	0.048	2.456	1.06	1111
VERDIG	4	1.919	0.149	7.753	1.23	1111
VERDOM	4	1.985	0.113	5.670	1.21	1111
VERDUS	4	1.911	0.120	6.277	1.17	1111
VUJYII	4	1.900	0.010	0.522	1.01	1121
VURJUN	4	1.948	0.009	0.474	1.01	1121
WABFIO	4	1.966	0.025	1.292	1.02	1111
WIKWUI	4	1.937	0.033	1.695	1.05	1111
WOYZOZ	4	1.931	0.024	1.226	1.02	1121
WURQOP	4	1.942	0.025	1.280	1.03	1211
XAFFIT	4	1.924	0.035	1.835	1.04	1121
XARLIM	4	1.908	0.098	5.124	1.12	1121
XARLUY	4	1.949	0.054	2.767	1.06	R
XARLUY01	4	1.944	0.034	1.753	1.03	1121
XIBWUA	4	1.925	0.029	1.516	1.03	1211
XIFHUP	4	1.931	0.018	0.911	1.02	1111
XILJUX	4	1.936	0.058	3.003	1.08	1241
YAPKIJ	4	1.959	0.073	3.745	1.14	1111
YEMZUL	4	1.908	0.000	0.000	1.00	1111
YIDYAW	4	1.965	0.070	3.539	1.08	1111
YIRRIA	4	1.933	0.012	0.597	1.01	1111
MOXCAE	4	1.945	0.039	1.998	1.05	1111
MOXCUY	4	1.927	0.000	0.000	1.00	1111
COZBUO	3	1.994	0.022	1.113	1.02	3125
DENGUY	3	1.932	0.026	1.349	1.03	3125
DOZYUM	3	1.923	0.017	0.858	1.02	3125
FUHQEE	3	1.823	0.021	1.130	1.02	3125
FUYWUR	3	1.895	0.014	0.758	1.01	3125
GACFEV	3	1.993	0.087	4.371	1.09	3125
GIDBAX	3	1.966	0.010	0.507	1.02	3125
IRIZIS	3	2.013	0.011	0.560	1.01	3125
JEVSAE	3	1.941	0.003	0.136	1.00	3125
JOSSIT	3	1.898	0.035	1.826	1.03	3125
KELQOH	3	1.958	0.011	0.568	1.02	3125
KEVQOR	3	1.913	0.020	1.066	1.03	3125
KIDRUK	3	1.945	0.022	1.134	1.02	3125
LONYES	3	1.887	0.014	0.742	1.01	3125

MUYXEJ	3	1.911	0.008	0.407	1.01	3125
NIGMOG	3	1.926	0.010	0.520	1.01	3125
OCEKAI	3	1.932	0.015	0.782	1.02	3125
QOZMEX	3	2.000	0.015	0.750	1.02	3125
REXTAQ	3	2.071	0.000	0.000	1.00	3125
REXTEU	3	1.989	0.000	0.000	1.00	3125
RIJKUQ	3	1.906	0.020	1.053	1.02	3125
TOKHEH	3	1.877	0.031	1.627	1.03	3125
XUPPED	3	1.861	0.000	0.000	1.00	3125
ZEPHUX	3	1.995	0.028	1.421	1.03	3125
SIHHEX	6	2.173	0.000	0.000	1.00	3125
YOGJIO	6	2.162	0.000	0.000	1.00	3125
YOGJOU	6	2.173	0.000	0.000	1.00	3125
AGIJUV	4	1.925	0.033	1.731	1.04	3125
AVAWAV	4	1.926	0.030	1.532	1.04	3125
AYIVIN	4	1.871	0.014	0.772	1.01	G
BANZOF	4	1.924	0.014	0.709	1.02	3125
BANZUL	4	1.927	0.016	0.816	1.02	3125
BEMMIQ	4	1.930	0.042	2.171	1.05	3125
BEQTAT	4	1.912	0.005	0.246	1.01	3125
BETPAS	4	1.926	0.004	0.210	1.00	3125
BEVBAG	4	1.906	0.016	0.821	1.02	3125
BEVBEK	4	1.918	0.017	0.871	1.02	3125
BEWYIM	4	1.924	0.013	0.691	1.02	3125
BEYROM01	4	1.911	0.013	0.692	1.02	3125
BISVEE	4	1.888	0.037	1.969	1.05	3125
BISZAE	4	1.920	0.011	0.581	1.01	3125
BISZUY	4	1.918	0.007	0.354	1.01	3125
BUCQIZ	4	1.929	0.036	1.860	1.04	3125
BUTXUJ	4	1.954	0.094	4.836	1.12	3125
CAFQOP	4	1.917	0.056	2.930	1.07	3125
CAWWAY	4	1.918	0.020	1.041	1.02	3125
CAXGOY	4	1.951	0.093	4.749	1.19	3125
CIFYAS	4	1.902	0.017	0.910	1.02	3125
CESDAF	4	1.916	0.067	3.509	1.08	3125
CIQNUL	4	1.897	0.005	0.249	1.01	3125
CIQQEY	4	1.930	0.013	0.657	1.02	3125
CIWQII	4	1.913	0.031	1.643	1.04	3125
COSQIK	4	1.941	0.009	0.440	1.01	3125
CUSFEB	4	1.923	0.010	0.544	1.01	3125
CUSFOL	4	1.925	0.141	7.337	1.20	3125
DAGKOL	4	1.920	0.017	0.909	1.02	3125
DEZQOP	4	1.914	0.009	0.474	1.01	3125
DEZQUV	4	1.913	0.013	0.694	1.02	3125
DIBYES	4	1.914	0.047	2.453	1.06	3125
DOFHOW	4	1.905	0.038	2.017	1.05	3125
DONPUS	4	1.907	0.007	0.373	1.01	3125
DONWUZ	4	1.921	0.015	0.799	1.02	3125
DONXAG	4	1.919	0.013	0.676	1.02	3125
DOQTEI	4	1.909	0.006	0.313	1.01	3125
DOTYEQ	4	1.952	0.085	4.335	1.10	3125
EFEFEB	4	1.900	0.037	1.964	1.05	3125
EGUDAL	4	1.920	0.030	1.543	1.04	3125
EGUDEP	4	1.917	0.014	0.726	1.02	3125
EHEHEE	4	1.946	0.010	0.488	1.01	3125
ELUWIR	4	1.913	0.010	0.513	1.01	3125
ETANIW	4	1.924	0.014	0.753	1.02	3125
EXUZEC	4	1.941	0.015	0.768	1.02	3125
FAFZUI	4	1.905	0.022	1.177	1.02	3125
FAMLOV	4	1.940	0.052	2.670	1.06	3125
FAMTIX	4	1.915	0.009	0.445	1.01	3125

FAPVEY	4	1.900	0.114	6.010	1.22	3125
FERVII	4	1.921	0.023	1.209	1.04	3125
FITLOK	4	1.900	0.003	0.182	1.00	3125
FONJIB	4	1.882	0.024	1.288	1.02	3125
FOZYIC	4	1.925	0.023	1.189	1.03	3125
GEVJIB	4	1.909	0.010	0.501	1.01	3125
GEVJUM	4	1.936	0.065	3.360	1.08	3125
GEVKAT	4	1.911	0.055	2.865	1.07	3125
GEVKEX	4	1.920	0.031	1.592	1.04	3125
GIFVIA	4	1.950	0.041	2.122	1.05	3125
GILHEO	4	1.925	0.022	1.128	1.02	3125
GILHIS	4	1.922	0.008	0.408	1.01	3125
GIXKED	4	1.925	0.013	0.659	1.02	3125
HAJSIU	4	1.917	0.058	3.038	1.08	3125
HAKVEU	4	1.935	0.020	1.022	1.03	3125
HELKAK	4	1.890	0.033	1.744	1.06	3125
HILXIJ	4	1.919	0.032	1.669	1.06	3125
HIMCIP	4	1.877	0.032	1.682	1.04	3125
HOBZUU	4	1.927	0.022	1.139	1.05	3125
HOJWUY	4	1.927	0.010	0.544	1.01	3125
HOJXAF	4	1.940	0.032	1.668	1.04	3125
HOJXEJ	4	1.937	0.024	1.229	1.03	3125
HOKHAR	4	1.922	0.019	1.002	1.03	3125
HOKQIH	4	1.914	0.028	1.462	1.06	3125
HOMMUS	4	1.907	0.012	0.608	1.01	3125
HOMNAZ	4	1.903	0.007	0.375	1.01	3125
HOMNED	4	1.908	0.012	0.635	1.01	3125
HOMPIJ	4	1.906	0.029	1.543	1.04	3125
HOXBOL	4	1.941	0.049	2.511	1.06	3125
HUCGOB	4	1.902	0.025	1.316	1.03	3125
ILEWAX	4	1.928	0.024	1.233	1.03	3125
ILEWEB	4	1.936	0.026	1.317	1.03	3125
IMEQAS	4	1.920	0.013	0.668	1.02	3125
IMUMAE	4	1.866	0.052	2.782	1.06	G
INOBES	4	1.946	0.008	0.386	1.01	3125
IQEHOB	4	1.925	0.010	0.518	1.01	3125
IQEHUH	4	1.954	0.032	1.617	1.04	3125
JABVIS	4	1.907	0.006	0.334	1.01	3125
JASPID	4	1.928	0.023	1.199	1.03	3125
JASQAW	4	1.910	0.025	1.301	1.03	3125
JEMKIV	4	1.884	0.009	0.460	1.01	3125
JENQUP	4	1.918	0.018	0.947	1.02	3125
JENRIE	4	1.906	0.012	0.627	1.02	3125
JIWRIQ	4	1.902	0.024	1.281	1.03	R
JIWRIQ01	4	1.902	0.024	1.281	1.03	3125
JIXJAB	4	1.967	0.089	4.531	1.11	R
JIXJAB10	4	1.967	0.089	4.531	1.11	3125
JOQVOA	4	1.906	0.012	0.620	1.01	3125
JOQVUG	4	1.904	0.005	0.252	1.01	3125
JURPER	4	1.926	0.058	3.028	1.05	3125
JUYSIF	4	1.920	0.013	0.694	1.02	3125
JUYSOL	4	1.902	0.023	1.222	1.03	R
JUYSOL01	4	1.880	0.028	1.488	1.03	3125
KALVUP	4	1.929	0.047	2.413	1.06	3125
KERHAQ	4	1.994	0.151	7.584	1.20	3125
KONRUA	4	1.896	0.029	1.517	1.04	3125
KONRUA01	4	1.896	0.029	1.517	1.04	3125
LECXUN	4	1.935	0.021	1.070	1.03	3125
LEKVAZ	4	1.925	0.009	0.471	1.01	3125
LILQAY	4	1.909	0.009	0.454	1.01	3125
LIPKIE	4	1.908	0.009	0.454	1.01	3125

