Solutions:

S1. Consider a positive ion in the NaCl is surrounded by 26 neighbors (see Fig.1) . The first group of **6** *nearest* "central" neighbors have negative charges. They are located in distance **r** from the considered ion and their contribution is attractive:

$$V_{C0'}(r) = -6 \cdot k\frac{e^2}{r}$$

The next group of "central" neighbors are **12** ions standing in distance $\sqrt{r^2+r^2}=\sqrt{2}r$. All they have positive charge and act repulsively

$$V_{C0''}(r) = +\frac{12}{\sqrt{2}} \cdot k\frac{e^2}{r}$$

Easily to guess that the "vertex" **8** negative ions standing in distance $\sqrt{r^2+r^2+r^2}=\sqrt{3}r$ produce an attractive potential:

$$V_{C0'''}(r) = -\frac{8}{\sqrt{3}} \cdot k\frac{e^2}{r}$$

Having done summation of these contributions, we obtain the zero-order Coulomb potential

$$V_{C0}(r) = V_{C0'}(r) + V_{C0''}(r) + V_{C0'''}(r) = -\alpha_0 \cdot k\frac{e^2}{r}$$

where the approximate Madelung constant reads

$$\alpha_0 = 6 - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} \approx 2.134$$

S2. The net potential energy is the sum of attractive and repulsive exponential parts and reads

$$V_1(r) = V_{att} + V_{rep1} = -\alpha \cdot k\frac{e^2}{r} + \lambda \cdot e^{-r/\rho}$$

The condition for the equilibrium position r=r_0 is

$$F(r_0) = \frac{dV_1}{dr}(r_0) = -\alpha \cdot k\frac{e^2}{r_0^2} + \frac{\lambda}{\rho}e^{-r_0/\rho} = 0$$

Then, r_0 may be defined from

$$e^{-r_0/\rho} = \rho \cdot \frac{\alpha \cdot k \cdot e^2}{\lambda \cdot r_0^2}$$

The equilibrium potential is:

$$V_1(r_0) = -\alpha \cdot k\frac{e^2}{r_0}\left(1 - \frac{\rho}{r_0}\right)$$

S3. The dissociation energy corresponding to an ion (pair of atoms) is

$$E_{pair} = \frac{E_{dis}}{N_A} = \frac{-764\ [kJ/mole]}{6.022\cdot 10^{23}[1/mole]} \approx -1.269\cdot 10^{-18}[J]$$

This energy will be spent to overcome the potential energy $E_{pair} = V_1(r_0) = -k\cdot\alpha\frac{e^2}{r_0}\left(1-\frac{\rho}{r_0}\right)$

Then,

$$\frac{\rho}{r_0} = 1 + \frac{r_0 E_{pair}}{k\alpha e^2} \approx 1 - \frac{0.282\cdot 10^{-9}\cdot 1.269\cdot 10^{-18}}{9\cdot 10^9\cdot 1.7476\cdot\left(1.6\cdot 10^{-19}\right)^2} \approx 0.112...$$

Subsequently,

$$\rho = 0.112\cdot r_0 \approx 0.0316\cdot 10^{-9}[m]$$

This result is in good agreement with experimental data (see Table 2).

Crystal	r [nm]	ρ [nm]	E_{dis} $[kJ/mole]$
NaCl	0.282	0.032	-764.4
LiF	0.214	0.029	-1014.0
RbBr	0.345	0.034	-638.8

Table 2
Properties of Salt Crystals with the NaCl Structure [C.Kittel, "Introduction to Solid State Physics", N.Y., Wiley (1976) p.92]

S4. The repulsive inverse-power part leads to the following net potential

$$V_2(r) = V_{att} + V_{rep2} = -\alpha\cdot k\frac{e^2}{r} + \frac{b}{r^n}$$

The equilibrium position r= r_0 is defined from the zero-force condition

$$F(r_0) = \frac{dV_2(r_0)}{dr} = -\alpha\cdot k\frac{e^2}{r_0^2} - \frac{nb}{r_0^{n+1}} = 0$$

The equation for r_0 reads $r_0^{n-1} = \dfrac{b\cdot n}{\alpha\cdot k\cdot e^2}$

Then, $$V_2(r_0) = -\alpha\cdot k\frac{e^2}{r_0}\left(1-\frac{1}{n}\right) = V_{Coulomb}(r_0) + V_{Pauli}(r_0)$$

Here, the first term corresponds to the Coulomb potential and the second – to the Pauli's.

