

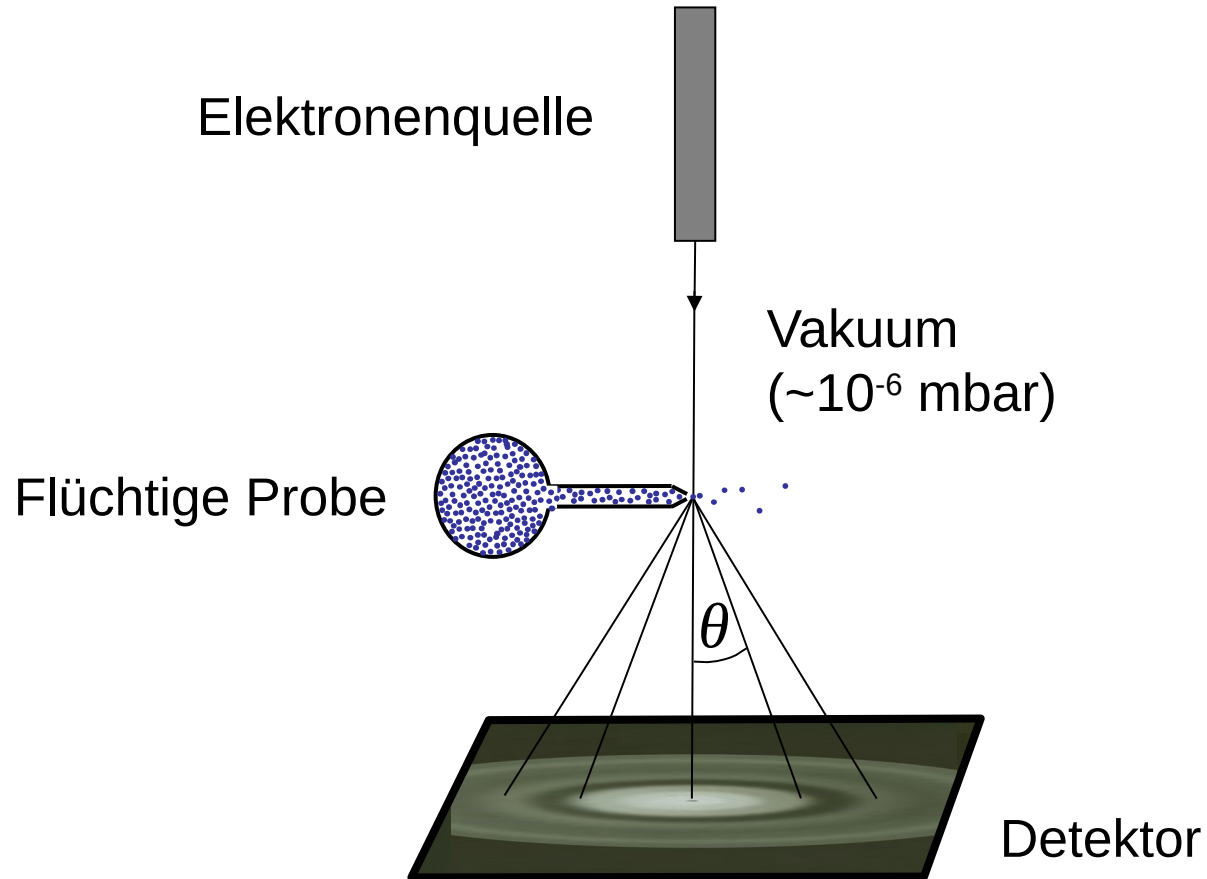
Nachrichten aus GED-Labor

Yury V. Vishnevskiy

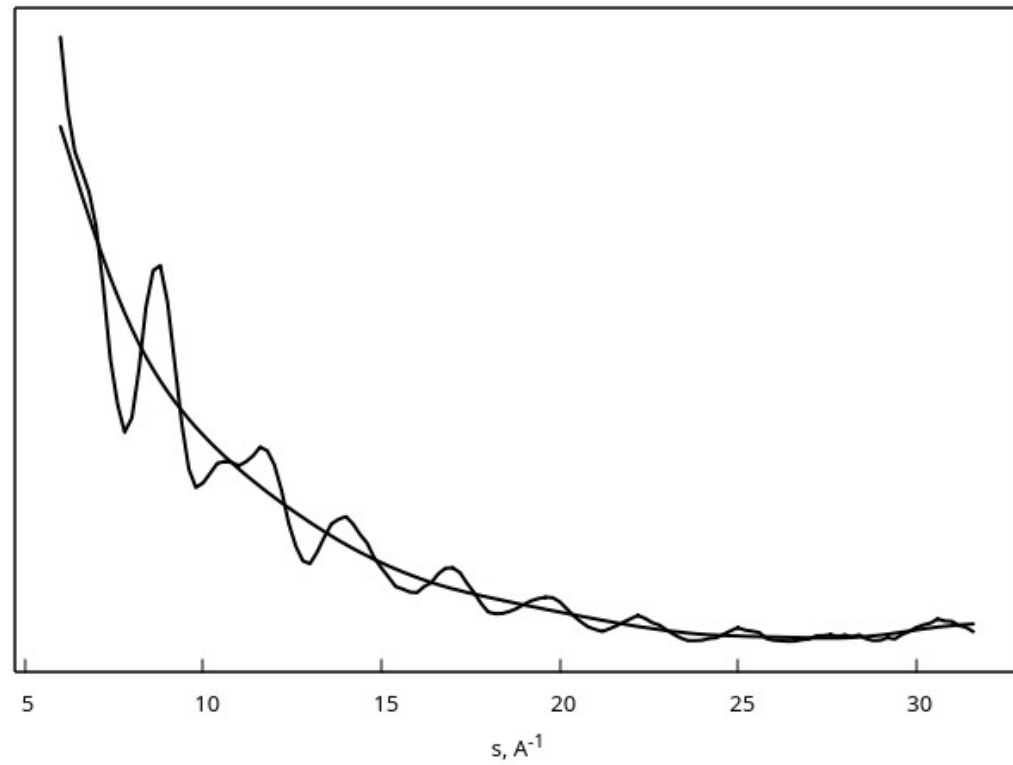
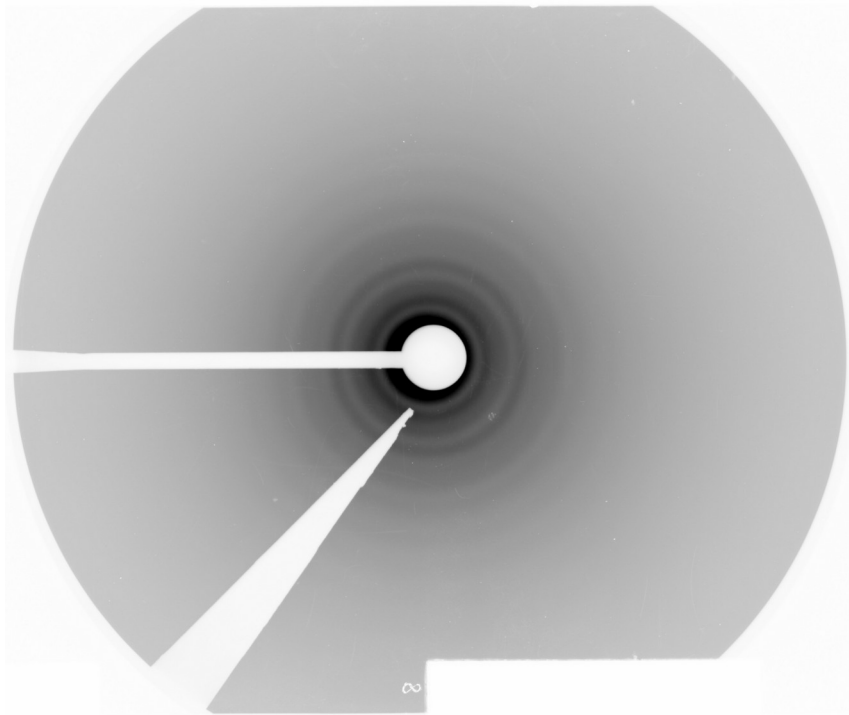
Uni-Bielefeld