LIZYUO	4	1.912	0.039	2.038	1.05	3125
LOLNIJ	4	1.931	0.032	1.635	1.04	3125
LOLPAD	4	1.935	0.068	3.505	1.08	3125
MANWAA	4	1.914	0.006	0.339	1.01	3125
MAYLED	4	1.910	0.018	0.967	1.02	3125
MAYLON	4	1.923	0.070	3.631	1.08	3125
MECFAC	4	1.921	0.000	0.000	1.00	3125
MESDIY	4	1.901	0.100	5.256	1.14	3125
MIDCUY	4	1.912	0.053	2.749	1.06	3125
MIDFIP	4	1.936	0.054	2.802	1.07	3125
MIDFOV	4	1.930	0.076	3.964	1.10	3125
MOQWOE	4	1.925	0.002	0.090	1.00	3125
MOQWUK	4	1.912	0.003	0.181	1.00	3125
MURJAK	4	1.923	0.008	0.441	1.01	3125
MUYWUY	4	1.917	0.014	0.710	1.02	3125
MUYXEJ	4	1.920	0.013	0.651	1.01	3125
NADHEF	4	1.914	0.009	0.448	1.01	3125
NAPREV	4	1.922	0.030	1.568	1.04	3125
NAXXIT	4	1.920	0.042	2.163	1.08	3125
NEDZOM	4	1.912	0.031	1.634	1.05	3125
NEGCOS	4	1.922	0.015	0.781	1.01	3125
NEHGOW	4	1.923	0.006	0.299	1.01	3125
NEHXED	4	1.924	0.035	1.829	1.04	3125
NEWQUB	4	1.927	0.003	0.136	1.00	3125
NIFNEW	4	1.917	0.017	0.881	1.02	3125
NIRTUE	4	1.913	0.012	0.607	1.02	3125
NIRVAM	4	1.911	0.013	0.663	1.02	3125
NOBZEJ	4	1.922	0.010	0.541	1.01	3125
NOJLIH	4	1.917	0.045	2.339	1.08	3125
NOYGAJ	4	1.928	0.011	0.572	1.01	3125
OBUXIT	4	1.922	0.014	0.735	1.02	3125
OCEJOV	4	1.915	0.038	1.975	1.05	3125
ODUDEW	4	1.981	0.107	5.396	1.11	3125
OFAGUY	4	1.922	0.035	1.815	1.04	3125
OGOCIW	4	1.914	0.030	1.557	1.04	3125
OHOHEY	4	1.918	0.023	1.173	1.02	3125
OLAJUG	4	1.921	0.030	1.576	1.04	3125
OLEZAG	4	1.901	0.019	0.976	1.02	3125
OLIPAA	4	1.928	0.008	0.427	1.01	3125
OMIBIV	4	1.918	0.015	0.768	1.02	3125
OMICOC	4	1.923	0.010	0.524	1.01	3125
OMITEJ	4	1.925	0.015	0.772	1.02	3125
OMITIN	4	1.920	0.010	0.545	1.01	3125
PATKUQ	4	1.916	0.009	0.478	1.01	3125
PAWKIH	4	1.904	0.013	0.659	1.02	3125
PAZSIS	4	1.929	0.014	0.748	1.01	3125
PEPGOH	4	1.923	0.057	2.987	1.07	3125
POBYEK	4	1.922	0.002	0.115	1.00	3125
PUYHEW	4	1.923	0.044	2.292	1.05	3125
QACVOF	4	1.939	0.000	0.000	1.00	3125
QECYEC	4	1.905	0.011	0.584	1.01	3125
QEPSEJ	4	1.904	0.010	0.512	1.01	3125
QEWQAL	4	1.905	0.000	0.000	1.00	3125
QEWQIT	4	1.927	0.038	1.984	1.05	3125
QEWQOZ	4	1.904	0.003	0.182	1.00	3125
QEXCIG	4	1.908	0.018	0.954	1.02	3125
QICDOV	4	1.894	0.082	4.320	1.10	3125
QIVDII	4	1.919	0.020	1.032	1.03	3125
QOMCOK	4	1.919	0.056	2.922	1.07	3125
QOPRES	4	1.918	0.016	0.842	1.02	3125
QOPRIW	4	1.935	0.055	2.860	1.07	3125

QUNHAI	4	1.930	0.008	0.411	1.01	3125
RAJLET	4	1.917	0.020	1.062	1.02	3125
RAJMAQ	4	1.937	0.093	4.817	1.12	3125
RANNAV	4	1.930	0.056	2.922	1.07	3125
RANNEZ	4	1.886	0.099	5.272	1.13	3125
RAPQUU	4	1.931	0.020	1.050	1.02	3125
RARSUZ	4	1.923	0.016	0.825	1.02	3125
RARXIS	4	1.917	0.018	0.956	1.02	3125
RARXOY	4	1.911	0.017	0.892	1.02	3125
RAVWER	4	1.923	0.009	0.487	1.01	3125
REJYUA	4	1.924	0.013	0.658	1.01	3125
REJYUA01	4	1.908	0.019	0.988	1.02	3125
RELQEF	4	1.906	0.067	3.509	1.07	3125
RENXIR	4	1.912	0.008	0.393	1.01	3125
REPBUJ	4	1.897	0.012	0.624	1.02	3125
REPHID	4	1.910	0.075	3.915	1.14	3125
RESBIA	4	1.921	0.016	0.858	1.02	R
RESBIA01	4	1.919	0.023	1.197	1.03	3125
REVGII	4	1.918	0.012	0.632	1.01	3125
REZBAZ	4	1.909	0.025	1.314	1.03	3125
RIQJAD	4	1.924	0.025	1.278	1.03	3125
RIVDIJ	4	1.765	0.000	0.000	1.00	G
RIVKUD	4	1.923	0.067	3.496	1.08	3125
RIVLAK	4	1.903	0.106	5.556	1.18	3125
RUFFON	4	1.910	0.017	0.865	1.02	3125
RUQRAW	4	1.925	0.013	0.696	1.01	3125
RUYBIW	4	1.917	0.006	0.307	1.01	3125
SADROF	4	1.911	0.032	1.686	1.04	3125
SADRUL	4	1.911	0.025	1.298	1.03	3125
SADSAS	4	1.918	0.049	2.552	1.06	3125
SAFPEV	4	1.926	0.012	0.630	1.01	3125
SIGTOS	4	1.923	0.014	0.703	1.02	3125
SIGYEM	4	1.927	0.065	3.353	1.08	3125
SOZJUM	4	1.917	0.011	0.595	1.01	3125
SUHWEX	4	1.931	0.022	1.142	1.03	3125
TARSAG	4	1.898	0.018	0.943	1.02	3125
TARSEK	4	1.913	0.010	0.502	1.01	3125
TAZTAP	4	1.914	0.002	0.121	1.00	3125
TEBHAK	4	1.926	0.008	0.436	1.01	3125
TEBJEP	4	1.902	0.030	1.570	1.04	3125
TEQGIF	4	1.917	0.051	2.684	1.06	R
TEQGIF01	4	1.917	0.051	2.684	1.06	3125
TIGFAQ	4	1.899	0.000	0.000	1.00	3125
TOJSOB	4	1.918	0.016	0.824	1.02	3125
TOVQEA	4	1.905	0.072	3.781	1.08	3125
TUMPAS	4	1.922	0.006	0.337	1.01	3125
TURSEE	4	1.909	0.018	0.939	1.02	3125
UCESAX	4	1.918	0.051	2.670	1.08	R
UCESAX01	4	1.934	0.014	0.747	1.01	3125
VAGGOZ	4	1.939	0.015	0.798	1.02	3125
VAXMAJ	4	1.921	0.038	1.972	1.04	3125
VAZSUK	4	1.910	0.022	1.135	1.03	3125
VAZTAR	4	1.920	0.018	0.959	1.02	3125
VEHREG	4	1.912	0.026	1.342	1.04	3125
VEQYUL	4	1.909	0.009	0.474	1.01	3125
VEQZAS	4	1.921	0.017	0.906	1.02	3125
VIHHIE	4	1.920	0.021	1.096	1.03	3125
VIPVAR	4	1.901	0.028	1.462	1.03	3125
VUZKOQ	4	1.915	0.040	2.084	1.05	3125
WAGFIU	4	1.907	0.001	0.030	1.00	3125
WASSIT	4	1.915	0.013	0.699	1.01	3125

WEKNAC	4	1.902	0.019	1.004	1.03	3125
WEWKIS	4	1.942	0.077	3.958	1.09	3125
WIDWOV	4	1.936	0.076	3.902	1.10	3125
WIMLIN	4	1.929	0.039	2.011	1.05	3125
WIMLOT	4	1.926	0.051	2.670	1.10	3125
WISXIF	4	1.930	0.030	1.571	1.04	3125
WUSXOX	4	1.942	0.043	2.201	1.05	3125
XAFFIT	4	1.924	0.035	1.835	1.04	3125
XANRIN	4	1.922	0.020	1.064	1.03	3125
XEBSAY	4	1.927	0.017	0.891	1.02	3125
XIGJUS	4	1.929	0.069	3.591	1.09	3125
XIGKED	4	2.002	0.025	1.238	1.03	G
XIGKIH	4	1.834	0.113	6.151	1.15	3125
XUPPAZ	4	1.901	0.004	0.199	1.00	3125
XUPPED	4	1.906	0.014	0.757	1.02	3125
XUTNIJ	4	1.914	0.009	0.483	1.01	3125
XUTNOP	4	1.926	0.020	1.041	1.02	3125
YADXAC	4	1.937	0.001	0.060	1.00	3125
YALKAY	4	1.921	0.008	0.406	1.01	3125
YELDAU	4	1.910	0.018	0.920	1.02	3125
YEVSUN	4	1.918	0.016	0.812	1.02	3125
YIGSAI	4	1.911	0.007	0.387	1.01	3125
YIQPIX	4	1.916	0.026	1.340	1.03	3125
YITSAW	4	1.949	0.012	0.626	1.01	3125
YOKMUH	4	1.926	0.038	1.989	1.04	3125
YUPJIC	4	1.904	0.040	2.092	1.06	3125
ZABFIR	4	1.913	0.025	1.313	1.03	3125
ZAZPAR	4	1.918	0.016	0.813	1.01	3125
ZIMFIK	4	1.913	0.014	0.743	1.02	3125
ZIWZEK	4	1.909	0.002	0.115	1.00	3125
ZOJLIT	4	1.925	0.020	1.015	1.02	3125
ZUQTOU	4	1.909	0.040	2.071	1.06	3125
ZURVUD	4	1.931	0.017	0.889	1.02	3125
SEJNAW	4	1.907	0.031	1.605	1.03	1111
ASITUR	4	1.953	0.014	0.700	1.02	1112
YIDJAW	4	1.965	0.070	3.539	1.08	1111
260275	4	1.927	0.000	0.000	1.00	1111
79472	4	1.935	0.016	0.827	1.02	1114
170007	4	1.944	0.105	5.413	1.12	1114
260274	4	1.945	0.039	1.998	1.05	1114
58839	4	1.949	0.000	0.000	1.00	1114
109876	4	1.949	0.032	1.624	1.05	1114
173218	4	1.956	0.040	2.037	1.06	1114
173217	4	1.957	0.026	1.345	1.04	1114
1521	4	1.968	0.027	1.392	1.03	1114
16441	4	1.967	0.032	1.648	1.05	1114
260273	4	1.970	0.058	2.935	1.11	1114
173216	4	2.001	0.014	0.688	1.02	G
170712	6	2.150	0.053	2.486	1.06	1114
416608	6	2.120	0.001	0.026	1.00	1114
1321	6	2.124	0.003	0.155	1.00	1114
1913	6	2.128	0.005	0.232	1.00	1114
260045	6	2.126	0.043	2.036	1.04	1114
417413	6	2.126	0.043	2.036	1.04	1114
32534	6	2.129	0.004	0.206	1.00	1114
33776	6	2.137	0.051	2.384	1.04	1114
1914	6	2.140	0.004	0.179	1.00	1114
73706	6	2.142	0.007	0.332	1.01	1114
34387	6	2.195	0.063	2.890	1.08	G
DOFFIN	4	1.957	0.130	6.623	1.15	3141
DOFKIS	4	2.149	0.312	14.512	1.42	3141

DOFKOY	4	2.014	0.218	10.815	1.26	3141
LIZLUB	4	1.908	0.035	1.846	1.03	3141
MAJPAO	4	2.083	0.031	1.467	1.03	3141
QOHGID	4	1.952	0.021	1.093	1.02	3141
AGONEP	6	2.133	0.063	2.974	1.08	3141
BEPBUU	6	2.125	0.057	2.689	1.07	3141
CALQEM	6	2.135	0.062	2.907	1.09	3141
CAWQUM	6	2.193	0.071	3.221	1.07	G
CAWVUR	6	2.156	0.052	2.433	1.06	3141
CEHVAM	6	2.168	0.077	3.551	1.10	3141
COLGEP	6	2.139	0.048	2.242	1.05	3141
DADYEM	6	2.137	0.025	1.163	1.02	3141
DEHTUG	6	2.120	0.052	2.448	1.09	3141
DEHVAO	6	2.120	0.104	4.916	1.14	3141
DEHVIW	6	2.122	0.052	2.460	1.07	3141
DOFJEN	6	2.147	0.050	2.307	1.06	3141
DOFQAQ	6	2.122	0.039	1.852	1.06	3141
ETAGIP	6	2.119	0.046	2.150	1.06	3141
ETAHEM	6	2.168	0.053	2.463	1.06	3141
ETAHIQ	6	2.135	0.096	4.489	1.15	3141
ETAHUC	6	2.224	0.105	4.731	1.16	3141
ETAJAK	6	2.225	0.104	4.696	1.13	3141
ETAJIS	6	2.118	0.056	2.620	1.09	3141
GIBVUI	6	2.133	0.073	3.401	1.08	3141
GIMWEE	6	2.120	0.040	1.881	1.05	3141
GUMHEB	6	2.139	0.054	2.513	1.07	3141
GUMHIF	6	2.144	0.102	4.772	1.13	3141
HAZVIO	6	2.146	0.040	1.847	1.05	3141
HEQRES	6	2.119	0.021	0.974	1.02	3141
HIKLAP	6	2.103	0.034	1.614	1.04	3141
HIMRIF	6	2.125	0.037	1.728	1.04	3141
HITHAT	6	2.122	0.014	0.676	1.02	3141
HODGUC	6	2.116	0.043	2.020	1.06	3141
HODHAJ	6	2.162	0.049	2.263	1.06	3141
HOFYAC	6	2.136	0.056	2.614	1.08	3141
HOTKEG	6	2.149	0.111	5.182	1.15	3141
JEFGUX	6	2.150	0.064	2.959	1.08	3141
JIRJEA	6	2.175	0.030	1.375	1.04	3141
JOGMIB	6	2.117	0.102	4.837	1.10	3141
KALWAW	6	2.133	0.031	1.473	1.04	3141
KESKUO	6	2.123	0.052	2.450	1.10	3141
KEYJAZ	6	2.137	0.045	2.103	1.04	3141
KOMCEV	6	2.135	0.093	4.335	1.13	3141
KOYDEH	6	2.161	0.081	3.758	1.10	3141
LELSAX	6	2.152	0.095	4.398	1.12	3141
LIGSIE	6	2.133	0.045	2.116	1.08	3141
LIGSOK	6	2.126	0.043	2.020	1.05	3141
LIZLEL	6	2.110	0.112	5.293	1.22	3141
LIZLUB	6	2.135	0.039	1.836	1.05	3141
LOLNOP	6	2.138	0.029	1.365	1.04	3141
LOLNOP01	6	2.137	0.036	1.677	1.04	3141
MIMFOD	6	2.127	0.030	1.427	1.05	3141
MUXLIA	6	2.119	0.034	1.589	1.06	3141
MUYXAF	6	2.132	0.033	1.549	1.04	3141
MUYXIN	6	2.145	0.045	2.096	1.06	3141
NOMGOM	6	2.114	0.040	1.913	1.05	3141
NUFPAF	6	2.107	0.036	1.720	1.04	3141
OCEJUB	6	2.122	0.053	2.500	1.08	3141
OHAJAI	6	2.181	0.041	1.875	1.04	3141
OJINAW	6	2.129	0.073	3.422	1.09	3141
OKUTIX	6	2.146	0.028	1.317	1.04	3141

