



Chimie au coeur des atomes

Trond Saue

Laboratoire de Chimie et Physique Quantiques

Université de Toulouse 3 (Paul Sabatier)

118 route de Narbonne, F-31062 Toulouse, France

e-mail: trond.saue@irsamc.ups-tlse.fr



Periodic table (1871)

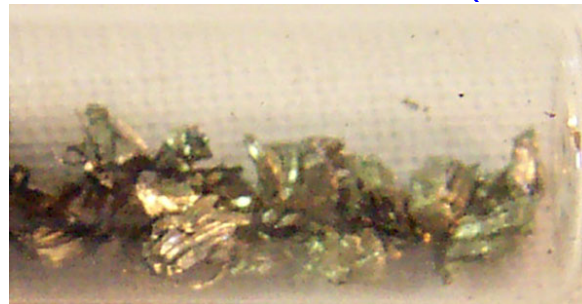
T a b e l l e II.

Reihen n.	Gruppe I.	Gruppe II.	Gruppe III.	Gruppe IV.	Gruppe V.	Gruppe VI.	Gruppe VII.	Gruppe VIII.
	— R ⁰	— RO	— R ⁰ 3	RH ⁴ RO ²	RH ⁵ R ⁰ 5	RH ⁶ RO ³	RH R ⁰ 7	— RO ⁴
1	H=1							
2	Li=7	Be=9,4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27,3	Si=28	P=31	S=32	Cl=35,5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59, Ni=59, Cu=63.
5	(Cu=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	?Yt=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104, Pd=106, Ag=108.
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	J=127	
8	Cs=133	Ba=137	?Di=138	?Ce=140	—	—	—	— — — —
9	(—)	—	—	—	—	—	—	
10	—	—	?Er=178	?La=180	Ta=182	W=184	—	Os=195, Ir=197, Pt=198, Au=199.
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	—	—	
12	—	—	—	Th=231	—	U=240	—	— — — —

eka-aluminium:
gallium (1875)



eka-boron: scandium (1879)



eka-silicon:
germanium (1886)





Goldschmidt and Einstein in Norway 1920

Relativistic effects

- scalar effects
- spin-orbit interaction

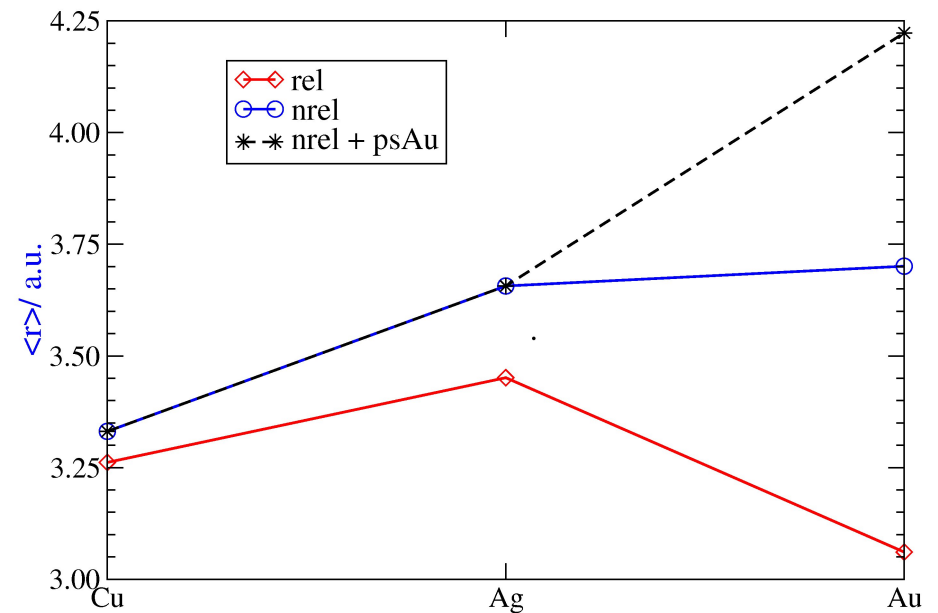
Lorentz factor:

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Lanthanide contraction

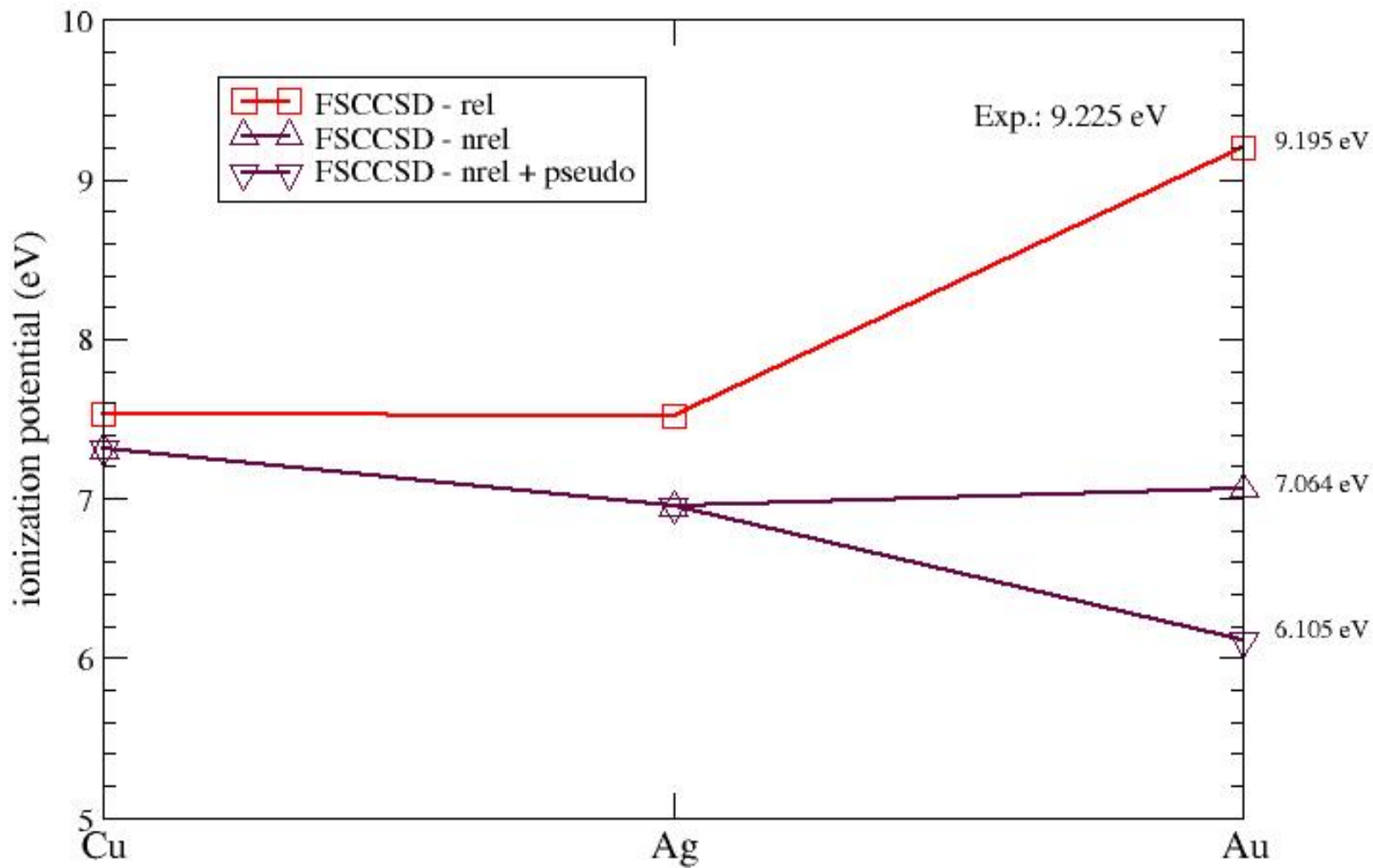
V.M. Goldschmidt, T. Barth, G. Lunde:
 Norske Vidensk. Selsk. Skrifter I Mat. Naturv. Kl. 7, 1 (1925)
 D. R. Lloyd, J. Chem. Ed. **63** (1986) 503

- La^{3+} - Lu^{3+} (117.2 - 100.1 pm)
- Ca^{2+} - Zn^{2+} (114 - 88 pm)
- Cu (138 pm) < Au (144 pm) < Ag (153 pm)



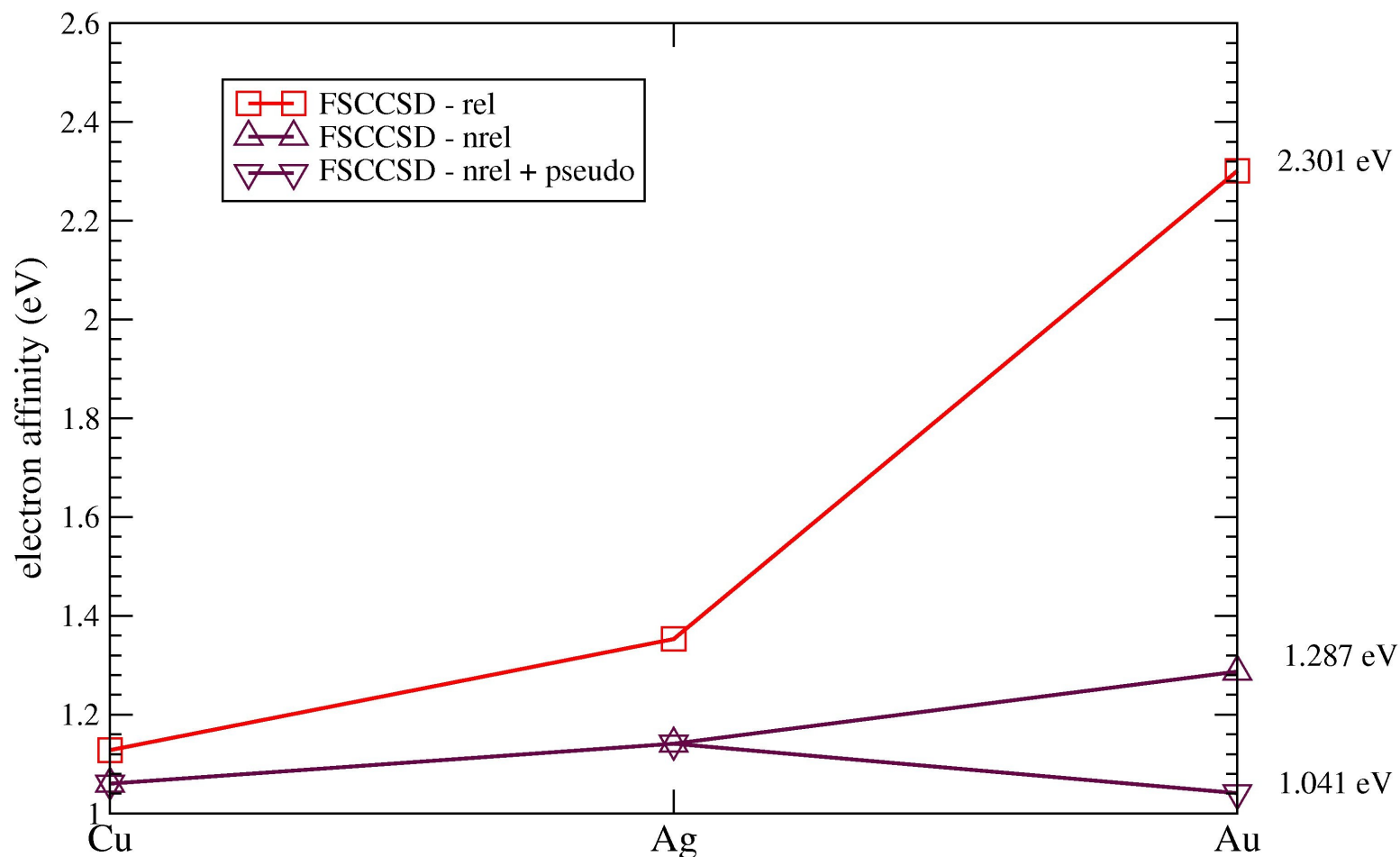
Ionisation energy of gold

O. Fossgaard, O. Gropen, E. Eliav and T. Saue, J. Chem. Phys. **119** (2003) 9355



Electron affinity of gold

O. Fossgaard, O. Gropen, E. Eliav and T. Saue, J. Chem. Phys. **119** (2003) 9355

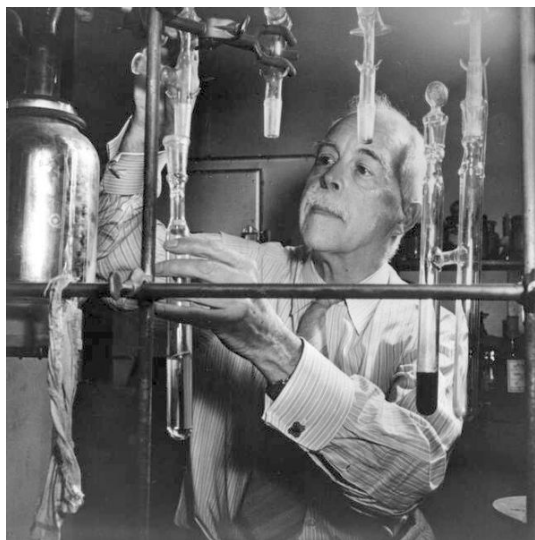


- ✓ Gold and caesium are extremes on the electron affinity scale — 2.309 eV vs. 0.472 eV.
- ✓ CsAu is a semi-conductor with a CsCl crystal structure in the solid state; it forms an ionic melt. The oxidation state of gold is -I.

THE ATOM AND THE MOLECULE.

BY GILBERT N. LEWIS.

Received January 26, 1916.

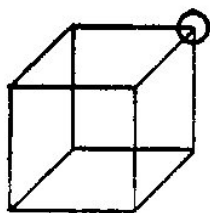


1. In every atom is an essential *kernel* which remains unaltered in all ordinary chemical changes and which possesses an excess of positive charges corresponding in number to the ordinal number of the group in the periodic table to which the element belongs.

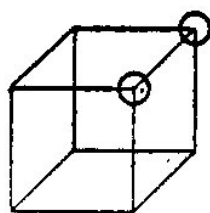
2. The atom is composed of the kernel and an *outer atom* or *shell*, which, in the case of the neutral atom, contains negative electrons equal in number to the excess of positive charges of the kernel, but the number of electrons in the shell may vary during chemical change between 0 and 8.

3. The atom tends to hold an even number of electrons in the shell, and especially to hold eight electrons which are normally arranged symmetrically at the eight corners of a cube.¹

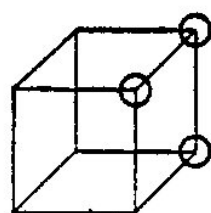
4. Two atomic shells are mutually interpenetrable.



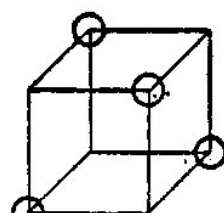
Li



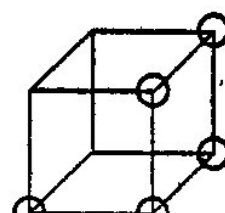
Be



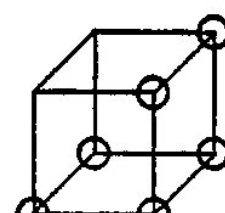
B



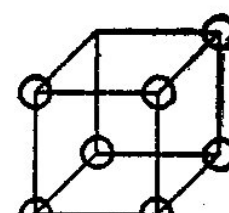
C



N



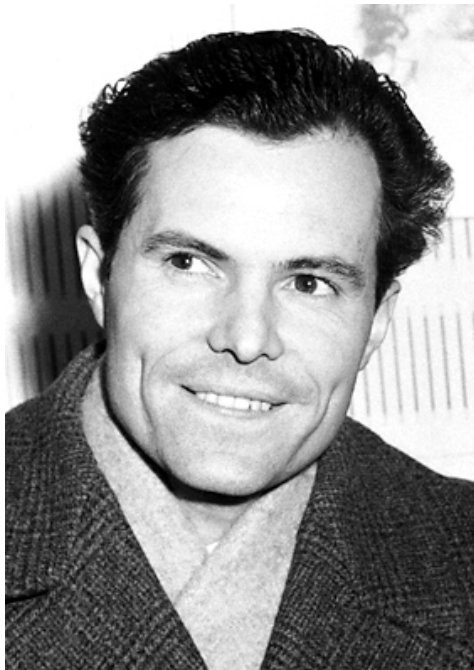
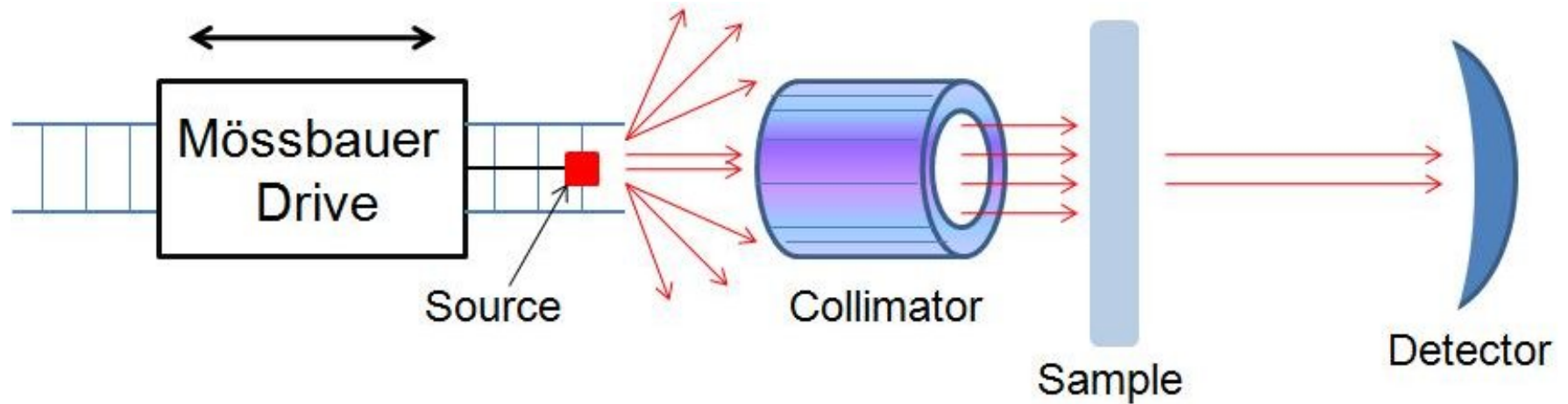
O



F

Although chemistry is associated with the valence region of an atom, a wealth of chemical information can be extracted from probing the core region of atoms.

Mössbauer spectroscopy



Rudolf Mössbauer

(January 31, 1929 - September 14, 2011)

- Recoil-free, resonant absorption and emission of gamma rays in solids
- The energy E_γ of the nuclear γ -transition is modified by the local chemical environment
- Isomer shift (mm/s):

$$\delta = \frac{c}{E_\gamma} (\Delta E_\gamma^a - \Delta E_\gamma^s)$$

Isomer shift

- Modification of nuclear γ -transition by electrostatic interaction between electronic and nuclear charge distributions

$$\Delta E_\gamma = E^{el}(R_{ex}) - E^{el}(R_0); \quad R - \text{radial size parameter}$$

- Electrostatic interaction:

$$E^{el}(R) = \int \rho_e(\mathbf{r}_e) \phi_n(\mathbf{r}_e; R) d^3r_e; \quad \phi_n(\mathbf{r}_e; R) = \int \frac{\rho_n(\mathbf{r}_n)}{r_{en}} d^3r_n$$

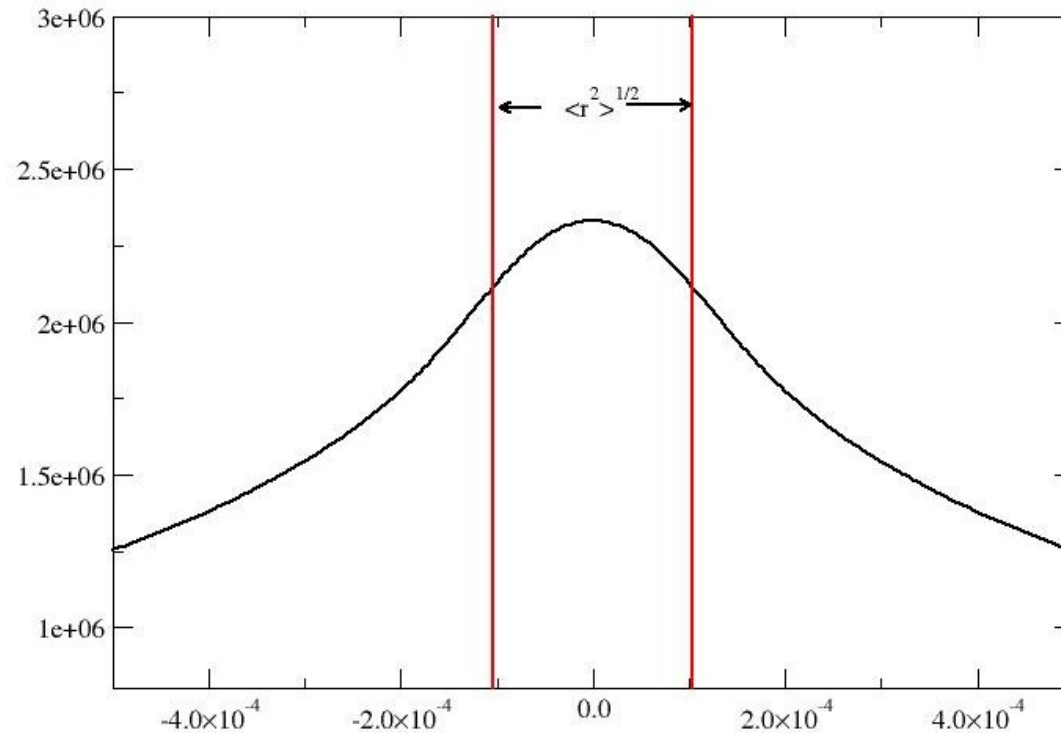
- Approximations:

$$\begin{aligned} \Delta E_\gamma &= \left. \frac{\partial E^{el}}{\partial R} \right|_{R=R_0} \Delta R; \quad \Delta R = R_{ex} - R_0 \\ &= \left[\int \rho_e(\mathbf{r}_e) \frac{\partial \phi_n(\mathbf{r}_e; R)}{\partial R} d^3r_e + \int \underbrace{\frac{\partial \rho_e(\mathbf{r}_e)}{\partial R}}_{\approx 0} \phi_n(\mathbf{r}_e; R) d^3r_e \right]_{R=R_0} \Delta R \end{aligned}$$

Contact density

$$\Delta E_\gamma \approx \int \rho_e(\mathbf{r}_e) \frac{\partial \phi_n(\mathbf{r}_e; R)}{\partial R} d^3 r_e \Delta R$$

$$\approx \bar{\rho}_e \int \frac{\partial \phi_n(\mathbf{r}_e; R)}{\partial R} d^3 r_e \Delta R \quad \approx \rho_e(0) \int \frac{\partial \phi_n(\mathbf{r}_e; R)}{\partial R} d^3 r_e \Delta R$$



Is the contact density a good approximation to the effective density for heavy elements ?

