Nachrichten aus GED-Labor

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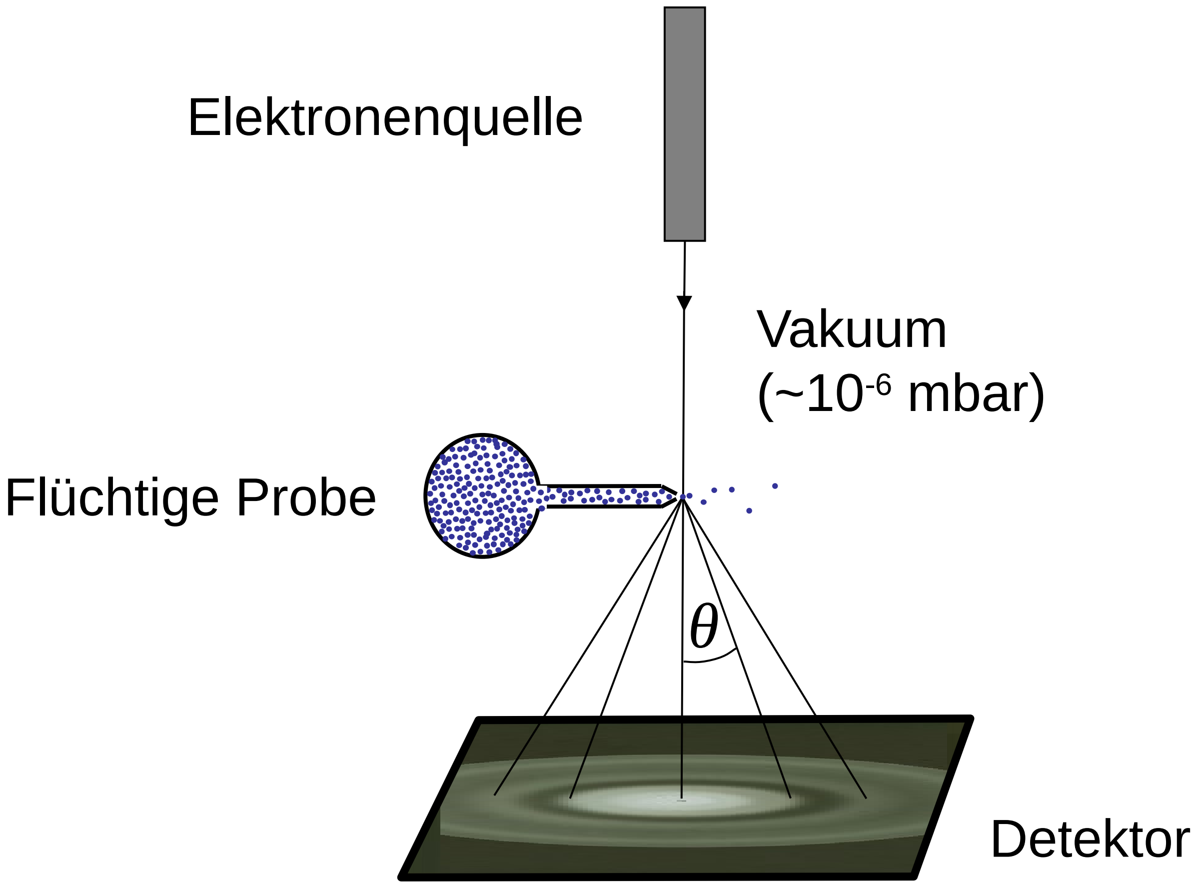
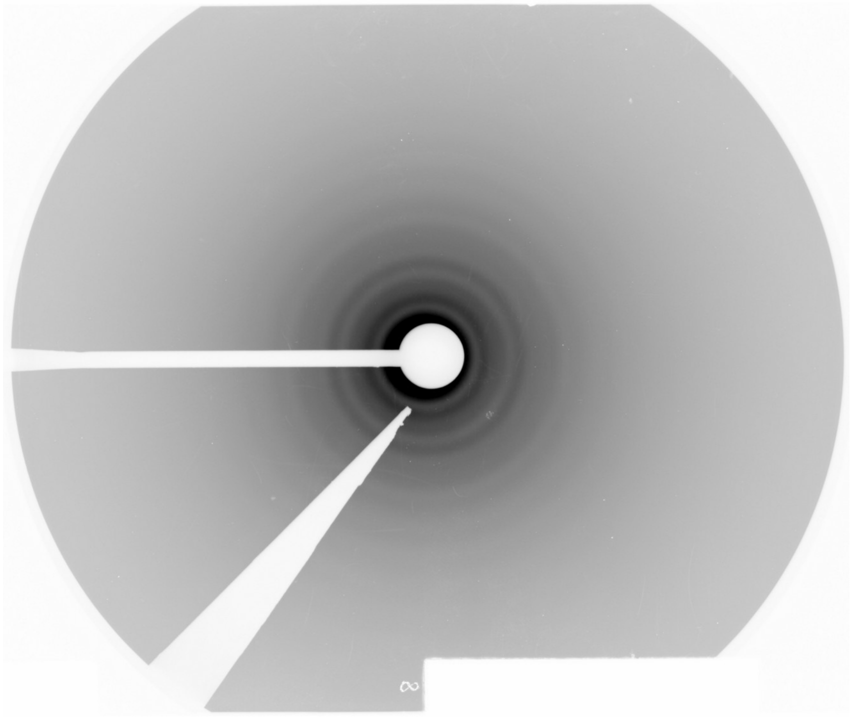
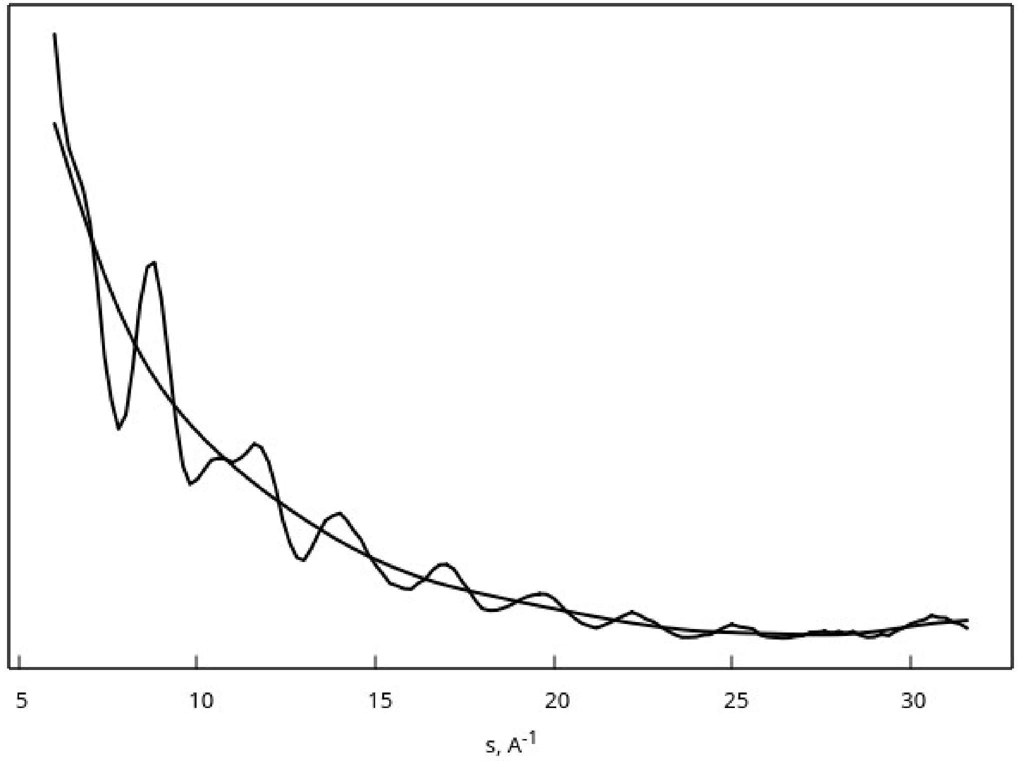
GED: prinzipielles Schema