2026

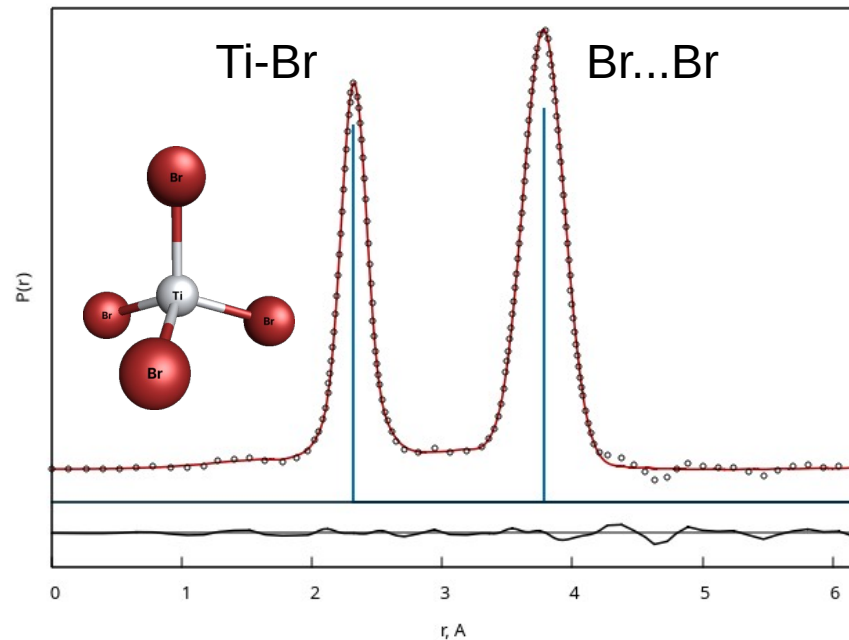
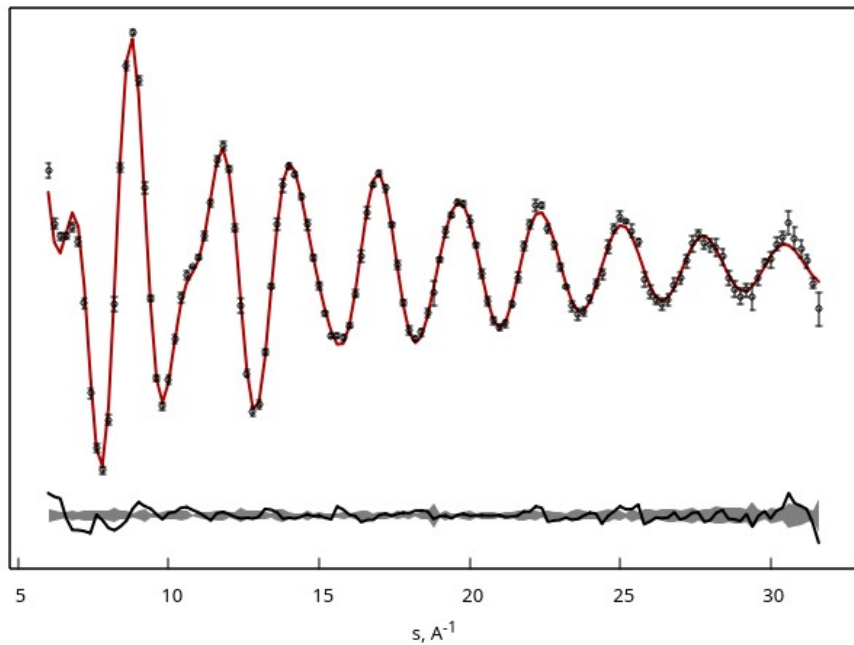
GED: prinzipielles Schema