B. Fricke B and J. T. Waber, Phys Rev B **5** (1972) 3445

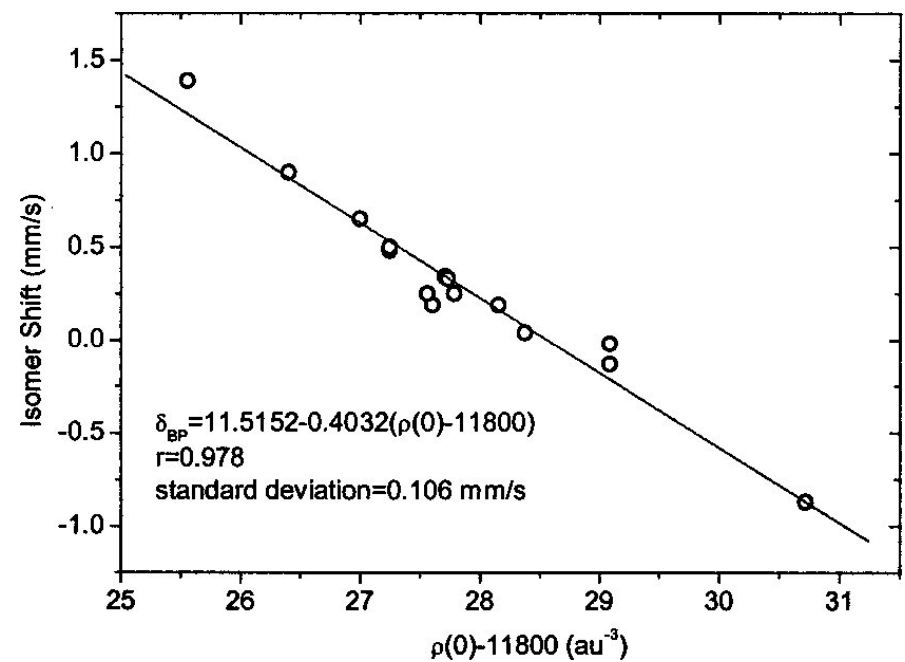
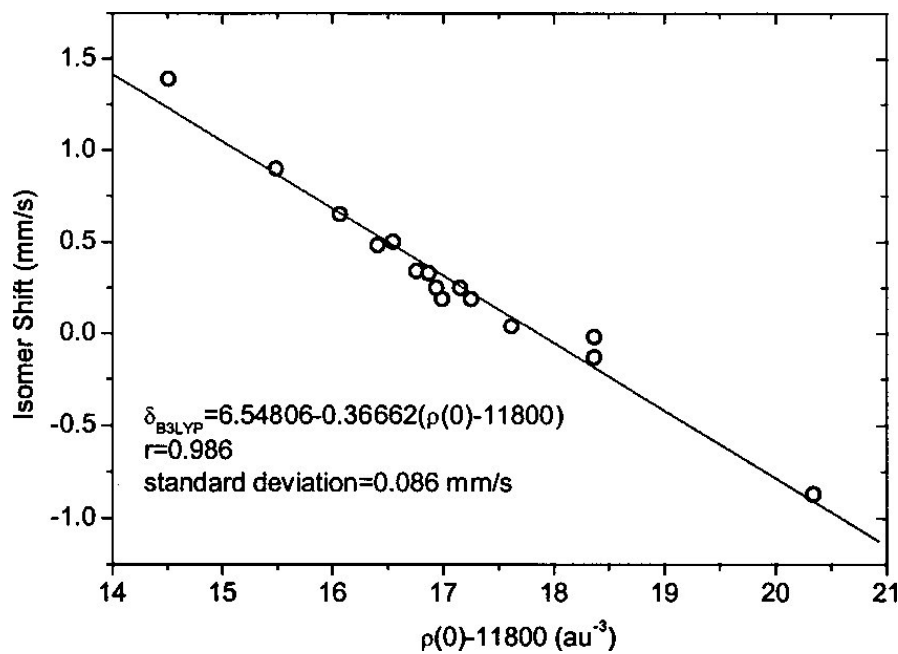
A DFT approach to the calculation of Mössbauer spectra

F. Neese, Inorganica Chimica Acta **337** (2002) 181

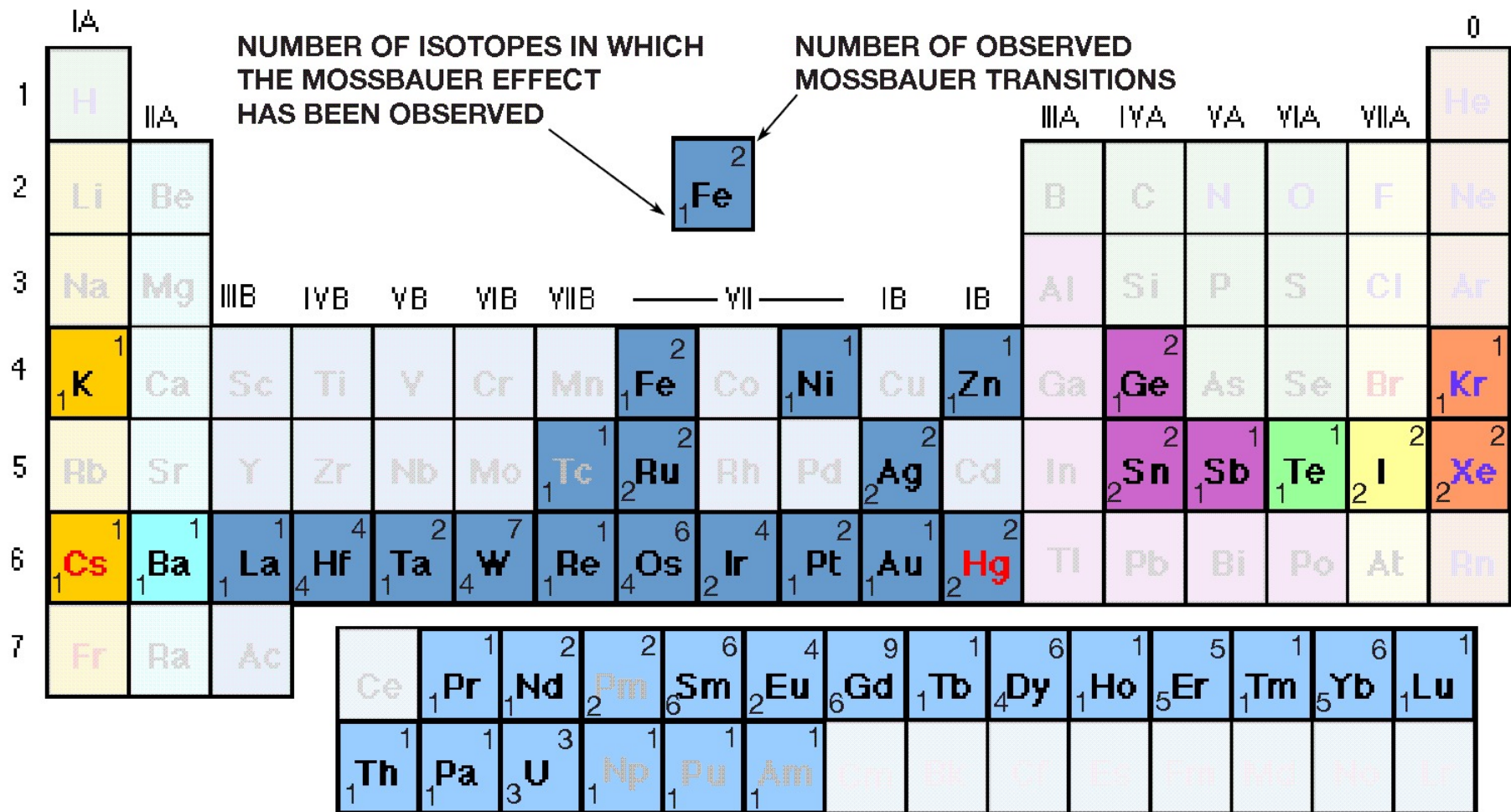
The isomer shift is written as

$$\delta = a [\rho^A(0) - b]$$

where a and b are parameters to determine from calibration.



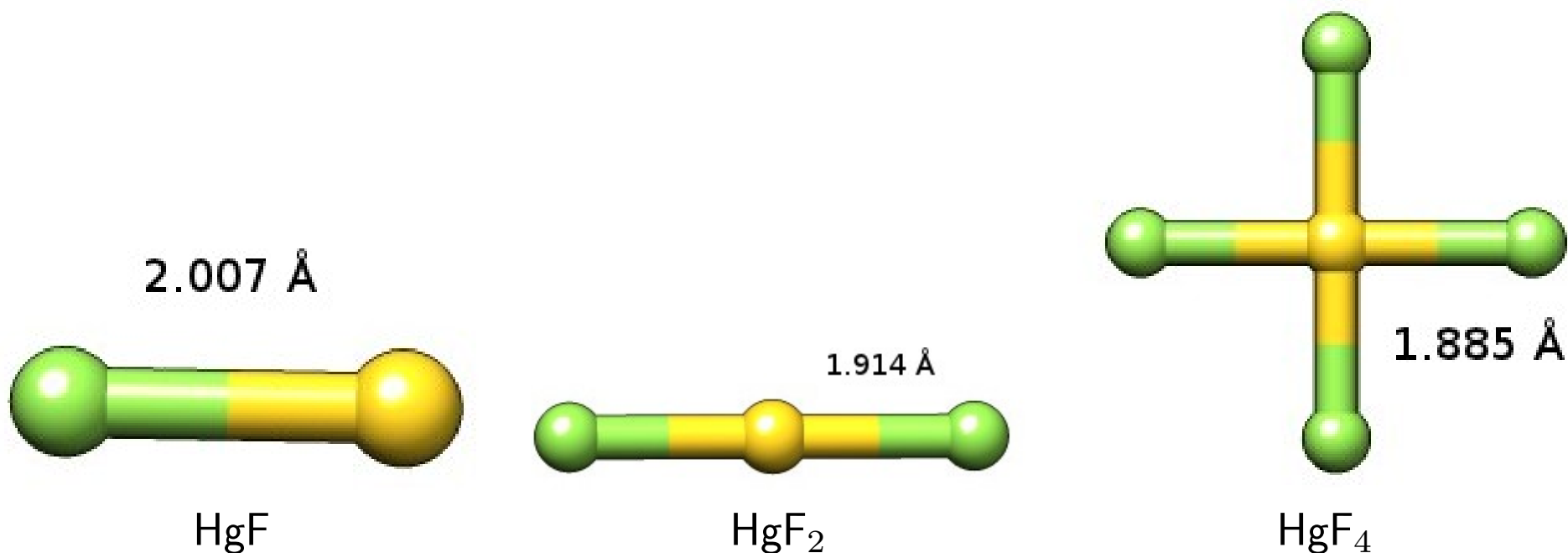
Mössbauer spectroscopy for heavy elements



Relativistic effects are particularly pronounced in the core region of atoms !

Contact densities in mercury fluorides

S. Knecht, S. Fux, R. van Meer, L. Visscher, M. Reiher and T. Saue,
Theor. Chem. Acc. **129** (2011) 631

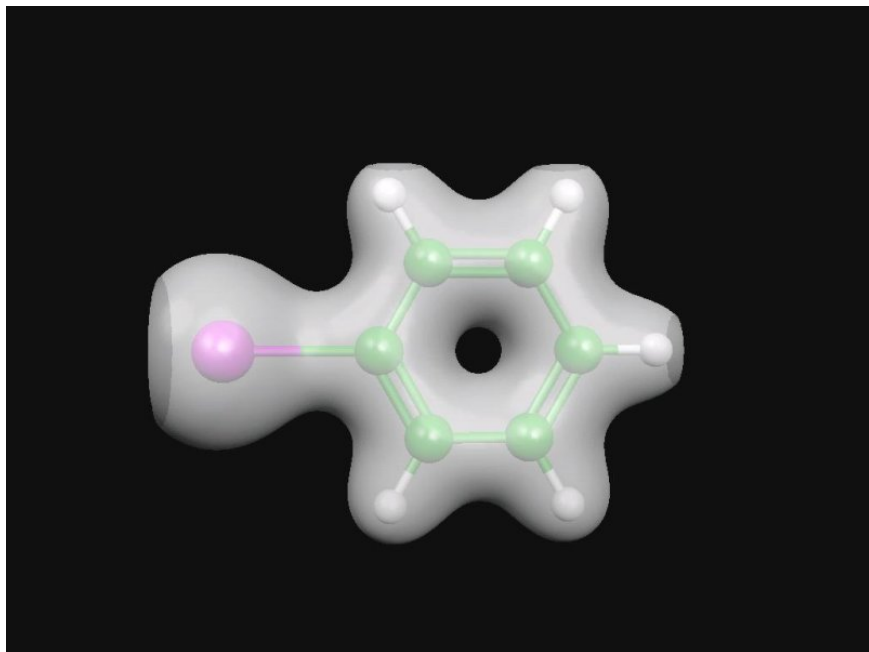


The series HgF_n ($n = 0, 1, 2, 4$) was selected for a relativistic benchmark study.

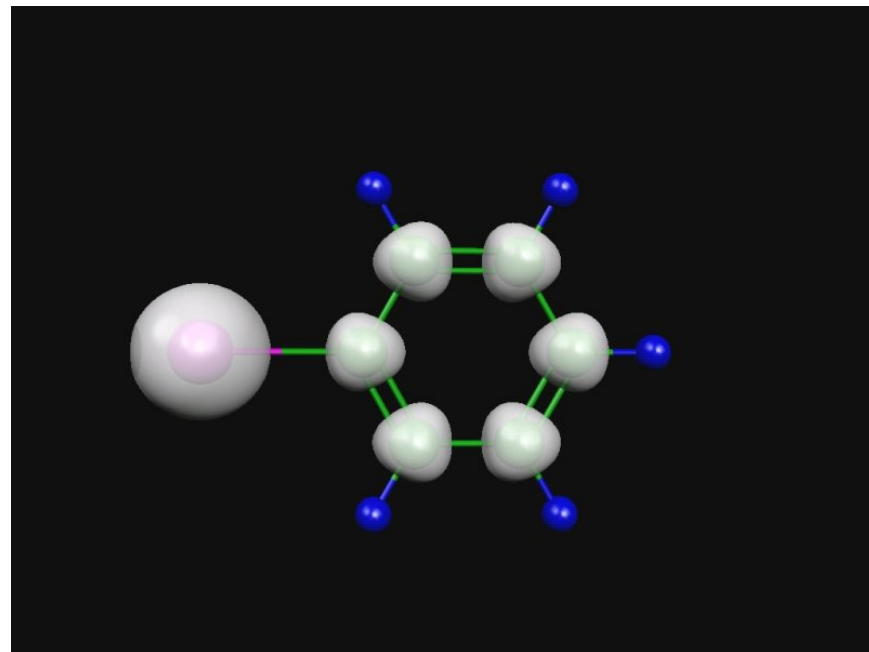
X. Wang, L. Andrews, S. Riedel and M. Kaupp,
Mercury Is a Transition Metal: The First Experimental Evidence for HgF₄,
Angew. Chem. **119** (2007) 8523

Electron density of iodobenzene

$$\rho^{4c}(\mathbf{r}) = \rho^L(\mathbf{r}) + \rho^S(\mathbf{r})$$



$\rho^L(\mathbf{r})$
(isosurface=0.01)



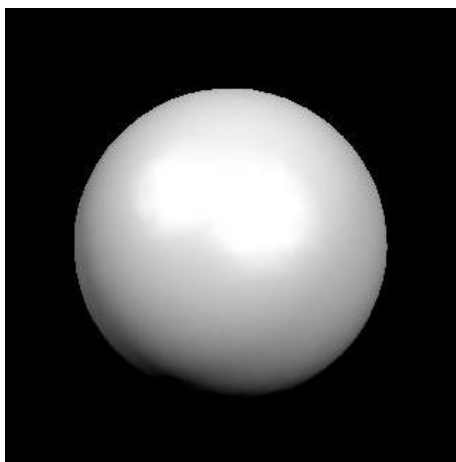
$\rho^S(\mathbf{r})$
(isosurface=0.0001)

$$\rho^{4c}(\mathbf{P}) = -e \sum_i \langle \psi_i^{4c} | \delta(\mathbf{r} - \mathbf{P}) | \psi_i^{4c} \rangle = -e \sum_i \psi_i^{4c\dagger}(\mathbf{P}) \psi_i^{4c}(\mathbf{P})$$

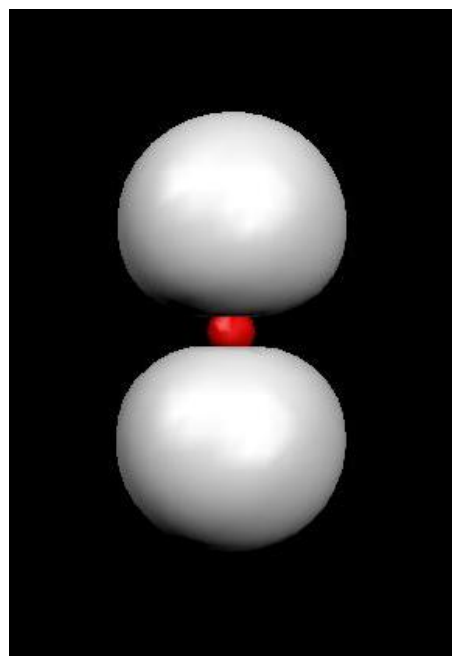
Relativistic atomic orbitals

$$\psi^{\text{NR}}(r, \theta, \phi) = R(r)Y_{lm}(\theta, \phi) \Rightarrow \psi^{\text{R}}(r, \theta, \phi) = \begin{bmatrix} R^L(r)\chi_{\kappa, m_j}(\theta, \phi) \\ iR^S(r)\chi_{-\kappa, m_j}(\theta, \phi) \end{bmatrix}$$

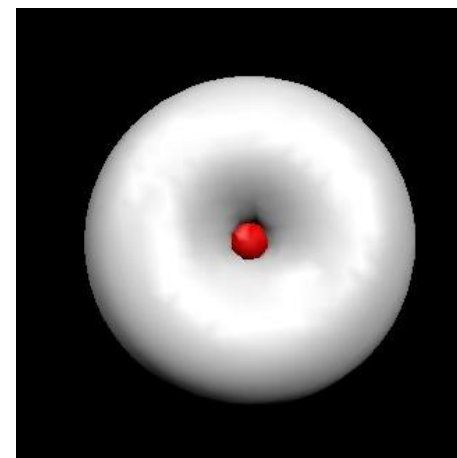
	$s_{1/2}$	$p_{1/2}$	$p_{3/2}$	$d_{3/2}$	$d_{5/2}$
j	1/2	1/2	3/2	3/2	5/2
κ	-1	+1	-2	+2	-3



$2(s, p)_{1/2, 1/2}$
(z-axis anywhere)



$2(p, d)_{3/2, 1/2}$
(z-axis in plane)



$2(p, d)_{3/2, 3/2}$
(z-axis out of plane)

Atomic contact density

$$\begin{aligned}\rho^{Hg}(0) &= \sum_i \langle \psi_i^{Hg} | \delta(\mathbf{r}) | \psi_i^{Hg} \rangle \\ &= \sum_i \left[\left\langle R_i^L \left| \frac{\delta(r)}{4\pi r^2} \right| R_i^L \right\rangle_r \langle \chi_{\kappa,m} | \chi_{\kappa,m} \rangle_{(\theta,\phi)} + \right. \\ &\quad \left. + \left\langle R_i^S \left| \frac{\delta(r)}{4\pi r^2} \right| R_i^S \right\rangle_r \langle \chi_{-\kappa,m} | \chi_{-\kappa,m} \rangle_{(\theta,\phi)} \right] \\ &= \frac{1}{4\pi} \sum_i [R_i^L(0) R_i^L(0) + R_i^S(0) R_i^S(0)]\end{aligned}$$

Let us look at small r solutions of relativistic atomic orbitals

Small r solutions

- We consider radial solutions at small r :

$$R^L = r^{\gamma-1} (p_0 + p_1 r + p_2 r^2 + \dots)$$

$$R^S = r^{\gamma-1} (q_0 + q_1 r + q_2 r^2 + \dots)$$

- Point nucleus: $\gamma = +\sqrt{\kappa^2 - Z^2/c^2} < |\kappa|$ (singularity at the nucleus for $|\kappa| = 1$)
- Extended nuclei: $\gamma = |\kappa|$
 - $\kappa < 0$: $q_0 = p_1 = 0$ (for $s_{1/2}$ - orbitals ($\kappa = -1$) $R^L(0) = p_0$ and $R^S(0) = 0$)
 - $\kappa > 0$: $p_0 = q_1 = 0$ (for $p_{1/2}$ - orbitals ($\kappa = 1$) $R^L(0) = 0$ and $R^S(0) = q_0$)

In the relativistic case the contact density has contributions from the large components of $s_{1/2}$ orbitals and the small components of $p_{1/2}$ components.