OKUTOD	6	2.134	0.033	1.529	1.04	3141
PALMEV	6	2.139	0.068	3.193	1.13	3141
PALMOF	6	2.139	0.040	1.867	1.05	3141
PALSUQ	6	2.160	0.041	1.917	1.04	3141
PAQCIU	6	2.144	0.071	3.308	1.09	3141
PIPFID	6	2.131	0.055	2.581	1.07	3141
POJPAF	6	2.117	0.038	1.792	1.04	3141
PONKEJ	6	2.131	0.050	2.337	1.06	3141
PUMGEJ	6	2.139	0.018	0.855	1.03	3141
QEBBEE	6	2.133	0.074	3.463	1.13	3141
QECTAT	6	2.123	0.017	0.802	1.02	3141
QECTEX	6	2.141	0.063	2.964	1.08	3141
QODZAL	6	2.127	0.064	2.995	1.12	3141
QOHJAY	6	2.150	0.072	3.347	1.13	3141
QOMDIF	6	2.072	0.072	3.462	1.09	G
QOMDOL	6	2.154	0.075	3.464	1.11	3141
REDVAY	6	2.162	0.132	6.094	1.16	3141
SEVXIB	6	2.129	0.031	1.469	1.04	3141
SIRHOR	6	2.129	0.037	1.749	1.05	3141
SIVSAS	6	2.126	0.047	2.191	1.07	3141
TIDYOU	6	2.122	0.045	2.122	1.09	3141
TILLUV	6	2.140	0.050	2.346	1.06	3141
TOQFEL	6	2.132	0.038	1.777	1.04	3141
TUJNER	6	2.143	0.049	2.286	1.06	3141
TUVBER	6	2.154	0.051	2.350	1.06	3141
TUVBOB	6	2.132	0.045	2.104	1.05	3141
UFEHOD	6	2.130	0.035	1.623	1.06	3141
UFUCII	6	2.145	0.050	2.339	1.07	3141
VULKOC	6	2.192	0.118	5.396	1.17	3141
VULKOC01	6	2.192	0.120	5.465	1.17	R
WAGFOA	6	2.115	0.053	2.513	1.07	3141
WAGFUG	6	2.136	0.036	1.698	1.05	3141
WEKMEF	6	2.135	0.046	2.158	1.07	3141
WIHFAU	6	2.162	0.102	4.725	1.13	3141
WOCXAO	6	2.133	0.085	3.982	1.16	3141
XEDQEC	6	2.130	0.073	3.440	1.14	3141
XIGJOM	6	2.127	0.052	2.460	1.08	3141
XIGKAZ	6	2.120	0.088	4.158	1.10	3141
XIVQAU	6	2.137	0.023	1.065	1.02	3141
YADNOG	6	2.147	0.069	3.225	1.12	3141
YEVTAU	6	2.122	0.017	0.801	1.02	3141
YIQMEQ	6	2.135	0.043	2.029	1.06	3141
YIYVAE	6	2.143	0.142	6.639	1.19	3141
YIYVEI	6	2.146	0.136	6.339	1.15	3141
ZIBSEI	6	2.133	0.069	3.232	1.10	3141
ZIKDEC	6	2.130	0.049	2.311	1.09	3141
ZIXWAE	6	2.352	0.060	2.572	1.12	3141

Table S1b. *Considered sodium-oxygen structures of different classes as described in appendix 2. Structures in which $d_{max}/d_{min} > 1.10$ has not been used in the calculations of the main report. Structures denoted letters have been found in the Cambridge Crystallographic Data Centre database while structures denoted by numbers have been found in the Inorganic Crystal Structure Database.*

Structure	N_c	Distance Å	Stdev Å	Stdev %	d_{max}/d_{min}	Classif.
WABPIZ	4	2.217	0.000	0.000	1.00	1111
GIXBAQ	4	2.224	0.000	0.000	1.00	1111
FAZYAH	5	2.336	0.059	2.508	1.06	1111
WADKAO	6	2.424	0.070	2.885	1.08	2214
WADKAO	5	2.351	0.075	3.177	1.08	2214

QQQETG01	5	2.356	0.256	10.856	1.33	1112
QQQETG01	6	2.378	0.033	1.405	1.03	1212
LALLEP	5	2.358	0.076	3.229	1.08	1213
IBUHOD	5	2.366	0.047	1.987	1.05	1113
UGUFAD	5	2.382	0.054	2.274	1.05	1113
KOBBOS	5	2.383	0.033	1.374	1.03	2211
KOBBOS	4	2.319	0.041	1.753	1.04	2211
XORHER	5	2.386	0.061	2.562	1.06	1213
FABCOA	5	2.399	0.061	2.529	1.06	2223
PEJWAC	6	2.359	0.041	1.756	1.05	1111
BETFIQ	5	2.360	0.054	2.307	1.05	2213
XUKWOP	6	2.379	0.000	0.000	1.00	1111
FEJMOX	5	2.370	0.047	1.981	1.05	1114
FEJMOX	6	2.411	0.084	3.481	1.13	1114
HUQPAK	5	2.426	0.030	1.248	1.03	2234
HUQPAK	6	2.400	0.036	1.480	1.04	1112
QASHOH	6	2.400	0.049	2.036	1.06	1113
AWOPEH	6	2.500	0.122	4.885	1.18	2214
MAJKUE	6	2.402	0.048	2.018	1.05	1113
ENOBUE	6	2.405	0.072	2.997	1.09	2234
AYINEB	6	2.407	0.030	1.229	1.03	1114
NAACET05	6	2.407	0.052	2.147	1.07	2214
LUPQES	6	2.408	0.031	1.300	1.03	2214
NAPHSX01	5	2.391	0.095	3.993	1.14	2234
NAPHSX01	6	2.408	0.050	2.077	1.05	1112
BARJOU	6	2.423	0.069	2.854	1.11	2214
BARJOU	6	2.418	0.119	4.915	1.14	2232
PAVKOM	6	2.414	0.041	1.696	1.05	1213
PAVKOM	6	2.291	0.007	0.303	1.01	2124
GUFROO	6	2.374	0.050	2.089	1.04	2234
GUFROO	7	2.528	0.130	5.139	1.14	2234
GUFROO	6	2.421	0.086	3.564	1.11	2214
FIJNES	6	2.434	0.061	2.511	1.07	1114
KIQHUN01	6	2.421	0.087	3.585	1.11	R
LUQBII	6	2.421	0.065	2.669	1.07	1111
LUQBII	6	2.459	0.230	9.362	1.25	2211
SAQGIA	6	2.421	0.072	2.972	1.09	2231
WOPJOA	6	2.441	0.123	5.042	1.20	1114
WOPJOA	6	2.457	0.055	2.245	1.06	2214
YUHJOA	6	2.421	0.055	2.279	1.07	1114
MUXRIG	6	2.422	0.073	2.997	1.10	2231
MUXRIG	6	2.424	0.071	2.914	1.08	1114
XAFFEQ	6	2.424	0.032	1.332	1.03	2214
DALVAO	4	2.367	0.010	0.409	1.01	2314
DALVAO	6	2.409	0.041	1.694	1.06	1114
DALVAO	6	2.442	0.112	4.582	1.12	2214
ECEPIL	6	2.425	0.062	2.548	1.07	1113
MEQVAF	6	2.427	0.090	3.706	1.11	2214
MEQVAF	6	2.384	0.032	1.343	1.03	1114
VOKNEO	6	2.446	0.027	1.107	1.02	2214
VOKNEO	6	2.416	0.043	1.800	1.05	1114
YARZAT	6	2.436	0.086	3.548	1.18	2214
KIQHUN01	6	2.429	0.102	4.211	1.13	2214
MIGKUI	6	2.429	0.040	1.665	1.04	2211
FIPQUQ	6	2.430	0.037	1.515	1.04	1112
TUTJAT	6	2.430	0.045	1.842	1.05	2214
XAJGAQ	6	2.427	0.055	2.280	1.07	2211
XAJGAQ	6	2.433	0.057	2.362	1.06	1114
KUDJOI	6	2.432	0.046	1.879	1.06	1114
NADGUV	6	2.432	0.030	1.237	1.03	1113
HIXROV	6	2.433	0.041	1.690	1.05	2211

LAHPEQ	6	2.441	0.071	2.903	1.11	2214
LAHPEQ	5	2.341	0.108	4.624	1.13	2214
QUQKES	6	2.434	0.000	0.000	1.00	1111
ICAGIC	6	2.437	0.132	5.407	1.12	1214
ILOKID	5	2.365	0.059	2.495	1.07	1214
ILOKID	6	2.437	0.049	2.031	1.06	1114
GUFRII	6	2.439	0.055	2.244	1.06	2214
AVUNUA	6	2.440	0.099	4.067	1.12	1114
IPEGAL	6	2.445	0.047	1.919	1.07	2214
VOPKAM	6	2.443	0.063	2.593	1.07	2214
QOGHUP	6	2.444	0.065	2.664	1.11	1214
FIJNAO	6	2.445	0.105	4.312	1.13	2244
ASABEB	6	2.446	0.071	2.917	1.08	1114
BIHMUB	6	2.428	0.099	4.059	1.12	1114
LUQCIJ	6	2.449	0.080	3.270	1.07	2214
	6	2.443	0.111	4.527	1.10	2214
VOFVER	6	2.449	0.064	2.620	1.07	2211
EJAMEH	6	2.452	0.068	2.756	1.08	2214
EJAMEH	6	2.462	0.025	0.996	1.04	1114
EJAMEH	5	2.430	0.099	4.079	1.10	1114
EJAMEH	5	2.418	0.113	4.684	1.11	1214
WOWKEX	6	2.454	0.094	3.836	1.11	2214
ASIVAZ	6	2.410	0.042	1.733	1.06	1114
EBUMUK	6	2.461	0.149	6.075	1.16	1113
JUPKUA	6	2.464	0.155	6.271	1.18	2213
UDIQED	6	2.469	0.119	4.823	1.14	2212
AYUWUM	6	2.451	0.074	3.013	1.07	2214
AYUWUM	6	2.474	0.067	2.725	1.08	1114
AYUWUM	5	2.404	0.146	6.072	1.14	2214
QOBKOH	6	2.470	0.118	4.785	1.14	2214
REQKON01	6	2.470	0.101	4.103	1.10	1211
ECEPEH	5	2.365	0.076	3.229	1.08	2211
ECEPEH	6	2.469	0.090	3.643	1.12	1114
FASCEI	6	2.435	0.000	0.000	1.00	2121
FASCEI	6	2.477	0.001	0.030	1.00	1111
ROPYAW	7	2.805	0.282	10.052	1.30	2214
ROPYAW	5	2.399	0.029	1.188	1.03	1314
JABHUP	6	2.383	0.013	0.532	1.01	1125
VAXMUC	6	2.113	0.015	0.701	1.02	G
OLAXEE	6	2.353	0.022	0.929	1.02	3125
OLAXII	6	2.356	0.020	0.836	1.02	3125
VEXXIG	6	2.360	0.024	1.018	1.02	3125
BECVUA	6	2.363	0.051	2.151	1.05	3125
PEJROL	6	2.366	0.014	0.573	1.02	3125
QAYWUI	6	2.366	0.064	2.685	1.07	3125
RAGTIC	6	2.369	0.020	0.840	1.03	3125
PAGNAN	6	2.386	0.038	1.580	1.03	4221
PAGNAN	6	2.378	0.030	1.277	1.03	3125
SUMTAV	6	2.373	0.019	0.814	1.02	3125
WESHIL	6	2.378	0.026	1.092	1.02	3125
DIJJAH	6	2.383	0.047	1.957	1.04	3125
GELREV	6	2.385	0.006	0.262	1.01	3125
IBUTOO	6	2.386	0.000	0.000	1.00	3125
TEDBEK	6	2.389	0.024	0.991	1.03	3125
TEDBEK	5	2.326	0.015	0.631	1.02	3125
HOJFIV	6	2.391	0.054	2.253	1.05	3125
AYOWOA	6	2.398	0.046	1.904	1.04	3125
TIRQAM	6	2.399	0.001	0.026	1.00	3125
GAHDUO	6	2.404	0.025	1.023	1.02	3125
HIZMIM	6	2.404	0.028	1.170	1.03	3125
JOGDOY	6	2.409	0.042	1.746	1.04	3125

