Isomer effect in electron collisions with small hydrocarbons

Márcio H. F. Bettega

Departamento de Física, Universidade Federal do Paraná,

Caixa Postal 19044, 81531-990, Curitiba Paraná, Brazil

Adriana R. Lopes, Sérgio d'A. Sanchez,

Márcio T. do N. Varella, Marco A. P. Lima, Luiz G. Ferreira

Instituto de Física "Gleb Wataghin",

Universidade Estadual de Campinas, Caixa Postal 6165, 13083-970,

Campinas, São Paulo, Brazil

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  - C_3H_6: propene and cyclopropane.
  - C_4H_6: 1,3-butadiene, 2-butyne and cyclobutene.
  - C_4H_8: isobutene, trans-2- and cis-2-butene, syn-1- and skew-1-butene.
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- Previous experimental works motivated us to perfom this systematic study.

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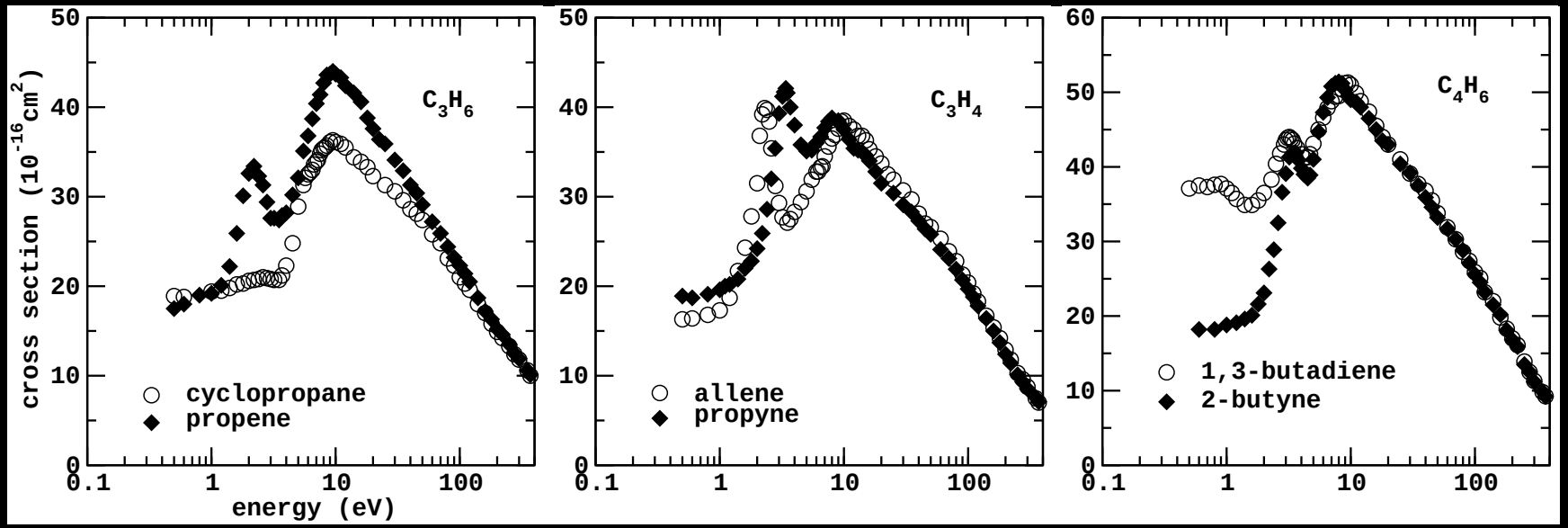
Total cross sections: C. Szmytkowski, S. Kwitnewski, JPB **35**, 2612 (2002); JPB **35**, 3781 (2002); JPB **36**, 2129 (2003).



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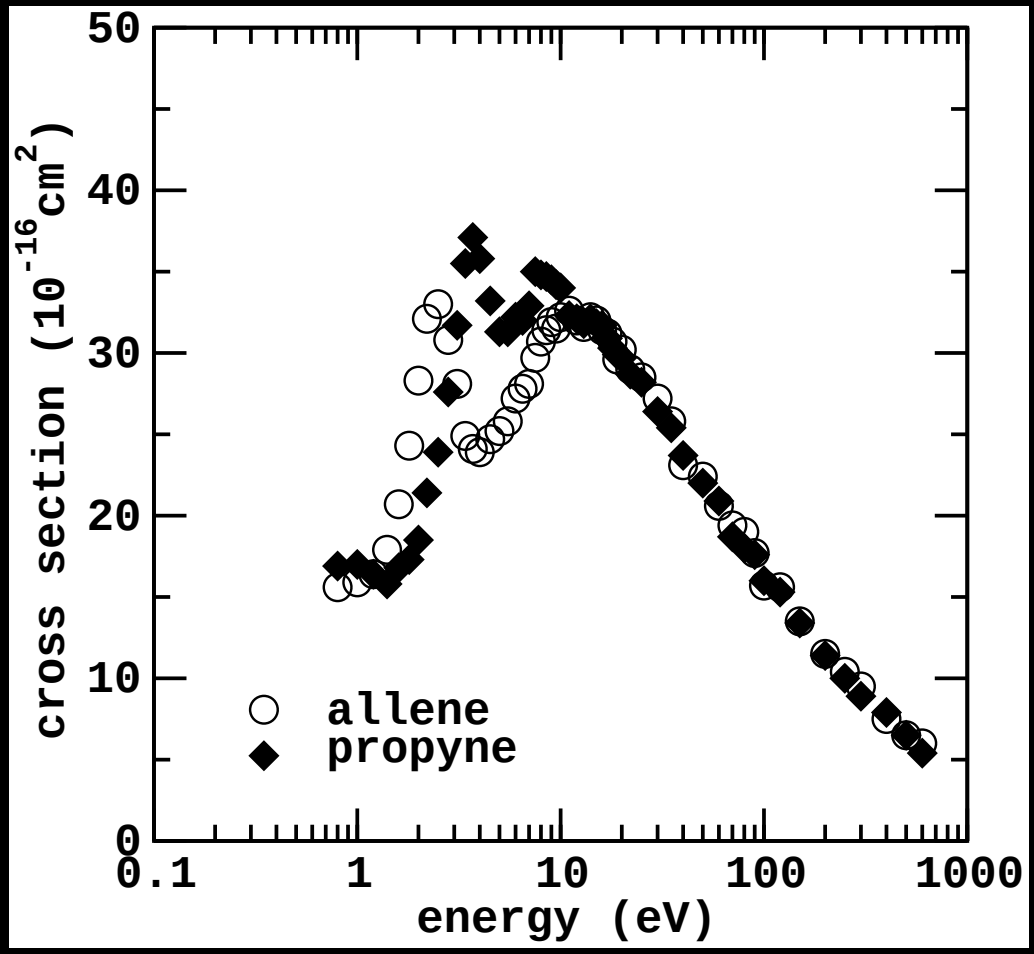
Total cross sections: C. Makochekanwa, H. Kawate, O. Sueoka, M. Kimura, M. Kitajima, M. Hoshino and H. Tanaka, CPL **368**, 82 (2003).