- Non-relativistic case: $R(r) = r^l (a_0 + a_1 r + a_2 r^2 + \dots)$

(a_1 is zero for extended nuclei, thus removing the cusp)

Relativistic effects on absolute and relative $\rho^{Hg}(0)$ (a.u.)

Contact density (a_0^{-3}):		absolute	relative to Hg		
Method	Hamiltonian	Hg	HgF	HgF ₂	HgF ₄
HF	DC	2363929.12	-114.48	-127.92	-98.09
HF	NR	361818.93	-11.92	-13.35	-6.77
		-84.69%	-89.59%	-89.56%	-93.10%

Correlation effects on absolute and relative $\rho^{Hg}(0)$ (a.u.)

Contact density (a_0^{-3}):		absolute	relative to Hg		
Method	Hamiltonian	Hg	HgF	HgF ₂	HgF ₄
CCSD(T)[cv]	DC	2363990.74	-95.11	-110.46	-103.70
HF	DC	2363929.12	-114.48	-127.92	-98.09
LDA	DC	2362802.35	-74.38	-99.03	-113.69
BP86	DC	2373796.03	-74.35	-98.52	-114.00
BLYP	DC	2373687.69	-72.82	-95.88	-111.48
B3LYP	DC	2370863.15	-85.86	-105.87	-113.54
CAMB3LYP	DC	2371811.55	-95.79	-113.92	-116.38
PBE	DC	2372713.57	-75.11	-98.74	-113.42
PBE0	DC	2370507.83	-91.30	-111.07	-115.62

- Compared to CCSD(T), our selection of density functionals give errors on the order of 0.5% in the absolute contact density, which is two orders of magnitude larger than the relative shifts in density
- DFT is not able to qualitatively reproduce the non-monotonic decrease of the contact density of the heavier atom mercury that we obtain from our benchmark CCSD(T) calculations and even at the HF level.
- How can the non-monotonic trend be explained ?

Projection analysis of expectation values

R. Bast, A. Koers, A. Severo Pereira Gomes, M. Iliaš, L. Visscher, P. Schwerdtfeger and T. Saue,

Phys. Chem. Chem. Phys. **13** (2011) 854

Consider the expectation value of some operator $\hat{\Omega}$ at the HF or KS level

$$\langle \Psi | \hat{\Omega} | \Psi \rangle = \sum_i^{N_{occ}} \langle \psi_i | \hat{\Omega} | \psi_i \rangle$$

Molecular orbitals (MOs) are expanded in atomic (or fragment) orbitals (AOs):

$$|\psi_i\rangle = \sum_{Ap} |\psi_p^A\rangle c_{pi}^A + |\psi_i^{\text{pol}}\rangle$$

giving

$$\langle \Psi | \hat{\Omega} | \Psi \rangle = \underbrace{\sum_{pqB} \sum_i^{N_{occ}} \langle \psi_p^B | \hat{\Omega} | \psi_q^B \rangle c_{pi}^{B*} c_{qi}^B}_{\text{intra-atomic}} + (\text{inter-atomic: } B \neq C) + (\text{pol})$$

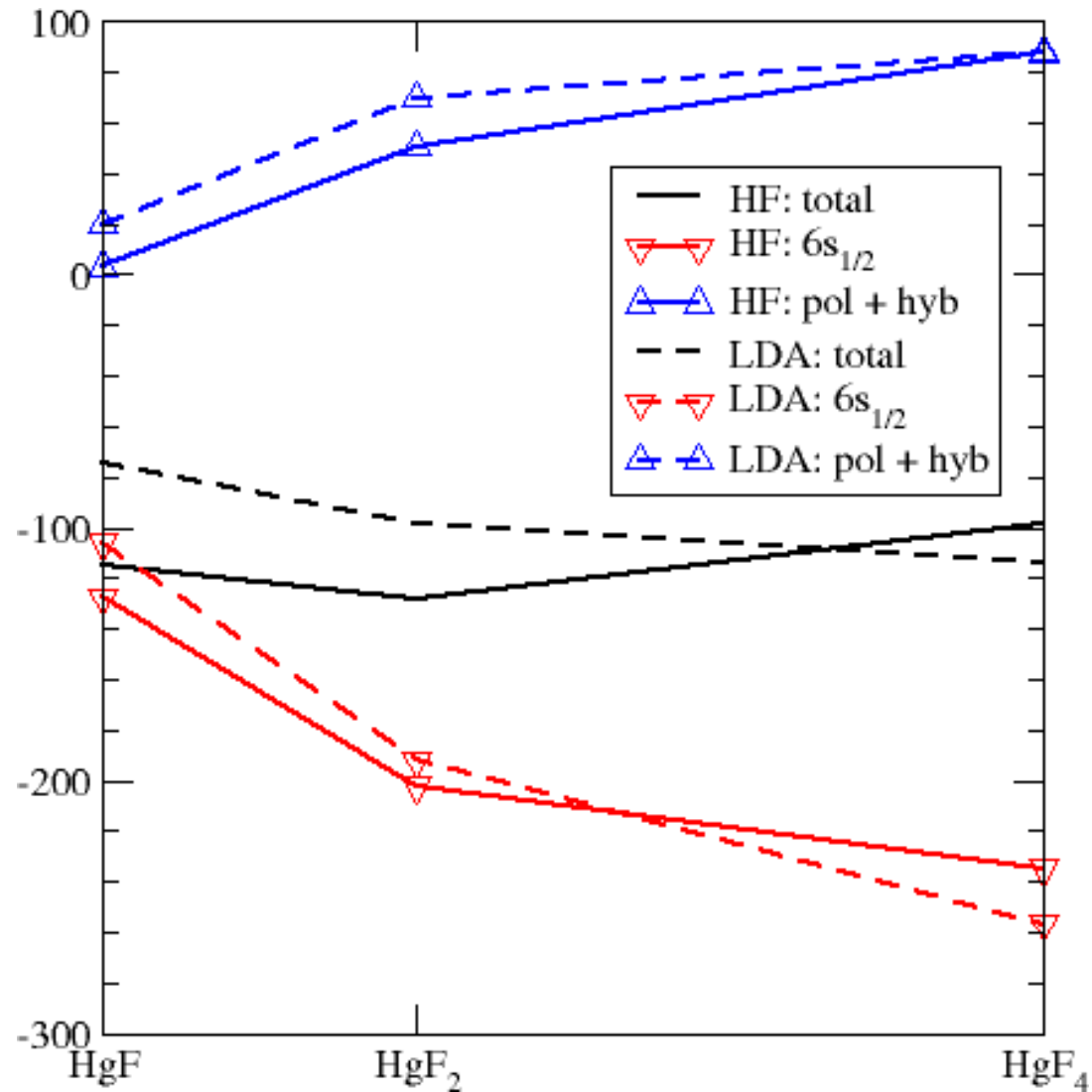
Projection analysis of ρ^{Hg} in the series HgF_n ($n=1,2,4$)

(HF/TZ+2s1p; a_0^{-3})

	HgF	HgF ₂	HgF ₄
Intra-atomic contribution			
Hg	-120.33	-161.99	-168.41
diagonal	-117.32	-178.30	-185.46
core	10.05	23.85	49.14
6s _{1/2}	-127.37	-202.15	-234.60
6p _{1/2}	0.06	0.01	0.01
hybrid	-3.01	16.32	17.06
F	0.00	0.00	0.00
Inter-atomic contribution			
	-0.07	-0.33	-0.53
Polarization contribution			
	5.93	34.39	70.84
Total			
	-114.48	-127.92	-98.09

HgF₄: Successively adding the mercury 7s_{1/2}, 8s_{1/2} and 9s_{1/2} orbitals reduces the polarization contribution from 70.84 to 52.07, 10.98 and -2.89 a_0^{-3} , respectively.

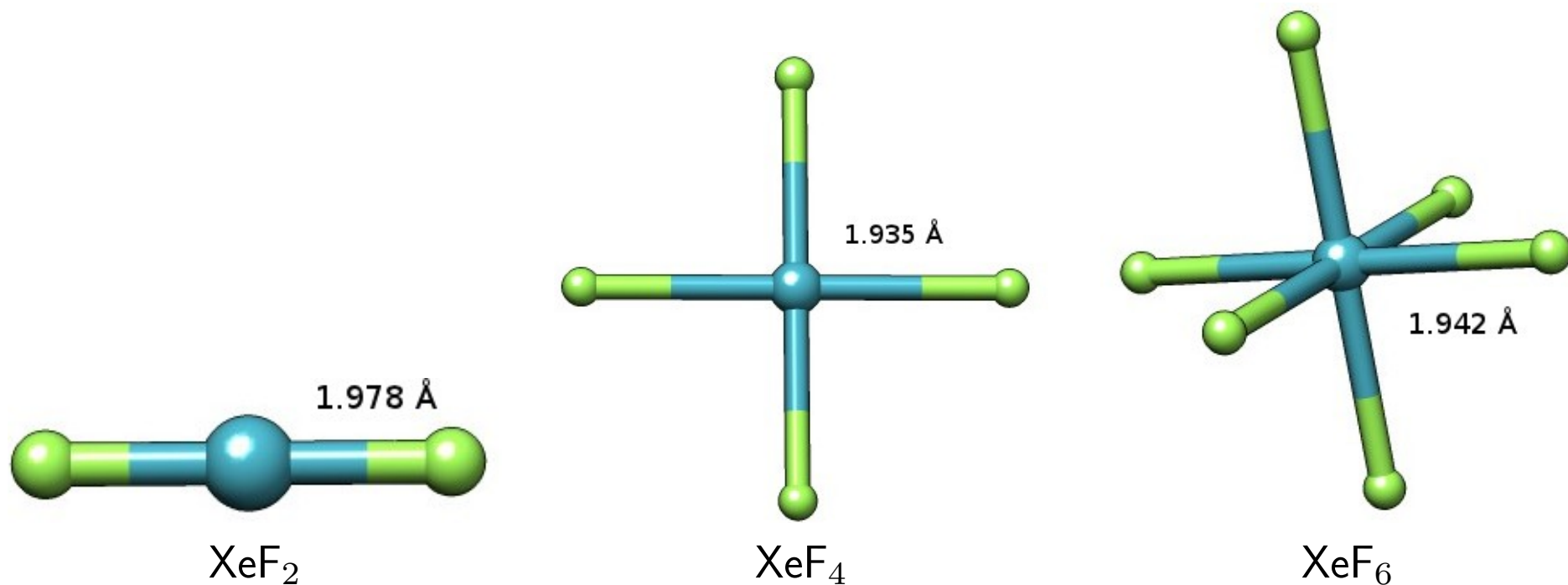
Projection analysis of ρ^{Hg} in the series HgF_n ($n=1,2,4$)



At the HF level the decreasing $6s_{1/2}$ population along the series is offset by increasing polarization and hybridization.

Contact densities in xenon fluorides

S. Knecht and T. Saue, in preparation



Are there systems dominated by the small component density of $p_{1/2}$ orbitals ?

Absolute and relative contact densities in xenon fluorides

S. Knecht and T. Saue, in preparation

Method	Hamiltonian	Xe	XeF ₂	XeF ₄	XeF ₆
HF	DC	272903.24	14.89	34.15	66.09
HF	DCG	272150.70	14.80	33.97	65.84
CCSD(T)[v]	DC(mmf)	272903.64	12.01	27.28	-
CCSD(T)[cv]	DC(mmf)	272907.38	12.54	28.40	50.83
CCSD(T)[cv]	DC	272907.38	12.54	28.40	-
LDA	DC	272469.70	12.53	28.19	49.00
B3LYP	DC	273440.68	13.34	30.21	53.69
CAMB3LYP	DC	273540.61	14.24	32.03	57.11
PBE	DC	273600.59	12.46	28.13	49.42
PBE0	DC	273424.05	13.25	29.98	53.68
HSE	DC	273425.88	13.10	29.70	53.18

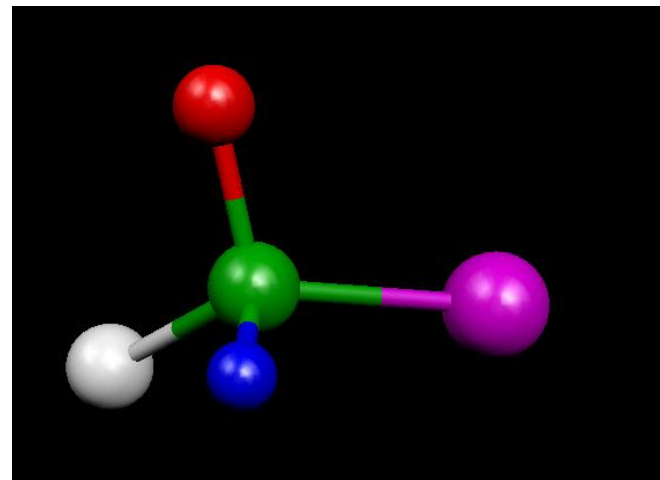
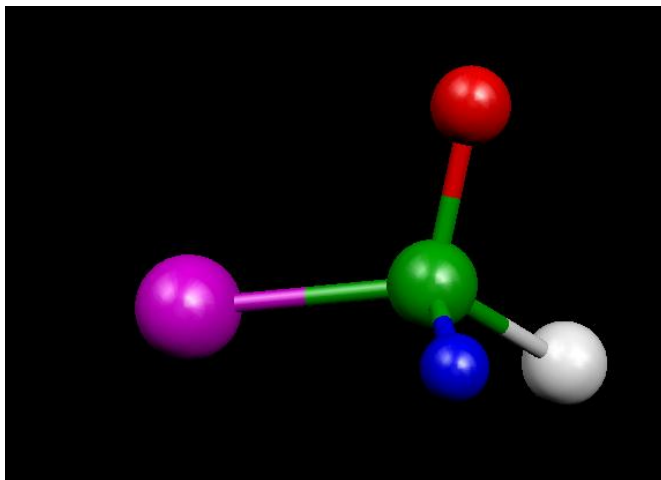
- DFT shows good performance
- Relative contact densities dominated by overlap effects

Chiral molecules

The word chirality (handedness) was introduced by Lord Kelvin (1873).

The first paper in chemistry using the word chirality dates from 1962

Carl Djerassi, Ruth Records, E. Bunnenberg, Kurt Mislow and Albert Moscowitz, J. Am. Chem. Soc. 84 (1962) 870



Enantiomers of chiral molecules are related by the parity operation

$$\hat{P}\Psi_L = \Psi_R$$

The Hamiltonian of (electromagnetic) quantum chemistry commutes with the parity operator

$$[\hat{H}, \hat{P}] = 0$$

and so the enantiomers are degenerate, that is, they have the same energy.

Pasteur and the universal chiral force



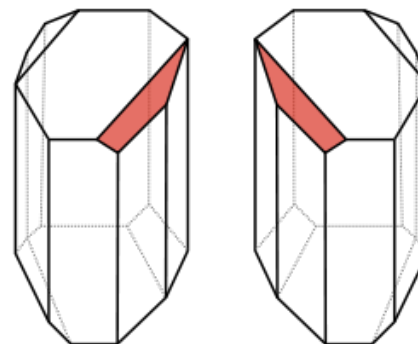
Biomolecular homochirality:

Life on earth has many homochiral features, e.g. amino acids and sugars consist (almost) exclusively of the L- and the D-form, respectively.

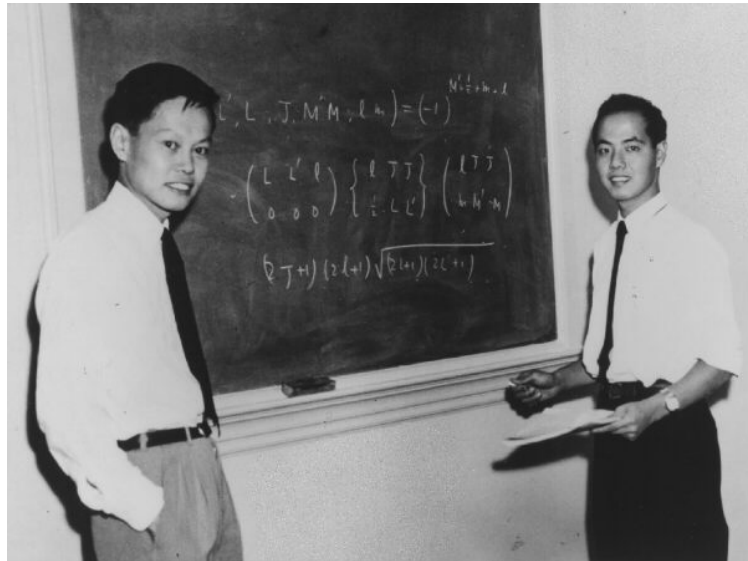
L'univers est un ensemble dissymétrique, et je suis persuadé que la vie, telle qu'elle se manifeste à nous, est fonction de la dissymétrie de l'univers ou des conséquences qu'elle entraîne.



Louis Pasteur manually separated left- and right-handed crystals of chemically synthesized tartaric acid and showed that they were optically active, rotating the plane of light the opposite way.



Parity violation in weak interactions



In 1956 Lee and Yang suggested that parity may not be conserved in processes involving the weak force

PHYSICAL REVIEW VOLUME 104, NUMBER 1 OCTOBER 1, 1956

Question of Parity Conservation in Weak Interactions*

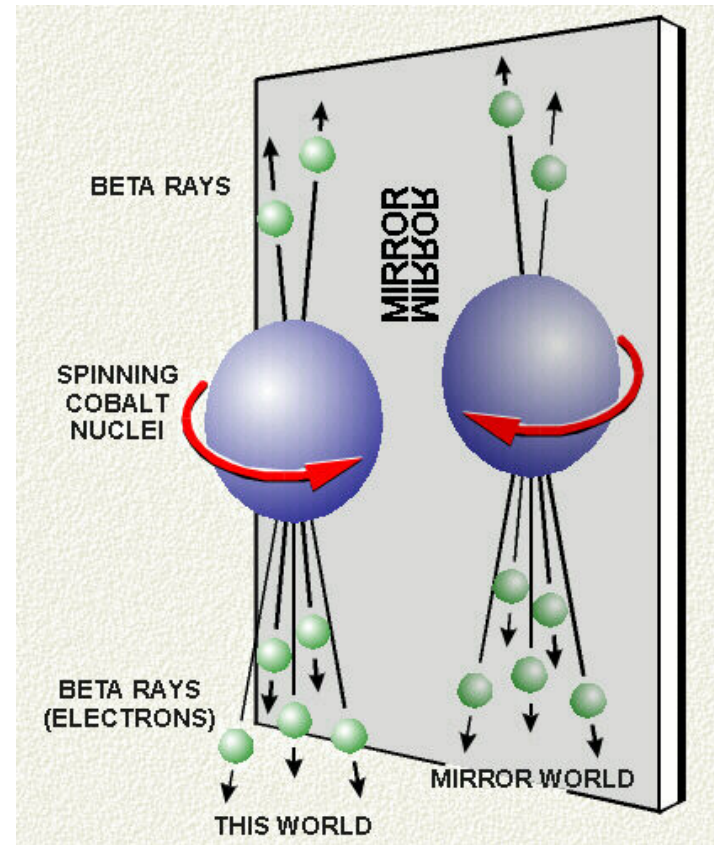
T. D. LEE, *Columbia University, New York, New York*

AND

C. N. YANG, *Brookhaven National Laboratory, Upton, New York*

(Received June 22, 1956)

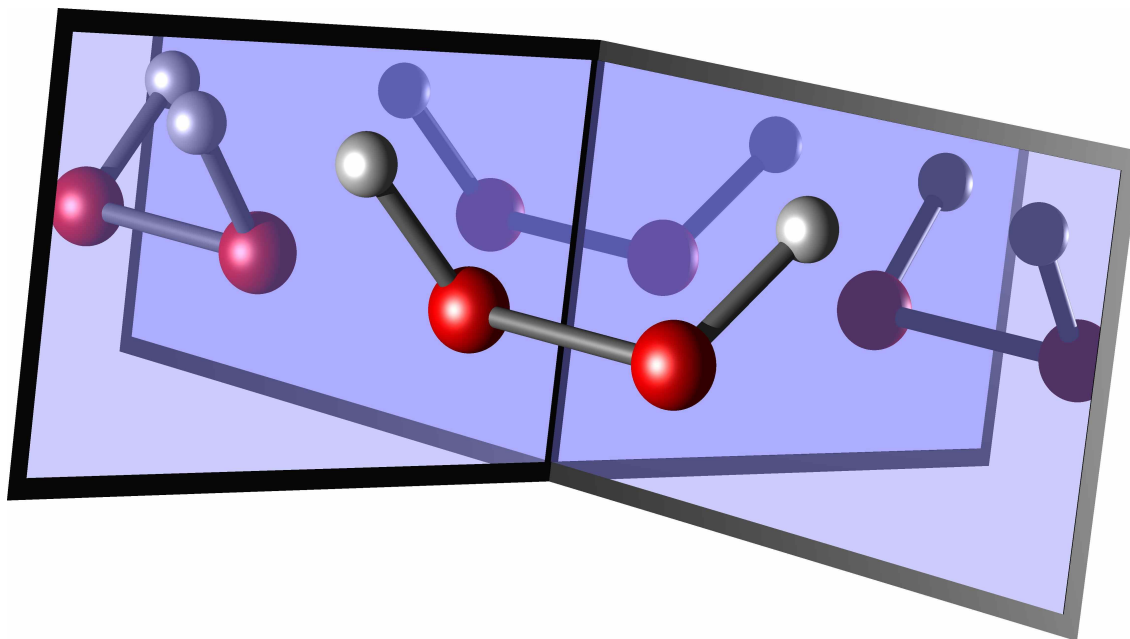
The question of parity conservation in β decays and in hyperon and meson decays is examined. Possible experiments are suggested which might test parity conservation in these interactions.