MICPUJ	6	2.409	0.002	0.086	1.00	3125
WIMLUZ	6	2.395	0.022	0.936	1.03	3125
FIGQER	6	2.411	0.022	0.927	1.02	3125
TEDBAG	6	2.414	0.000	0.000	1.00	3125
TEDBAG	5	2.315	0.067	2.895	1.05	3125
NUGLAC	6	2.423	0.043	1.791	1.04	3125
YELBUN	6	2.425	0.094	3.859	1.08	3125
YELBUN	5	2.253	0.050	2.237	1.04	G
XIHJON	6	2.435	0.095	3.910	1.12	3125
GULQIN	6	2.453	0.012	0.506	1.01	3125
GULQIN	5	2.326	0.047	2.041	1.04	3125
GULQAF	6	2.458	0.015	0.616	1.01	3125
XAJQEE	6	2.463	0.027	1.090	1.02	3125
OGODAP	6	2.472	0.000	0.000	1.00	3125
OGODAP	4	2.336	0.000	0.000	1.00	3125
GORKON	6	2.499	0.094	3.745	1.10	3125
JOGFEQ	6	2.341	0.037	1.599	1.06	3141
MATCUG	6	2.339	0.027	1.138	1.03	3141
WOTVOQ	6	2.354	0.012	0.530	1.01	3141
TIFJIB	6	2.356	0.041	1.734	1.05	3141
WIVKAN	6	2.373	0.053	2.234	1.09	3141
PAPPAY	6	2.355	0.073	3.081	1.16	3141
XAVXOH	6	2.360	0.037	1.582	1.05	3141
BINGEL	6	2.364	0.045	1.916	1.05	3141
TUJMUG	6	2.368	0.024	0.999	1.03	3141
WEDNUP	6	2.374	0.016	0.655	1.01	3141
PAPPEC	6	2.376	0.051	2.136	1.08	3141
ROMXUM	6	2.411	0.045	1.848	1.05	3141
WIVKOB	6	2.417	0.079	3.267	1.08	3141
DIVQII	6	2.420	0.211	8.739	1.27	3141
UKOPIT	6	2.486	0.001	0.021	1.00	3141
XIVGEP	7	2.558	0.183	7.170	1.22	2231
AFELUT	4	2.342	0.053	2.268	1.04	2211
AJIZEY	4	2.226	0.016	0.704	1.01	1121
ASACOM	4	2.318	0.154	6.625	1.12	1311
ASACOM	6	2.415	0.068	2.814	1.06	1211
EXOVOC	4	2.308	0.067	2.906	1.07	2211
FACLAW	4	2.252	0.058	2.584	1.06	1231
FALZOI	4	2.637	0.004	0.152	1.00	1111
FILRAU	4	2.351	0.122	5.181	1.13	2211
JUTFIN	4	2.293	0.019	0.830	1.02	3125
JUZGUG	4	2.333	0.042	1.782	1.04	1121
JUZHAN	4	2.404	0.066	2.729	1.06	1211
LOCHER	4	2.412	0.018	0.746	1.02	N
MAZQEJ	4	2.316	0.029	1.236	1.03	3128
NONPUC	4	2.321	0.045	1.930	1.05	4228
PVANSB	4	2.304	0.064	2.783	1.05	1247
QEXQIT	4	2.279	0.093	4.066	1.16	1124
REDBAD	4	2.298	0.021	0.915	1.02	2211
RODPOP	4	2.290	0.048	2.114	1.05	2211
SOHWIW	4	2.292	0.024	1.043	1.02	3221
UDUJIM	4	2.336	0.019	0.820	1.02	3121
VERDUS	4	2.296	0.025	1.075	1.02	1111
VIMWOE	4	2.301	0.098	4.246	1.11	3221
WIGJOL	4	2.432	0.078	3.217	1.07	1211
WIPDEF	4	2.599	0.000	0.000	1.00	1111
XEKPAE	4	2.297	0.054	2.339	1.06	3221
YAFVEH	4	2.316	0.067	2.903	1.07	2211
YITWAZ	4	2.234	0.073	3.246	1.07	1123
YUXXOE	4	2.338	0.019	0.825	1.02	1221
ZUSVUE	4	2.235	0.023	1.043	1.02	1121

FOPYUF	4	2.963	0.042	1.403	1.02	2314
AVIZEK	8	2.507	0.080	3.199	1.08	R
AVIZEK01	8	2.506	0.079	3.153	1.08	2241
EHUCUF	8	2.603	0.102	3.933	1.12	1241
IXELUS	8	2.541	0.087	3.408	1.12	2241
MARWUY	8	2.576	0.025	0.967	1.03	2214
MEDBIH	8	2.566	0.073	2.828	1.07	2244
NEXDOK	8	2.501	0.000	0.000	1.00	1144
QIYPAQ	8	2.511	0.063	2.493	1.08	2121
YEVDIN	8	2.562	0.126	4.919	1.17	2234
WEGCUG	7	2.524	0.107	4.258	1.11	1214
CASWUP	7	2.543	0.160	6.303	1.16	2214
SEKNUS	7	2.514	0.105	4.165	1.12	2224
DARPAO	5	2.437	0.055	2.256	1.06	N
DARPAO	6	2.445	0.113	4.641	1.18	1114
DEHNAG	5	2.386	0.048	2.011	1.04	1213
FOCTIB	5	2.359	0.043	1.814	1.05	1211
GOLSIJ	5	2.328	0.061	2.636	1.07	1213
HEFYOH	5	2.404	0.072	3.003	1.06	1113
HEFYOH	6	2.436	0.084	3.444	1.09	1113
JAZYIS10	5	2.326	0.075	3.224	1.08	1244
MISFOK	5	2.372	0.044	1.838	1.05	1114
MISFUQ	5	2.378	0.074	3.118	1.08	1113
MITGUS	5	2.344	0.061	2.604	1.07	1111
NIDKUH	5	2.305	0.084	3.639	1.09	1211
QITCUS	5	2.381	0.087	3.633	1.10	1113
QUBWAL	6	2.375	0.098	4.124	1.13	2244
QUBWAL	5	2.329	0.036	1.536	1.04	1214
QUBWAL	6	2.435	0.213	8.734	1.27	1214
RIKYIT	5	2.336	0.084	3.614	1.10	1124
SICHIW	5	2.404	0.114	4.737	1.19	1113
UKECOC	5	2.322	0.066	2.858	1.07	1121
VOYYIR	6	2.430	0.063	2.599	1.08	2214
WEGDER	5	2.355	0.069	2.940	1.08	1244
WUZNEK	5	2.332	0.136	5.845	1.16	1212
WUZNEK	6	2.537	0.286	11.265	1.33	1213
WUZNEK	4	2.709	0.194	7.148	1.17	1213
WUZNIO	5	2.360	0.134	5.686	1.22	1214
XAHZOV	5	2.385	0.121	5.069	1.14	1141
XEDDOL	5	2.326	0.080	3.454	1.08	1124
XEDDOL	6	2.378	0.088	3.702	1.17	1124
ZOGTEV	5	2.382	0.065	2.719	1.06	1123
ASIVAZ	6	2.443	0.090	3.678	1.11	2214
ASIVAZ	5	2.369	0.033	1.379	1.04	2214
AYOLIJ	6	2.419	0.031	1.275	1.03	1213
CEYXIO	6	2.449	0.042	1.697	1.04	1214
CICWOB	6	2.438	0.016	0.669	1.01	1114
CIYGAT	6	2.389	0.012	0.487	1.01	1214
DARNIU	6	2.423	0.075	3.095	1.11	1114
DARNOA	6	2.426	0.083	3.406	1.13	1114
DIXGIB	6	2.427	0.127	5.239	1.14	1214
DOGQOG	6	2.449	0.093	3.809	1.12	2234
DOGQOG	6	2.431	0.094	3.857	1.19	1114
EDIFOM	6	2.456	0.001	0.021	1.00	1141
ENERIY	6	2.447	0.178	7.258	1.28	2224
GEFRUF	6	2.070	0.100	4.837	1.16	1111
GIYWAM	5	2.415	0.108	4.462	1.13	2214
GIYWAM	6	2.392	0.039	1.615	1.04	1114
GIYWAM	5	2.458	0.122	4.974	1.12	1114
HAYQUU	6	2.402	0.033	1.360	1.03	1114
IDAPEJ	5	2.365	0.047	1.991	1.07	2214

IDAPEJ	6	2.423	0.076	3.122	1.11	1114
IDAPIN	6	2.438	0.136	5.579	1.14	1214
IDAPOT	6	2.438	0.143	5.871	1.14	1214
IVUCOR	6	2.415	0.224	9.278	1.25	1221
JIDKOW	6	2.410	0.046	1.909	1.04	1123
JUXTAX	6	2.402	0.078	3.233	1.07	1121
KOJBAN	6	2.442	0.094	3.838	1.12	1114
KOJBER	6	2.438	0.079	3.233	1.10	1114
KOJBIV	6	2.432	0.102	4.214	1.12	1114
KOJBOB	6	2.436	0.100	4.088	1.12	1114
LAYCAQ	6	2.457	0.048	1.957	1.06	1114
LEMJET	6	2.480	0.051	2.069	1.04	2214
MIVBAV	6	2.473	0.273	11.024	1.32	1111
NAWDIY	6	2.295	0.010	0.434	1.01	2244
NERLIG	6	2.397	0.057	2.391	1.07	1234
QEXYOH	6	2.371	0.004	0.189	1.00	1141
QITDED	6	2.390	0.016	0.683	1.01	1114
REHGEQ	6	2.351	0.027	1.161	1.03	1121
RIGRIJ	6	2.469	0.171	6.924	1.18	S
RIQVIX	6	2.341	0.020	0.853	1.02	1144
SIRGOQ	6	2.417	0.033	1.351	1.04	1113
SOQZAA	6	2.466	0.086	3.477	1.12	1144
TAGMIY	6	2.391	0.055	2.314	1.07	1224
TERDIE	6	2.303	0.017	0.723	1.02	1146
TOPYUS	6	2.392	0.040	1.690	1.04	1224
VEKVOX	6	2.456	0.241	9.803	1.28	1113
VIQCAA	6	2.415	0.045	1.873	1.07	1214
WEGDAN	6	2.489	0.098	3.923	1.10	1244
WEVNOB	6	2.405	0.081	3.387	1.08	1123
WUZNEK	6	2.537	0.286	11.265	1.33	1224
XEPHIK	6	2.408	0.056	2.323	1.06	1113
XIJFOM	6	2.407	0.065	2.703	1.08	1114
XONQAS	6	2.430	0.039	1.614	1.04	1144
YIVSAY	6	2.498	0.108	4.316	1.10	1234
POWGOY	6	2.489	0.049	1.957	1.04	2214
POWGOY	6	2.459	0.125	5.076	1.15	1214
JUTFIN	4	2.293	0.019	0.830	1.02	3221
MIBXOK	4	2.344	0.061	2.589	1.06	1141
QEXQAL	4	2.277	0.027	1.192	1.03	1221
WODXAO	4	2.334	0.015	0.634	1.01	S
YAWVEY	4	2.222	0.000	0.000	1.00	S
YOBPIO	4	2.341	0.003	0.148	1.00	S
YUCKUC	4	2.338	0.007	0.311	1.01	3125
ACOFII	5	2.340	0.007	0.304	1.01	3125
ASAZUP	5	2.321	0.037	1.595	1.03	3125
DAWNOF	5	2.356	0.022	0.939	1.02	3125
FIMPEX	5	2.291	0.047	2.037	1.05	3125
GOSBAR	5	2.338	0.039	1.668	1.04	3125
JANLIU	5	2.320	0.024	1.016	1.03	3125
OBIMOB	5	2.301	0.015	0.656	1.02	4125
PAPLIC	5	2.326	0.030	1.309	1.05	3125
XIPTAR	5	2.304	0.020	0.888	1.02	3125
COFWIE	6	2.374	0.028	1.194	1.02	3125
JIWTUF	6	2.394	0.002	0.072	1.00	3125
RAGTIC	6	2.369	0.020	0.840	1.03	3125
SOPFEJ	6	2.373	0.046	1.943	1.04	3125
VICXIO	6	2.389	0.020	0.833	1.02	3125
YUFWUR	6	2.403	0.018	0.756	1.02	3125
161174	6	2.405	0.017	0.706	1.01	1111
413337	6	2.351	0.048	2.053	1.05	1113
416437	6	2.370	0.038	1.602	1.04	1113

