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Cohesive and thermoelastic properties of $(KCN)_x (KCl)_{1-x}$

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Abstract

The thermal and elastic properties of $(KCN)_x(KCl)_{1-x}$ are investigated by means of Extended Three Body Force Shell Model (ETSM). The motion of constituent atoms or molecules or the nature of binding forces of a crystal can be investigated by exploring the mechanical properties of pure and mixed crystals like anharmonic elastic properties. We have chosen different compositions at different temperature to show that anharmonic elastic properties are temperature dependent rather than composition dependent and the purpose of study is to test the mechanical stabilities of the potential. Moreover, the thermodynamic properties such as molecular force constant (f), Reststrahlen frequency (υ_o), cohesive energy (ϕ), Debye temperature (θ_D) and Gruneisen parameter (γ) have also been discussed.

Keywords: Elastic constants, Cohesive energy, Thermodynamic properties

1. Introduction

In past few years, the cohesive and thermoelastic properties of orientationally disordered alkali metal cyanides have been of interest to the experimental as well as theoretical workers on this field. The lattice mechanics of many ODMs have been reported satisfactorily by means of ETSM. This model which was designed by incorporating Translational-Rotational coupling effect in the framework of Three Body Force Shell Model was found to be excellent in explaining the static, dynamic, dielectric and optic properties of ODMs. Inspired by the great success of ETSM [1] in explaining these properties of ODMs we thought it appropriate to extend the investigation to thermoelastic and cohesive behaviour of $(KCN)_x(KCl)_{1-x}$ which belongs to the mixed alkali halide-cyanide family.

When the Cl^- ion of an alkali halide system is replaced by a CN^- ion, a $(KCN)_x(KCl)_{1-x}$ system is generated. Here, the substitution of the spherical Cl^- ions by the dump-bell shaped CN^- ions strongly lower the transition temperature of the system. This mixed system shows glassy state at very low temperature and over a wide range of concentration. This system which exhibits rich (X, T) phase diagram [2], above a critical concentration of x_c =0.08, undergo structural change from cubic phase to monoclinic or orthorhombic phases at room temperature [2]. The structural changes result in linear TR coupling orientational degree of freedom of the cyanide molecules and the translational modes. Also, the requirement of application of ETSM to $(KCN)_x(KCl)_{1-x}$ evolved from the fact that the K^+ ions and the CN^- ions has larger ionic size difference which makes the three-body interactions (TBI) more effective in this crystal. The formulation of ETSM is given in 2. We present the results and related discussions about the thermoelastic and coheisive properties in section 3. Concluding remarks are given in Section 4.

2. Potential model and method of calculations

The formalism of the Extended Three Body Force Shell Model has been derived from the following interatomic interaction [3-6]

$$\Phi = \frac{e^2}{2}\Sigma Z_k Z_{k'} r_{kk'}^{-1}[1+\Sigma_{kk}f(r_{kk'})]-\Sigma_{kk'}c_{kk}r_{kk'}^{-6}-\Sigma_{kk'}d_{kk'}r_{kk'}^{-8}+b\,\Sigma_{kk'}\beta_{kk'}\exp(r_k+r_{k'}-r_{kk'}/\rho)+\phi^{TR} \quad (1)$$

Here, the first term is attractive long range (LR) coulomb interactions energy and the second term is the three body interaction potential. The third and fourth term represents the contributions of van derWaals (vdW) attraction for the dipole-dipole interaction and dipole-quadrupole interactions and the fifth term is short range (SR) overlap repulsive energy represented by the Hafemeister–Flygare type (HF) interaction extended up to the second neighbor. $\emptyset^{TR}$ is the contribution due to ranslational rotational coupling. In expression (1), other symbols involved are the same as those defined in our earlier papers [3-6]. b_i and ρ_i are the hardness and range parameters for the i^{th} cation–anion pair (i = 1, 2) respectively and $\beta_i^{kk'}$ is the Pauling coefficient [7] given by

$$\beta_i^{kk'} = 1 + (Z_k / N_k) + (Z_{k'} / N_{k'}) \quad (2)$$

Z_k ($Z_{k'}$) and N_k (N_k') are the valence and the number of electrons in the outermost orbit of the k (k′) ion respectively. The contributions of van der Waals (vdW) attraction for the dipole-dipole interaction is determined by using the Slater- Kirkwood Variational (SKV) method [8]. The model parameters, hardness (b) and range (ρ) are determined from the equilibrium condition.