In 1957 Wu and co-workers observed parity violation in the β -decay of the ^{60}Co nucleus.

Parity-violation in molecular systems

M.Quack, Ang. Chem. Int. Ed. **41**(2002) 4618, J. K. Laerdahl and P. Schwerdtfeger, Phys. Rev. A **60** (1999) 4439



The Hamiltonian of *electroweak* quantum chemistry has a parity-violating (PV) component H_{pv}^{PV} and thus induces a minute energy difference between left- and right-handed molecules

$$E_{pv;L}^{PV} = \langle \Psi_L | \hat{H}_{pv}^{PV} | \Psi_L \rangle = \langle \hat{P}\Psi_L | \hat{P}\hat{H}_{pv}^{PV}\hat{P}^{-1} | \hat{P}\Psi_L \rangle = - \langle \Psi_R | \hat{H}_{pv}^{PV} | \Psi_R \rangle = -E_{pv;R}^{PV}$$

Could this explain the origin of biochirality ?

The goal of the ANR project NCPCHEM is to detect the effect of parity violation in vibrational spectra.

Electroweak chemistry

$$E_{PV} = \sum_K E_{PV}^K; \quad E_{PV}^K = \frac{G_F}{2\sqrt{2}} Q_W^K \sum_i \langle \psi_i | \gamma_5 \rho_K | \psi_i \rangle$$

✓ Weak charge: $Q_{W;A} = -N_A + Z_A (1 - 4 \sin^2 \theta_W)$; $\sin^2 \theta_W = 0.2319$

✓ Normalized nucleon density: ρ_A

$$\checkmark \gamma_5 = \begin{bmatrix} 0_2 & I_2 \\ I_2 & 0_2 \end{bmatrix}$$

✓ Fermi coupling constant: $G_F = 2.22255 \cdot 10^{-14}$ a.u. **very weak !**

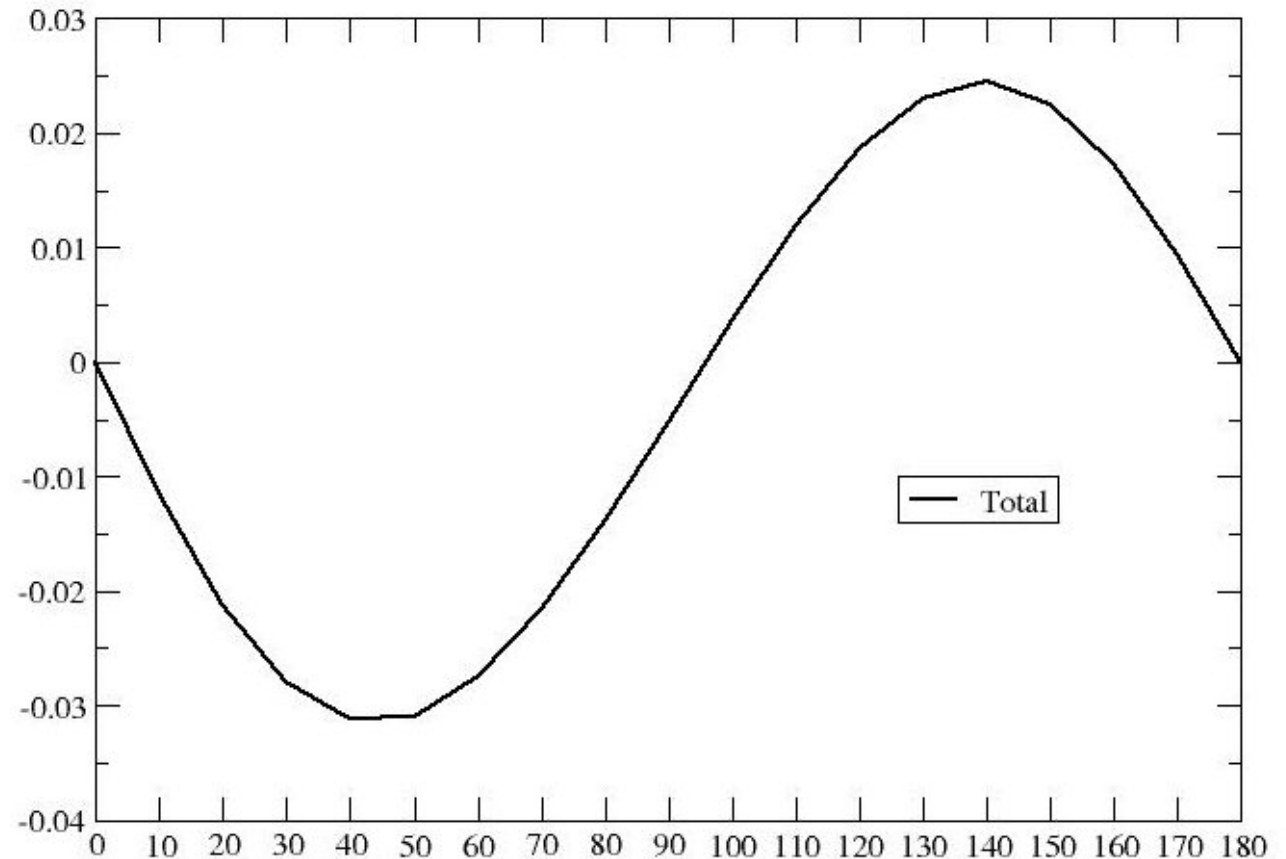
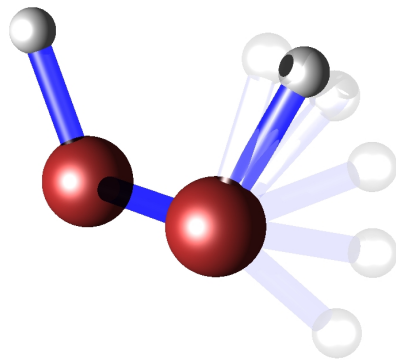
$$\checkmark E_{PV}^K \propto Z_K^5$$

✓ $E_{PV}^K = 0$, unless spin-orbit coupling is present.

Look for chiral compounds with heavy elements !

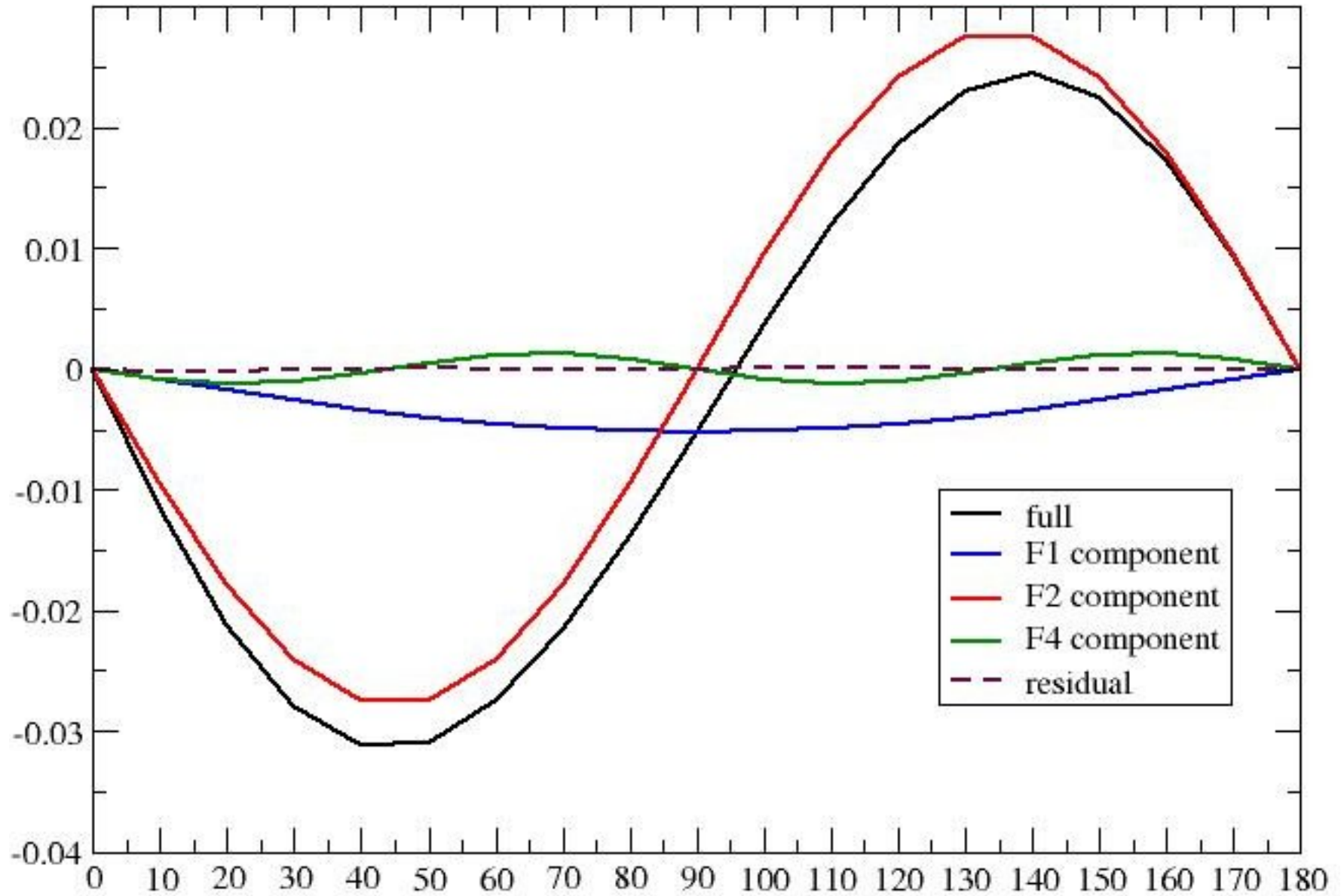
H_2X_2 (X=O, S, Se, Te, Po) — a toy system

S. F. Mason and G. E. Tranter, Mol. Phys. **53** (1984) 1091



We focus on the PV-contribution E_{PV}^{Te} from one tellurium atom of H_2Te_2 as a function of dihedral angle.

Fourier decomposition

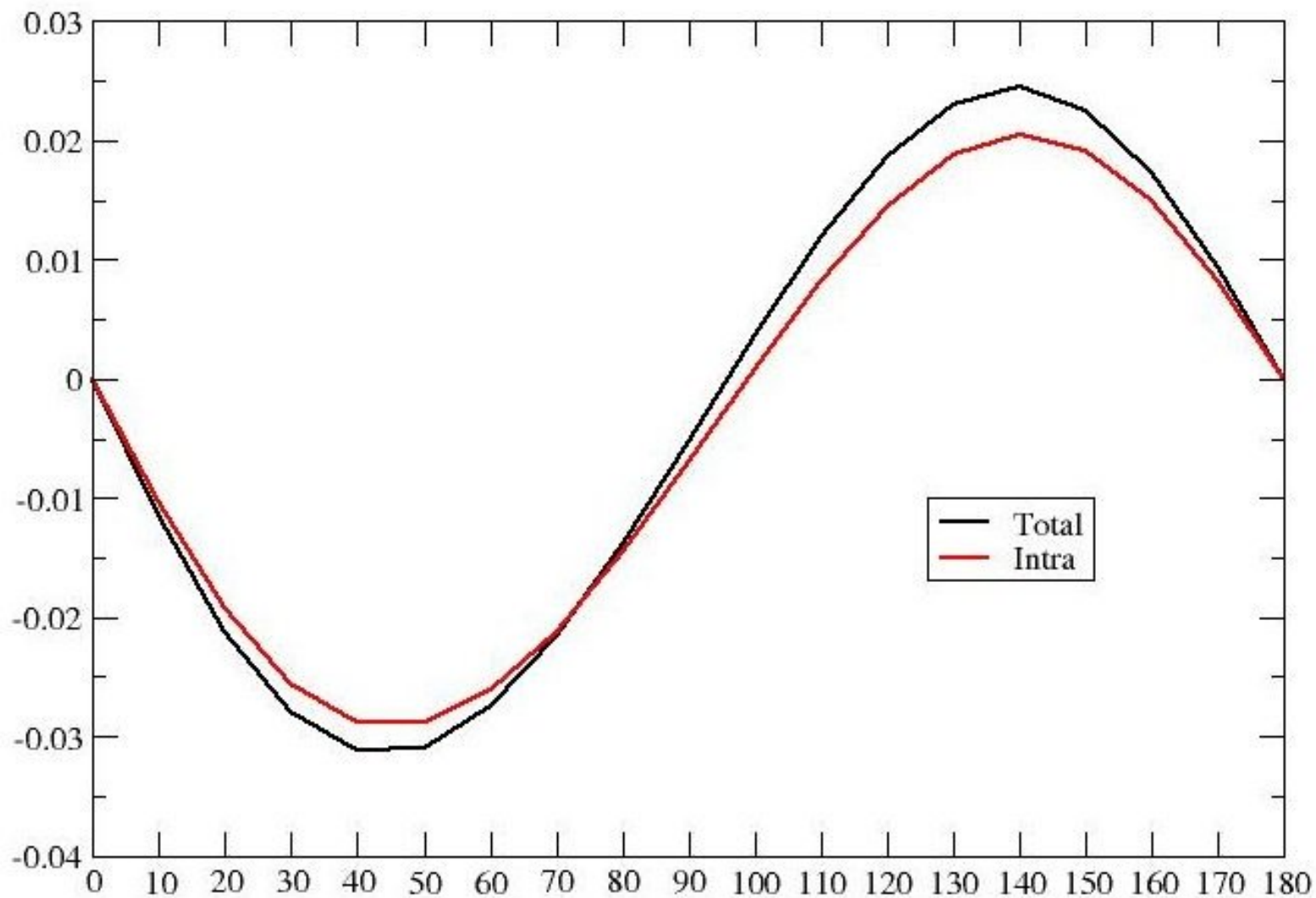


$$K_{PV}^X(\gamma) = \sum_{n=1}^{\infty} F_n \sin(n\gamma)$$

Projection analysis of H_2X_2 compounds

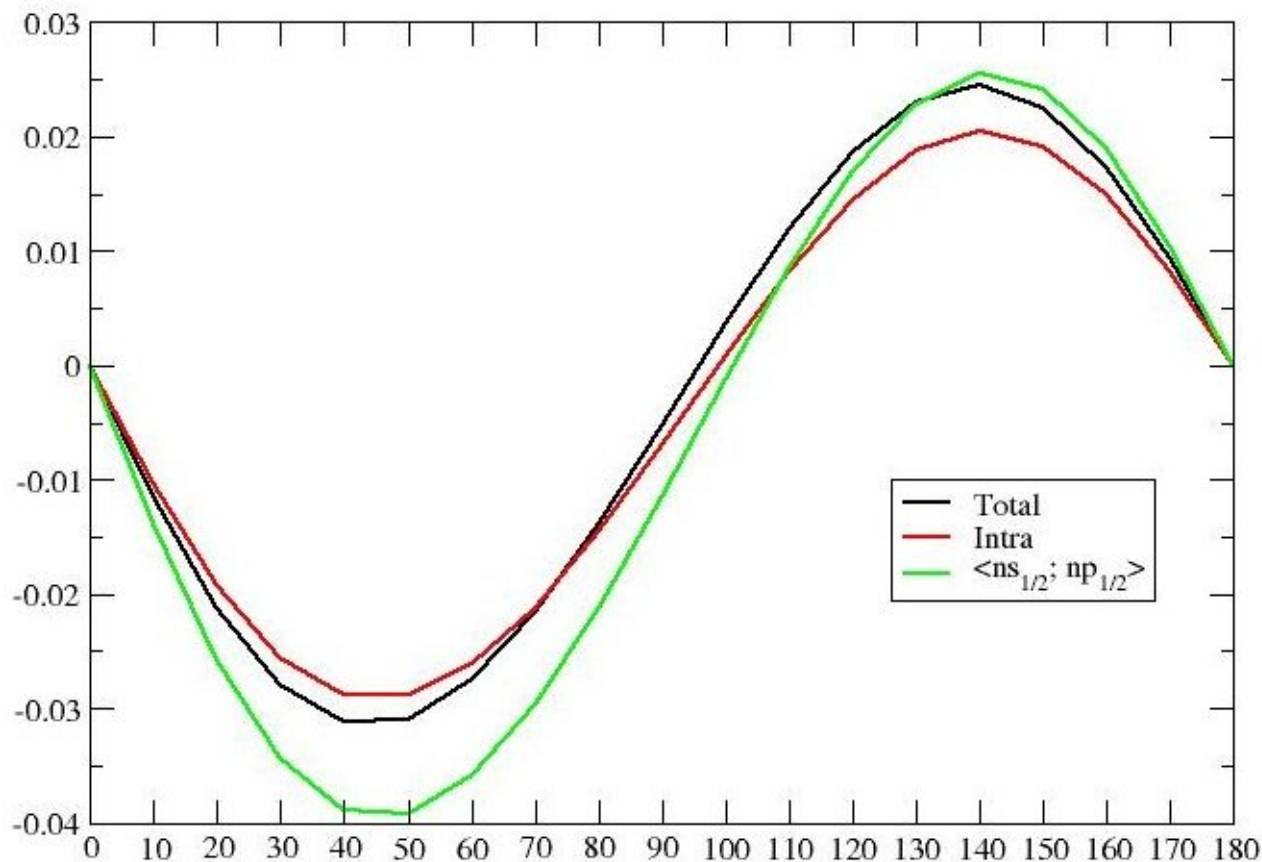
R. Bast, A. Koers, A. Severo Pereira Gomes, M. Iliáš, L. Visscher, P. Schwerdtfeger and T. Saue,

Phys. Chem. Chem. Phys. **13** (2011) 854



E_{PV}^{Te} is completely dominated by intra-atomic contributions from the same center.