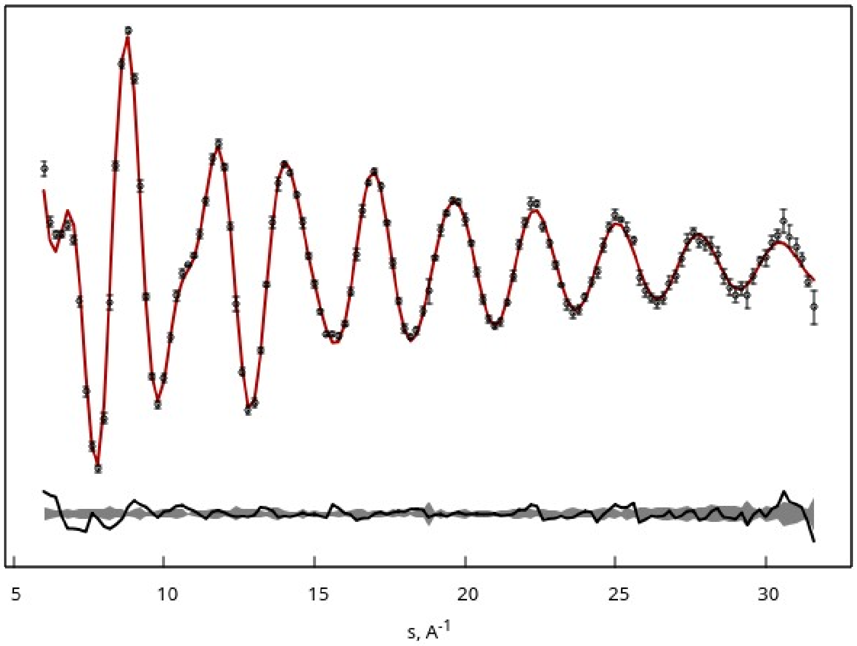


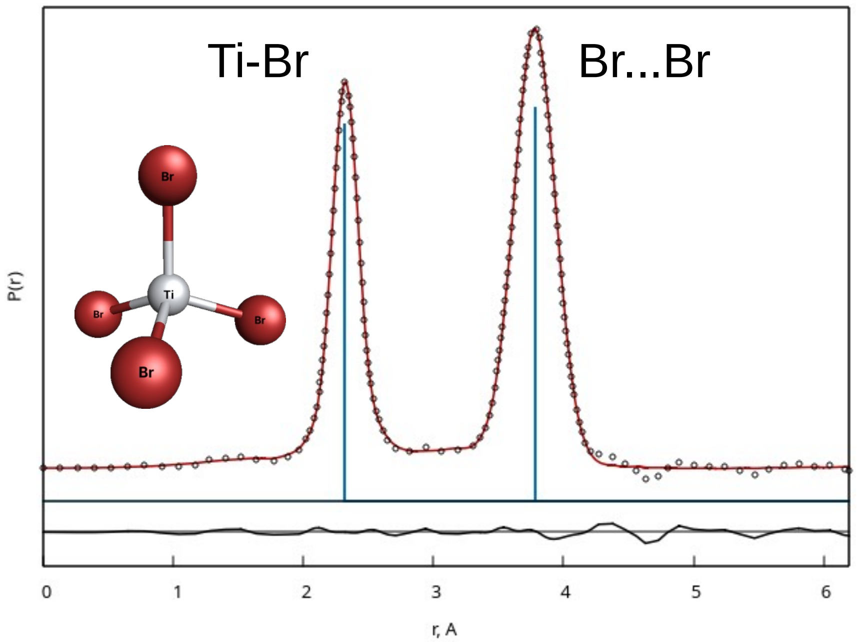
Erste Daten: $TiBr_4$





Erste Daten: $TiBr_4$





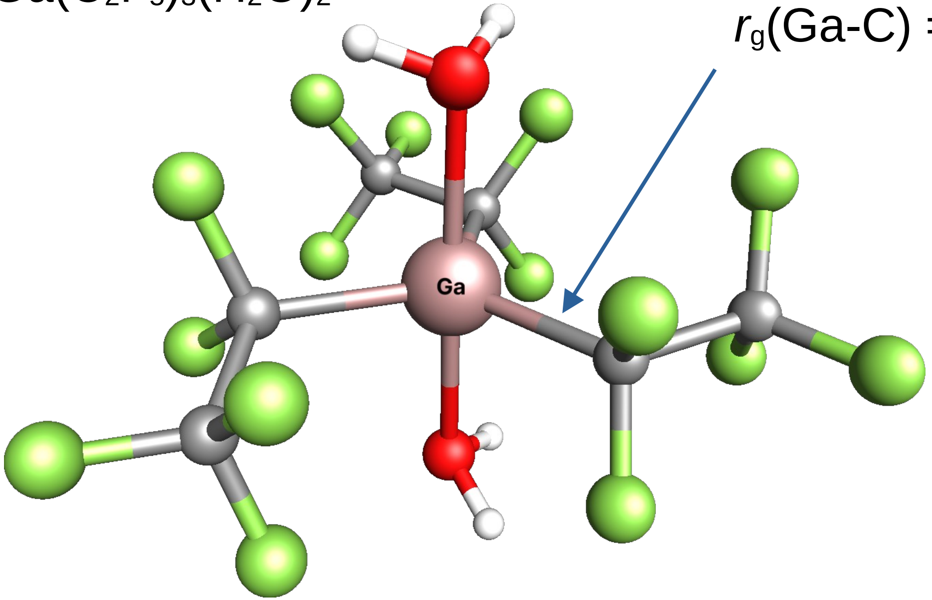
Parameter	GED	Theorie
r_e(Ti-Br), Å	2.3100(5)	2.3087
l(Ti-Br), Å	0.063(1)	0.053
l(Br...Br), Å	0.143(1)	0.150

wR = 7.9 %

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