$$\left[d\phi/dr\right]_{r=r_0} = 0 \tag{3}$$

and the bulk modulus

$$B = 1/9 K r_0 \left[d^2\phi/dr^2\right]_{r=r_0} \tag{4}$$

where K is the crystal-structure-dependent constant and r_0 is the equilibrium nearest neighbour distance. The expressions for calculating the thermodynamic properties like Debye temperature (θ_D), Reststrahlen frequency (υ), molecular force constant (f), and Gruneisen parameter (γ) are taken from our earlier papers [3-6]. The present model (ETSM)) described above for the $(KCN)_x(KCl)_{1-x}$ contains three model parameters (b, ρ and f(r)), which are used to determine the second- order (SOECs), third order (TOECs) and fourth order (FOECs) elastic constants [9] of $(KCN)_x(KCl)_{1-x}$.

3 Results and discussions

We have obtained the model parameters (b, ρ and *f(r)*) as a function of temperature using input data (Table 1) taken from Ref. [9-10] and the van der Walls coefficients. The model parameters computed for $(KCN)_x(KCl)_{1-x}$ for the concentrations x=0, 0.025,0.05,0.07,0.5,0.7 are given in Table 2. Using the model parameters we have calculated the second order (SOEC), third order (TOEC) and fourth order (FOEC) elastic constants of $(KCN)_x(KCl)_{1-x}$ at 175K≤T≤245K for the composition x=0.025,0.05, 0.07,0.5,0.7 and are presented in Table 3-8. The values of SOECs are plotted in Figures 1-3. The values of c_{11} and c_{12} decreases with increase in temperature and they show quasilinear dependence on temperature. Due to lack of experimental results the values of c_{11} and c_{12} could not be compared. Our calculated results on shear elastic constant c_{44} (Figure 3) are in good agreement with the measured values obtained by Kwiecien and Garland [11]. Also a gradual increase in c_{44} with increase in temperature is observed. It is interesting to note that a softening of c_{44} with lowering of temperature is observed which might be due to the effective coupling of CN^- ions which indicates a phase transition at lower temperature or the collective behaviour of coupled impurity. The values of c_{44} are found to be 100 times lesser than the values of c_{11} and c_{12} in these compounds. The computed values of third and fourth order elastic constants are presented in Table 3-8. Our results on anharmonic elastic constants show that the magnitudes all the values of TOECS decreases with increase in temperature near room temperature. Its variation plays a significant role in explaining the anharmonic properties. The variation of TOECs follows the same trend for all compositions.

The values of all the FOECs also decrease in magnitude with increase in temperature. These values could not be compared due to the lack of experimental data. The thermophysical properties of $(KCN)_x$ $(KCl)_{1-x}$ cohesive energy ϕ, compressibility β , molecular force constant f and Restrahalen frequency υ_o, the Debye temperature θ_D and Gruniesen parameter γ, α_v / c_v are calculated for concentrations x = 0.5, 0.7 and 0.95 for temperature range 175K ≤T≤ 245K and are listed in Table 9. From Table 9 it is clear that cohesive energy ϕ, compressibility β, molecular force constant f and Restrahalen frequency υ_o are decreasing with increase in temperature but are increasing with increase in concentration of CN^- ions. The experimental values of cohesive energy for pure KCN and KCl are -674kJ/mol and -813kJ/mol [12] respectively. The negative values of cohesive energy show that the stability of these compounds is intact.

The calculated values of Reststrahlen frequency by ETSM are closer with the available value of υ= 8.58THz [13]. Our values of compressibility β and molecular force constant f are closer to the reported values of 6.95 × 10^{-12} $dynes^{-1}cm^2$ and 2.82 10^4 dynes/cm respectively for pure KCN crystals [12] at 300K. Also the Debye temperature Θ_D and α_v / c_v decrease with increase in temperature and Gruneisen parameter increases with increase in temperature. Here, it is noteworthy that the Gruneisen parameters for $(KCN)_x$ $(KCl)_{1-x}$ lie in between 2 and 3 which is usually found in ODM. The Debye temperature calculated by us is elastic constant dependent and hence is more accurate.

