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116

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Characteristic Frequencies and Amplitudes of Free Normal Oscillations in KCl Crystals

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Results are presented for a calculation of the characteristic frequencies and amplitudes of free normal oscillations of the ions of a KCl crystal. These calculations are carried out for values of the wave vector k which uniformly cover the cell of the reciprocal lattice by 729 points, with account taken of polarization deformation of the electron shells of the ions. A comparison is made with the results obtained by other authors.[1,2]

KNOWLEDGE of the characteristic frequencies and amplitudes of the free normal oscillations of the ions of a crystal is necessary in the solution of a number of problems, for example, in the determination of heat capacity, the interaction of a conduction electron with the vibrations of the lattice, the energy of interaction of point charges placed in a crystal, computation of the energy levels of the local states of an electron or hole with small radius of the state, etc.[3]

The frequencies $\omega_{\mathbf{k}}^{\alpha}$ for certain wave numbers k were found by Iona.[1] The amplitudes were not of interest since he computed the heat capacity. In determining the frequencies, Iona considered a model of a point lattice with ions of equal mass. Tolpygo and Zaslavskaia[2] computed the frequencies and amplitudes of the normal vibrations of a KCl crystal for 8 values of the vector k which, in particular, were obtained in Ref. 1 by considering the deformation of the electron shells of the ions, according to the method proposed earlier by Tolpygo.[4,5]

However, part of the exchange integral of the interaction of two (opposite) neighbors, which depends on the polarization, was thrown away in Ref. 2, without any justification. This can be avoided.[6] Moreover, knowledge of the frequencies for only 125 points of the reciprocal lattice is insufficient for the following quantitative analysis.