Erste Daten: TiBr_4



Erste Daten: TiBr₄

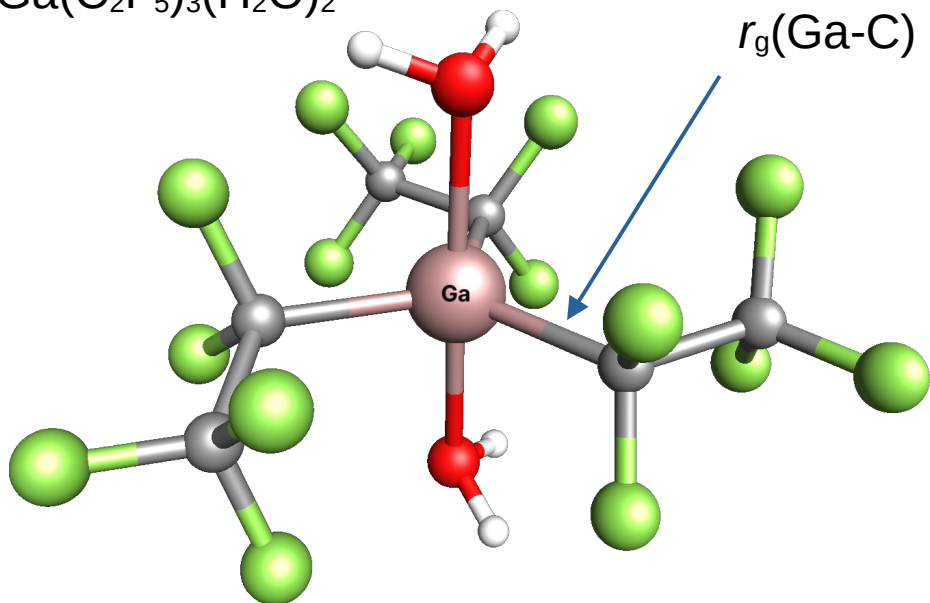
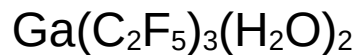


| Parameter | GED | Theorie |
|-------------------------------|-----------|---------|
| $r_e(\text{Ti-Br}), \text{Å}$ | 2.3100(5) | 2.3087 |
| $l(\text{Ti-Br}), \text{Å}$ | 0.063(1) | 0.053 |
| $l(\text{Br...Br}), \text{Å}$ | 0.143(1) | 0.150 |

$wR = 7.9 \%$

ae-CCSD(T)/cc-pwCVQZ-PP
PBE0-D3BJ/def2-QZVPP

Alte GED Daten und verdächtige $r(\text{Ga-C})$ aus Theorie



$$r_g(\text{Ga-C}) = 2.004(10) \text{ \AA} \quad \text{GED [1]}$$
$$2.072 \quad \text{Theorie [2]}$$

Vgl. GaMe_3 $r_g(\text{Ga-C}) = 1.967 \text{ \AA}$ GED [3]
1.982 Theorie [2]

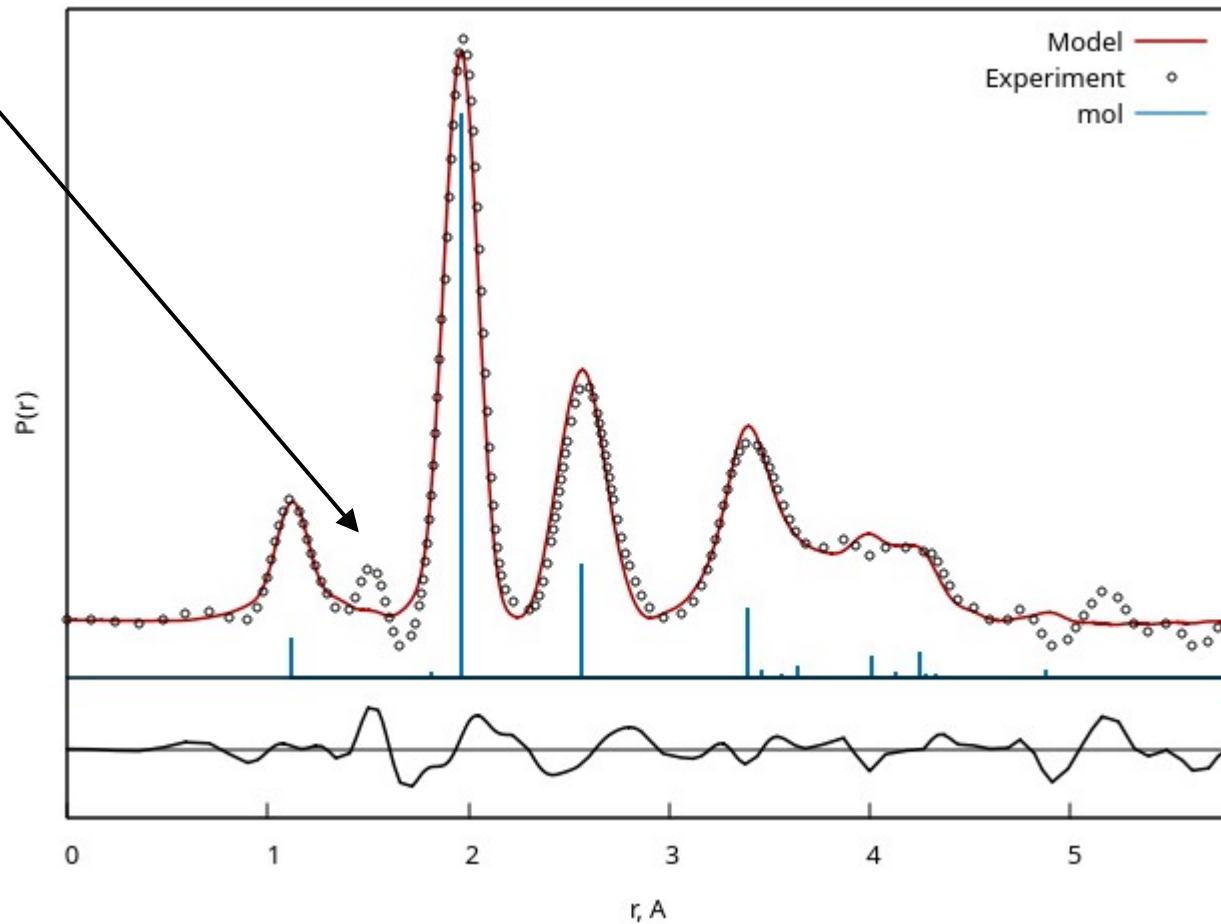
[1] K. Tölke, S. Porath, Y. V. Vishnevskiy, B. Neumann, H.-G. Stammer, N. W. Mitzel, B. Hoge, *Eur. J. Inorg. Chem.* **2024**, 27, e202300759.

[2] PBE0-D3BJ/def2-QZVPP

[3] B. Beagley, D. G. Schmidling, *J. Mol. Struct.* **1974**, 21, 437–444.

GaMe₃: GED@Bielefeld, Versuch 1

Verunreinigung
mit C-C ?