4. Conclusions

The elastic and thermodynamic properties of the orientationally disordered $(KCN)_x(KCl)_{1-x}$ mixed crystal are investigated with the help of ETSM. Our calculated results on shear elastic constant c_{44} are in fairly good agreement with the available experimental data. Also, the values of cohesive energy, compressibility and molecular force constant obtained from ETSM are in good agreement with the experimental values of these parameters for pure KCN crystals. Our comments on the other results are restricted until the report of experimental data on them but these results will serve as a guide to the experimental workers in future. A successful description of mechanical properties achieved for such complicated $(KCN)_x(KCl)_{1-x}$ can be considered remarkable in view of the inherent simplicity of the ETSM and its less parametric nature.

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Table 1. Input Data for $(KCN)_x(KCl)_{1-x}$ at different concentrations.

Prop.	x = 0	x = 0.025	x = 0.05	x = 0.07	x = 0.5	x = 0.70
r_o	2.846	2.848	2.850	2.852	2.854	2.856
r_-	1.528	1.529	1.531	1.534	1.582	1.601
r_+	1.43	1.42	1.41	1.40	1.33	1.28
$\alpha +$	1.24	1.20	1.19	1.18	1.07	1.04
$\alpha -$	2.74	2.714	2.688	2.664	2.213	2.112
c_{11}	3.652	1.732	1.867	1.891	2.872	5.436
c_{12}	0.631	1.073	1.062	1.051	0.891	1.823
c_{44}	0.57	1.421	1.502	1.588	0.387	0.324
υ_{TO}	3.420	3.444	3.530	3.758	3.921	0.998
ϵ_0	4.23	4.302	4.341	4.362	4.602	4.718
ϵ_∞	1.928	1.937	1.934	1.931	1.871	1.853
C	1045.11	618.36	628.14	100.01	862.47	788.24
D	448.20	451.638	442.176	437.68	356.18	286.67

c+-	117.13	118.016	117.235	116.386	99.76	73.248
c++	58.8	59.23	58.341	58.482	58.211	57.986
c--	262.31	256.84	254.23	251.67	201.017	168.23
d+-	61.1	60.28	59.97	59.43	49.23	45.76
d++	22.48	22.21	22.14	22.04	21.87	21.43
d- -	161.28	159.37	157.65	155.88	116.718	104.28

Table 2. Model parameters for $(KCN)_x(KCl)_{1-x}$ with temperature range 175K≤T≤245 K for different concentrations.

x	T	Model parameters		
		b(10^{-12} ergs)	ρ(A^o)	f(r)
0	175	0.378	0.312	0.200
	185	0.379	0.312	0.200
	195	0.381	0.312	0.200
	205	0.382	0.312	0.200
	215	0.384	0.313	0.200
	225	0.386	0.313	0.200
	235	0.387	0.313	0.200
	245	0.389	0.313	0.200
0.025	175	0.334	0.314	0.199
	185	0.336	0.314	0.199
	195	0.338	0.314	0.199
	205	0.339	0.314	0.199
	215	0.340	0.315	0.199
	225	0.341	0.315	0.199
	235	0.343	0.316	0.199
	245	0.345	0.316	0.199
0.05	175	0.330	0.313	0.206
	185	0.331	0.313	0.206
	195	0.333	0.313	0.206
	205	0.334	0.313	0.206
	215	0.336	0.313	0.206
	225	0.337	0.314	0.206
	235	0.338	0.314	0.206
	245	0.340	0.314	0.206
0.07	175	0.318	0.313	0.082
	185	0.320	0.314	0.082

