

Robinson

Note Title

3/1/2005

controversy?

⇒ bonding in digallium

Cotton: Organomet., 1998 17 128-130

"Remarks on Ga-Fe bond in ..."
quote from paper: "unfounded and,
in a word, wrong!"

~~Votrial
in the
literature~~

⇒ simplify

★ Which Lewis structure best represents
the molecule's bonding?

translate MO theory into Lewis picture?

ELF has emerged as such a vehicle.

- * topological approach
- * Electron Localization function
- * Lewis electron-pair bond
- * Direct space mapping of Pauli principle

* function, continuous in 3D space
similar to ρ (rho), called η (ELF)

* gradient vector field of η
for topological analysis.

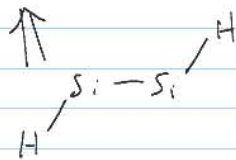
* nuclei aren't the sole attractors of
ELF basins
attractors: core, lone pair, bond.

* ELF is relative to homogeneous electron
gas "box of electrons"

* η runs from 0 to 1, 0.5 = HEG

HeCH vs HSiSiH

↑
linear



? Lewis

