

LONG-RANGE INTERACTIONS BETWEEN MOLECULES

ADRIAN BATISTA

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CHEMISTRY

INTRODUCTION

Gas-Phase Molecular Dynamics

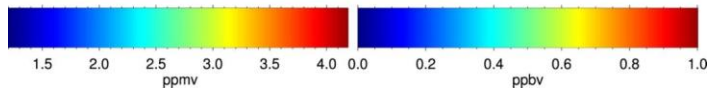
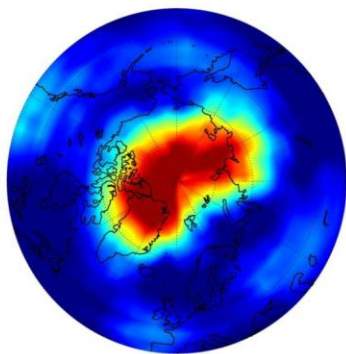
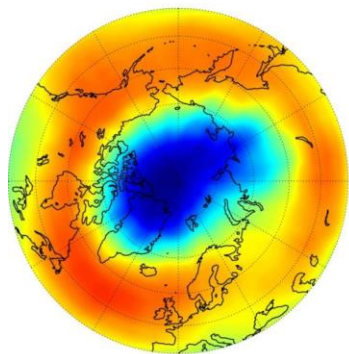
Atmospheric Chemistry

Astrochemistry

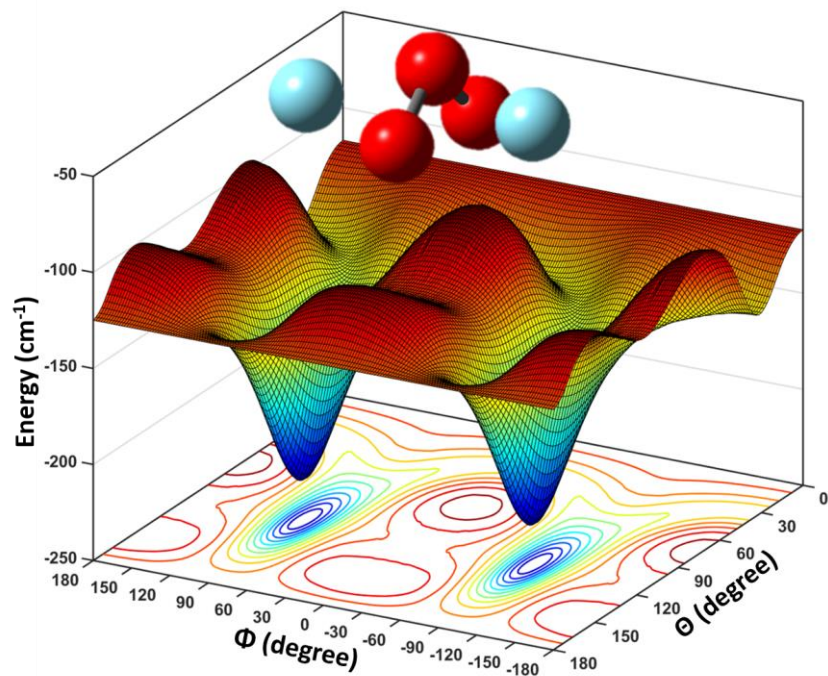
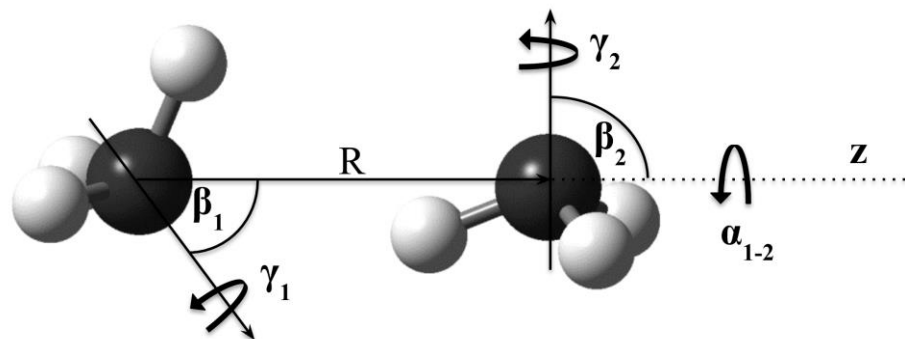
Combustion (Automobile & Aircraft Industries)