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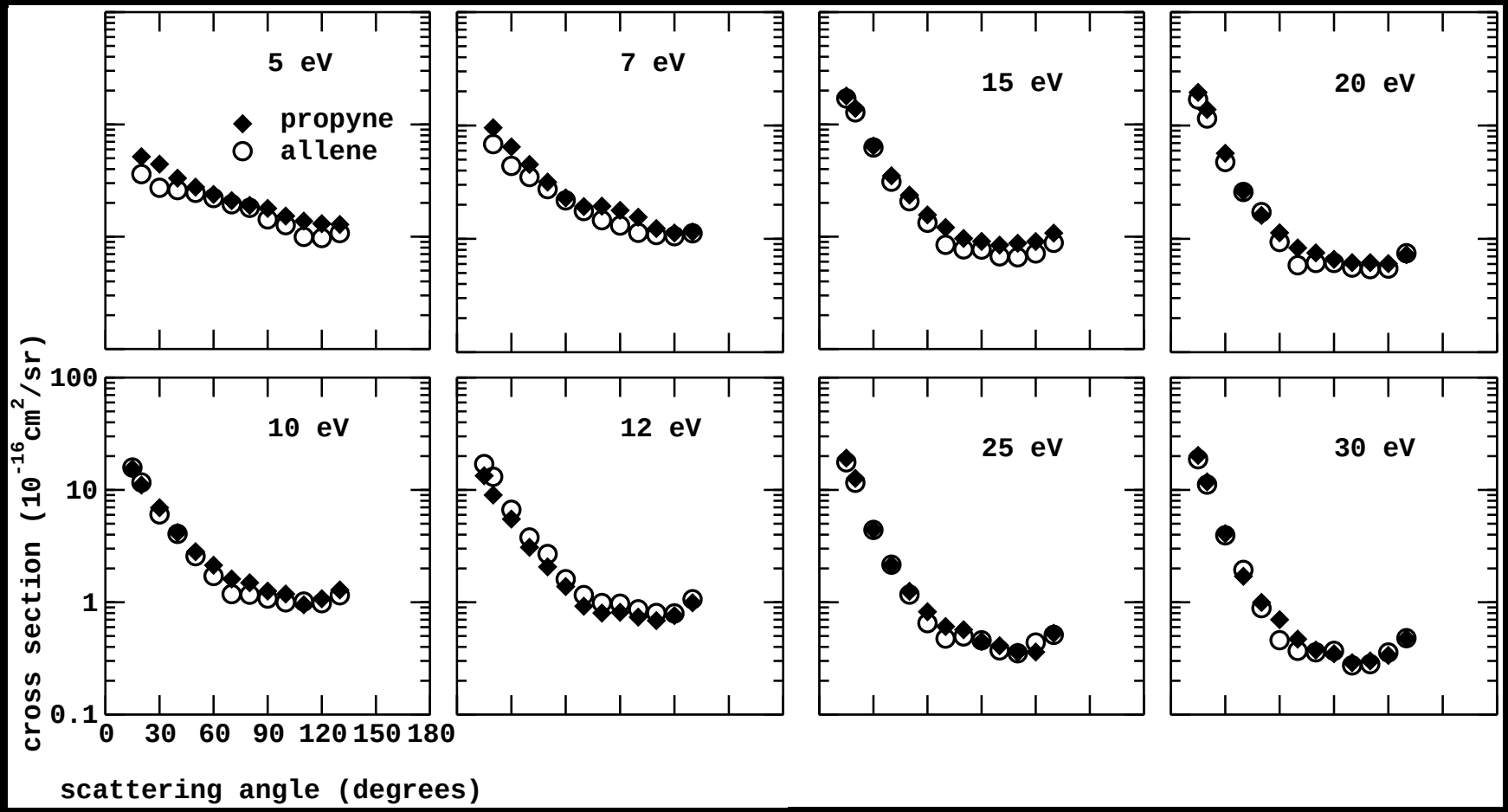
Differential cross sections: Y. Nakano, M. Hoshino, M. Kitajima, H. Tanaka, M. Kimura, PRA **66**, 032714 (2002).



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- C_3H_6 isomers (theory): C. Winstead, Q. Sun, and V. McKoy, JCP **96**, 4246 (1992).
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SMC method

Takatsuka and McKoy, PRA **24**, 2473 (1981)
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  Bettega, Ferreira and Lima, PRA **47**, 1111 (1993).

Results

- Elastic integral, differential and momentum transfer cross sections at the static-exchange (SE) approximation.

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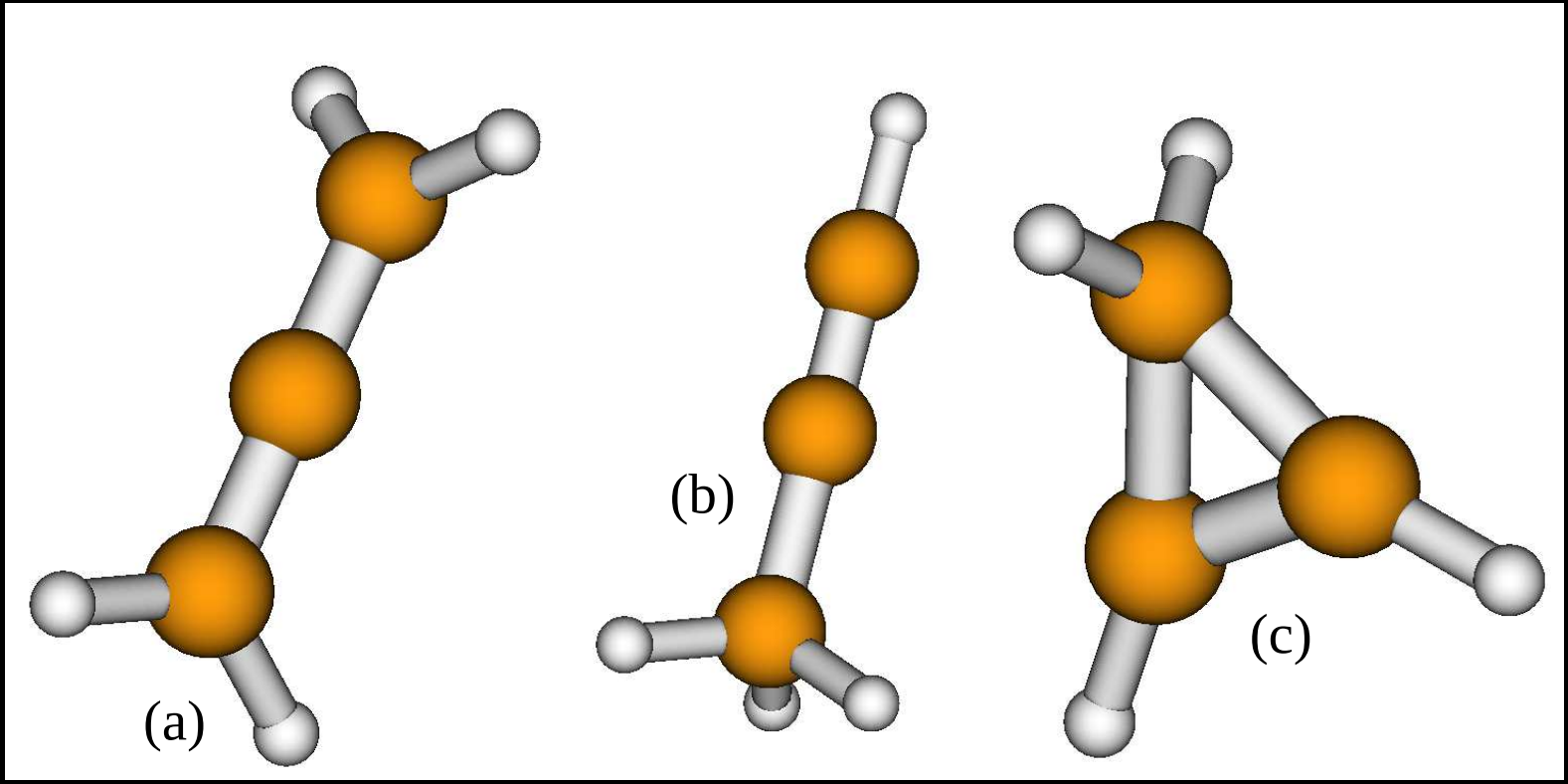
  - C_3H_4 isomers: Lopes and Bettega, PRA **67**, 032711 (2003).
  - C_4H_6 isomers: Lopes *et al.*, PRA **69**, 014702 (2004).
  - C_4H_8 and C_4H_{10} isomers: Lopes *et al.*, JPB **37**, 997 (2004).
  - C_3H_4 (SEP): Sanchez *et al.*, PRA **71** , 062702 (2005).
  - C_3H_4 (rotational excitation): Lopes *et al.*, to be submitted.
  - C_3H_6 (SE and SEP): Bettega *et al.*, to be submitted.