280960	6	2.416	0.056	2.324	1.10	1114
249161	6	2.400	0.022	0.904	1.02	1113
249323	6	2.390	0.044	1.861	1.05	1114
280442	6	2.402	0.068	2.830	1.07	1114
413819	6	2.417	0.055	2.264	1.10	1114
281590	6	2.361	0.031	1.314	1.03	1114
411045	6	2.428	0.039	1.587	1.05	1114
418940	6	2.474	0.109	4.403	1.12	1114
14302	6	2.419	0.047	1.940	1.06	1114
418569	6	2.412	0.085	3.538	1.11	1114
GOHWIK	6	2.341	0.054	2.286	1.06	3141
GOHWOQ	6	2.369	0.072	3.042	1.07	3141
HUPZOH	6	2.345	0.019	0.822	1.02	3141
MIPCIY	6	2.358	0.039	1.641	1.05	3141
PALTEB	6	2.373	0.020	0.848	1.02	3141
TIWVUR	6	2.368	0.028	1.184	1.03	3141
UFUCEE	6	2.373	0.078	3.271	1.09	3141
UFUCUU	6	2.329	0.088	3.783	1.11	3141
VIQSIY	6	2.405	0.093	3.862	1.08	3141
WIMCIE	6	2.376	0.041	1.717	1.05	3141
ZEBSUU	6	2.485	0.091	3.656	1.09	3141

Table S1c. *Considered potassium-oxygen structures of different classes as described in appendix 2. Structures in which $d_{max}/d_{min} > 1.10$ has not been used in the calculations of the main report. Structures denoted letters have been found in the Cambridge Crystallographic Data Centre database while structures denoted by numbers have been found in the Inorganic Crystal Structure Database.*

Structure	N_c	Distance Å	Stdev Å	Stdev %	d_{max}/d_{min}	Classif.
GOGBUZ	5	2.797	0.096	3.440	1.08	1414
IZIVOC	5	2.851	0.080	2.798	1.09	1112
IBUKAS	6	2.797	0.039	1.403	1.03	2414
KAMYED	6	2.787	0.123	4.404	1.16	2224
KAMYED	6	2.850	0.126	4.423	1.12	2444
VOWKIB	6	2.813	0.137	4.865	1.13	2214
RUGXAS	6	2.830	0.182	6.415	1.16	2244
GUGNUR	6	1.611	0.065	4.054	1.11	1111
ECENIJ01	7	2.810	0.112	3.979	1.11	R
ECENIJ01	6	2.887	0.080	2.774	1.06	R
ECENIJ02	6	2.871	0.057	1.970	1.04	R
ECENIJ02	7	2.812	0.127	4.512	1.12	R
ECENIJ03	6	2.878	0.082	2.859	1.07	2214
ECENOP	6	2.880	0.087	3.005	1.07	2214
ECENOP	7	2.792	0.109	3.911	1.11	2214
EJALUW	6	2.884	0.071	2.453	1.06	2214
EJALUW	7	2.803	0.114	4.067	1.11	2214
EJALIK	6	2.885	0.065	2.254	1.05	2214
EJALIK	7	2.818	0.147	5.218	1.13	2214
BEVQOJ	8	2.816	0.019	0.683	1.01	2214
XUQQOP	8	2.843	0.057	2.015	1.05	2214
RIZQIA	8	2.848	0.094	3.304	1.11	2214
KAMYIH	8	2.870	0.250	8.726	1.33	2214
IQUNAJ	8	2.859	0.016	0.542	1.01	2214
QAJDEL	8	2.854	0.116	4.071	1.10	2214
OJONUW	8	2.864	0.030	1.045	1.02	2214
VENDUN01	7	2.799	0.107	3.806	1.10	R
VENDUN01	8	2.951	0.123	4.157	1.11	R
GUQTUH	8	2.463	0.098	3.982	1.12	1234
IKOMEA	8	2.495	0.153	6.135	1.21	2234

MEQZOX	10	2.929	0.084	2.859	1.09	2234
MEQZOX	9	2.902	0.113	3.894	1.13	2234
RUGXAS	7	2.781	0.061	2.201	1.06	2234
IBUKAS	7	2.576	0.118	4.599	1.15	2214
KAMYON	8	2.950	0.237	8.049	1.27	2244
ABOBEY	8	2.885	0.189	6.541	1.20	2244
CASNAM	8	2.892	0.102	3.512	1.11	2234
LOTWOG	8	2.859	0.097	3.378	1.10	2224
RIPYUL	8	2.577	0.219	8.493	1.22	2214
NASWEK	7	2.859	0.163	5.707	1.15	2234
QENCUI	7	2.790	0.103	3.699	1.13	2244
QISXAS	7	2.868	0.125	4.353	1.13	2234
QOGRUA	7	2.858	0.141	4.919	1.16	2244
RIVCUV	7	2.869	0.193	6.717	1.18	1124
WODGOM	7	2.433	0.088	3.634	1.12	2214
XIZFOC	7	2.884	0.203	7.025	1.21	2234
FOTBOG	7	2.771	0.053	1.914	1.05	2244
KAMYON	9	2.894	0.135	4.666	1.16	2234
KAMYON	8	2.934	0.207	7.055	1.27	2234
LETGAT	9	2.939	0.157	5.336	1.18	2234
GITCIV	4	2.694	0.011	0.424	1.01	S
IMABIH	4	1.910	0.026	1.375	1.03	3125
IMABON	4	1.944	0.179	9.209	1.25	3125
IMABUT	4	1.887	0.034	1.788	1.04	3125
FOFZEG	5	2.726	0.026	0.945	1.02	3125
RIVLEO	5	2.327	0.028	1.196	1.03	3125
CEDLIH	6	2.672	0.025	0.920	1.02	3125
DORDAQ	6	2.705	0.013	0.495	1.01	3125
GAGLIK	6	2.678	0.022	0.813	1.02	3125
GAGLOQ	6	2.671	0.020	0.739	1.02	3125
GAGLUW	6	2.684	0.027	1.021	1.03	3125
GELROF	6	2.724	0.037	1.365	1.03	3125
HIWLAA	6	2.699	0.076	2.834	1.08	3125
HIWLEE	6	2.705	0.035	1.278	1.04	3125
ITAKAP	6	2.722	0.034	1.258	1.03	3125
JARKUJ	6	2.717	0.070	2.580	1.08	3125
NUVXUX	6	2.665	0.044	1.655	1.04	3125
PUCMAB	6	2.708	0.016	0.601	1.01	3125
ROJYIZ	6	2.755	0.055	1.984	1.06	3125
TOJNOW	6	2.579	0.000	0.000	1.00	G
TOPDIL	6	2.698	0.030	1.112	1.03	3125
TOSPUM	6	2.398	0.042	1.746	1.04	G
ULETUA	6	2.650	0.040	1.520	1.03	3125
WADGOX	6	2.741	0.035	1.262	1.03	3125
XEKNIK	6	2.746	0.092	3.348	1.09	3125
TOJSUH	7	2.782	0.051	1.828	1.05	3125

Table S1d. *Considered rubidium-oxygen structures of different classes as described in appendix 2. Structures in which $d_{max}/d_{min} > 1.10$ has not been used in the calculations of the main report. Structures denoted letters have been found in the Cambridge Crystallographic Data Centre database while structures denoted by numbers have been found in the Inorganic Crystal Structure Database.*

Structure	N_c	Distance Å	Stdev Å	Stdev %	d_{max}/d_{min}	Classif.
EVEHAO	6	2.899	0.126	4.333	1.12	2229
PROMYC10	6	2.902	0.068	2.356	1.08	1147
BEVQUP	8	2.948	0.052	1.759	1.03	2214
YINWUO	6	2.925	0.065	2.219	1.05	2244
NIPPAE	12	3.082	0.044	1.423	1.03	2144

65210	8	3.051	0.020	0.666	1.01	2234
61048	6	3.011	0.163	5.413	1.16	2124
47115	6	2.985	0.051	1.723	1.04	2234
45253	7	3.210	0.328	10.211	1.23	2124
82109	8	3.005	0.055	1.834	1.04	2244
66710	12	3.187	0.167	5.251	1.16	R
66711	12	3.195	0.169	5.293	1.17	R
66712	11	3.189	0.163	5.103	1.16	R
66713	12	3.163	0.183	5.790	1.19	R
66709	12	3.198	0.216	6.753	1.24	2144
60578	6	2.983	0.255	8.566	1.28	2144
35102	8	3.082	0.047	1.530	1.04	2144
35103	8	3.122	0.059	1.904	1.06	R
16338	10	3.003	0.103	3.429	1.08	2144

Table S1e. *Considered cesium-oxygen structures of different classes as described in appendix 2. Structures in which $d_{max}/d_{min} > 1.10$ has not been used in the calculations of the main report. Structures denoted letters have been found in the Cambridge Crystallographic Data Centre database while structures denoted by numbers have been found in the Inorganic Crystal Structure Database.*

Structure	N_c	Distance Å	Stdev Å	Stdev %	d_{max}/d_{min}	Classif.
UFIHEX	6	3.016	0.012	0.404	1.01	1249
NEXQUC	7	3.228	0.162	5.024	1.15	1239
OKEFUF	10	3.277	0.090	2.756	1.09	1139
NIPPOS	12	3.177	0.040	1.259	1.03	2144
36016	12	3.450	0.000	0.000	1.00	R
15274	7	3.291	0.324	9.848	1.28	2129
152234	9	3.213	0.075	2.328	1.10	2149
50327	6	3.155	0.077	2.432	1.06	R
50328	6	3.189	0.033	1.039	1.02	2149
64600	9	3.246	0.072	2.228	1.07	D
64601	9	3.236	0.077	2.392	1.08	2149
60579	12	3.292	0.157	4.775	1.18	2149
38068	10	3.274	0.098	2.994	1.10	2149
16339	12	3.106	0.079	2.547	1.08	2149
35555	12	3.359	0.000	0.000	1.00	2149
280909	12	3.364	0.034	1.010	1.02	2219
36634	12	3.504	0.273	7.797	1.24	2219
36633	12	3.431	0.300	8.741	1.32	2219
36015	12	3.450	0.000	0.000	1.00	2219
72507	9	3.228	0.045	1.394	1.04	2149
16340	10	2.970	0.052	1.747	1.04	R
DOWDAU	7	3.021	0.129	4.255	1.14	2247
NEWRIQ	8	3.291	0.123	3.750	1.09	1339
OBIXOM	8	3.275	0.113	3.460	1.07	1339
JAQHEP	4	3.504	0.037	1.055	1.02	1439
YEDZUD	8	3.277	0.241	7.359	1.18	2244