Let us consider an ideal crystal of KCl. We denote the dipole moment of the electron shell s_1 of the lth ion by $\mathbf{P}_s^l$, and the dipole moment, due to a shift $\mathbf{u}_s^l$ of this ion from its equilibrium position, by $\mathbf{p}_s^l = e_s \mathbf{u}_s^l$ (e_s = charge of the sth ion). For the

Characteristic frequencies and amplitudes of free normal oscillations of KCl crystals*

$\frac{k_x}{\pi}; \frac{k_y}{\pi}; \frac{k_z}{\pi}$	Ω^2	ω, sec^{-1}	$p_{1x}\|\pi_{1x}$	$p_{1y}\|\pi_{1y}$	$p_{1z}\|\pi_{1z}$	$p_{2x}\|\pi_{2x}$	$p_{2y}\|\pi_{2y}$	$p_{2z}\|\pi_{2z}$
1	2	3	4	5	6	7	8	9
0, 0, 1/4	5,7641	3,7209	0	0	4741	0	0	5259
			0	0	4195	0	0	1039
	2,9250	2,6506	4760	0	0	5240	0	0
			5378	0	0	5818	0	0
	2,9250	2,6506	0	4760	0	0	5240	0
			0	5378	0	0	5818	0
	0,5292	1,1274	0	0	—5008	0	0	4978
			0	0	—5102	0	0	5063
	0,0772	0,4305	—4991	0	0	4998	0	0
			—4952	0	0	4791	0	0
	0,0772	0,4305	0	—4991	0	0	4998	0
			0	—4952	0	0	4791	0
0, 0, 1/2	4,0051	3,1016	0	0	4632	0	0	5365
			0	0	4083	0	0	1419
	2,9918	2,6807	4767	0	0	5233	0	0
			5431	0	0	5885	0	0
	2,9918	2,6807	0	4767	0	0	5233	0
			0	5431	0	0	5885	0
	1,7459	2,0478	0	0	—5109	0	0	4864
			0	0	—5450	0	0	5281
	0,2424	0,7631	—4984	0	0	5005	0	0
			—4860	0	0	4326	0	0
	0,2424	0,7631	0	—4984	0	0	5005	0
			0	—4860	0	0	4326	0
1/4, 1, 1	2,8706	2,6259	4287	0	0	5672	0	0
			5025	0	0	5872	0	0
	0,3797	0,9550	0	0	4980	0	0	5009
			0	0	4782	0	0	3890
	0,3797	0,9550	0	4980	0	0	5009	0
			0	4782	0	0	3890	0
	2,2084	2,3032	—5402	0	0	4502	0	0
			—4945	0	0	0785	0	0
	3,0574	2,7100	0	0	—4770	0	0	5230
			0	0	—5482	0	0	5955
	3,0574	2,7100	0	—4770	0	0	5230	0
			0	—5482	0	0	5955	0
0, 0, 1	1,4696	1,8788	0	0	5029	0	0	4955
			0	0	4509	0	0	1395
	3,0840	2,7217	4771	0	0	5229	0	0
			5502	0	0	5985	0	0
	3,0840	2,7217	0	4771	0	0	5229	0
			0	5502	0	0	5985	0
	3,2821	2,8077	0	0	—4719	0	0	5281
			0	0	—5571	0	0	6016
	0,4296	1,0158	—4980	0	0	5010	0	0
			—4758	0	0	3716	0	0
	0,4296	1,0158	0	—4980	0	0	5010	0
			0	—4753	0	0	3716	0
0, 1/4, 1/4	5,7036	3,7013	0	3433	3433	0	3636	3636
			0	3051	3051	0	0824	0824
	2,9532	2,6633	4762	0	0	5238	0	0
			5399	0	0	5842	0	0
	2,5435	2,4717	0	3300	—3300	0	3770	—3770
			0	3620	—3620	0	3960	—3960
	0,7391	1,3324	0	—3463	—3463	0	3605	3605
			0	—3461	—3461	0	3397	3397