Results: C_3H_4 isomers



Geometrical structure of the C_3H_4 isomers: (a) allene (D_{2d}), (b) propyne (C_{3v}), and (c) cyclopropene (C_{2v}).

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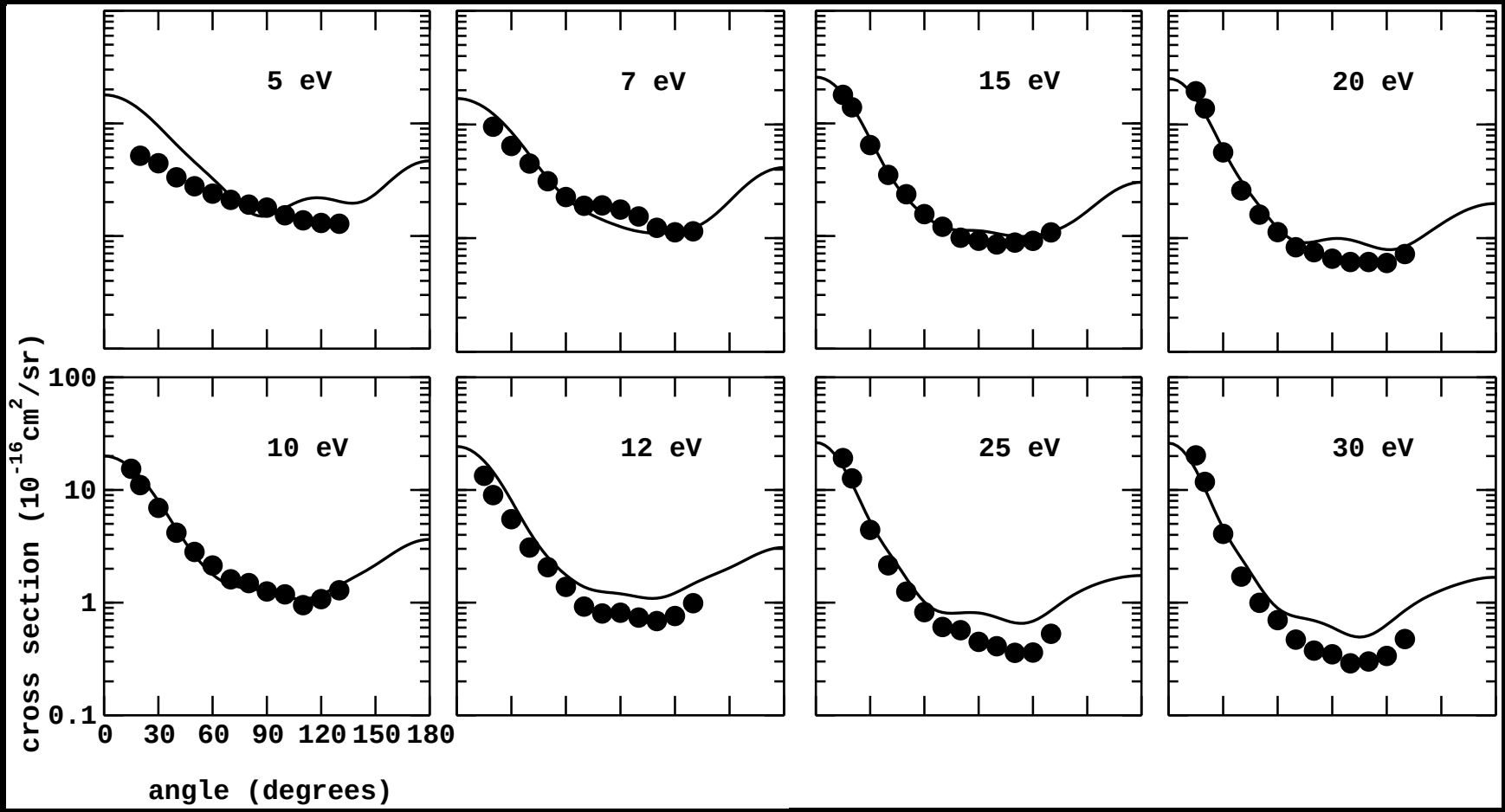
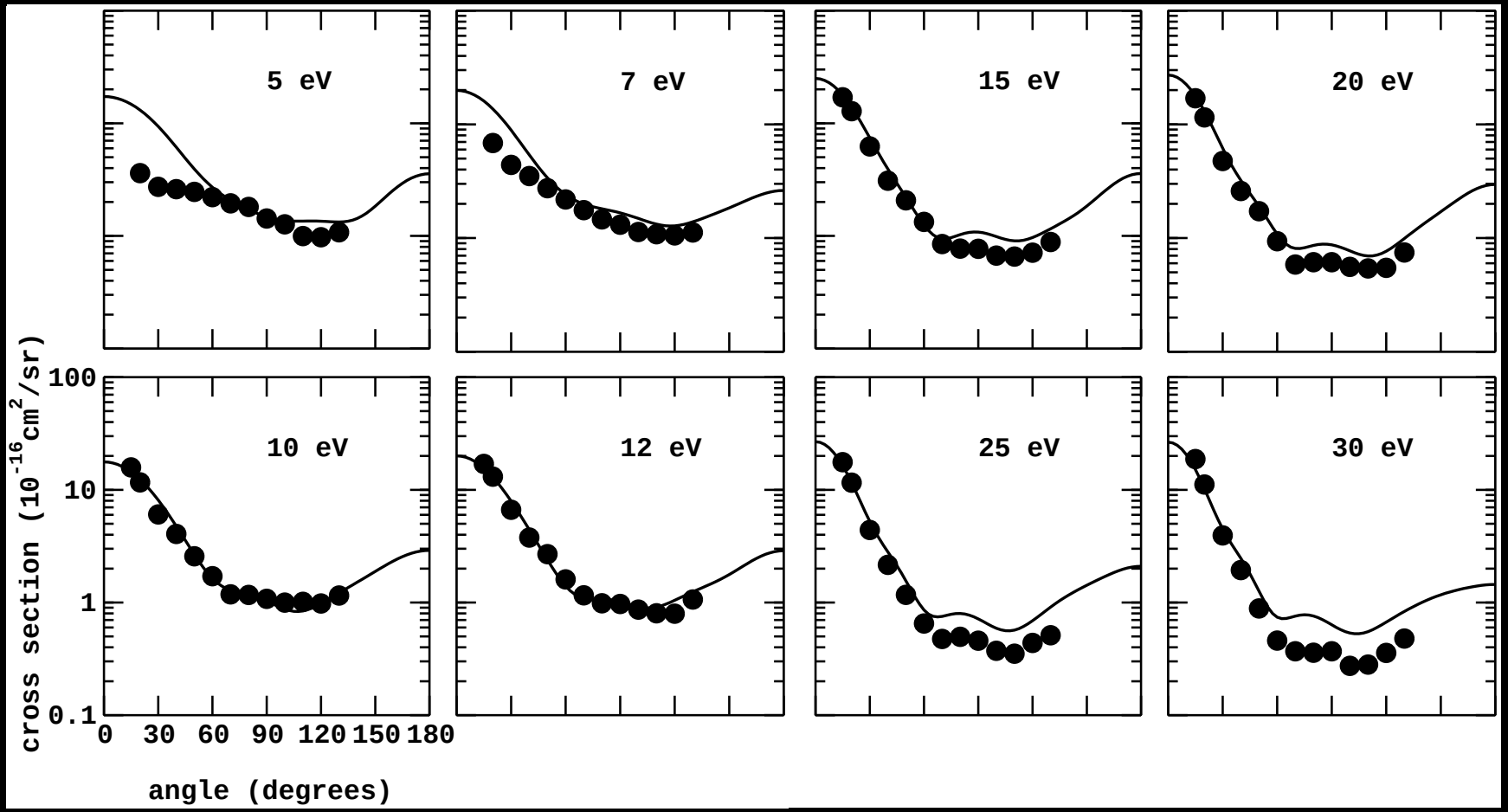


