```
(* C2H6 Molekül nach Kimball, nichtüberlappend,
 parametrisiert mit G2//6-311g *)

Clear[k1, k2, k3, s1, s2, s3]; n = 2.;

(* Terme aus 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; z = 6.; ad = 8. / 3.; zd = 2. / 3.; vd = 4. / 3.;
q = P + Q; r = P + R; q2 = q * q; r2 = r * r; r2p2 = r2 * p2;
r2p = r2 * p; qr = q * r; qrp = qr * p;

Vee = 3.0 * n * s1 / P + (n - 1.0) * 3.0 * s2 / Q
   + (n + 1.0) * 6.0 * s3 / R + 8.0 / Sqrt[q2]
   + 24.0 / Sqrt[zd * qr + q2 + r2]
   + 24.0 / Sqrt[r2] + 4.0 / Sqrt[4.0 * q2] + 24.0 / Sqrt[vd * qr + 4.0 * q2 + r2]
   + 24.0 / Sqrt[ad * r2] + 12.0 / Sqrt[ad * qr + 4.0 * q2 + 4.0 * r2]
   + 24.0 / Sqrt[ad * qr + 4.0 * q2 + vd * r2];

Vne = -2.0 * (n + 1.0) * (3.0 - ((p - 1.0) * (1.0 + P / R)) ^2) / R - 3.0 * n * z / P
   - 4.0 * z / Sqrt[q2] - 12.0 / Sqrt[zd * qrp + r2p2 + q2]
   - 12.0 * z / Sqrt[r2] - 12.0 / Sqrt[r2p2] - 4.0 * z / Sqrt[4.0 * q2]
   - 12.0 * z / Sqrt[vd * qr + 4.0 * q2 + r2] - 12.0 / Sqrt[vd * qrp + r2p2 + 4.0 * q2]
   - 24.0 / Sqrt[zd * r2p + r2p2 + r2]
   - 12.0 / Sqrt[vd * qr + vd * qrp + 2.0 * r2p + r2p2 + 4.0 * q2 + r2]
   - 24.0 / Sqrt[vd * qr + vd * qrp - zd * r2p + r2p2 + 4.0 * q2 + r2];

Vnn = 6.0 * z / Sqrt[r2p2] + z * z / Sqrt[4.0 * q2]
   + 6.0 * z / Sqrt[vd * qrp + r2p2 + 4.0 * q2] + 6.0 / Sqrt[ad * r2p2]
   + 3.0 / Sqrt[ad * qrp + 4.0 * r2p2 + 4.0 * q2]
   + 6.0 / Sqrt[ad * qrp + vd * r2p2 + 4.0 * q2];

func = T + Vne + Vee + Vnn;

(* Parameterliste c *)

c = {k1 -> 1.02246687, k2 -> 1.37426345, k3 -> 1.20537762, s1 -> 0.30582536,
  s2 -> 0.30677632, s3 -> 0.35441063};

func = func /. c;
```

```
N[t = FindMinimum[func, {P, 0.26141206}, {Q, 1.178240}, {R, 1.2709725},
  {X, 1.3575745}], 10]
```

$$\{-79.63122262, \{P \to 0.2614120646, Q \to 1.1782401, R \to 1.270972504, X \to 1.357574642\}\}$$

```
u = t[[2]];

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

$$-271.1254022$$

```
N[Vee /. u /. c, 9]
```

$$69.6604882$$

```
N[Vnn /. u, 8]
```

$$42.202469$$

```
ch = X * (P + R) /. u;

dch = ch * 0.529177 (* C-H Abstand *)
```

$$1.10086$$

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

$$1.52366$$