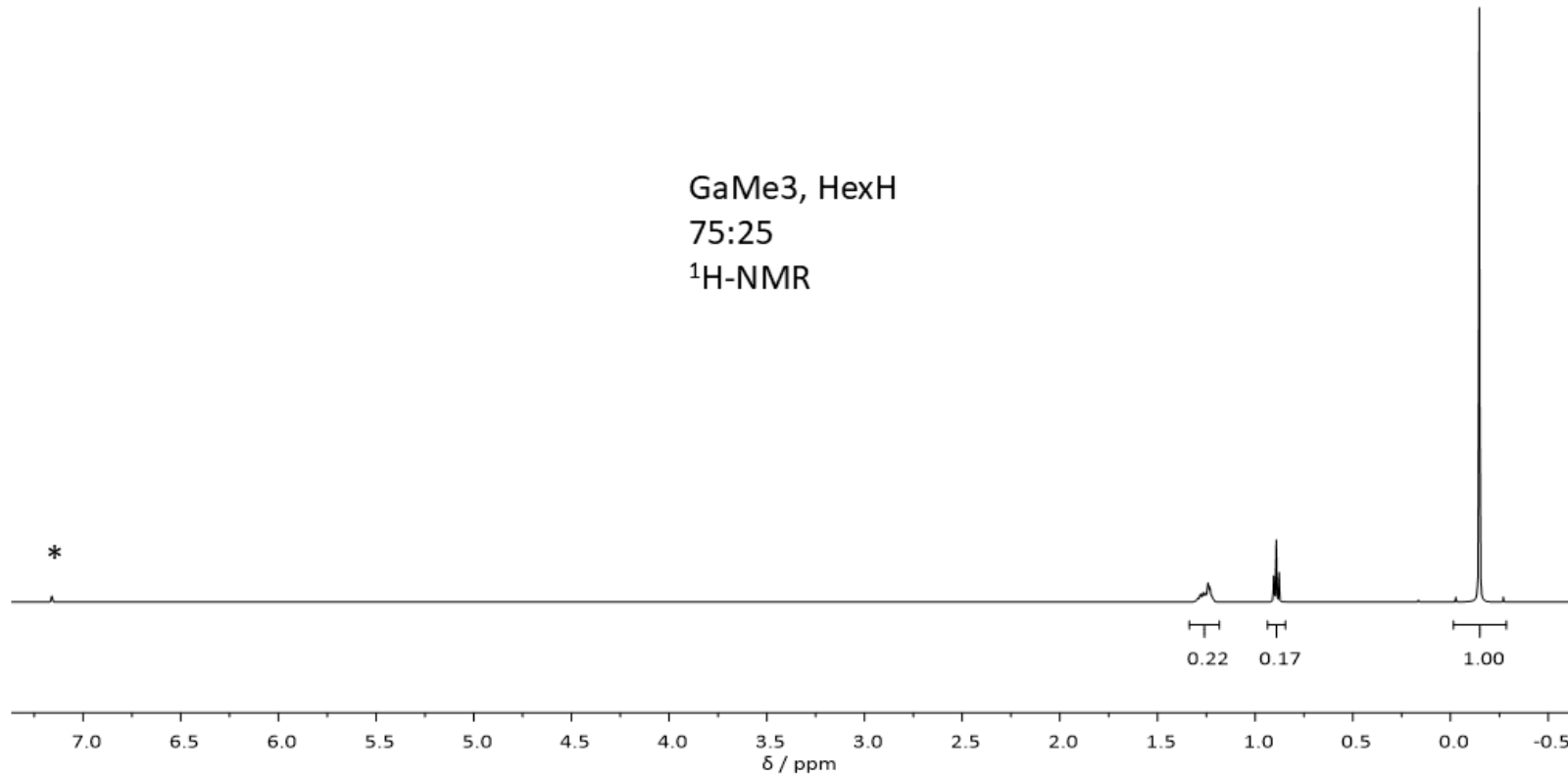


GaMe₃: GED@Bielefeld, Versuch 1

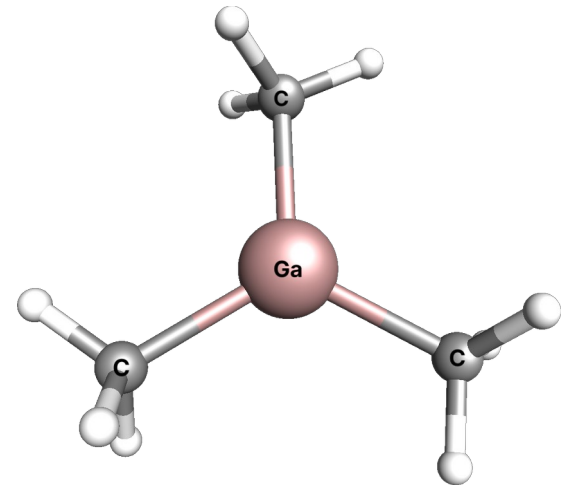
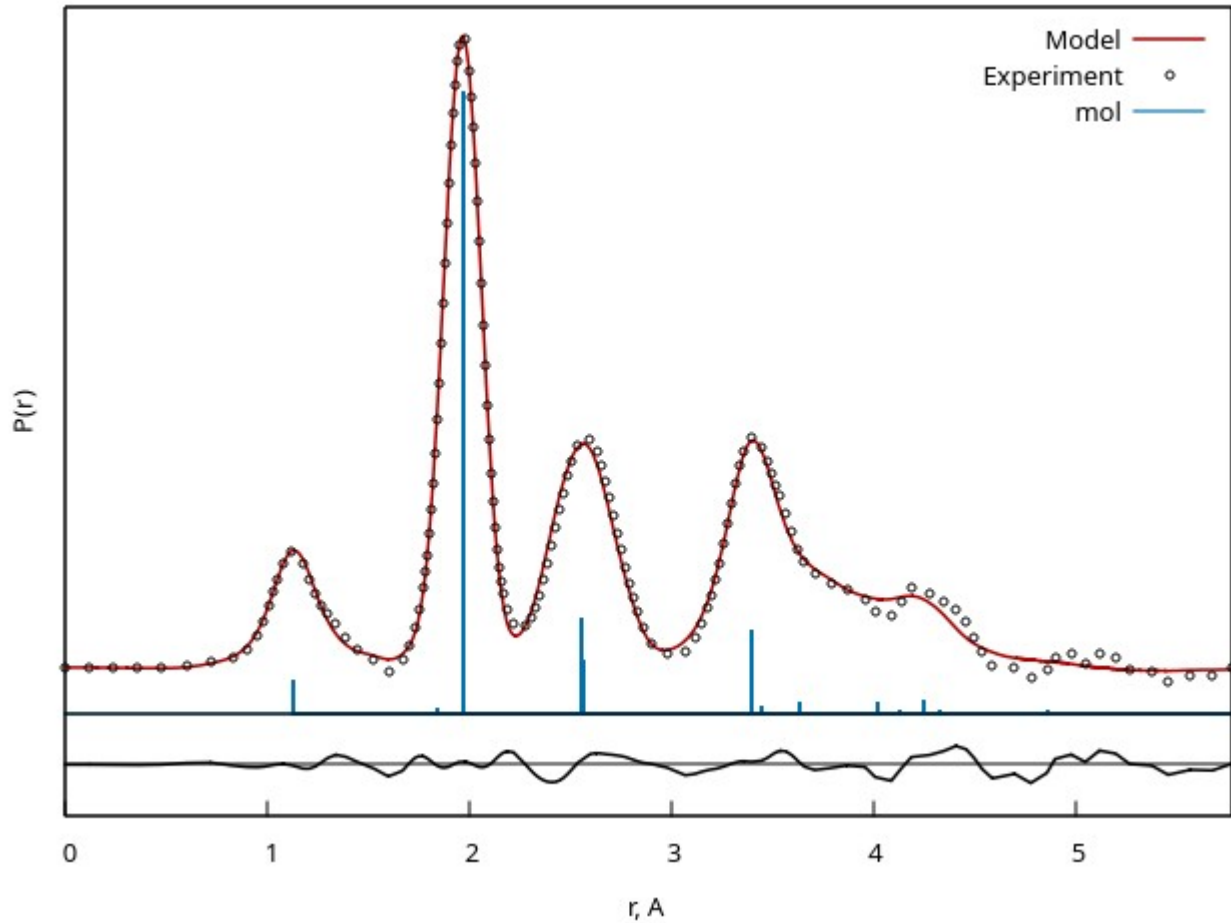
Verunreinigung ist n-Hexan 25%.