Differential cross sections for propyne. Solid lines, our results at the SE approximation; circles, experimental data of Nakano *et al.*.

Results: C_3H_4 isomers



Differential cross sections for allene. Solid lines, our results at the SE approximation; circles, experimental data of Nakano *et al.*.

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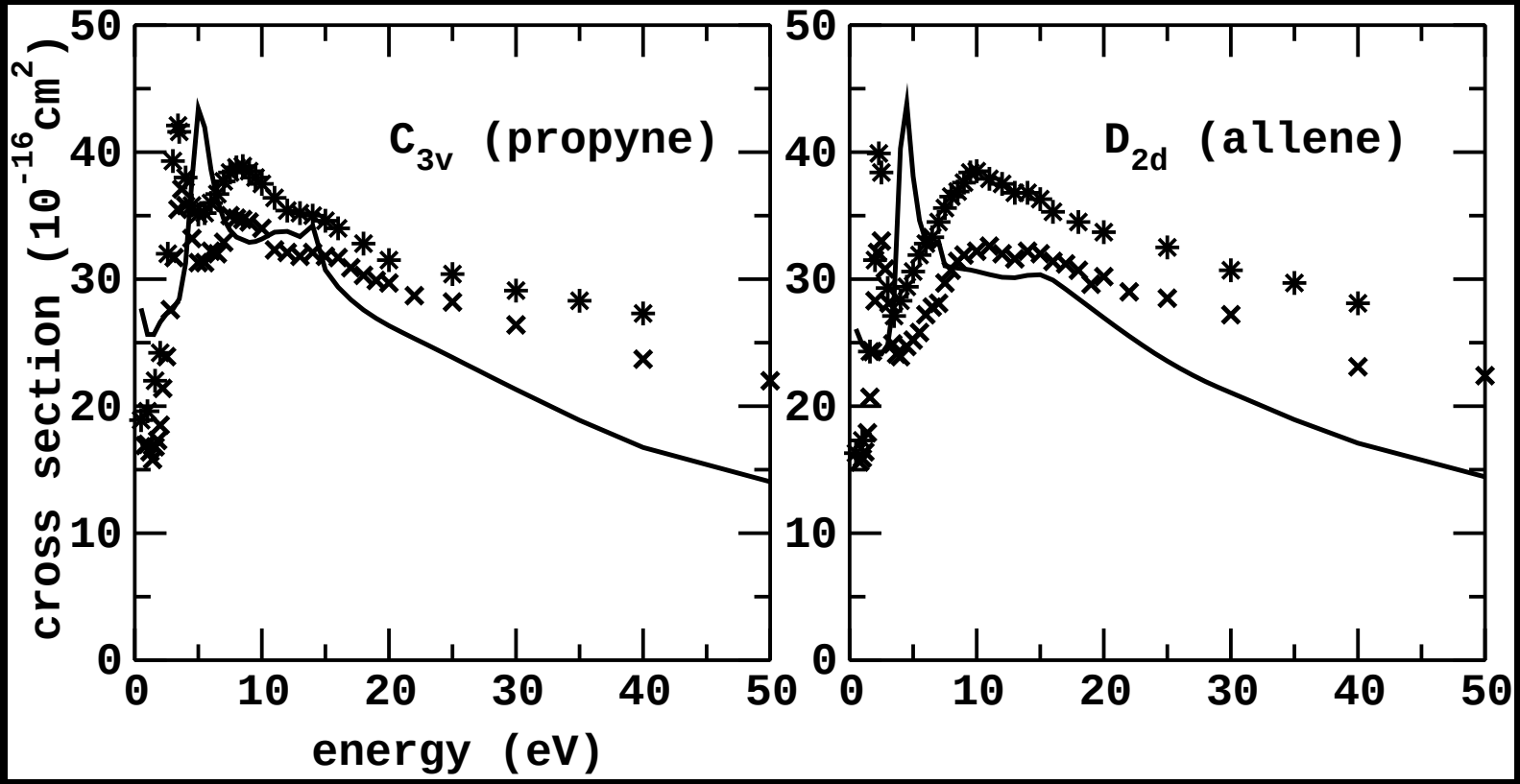
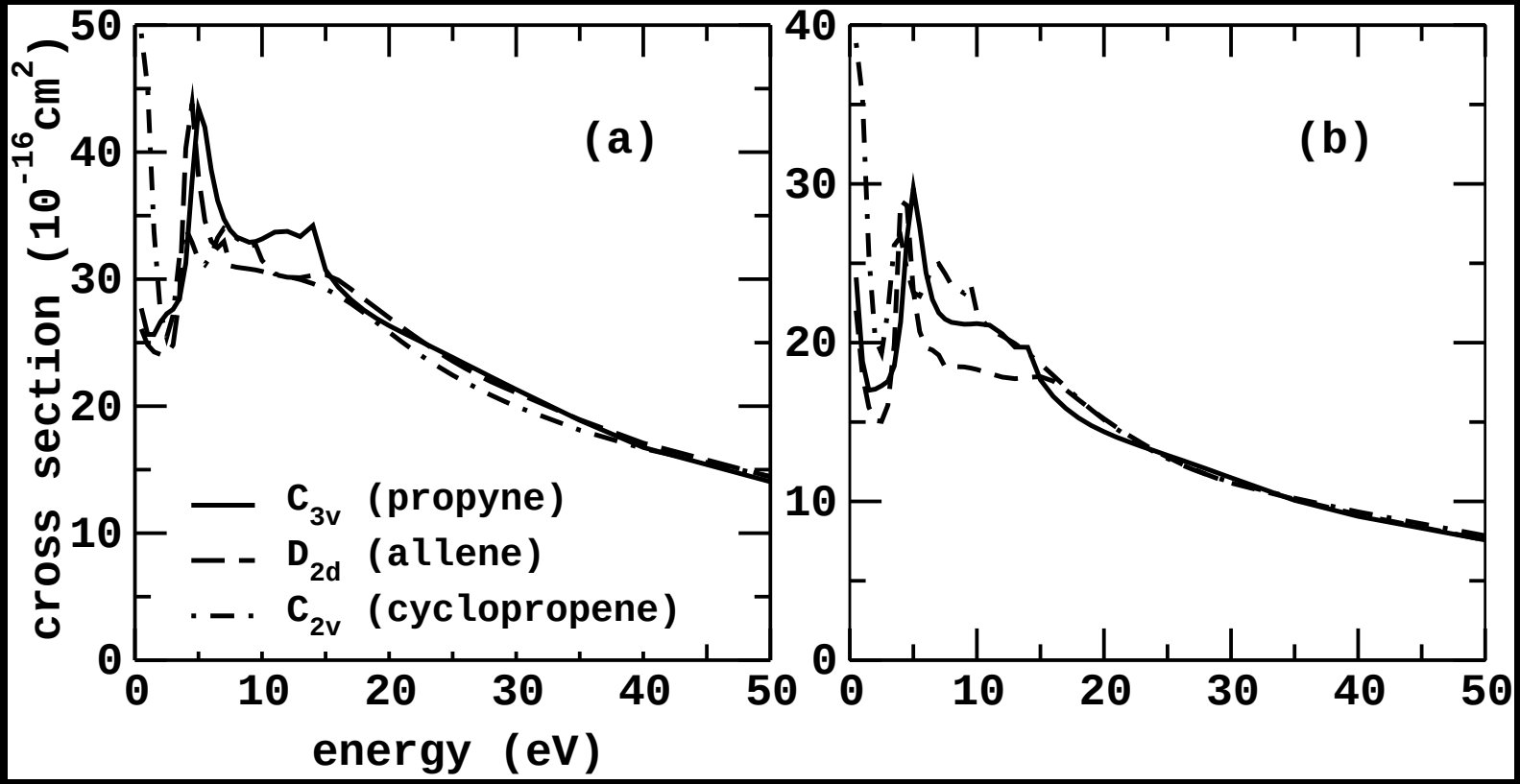