```
N[- (Vne + Vee + Vnn) / T /. u /. c, 9] (* Virial Theorem *)
```

$$2.00000001$$

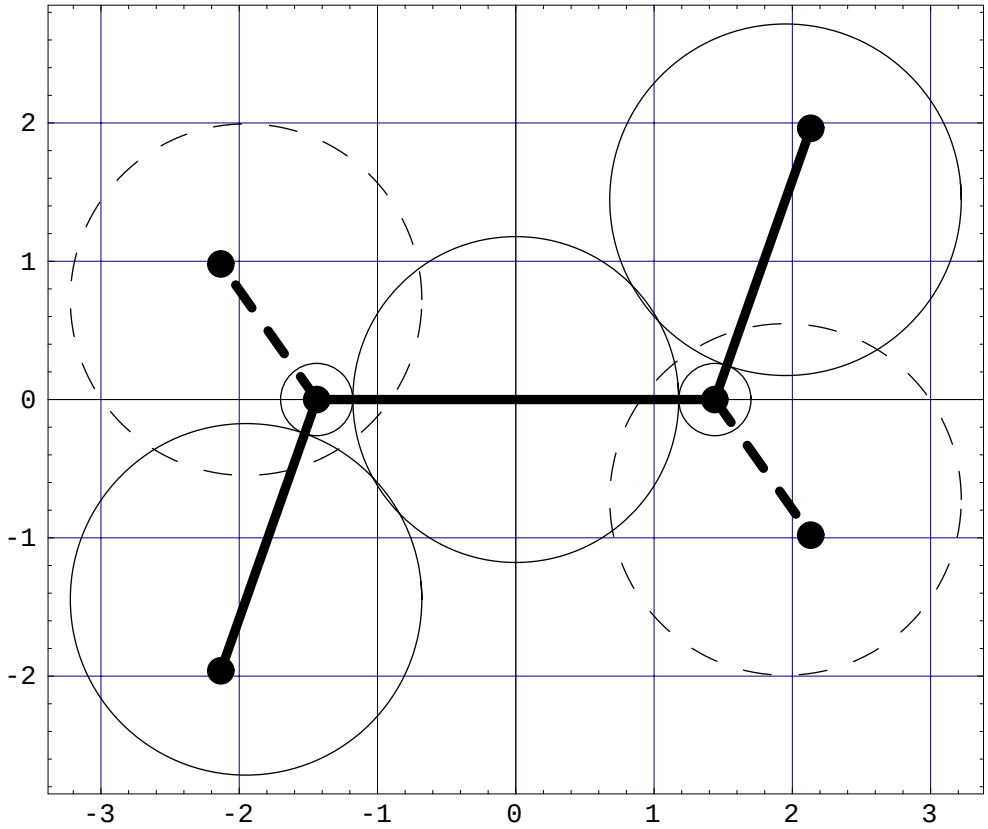
```
(-t[[1]] - n * 37.784301 - n - 1.0) * 627.50956
(* Atomisierungsenergie 0 K in kcal/mol *)
```

$$666.805$$

```
plot1 = Graphics[{Circle[{-(P + Q), 0}, P], Disk[{-(P + Q), 0}, 0.1],
   Circle[{P + Q, 0}, P], Disk[{P + Q, 0}, 0.1],
   Circle[{0, 0}, Q],
Circle[{-(P + Q) - (P + R) / 3. , -(P + R) * Sqrt[8. / 9.]}, R],
    Disk[{-(P + Q) - p * (P + R) / 3. , -p * (P + R) * Sqrt[8. / 9.]}, 0.1],
      Circle[{P + Q + (P + R) / 3. , (P + R) * Sqrt[8. / 9.]}, R],
    Disk[{(P + Q) + p * (P + R) / 3. , p * (P + R) * Sqrt[8. / 9.]}, 0.1],
      {Dashing[{0.03, 0.03}],
     Circle[{(P + Q) + (P + R) / 3., -(P + R) * Sqrt[2. / 9.]}, R],
    Disk[{P + Q + p * (P + R) / 3., -p * (P + R) * Sqrt[2.] / 3.}, 0.1],
     Circle[{-(P + Q) - (P + R) / 3., (P + R) * Sqrt[2. / 9.]}, R],
   Disk[{-(P + Q) - p * (P + R) / 3., p * (P + R) * Sqrt[2.] / 3.}, 0.1]},
   {Thickness[0.01], Line[{{-(P + Q), 0}, {P + Q, 0}}],
    Line[{{P + Q, 0}, {P + Q + p * (P + R) / 3., p * (P + R) * Sqrt[8. / 9.]}}],
     Line[{{-(P + Q), 0}, {-(P + Q) - p * (P + R) / 3., -p * (P + R) * Sqrt[8. / 9.]}}],
    {Dashing[{0.03, 0.03}],
       Line[{{P + Q, 0}, {P + Q + p * (P + R) / 3., -p * (P + R) * Sqrt[2. / 9.]}}],
      Line[{{-(P + Q), 0}, {-(P + Q) - p * (P + R) / 3., p * (P + R) * Sqrt[2. / 9.]}}]}]}]}]
   /. u
```

- Graphics -

```
Show[plot1, {AspectRatio -> Automatic, PlotRange -> All,
  Axes -> True, GridLines -> Automatic, Frame -> True}]
```



- Graphics -