	195	0.321	0.315	0.082
	205	0.323	0315	0.082
	215	0.325	0.315	0.082
	225	0.326	0.315	0.082
	235	0.327	0.316	0.082
	245	0.328	0.316	0.082
0.5	175	0.439	0.295	0.051
	185	0.443	0.296	0.051
	195	0.445	0.296	0.051
	205	0.448	0.296	0.051
	215	0.451	0.296	0.051
	225	0.453	0.297	0.051
	235	0.456	0.297	0.051
	245	0.459	0.297	0.051
0.70	175	0.412	0.275	0.022
	185	0.416	0.275	0.022
	195	0.419	0.275	0.022
	205	0.422	0.276	0.022
	215	0.424	0.276	0.022
	225	0.428	0.276	0.022
	235	0.433	0.277	0.022
	245	0.435	0.277	0.022

Table 3. TOECs and FOECs of $(KCN)_x(KCl)_{1-x}$ (in units of 10^{12}dynes / cm^2) for x = 0

Props	175K	185K	195K	205K	215K	225K	235K	245K
C_{111}	-11.164	-11.142	-11.123	-11.104	-10.986	-10.966	-10.945	-10.931
C_{112}	-0.954	-0.953	-0.952	-0.951	-0.948	-0.946	-0.944	-0.942
C_{116}	-0.225	-0.225	-0.224	-0.224	-0.224	-0.223	-0.223	-0.223
C_{123}	0.321	0.320	0.319	0.318	0.317	0.316	0.315	0.314
C_{144}	0.204	0.204	0.203	0.203	0.202	0.202	0.201	0.201
C_{456}	0.153	0.153	0.153	0.153	0.152	0.152	0.151	0.151
C_{1111}	170.213	169.928	169.568	169.123	168.881	168.531	168.265	167.976
C_{1112}	6.438	6.386	6.365	6.321	6.296	6.271	6.253	6.231
C_{1166}	0.312	0.309	0.307	0.305	0.304	0.303	0.302	0.302
C_{1122}	6.236	6.227	6.202	6.188	6.175	6.163	6.150	6.134
C_{1266}	1.263	1.260	1.258	1.255	1.252	1.250	1.248	1.246
C_{4444}	0.522	0.521	0.521	0.521	0.520	0.520	0.519	0.519
C_{1123}	-1.114	-1.112	-1.110	-1.108	-1.106	-1.104	-1.102	-1.100
C_{1144}	-0.714	-0.713	-0.712	-0.711	-0.710	-0.709	-0.708	-0.707
C_{1244}	-0.437	-0.436	-0.435	-0.434	-0.433	-0.432	-0.431	-0.430
C_{1456}	-0.248	-0.248	-0.247	-0.247	-0.246	-0.246	-0.245	-0.245
C_{4466}	-1.431	-1.429	-1.427	-1.427	-1.424	-1.421	-1.418	-1.412

Table 4. TOECs and FOECs (in units of 10^{12}dyns/Cm^2) for X = 0.025 of $(KCN)_x(KCl)_{1-x}$

Props	175K	185K	195K	205K	215K	225K	235K	245K
C_{111}	-11.688	-11.665	-11.646	-11.625	-11.601	-11.572	-11.534	-11.506
C_{112}	-0.856	-0.854	-0.852	-0.850	-0.847	-0.845	-0.843	-0.841
C_{116}	-0.107	-0.107	-0.107	-0.107	-0.107	-0.107	-0.107	-0.107
C_{123}	+0.274	0.274	0.274	0.273	0.273	0.272	0.272	0.272
C_{144}	0.164	0.164	0.164	0.163	0.163	0.162	0.162	0.162
C_{456}	0.112	0.112	0.112	0.112	0.111	0.111	0.111	0.111
C_{1111}	178.034	177.634	177.321	177.108	176.847	176.26	175.768	175.377
C_{1112}	5.924	5.913	5.901	5.890	5.882	5.874	5.865	5.853
C_{1166}	0.045	0.045	0.044	0.044	0.044	0.043	0.043	0.043
C_{1122}	5.861	5.852	5.844	5.831	5.825	5.816	5.807	5.791
C_{1266}	1.011	1.009	1.007	1.005	1.003	1.001	0.999	0.099
C_{4444}	0.098	0.098	0.098	0.098	0.099	0.099	0.099	0.099
C_{1123}	-0.997	-0.995	-0.994	-0.992	-0.990	-0.989	-0.981	-0.985
C_{1144}	-0.612	-0.611	-0.610	-0.609	-0.608	-0.607	-0.606	-0.605
C_{1244}	-0.345	-0.345	-0.344	-0.344	-0.343	-0.343	-0.342	-0.342
C_{1456}	-0.161	0.161	-0.161	-0.160	-0.160	-0.160	-0.159	-0.159
C_{4466}	-1.432	-1.430	-1.428	-1.425	-1.422	-1.418	-1.414	-1.410