MIPAS O3 20110318 50.00 hPa

MIPAS CLO am 20110318 50.00 hPa

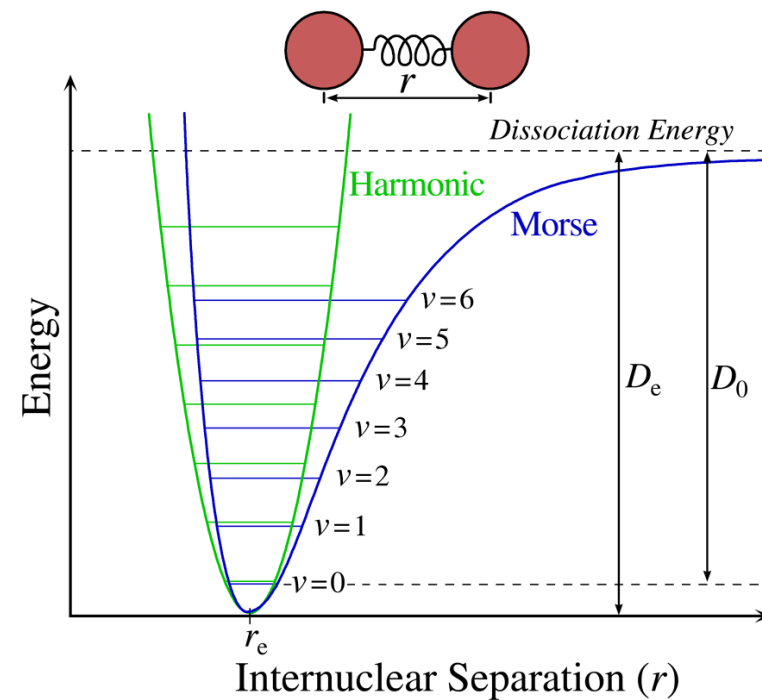


INTRODUCTION



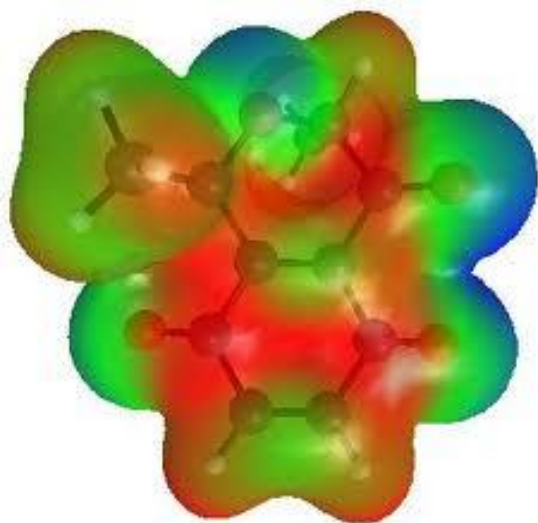
Potential Energy Surface

- Energy as a function of molecular geometry



$$\vec{F} = -\nabla V(X)$$

... BUT, WHAT DO YOU MEAN BY *MULTIPOLES* ?



Representation of the
electron density of the
molecule

Charge

$$q = q_1 + q_2 + \dots$$

Dipole

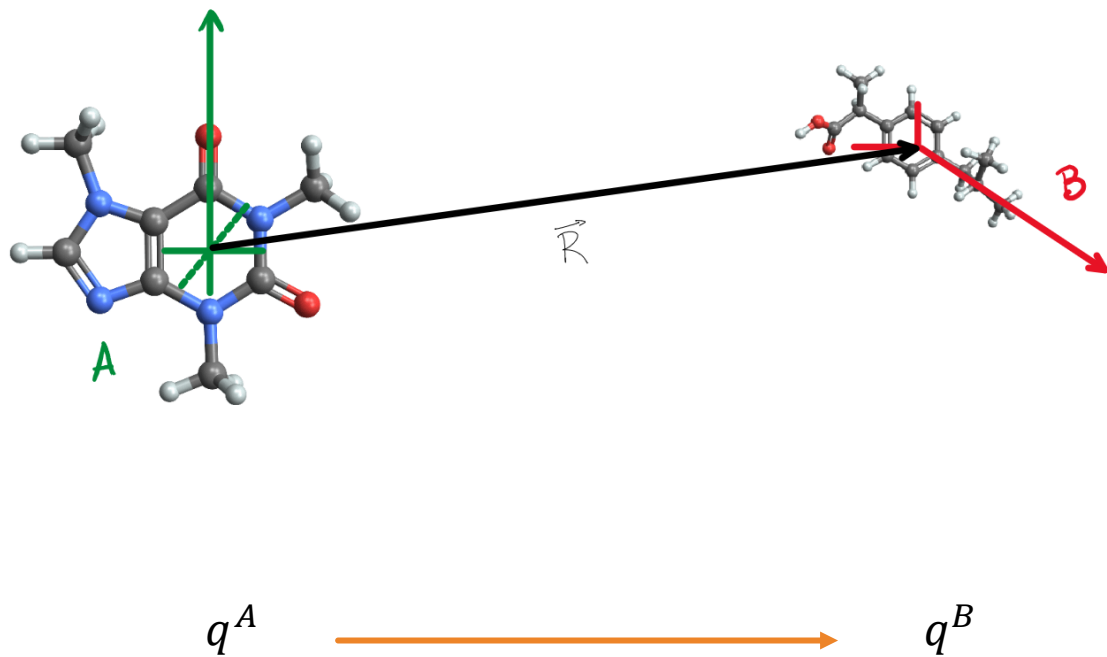
$$\mu_i = q_1 \cdot r_{i_1} + q_2 \cdot r_{i_2} + \dots$$

Quadrupole

$$\Theta_{ij} = \frac{1}{2} \left[q_1 \left(3 \cdot r_{i_1} \cdot r_{j_1} - r_1^2 \right) + q_2 \left(3 \cdot r_{i_2} \cdot r_{j_2} - r_2^2 \right) + \dots \right]$$

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. .
. . .

METHODOLOGY



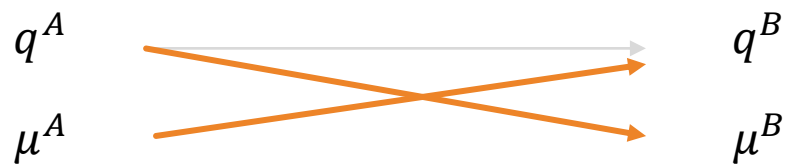
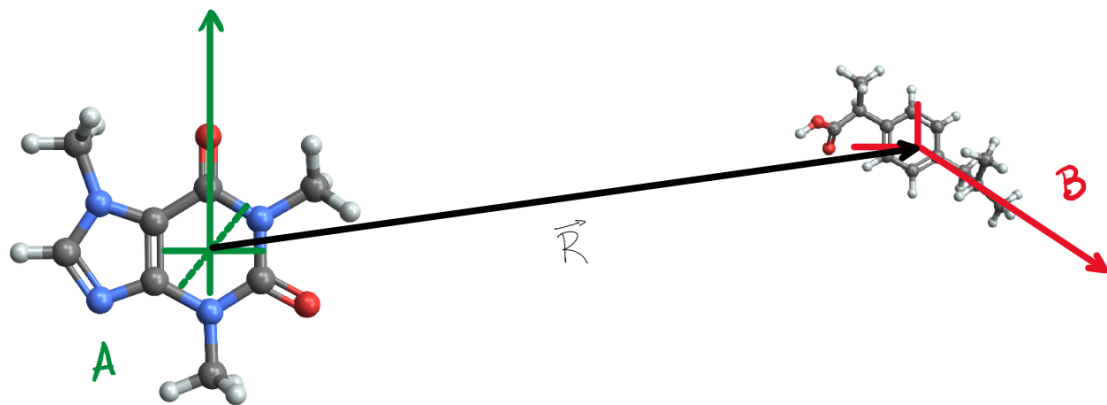
Multipole Expansion