Appendix 2: Preparation of solutions

Table S2. *Composition of the studied solutions*

Salt	Conc. in ~4 w% D_2O mol/l	Density in ~4w% D_2O g/ml	Weight% D_2O g/g*100	Conc in H_2O mol/l	Density in H_2O g/ml	Conc. in DMSO mol/l	Method
CsI	1.001	1.2016	4.000	1.003	1.1984	-	DDIR
CsI	0.899	1.1845	4.000	0.902	1.1785	-	DDIR
CsI	0.804	1.1625	4.000	0.805	1.1589	-	DDIR
CsI	0.698	1.141	4.000	0.700	1.1380	-	DDIR
CsI	0.602	1.1218	4.000	0.602	1.1181	-	DDIR
CsI	0.501	1.1017	4.000	0.500	1.0978	-	DDIR
CsI	0.400	1.0814	4.000	0.400	1.0778	-	DDIR
CsI	0.296	1.0605	4.000	0.300	1.0575	-	DDIR
CsI	0.202	1.0416	4.000	0.202	1.0379	-	DDIR
CsI	0.102	1.0214	4.000	0.101	1.0175	-	DDIR
RbI	0.900	1.1454	3.995	0.899	1.1416	-	DDIR
RbI	0.801	1.1297	3.995	0.804	1.1262	-	DDIR
RbI	0.701	1.1136	3.995	0.700	1.1097	-	DDIR
RbI	0.602	1.0978	3.995	0.601	1.0939	-	DDIR
RbI	0.500	1.0815	3.995	0.499	1.0775	-	DDIR
RbI	0.400	1.0654	3.995	0.401	1.0616	-	DDIR
RbI	0.300	1.0493	3.995	0.300	1.0457	-	DDIR
RbI	0.200	1.0332	3.995	0.199	1.0293	-	DDIR
RbI	0.100	1.012	3.995	0.101	1.0135	-	DDIR
KI	0.999	1.1212	3.999	1.000	1.1165	-	DDIR
KI	0.893	1.1077	3.999	0.903	1.1052	-	DDIR
KI	0.804	1.0971	3.999	0.803	1.0931	-	DDIR
KI	0.703	1.0882	3.999	0.699	1.0809	-	DDIR
KI	0.603	1.0732	3.999	0.602	1.0692	-	DDIR
KI	0.502	1.0611	3.999	0.500	1.0572	-	DDIR
KI	0.400	1.0489	3.999	0.400	1.0451	-	DDIR
KI	0.296	1.0365	3.999	0.300	1.0331	-	DDIR
KI	0.200	1.025	3.999	0.200	1.0212	-	DDIR
KI	0.100	1.0132	3.999	0.100	1.0092	-	DDIR
$NaClO_4$	1.001	1.0786	3.960	1.001	1.0751	-	DDIR
$NaClO_4$	0.905	1.0701	3.960	0.901	1.0673	-	DDIR
$NaClO_4$	0.809	1.0633	3.960	0.800	1.0596	-	DDIR
$NaClO_4$	0.707	1.0555	3.960	0.699	1.0519	-	DDIR
$NaClO_4$	0.603	1.0478	3.960	0.601	1.0442	-	DDIR
$NaClO_4$	0.505	1.04	3.960	0.501	1.0365	-	DDIR
$NaClO_4$	0.403	1.0321	3.960	0.399	1.0285	-	DDIR
$NaClO_4$	0.299	1.024	3.960	0.300	1.0207	-	DDIR
$NaClO_4$	0.201	1.0165	3.960	0.201	1.0129	-	DDIR
$NaClO_4$	0.101	1.0086	3.960	0.100	1.0050	-	DDIR
$LiClO_4$	1.001	1.0625	3.999	1.000	1.0589	-	DDIR
$LiClO_4$	0.895	1.056	3.999	0.904	1.053	-	DDIR
$LiClO_4$	0.803	1.0505	3.999	0.801	1.0467	-	DDIR
$LiClO_4$	0.701	1.0442	3.999	0.702	1.0406	-	DDIR
$LiClO_4$	0.602	1.0382	3.999	0.603	1.0345	-	DDIR
$LiClO_4$	0.501	1.0319	3.999	0.501	1.0282	-	DDIR
$LiClO_4$	0.401	1.0258	3.999	0.401	1.0221	-	DDIR
$LiClO_4$	0.297	1.0194	3.999	0.301	1.0158	-	DDIR
$LiClO_4$	0.200	1.0134	3.999	0.200	1.0096	-	DDIR

$LiClO_4$	0.101	1.0072	3.999	0.101	1.0034	-	DDIR
NaI	0.815	1.0926	4.000	0.816	1.0891	-	DDIR
NaI	0.730	1.0832	4.000	0.736	1.08	-	DDIR
NaI	0.655	1.0747	4.000	0.656	1.071	-	DDIR
NaI	0.571	1.0653	4.000	0.572	1.0615	-	DDIR
NaI	0.491	1.0563	4.000	0.491	1.0525	-	DDIR
NaI	0.409	1.0471	4.000	0.408	1.0432	-	DDIR
NaI	0.327	1.0378	4.000	0.327	1.034	-	DDIR
NaI	0.241	1.0283	4.000	0.244	1.0248	-	DDIR
NaI	0.163	1.0194	4.000	0.163	1.0155	-	DDIR
NaI	0.082	1.0103	4.000	0.082	1.0064	-	DDIR
NaI	-	-	-	2.0073	1.1981	1.017	LAXS
CsI	-	-	-	1.7307	1.3431	1.000	LAXS
CsOH	-	-	-	1.8018	1.2312		LAXS
KI	-	-	-	2.0015	1.2356	1.017	LAXS

Appendix 3: Introduced system for central atom classification based on ligands.

If the statement of more than one digit is true for each subsection, the higher number is chosen.

***Table S3**: Classification of investigated crystal structures.*

	Type	Structure	Teeth	Bridging	Comment
Neutral	1				Neutral ligands
Anion	2				At least one anionic ligand
Eter	3				At least one ether oxygen ligand
Anionic and eter	4				At least one of each
Oxide	5				At least one oxide oxygen ligand
Other	8				
Homoleptic		1			Identical ligand atoms
Heteroleptic		2			Not identical ligand atoms
Steric obstacle, non π		3			Severe. Ignore homo/hetero
Steric obstacle π-intera.		4			Severe. Ignore homo/hetero
Homoleptic c.e. struct.		5			Ex. crown ethers with equal O:s
Heteroleptic c.e. struct.		6			Ex. other crown ether types
Not considered		9			
Hydrate, all monodentate			1		All ligands monod., not just H_2O
Complex, all monodentate			2		All ligands monodentate
Hydrate, multidentate			3		At least some multidentate ligand
Complex, multidentate			4		At least some multidentate ligand
Not considered			9		
Nonbridging ligands				1	Ex. $Cs(H_2O)_8$
One ligand bridging				2	Ex. $(H_2O)_7$-Cs-O(H_2)-Cs-$(H_2O)_7$
Two ligand bridging				3	
Ligand multibridging				4	
Exo-cyclic ligand				5	Ex. $K^+(THF)_6$
M+ bridges rings				6	Between ring structures
M+ centered in ring				7	Centered in ring structures
Not considered				9	

Consider the example figure ECENOP (1) which is shown in Figure S1. There are two different potassium ions in this structure, one with coordination number 7 and the other with coordination number 6. In this case both are classified as 2214 atoms, since:

- At least one ligand is anionic → 2
- Not all ligands are the equivalent → 2
- At least one ligand is H_2O. All ligands are approaching K^+ with only one ligand atom → 1
- More than two ligands are bridging to another K^+. → 4

When two or more atoms in a structure share both class and coordination number, they are being considered equivalent and presented average distances and standard deviations refer to all bonds. This classification system may appear complicated at a first glance, but an organization of available structures is necessary in order to judge the relevance of structures. Furthermore, it is not necessary to master the classification system in detail in order to see the

potential in extracting relevant structures. A given interval of classes, 1111-1224, should be interpreted as if the second number can vary between 1 and 2 and so on. Hence the hypothetical structure of class 1144 is not a part of the interval 1111-1224

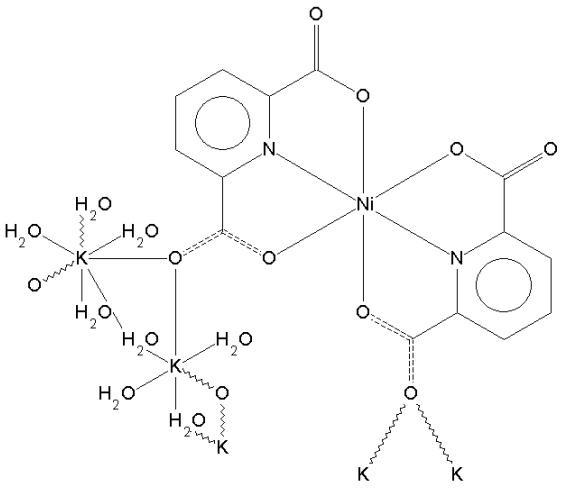

Figure S1: *Example structure ECENOP* (1)*. The Figure based on the cif file deponated at CCDC.*

Appendix 4

Table S4: *Obtained Li-O distances depending on data selection for coordination numbers 4 and 6.*

Li^+			CN = **4**			CN = **6**		
Structures from	to	Description	Number Obs.	d_{M-O} (Å)	Stddev (Å)	Number Obs.	d_{M-O} (Å)	Stddev (Å)
1111	1111	Neutral, homoleptic, nonbridging hydrates	24	1.936	0.016	0		
1112	1114	Neutral, homoleptic, bridging hydrates	12	1.954	0.010	10	2.132	0.010
1111	**1114**	**Neutral homoleptic hydrates**	**36**	**1.942**	**0.017**	**10**	**2.132**	**0.010**
1121	1124	Neutral homoleptic non-eter, non-hydrate	30	1.939	0.025	0		
1111	**1124**	**Neutral homoleptic non-eter solvates**	**66**	**1.941**	**0.021**	**10**	**2.132**	**0.010**
1211	1224	Neutral heteroleptic monodentate non-eter	14	1.943	0.018	0		
1111	**1224**	**Neutral monodentate non-eter solvates**	**80**	**1.941**	**0.020**	**10**	**2.132**	**0.010**
1131	1244	Neutral multidentate non-eter solvates	3	1.916	0.018	0		
1111	**1244**	**Neutral non-eter solvates**	**83**	**1.940**	**0.021**	**10**	**2.132**	**0.010**
3125	3125	THF-solvates	242	1.918	0.013	3	2.169	0.006
3141	3141	1,2-Dimethoxyethane	0			75	2.134	0.015

Table S5: *Obtained Na-O distances depending on data selection for coordination numbers 5 and 6.*

Na^+			CN = **5**			CN = **6**		
Structures from	to	Description	Number Obs.	d_{M-O} (Å)	Stddev (Å)	Number Obs.	d_{M-O} (Å)	Stddev (Å)
1111	1111	Neutral, homoleptic, nonbridging hydrates	2	2.340	0.006	6	2.412	0.042
1112	1114	Neutral, homoleptic, bridging hydrates	7	2.379	0.012	39	2.415	0.026
1111	**1114**	**Neutral homoleptic hydrates**	**9**	**2.370**	**0.020**	**45**	**2.415**	**0.028**
1121	1124	Neutral homoleptic non-eter, non-hydrate	4	2.341	0.028	4	2.392	0.027
1111	**1124**	**Neutral homoleptic non-eter solvates**	**13**	**2.361**	**0.026**	**49**	**2.413**	**0.028**
1211	1224	Neutral heteroleptic monodentate non-eter	8	2.352	0.029	9	2.407	0.022
1111	**1224**	**Neutral monodentate non-eter solvates**	**21**	**2.358**	**0.027**	**58**	**2.412**	**0.027**
1131	1244	Neutral multidentate non-eter solvates	2	2.341	0.021	5	2.399	0.046
1111	**1244**	**Neutral non-eter solvates**	**23**	**2.356**	**0.026**	**63**	**2.411**	**0.029**
3125	3125	THF-solvates	11	2.324	0.017	36	2.395	0.030
3141	3141	1,2-Dimethoxyethane				26	2.377	0.039

Classification have been made in accordance with appendix 3

Appendix 5

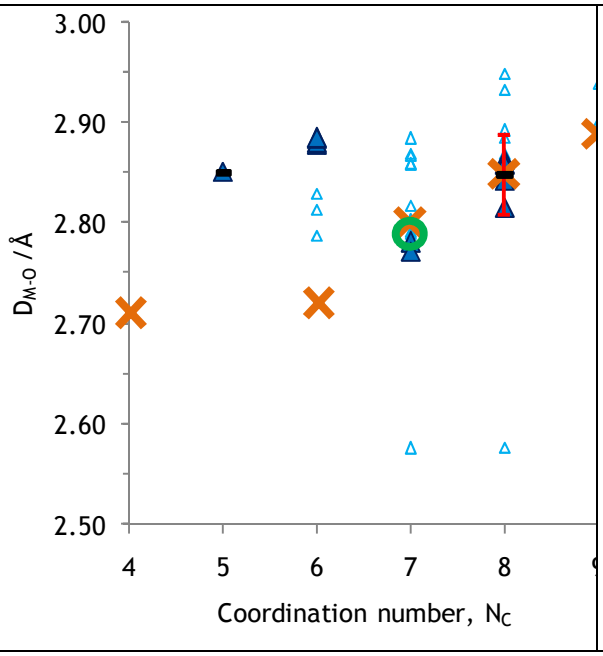

Figure S2. Crystal structures of not very representative ionic non-ether K^+ complexes. The error bar corresponds to ± two standard deviations. The sums of the radii given by Shannon and the oxygen radius are shown as orange crosses. Blue filled triangles represent geometrically approved atoms while open triangles represent atoms with geometrical flaws, i.e. where the longest bond exceed 110% of the shortest bond. A green circle represent the experimental M-O distance determined by LAXS for 7-coordination.