Dominant intra-atomic contribution



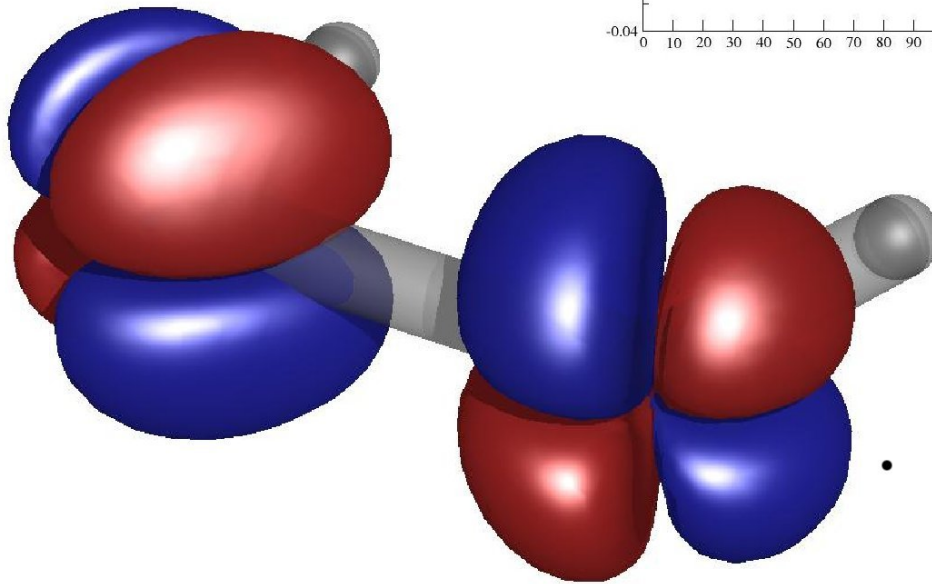
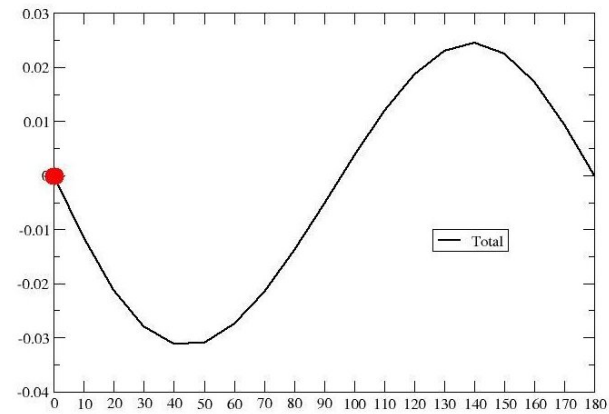
HF	H_2O_2	H_2S_2	H_2Se_2	H_2Te_2	H_2Po_2
Full	-6.729E-06	-7.435E-05	-3.163E-03	-2.787E-02	-7.955E-01
Intra	-5.879E-06	-6.876E-05	-2.717E-03	-2.459E-02	-6.334E-01
$\langle ns_{1/2} \hat{H}_{pv}^X np_{1/2} \rangle$	-8.819E-06	-8.548E-05	-3.773E-03	-3.216E-02	-7.728E-01

A non-zero contribution requires an imaginary phase in the mixing coefficient between $s_{1/2}$ and $p_{1/2}$.

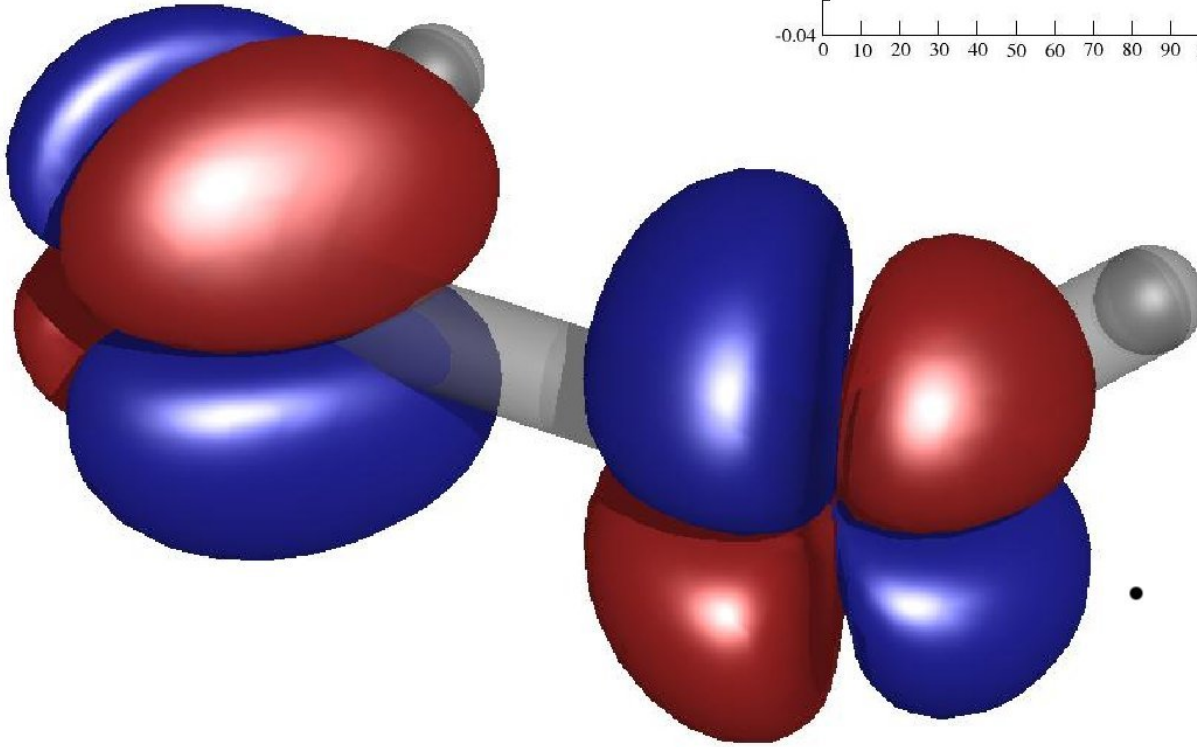
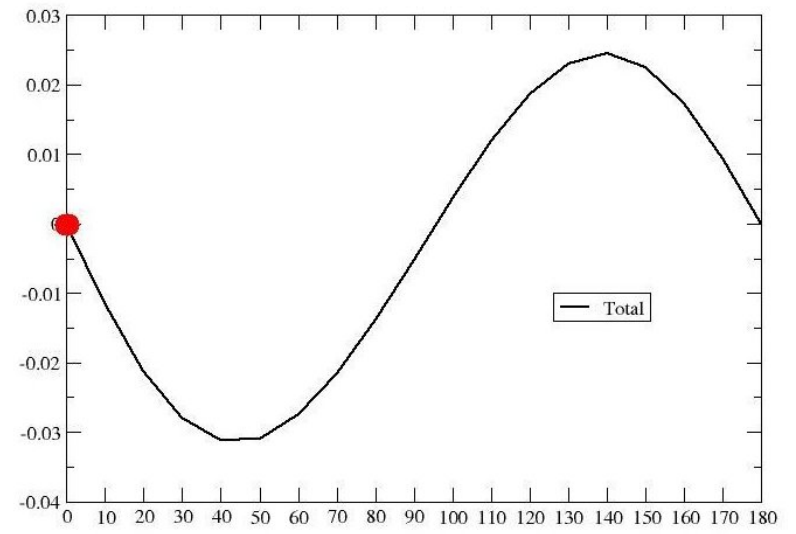
A real-space approach

$$E_{PV}^A = \frac{G}{2\sqrt{2}} Q_W^A \sum_i \langle \psi_i | \gamma_5 \rho_A | \psi_i \rangle = \frac{G}{2\sqrt{2}} Q_W^A \int \gamma^5(\mathbf{r}) \rho_A(\mathbf{r}) d\tau; \quad \gamma_5 = \begin{bmatrix} 0_2 & I_2 \\ I_2 & 0_2 \end{bmatrix}$$

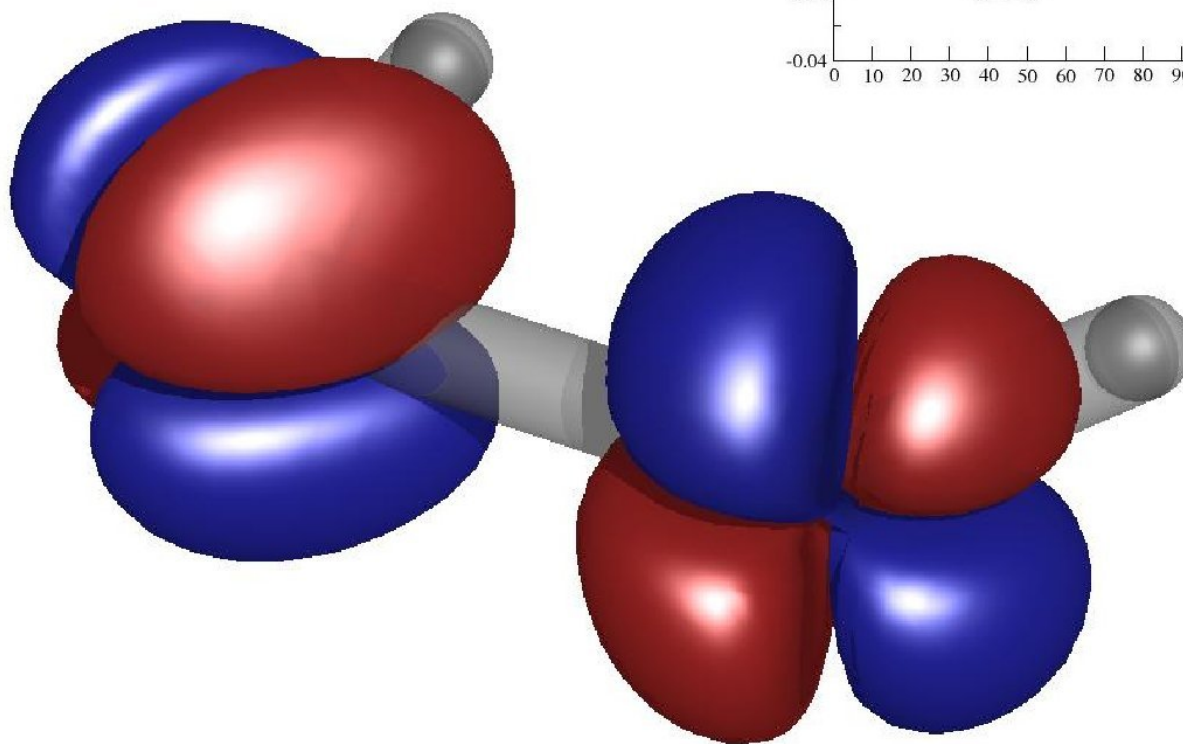
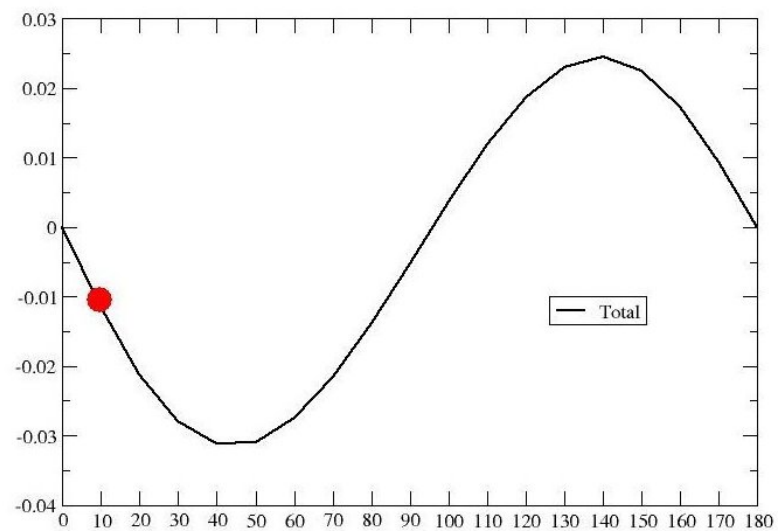
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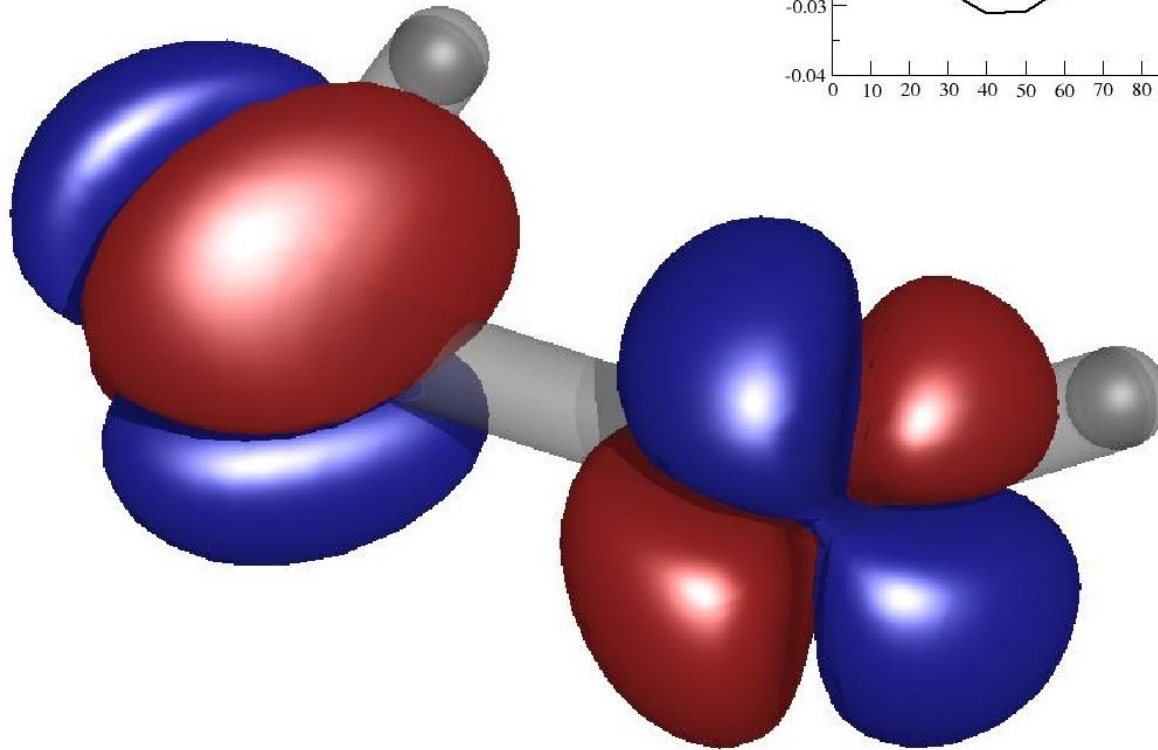
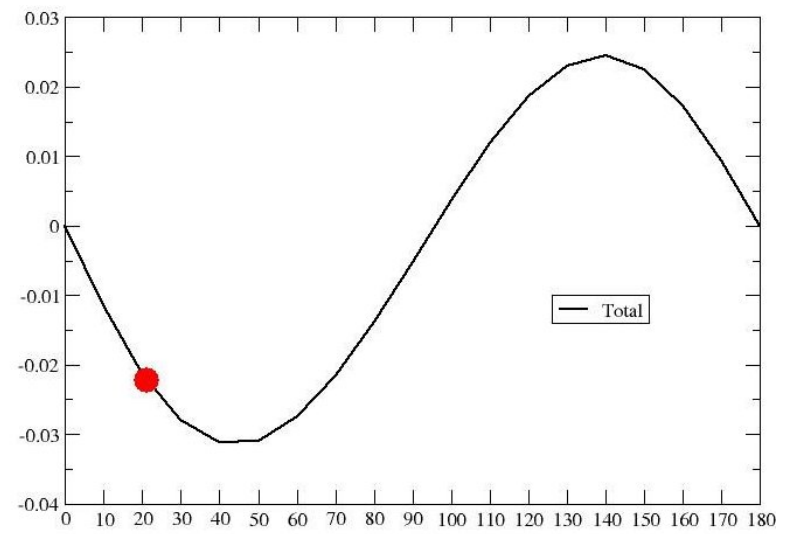


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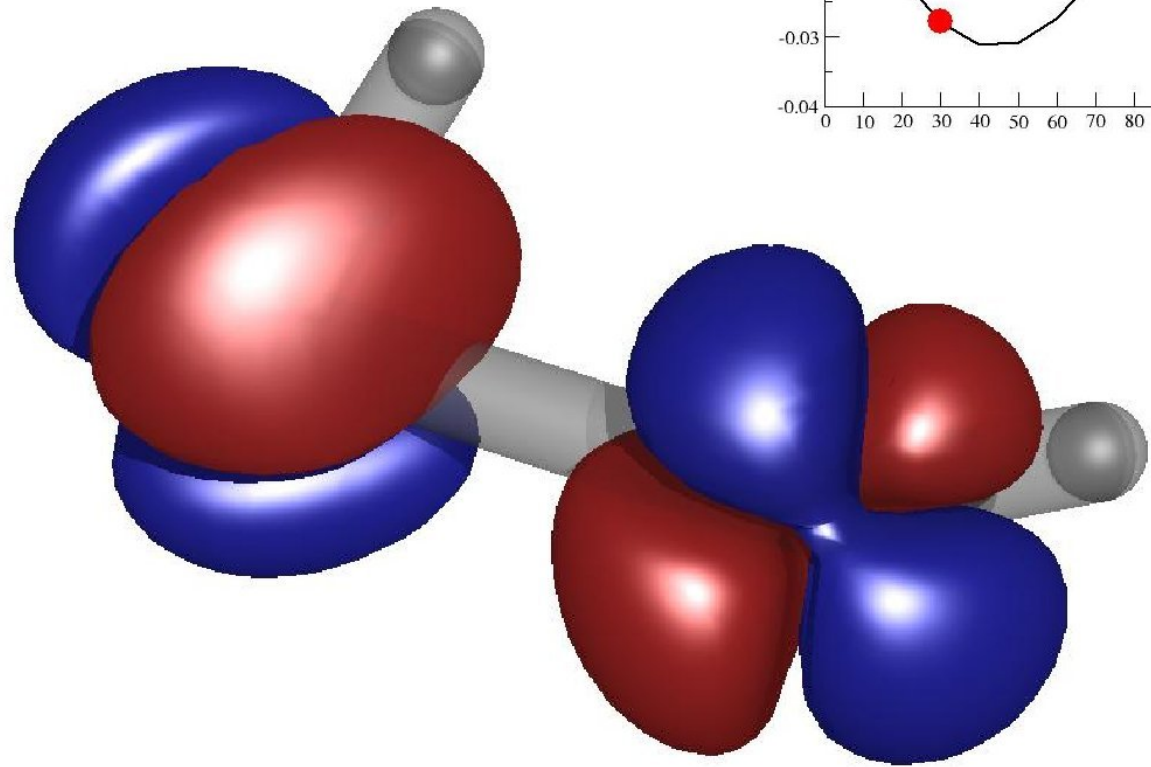
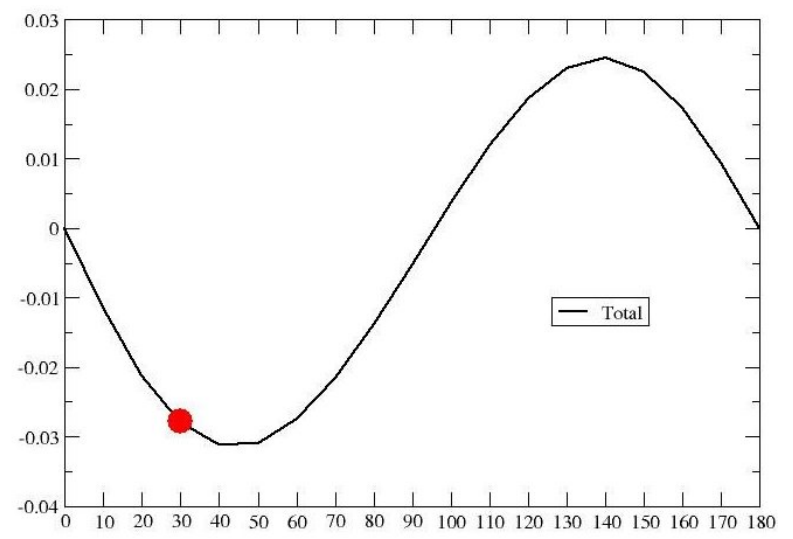