Charge - Charge

$$U_{qq} = \frac{q^B q^A}{4\pi\epsilon_0 R}$$

⋮

METHODOLOGY



Multipole Expansion

Charge - Charge

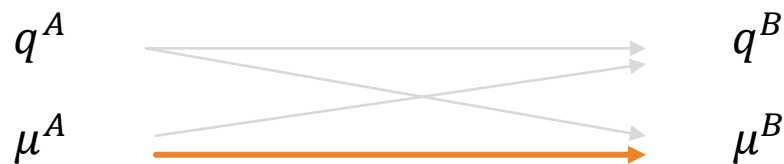
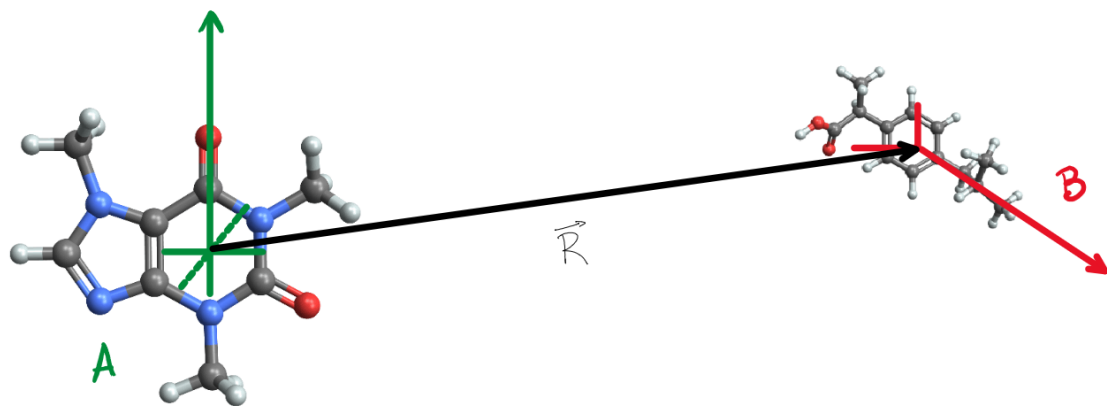
$$U_{qq} = \frac{q^B q^A}{4\pi\epsilon_0 R}$$

Charge - Dipole

$$U_{q\mu} = \frac{\mu^A q^B \cos \beta_1}{4\pi\epsilon_0 R^2}$$

⋮

METHODOLOGY



Multipole Expansion

Charge - Charge

$$U_{qq} = \frac{q^B q^A}{4\pi\epsilon_0 R}$$

Charge - Dipole

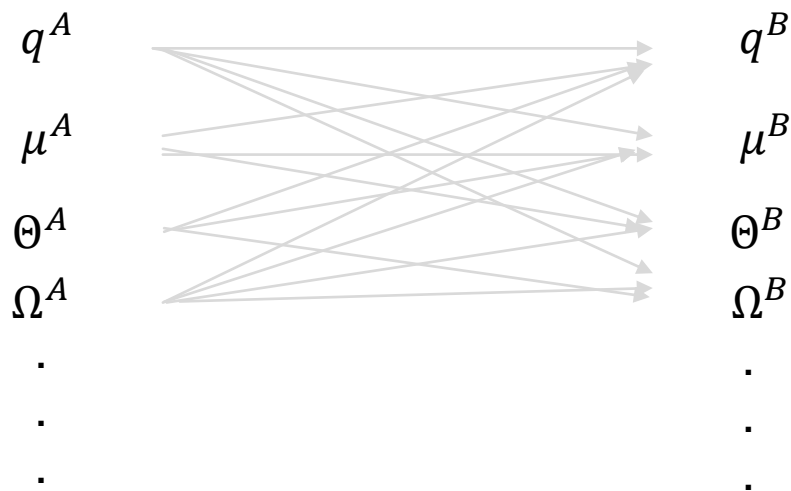
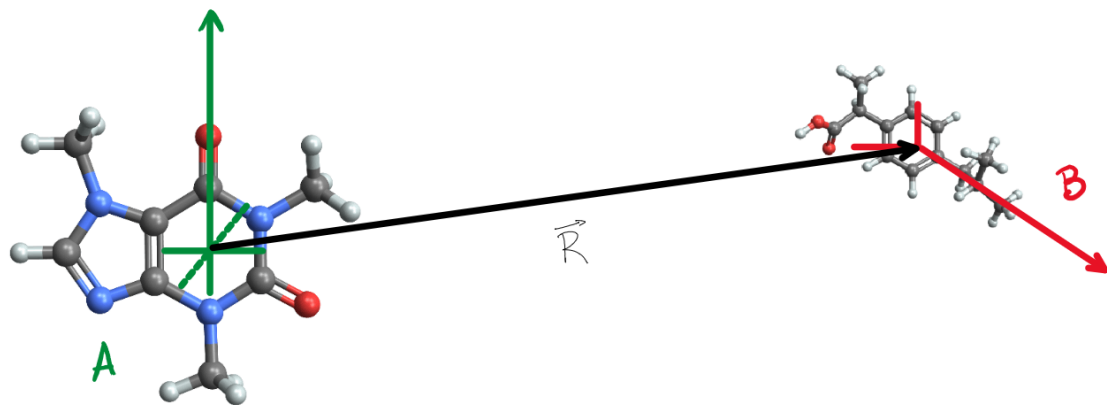
$$U_{q\mu} = \frac{\mu^A q^B \cos\beta_1}{4\pi\epsilon_0 R^2}$$