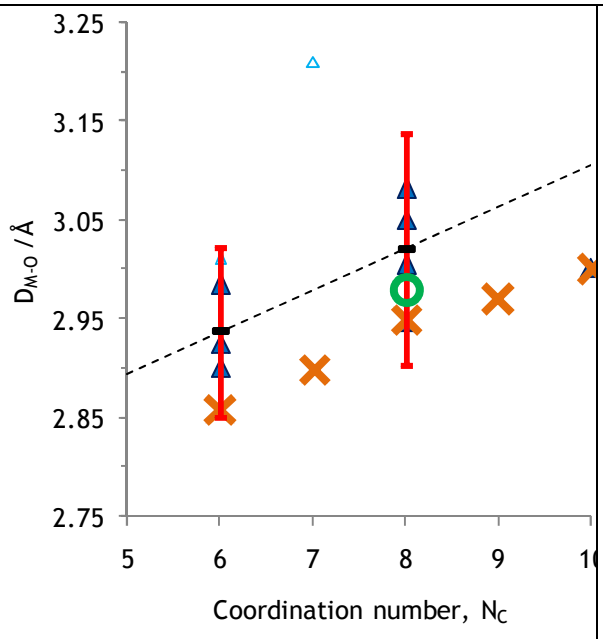

Figure S3. Crystal structures of not very representative ionic, non-ether, Rb^+ complexes. Error bars correspond to ± two standard deviations. The sums of the radii given by Shannon and the oxygen radius are shown as orange crosses. The dashed line is drawn between mean values for 6- and 8-coordination, and should be taken as a guide for the eye rather than a proposed relationship. A green circle represent the experimental M-O distance determined by LAXS for 8-coordination, ref. 60. Blue filled triangles represent geometrically approved atoms while open triangles represent atoms with geometrical flaws, i.e. where the longest bond exceed 110% of the shortest bond.

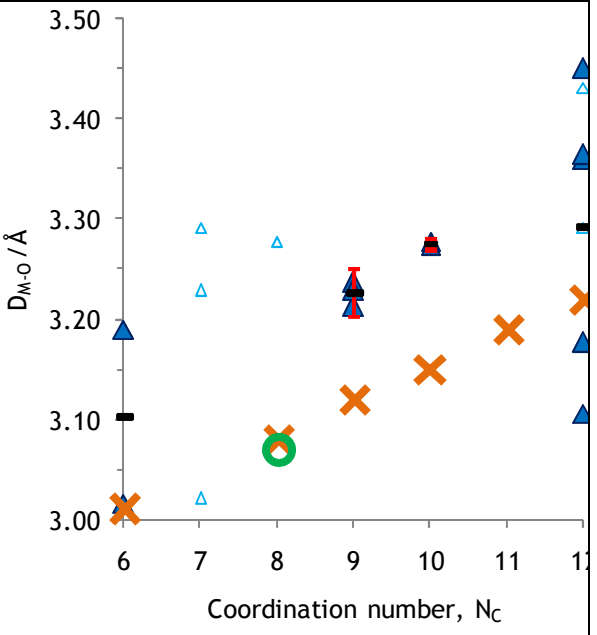

Figure S4. Crystal structures of not very representative ionic, non-ether, Cs^+ solvates. Error bars correspond to ± two standard deviations. The sums of the radii given by Shannon and the oxygen radius are shown as orange crosses. Blue filled triangles represent geometrically approved atoms while open triangles represent atoms with geometrical flaws, i.e. where the longest bond exceed 110% of the shortest bond. A green circle represent the experimental M-O distance determined by LAXS for 8-coordination.

Appendix 6

Table S6: *Hydration enthalpies utilized for evaluation of hydration enthalpies vs inverse MO-distance, main report*

Li^+	519	$kJmol^{-1}$
Na^+	409	$kJmol^{-1}$
K^+	322	$kJmol^{-1}$
Rb^+	293	$kJmol^{-1}$
Cs^+	264	$kJmol^{-1}$

Table S7: *Distances used for evaluation of hydration enthalpies vs MO-distance, main report. Values from crystal structure search is printed in bold and values approximated from THF structures (see main article) are underlined. Other values are Shannon radii+1.34 Å. for water oxygen. Coordination number 6 is unlikely for Rb^+ and Cs^+, as is coordination number 8 for Li^+, and these values were not applied in the final evaluation in the main report.*

N_C	4	5	6	7	8	9	10	11	12	14
Li^+	**1.942**		**2.132**		*(2.26)*					
Na^+	2.33	**2.358**	**2.415**	2.46	2.52	2.58			2.68	
K^+	2.71		**2.72**	**2.8**	2.85	2.89	2.93		2.98	
Rb^+			*(2.86)*	2.9	2.95	2.97	3	3.03	3.06	3.17
Cs^+			*(3.01)*		3.08	3.12	3.15	3.19	3.22	

Appendix 7 - LAXS results

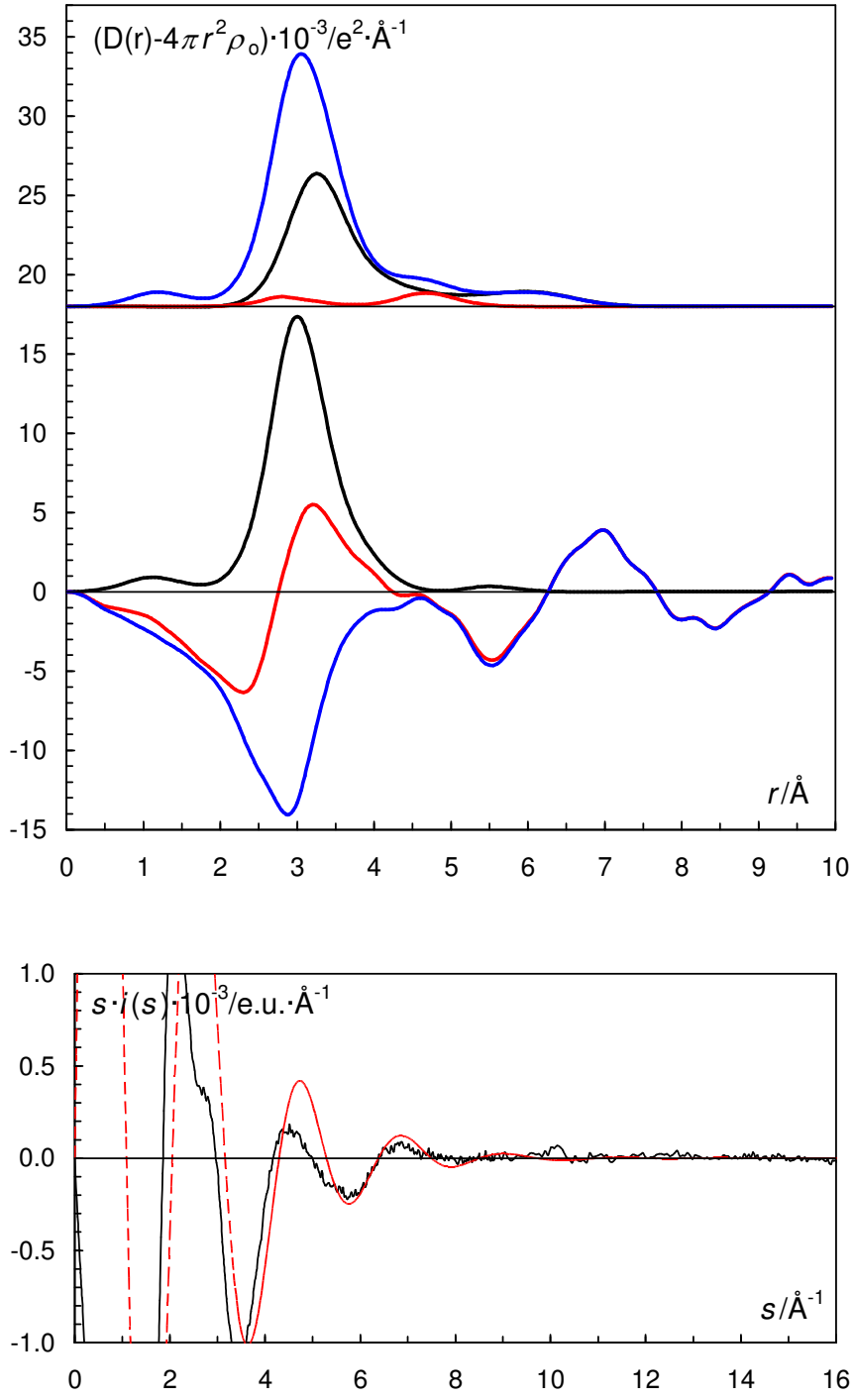

Figure S5. (Top) LAXS radial distribution curves for a 1.802 mol·dm^{-3} aqueous solution of cesium hydroxide. Upper part: Separate model contributions (offset: 18) of the hydrated cessium ion (black line), the hydrated hydoxide ion (red line) and the aqueous bulk (blue line). (Middle) Experimental RDF: D(r)-4πr^{2}ρ$_O$ (red line), sum of model contributions (black line) and the difference between experimental and calculated functions (blue line). (Bottom) Reduced LAXS intensity functions s·i(s) (solid line); model s·i$_{calc}$(s) (dashed line).

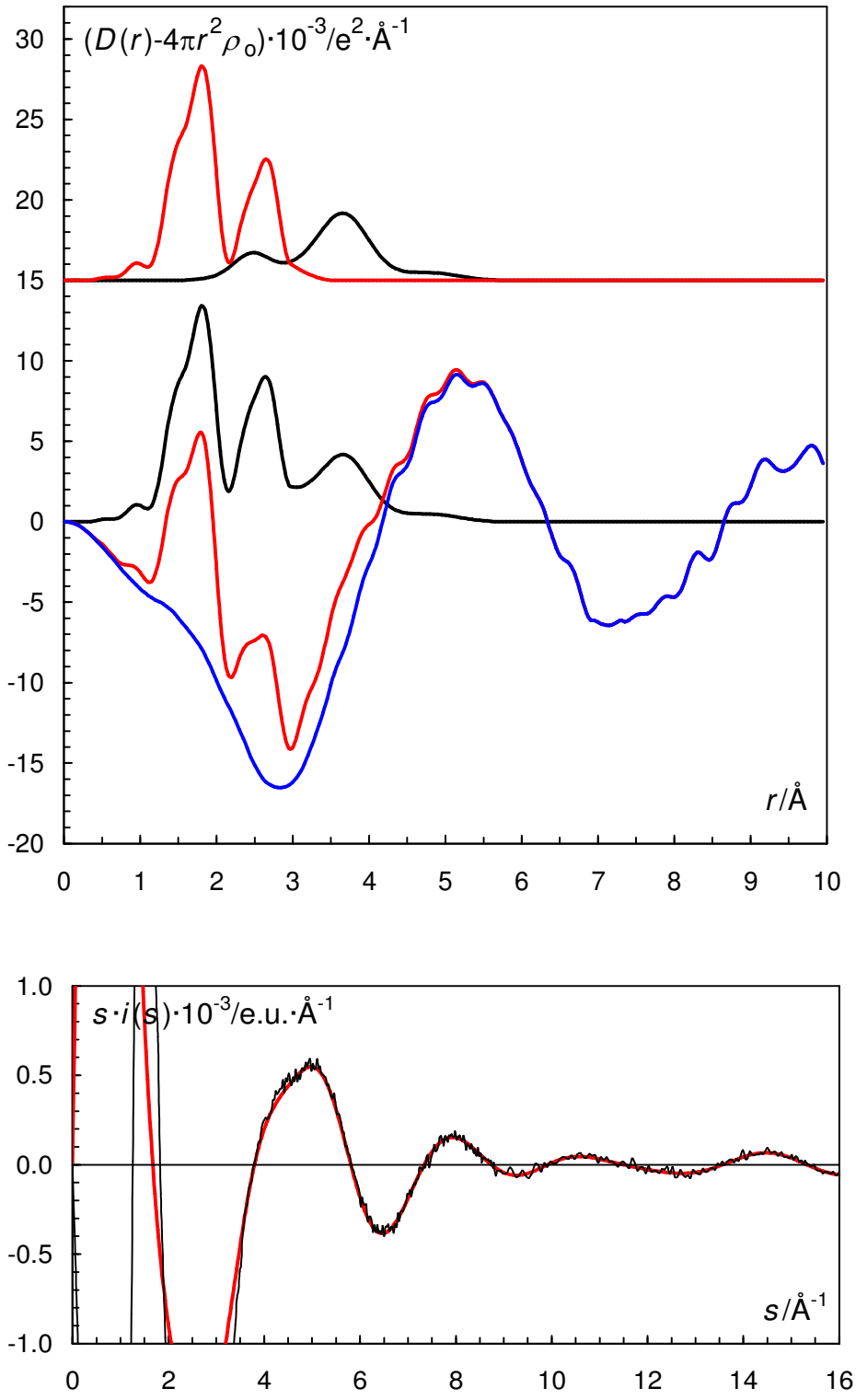

Figure S6. (Top) LAXS radial distribution curves for a 1.017 mol·dm^{-3} dimethylsulfoxide solution of sodium iodide. Upper part: Separate model contributions (offset: 15) of the dimethylsulfoxide solvated sodium ion (black line) and the dimethylsulfoxide molecule (blue line). (Middle) Experimental RDF: D(r)-4πr^{2}ρ$_o$ (red line), sum of model contributions (black line) and the difference between experimental and calculated functions (blue line). (Bottom) Reduced LAXS intensity functions s·i(s) (solid line); model s·i$_{calc}$(s) (dashed line).

