```
(* C3H8 Molekül nach Kimball, nicht überlappend,
   parametrisiert mit G2//6-311g *)

Clear[k1,k2,k3,s1,s2,s3];  n=3.;

(* Terme automatisch mit ChemEdu/Kimball/Alkan.sys *)

T=2.25*n*k1/P^2+(n-1.0)*2.25*k2/Q^2+4.5*(n+1.0)*k3/R^2;

p=X;  p2=p*p;  q=P+Q;  r=P+R;  q2=q*q;  r2=r*r;
r2p2=r2*p2;  r2p=r2*p;  qr=q*r; qrp=qr*p; z=6.; z2=z*z;
dd=32.0/3.0;  cd=19.0/3.0;  sd=16.0/3.0;
jd=10.0/3.0;  ad=8.0/3.0;  vd=4.0/3.0;  zd=2.0/3.0;

Vne = -3.0*n*z/P-2.0*(n+1.0)*(3.0-((p-1.0)*(1.0+P/R))^2)/R-
      16.0*z/r -16.0/r/p-8.0*z/2.0/q-
      20.0*z/Sqrt[vd*qr+4.0*q2+r2]-
      20.0/Sqrt[vd*qrp+r2p2+4.0*q2]-8.0*z/Sqrt[q2]-
      28.0/Sqrt[zd*r2p+r2p2+r2]-
      32.0/Sqrt[vd*qr+vd*qrp-zd*r2p+r2p2+4.0*q2+r2]-
      16.0/Sqrt[vd*qr+vd*qrp+2.0*r2p+r2p2+4.0*q2+r2]-
      20.0/Sqrt[zd*qrp+r2p2+q2]-4.0*z/Sqrt[dd*q2]-
       8.0*z/Sqrt[dd*q2+r2]-8.0/Sqrt[r2p2+dd*q2]-
       4.0*z/Sqrt[cd*q2]-4.0*z/Sqrt[sd*qr+dd*q2+r2]-
       4.0/Sqrt[sd*qrp+r2p2+dd*q2]-
       8.0/Sqrt[zd*r2p+r2p2+dd*q2+r2]-
       8.0/Sqrt[-2.0*r2p+r2p2+dd*q2+r2]-
       8.0/Sqrt[sd*qrp+zd*r2p+r2p2+dd*q2+r2]-
       8.0/Sqrt[zd*qrp+r2p2+cd*q2]-
       8.0/Sqrt[sd*qr+zd*r2p+r2p2+dd*q2+r2]-
       4.0/Sqrt[jd*qrp+r2p2+cd*q2]-
       4.0/Sqrt[sd*qr+sd*qrp+zd*r2p+r2p2+dd*q2+r2];

Vee =   3.0*n*s1/P+(n-1.0)*3.0*s2/Q+(n+1.0)*6.0*s3/R+32.0/r+
        8.0/2.0/q+40.0/Sqrt[vd*qr+4.0*q2+r2]+16.0/q+
       28.0/Sqrt[ad*r2]+32.0/Sqrt[ad*qr+4.0*q2+vd*r2]+
       16.0/Sqrt[ad*qr+4.0*q2+4.0*r2]+40.0/Sqrt[zd*qr+q2+r2]+
       12.0/Sqrt[dd*q2]+16.0/Sqrt[dd*q2+r2]+8.0/Sqrt[cd*q2]+
        8.0/Sqrt[sd*qr+dd*q2+r2]+8.0/Sqrt[dd*q2+ad*r2]+
       16.0/Sqrt[zd*qr+cd*q2+r2]+16.0/Sqrt[sd*qr+dd*q2+ad*r2]+
        4.0/Sqrt[ad*q2]+8.0/Sqrt[jd*qr+cd*q2+r2]+
        4.0/Sqrt[dd*qr+dd*q2+ad*r2];

Vnn =   8.0*z/r/p+2.0*z2/2.0/q+10.0*z/Sqrt[vd*qrp+r2p2+4.0*q2]+
        7.0/Sqrt[ad*r2p2]+8.0/Sqrt[ad*qrp+vd*r2p2+4.0*q2]+
        4.0/Sqrt[ad*qrp+4.0*r2p2+4.0*q2]+2.0/Sqrt[dd*q2]+
        z2/Sqrt[dd*q2]+4.0*z/Sqrt[r2p2+dd*q2]+
        2.0*z/Sqrt[sd*qrp+r2p2+dd*q2]+2.0/Sqrt[ad*r2p2+dd*q2]+
        4.0/Sqrt[sd*qrp+ad*r2p2+dd*q2]+
        1.0/Sqrt[dd*qrp+ad*r2p2+dd*q2];
```

```
func=T+Vne+Vee+Vnn;

(* Parameterliste c *)

c={k1 -> 1.02248824, k2 -> 1.37439662, k3 -> 1.20536809,
s1 -> 0.30582289, s2 -> 0.30680633, s3 -> 0.35440675 };

func = func /. c;

N[t = FindMinimum[func, {P,0.26134285}, {Q, 1.18367097},
                        {R, 1.2729},{X, 1.356986}], 10]
```

```
{-118.8560742,
 {P → 0.2613428497, Q → 1.183670966, R → 1.272899932, X → 1.356985998}}
```

```
u = t[[2]];
N[Vne /. u, 10]
```

```
-444.3496745
```

```
N[Vee /. u /. c, 10]
```

```
123.9627817
```

```
N[Vnn /. u, 10]
```

```
82.67474444
```

```
ch = X * (P + R) /. u;
dch = ch * 0.529177   (* C-H Abstand *)
```

```
1.10172
```

```
cc = 2. * (P + Q) /. u;
dcc = cc * 0.529177   (* C-C Abstand *)
```

```
1.52934
```

```
N[-(Vne + Vee + Vnn) / T /. u /. c, 10]  (* Virial Theorem *)
```

```
2.
```

```
(-t[[1]] - n * 37.784301 - n - 1.0) * 627.50956
(* Atomisierungsenergie bei 0 K in kcal/mol *)
```

```
943.254
```