Ga-NMR in $BaGa_4$

- This exercise should be done WITHOUT w2web in a terminal window !
- *mkdir BaGa4; cd BaGa4*
- *makestruct* (and type in the following information)
  - *$BaGa_4$: SG 139 (I4/mmm), a,a,c= 4.566 4.566 10.775 Ang*
  - *Ba (0,0, 0), Ga1(0.5,0, 0.75), Ga2 (0,0, 0.38)*
- *cp init.struct BaGa4.struct*
- *init_lapw -b -numk 10000 –fermit 0.004* (batch mode)
- edit .machines (insert 2 lines with 1:psi3X)
- *run_lapw -p -fc 1 -cc 0.0001; save_lapw rkm7_10k_4mry*
- *tail *scf* and verify that the forces are “small” (no struct opt. necessary)
- *x_nmr_lapw -mode in1* (and view the resulting *in1c_nmr file)
- *x_nmr_lapw –p –metal*
  - *check BaGa4.outputnmr_integ for σ_{iso} of both Ga atoms*
  - *grep :EFG002 *scf*
  - *grep :EFG003 *scf*

- R.Laskowski et al., J. Phys. Chem. C 2017, 121, 753−760
- * These calc. will take some time, continue next page while run/x_nmr is running

NMR continued ..

- *mkdir spin; cp BaGa4.struct spin/spin.struct; cp .machines spin; cd spin*
- *instgen_lapw –nm; init_lapw –b –sp –numk 10000 –fermit 0.004*
- *runsp_c_lapw –p; save non-magnetic*
- *cp $WIENROOT/SRC_templates/case.vorbup_100T spin.vorbup* (and for dn)
- *runsp_lapw –p –orbc –cc 0.000005; save_lapw rkm7_10k_4mry*
- *grepline :hff002/3 ´rkm*scf´ 3* σ_c=HFF*1000 *(for a 100T field)*
- compare with experiment: (F.Haarmann et al. Chem. Eur. J. 2011, 17, 7560 – 7568)
- *cp $WIENROOT/SRC_templates/case.indm spin.indm;*
- *edit *indm: set atom2+3; l=1-3; 3 5 in last line*
- *x lapwdm –p –up/dn; cat *scfdmup/dn;* $\sigma_{sd}=(tot_{up}-tot_{dn})*10000$

case	V_{zz}(exp)	V_{zz}(th)	δ_{iso}(exp)	δ_{iso}(th)
Ga1	5.99		3010	
Ga2	1.20		840	

- $\sigma_{iso}(th)= \sigma_{orb}- \sigma_c- \sigma_{sd}$
- *Estimate* $\delta_{iso}(th)=(\sigma_{itot}th)-\sigma_{ref}(th))$; *estimate* $\sigma_{ref}(th)$ *to obtain "best" agreement with exp. (usually one would either calculate the reference compound or do several Ga compounds)*
- *In metals the results are* ***very*** *sensitive to k-mesh and smearing and careful convergence are necessary (up to 1 000 000 k-points).*