Alte GED Daten und verdächtige r(Ga-C) aus Theorie

$Ga(C_2F_5)_3(H_2O)_2$



r_g(Ga-C) = 2.004(10) Å GED [1]
2.072 Theorie [2]

Vgl. $GaMe_3$ r_g(Ga-C) = 1.967 Å GED [3]
1.982 Theorie [2]

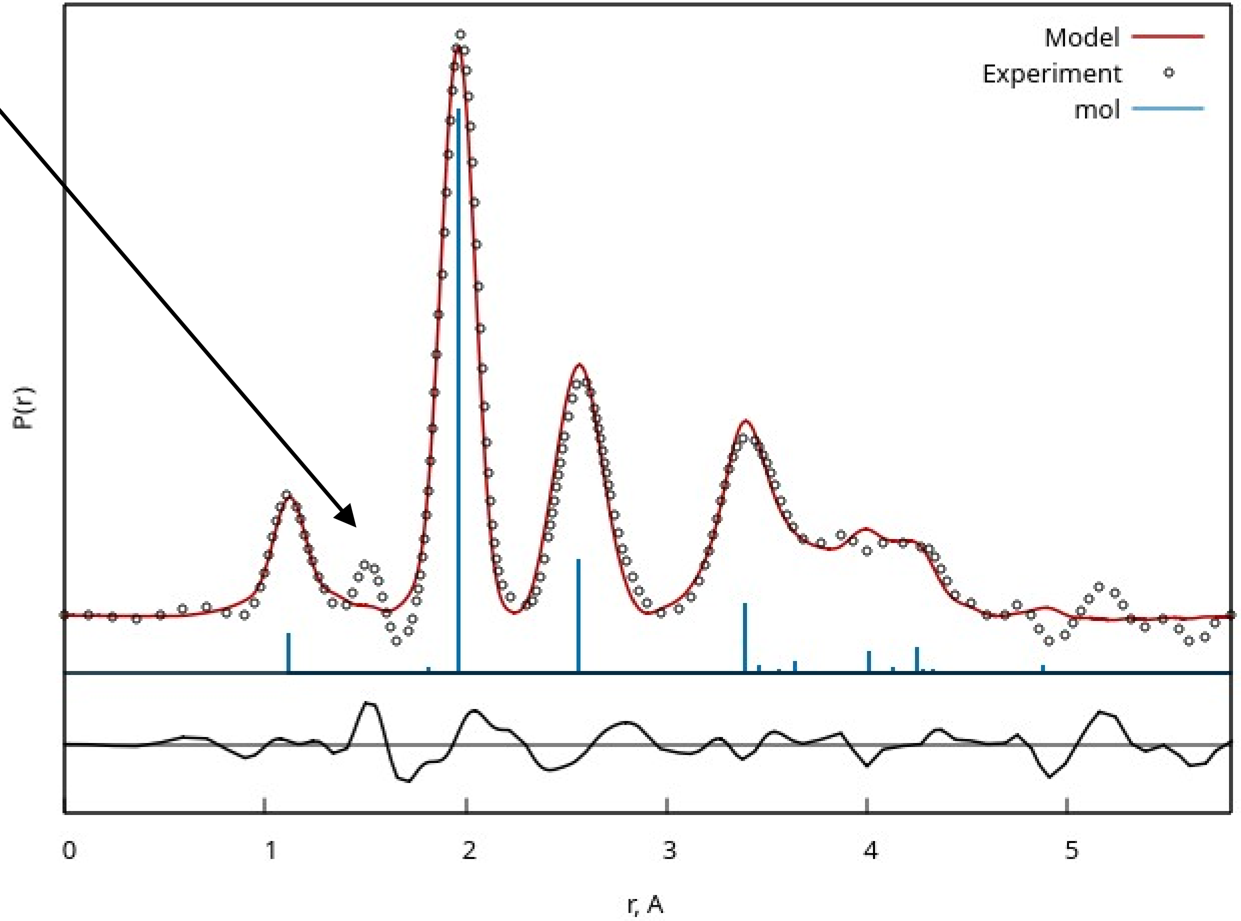
[1] K. Tölke, S. Porath, Y. V. Vishnevskiy, B. Neumann, H.-G. Stammler, N. W. Mitzel, B. Hoge, *Eur. J. Inorg. Chem.* **2024**, 27, e202300759.