Table 5. TOECS and FOECS for $(KCN)_x(KCl)_{1-x}$(in units of 10^{12}dyns/Cm^2) for x = 0.05

Props	175K	185K	195K	205K	215K	225K	235K	245K
C_{111}	-12.067	-12.056	-12.043	-12.031	-12.025	-12.014	-12.062	-11.992
C_{112}	-0.864	-0.862	-0.860	-0.858	-0.857	-0.856	-0.853	-0.850
C_{116}	-0.136	-0.136	-0.134	-0.134	-0.132	-0.132	-0.130	-0.130
C_{123}	0.228	0.228	0.228	0.226	0.226	0.226	0.224	0.224
C_{144}	0.184	0.184	0.184	0.183	0.183	0.183	0.182	0.182
C_{456}	0.102	0.102	0.101	0.101	0.100	0.100	0.099	0.099
C_{1111}	180.026	179.864	179.532	179.281	178.864	178.462	178.125	177.735
C_{1112}	5.938	5.930	5.921	5.910	5.898	5.888	5.876	5.865
C_{1166}	-0.211	-0.211	-0.211	-0.210	-0.210	-0.210	-0.210	-0.209
C_{1122}	5.537	5.528	5.517	5.506	5.494	5.483	5.472	5.461
C_{1266}	0.713	0.712	0.711	0.710	0.709	0.708	0.707	0.706
C_{4444}	-0.214	0.214	-0.213	-0.213	-0.212	-0.212	-0.211	-0.211
C_{1123}	-0.929	-0.927	-0.925	-0.923	-0.921	-0.919	-0.917	-0.915
C_{1144}	-0.547	-0.546	-0.545	-0.544	-0.543	-0.542	-0.541	-0.540
C_{1244}	-0.287	-0.287	-0.286	-0.286	-0.285	-0.285	-0.284	-0.284
C_{1456}	-0.101	0.101	-0.101	-0.101	-0.101	-0.101	-0.101	-0.101
C_{4466}	-1.278	-1.275	-1.272	-1.270	-1.268	-1.266	-1.24	-1.22

Table 6. TOECS and FOECS (in units of 10^{12}dyns/Cm^2) for $(KCN)_x(KCl)_{1-x}$for x = 0.07

Props	175K	185K	195K	205K	215K	225K	235K	245K
C_{111}	-12.878	-12.867	-12.88	-12.845	-12.836	-12.823	-12.814	-12.805
C_{112}	-0.802	-0.801	-0.799	-0.797	-0.795	-0.792	-0.788	-0.784
C_{116}	-0.061	-0.061	-0.069	-0.069	-0.068	-0.068	-0.068	-0.068
C_{123}	0.241	0.241	0.241	0.241	0.240	0.240	0.240	0.240
C_{144}	0.138	0.138	0.1380.138	0.138	0.137	0.137	0.137	0.137
C_{456}	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
C_{1111}	184.628	184.316	184.028	183.756	183.448	183.127	182.967	182.645
C_{1112}	6.063	6.052	6.041	6.033	6.024	6.016	6.005	5.991
C_{1166}	-0.234	-0.233	-0.232	-0.231	-0.230	-0.229	-0.228	-0.227
C_{1122}	5.678	5.666	5.654	5.643	5.636	5.624	5.615	5.608
C_{1266}	0.660	0.660	0.660	0.659	0.659	0.658	0.658	0.657
C_{4444}	0.251	0.251	0.250	0.250	0.249	0.249	0.248	0.248
C_{1123}	0.958	0.956	0.954	0.952	0.951	0.949	0.948	0.946
C_{1144}	-0.562	-0.561	-0.560	-0.558	-0.556	-0.555	-0.553	-0.551
C_{1244}	-0.282	-0.282	-0.281	-0.281	-0.280	-0.280	-0.279	-0.279
C_{1456}	-0.102	-0.102	-0.102	-0.102	-0.102	-0.101	-0.101	-0.101
C_{4466}	-1.324	1.322	-1.319	-1.316	-1.313	-1.310	-1.307	-1.304