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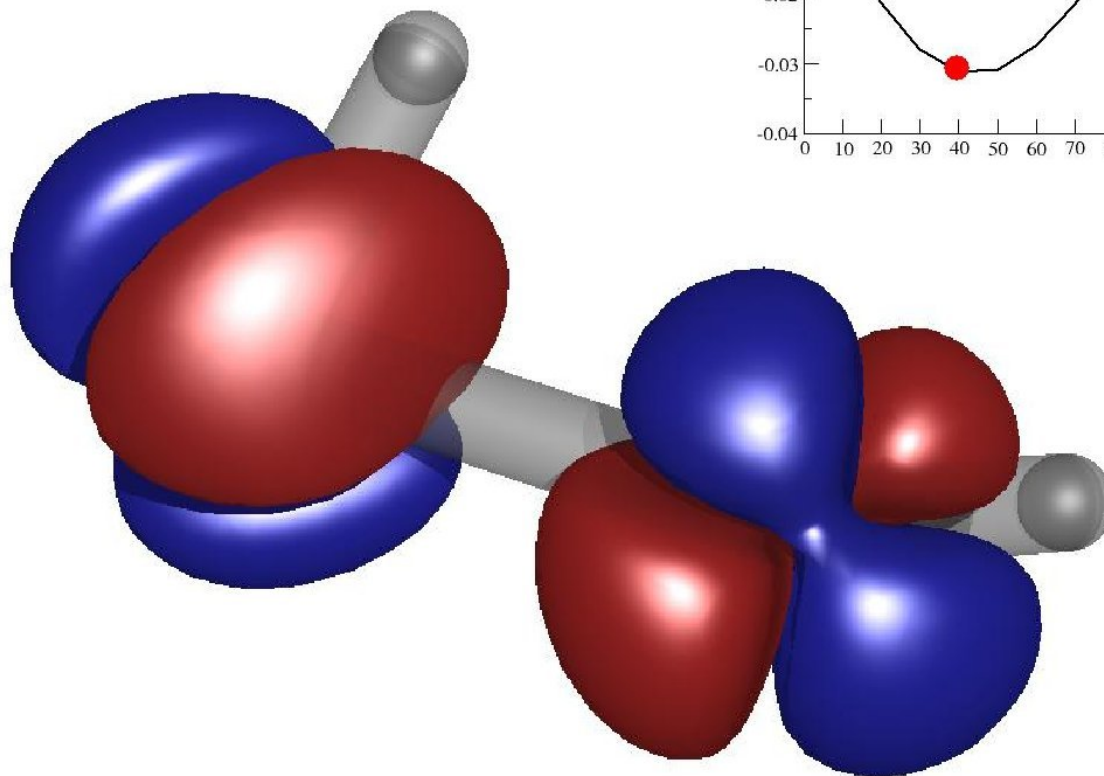
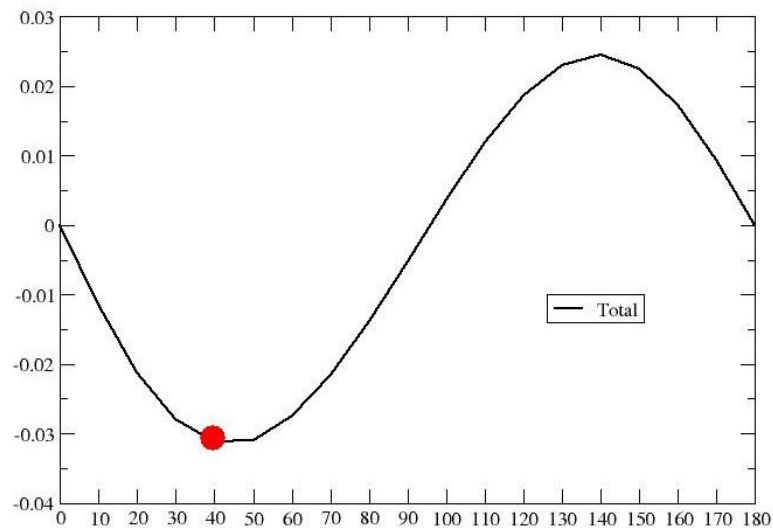




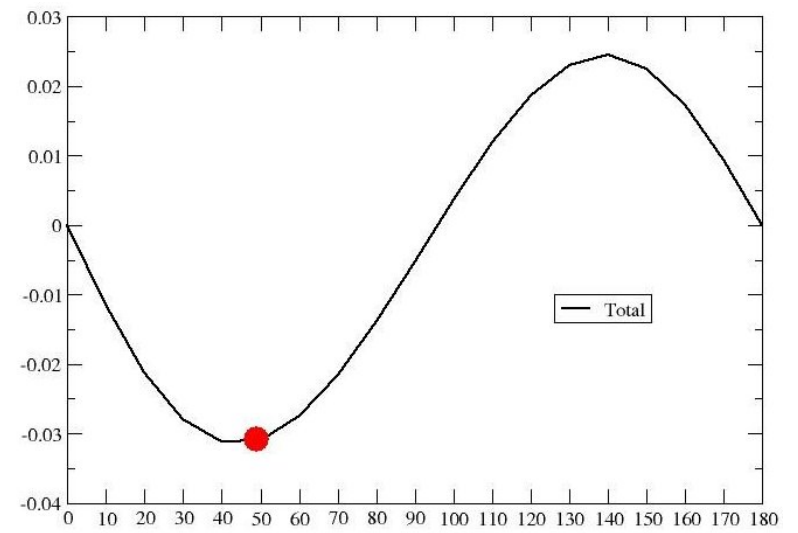
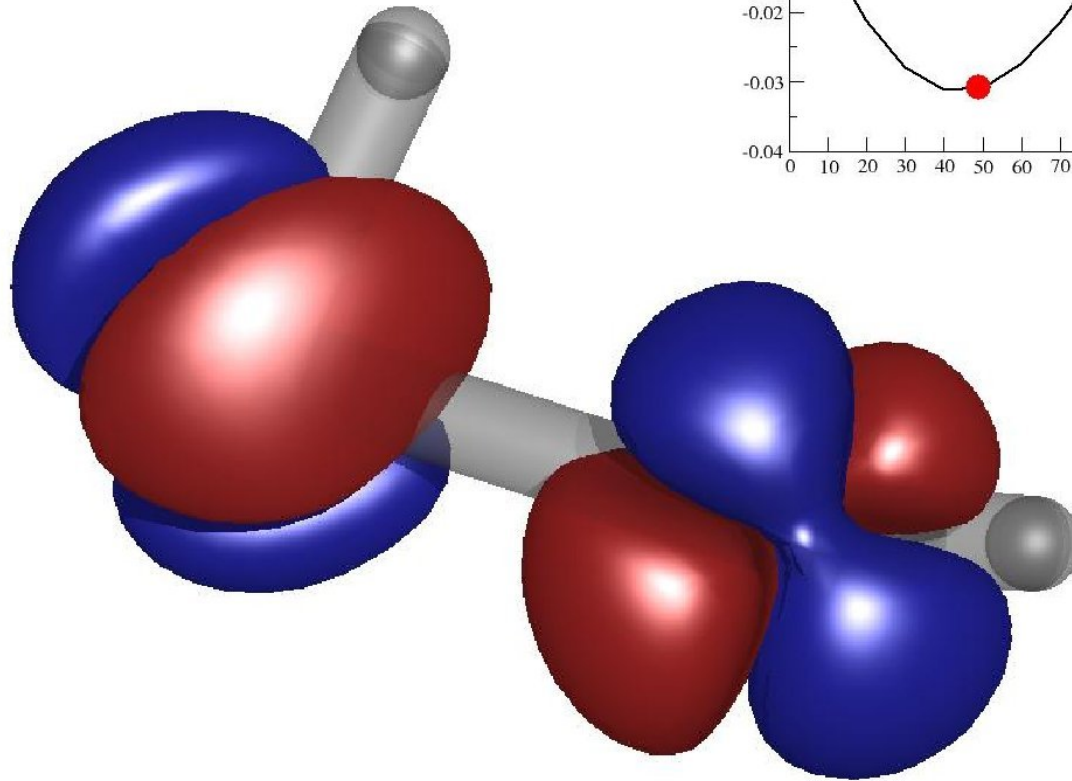
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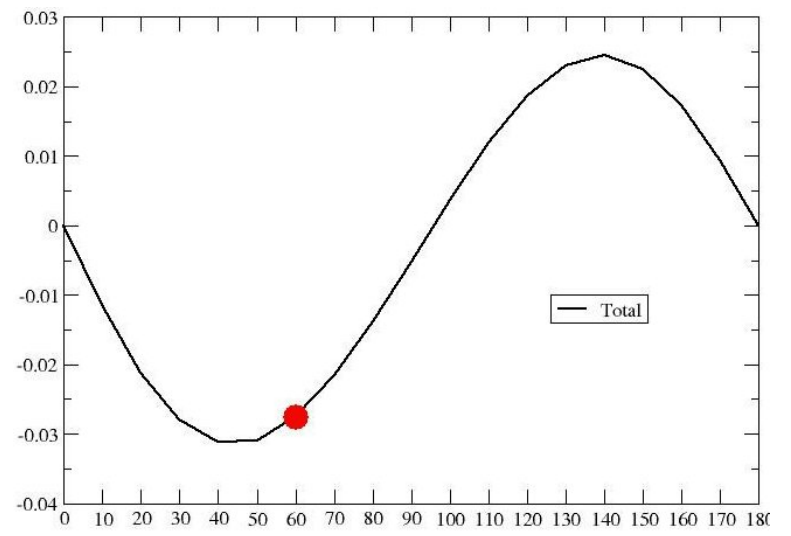
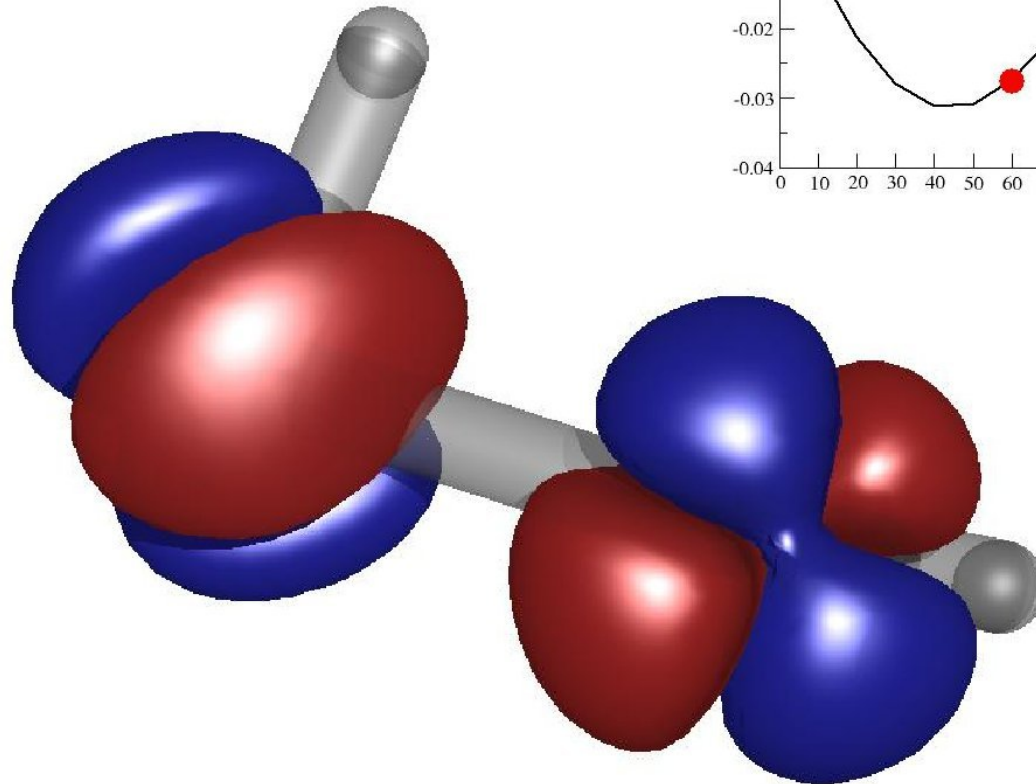
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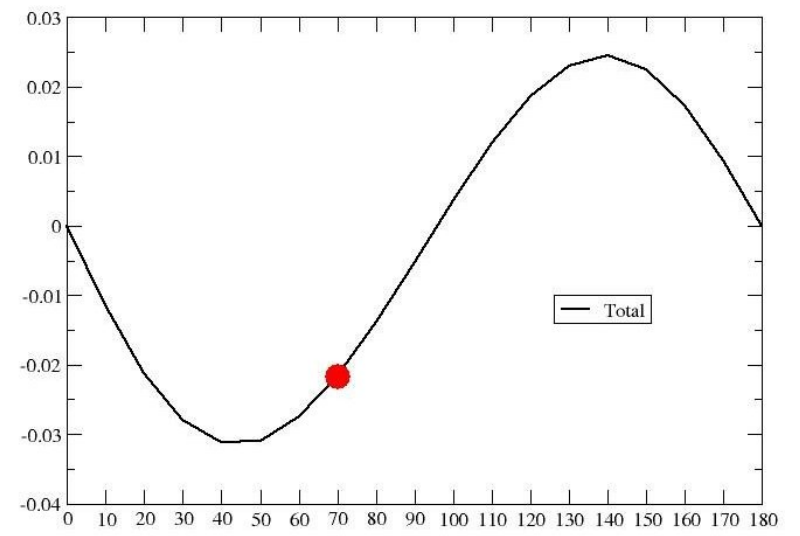
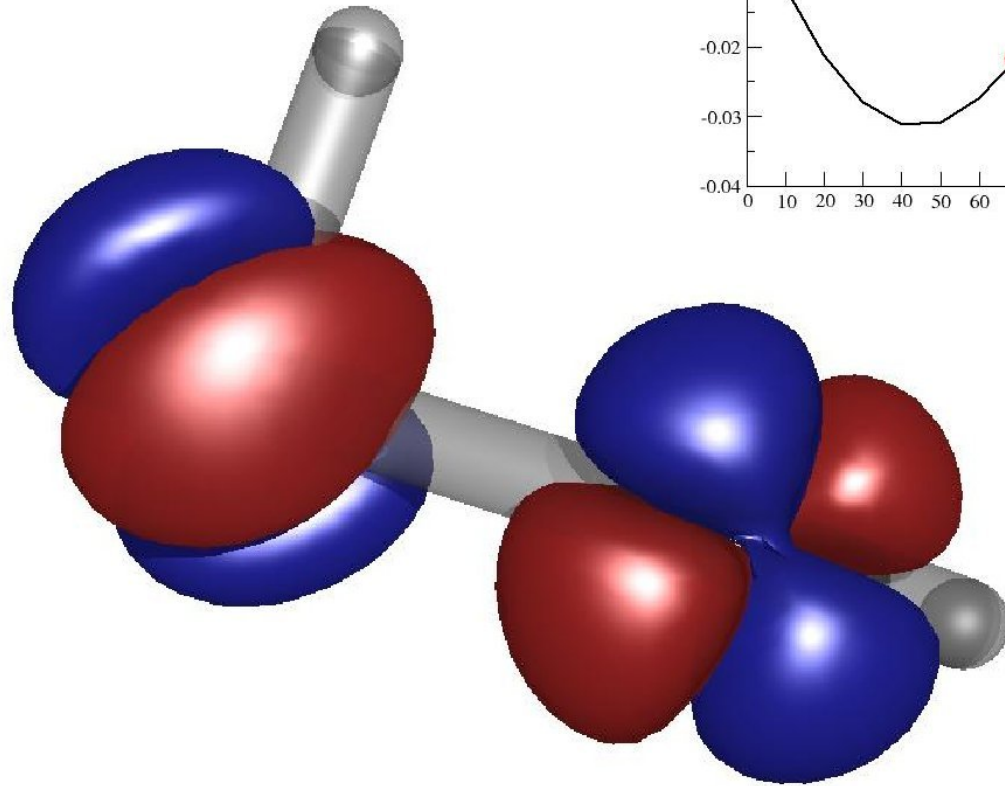
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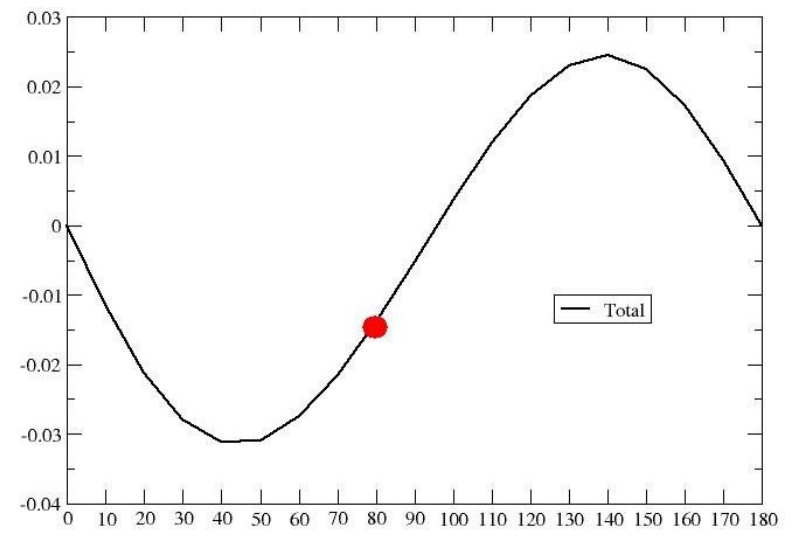
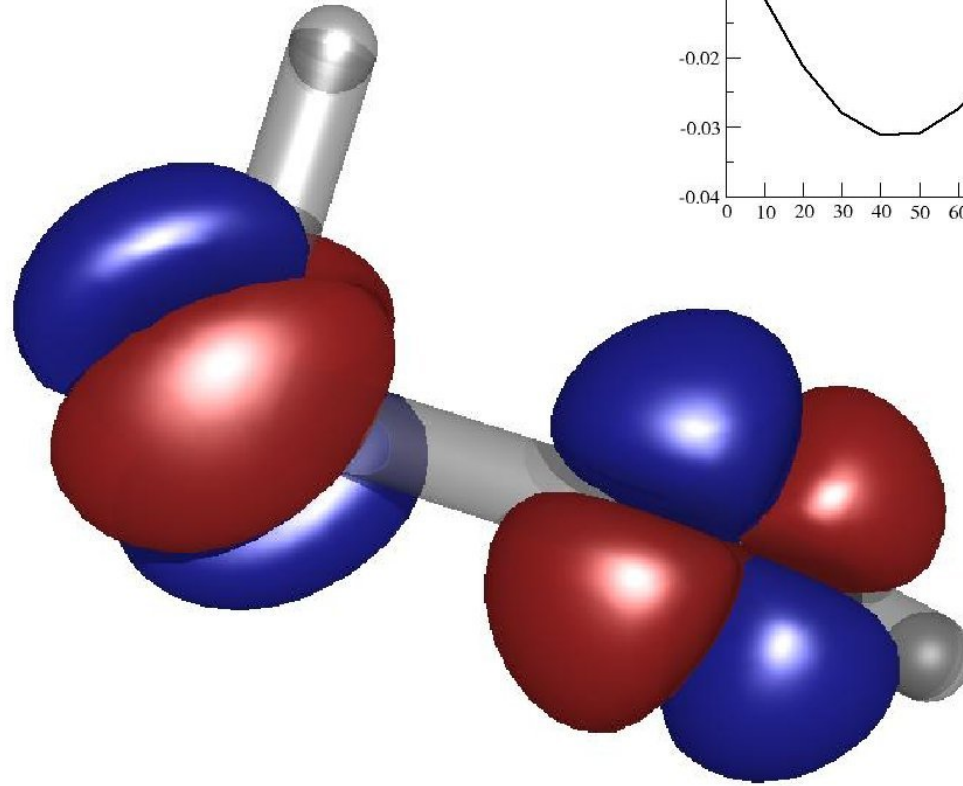


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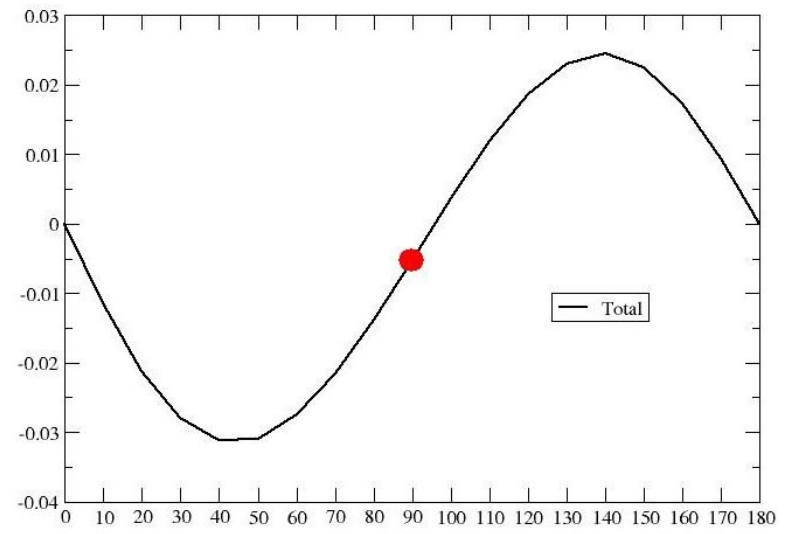
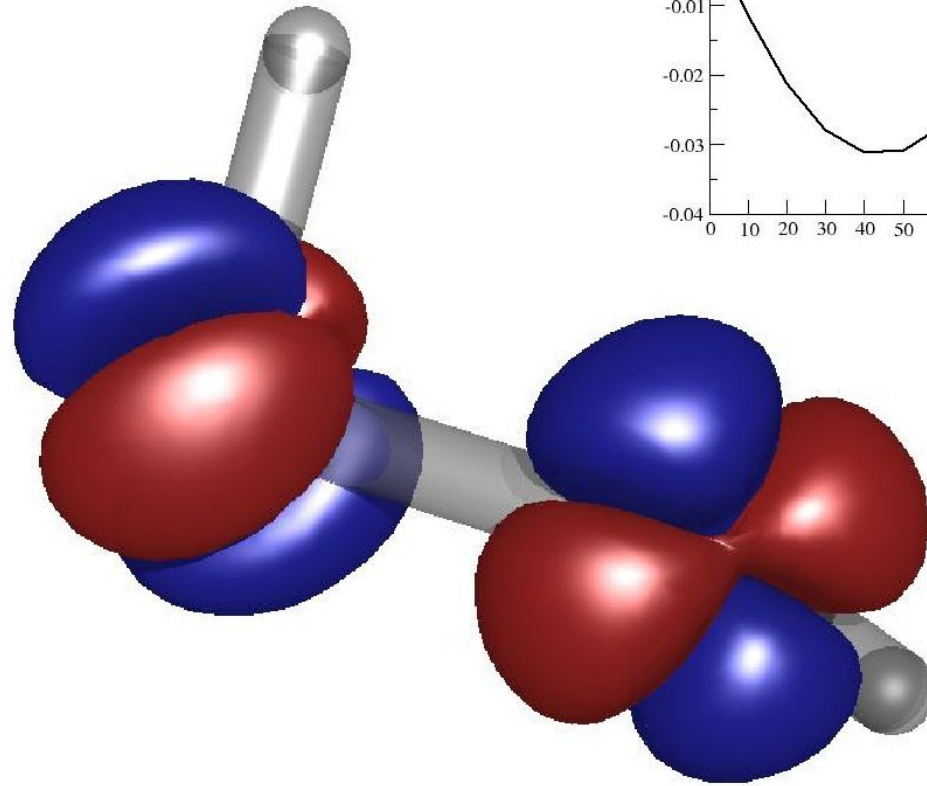