[2] PBE0-D3BJ/def2-QZVPP

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

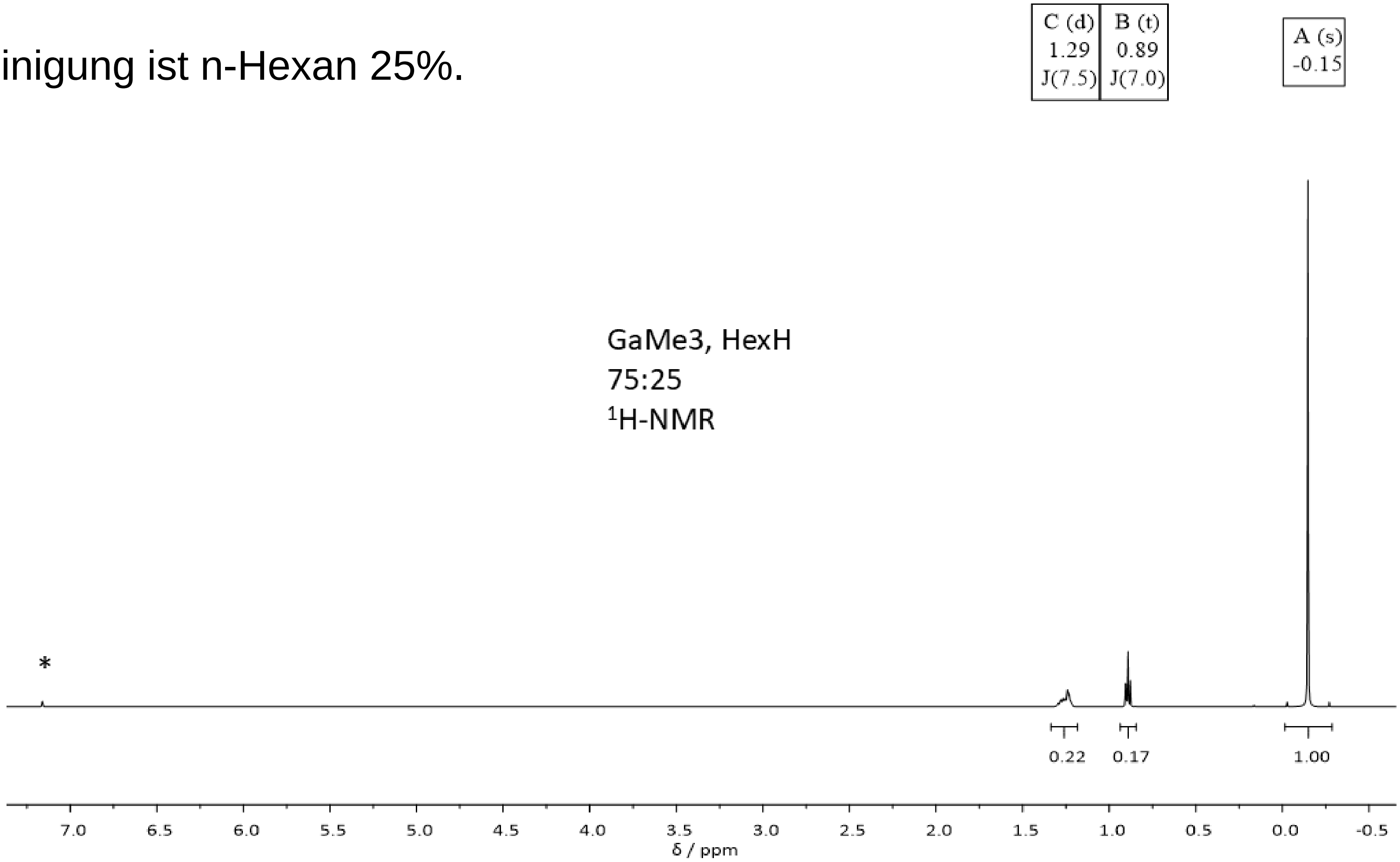
$GaMe_3$: GED@Bielefeld, Versuch 1

Verunreinigung
mit C-C ?

