Diamond as {[C(+4)(2e)4/2}∞G}, structure of beta-Cristobalite, ES 1963/2012

```
Clear[k1,k2,sig1,sig2,c,Z,R1,R2];
c = {k1 -> 1.02118, k2 -> 1.3513, sig1 -> 0.306, sig2 -> 0.30515};
```

Prefacts as for hydrocarbons
```
Z=6.0; M=4.4394; EC=-1030.08;
```

He and Neon shell
```
T = 2.25*k1/R1^2+4.5*k2/R2^2 /. c;
Vee=3.0*sig1/R1+6.0*sig2/R2 /. c;
Vne=-3.0*Z/R1;
```
Madelung lattice energy
```
MadE = - M*(Z-2.0)/(R1+R2);
```

Total energy, to be minimized
```
Etot = T + Vee + Vne + MadE ;

t = FindMinimum[Etot, {R1,0.26}, {R2,1.2},{Method -> Automatic},{MaxIterations -> 500}]
```

Virial Ratio
```
N[-(Vee+Vne+MadE)/T /. c /. t[[2]],10]
```
Lattice constant, angstrom
```
N[2*0.529177*(R1+R2) /. t[[2]],10]
```
Lattice energy at 0 K, eV
```
Del = t[[1]]*27.2114-EC
```
Sublimation energy at 0 K, kJ/mol, kcal/mol
```
-Del*96.48532
-Del*23.06055
```
$\{-38.1253, \{R1 \to 0.260386, R2 \to 1.19799\}\}$

2.

1.54348

-7.36285

710.407

169.791