Dipole - Dipole

$$U_{\mu\mu} = \frac{\mu^A \mu^B}{4\pi\epsilon_0 R^3} (2\cos\beta_1 \cos\beta_2 - \sin\beta_1 \sin\beta_2 \cos\alpha)$$

⋮

METHODOLOGY



Multipole Expansion

Charge - Charge

$$U_{qq} = \frac{q^B q^A}{4\pi\epsilon_0 R}$$

Charge - Dipole

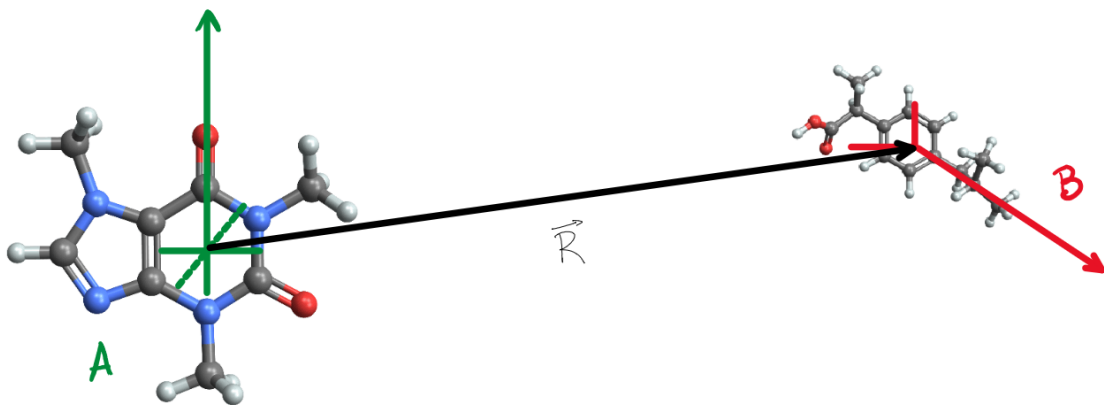
$$U_{q\mu} = \frac{\mu^A q^B \cos \beta_1}{4\pi\epsilon_0 R^2}$$

Dipole - Dipole

$$U_{\mu\mu} = \frac{\mu^A \mu^B}{4\pi\epsilon_0 R^3} (2\cos\beta_1 \cos\beta_2 - \sin\beta_1 \sin\beta_2 \cos\alpha)$$

⋮

METHODOLOGY


 q^A
 μ^A
 Θ^A
 Ω^A
 \cdot
 \cdot
 \cdot
 q^B
 μ^B
 Θ^B
 Ω^B
 \cdot
 \cdot
 \cdot

Multipole Expansion

Quadrupole - Quadrupole

$$U_{\Theta\Theta} = -\frac{1}{12\pi R^5 \epsilon_0} (\Theta_{yy}^A + 2\Theta_{zz}^A)(\Theta_{yy}^B + 2\Theta_{zz}^B) ((17 \cos^2 \beta_1 - 5) \cos^2 \beta_2 + 2 \cos \alpha (\cos \alpha \sin^2 \beta_1 \sin^2 \beta_2 - 2 \sin 2\beta_1 \sin 2\beta_2))$$

$$+ \Theta_{xz}^A \Theta_{xy}^B \cos 2\gamma_2 ((\cos \beta_2 \sin(2\alpha) \sin 2\beta_1 + 18 \cos 2\beta_1 \sin \alpha \sin \beta_2) \sin \gamma_1 - 2 \cos \gamma_1 (\cos(2\alpha) \cos \beta_2 \sin \beta_1 + 9 \cos \alpha \cos \beta_1 \sin \beta_2))$$

$$+ \Theta_{xz}^A (\Theta_{yy}^B + 2\Theta_{zz}^B) (\cos \gamma_1 (8 \cos \beta_1 \sin \alpha \sin 2\beta_2 - 2 \sin(2\alpha) \sin \beta_1 \sin^2 \beta_2) + (-36 \cos \beta_1 \sin \beta_1 \cos^2 \beta_2$$

$$+ \sin 2\beta_1 (35 \cos^2 \beta_2 - 2 \cos^2 \alpha \sin^2 \beta_2) + 8 \cos \alpha \cos 2\beta_1 \sin 2\beta_2) \sin \gamma_1)$$

$$+ \Theta_{yz}^A (\Theta_{yy}^B + 2\Theta_{zz}^B) (\cos \gamma_1 (-36 \cos \beta_1 \sin \beta_1 \cos^2 \beta_2 + \sin 2\beta_1 (35 \cos^2 \beta_2 - 2 \cos^2 \alpha \sin^2 \beta_2) + 8 \cos \alpha \cos 2\beta_1 \sin 2\beta_2) + 2(\sin(2\alpha) \sin \beta_1 \sin^2 \beta_2$$

$$- 4 \cos \beta_1 \sin \alpha \sin 2\beta_2) \sin \gamma_1) + (2\Theta_{yy}^A + \Theta_{zz}^A) (\Theta_{yy}^B + 2\Theta_{zz}^B) ((17 \cos^2 \gamma_1 \sin^2 \beta_1 - 5) \cos^2 \beta_2 + 2 \sin^2 \alpha \sin^2 \beta_2 \sin^2 \gamma_1$$

$$+ 2 \cos \alpha \cos^2 \gamma_1 (\cos \alpha \cos^2 \beta_1 \sin^2 \beta_2 + 2 \sin 2\beta_1 \sin 2\beta_2) - (\cos \beta_1 \sin(2\alpha) \sin^2 \beta_2 + 4 \sin \alpha \sin \beta_1 \sin 2\beta_2) \sin 2\gamma_1)$$