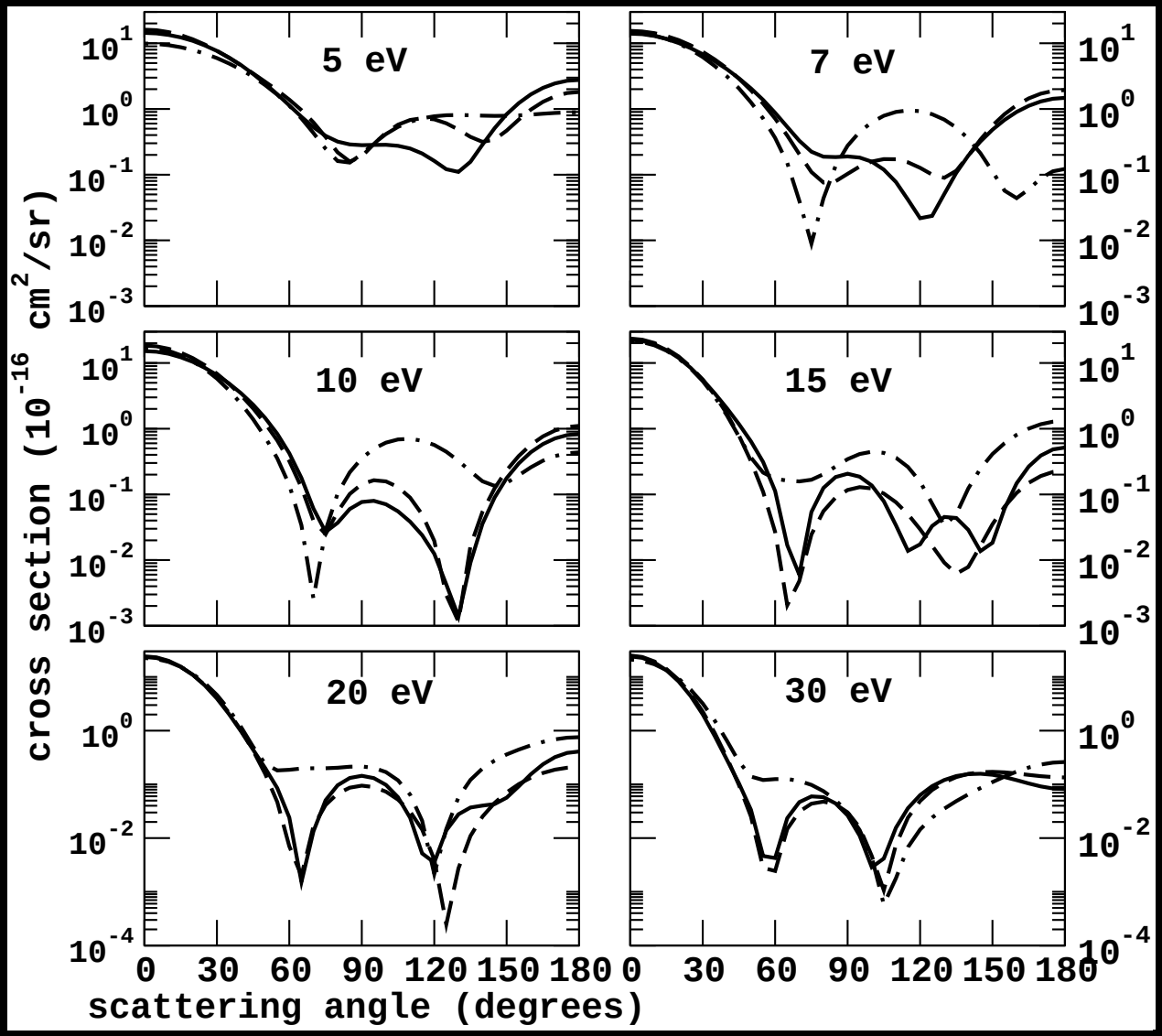
Integral cross section for C_3H_4 isomers propyne and allene. Solid lines, our results at the SE approximation; stars, total cross section of Szmytkowski and Kwitnewski; crosses, total cross section of Makochekanwa *et al.*.