| | |
|--------|--------|
| C (d) | B (t) |
| 1.29 | 0.89 |
| J(7.5) | J(7.0) |

| |
|-------|
| A (s) |
| -0.15 |



GaMe₃: unsere neue GED Daten



$r_g(\text{Ga-C}) = 1.966(1) \text{ \AA}$
Vgl.: 1.967(2) Beagley et al.

Quelle des Fehlers: Hypothese

def2- Basen-Sätze:

| | | | | | | | | | | | | | | | | | | | | | | | | | | |
|--|---|---|---|--|--|---|---|--|--|--|--|---|---|--|---|---|--|--|---|---|--|---|---|---|---|--|
| 1 1.0080 H Hydrogen Nonmetal | | | | | | | | | | | | | | | | | 2 4.00260 He Helium Noble Gas | | | | | | | | | |
| 3 7.0 Li Lithium Alkali Metal | 4 9.012183 Be Beryllium Alkaline Earth Me... | | | | | | | | | | | 5 10.81 B Boron Metalloid | 6 12.011 C Carbon Nonmetal | 7 14.007 N Nitrogen Nonmetal | 8 15.999 O Oxygen Nonmetal | 9 18.9984... F Fluorine Halogen | 10 20.180 Ne Neon Noble Gas | | | | | | | | | |
| 11 22.989... Na Sodium Alkali Metal | 12 24.305 Mg Magnesium Alkaline Earth Me... | | | | | | | | | | | 13 26.981... Al Aluminum Post-Transition M... | 14 28.085 Si Silicon Metalloid | 15 30.973... P Phosphorus Nonmetal | 16 32.07 S Sulfur Nonmetal | 17 35.45 Cl Chlorine Halogen | 18 39.9 Ar Argon Noble Gas | | | | | | | | | |
| 19 39.0983 K Potassium Alkali Metal | 20 40.08 Ca Calcium Alkaline Earth Me... | 21 44.95591 Sc Scandium Transition Metal | 22 47.867 Ti Titanium Transition Metal | 23 50.9415 V Vanadium Transition Metal | 24 51.996 Cr Chromium Transition Metal | 25 54.93804 Mn Manganese Transition Metal | 26 55.84 Fe Iron Transition Metal | 27 58.93319 Co Cobalt Transition Metal | 28 58.693 Ni Nickel Transition Metal | 29 63.55 Cu Copper Transition Metal | 30 65.4 Zn Zinc Transition Metal | 31 69.723 Ga Gallium Post-Transition M... | 32 72.63 Ge Germanium Metalloid | 33 74.92159 As Arsenic Metalloid | 34 78.97 Se Selenium Nonmetal | 35 79.90 Br Bromine Halogen | 36 83.80 Kr Krypton Noble Gas | | | | | | | | | |
| 37 85.468 Rb Rubidium Alkali Metal | 38 87.62 Sr Strontium Alkaline Earth Me... | 39 88.90584 Y Yttrium Transition Metal | 40 91.22 Zr Zirconium Transition Metal | 41 92.90637 Nb Niobium Transition Metal | 42 95.95 Mo Molybdenum Transition Metal | 43 96.90636 Tc Technetium Transition Metal | 44 101.1 Ru Ruthenium Transition Metal | 45 102.9055 Rh Rhodium Transition Metal | 46 106.42 Pd Palladium Transition Metal | 47 107.868 Ag Silver Transition Metal | 48 112.41 Cd Cadmium Transition Metal | 49 114.818 In Indium Post-Transition M... | 50 118.71 Sn Tin Post-Transition M... | 51 121.760 Sb Antimony Metalloid | 52 127.6 Te Tellurium Metalloid | 53 126.9045 I Iodine Halogen | 54 131.29 Xe Xenon Noble Gas | | | | | | | | | |
| 55 132.90... Cs Cesium Alkali Metal | 56 137.33 Ba Barium Alkaline Earth Me... | | | | | | | | | | | 72 178.49 Hf Hafnium Transition Metal | 73 180.9479 Ta Tantalum Transition Metal | 74 183.84 W Tungsten Transition Metal | 75 186.207 Re Rhenium Transition Metal | 76 190.2 Os Osmium Transition Metal | 77 192.22 Ir Iridium Transition Metal | 78 195.08 Pt Platinum Transition Metal | 79 196.96... Au Gold Transition Metal | 80 200.59 Hg Mercury Transition Metal | 81 204.383 Tl Thallium Post-Transition M... | 82 207 Pb Lead Post-Transition M... | 83 208.98... Bi Bismuth Post-Transition M... | 84 208.98... Po Polonium Metalloid | 85 209.98... At Astatine Halogen | 86 222.01... Rn Radon Noble Gas |
| 87 223.01... Fr Francium Alkali Metal | 88 226.02... Ra Radium Alkaline Earth Me... | | | | | | | | | | | 104 267.1... Rf Rutherfordium Transition Metal | 105 268.1... Db Dubnium Transition Metal | 106 269.1... Sg Seaborgium Transition Metal | 107 270.1... Bh Bohrium Transition Metal | 108 269.1... Hs Hassium Transition Metal | 109 277.1... Mt Meitnerium Transition Metal | 110 282.1... Ds Darmstadtium Transition Metal | 111 282.1... Rg Roentgenium Transition Metal | 112 286.1... Cn Copernicium Transition Metal | 113 286.1... Nh Nihonium Post-Transition M... | 114 290.1... Fl Flerovium Post-Transition M... | 115 290.1... Mc Moscovium Post-Transition M... | 116 293.2... Lv Livermorium Post-Transition M... | 117 294.2... Ts Tennessine Halogen | 118 295.2... Og Oganesson Noble Gas |
| | | 57 138.9055 La Lanthanum Lanthanide | 58 140.116 Ce Cerium Lanthanide | 59 140.90... Pr Praseodymium Lanthanide | 60 144.24 Nd Neodymium Lanthanide | 61 144.91... Pm Promethium Lanthanide | 62 150.4 Sm Samarium Lanthanide | 63 151.964 Eu Europium Lanthanide | 64 157.2 Gd Gadolinium Lanthanide | 65 158.92... Tb Terbium Lanthanide | 66 162.500 Dy Dysprosium Lanthanide | 67 164.93... Ho Holmium Lanthanide | 68 167.26 Er Erbium Lanthanide | 69 168.93... Tm Thulium Lanthanide | 70 173.05 Yb Ytterbium Lanthanide | 71 174.9668 Lu Lutetium Lanthanide | | | | | | | | | | |
| | | 89 227.02... Ac Actinium Actinide | 90 232.038 Th Thorium Actinide | 91 231.03... Pa Protactinium Actinide | 92 238.0289 U Uranium Actinide | 93 237.04... Np Neptunium Actinide | 94 244.06... Pu Plutonium Actinide | 95 243.06... Am Americium Actinide | 96 247.07... Cm Curium Actinide | 97 247.07... Bk Berkelium Actinide | 98 251.07... Cf Californium Actinide | 99 252.0830 Es Einsteinium Actinide | 100 257.0... Fm Fermium Actinide | 101 258.0... Md Mendelevium Actinide | 102 259.1... No Nobelium Actinide | 103 266.1... Lr Lawrencium Actinide | | | | | | | | | | |