$$+ \Theta_{xy}^A (\Theta_{yy}^B + 2\Theta_{zz}^B) (34 \cos^2 \beta_2 \cos \gamma_1 \sin \gamma_1 \sin^2 \beta_1 + 16 \cos \beta_2 \sin \beta_2 (\cos 2\gamma_1 \sin \alpha + \cos \alpha \cos \beta_1 \sin 2\gamma_1) \sin \beta_1$$

$$+ 2 \sin^2 \beta_2 (\cos \beta_1 \cos 2\gamma_1 \sin(2\alpha) + (\cos^2 \alpha \cos^2 \beta_1 - \sin^2 \alpha) \sin 2\gamma_1))$$

$$- \frac{1}{2} (\Theta_{yy}^A + 2\Theta_{zz}^A) \Theta_{yz}^B (\cos \gamma_2 ((4 \cos^2 \alpha \sin^2 \beta_1 - 17 \cos 2\beta_1 - 7) \sin 2\beta_2 - 16 \cos \alpha \cos 2\beta_2 \sin 2\beta_1) + 4(\sin(2\alpha) \sin^2 \beta_1 \sin \beta_2 - 4 \cos \beta_2 \sin \alpha \sin 2\beta_1) \sin \gamma_2)$$

$$+ \frac{1}{2} \Theta_{xz}^A \Theta_{yz}^B (\cos \gamma_2 (-36 \cos \beta_1 \cos 2\beta_2 \cos \gamma_1 \sin \alpha - 36 \cos \alpha \cos 2\beta_1 \cos 2\beta_2 \sin \gamma_1 + \sin 2\beta_2 (2 \cos \gamma_1 \sin(2\alpha) \sin \beta_1 + (\cos(2\alpha) + 33) \sin 2\beta_1 \sin \gamma_1))$$

$$+ 2(18 \cos \alpha \cos \beta_1 \cos \beta_2 \cos \gamma_1 - 2 \cos(2\alpha) \sin \beta_1 \sin \beta_2 \cos \gamma_1 + (\sin(2\alpha) \sin 2\beta_1 \sin \beta_2 - 18 \cos 2\beta_1 \cos \beta_2 \sin \alpha) \sin \gamma_1) \sin \gamma_2)$$

$$+ \frac{1}{4} \Theta_{xy}^A \Theta_{yz}^B (-\cos \gamma_2 \sin 2\beta_2 (4 \cos \beta_1 \cos 2\gamma_1 \sin(2\alpha) + (\cos(2\alpha) (\cos 2\beta_1 + 3) - 66 \sin^2 \beta_1) \sin 2\gamma_1)$$

$$- 36 \cos 2\beta_2 \cos \gamma_2 (2 \cos 2\gamma_1 \sin \alpha \sin \beta_1 + \cos \alpha \sin 2\beta_1 \sin 2\gamma_1) + 2(4 \cos 2\gamma_1 (9 \cos \alpha \cos \beta_2 \sin \beta_1$$

$$+ \cos(2\alpha) \cos \beta_1 \sin \beta_2) - (18 \cos \beta_2 \sin \alpha \sin 2\beta_1 + (\cos 2\beta_1 + 3) \sin(2\alpha) \sin \beta_2) \sin 2\gamma_1) \sin \gamma_2)$$

$$+ \Theta_{xy}^A \Theta_{xz}^B (\cos \gamma_2 (\sin \alpha (9 \cos \beta_2 \sin 2\beta_1 + \cos \alpha (\cos 2\beta_1 + 3) \sin \beta_2) \sin 2\gamma_1 - 2 \cos 2\gamma_1 (9 \cos \alpha \cos \beta_2 \sin \beta_1 + \cos(2\alpha) \cos \beta_1 \sin \beta_2))$$

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 \cdot

Multipole Expansion

$$\begin{aligned}
 q^A q^B & \\
 q^A \mu^B & + q^B \mu^A \\
 q^A \Theta^B & + \mu^B \mu^A + q^B \Theta^A \\
 q^A \Omega^B & + \mu^A \Theta^B + \mu^B \Theta^A + q^B \Omega^A \\
 q^A \Phi^B & + \mu^A \Omega^B + \Theta^A \Theta^B + \mu^B \Omega^A + q^B \Phi^A \\
 q^A \xi^{(5)B} & + \mu^A \Phi^B + \Theta^A \Omega^B + \Theta^B \Omega^A + \mu^B \Phi^A + q^B \xi^{(5)A} \\
 q^A \xi^{(6)B} & + \mu^A \xi^{(5)B} + \Theta^A \Phi^B + \Omega^A \Omega^B + \Theta^B \Phi^A + \mu^B \xi^{(5)A} + q^B \xi^{(6)A} \\
 q^A \xi^{(7)B} & + \mu^A \xi^{(6)B} + \Theta^A \xi^{(5)B} + \Omega^A \Phi^B + \Phi^A \Omega^B + \Theta^B \xi^{(5)A} + \mu^B \xi^{(6)A} + q^B \xi^{(7)A}
 \end{aligned}$$