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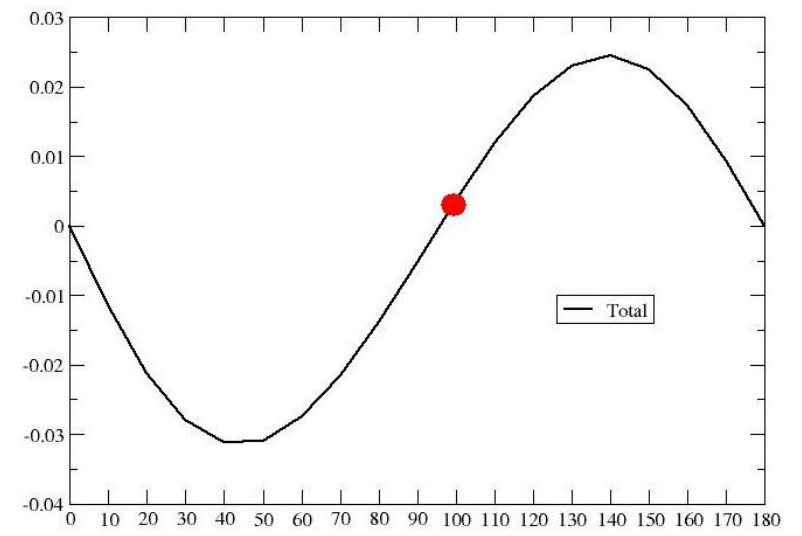
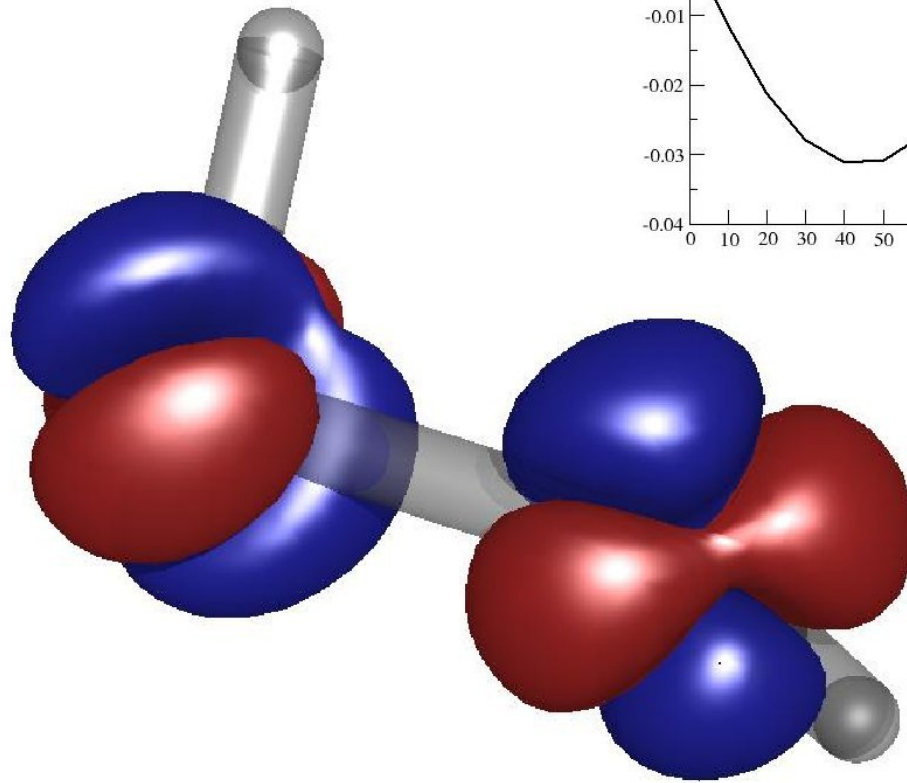




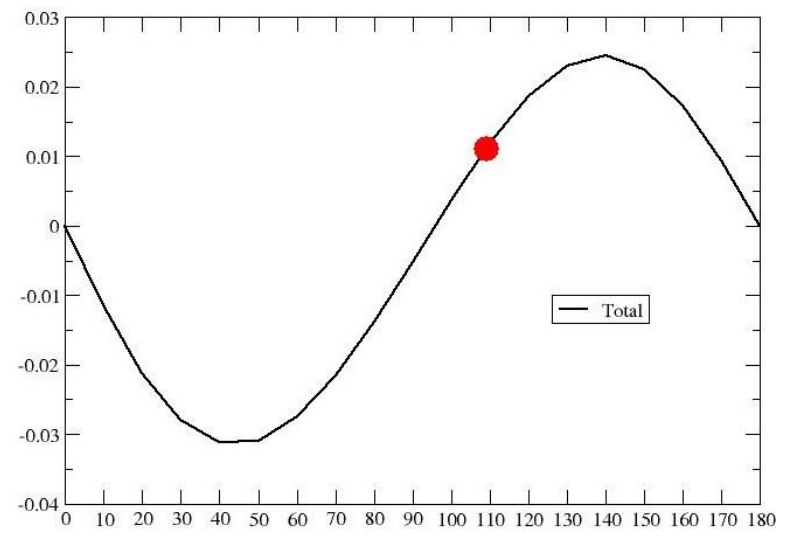
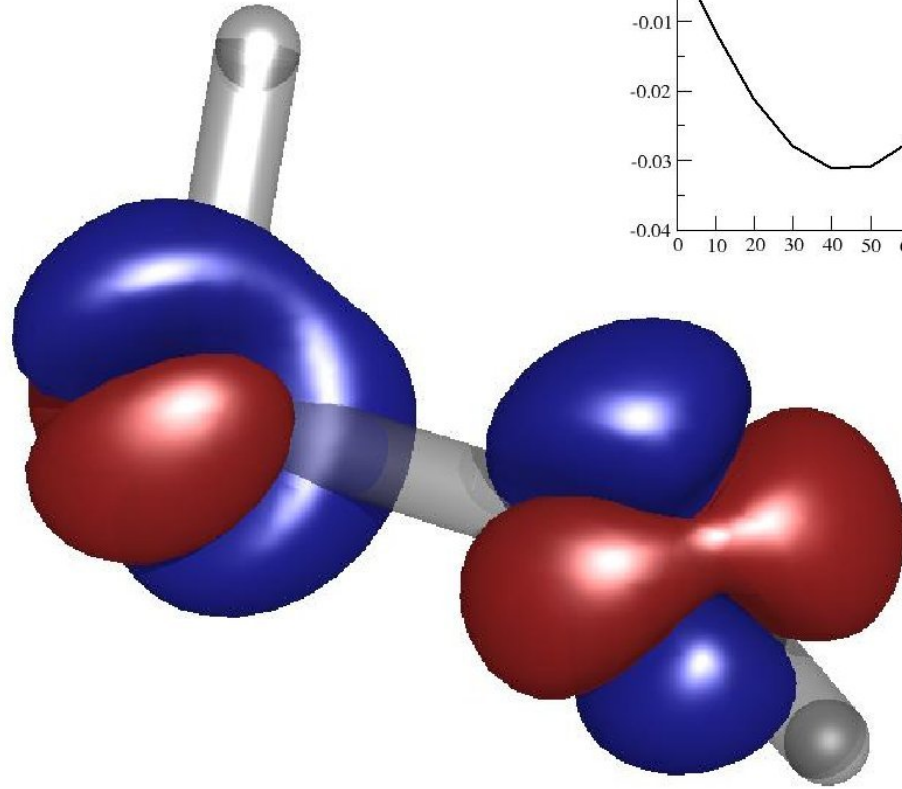
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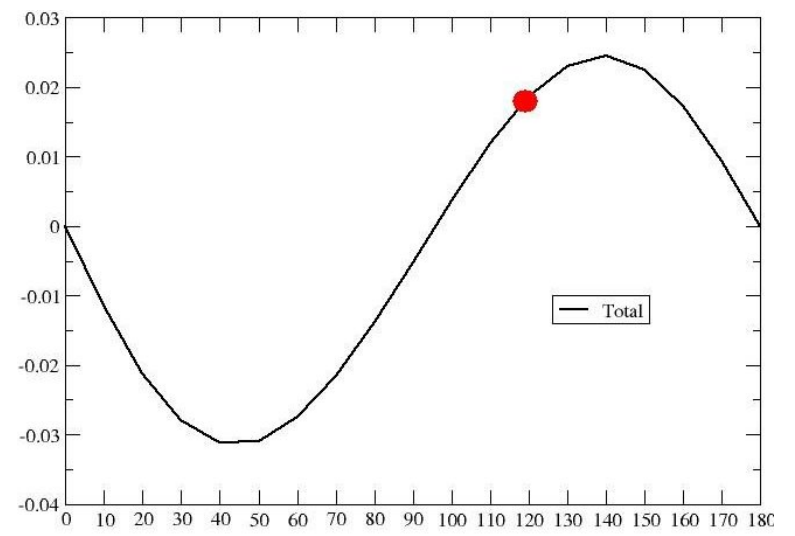
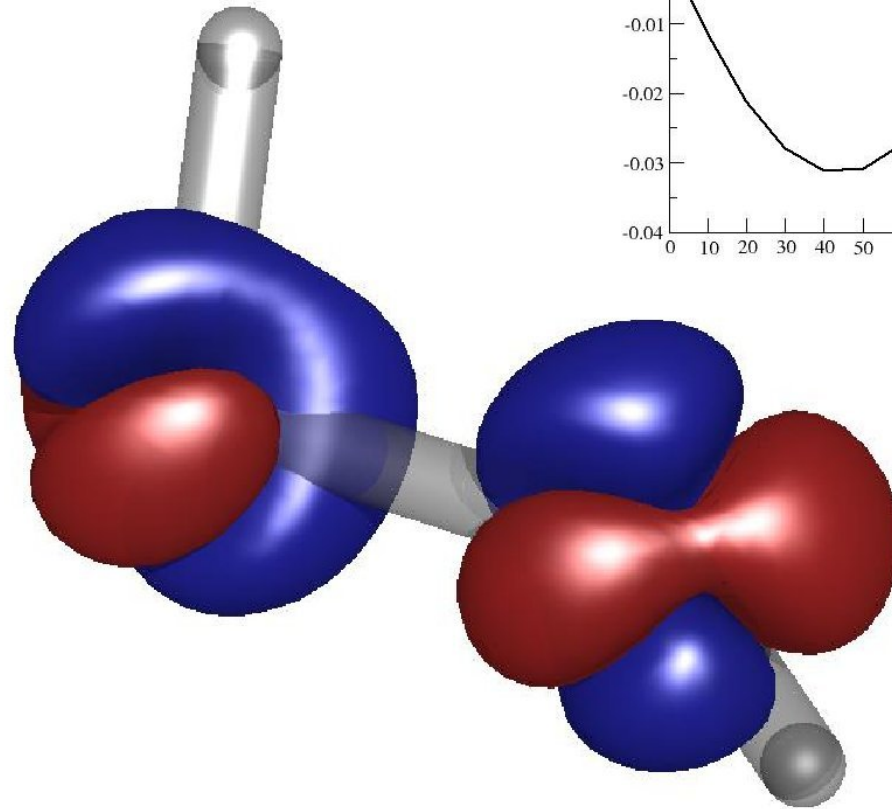
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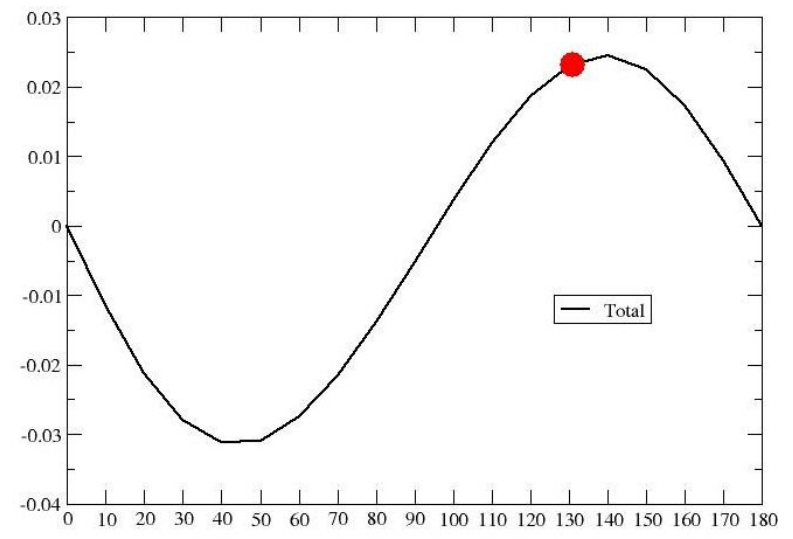
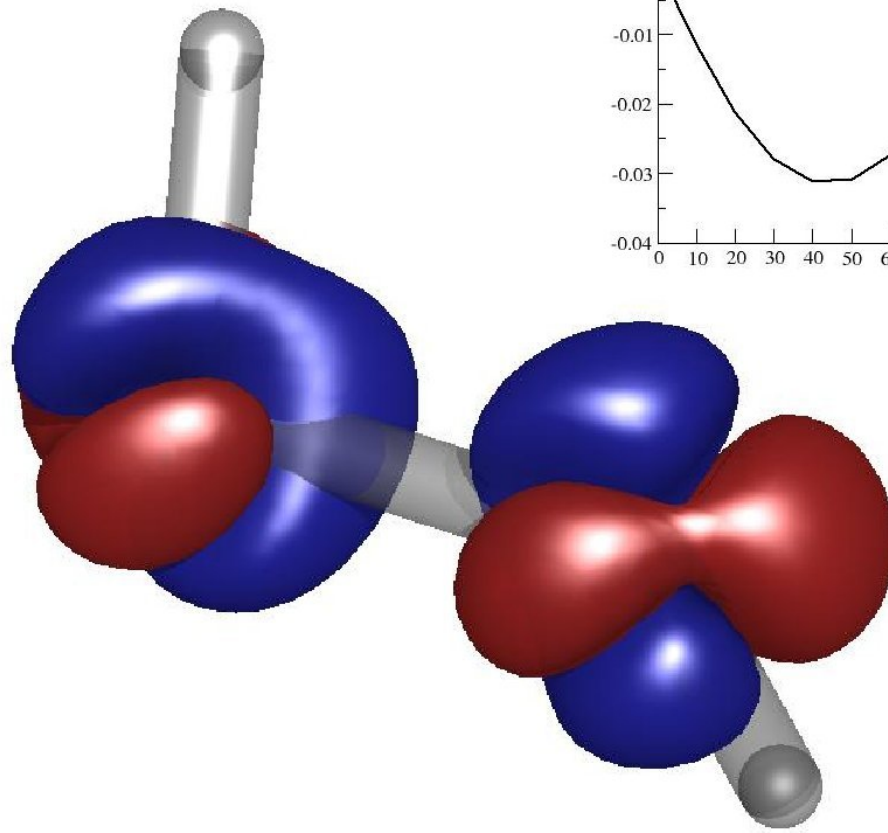
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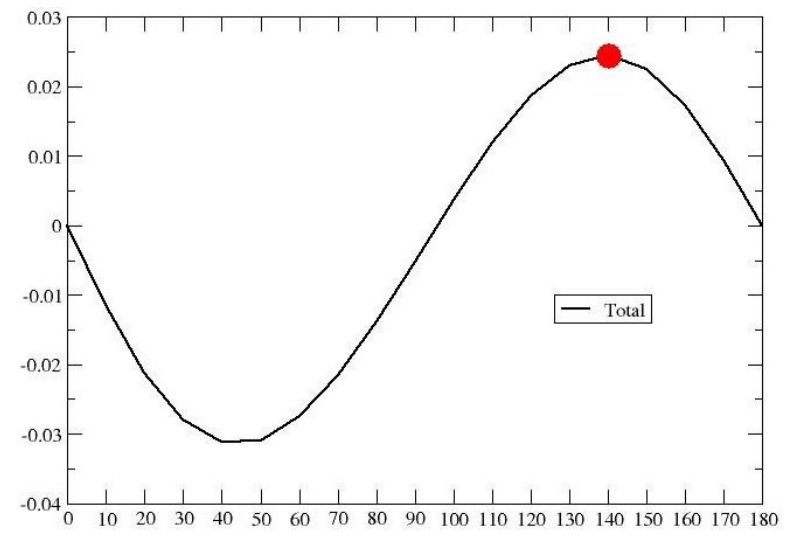
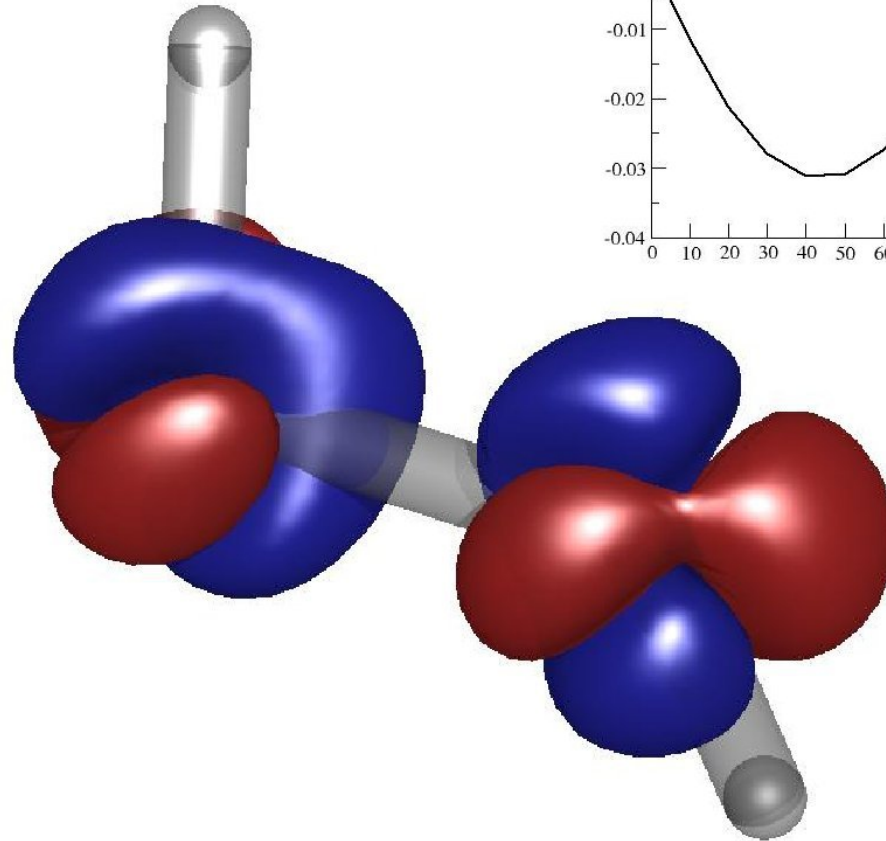
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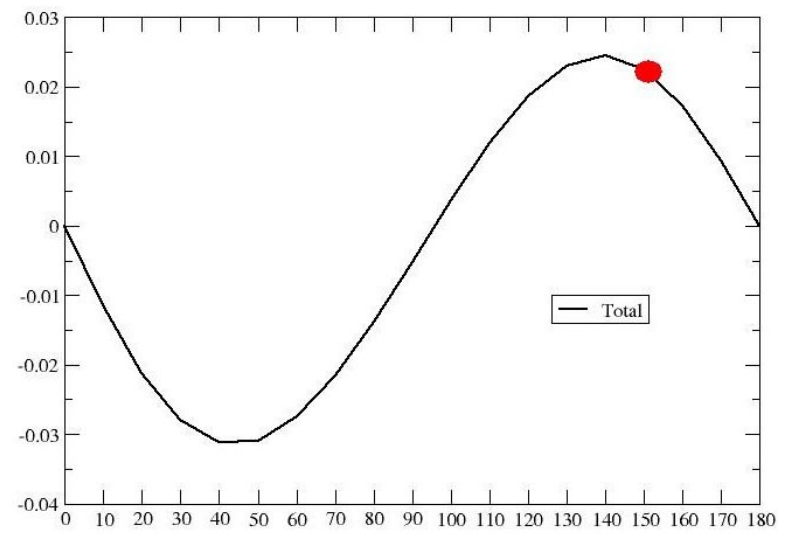
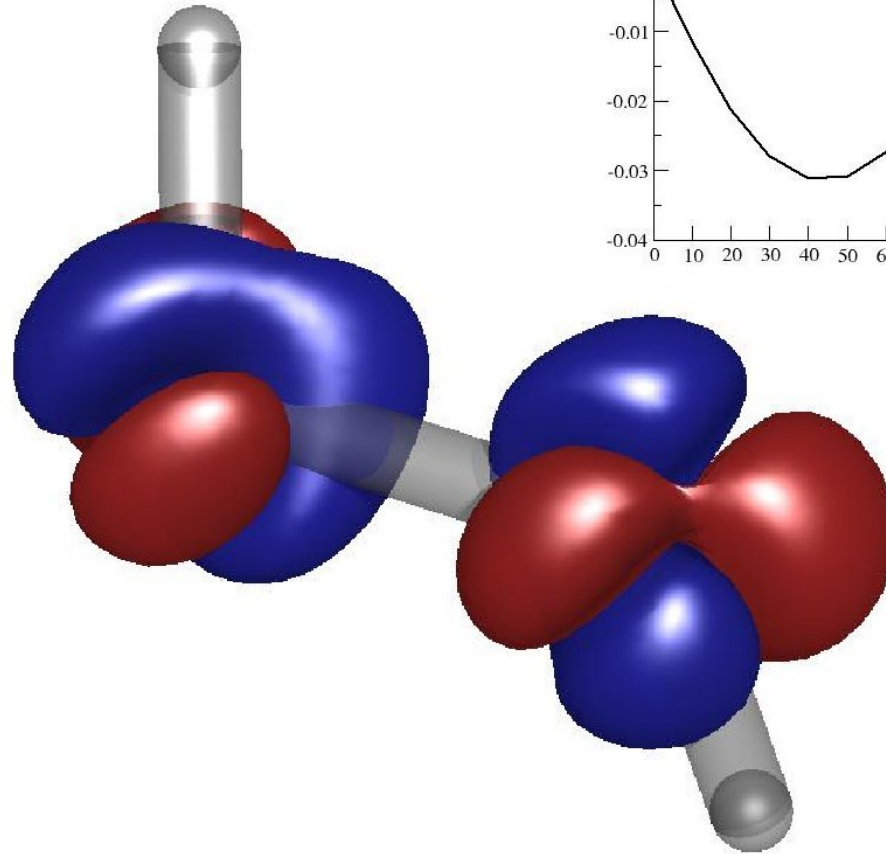
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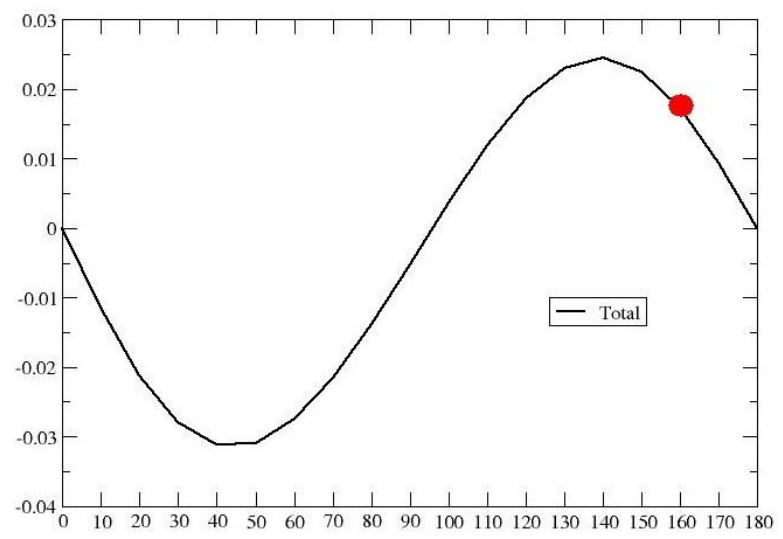
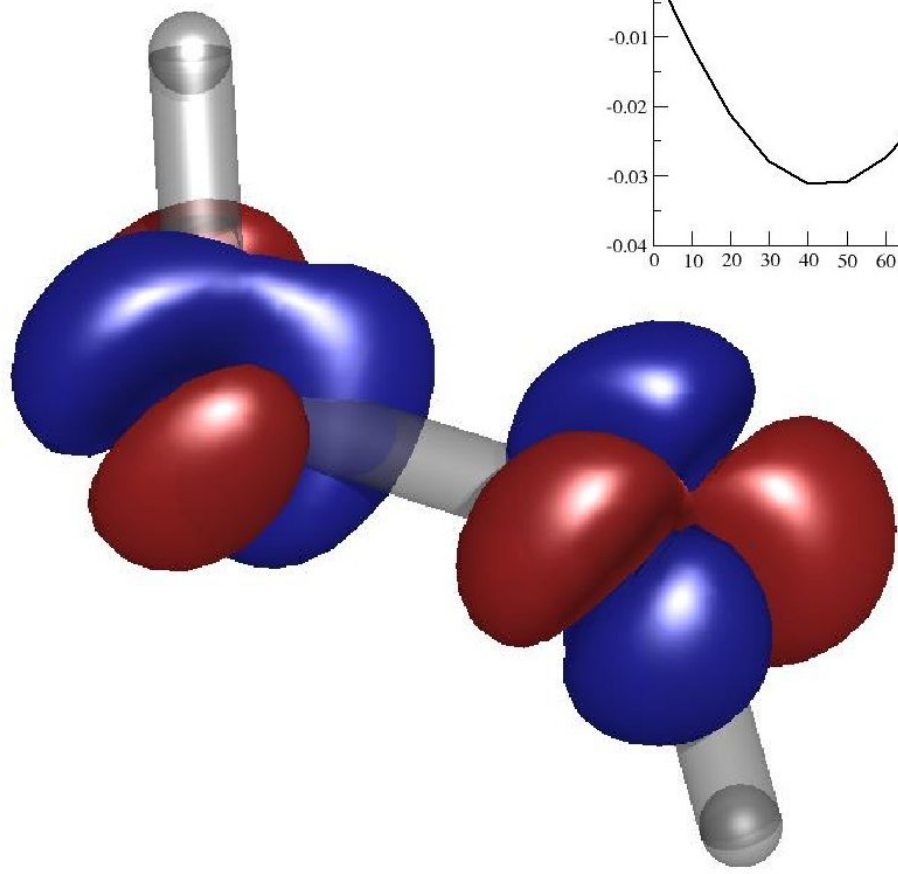
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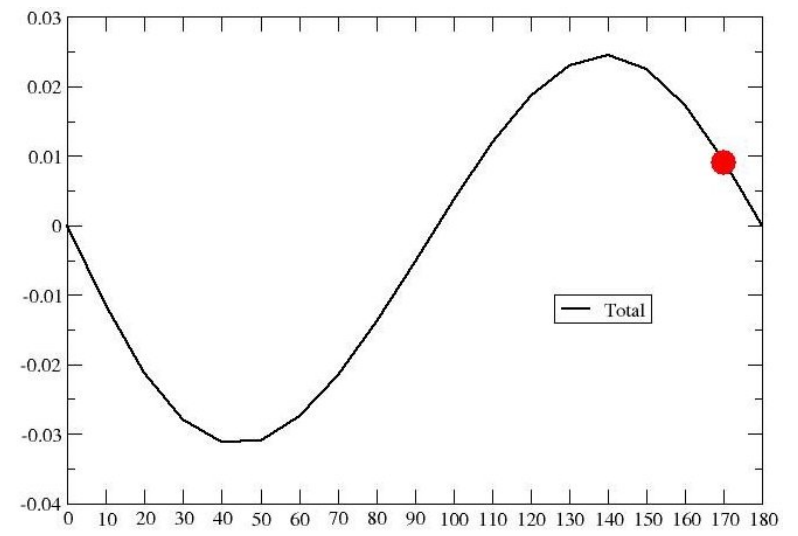
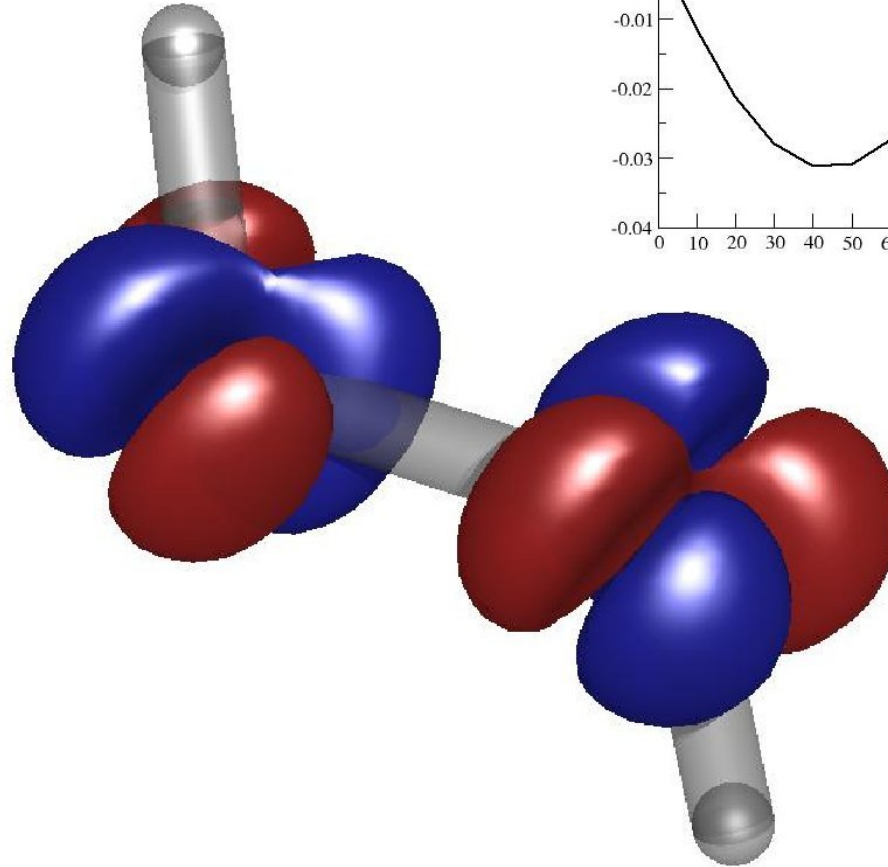
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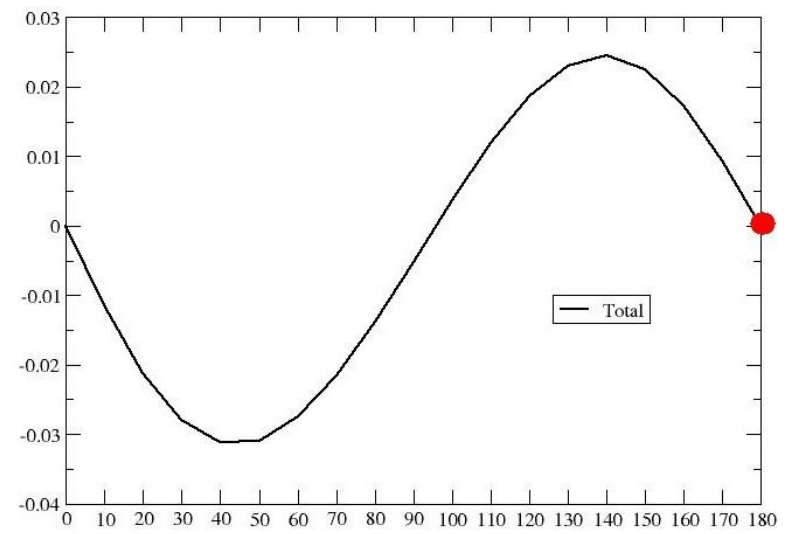
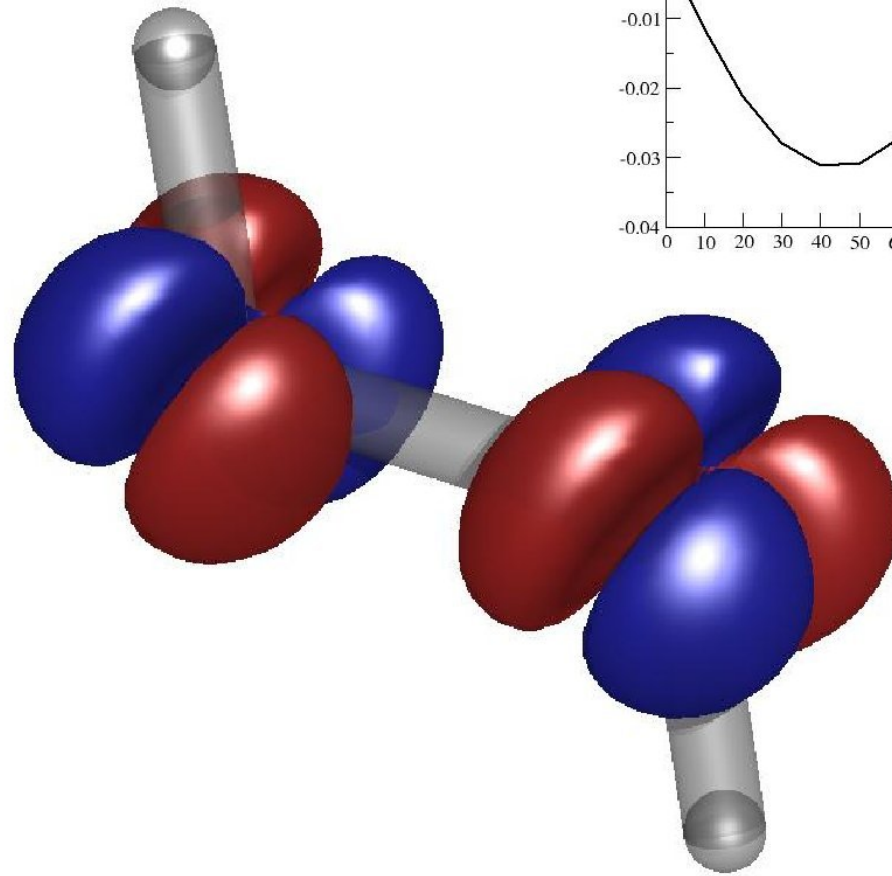
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170