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*ω in Column 3 has been multiplied by 10^{-13} and the components of the vectors P and $\pi = p + P$ in Columns 4-9 been multiplied by 19^4.

$\frac{k_x}{\pi}$; $\frac{k_y}{\pi}$; $\frac{k_z}{\pi}$	Ω^2	ω, sec^{-1}	p_{1x}/π_{1x}	p_{1y}/π_{1y}	p_{1z}/π_{1z}	p_{2x}/π_{2x}	p_{2y}/π_{2y}	p_{2z}/π_{2z}
1	2	3	4	5	6	7	8	9
0, $^1/_4$, $^1/_2$	0,1742	0,6469	—4988	0	0	5000	0	0
			—4909	0	0	4558	0	0
	0,4545	1,0449	0	—3590	3590	0	3465	—3465
			0	—3667	3667	0	3536	—3536
	4,3779	3,2428	0	3311	3627	0	3290	3876
			0	3238	3145	0	2033	0628
	3,0203	2,6934	4765	0	0	5235	0	0
			5448	0	0	5902	0	0
	2,2960	2,3484	0	—3419	2801	0	—4070	3786
			0	—3873	2718	0	—4639	2869
	1,8262	2,0944	0	0717	5007	0	—1283	—4752
			0	0616	5293	0	—0891	—4957
0, $^1/_4$, $^3/_4$	0,3825	0,9585	—4985	0	0	5004	0	0
			—4814	0	0	4022	0	0
	0,7033	1,2997	0	—4938	1219	0	4838	—0712
			0	—4928	1362	0	4354	—1095
	3,1463	2,7490	0	4446	1574	0	4725	2364
			0	4788	1247	0	4563	0485
	3,0864	2,7228	4765	0	0	5235	0	0
			5494	0	0	5964	0	0
	1,8225	2,0923	0	1360	—4621	0	2545	—4515
			0	1712	—4225	0	3007	—1804
	2,8694	2,6253	0	—0777	—4792	0	—0006	5144
			0	—0766	—5432	0	—0373	5748
0, $^1/_4$, 1	0,5583	1,1580	—4985	0	0	5004	0	0
			—4735	0	0	3522	0	0
	0,8675	1,4435	0	—5034	0882	0	4862	0073
			0	—4944	0972	0	3884	—0430
	2,8859	2,6328	0	4744	0	0	5256	0
			0	5241	0	0	5461	0
	3,1134	2,7347	4764	0	0	5236	0	0
			5512	0	0	5990	0	0
	1,3540	1,8034	0	0	5018	0	0	4967
			0	0	4530	0	0	1693
	3,2549	2,7961	0	0	—4730	0	0	5269
			0	0	—5564	0	0	6011
0, $^1/_2$, $^1/_2$	0,6222	1,2225	—4986	0	0	5002	0	0
			—4706	0	0	3324	0	0
	0,9439	1,5057	0	—5006	0	0	4981	0
			0	—4861	0	0	3839	0
	3,7106	2,9854	0	3677	3677	0	3364	3364
			0	3358	3358	0	1210	1210
	3,0886	2,7237	4759	0	0	5240	0	0
			5486	0	0	5944	0	0
	1,7309	2,0390	0	1289	—1289	0	4938	—4938
			0	1255	—1255	0	4826	—4826
	2,2163	2,3073	0	—3203	—3203	0	3861	3861
			0	—3287	—3287	0	3340	3340
$^1/_4$, $^1/_2$, 1	0,6820	1,2799	—4991	0	0	4998	0	0
			—4717	0	0	3334	0	0
	1,4946	1,8947	0	—4703	4703	0	1353	—1353
			0	—4965	4965	0	1718	—1718
	2,9320	2,6538	4761	1605	0	4819	1175	0
			5278	1555	0	5287	0714	0
	0,9330	1,4970	0	0	5000	0	0	4988
			0	0	4639	0	0	2703
	1,9385	2,1578	0825	—4072	0	1916	—5453	0
			1120	—4200	0	2211	—5104	0
	2,5349	2,4675	—2146	—4319	0	2878	4302	0
			—1816	—4263	0	1061	3155	0
	3,1558	2,7532	0	0	—4750	0	0	5250
			0	0	—5522	0	0	5986