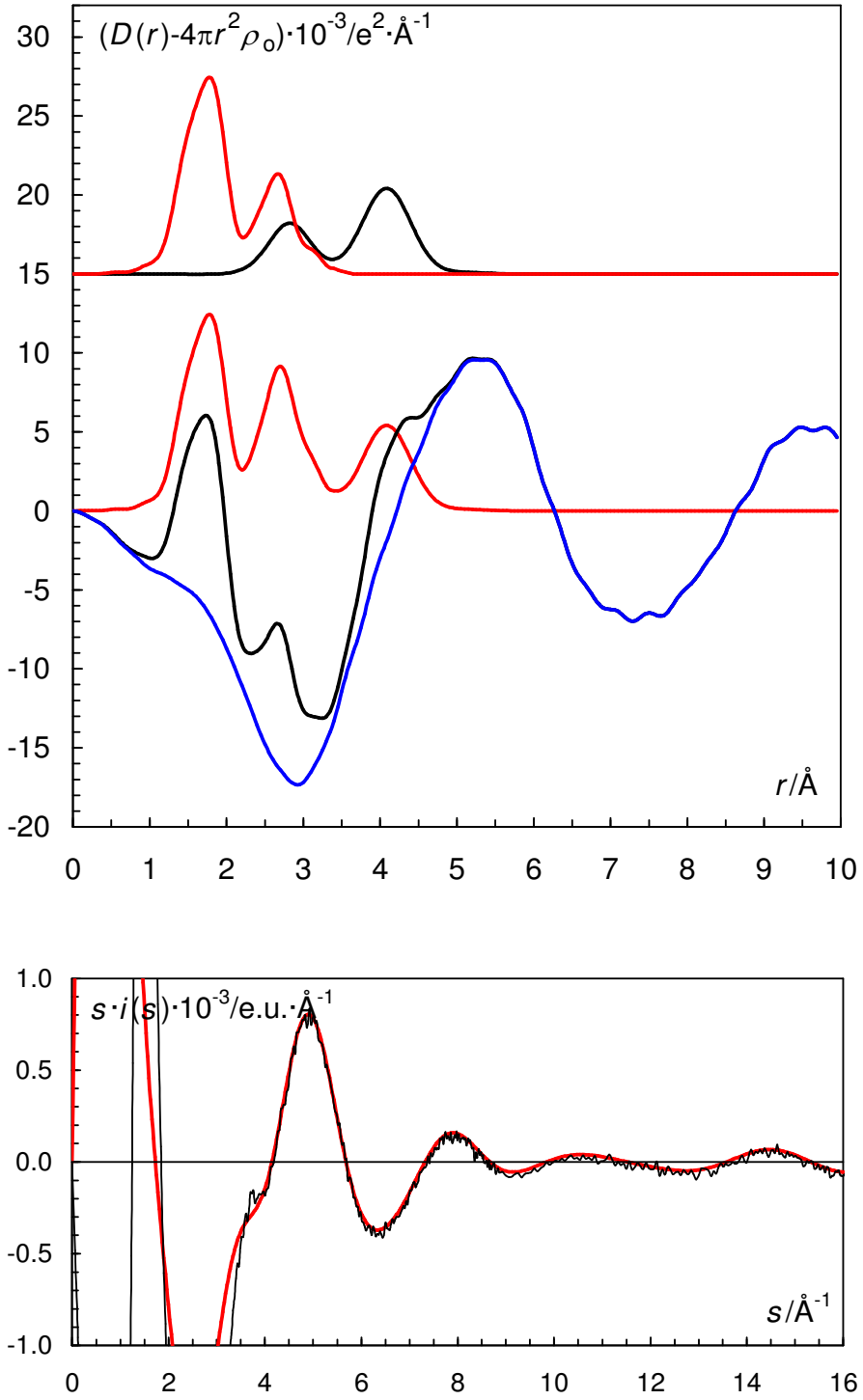

Figure S7. (Top) LAXS radial distribution curves for a 1.017 mol·dm^{-3} dimethylsulfoxide solution of potassium iodide. Upper part: Separate model contributions (offset: 15) of the dimethylsulfoxide solvated potassium ion (black line) and the dimethylsulfoxide molecule (blue line). (Middle) Experimental RDF: D(r)-4πr^{2}ρ$_o$ (red line), sum of model contributions (black line) and the difference between experimental and calculated functions (blue line). (Bottom) Reduced LAXS intensity functions s·i(s) (solid line); model s·i$_{calc}$(s) (dashed line).

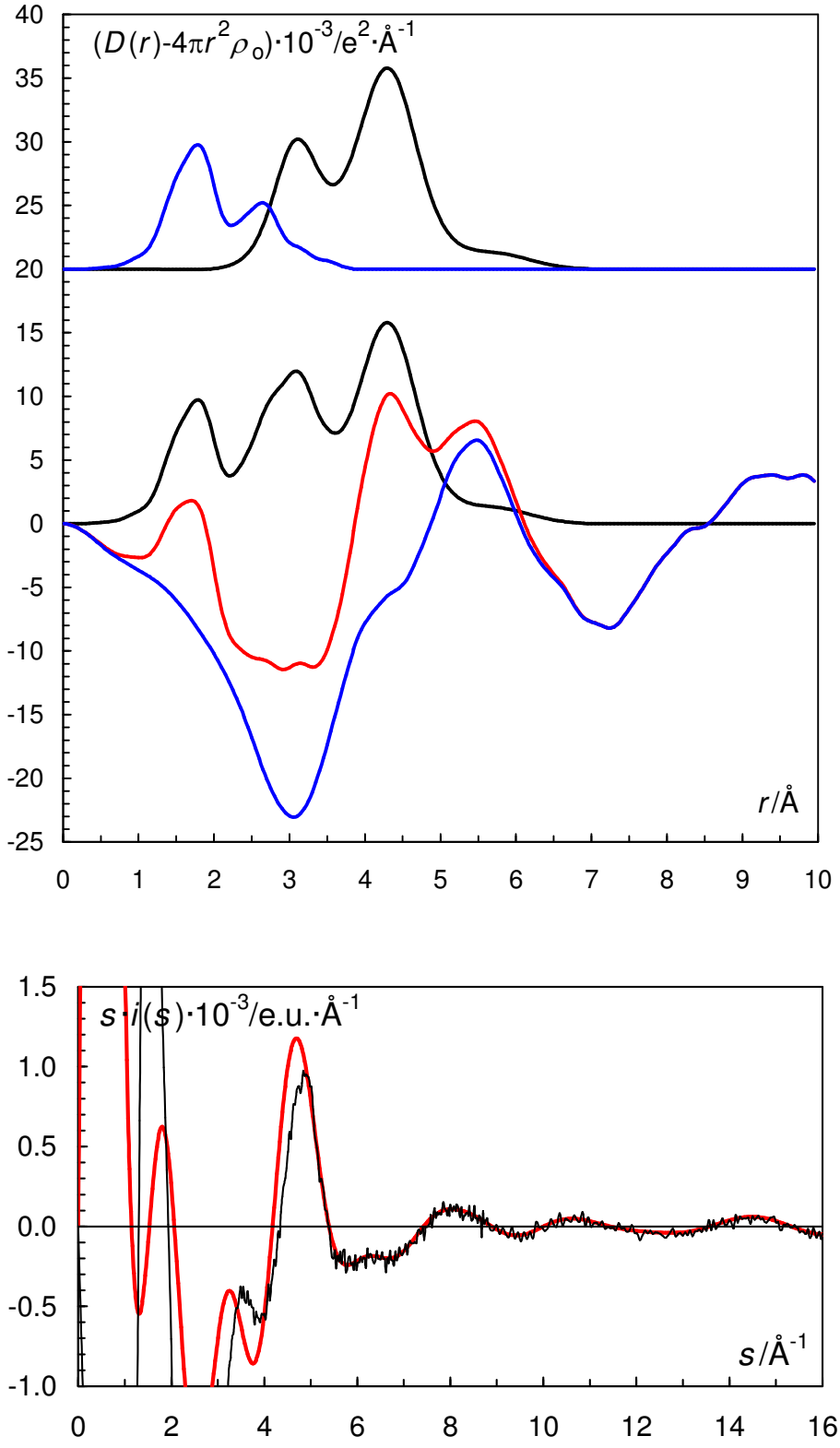

Figure S8. LAXS radial distribution curves for a 1.000 mol·dm^{-3} dimethylsulfoxide solution of cesium iodide. Upper part: Separate model contributions (offset: 20) of the dimethylsulfoxide solvated cesium ion (black line) and the dimethylsulfoxide molecule (blue line). (Middle) Experimental RDF: D(r)-4πr^{2}ρ$_o$ (red line), sum of model contributions (black line) and the difference between experimental and calculated functions (blue line). (Bottom) Reduced LAXS intensity functions s·i(s) (solid line); model s·i$_{calc}$(s) (dashed line).

Appendix 8 - Additional DDIR figures

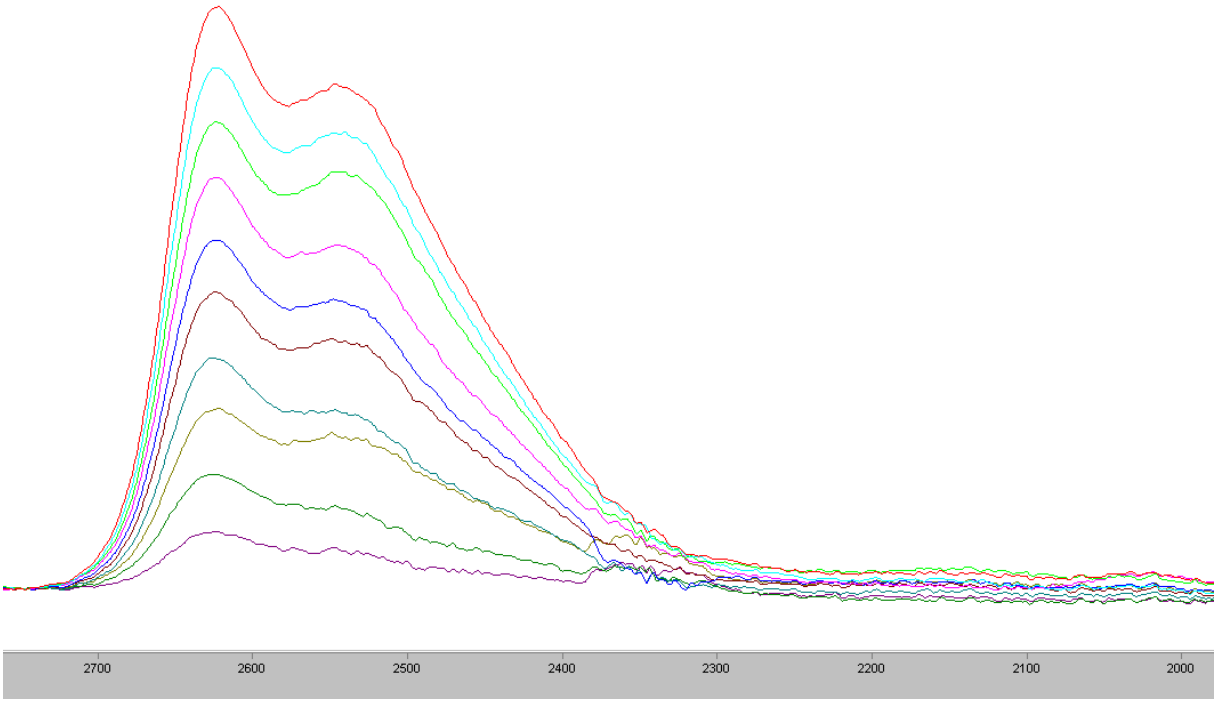

Figure S9: Affected spectra of Lithium perchlorate at different concentrations, as calculated the old method of assuming an affected number N prior to spectrum generation. The highest spectrum represent 1.0M and each consecutive spectrum represent a concentration 0.1M lower than the previous one, down to 0.1M. For the simple purpose of comparing the spectrum shape, high accuracy of N is not important.