Table 7. TOECs and FOECs of $(KCN)_x(KCl)_{1-x}$ (in units of 10^{12} dynes/cm^2) at x=0.5

Props	175K	185K	195K	205K	215K	225K	235K	245K
C_{111}	-1.531	-1.528	-1.525	-1.520	-1.514	-1.507	-1.500	-1.491
C_{112}	-0.612	-0.609	-0.607	-0.605	-0.603	-0.601	-0.600	-0.599
C_{116}	-0.231	-0.231	-0.230	-0.230	-0.229	-0.229	-0.228	-0.228
C_{123}	0.2162	0.2153	0.2146	0.2139	0.2136	0.2130	0.2123	0.2116
C_{144}	0.1640	0.1639	0.1638	0.1636	0.1627	0.1616	0.1608	0.1600
C_{456}	0.1364	0.1362	0.1357	0.1352	0.1348	0.1342	0.1336	0.1328
C_{1111}	153.298	153.674	161.267	159.678	158.937	156.744	160.248	165.238
C_{1112}	3.621	4.625	4.601	4.595	4.585	4.594	4.741	4.797
C_{1166}	0.723	0.612	0.674	0.653	0.654	0.652	0.650	0.648
C_{1122}	3.734	3.621	3.648	3.634	3.630	3.620	3.631	3.819
C_{1266}	1.458	1.388	1.428	1.421	1.423	1.419	1.425	1.455
C_{4444}	0.802	0.748	0.775	0.772	0.772	0.770	0.770	0.768
C_{1123}	-0.592	-0.590	-0.589	-0.580	-0.578	-0.576	-0.574	-0.572
C_{1144}	-0.414	-0.413	-0.412	-0.411	-0.409	-0.408	-0.406	-0.405
C_{1244}	-0.301	-0.300	-0.299	-0.298	-0.297	-0.296	-0.295	-0.291
C_{1456}	-0.220	-0.219	-0.218	-0.217	-0.216	-0.215	-0.214	-0..215
C_{4466}	-0.835	-0.832	-0.829	-0.826	-0.823	-0.820	-0.817	-0.814

Tables 8. TOECS and FOECS (in units of 10^2 dynes / cm^2) for x = 0.70 of $(KCN)_x$ $(KCl)_{1-x}$

Props	175K	185 K	195 K	205 K	215 K	225K	235K	245K
C_{111}	-1.634	-1.631	-1.628	-1.625	-1.623	-1.620	-1.617	-1.614
C_{112}	-0.704	-0.704	-0.700	-0.697	-0.694	-0.692	-0.690	-0.687
C_{116}	-0.198	-0.197	-0.196	-0.196	-0.195	-0.194	-0.194	-0.196
C_{123}	0.2486	0.2481	0.2476	0.2470	0.2467	0.2464	0.2462	0.2461
C_{144}	0.1767	0.1764	0.1761	0.1757	0.1752	0.1748	0.1744	0.1741
C_{456}	0.1421	0.1417	0.1413	0.1410	0.1407	0.1404	0.1403	0.1402
C_{1111}	205.168	204.841	204.431	203.981	203.361	202.718	202.515	202.111
C_{1112}	4.632	4.630	4.617	4.608	4.600	4.598	4.596	4.594
C_{1166}	0.421	0.418	0.417	0.416	0.415	0.414	0.413	0.412
C_{1122}	4.428	4.4225	4.217	4.210	4.202	4.193	4.182	4.176
C_{1266}	1.142	1.140	1.137	1.135	1.132	1.130	1.127	1.125
C_{4444}	0.478	0.476	0.475	0.474	0.473	0.472	0.471	0.470
C_{1123}	-0.717	-0.175	-0.173	-0.711	-0.710	-0.708	-0.706	-0.704
C_{1144}	-0.482	-0.482	-0.481	-0.481	-0.480	-0.479	-0.479	-0.478
C_{1244}	-0.314	-0.314	-0.313	-0.313	-0.312	-0.312	-0.311	-0.311
C_{1456}	-0.201	-0.201	-0.201	-0.200	-0.200	-0.200	-0.199	-0.199
C_{4466}	-1.023	-1.020	-1.018	-1.016	-1.013	-1.013	-1.011	-1.008

Table 9. Thermal and Cohesive properties of $(KCN)_x(KCl)_{1-x}$ within temperature range 175 K ≤T≤ 245 K.