Induction Expansion

$$\begin{aligned}
 (q^A)^2 \alpha_{\mu\mu}^B & + (q^B)^2 \alpha_{\mu\mu}^A \\
 (q^A)^2 \alpha_{\mu\Theta}^B & + (q^A \mu^A) \alpha_{\mu\mu}^B + (q^B \mu^B) \alpha_{\mu\mu}^A + (q^B)^2 \alpha_{\mu\Theta}^A \\
 (q^A)^2 \alpha_{\mu\Omega}^B & + (q^A)^2 \alpha_{\Theta\Theta}^B + (q^A \mu^A) \alpha_{\mu\Theta}^B + (q^A \mu^A) \alpha_{\Theta\mu}^B + (q^A \Theta^A) \alpha_{\mu\mu}^B + (\mu^A)^2 \alpha_{\mu\mu}^B + (q^B)^2 \alpha_{\mu\Omega}^A \\
 & + (q^B)^2 \alpha_{\Theta\Theta}^A + (q^B \mu^B) \alpha_{\mu\Theta}^A + (q^B \mu^B) \alpha_{\Theta\mu}^A + (q^B \Theta^B) \alpha_{\mu\mu}^A + (\mu^B)^2 \alpha_{\mu\mu}^A \\
 (q^A)^2 \alpha_{\mu\Phi}^B & + (q^A)^2 \alpha_{\Theta\Omega}^B + (q^A \mu^A) \alpha_{\mu\Omega}^B + (q^A \mu^A) \alpha_{\Omega\mu}^B + (q^A \mu^A) \alpha_{\Theta\Theta}^B + (q^A \Theta^A) \alpha_{\mu\Theta}^B + (q^A \Theta^A) \alpha_{\Theta\mu}^B \\
 & + (q^A \Omega^A) \alpha_{\mu\mu}^B + (\mu^A)^2 \alpha_{\mu\Theta}^B + (\mu^A \Theta^A) \alpha_{\mu\mu}^B + (q^B)^2 \alpha_{\mu\Phi}^A + (q^B)^2 \alpha_{\Theta\Omega}^A + (q^B \mu^B) \alpha_{\mu\Omega}^A + (q^B \mu^B) \alpha_{\Omega\mu}^A \\
 & + (q^B \mu^B) \alpha_{\Theta\Theta}^A + (q^B \Theta^B) \alpha_{\mu\Theta}^A + (q^B \Theta^B) \alpha_{\Theta\mu}^A + (q^B \Omega^B) \alpha_{\mu\mu}^A + (\mu^B)^2 \alpha_{\mu\Theta}^A + (\mu^B \Theta^B) \alpha_{\mu\mu}^A \\
 (q^A)^2 \alpha_{\mu\xi^{(5)}}^B & + (q^A)^2 \alpha_{\Theta\Phi}^B + (q^A)^2 \alpha_{\Omega\Omega}^B + (q^A \mu^A) \alpha_{\mu\Phi}^B + (q^A \mu^A) \alpha_{\Phi\mu}^B + (q^A \mu^A) \alpha_{\Theta\Omega}^B + (q^A \mu^A) \alpha_{\Omega\Theta}^B \\
 & + (q^A \Theta^A) \alpha_{\mu\Omega}^B + (q^A \Theta^A) \alpha_{\Omega\mu}^B + (q^A \Theta^A) \alpha_{\Theta\Theta}^B + (q^A \Omega^A) \alpha_{\mu\Theta}^B + (q^A \Omega^A) \alpha_{\Theta\mu}^B + (q^A \Phi^A) \alpha_{\mu\mu}^B + (\mu^A)^2 \alpha_{\mu\Omega}^B \\
 & + (\mu^A)^2 \alpha_{\Theta\Theta}^B + (\mu^A \Theta^A) \alpha_{\mu\Theta}^B + (\mu^A \Theta^A) \alpha_{\Theta\mu}^B + (\mu^A \Omega^A) \alpha_{\mu\mu}^B + (\Theta^A)^2 \alpha_{\mu\mu}^B + (q^B)^2 \alpha_{\mu\xi^{(5)}}^A + (q^B)^2 \alpha_{\Theta\Phi}^A \\
 & + (q^B)^2 \alpha_{\Omega\Omega}^A + (q^B \mu^B) \alpha_{\mu\Phi}^A + (q^B \mu^B) \alpha_{\Phi\mu}^A + (q^B \mu^B) \alpha_{\Theta\Omega}^A + (q^B \mu^B) \alpha_{\Omega\Theta}^A + (q^B \Theta^B) \alpha_{\mu\Omega}^A + (q^B \Theta^B) \alpha_{\Omega\mu}^A \\
 & + (q^B \Theta^B) \alpha_{\Theta\Theta}^A + (q^B \Omega^B) \alpha_{\mu\Theta}^A + (q^B \Omega^B) \alpha_{\Theta\mu}^A + (q^B \Phi^B) \alpha_{\mu\mu}^A + (\mu^B)^2 \alpha_{\mu\Omega}^A + (\mu^B)^2 \alpha_{\Theta\Theta}^A + (\mu^B \Theta^B) \alpha_{\mu\Theta}^A \\
 & + (\mu^B \Theta^B) \alpha_{\Theta\mu}^A + (\mu^B \Omega^B) \alpha_{\mu\mu}^A + (\Theta^B)^2 \alpha_{\mu\mu}^A
 \end{aligned}$$

Dispersion Expansion

$$\begin{aligned}
 D_{\mu\mu-\mu\mu} & \\
 D_{\mu\mu-\mu\Theta} & + D_{\mu\Theta-\mu\mu} \\
 D_{\mu\mu-\mu\Omega} & + D_{\mu\mu-\Theta\Theta} + D_{\mu\Theta-\mu\Theta} + D_{\mu\Omega-\mu\mu} + D_{\Theta\Theta-\mu\mu}
 \end{aligned}$$