$\frac{k_x}{\pi}$; $\frac{k_y}{\pi}$; $\frac{k_z}{\pi}$	Ω^2	ω, sec^{-1}	$p_{1x}\|\pi_{1x}$	$p_{1y}\|\pi_{1y}$	$p_{1z}\|\pi_{1z}$	$p_{2x}\|\pi_{2x}$	$p_{2y}\|\pi_{2y}$	$p_{2z}\|\pi_{2z}$
1	2	3	4	5	6	7	8	9
	1,2385	1,7247	—4430	3079	0	4134	—1803	0
			—4228	3269	0	2434	—2003	0
0, $^1/_2$, 1	2,1061	2,2492	0	0	0	0	7242	0
			0	0	0	0	6344	0
	3,1837	2,7653	4746	0	0	5254	0	0
			5537	0	0	6003	0	0
	1,0246	1,5688	0	0	5004	0	0	4983
			0	0	4610	0	0	2457
	2,0117	2,1982	0	6896	0	0	0	0
			0	7039	0	0	0	0
	1,0246	1,5688	—5004	0	0	4983	0	0
			—4610	0	0	2457	0	0
	3,1837	2,7653	0	0	—4746	0	0	5254
			0	0	—5537	0	0	6003
$^1/_8$, $^1/_8$, $^1/_8$	6,2719	3,8814	2778	2778	2778	2995	2995	2995
			2460	2460	2460	0588	0588	0588
	2,8116	2,5987	1934	1934	—3868	2148	2148	—4296
			2165	2165	—4330	2346	2346	—4692
	2,8116	2,5987	3350	—3350	0	3721	—3721	0
			3751	—3751	0	4063	—4063	0
	0,2649	0,7977	—2852	—2852	—2852	2917	2917	2917
			—2834	—2834	—2834	2806	2806	2806
	0,1375	0,5747	—2046	—2046	4092	2031	2031	—4062
			—2053	—2053	4106	2020	2020	—4040
	0,1375	0,5747	—3544	3544	0	3518	—3518	0
			—3556	3556	0	3498	—3498	0
$^1/_4$, $^1/_4$, $^1/_4$	5,6541	3,6852	2886	2886	2886	2880	2880	2880
			2571	2571	2571	0745	0745	0745
	2,5586	2,4790	1907	1907	—3814	2175	2175	—4350
			2101	2101	—4202	2306	2306	—4612
	2,5586	2,4790	3303	—3303	0	3767	—3767	0
			3640	—3640	0	3994	—3994	0
	1,0171	1,5630	—2743	—2743	—2743	3031	3031	3031
			—2675	—2675	—2675	2590	2590	2590
	0,5149	1,1121	—2071	—2071	4142	2002	2002	—4004
			—2100	—2100	4200	1970	1970	—3940
	0,5149	1,1121	—3587	3587	0	3468	—3468	0
			—3638	3638	0	3412	—3412	0
$^3/_8$,$^3/_8$, $^3/_8$	4,7177	3,3662	3148	3148	3148	2561	2561	2561
			2838	2838	2838	0931	0931	0931
	2,1547	2,2750	1819	1819	—3638	2256	2256	—4512
			1961	1961	—3922	2308	2308	—4616
	2,1547	2,2750	3151	—3151	0	3908	—3908	0
			3397	—3397	0	3997	—3997	0
	2,1110	2,2518	—2438	—2438	—2438	3305	3305	3305
			—2316	—2316	—2316	2316	2316	2316
	1,0405	1,5809	—2149	—2149	4297	1910	1910	—3820
			—2214	—2214	4428	1872	1872	—3745
	1,0405	1,5809	—3722	3722	0	3309	—3309	0
			—3835	3835	0	3243	—3243	0
$^1/_2$, $^1/_2$, $^1/_2$	3,8645	3,0467	3982	3982	3982	0	0	0
			3643	3643	3643	0	0	0
	1,7171	2,0308	0	0	0	2956	2956	—5912
			0	0	0	2947	2947	—5894
	1,7171	2,0308	0	0	0	5121	—5121	0
			0	0	0	5104	—5104	0
	3,0358	2,7004	0	0	0	4181	4181	4181
			0	0	0	2404	2404	2404
	1,5274	1,9154	2815	2815	—5630	0	0	0
			2952	2952	—5905	0	0	0
	1,5274	1,9154	4876	—4876	0	0	0	0
			5114	—5114	0	0	0	0
$^1/_8$, $^1/_8$, $^3/_8$	5,2132	3,5386	1984	1984	3956	2004	2004	4298
			1898	1898	3444	1014	1014	0693