X	T(K)	ϕ (KJ mol^{-1})	β (10^{-12}dyme/cm^2)	f (10^4dynes/cm)	Θ_D (K)	υ_o (THz)	α_v / c_v (10^3J)	γ
0.5	175	-621.581	4.153	9.361	218.69	7.285	1.709	1.878
	185	-621.238	4.141	9.354	213.44	7.279	1.709	1.878
	195	-620.861	4.018	9.342	208.26	7.263	1.709	1.879
	205	-620.642	3.994	9.336	203.43	7.251	1.709	1.880
	215	-620.546	3.986	9.328	198.86	7.245	1.708	1.880
	225	-620.412	3.979	9.321	193.67	7.234	1.708	1.880
	235	-620.281	3.964	9.317	188.48	7.218	1.708	1.880
	245	-619.981	3.957	9.312	187.36	7.206	1.708	1.881
0.7	175	-625.673	5.063	9.948	217.88	8.738	1.563	1.551
	185	-625.371	5.057	9.937	217.43	8.731	1.561	1.554
	195	-625.121	5.036	9.929	216.66	8.705	1.560	1.557
	205	-624.848	5.018	9.920	212.67	8.681	1.557	1.560
	215	-624.618	5.013	9.914	208.99	8.668	1.555	1.564
	225	-624.526	5.017	9.907	208.76	8.56	1.553	1.568
	235	-624.378	5.011	9.900	207.67	8.647	1.552	1.572
	245	-624.118	5.006	9.895	206.43	8.635	1.551	1.577
0.95	175	-618.243	7.021	11.134	215.36	10.138	1.143	1.013
	185	-618.012	7.015	11.123	214.95	10.131	1.141	1.016
	195	-617.834	6.994	11.111	214.16	9.704	1.140	1.019
	205	-617.623	6.973	11.103	210.38	9.680	1.137	1.021
	215	-617.581	6.968	11.091	206.43	9.664	1.135	1.024
	225	-617.348	6.952	11.083	206.14	9.653	1.133	1.028
	235	-617.214	6.941	11.076	205.78	9.642	1.132	1.032
	245	-617.036	6.934	11.067	204.53	9.631	1.131	1.037
Exp. KCN	300	-674	6.95	2.92	-	-	-	-