Hyperpolarizability Expansion

$$\begin{aligned}
 (q^A)^3 \beta_{\mu\mu\mu}^B & + (q^B)^3 \beta_{\mu\mu\mu}^A \\
 (q^A)^3 \beta_{\mu\mu\Theta}^B & + (q^A)^2 \mu^A \beta_{\mu\mu\mu}^B + (q^B)^3 \beta_{\mu\mu\Theta}^A + (q^A)^2 \mu^B \beta_{\mu\mu\mu}^A \\
 (q^A)^3 \beta_{\mu\mu\Omega}^B & + (q^A)^2 \beta_{\mu\Theta\Theta}^B + (q^A)^2 \mu^A \beta_{\mu\mu\Theta}^B + (q^A)^2 \Theta^A \beta_{\mu\mu\mu}^B + q^A (\mu^A)^2 \beta_{\mu\mu\mu}^B + (q^A)^4 \gamma_{\mu\mu\mu}^B \\
 (q^B)^3 \beta_{\mu\mu\Omega}^A & + (q^B)^3 \beta_{\mu\Theta\Theta}^A + (q^B)^2 \mu^B \beta_{\mu\mu\Theta}^A + (q^B)^2 \Theta^B \beta_{\mu\mu\mu}^A + q^B (\mu^B)^2 \beta_{\mu\mu\mu}^A + (q^B)^4 \gamma_{\mu\mu\mu}^A
 \end{aligned}$$

SOFTWARE

Example: $CF^+ - H_2$

Settings

Initial Setup | Multipoles A | Multipoles B | Polarizability A | Polarizability B | Dispersion | HyperPolarizability A | HyperPolarizability B

1 - Working Directory

Working Directory: Choose the working directory ...

Import Initialization File: Choose Initialization file File ...

2 - Choose Symmetry

Molecule A Symm.: C ∞ v (HF)

Molecule B Symm.: D ∞ h (H2)

Are the molecules identical? Off On

Total Charge: 1

Zero Potential: Fit

3- Import Data

Import Data: Choose Data File

R column: 2 Cos β 1 column: 3 Cos γ 1 column: 6

φ column: 5 Cos β 2 column: 4 Cos γ 2 column: 6

Whole Space: Off On Sampling(%): 100 Advanced Options

SOFTWARE

Example: $CF^+ - H_2$

Settings

Initial Setup | Multipoles A | Multipoles B | Polarizability A | Polarizability B | Dispersion | HyperPolarizability A | HyperPolarizability B

1 - Working Directory

Working Directory: Choose the working directory ...

Import Initialization File: Choose Initialization file File ...

2 - Choose Symmetry

Molecule A Symm.: C ∞ v (HF)

Molecule B Symm.: D ∞ h (H2)

Are the molecules identical? Off On

Total Charge: 1

Zero Potential: Fit

3 - Import Data

Import Data

R column: 2

ϕ column: 5

Cos β 2 column: 4

Cos γ 1 column: 1

Cos γ 2 column: 1

Energy: 6

Whole Space: Off On

Sampling(%): 100

Advanced Options

Choose Symmetry

- Spherical (Atom)
- C ∞ v (HF)
- D ∞ h (H2)
- C2v (H2O)
- Cs (HNO)
- C1 (NHFCI)

SOFTWARE

Example: $CF^+ - H_2$

Settings

R Filter (Å) 4000pts ?

- Multipole
 - M1
 - M2
 - M3
 - M4
 - M5
 - M6
 - M7
 - M8
- Dispersion
 - D6
 - D7
- Induction
 - I4
 - I5
 - I6
 - I7
 - I8
- HyperPolarizability
 - H6
 - H7

Run Fit

Results

index	Running	rmse	rSquared	zero	Q00_A	Q00_B	Q10_A	Q10_B	Q20_A	Q20_B	Q30_A	Q30_B	Q40_A	Q40_B	Q50_A	Q50_B
0	Initial Values	0	0	0	1	0	1	0	1	1	1	0	1	1	1	1
1	M-3-4-5-6/D-6/I-4-5-6/	0.0047267	1	-86995.846162858172	1.000000000000000	0	-0.455306054083	0.000000000000000	0.365388521197	0.488526737528	2.090954708832	0.000000000000000	1.000000000000000	0.042533446837	1.0	1.0

Choose symmetry

Symmetry of Molecule A: Symmetry of Molecule B:

Is Molecule A Charged: Off On Is Molecule B Charged: Off On

***** Multipoles *****

1st Order (~ R⁻¹) $q^A q^B$

2nd Order (~ R⁻²) $q^A \mu^B + q^B \mu^A$

3rd Order (~ R⁻³) $q^A \Theta^B + \mu^B \mu^A + q^B \Theta^A$

4th Order (~ R⁻⁴) $q^A \Omega^B + \mu^A \Theta^B + \mu^B \Theta^A + q^B \Omega^A$

5th Order (~ R⁻⁵) $q^A \Phi^B + \mu^A \Omega^B + \Theta^A \Theta^B + \mu^B \Omega^A + q^B \Phi^A$

6th Order (~ R⁻⁶) $q^A \xi^{(5)B} + \mu^A \Phi^B + \Theta^A \Omega^B + \Theta^B \Omega^A + \mu^B \Phi^A + q^B \xi^{(5)A}$

7th Order (~ R⁻⁷) $q^A \xi^{(6)B} + \mu^A \xi^{(5)B} + \Theta^A \Phi^B + \Omega^A \Omega^B + \Theta^B \Phi^A + \mu^B \xi^{(5)A} + q^B \xi^{(6)A}$

8th Order (~ R⁻⁸) $q^A \xi^{(7)B} + \mu^A \xi^{(6)B} + \Theta^A \xi^{(5)B} + \Omega^A \Phi^B + \Phi^A \Omega^B + \Theta^B \xi^{(5)A} + \mu^B \xi^{(6)A} + q^B \xi^{(7)A}$

***** Induction *****

4th Order (~ -R⁻⁴) $(q^A)^2 \alpha_{\mu\mu}^B + (q^B)^2 \alpha_{\mu\mu}^A$

5th Order (~ -R⁻⁵) $(q^A)^2 \alpha_{\mu\Theta}^B + (q^A \mu^A) \alpha_{\mu\mu}^B + (q^B \mu^B) \alpha_{\mu\mu}^A + (q^B)^2 \alpha_{\mu\Theta}^A$