$\frac{k_x}{\pi}$; $\frac{k_y}{\pi}$; $\frac{k_z}{\pi}$	Ω^2	ω, sec^{-1}	$p_{1x}\vert\pi_{1x}$	$p_{1y}\vert\pi_{1y}$	$p_{1z}\vert\pi_{1z}$	$p_{2x}\vert\pi_{2x}$	$p_{2y}\vert\pi_{2y}$	$p_{2z}\vert\pi_{2z}$
1	2	3	4	5	6	7	8	9
	2,6722	2,5335	—2745	—2745	2598	—3093	—3093	3042
			—3135	—3135	2656	—3548	—3548	2555
	2,8568	2,6196	3355	—3355	0	3716	—3716	0
			3781	—3781	0	4105	—4105	0
	1,1577	1,6676	0603	0603	4902	—0732	—0732	—4906
			0554	0554	5070	—0513	—0513	—4985
	0,3479	0,9141	—3456	—3456	1064	3479	3479	—0804
			—3403	—3403	1159	3132	3132	—1027
	0,2662	0,7996	—3539	3539	0	3523	—3523	0
			—3504	3504	0	3248	—3248	0
$^{1}/_{8}$, $^{1}/_{8}$, $^{5}/_{8}$	3,6436	2,9584	2762	2762	2833	2824	2824	3289
			2973	2973	2408	2690	2690	0488
	2,4466	2,4242	—1738	—1738	—0098	—1742	—1742	6301
			—2012	—2012	—0644	—2295	—2295	4862
	2,9195	2,6481	3358	—3358	0	3713	—3713	0
			3823	—3823	0	4168	—4168	0
	2,3509	2,3763	0900	0900	—6250	1693	1693	1358
			1071	1071	—1205	1701	1701	0469
	0,5538	1,1534	—3511	—3511	0680	3515	3515	—0180
			—3394	—3394	0779	2763	2763	—0519
	0,4206	1,0051	—3536	3536	0	3527	3527	0
			—3439	3439	0	2913	—2913	0
$^{1}/_{8}$, $^{1}/_{8}$, $^{7}/_{8}$	1,5740	1,9444	0208	0208	—5000	0621	0621	—4900
			0321	0321	—4508	0756	0756	—1530
	3,1454	2,7486	—3065	—3065	—2603	—3232	—3232	1833
			—3451	—3451	—2877	—3572	—3572	2727
	2,9626	2,6676	3359	—3359	0	3712	—3712	0
			3851	—3851	0	4214	—4214	0
	3,1730	2,7607	1393	1393	—3951	1687	1687	5025
			1595	1595	—4711	1719	1719	5310
	0,6889	1,2864	—3516	—3516	0397	3535	3535	0121
			—3352	—3352	0428	2518	2518	—0138
	0,5125	1,1095	—3535	3535	0	3527	—3527	0
			—3401	3401	0	2687	—2687	0
$^{1}/_{8}$, $^{3}/_{8}$, $^{3}/_{8}$	4,8928	3,4282	1762	3351	3351	1618	3289	3289
			1718	2990	2990	1046	0885	0885
	2,8394	2,6115	—4434	1156	1156	—4977	1235	1235
			—5059	1177	1177	—5603	1027	1027
	2,1521	2,2736	0	3151	—3151	0	3908	—3908
			0	3361	—3361	0	3905	—3905
	1,5453	1,9266	0873	3266	3266	—1010	—3679	—3679
			0789	3263	3263	—0548	—3216	—3216
	0,4866	1,0811	—4903	0740	0740	4902	—0590	—0590
			—4768	0794	0794	4035	—0695	—0695
	0,9646	1,5222	0	—3722	3722	0	3309	—3309
			0	—3879	3879	0	3442	—3442
$^{1}/_{8}$, $^{3}/_{8}$, $^{5}/_{8}$	3,6774	2,9720	1859	2366	1945	1825	2261	1858
			1998	2299	1687	1819	1469	0197
	2,8341	2,6091	—2692	1594	1052	—3331	1579	0816
			—3152	1636	0971	—3757	1411	0228
	1,7726	2,0634	—0027	1105	—2301	0522	3137	—3076
			0050	1317	—2139	0482	3292	—2284
	2,5126	2,4567	0432	0716	3038	—0321	—1196	—3728
			0397	0654	3328	0037	—0685	—3679
	0,7182	1,3134	—3334	0928	0229	3484	—0858	—0051
			—3164	0968	0258	2481	—0913	—0145
	1,3158	1,4778	0786	3447	—1776	—0750	—2808	0122
			0738	3512	—1912	—0354	—2363	0749
$^{1}/_{8}$, $^{3}/_{8}$, $^{7}/_{8}$	3,1397	2,7462	2359	0457	—3720	2761	1187	4667
			2724	0502	—4392	2904	0743	4930
	2,5648	2,4820	1453	—4425	—0903	1905	—4816	—0889
			1772	—4686	—0783	2278	—4621	—0055
	1,6012	1,9611	—1532	—4215	—0738	1715	4899	—1651