“all-electron” ohne ECP

← Relativistik !

mit ECP

Hypothese testen

$$\Delta r = r(\text{Theorie mit def2-}) - r(\text{Experiment})$$

?



13 26.981...
Al
Aluminum
Post-Transition M...

31 69.723
Ga
Gallium
Post-Transition M...

49 114.818
In
Indium
Post-Transition M...

30 65.4
Zn
Zinc
Transition Metal

32 72.63
Ge
Germanium
Metalloid

$\text{GaMe}_3 \Delta r(\text{Ga-C}) = \mathbf{0.015 \text{ \AA}}$
(GED Daten/Verfeinerung)

$\text{GaCN} \Delta r(\text{Ga-C}) = \mathbf{0.011 \text{ \AA}}$
(Lit. MW Daten,
unsere Verfeinerung)

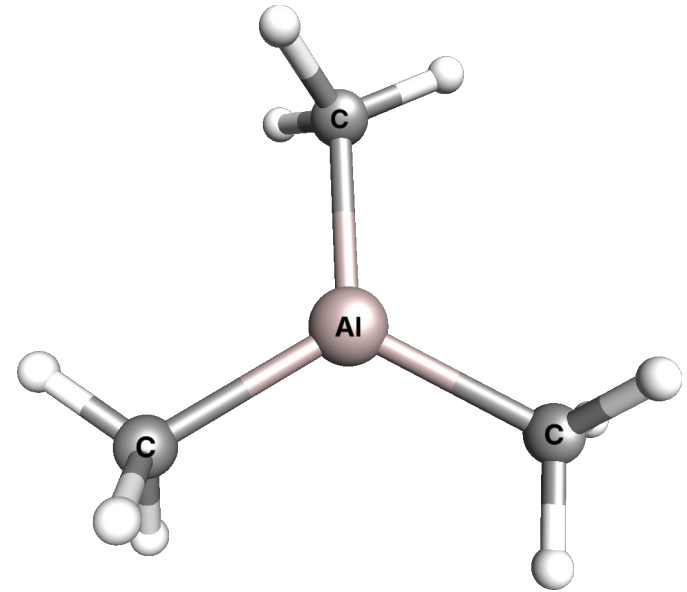
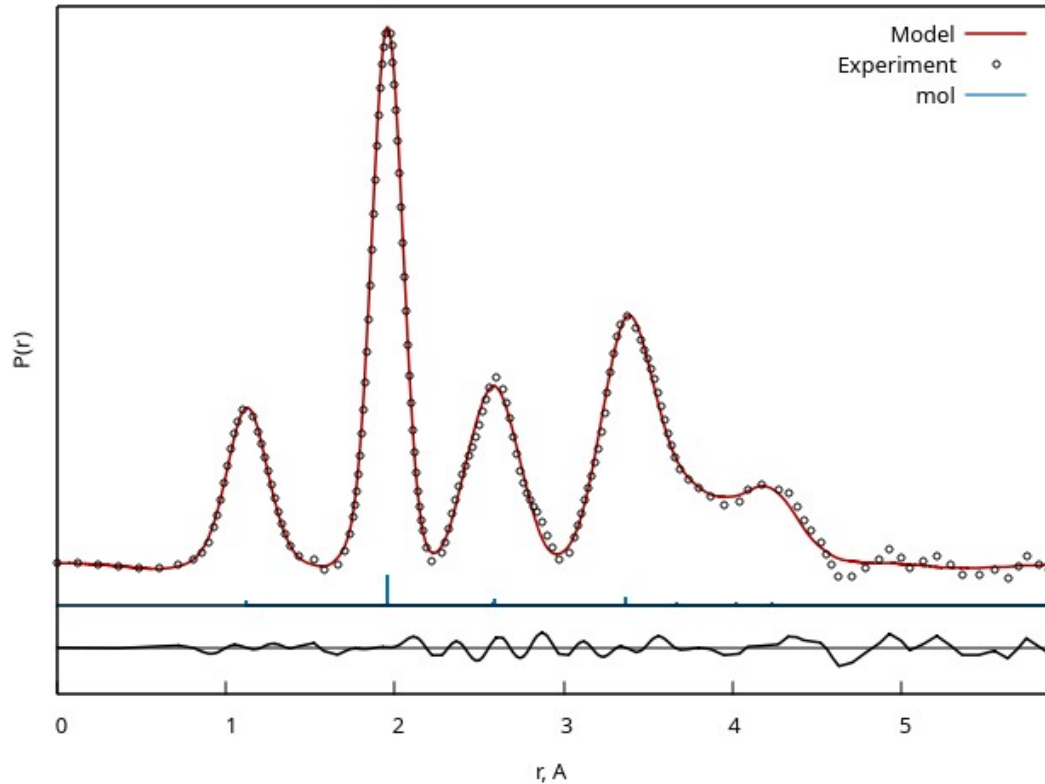
$\text{H}_3\text{C-GeH}_3 \Delta r(\text{Ge-C}) = \mathbf{0.009 \text{ \AA}}$
(Lit. MW Daten,
unsere Verfeinerung)