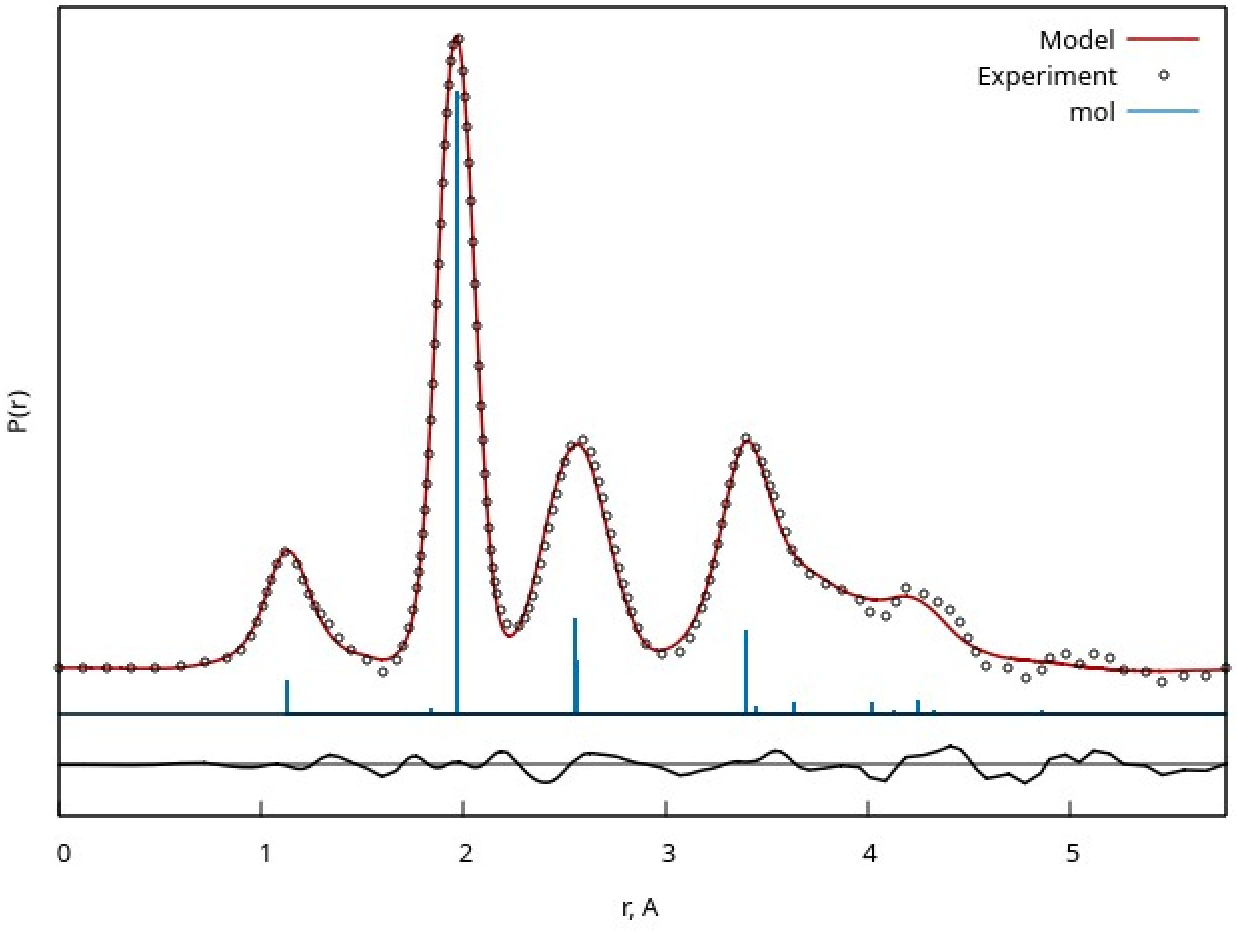


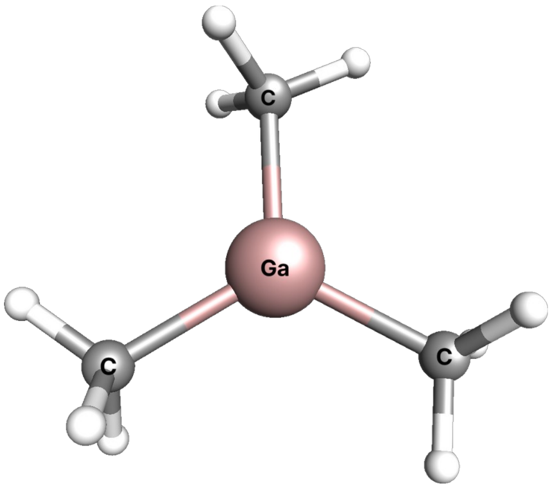
$GaMe_3$: GED@Bielefeld, Versuch 1

Verunreinigung ist n-Hexan 25%.