$\frac{k_x}{\pi}$; $\frac{k_y}{\pi}$; $\frac{k_z}{\pi}$	Ω^2	ω, sec⁻¹	$p_{1x}\|\pi_{1x}$	$p_{1y}\|\pi_{1y}$	$p_{1z}\|\pi_{1z}$	$p_{2x}\|\pi_{2x}$	$p_{2y}\|\pi_{2y}$	$p_{2z}\|\pi_{2z}$
1	2	3	4	5	6	7	8	9
			—1365	—4102	—0501	0801	4004	—1211
	3,1397	2,7462	2359	0457	—3720	2761	1187	4667
			2724	0502	—4392	2904	0743	4930
	1,2614	1,7407	0466	2075	—4856	—0159	—0154	—4627
			0484	2207	—4489	0110	0331	—1953
	0,8487	1,4278	—4722	1770	0155	4687	--1548	0077
			—4450	1824	0159	2927	—1517	—0008
3/8, 3/8, 5/8	3,7399	2,9972	3679	3679	3289	2087	2087	1400
			3517	3517	2969	1659	1659	—0355
	1,4874	1,8901	—2791	—2791	5075	0140	0140	2614
			—2936	—2936	5163	—0529	—0529	1316
	2,1539	2,2745	3131	—3131	0	3926	—3926	0
			3430	—3430	0	4143	—4143	0
	2,8663	2,6239	—0886	—0886	—3252	3062	3062	4505
			—0690	—0690	—3486	1695	1695	3723
	1,8057	2,0826	1321	1321	—0715	—3538	—3538	4795
			1146	1146	—1112	—3095	—3095	4859
	1,1310	1,6482	—3738	3738	0	3288	—3288	0
			—3799	3799	0	2949	—2949	0
1/8, 5/8, 5/8	3,1991	2,7720	4600	1817	1817	4555	0734	0734
			5182	1696	1696	5235	—0089	—0089
	2,3842	2,3930	1363	—2530	—2530	2006	—4015	—4015
			1723	—2273	—2273	2430	—2484	—2484
	1,1830	1,6856	0	3763	—3763	0	3257	—3257
			0	3791	—3791	0	2730	—2730
	2,9024	2,6404	0118	3650	3650	—1947	—3103	—3103
			—0162	3754	3754	—1202	—2890	—2890
	1,0648	1,5993	—4951	0854	0854	4860	—0305	—0305
			—4619	0946	0946	2618	—0601	—0601
	2,1517	2,2734	0	—3102	3102	0	3951	—3951
			0	—3441	3441	0	4254	—4254
1/4, 1/4, 1/2	4,5714	3,3137	2858	2858	3218	2588	2588	3101
			2748	2748	2773	1562	1562	0328
	2,1637	2,2797	—1885	—1885	3504	—2609	—2609	4177
			—2201	—2201	3458	—2979	—2979	3348
	2,5941	2,4962	3307	—3307	0	3763	—3763	0
			3684	—3684	0	4076	—4076	0
	1,9810	2,1813	1141	1141	4421	—1523	—1523	—4835
			1022	1022	4626	—0865	—0865	—4673
	0,9540	1,5138	—3278	—3278	2332	3226	3226	—1389
			—3218	—3218	2560	2600	2600	—1943
	0,6453	1,2450	—3584	3584	0	3473	—3473	0
			—3575	3575	0	3122	—3122	0
1/4, 1/4, 3/4	3,4212	2,8666	3381	3381	1858	3219	3219	1645
			3554	3554	1596	3015	3015	—0168
	1,6900	2,0148	0047	0047	3983	—2528	—2528	4708
			—0250	—0250	3561	—2488	—2488	2599
	2,6263	2,5116	3302	—3302	0	3768	—3768	0
			3721	—3721	0	4166	—4166	0
	2,9038	2,6410	—0488	—0488	—4679	0734	0734	5167
			—0404	—0404	—5284	0212	0212	5584
	1,2642	1,7425	—3480	—3480	2522	2986	2986	0945
			—3388	—3388	2605	1797	1797	—0314
	0,7531	1,3449	—3588	3588	0	3468	—3468	0
			—3529	3529	0	2837	—2837	0
1/4, 1/4, 1	3,1006	2,7290	3447	3447	0	3622	3622	0
			3751	3751	0	3626	3626	0
	1,2417	1,7270	0	0	5015	0	0	4971
			0	0	4561	0	0	1971
	0,7931	1,3802	—3590	3590	0	3466	—3466	0
			—3511	3511	0	2723	—2723	0
	1,4699	1,8790	—3449	—3449	0	3620	3620	0
			—3232	—3232	0	2240	2240	0