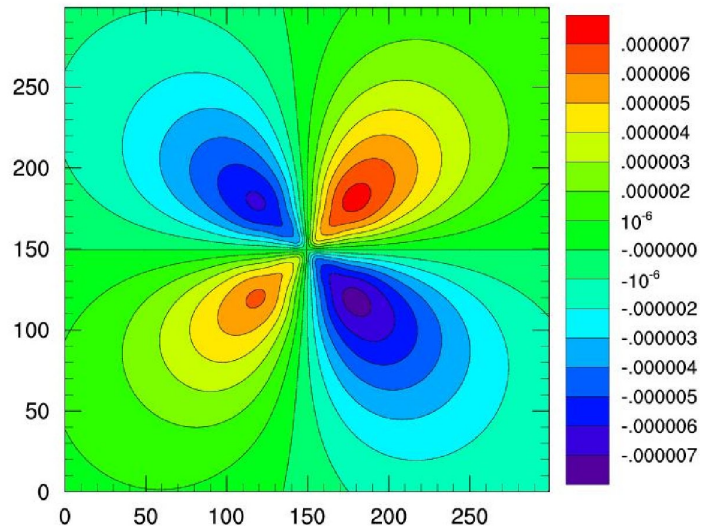


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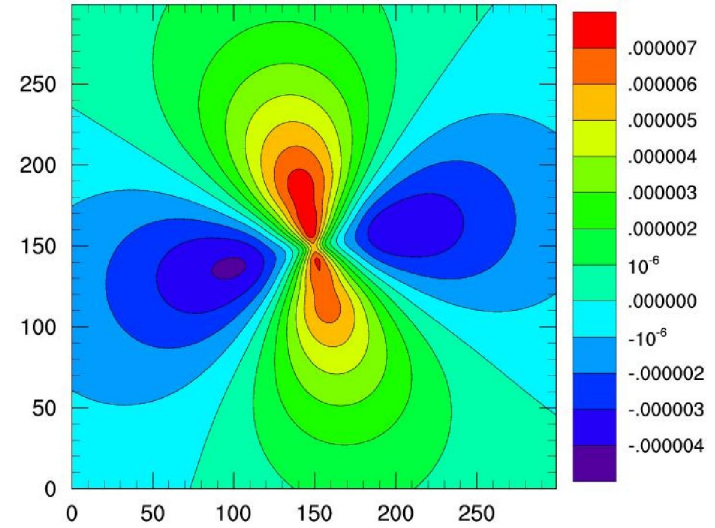


2D plots of the γ_5 density around the Te nucleus

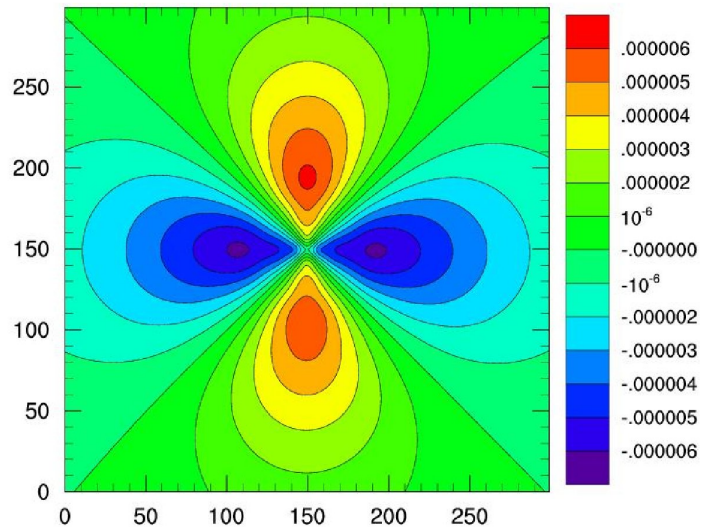
0 xy



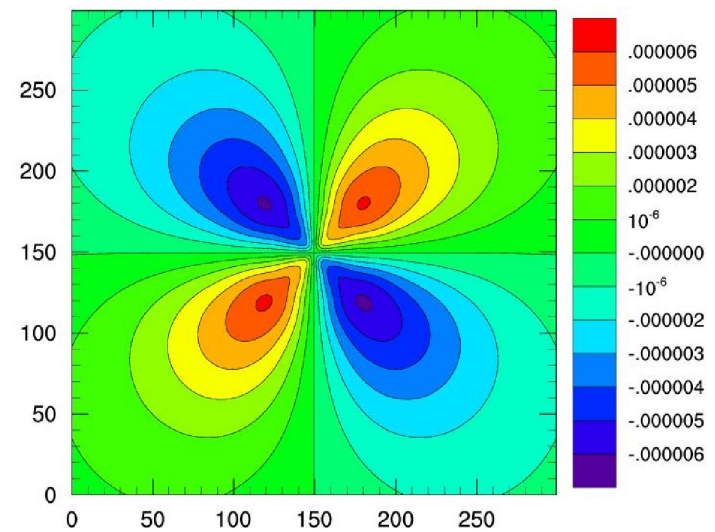
50 xz



90 xz



180 yz



Conclusions and perspectives

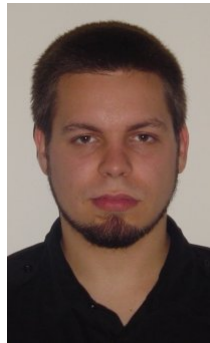
- Properties associated with the electronic density near or at the nucleus provide useful information about the local chemical environment
- A computational protocol for the simulation of **Mössbauer isomer shifts** for heavy elements has been developed
 - **Mercury fluorides:**
 - * DFT is not able to qualitatively reproduce the non-monotonic decrease of the contact density of the heavier atom mercury that we obtain from our benchmark CCSD(T) calculations and even at the HF level.
 - * Projection analysis shows that this non-monotonic trend is due to increasing polarization/hybridization of the valence $s_{1/2}$ orbital of mercury.
 - **Xenon fluorides:**
 - * DFT shows good performance
 - * Relative density shifts are dominated by overlap effects
- A detailed analysis of the mechanism of **parity violation** may shed light on the electronic structure of chiral molecules
- <http://dirac.chem.vu.nl>

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(Zürich)

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Christian Chardonnet (Paris)

Anne Amy-Klein (Paris)

Stanislav Komorovsky (Toulouse)

Jeanne Crassous (Rennes)

Benôit Darquié (Paris)

Christophe Daussey (Paris)

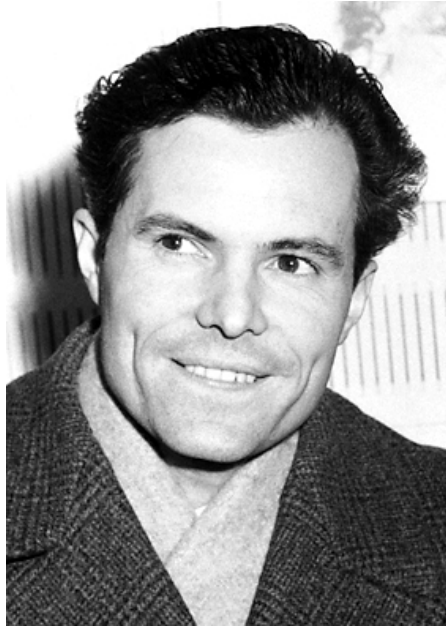
Aafke van Meteren (Toulouse)

Peter Schwerdtfeger (Auckland)

Pierre Asselin (Paris)

Thérèse Huet (Lille)

Explain it!



Rudolf Mössbauer

The most important thing is, that you are able to explain it!

You will have exams, there you have to explain it.

Eventually, you pass them, you get your diploma and you think, that's it!

– No, the whole life is an exam, you'll have to write applications, you'll have to discuss with peers...

So learn to explain it!

You can train this by explaining to another student, a colleague.

If they are not available, explain it to your mother – or to your cat!