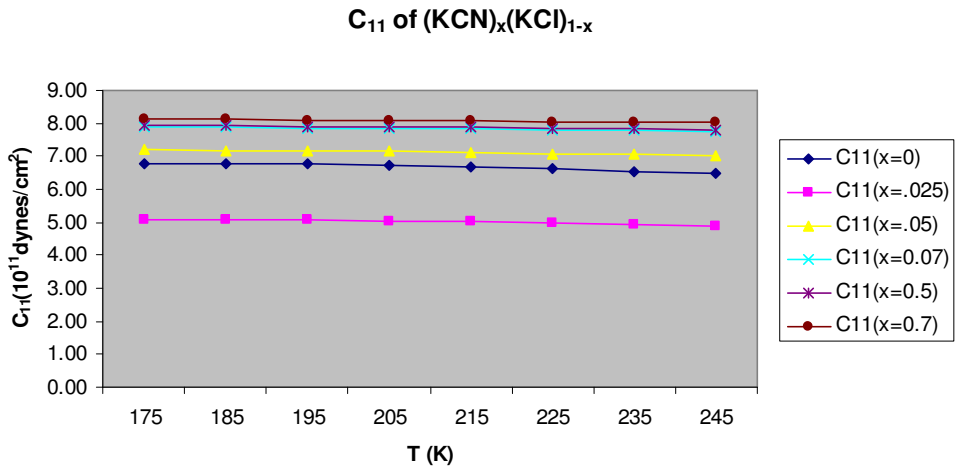

Figure 1. The variation of C_{11} with temperature for $(KCN)_x(KCl)_{1-x}$

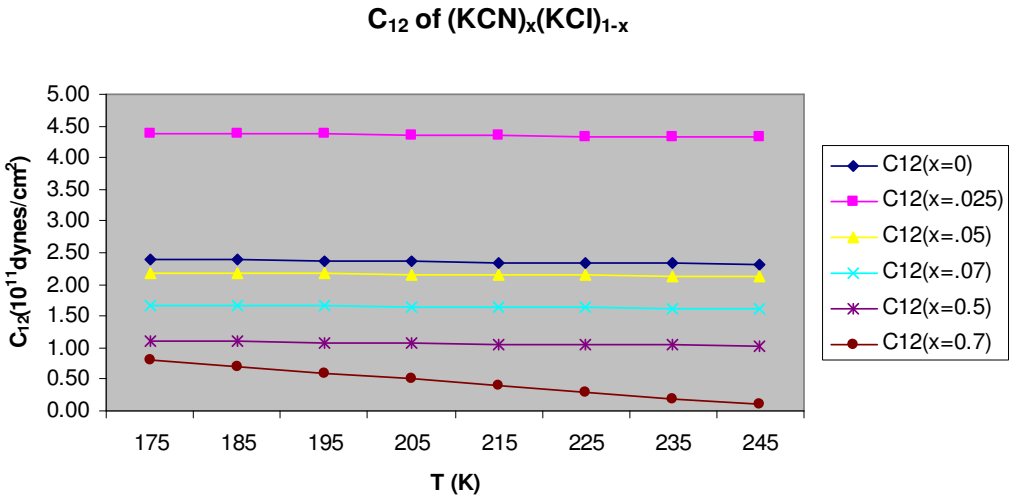

Figure 2. The variation of C_{12} with temperature for $(KCN)_x(KCl)_{1-x}$

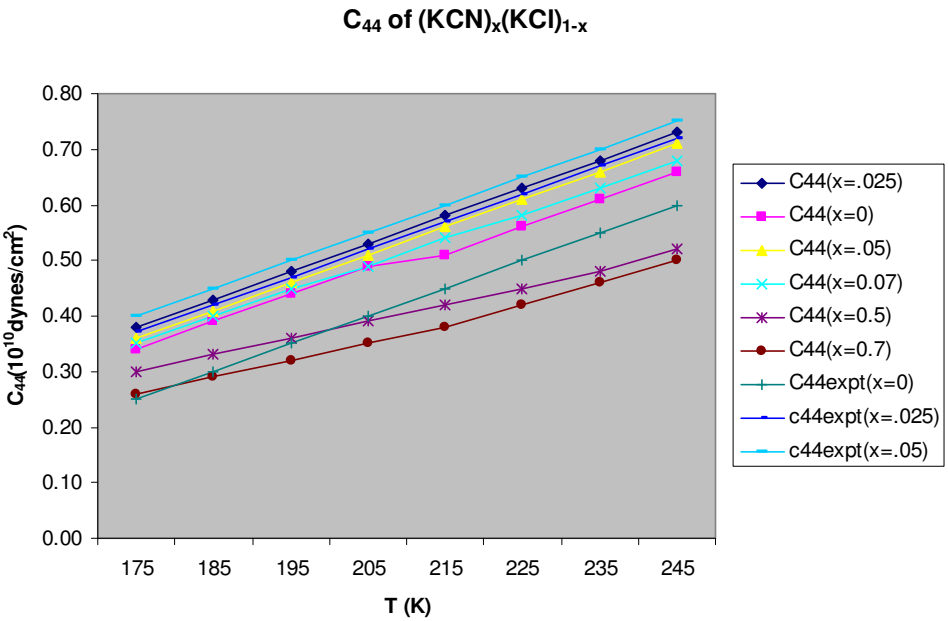

Figure 3. The variation of C_{44} with temperature for $(KCN)_x(KCl)_{1-x}$

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