On the Generation of Isomorphism Classes of Mappings

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Universität Bayreuth

Kolloquium über Kombinatorik,
16.–18. November 2006,
Magdeburg

Outline

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A chemical motivation

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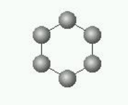
A chemical compound ...  cyclohexane

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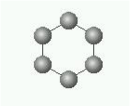
A chemical compound ...  cyclohexane

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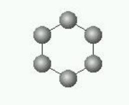
A chemical compound ...  cyclohexane

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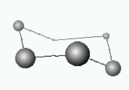

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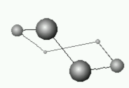

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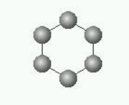
A chemical compound ...  cyclohexane

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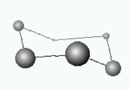

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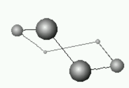

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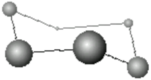
How do we get an overview over the *conformation space*?

Affine point configurations (Order types)



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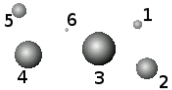

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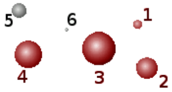

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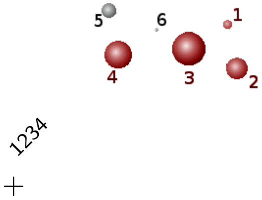

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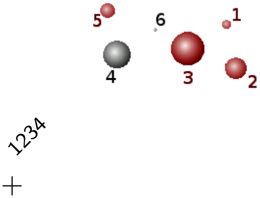

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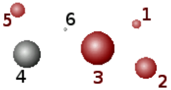

1234	1235
+	+

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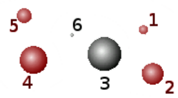

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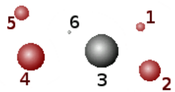

1234	1235	1245
+	+	0

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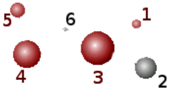

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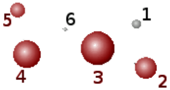

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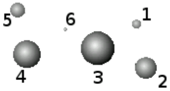

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+	+	0	−	−	+	+	0	−	+	+	0	+	+	+

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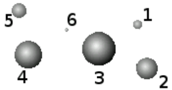

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- It is not practical to store full catalogues for larger n's.
- Generate chirotopes on purpose with individual parameters and restrictions!

Outline

1. Motivation: Chirotopes in chemistry
2. Generation of mappings
3. Generation of chirotopes

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Problem:

Generate a transversal of these isomorphism classes of mappings.

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- Backtrack generation

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Solution: Do not select the canonic elements, but another transversal.

Homomorphism principle (Laue, 1993)

Let G act on X and T be a G-transversal of X. Let further $\varphi : Y \to X$ be a G-homomorphism (i.e. $\varphi(g \cdot x) = g \cdot \varphi(x)$).

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Let G act on X and T be a G-transversal of X. Let further $\varphi : X \to Y$ be a G-homomorphism and $\psi : Y \to X$ a mapping with:

$$\varphi \circ \psi(y) = y \qquad \text{and} \qquad \psi(g \cdot y) \in g \cdot G_y \cdot \psi(y) \, .$$

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2. Select f_i iff $c_1(f_i) \in (G_i)_{f_i} \cdot i$.

Canonicity test during generation

Algorithm:

On level n_i of backtrack-tree, $i = 2, \ldots, n$, proceed with f_i iff

1. f_i is canonic w.r.t. the stabilizer group $(G_{i-1})_{f_{i-1}}$.

2. $c_1(f_i) \in (G_i)_{f_i} \cdot i$, where $c_1(f_i) = (g_{f_i}^{(G_i)})^{-1} \cdot 1$.

It remains a transversal of isomorphism classes of mappings.

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`http://www.mathe2.uni-bayreuth.de:/ralfg/origen.php`

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n:	3	4	5	6	7	8	9	10
rank 4:		1	3	12	206	181 472	—	—
Finschi (2001):					10.0s	250m		
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origen (2006):					0.6s	13s	13m	33h
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molecule:	C_6H_6	C_7H_7	C_8H_8	C_9H_9	$C_{10}H_{10}$
origen (2006):	13	18	30	46	78
time:			0.2s	4.9s	62s

Conclusions

Thank You!