SOFTWARE

Example: $CF^+ - H_2$

Long Range Fit

Settings

R Filter (Å) 4000pts

- Multipole
 - M1
 - M2
 - M3
 - M4
 - M5
 - M6
 - M7
 - M8
- Dispersion
 - D6
 - D7
- Induction
 - I4
 - I5
 - I6
 - I7
 - I8
- HyperPolarizability
 - H6
 - H7

Fitting Number

Number of points

R (Å)

β_1 (degrees)

β_2 (degrees)

φ (degrees)

ν_1 (degrees)

ν_2 (degrees)

Make Graphs

Export Graphs

Run Fit

Results

index	Running	rmse	rSquared	zero	Q00_A	Q00_B	Q10_A	Q10_B	Q20_A	Q20_B	Q30_A	Q30_B	Q40_A	Q40_B	Q50
0	Initial Values	0	0	0	1	0	1	0	1	1	1	0	1	1	1
1	M-3-4-5-6/D-6/I-4-5-6/	0.0047267	1	-86995.846162858172	1.00000000000000	0	-0.455306054083	0.00000000000000	0.365388521197	0.488526737528	2.090954708832	0.00000000000000	1.00000000000000	0.042533446837	1.0

Graphs | Data Set Analysis | Edit Table | Export | Testing | Log out | Expansion

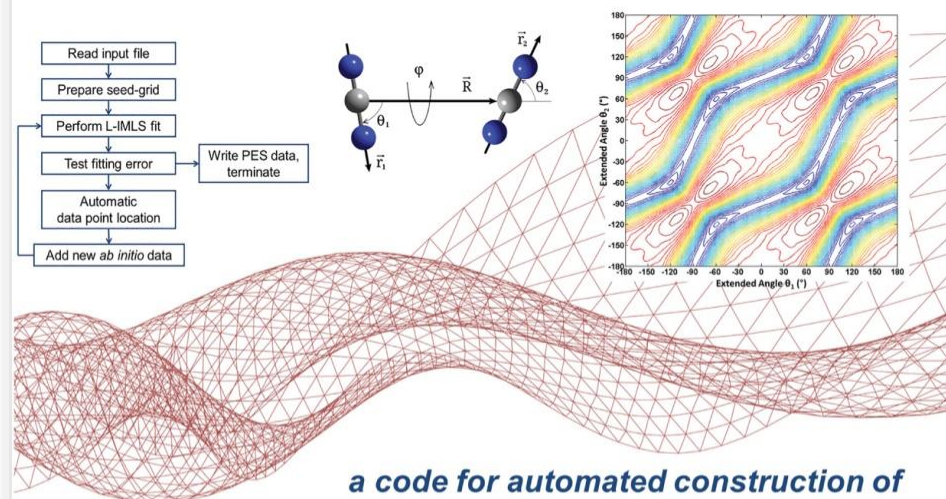
Total Energy considering :

- Multipole
 - M1
 - M2
 - M3
 - M4
 - M5
 - M6
 - M7
 - M8
- Dispersion
 - D6
 - D7
- Induction
 - I4
 - I5
 - I6
 - I7
 - I8
- HyperPolarization
 - H6
 - H7

ET | Combine | Table | EM1 | EM2 | EM3 | EM4 | EM5 | EM6 | EM7 | EM8 | ED6 | ED7 | E4 | E5 | E6 | E7 | E8 | H6

Combined Energy Interactions

AUTOSURF



*a code for automated construction of
Potential Energy Surfaces*

INTEGRATION

FIRST RESULTS

System	Collaborators	Interest Area
$PO^+ - H_2$ $PO^+ - He$	Otoniel Denis-Alpizar Universidad Autónoma de Chile, Chile.	Astro-Chemistry
$CO - CS$ $CO - HCN$ $CO - HNC$ $CO_2 - CO$	Martin Cordiner NASA, USA	Astro-Chemistry comets and icy satellites
$C_2H^- - H_2$ $C_4H^- - H_2$ $C_6H^- - H_2$	François Lique Institut de Physique de Rennes, France	Chemistry of Interstellar Medium (ISM)
$CO(v) - O_2$	Piotr Wcisło Nicolaus Copernicus University in Toruń, Poland	Atmospheric Chemistry

ACKNOWLEDGEMENTS

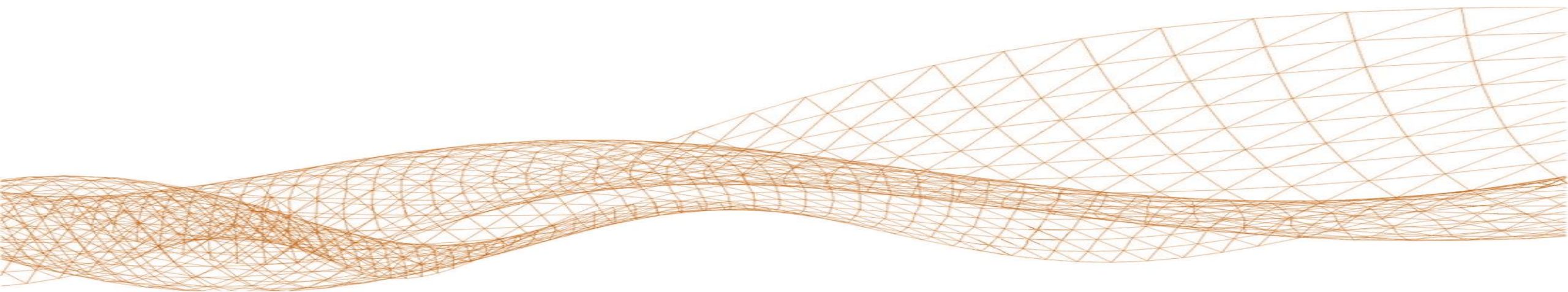


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THANK YOU!