Results: C_3H_4 isomers



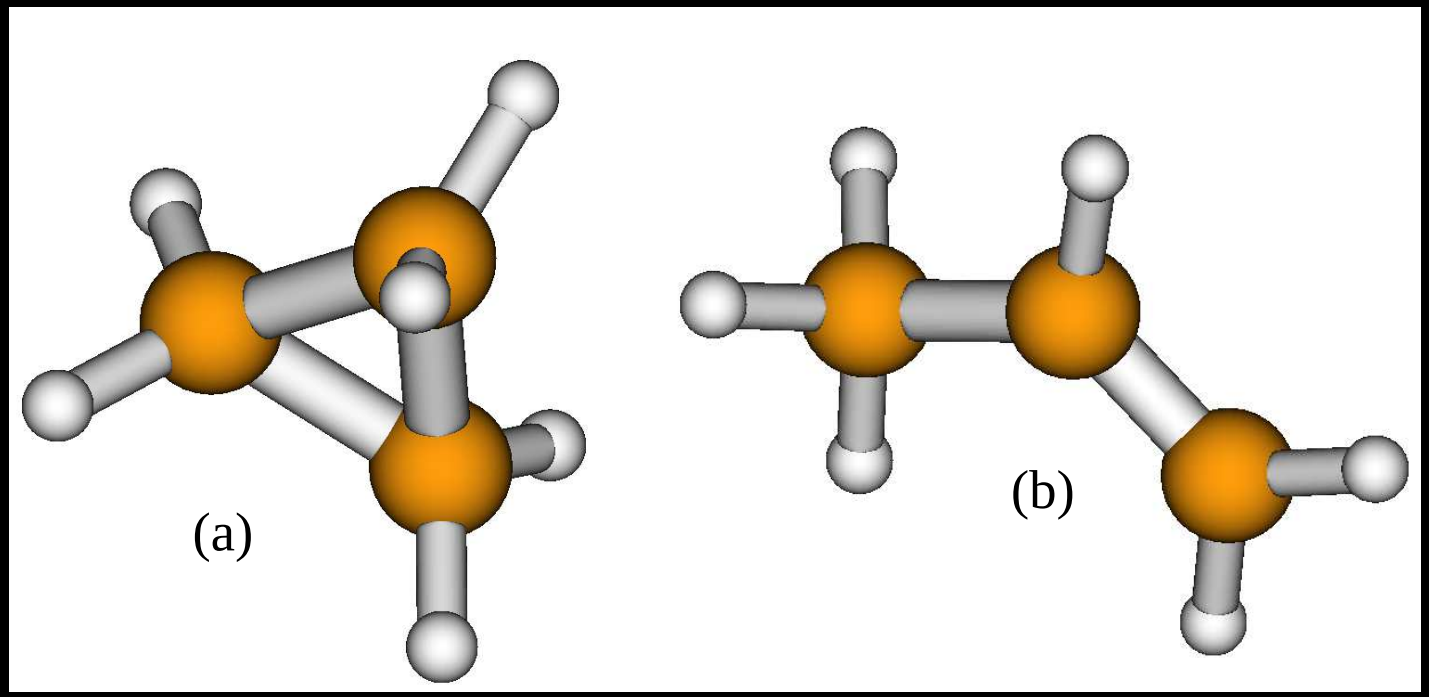
(a) Integral and (b) momentum transfer cross sections for C_3H_4 isomers at the SE approximation.

Results: C_3H_4 isomers



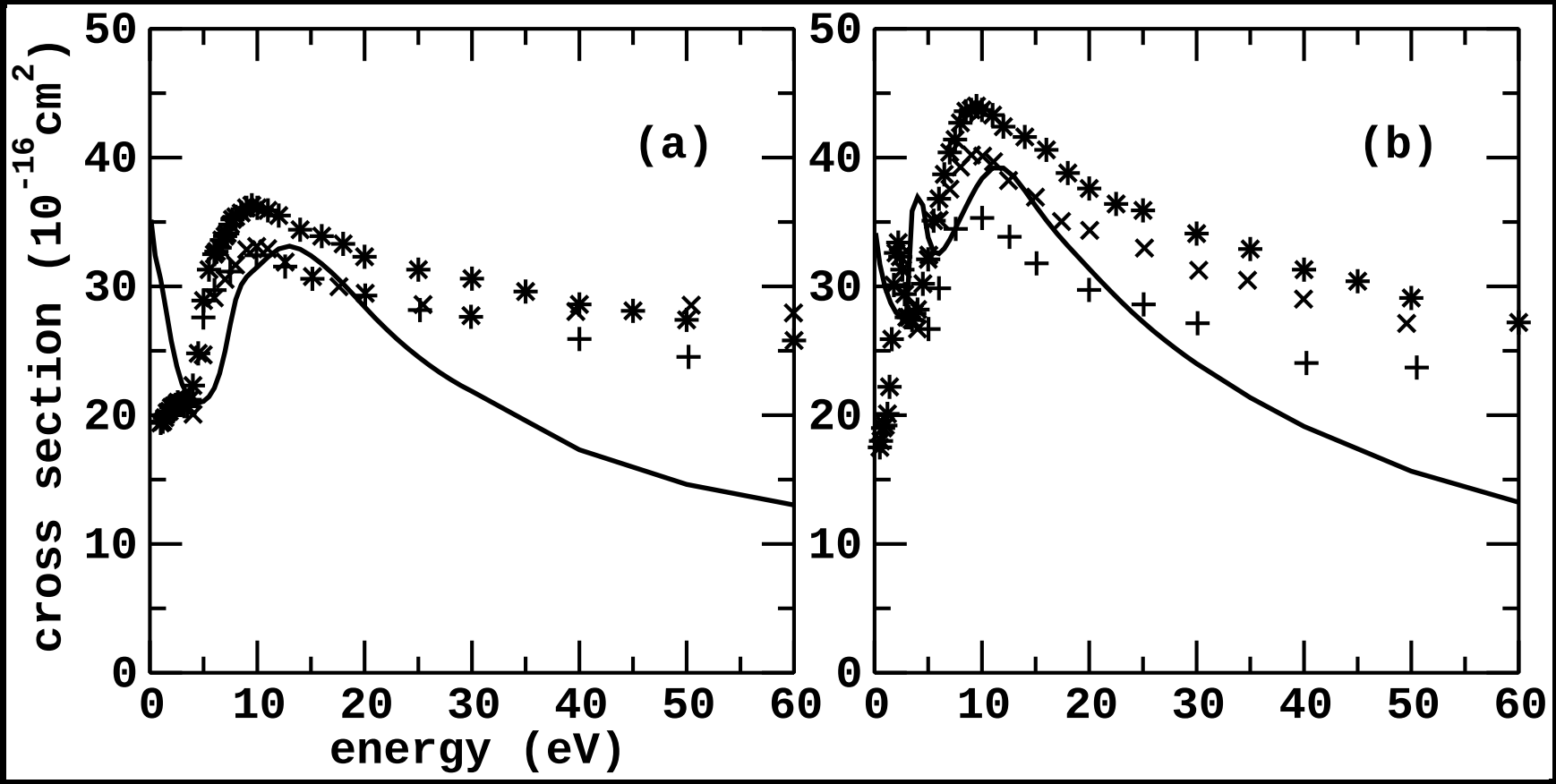
Differential rotationally elastic cross sections ($00 \rightarrow 00$) for allene (solid line), propyne (dashed line) and cyclopropene (dot-dashed line).