$\text{H-Zn-CH}_3 \Delta r(\text{Zn-C}) = \mathbf{0.015 \text{ \AA}}$
(Lit. MW Daten,
unsere Verfeinerung)

?

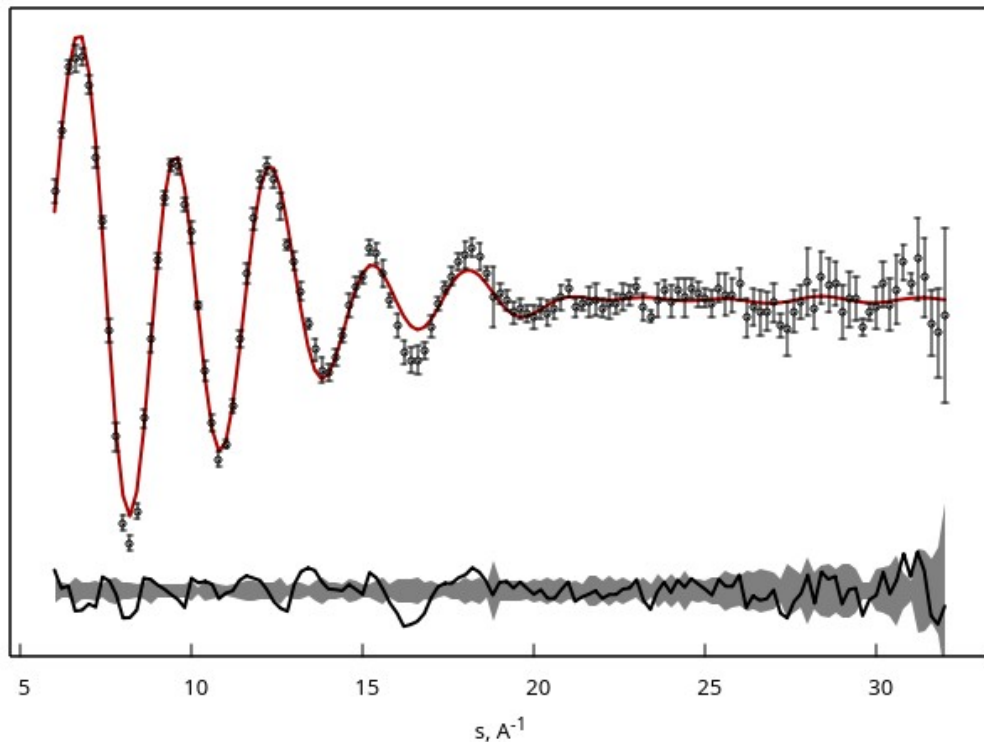


AlMe₃: unsere GED Daten



$r_a(\text{Al-C}) = 1.953(1) \text{ \AA}$
Vgl.: 1.957(3) Almenningen et al. [1]

