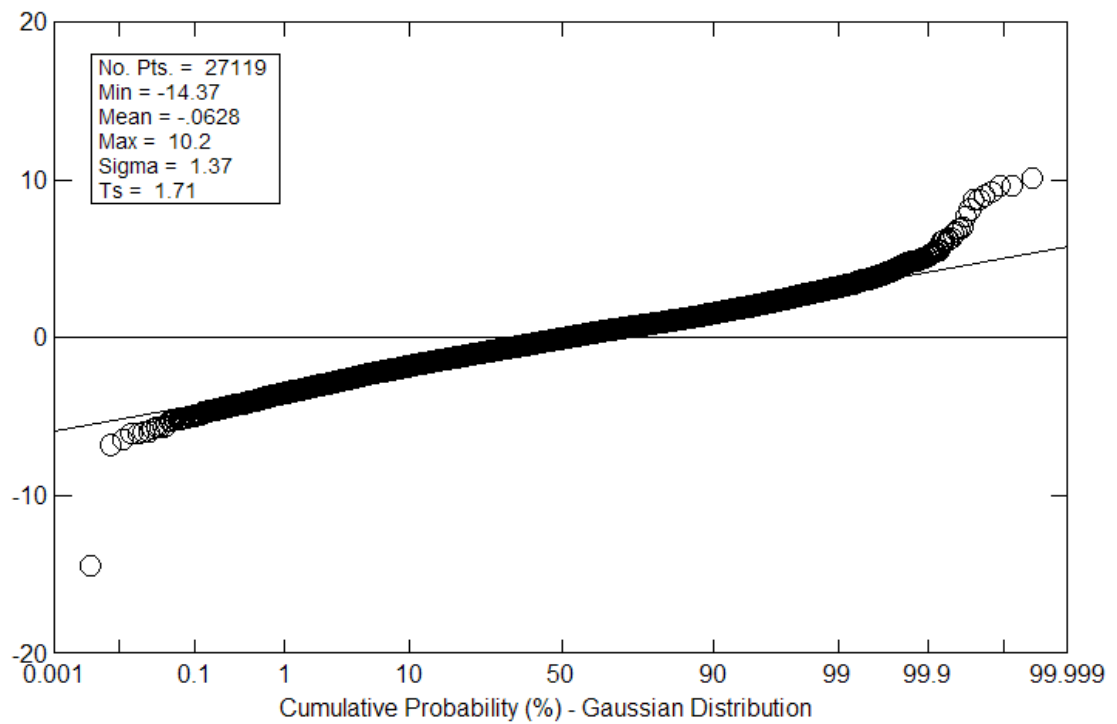


Fig. S1. Average $F_{\text{calc}}^2 / F_{\text{obs}}^2$ ratios. The average values of $\sin(\theta)/\lambda$ and $F_{\text{calc}}^2 / F_{\text{obs}}^2$ have been calculated for intervals of $\sin(\theta)/\lambda$ containing 1000 reflections each, except of the last one, which contained 1119 data.



04-29-14

Fig. S2. Cumulative probability distribution of $(F_{\text{calc}}^2 - F_{\text{obs}}^2) / \sigma(F_{\text{obs}}^2)$.

Table S1. Bonding distances (Å).

O(1)—N(1)	1.2254 (2)	C(3)—C(4)	1.3926 (2)
O(2)—N(1)	1.2353 (2)	C(4)—C(5)	1.3918 (1)
O(3)—N(2)	1.2244 (2)	C(5)—C(6)	1.3891 (2)
O(4)—N(2)	1.2324 (2)	C(11)—C(21)	1.4009 (2)
N(1)—C(4)	1.4550 (1)	C(11)—C(61)	1.4011 (1)
N(2)—C(41)	1.4547 (1)	C(21)—C(31)	1.3887 (2)
C(1)—C(2)	1.4011 (1)	C(31)—C(41)	1.3917 (2)
C(1)—C(6)	1.4000 (2)	C(41)—C(51)	1.3903 (2)
C(2)—C(3)	1.3866 (2)	C(51)—C(61)	1.3890 (2)
		C2-H2, C3-H3, C5-H5, C6-H6, C21-H21, C31- H31, C51-H51, C61-H61	1.09

Table S2. Experimental and theoretically calculated values of ellipticity and Hessian eigenvalues for the critical points of the bonds.