Results: C_3H_6 isomers



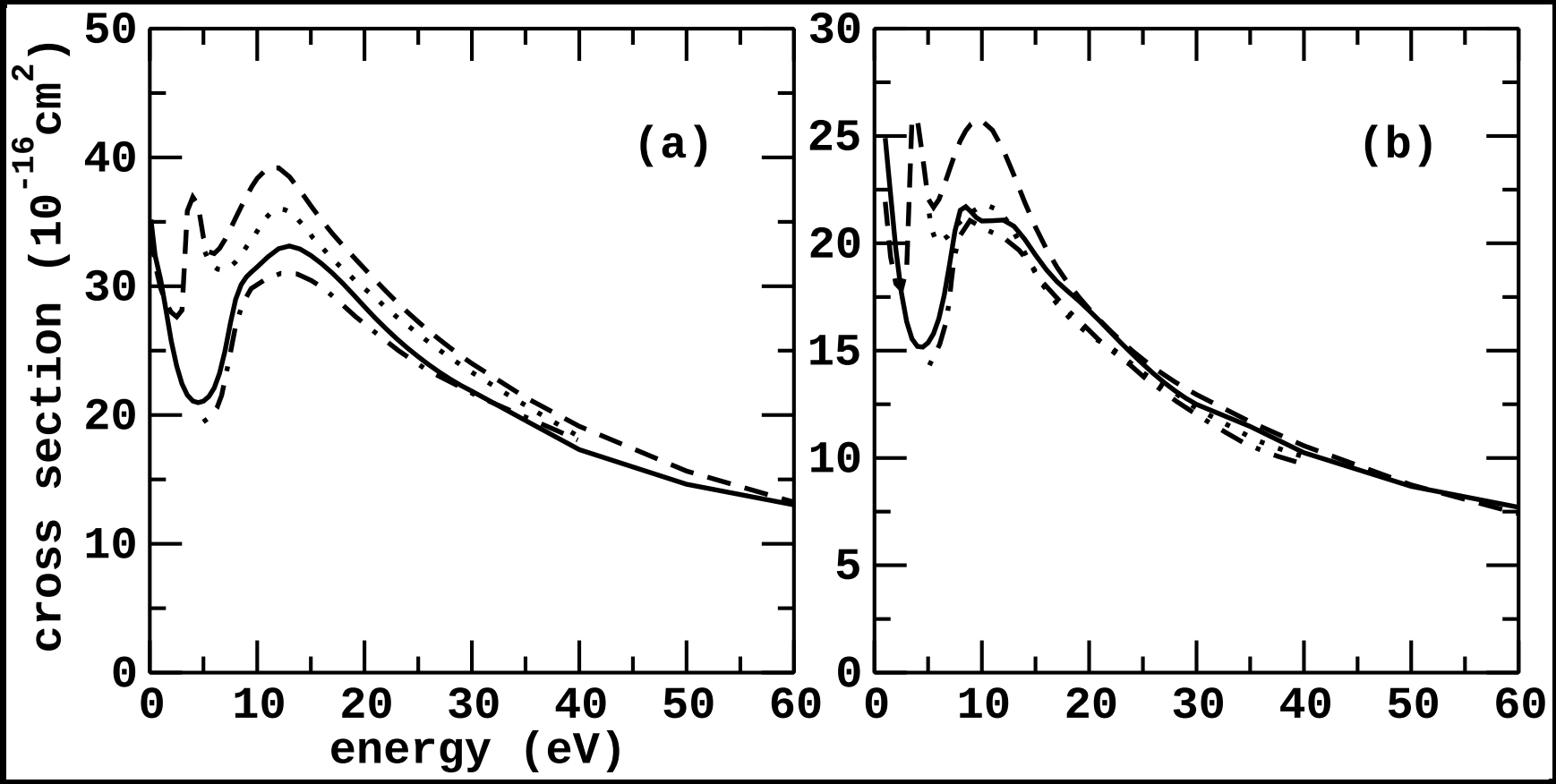
Geometrical structure of the C_3H_6 isomers: (a) cyclopropane (D_{3h}) and (b) propene (C_s).

Results: C_3H_6 isomers



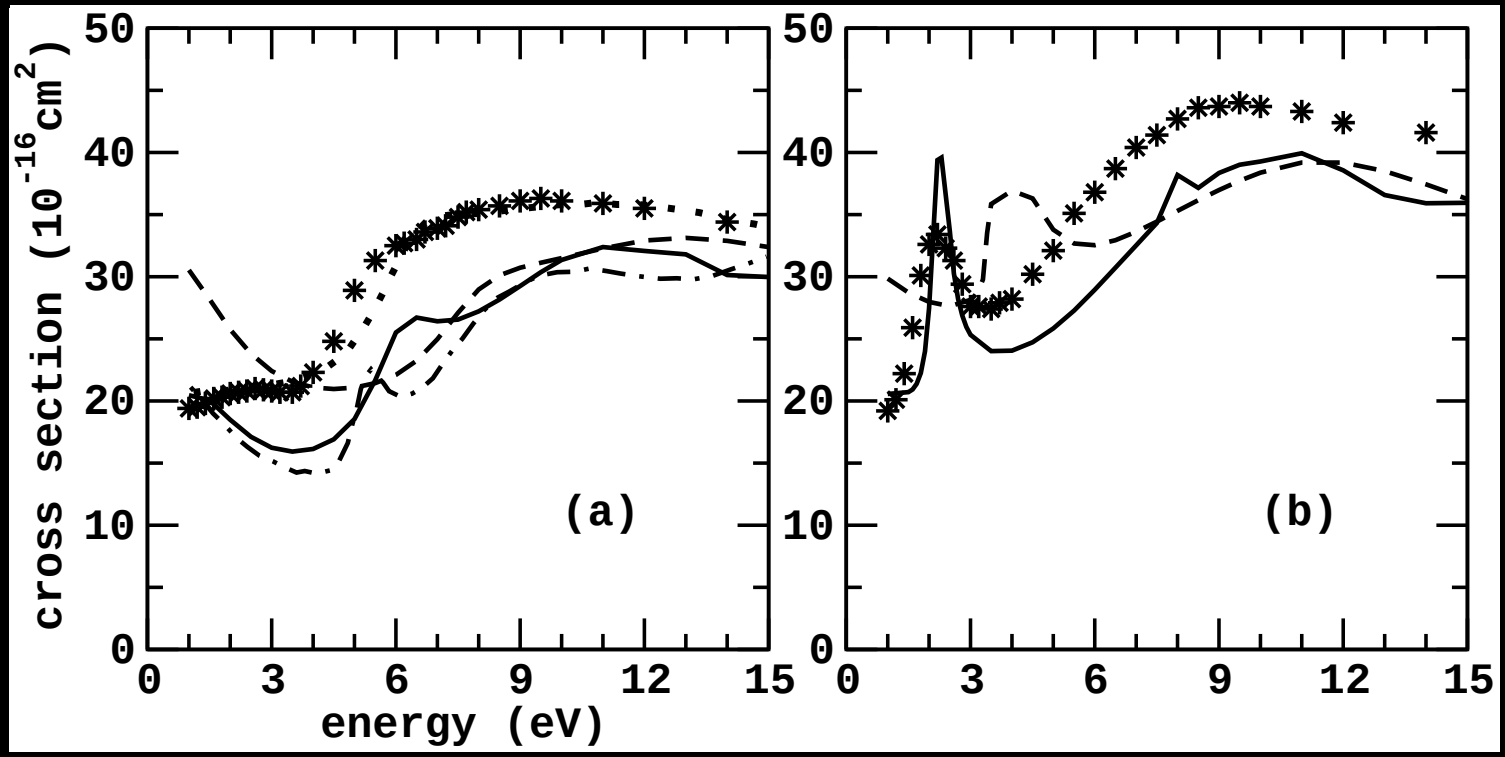
Integral cross sections for C_3H_6 isomers at the SE approximation. (a) Cyclopropane and (b) propene. Solid lines, our results at the SE approximation. Total cross sections: crosses, Floeder *et al.*; pluses, Nishimura and Tawara; stars, Szmytkowski and Kwitnewski.