$GaMe_3$: unsere neue GED Daten

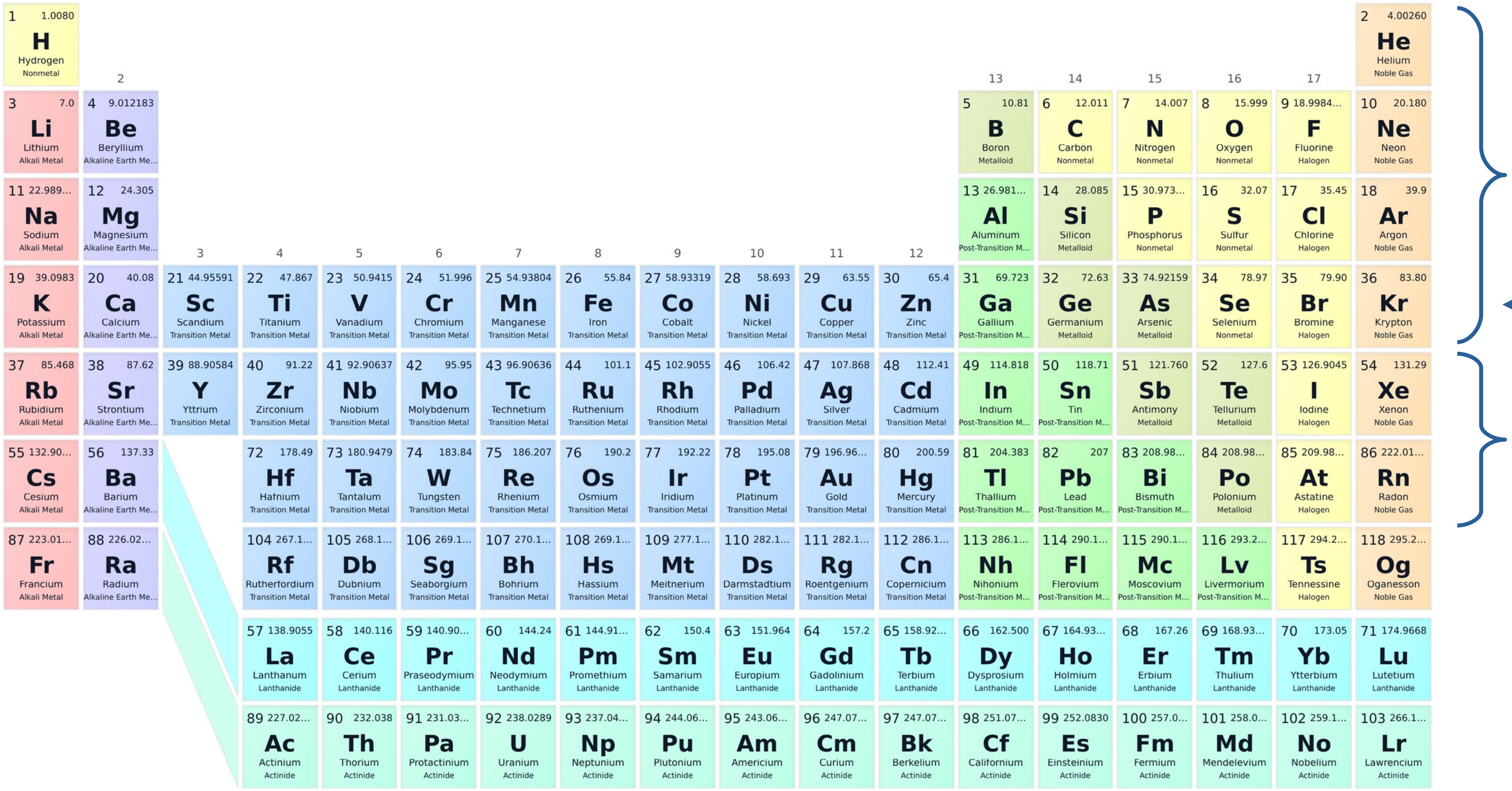




r_g(Ga-C) = 1.966(1) Å
Vgl.: 1.967(2) Beagley et al.

Quelle des Fehlers: Hypothese

def2- Basen-Sätze:



“all-electron” ohne ECP

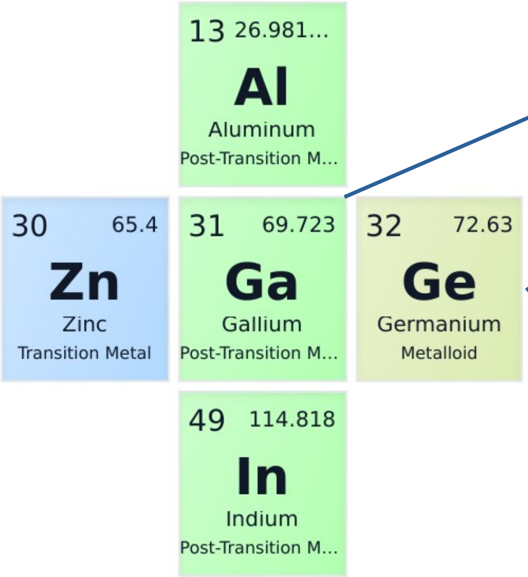
Relativistik !

mit ECP

Hypothese testen

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

?



?

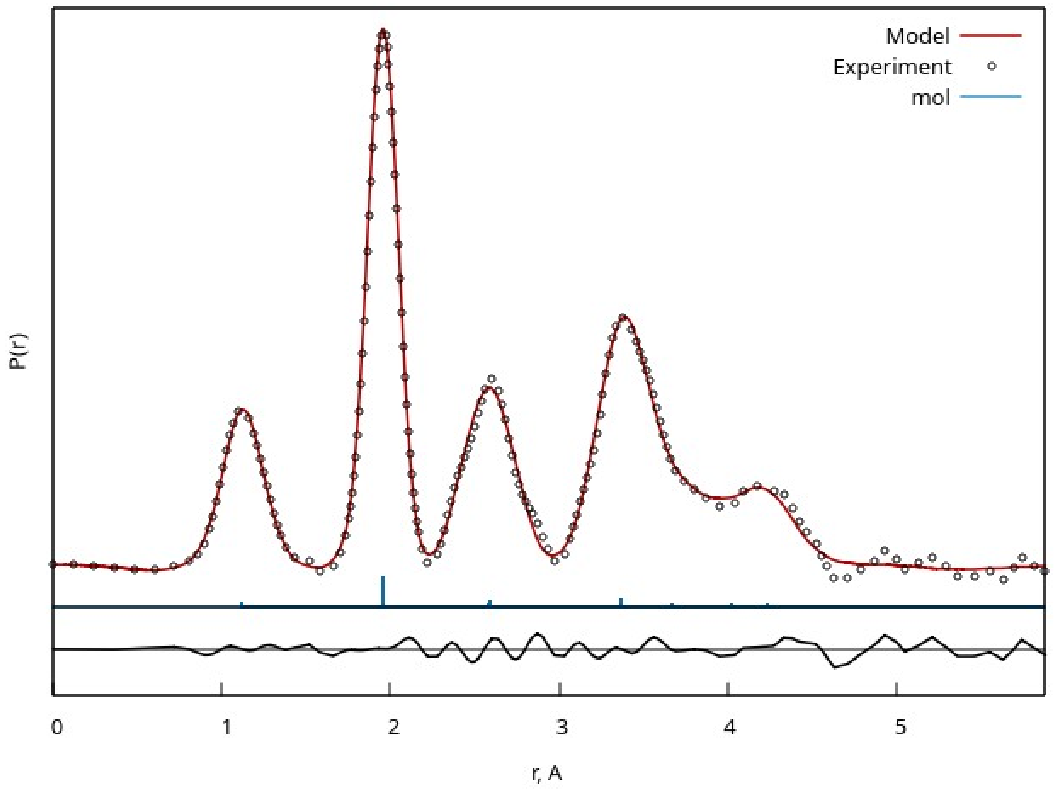
H-Zn-CH_3 Δr(Zn-C) = **0.015** Å
(Lit. MW Daten,
unsere Verfeinerung)