InMe₃: unsere GED Daten

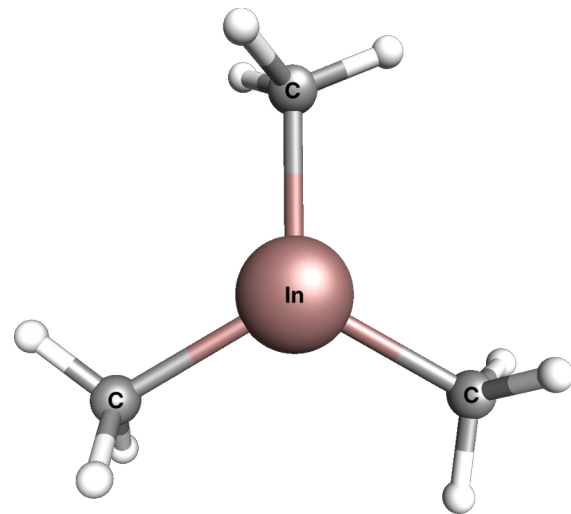
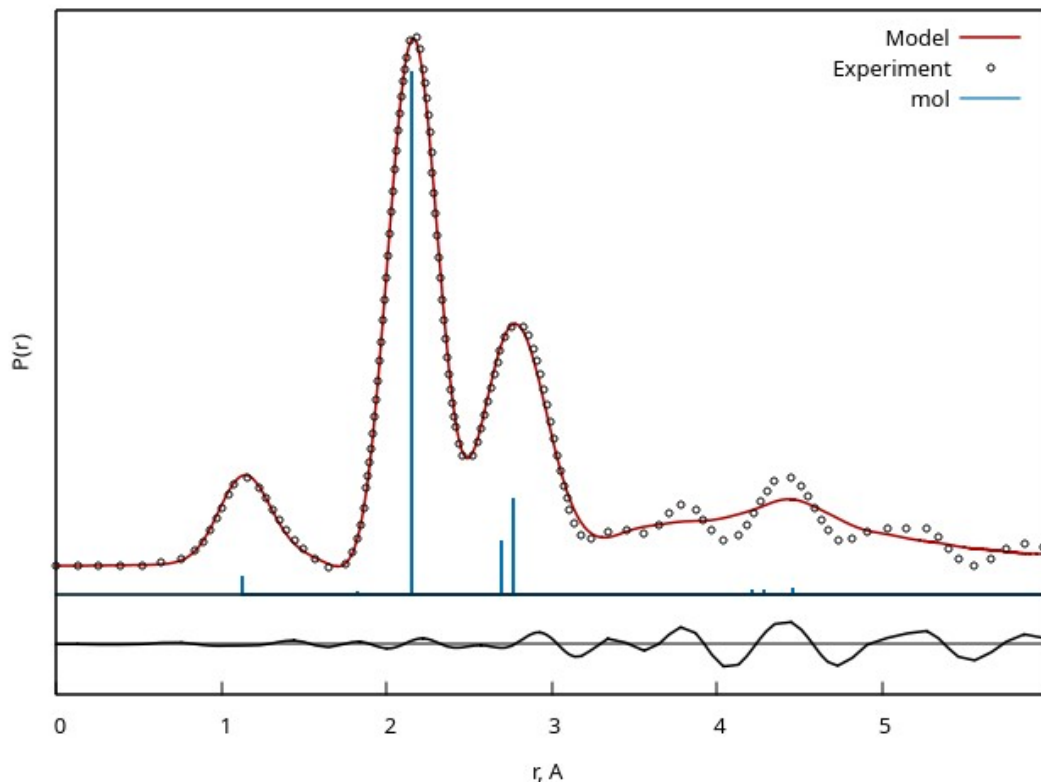


Kein Signal ab $s = 20 \text{ \AA}^{-1}$!

Gleiches Problem in:

T. Fjeldberg, A. Haaland, R. Seip, Q. Shen, J. Weidlein, V. P. Spiridonov, T. G. Strand, *Acta Chem. Scand.* **1982**, 36a, 495.

InMe₃: unsere GED Daten



$r_a(\text{In-C}) = 2.153(2) \text{ \AA}$
Vgl.: 2.161(3) Fjeldberg et al. [1]

[1] T. Fjeldberg, A. Haaland, R. Seip, Q. Shen, J. Weidlein, V. P. Spiridonov, T. G. Strand, *Acta Chem. Scand.* **1982**, 36a, 495.

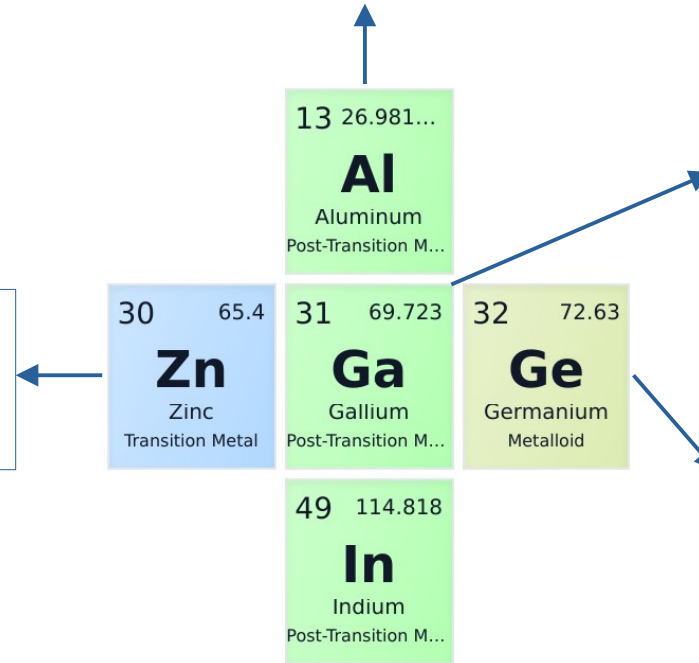
Theorie-Genauigkeit in Al → Ga → In und Zn → Ga → Ge

$\text{AlMe}_3 \Delta r(\text{Al-C}) = \mathbf{0.011 \text{ \AA}}$ oder $\mathbf{0.007 \text{ \AA}}$
(unsere Daten/Verfeinerung) (Lit.)

$\text{GaMe}_3 \Delta r(\text{Ga-C}) = \mathbf{0.015 \text{ \AA}}$
(unsere Daten/Verfeinerung)

$\text{GaCN} \Delta r(\text{Ga-C}) = \mathbf{0.011 \text{ \AA}}$
(Lit. MW Daten,
unsere Verfeinerung)

$\text{H-Zn-CH}_3 \Delta r(\text{Zn-C}) = \mathbf{0.015 \text{ \AA}}$
(Lit. MW Daten,
unsere Verfeinerung)



$\text{H}_3\text{C-GeH}_3 \Delta r(\text{Ge-C}) = \mathbf{0.009 \text{ \AA}}$
(Lit. MW Daten,
unsere Verfeinerung)

$\text{InMe}_3 \Delta r(\text{In-C}) = \mathbf{0.017 \text{ \AA}}$ oder $\mathbf{0.009 \text{ \AA}}$
(unsere Daten/Verfeinerung) (Lit.)

Statistik für *R*-Faktoren

| Substanz | Str. <i>R</i> -faktor, % | Exp. <i>R</i> -Faktor, % |
|-------------------|--------------------------|--------------------------|
| TiBr ₄ | 7.9 | 5.1 |
| GaMe ₃ | 8.6 | 5.2 |
| InMe ₃ | 9.5 | 5.2 |
| AlMe ₃ | 16.5 | 16.7 |

- Messdaten sind am meistens von hoher Qualität.
- Modelle müssen verbessert werden:
 - Dynamik von CH₃-Gruppen in AlMe₃, GaMe₃ und InMe₃.
 - Punkt-Beugung → Volumen-Beugung.