$\frac{k_x}{\pi}$; $\frac{k_y}{\pi}$; $\frac{k_z}{\pi}$	Ω^2	ω, sec^{-1}	$p_{1x}\|\pi_{1x}$	$p_{1y}\|\pi_{1y}$	$p_{1z}\|\pi_{1z}$	$p_{2x}\|\pi_{2x}$	$p_{2y}\|\pi_{2y}$	$p_{2z}\|\pi_{2z}$
1	2	3	4	5	6	7	8	9
$^1/_4$, $^1/_2$, $^1/_2$	3,2249	2,7832	0	0	—4734	0	0	5266
			0	0	—5550	0	0	6005
	2,6400	2,5182	3300	—3300	0	3770	—3770	0
			3737	—3737	0	4203	—4203	0
	3,9982	3,0990	3251	3286	3286	2438	2349	2349
			3229	2964	2964	2150	0639	0639
	2,3880	2,3950	3750	—0618	—0618	3230	—3582	—3582
			4169	—0583	—0583	4223	—2791	—2791
	1,7245	2,0352	0	0988	—0988	0	5014	—5014
			0	0966	—0966	0	4946	—4946
	2,5601	2,4798	—0499	3259	3259	—3891	—2609	—2609
			—0927	3248	3248	—3031	—1960	—1960
	0,9806	1,5347	—4765	1428	1428	4593	—0951	—0951
			—4640	1554	1554	3441	—1228	—1228
	1,5105	1,9048	0	—4775	4775	0	1037	—1037
			0	—5026	5026	0	1298	—1298
$^1/_4$, $^1/_2$, $^3/_4$	3,2170	2,7798	3930	3273	3930	1812	0	—1812
			4017	3113	4017	2821	0	—2821
	3,0400	2,7022	2279	0	—2279	4111	2679	4111
			2700	0	—2700	3454	1534	3454
	2,2260	2,3123	—0469	4791	—0469	—3650	0	3650
			—0935	4835	—0935	—3282	0	3282
	2,1023	2,2472	—2326	0	2326	—0631	6302	—0631
			—2490	0	2490	—1696	5521	—1696
	1,1963	1,6951	2849	—3727	2849	—3101	0	3101
			2673	—3977	2673	—2160	0	2160
	1,1627	1,6712	3630	0	—3630	—2986	2356	—2986
			3543	0	—3543	—1674	2744	—1674