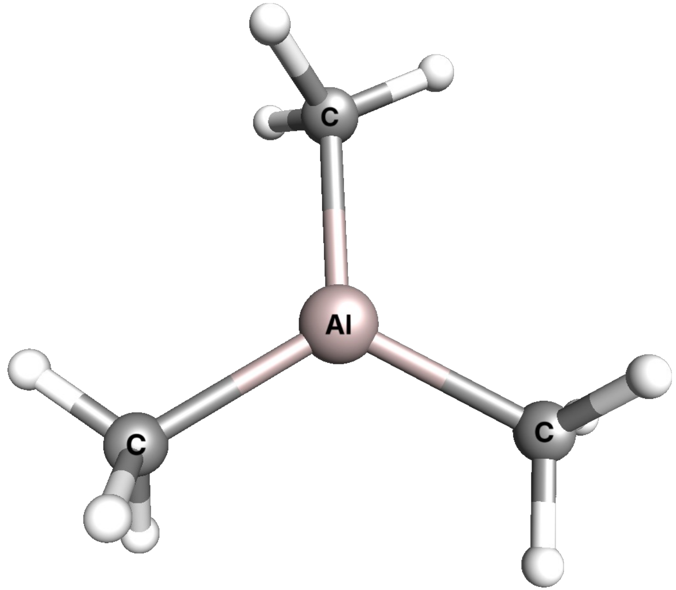
$GaMe_3$ Δr(Ga-C) = **0.015** Å
(GED Daten/Verfeinerung)

GaCN Δr(Ga-C) = **0.011** Å
(Lit. MW Daten,
unsere Verfeinerung)

H_3C-GeH_3 Δr(Ge-C) = **0.009** Å
(Lit. MW Daten,
unsere Verfeinerung)

$AlMe_3$: unsere GED Daten

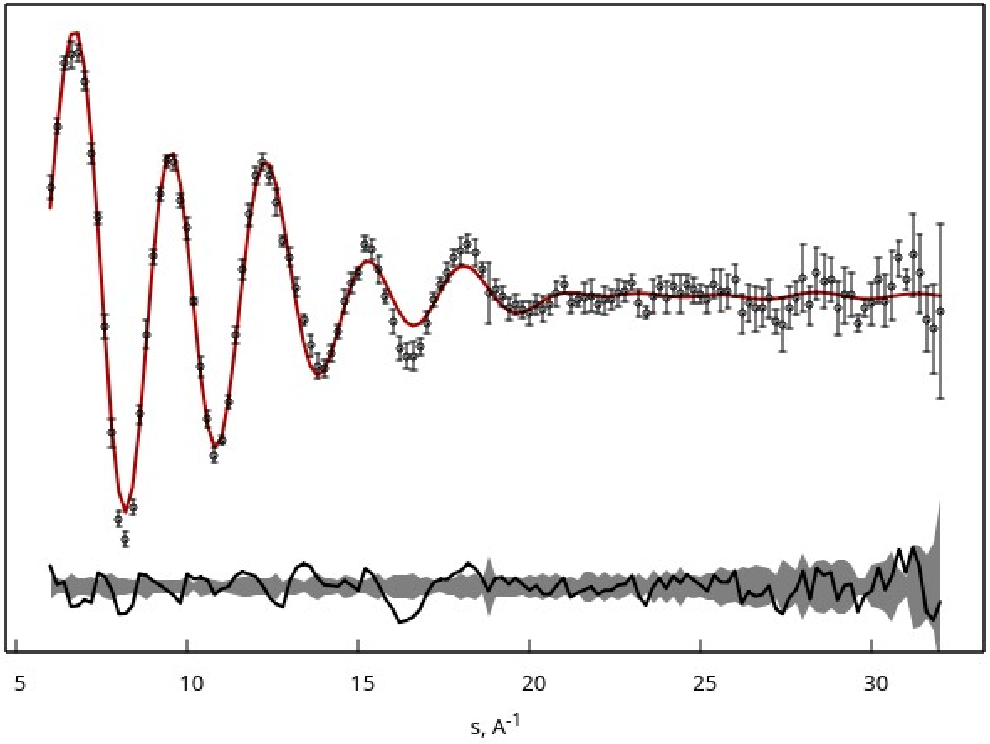




r_a(Al-C) = 1.953(1) Å
Vgl.: 1.957(3) Almenningen et al. [1]

[1] A. Almenningen, S. Halvorsen, A. Haaland, *Acta Chem. Scand.* **1971**, 25, 1937.