S5. Comparing with previous result (see **3.** and **4.**) we express the Born exponent

$$n = \frac{r_0}{\rho} \approx \frac{1}{0.112} \approx 9$$

With n=9 one finds that

$$V_{Coulomb}(r_0):V_{Pauli}(r_0)=1:(1/9)$$

The Coulomb and the Pauli potentials contribute to the net potential with a proportion 9:1. This result agrees well with experimental data (see, Table 3).

Ion type	n
Na^+, F^+	7
K^+, Cu^+, Cl^-	9
Au^+, I^+	12

Table 3. The experimental fit for the Born exponent.
[CRC Handbook of Physics, 2004]

S6. The ionization energy of the **Na** atom is **+5.14 eV** while the electron affinity of the **Cl** atom
is **-3.61 eV**. Subsequently, the electron transfer energy per atom is the half difference

$$E_{trans}\approx\frac{+5.14-3.61}{2}[\text{eV}]\approx+0.77[\text{eV}]$$

The total binding energy per atom in the NaCl crystal is:

$$E_{bind}=\frac{E_{pair}}{2}+E_{trans}=\frac{-1.269\cdot10^{-18}[\text{J}]}{2}+1.232\cdot10^{-19}[\text{J}]\approx\frac{-0.511\cdot10^{-18}[\text{J}]}{1.602\cdot10^{-19}[\text{J/eV}]}\approx-3.19[\text{eV}]$$

This estimate is in satisfactory agreement with the experimental result

$$E_{\exp}\approx-3.28[\text{eV}]$$

[*Marking Scheme*] Ionic Crystal, Yukawa-type Potential and Pauli Principle

Q	*Item*	*Answer*	*Points*
1.	*Attractive* Coulomb potential	$\boxed{V_{C0}(r)=V_{C0'}(r)+V_{C0''}(r)+V_{C0'''}(r)=-\alpha_0\cdot k\frac{e^2}{r}}$	*0.5*
	Madelung constant	$\alpha_0=6-\frac{12}{\sqrt{2}}+\frac{8}{\sqrt{3}}\approx 2.134$	*1.0*
2.	Equilibrium position	$F(r_0)=\frac{dV_1(r_0)}{dr}=-\alpha\cdot k\frac{e^2}{r_0^2}+\frac{\lambda}{\rho}e^{-r_0/\rho}=0$	*0.5*
	Net potential	$V_1(r_0)=-\alpha\cdot k\frac{e^2}{r_0}\left[1-\frac{\rho}{r_0}\right]$	*1.0*
3.	Pair energy	$E_{pair}=\frac{E_{dis}}{N_A}=\frac{\text{-764 }[kJ/mole]}{6.022\cdot 10^{22}[1/mole]}\approx -1.269\cdot 10^{-18}[J]$	*0.2*
	Equation for potential	$E_{pair}=V_1(r_0)=-k\alpha\frac{e^2}{r_0}\left[1-\frac{\rho}{r_0}\right]$	*0.9*
	Equation for range parameter	$\frac{\rho}{r_0}=1+\frac{r_0E_{pair}}{k\alpha e^2}\approx 1-\frac{0.282\cdot 10^{-9}\cdot 1.269\cdot 10^{-18}}{9\cdot 10^9\cdot 1.7476\cdot\left(1.6\cdot 10^{-19}\right)^2}\approx 0.112...$	*0.8*
	Range parameter	$\rho=0.112\cdot r_0\approx 0.0316\cdot 10^{-9}[m]$	*0.1*
4.	Equilibrium position	$F(r_0)=\frac{dV_2(r_0)}{dr}=-\alpha\cdot k\frac{e^2}{r_0^2}-\frac{nb}{r_0^{n+1}}=0$	*0.5*
	Equation for r_0	$r_0^{n-1}=\frac{b\cdot n}{\alpha\cdot k\cdot e^2}$	*0.5*
	Net potential	$V_2(r_0)=-\alpha\cdot k\frac{e^2}{r_0}\left[1-\frac{1}{n}\right]$	*1.0*
5.	Born exponent	$n=\frac{r_0}{\rho}\approx\frac{1}{0.112}\approx 9$	*1.2*
	Proportions	$V_{Coulomb}(r_0):V_{Pauli}(r_0)=1:(1/9)$	*0.3*
6.	Electron transfer energy	$E_{trans}\approx\frac{+5.14-3.61}{2}[\text{eV}]\approx +0.77[\text{eV}]$	*0.5*
	the total binding energy	$E_{bind}=\frac{E_{pair}}{2}+E_{trans}=\frac{\text{-1.269}\cdot 10^{-18}[\text{J}]}{2\cdot 1.602\cdot 10^{-19}[\text{J/eV}]}+0.77[\text{eV}]\simeq -3.19[\text{e}$	*1.0*
total			*10.0*