bond	experimental values				anion+5Na ⁺				anion			
	ϵ	λ_1	λ_2	λ_3	ϵ	λ_1	λ_2	λ_3	ϵ	λ_1	λ_2	λ_3
P1-O11	0.03	-6.42	-6.23	23.15	0.09	-8.088	-7.454	25.786	0.10	-7.904	-7.174	27.665
P1-O21	0.04	-6.54	-6.27	23.27	0.11	-8.066	-7.283	25.593	0.12	-7.851	-6.998	27.593
P1-O31	0.06	-11.24	-10.57	49.85	0.02	-10.635	-10.403	51.427	0.04	-10.379	-9.972	51.909
P1-O41	0.07	-11.18	-10.41	48.33	0.05	-11.006	-10.493	50.246	0.06	-10.254	-9.714	49.668
O1-N1	0.11	-29.53	-26.66	45.89	0.12	-30.798	-27.497	35.497	0.12	-30.726	-27.400	34.799
O2-N1	0.10	-29.25	-26.70	46.27	0.10	-29.159	-26.581	33.497	0.10	-28.846	-26.195	33.232
O3-N2	0.14	-31.18	-27.39	45.95	0.12	-30.750	-27.521	35.497	0.12	-30.774	-27.473	34.726
O4-N2	0.13	-29.92	-26.41	46.35	0.09	-29.352	-27.039	33.449	0.09	-29.039	-26.629	33.329
O11-C1	0.09	-15.53	-14.25	11.53	0.09	-14.830	-13.657	14.799	0.11	-15.047	-13.565	14.257
O21-C11	0.09	-15.17	-13.90	11.48	0.09	-14.920	-13.654	15.421	0.12	-15.373	-13.734	14.358
N1-C4	0.22	-13.38	-10.98	10.34	0.25	-14.565	-11.616	10.211	0.29	-14.551	-11.281	9.615
N2-C41	0.24	-13.27	-10.71	10.61	0.26	-14.703	-11.664	10.213	0.30	-14.712	-11.341	9.644
C1-C2	0.24	-16.41	-13.20	9.47	0.23	-16.100	-13.141	9.372	0.24	-16.469	-13.252	9.145
C2-C3	0.22	-16.19	-13.30	9.76	0.26	-16.640	-13.194	8.933	0.31	-16.876	-12.866	8.545
C3-C4	0.24	-15.95	-12.84	9.67	0.18	-15.609	-13.254	8.603	0.21	-15.770	-12.989	8.220
C4-C5	0.22	-16.18	-13.28	9.77	0.22	-16.079	-13.170	9.235	0.23	-16.231	-13.148	8.866

C5-C6	0.22	-16.16	-13.24	9.63	0.27	-16.452	-12.917	8.885	0.30	-16.720	-12.900	8.570
C1-C6	0.25	-16.50	-13.22	9.46	0.22	-15.638	-12.794	8.741	0.21	-15.852	-13.119	8.435
C11-C21	0.22	-16.30	-13.41	9.39	0.23	-16.038	-12.999	9.314	0.25	-16.406	-13.156	9.085
C21-C31	0.21	-15.78	-13.05	9.78	0.27	-16.696	-13.136	8.950	0.32	-16.951	-12.840	8.579
C31-C41	0.23	-15.90	-12.94	9.39	0.18	-15.667	-13.254	8.717	0.22	-15.828	-13.018	8.338
C41-C51	0.22	-16.30	-13.38	9.57	0.22	-16.074	-13.158	9.170	0.24	-16.228	-13.110	8.791
C51-C61	0.22	-16.19	-13.23	9.65	0.28	-16.631	-13.016	8.917	0.31	-16.920	-12.960	8.601
C11-C61	0.27	-16.19	-12.71	9.73	0.22	-15.594	-12.765	8.871	0.21	-15.843	-13.115	8.589
C2-H2	0.05	-17.12	-16.35	17.71	0.01	-19.508	-19.279	12.047	0.02	-18.893	-18.493	11.191
C3-H3	0.04	-17.73	-17.01	17.24	0.01	-20.016	-19.855	12.454	0.02	-19.349	-18.961	11.584
C5-H5	0.05	-16.42	-15.66	17.36	0.01	-19.433	-19.267	12.033	0.01	-19.436	-19.163	11.546
C6-H6	0.04	-17.92	-17.17	15.88	0.03	-18.207	-17.662	11.295	0.02	-19.619	-19.325	11.758
C21-H21	0.05	-16.73	-15.91	18.32	0.01	-19.419	-19.168	12.023	0.02	-18.908	-18.496	11.228
C31-H31	0.03	-17.32	-16.79	17.33	0.01	-19.951	-19.759	12.406	0.02	-19.320	-18.918	11.558
C51-H51	0.04	-17.21	-16.56	17.06	0.01	-19.590	-19.426	12.105	0.01	-19.515	-19.250	11.575
C61-H61	0.06	-16.98	-16.07	16.19	0.02	-18.664	-18.264	11.596	0.02	-19.674	-19.378	11.763
Na-O2	0.02	-0.35	-0.34	2.73	0.04	-0.479	-0.463	3.032	—	—	—	—
Na-X1_O4	0.01	-0.45	-0.45	3.45	0.05	-0.592	-0.566	3.730	—	—	—	—
Na-X1_O31	0.00	-0.76	-0.76	5.51	0.02	-0.782	-0.768	5.456	—	—	—	—
Na-X1_O41	0.02	-0.61	-0.60	4.44	0.01	-0.650	-0.641	4.478	—	—	—	—
Na-X2_O41	0.01	-0.44	-0.44	3.37	0.01	-0.508	-0.506	3.449	—	—	—	—