$InMe_3$: unsere GED Daten

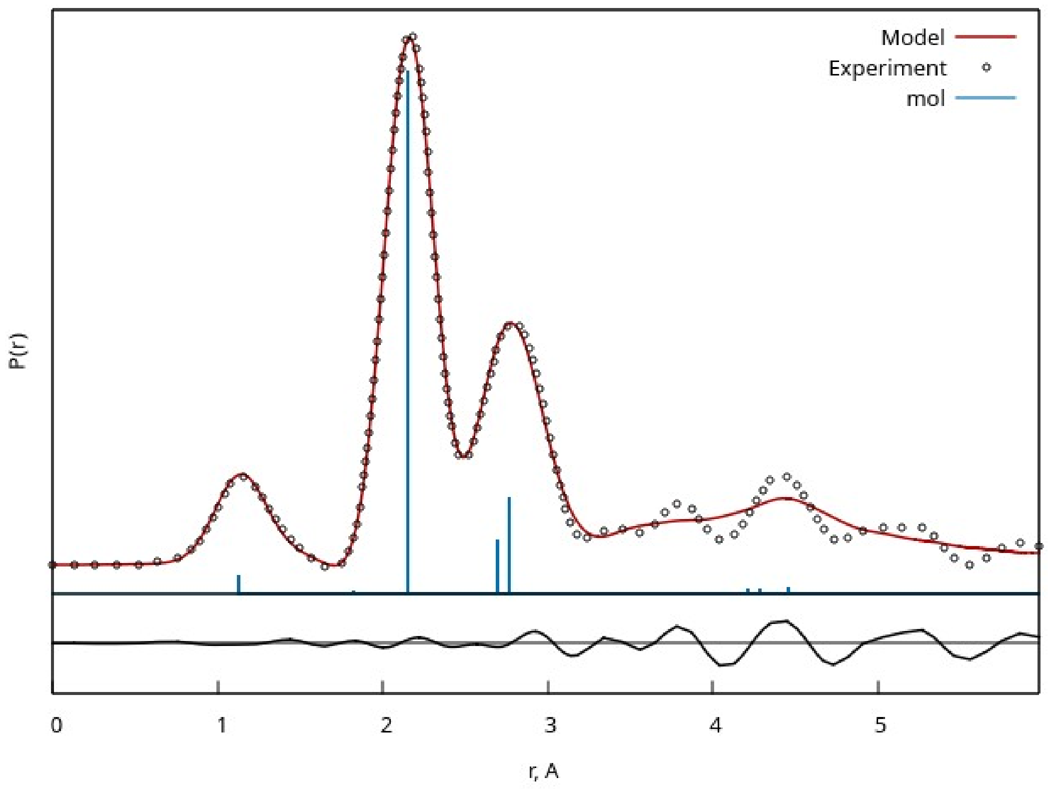


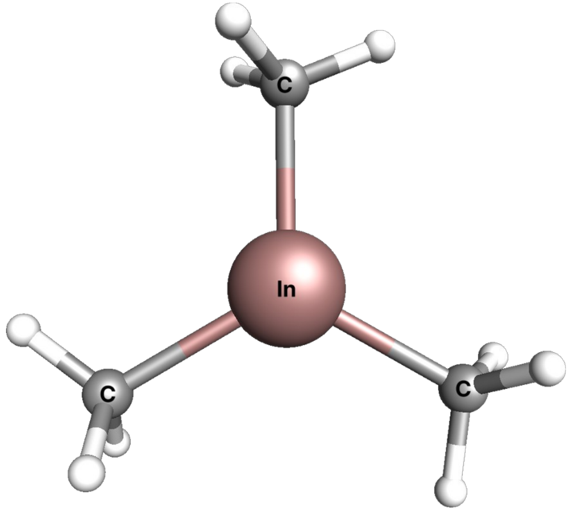
Kein Signal ab *s* = 20 Å^{-1} !

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.

$InMe_3$: unsere GED Daten





r_a(In-C) = 2.153(2) Å
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.

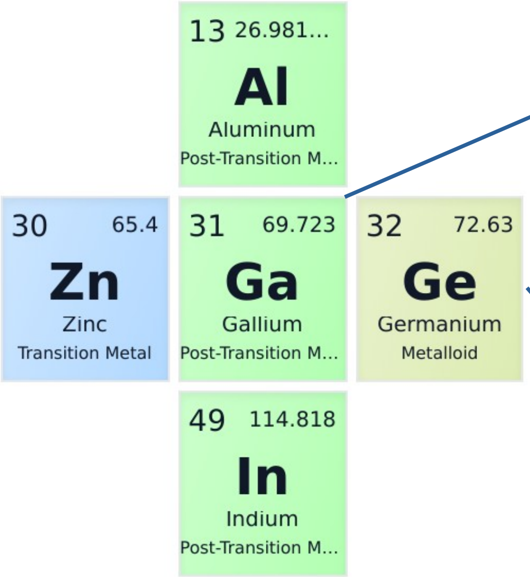
Theorie-Genauigkeit in Al→Ga→In und Zn→Ga→Ge

$AlMe_3$ Δ*r*(Al-C) = **0.011** Å oder **0.007** Å
(unsere Daten/Verfeinerung) (Lit.)

$GaMe_3$ Δ*r*(Ga-C) = **0.015** Å
(unsere Daten/Verfeinerung)

GaCN Δ*r*(Ga-C) = **0.011** Å
(Lit. MW Daten,
unsere Verfeinerung)

H-Zn-CH_3 Δ*r*(Zn-C) = **0.015** Å
(Lit. MW Daten,
unsere Verfeinerung)



H_3C-GeH_3 Δ*r*(Ge-C) = **0.009** Å
(Lit. MW Daten,
unsere Verfeinerung)

$InMe_3$ Δ*r*(In-C) = **0.017** Å oder **0.009** Å
(unsere Daten/Verfeinerung) (Lit.)

Statistik für *R*-Faktoren

Substanz	Str. *R*-faktor, %	Exp. *R*-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 CH_3-Gruppen in $AlMe_3$, $GaMe_3$ und $InMe_3$.
  - Punkt-Beugung → Volumen-Beugung.