ion K^+, let $s = 1$, and for Cl^-, $s = 2$.

As follows from Eq. (6) of Ref. 4, the energy of an ideal ionic crystal can be described by a quadratic function of the variables $\mathbf{p}^l_s$ and $\mathbf{P}^l_s$. The equations of free vibrations

$$m\ddot{u}^l_{sx} = -\partial U / \partial U^l_{sx}, \qquad (1)$$

$$-\partial U / \partial P^l_{sx} \ (s = 1, 2;\ x = x, y, z) = 0,$$

upon substitution in them of a solution in the form waves

$$\mathbf{p}^l = \mathbf{p}_\mathbf{k} \exp\{i(\omega_\mathbf{k} t + \mathbf{k}\mathbf{R}^l_s)\}; \qquad (2)$$

$$\mathbf{P}^l = \mathbf{P}_\mathbf{k} \exp\{i(\omega_\mathbf{k} t + \mathbf{k}\mathbf{R}^l_s)\};$$

lead to

$$\mathbf{p}_\mathbf{k}\mu_s\Omega^2_\mathbf{k} = A_\mathbf{k}\mathbf{p}_\mathbf{k} + B_\mathbf{k}\mathbf{P}_\mathbf{k}, \quad B^*_\mathbf{k}\,\mathbf{p}_\mathbf{k} + C_\mathbf{k}\mathbf{P}_\mathbf{k} = 0, \ (3)$$

where m_s is the ordinary mass and $\mu_s = m_s/\mu$ is the dimensionless mass of the ions, $\Omega_\mathbf{k} = e^{-2}\mu a^3\omega^2_\mathbf{k}$, $\mu = m_1m_2/(m_1 + m_2)$ is the reduced mass; $\mathbf{p}^l$ and $\mathbf{P}^l$ are the dimensionless six-component vectors with components p^l_{sx}/ae and P^l_{sx}/ae. The sixfold dimenless matrices $A_\mathbf{k}$, $B_\mathbf{k}$, and $C_\mathbf{k}$ are determined in Ref. 7 by the matrices $\Phi_\mathbf{k}$, the computed values of which have been tabulated by the author in Ref. 8. The matrices $C^{-1}_\mathbf{k}$ necessary for the solution of (3) have been listed there also. The extremely difficult calculation of the matrices $\Phi_\mathbf{k}$, for purposes of proof, was also carried out independently by Zaslavkaia and Tolpygo[9].

For the condition of solvability of the system, obtained from (3) after elimination of $\mathbf{P}_\mathbf{k}$, the six valus of the frequencies $\Omega^\alpha_\mathbf{k}(\alpha = 1, 2, \ldots, 6)$ were determined, and the mutually orthogonal eigenvectors $\mathbf{P}^\alpha_\mathbf{k}$ corresponding to them were also obtained. These were normalized in the Born fashion:

$$\mu_1\mathbf{p}^\alpha_{\mathbf{k}1}\mathbf{p}^\beta_{\mathbf{k}1} + \mu_2\mathbf{p}^\alpha_{\mathbf{k}2}\mathbf{p}^\beta_{\mathbf{k}2} = \delta_{\alpha,\beta}. \qquad (4)$$

The results of the calculations are shown in the Table. The frequencies and amplitudes at the point

K{0, 0, 0} can be taken from Ref. 2. The corresponding $(\Omega_{\mathbf{k}}^{\alpha})^2$ are listed along with each frequency $\omega_{\mathbf{k}}^{\alpha}$. The amplitude vectors of the dipole moments of the ionic displacements $\mathbf{p}_{\mathbf{k}}^{\alpha}$ and the total amplitude vectors $\pi_{\mathbf{k}}^{\alpha}=\mathbf{p}_{\mathbf{k}}^{\alpha}+\mathbf{P}_{\mathbf{k}}^{\alpha}$ are listed in adjacent columns. Wherever possible, a total of 10 steps were carried out.

The frequencies for each wave vector are divided into branches: the optical (longitudinal and transverse) and acoustical (longitudinal and transverse). The longitudinal optical branch was systematically described by Iona[1], with neglect of the polarization of the ions. Inasmuch as he considered the masses of the ions to be identical, the cell of this reciprocal lattice is a cube and threre are 3 branches altogether; on the other hand, the region of variation of **k** is different. Therefore, our optical and acoustical branches, of the same K according to Iona, actually belong to different **k**. The latter circumstance helped to distribute the resultant frequencies between the branches in doubtful cases. Determination of the branches was obtained by the monotonic variation of ω and **p**, which is not always unique. The division of the vibrations into longitudinal and transverse is also not unique. The latter has meaning only for symmetric directions of the wave vector relative to the coordinate axes. Thus, for example, for **k**{$\pi/8$; $3\pi/8$; $7\pi/8$}, the angle between **k** and $\mathbf{p}_1$ for the optical longitudinal branch amounts to more than 50°. This means that in the KCI crystal, the anisotropy is significant and therefore neglect of $\mathbf{P}_s$ in comparison with $\mathbf{p}_s$ is invalid.

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117