Results: C_3H_6 isomers



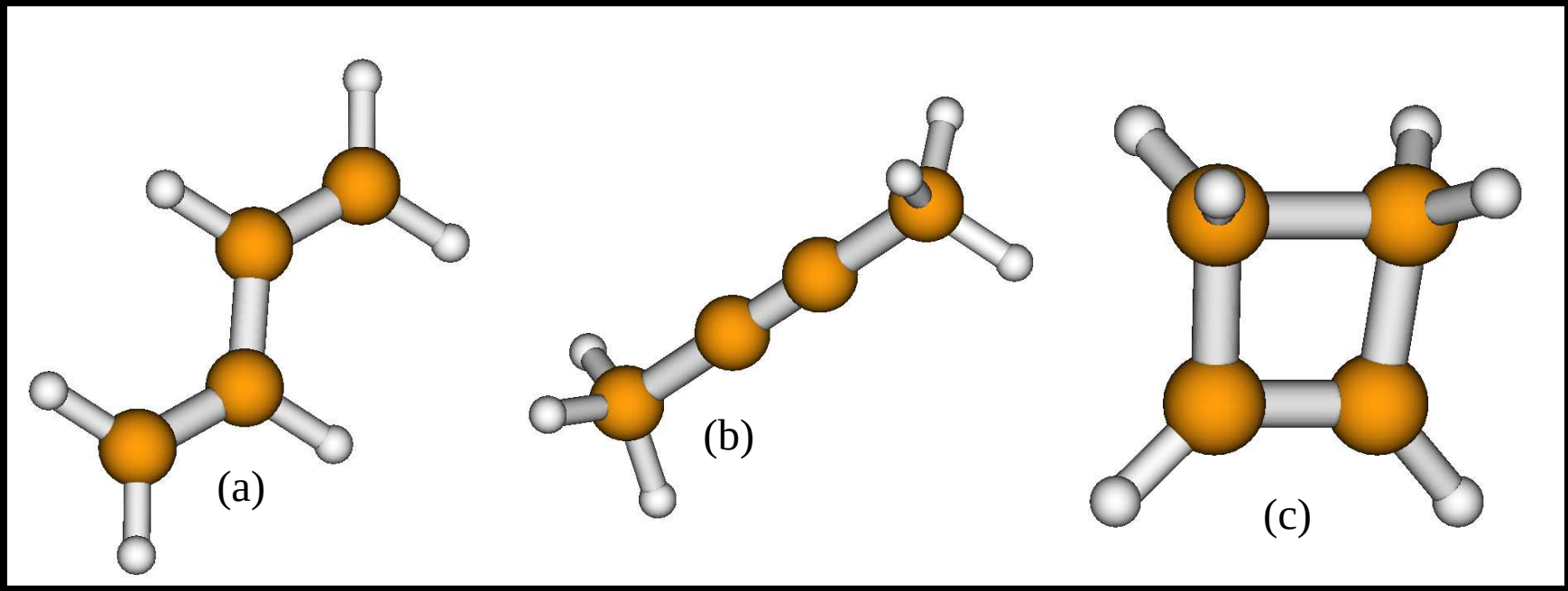
(a) Integral and (b) momentum transfer cross sections for C_3H_6 isomers at the SE approximation. Solid line (PP) and dot-dashed line (AE), cyclopropane; dashed line (PP) and dotted line (AE), propene.

Results: C_3H_6 isomers



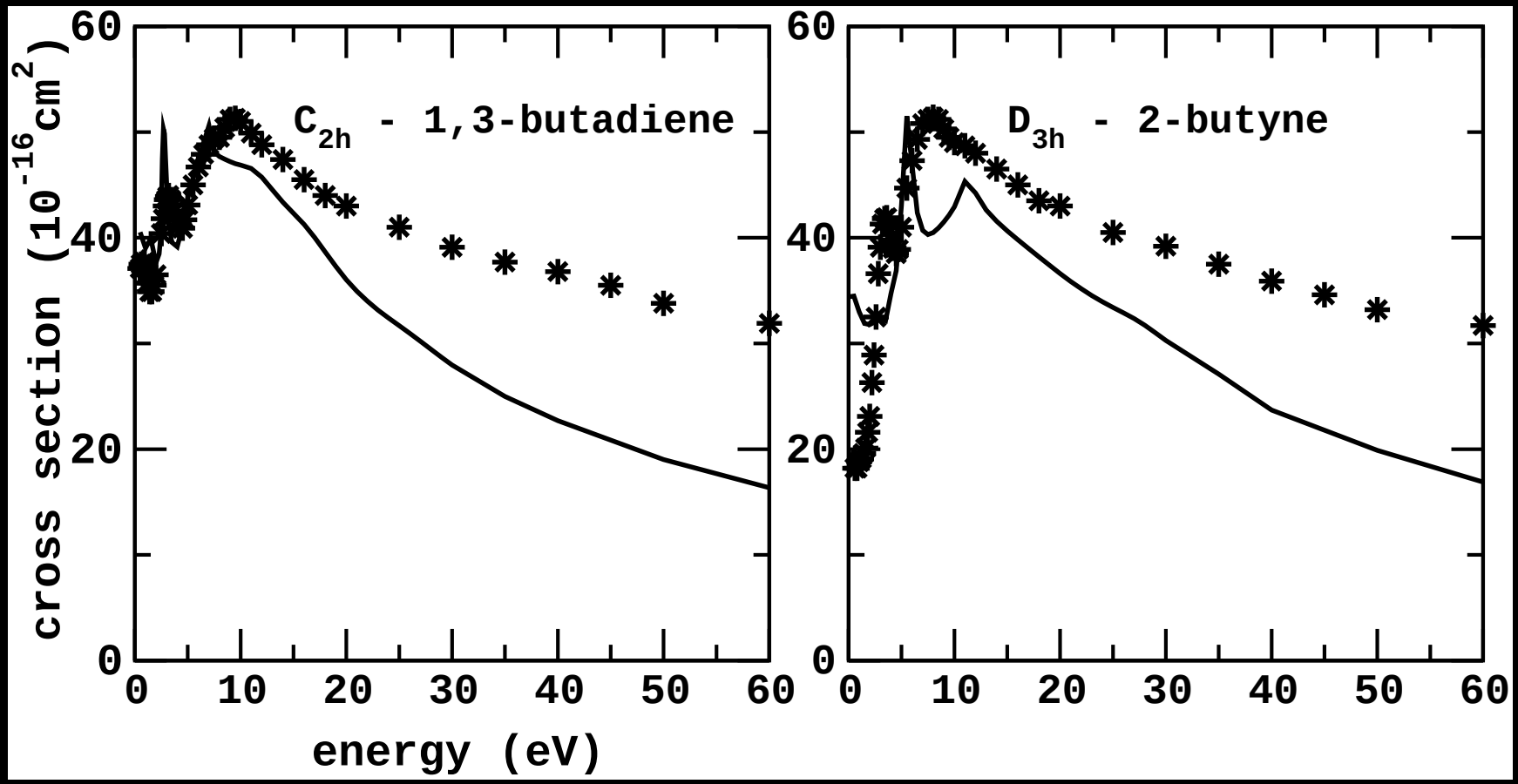
Integral cross sections for C_3H_6 isomers: (a) cyclopropane and (b) propene. Dashed lines, our results at the SE approximation; solid lines, our results at the SEP approximation; dotted line, results of Curik and Gianturco at the SEP approximation; dot-dashed lines, results of Beyer *et al.* at the SEP approximation; stars, total cross section of Szmytkowski and Kwitnewski.

Results: C_4H_6 isomers



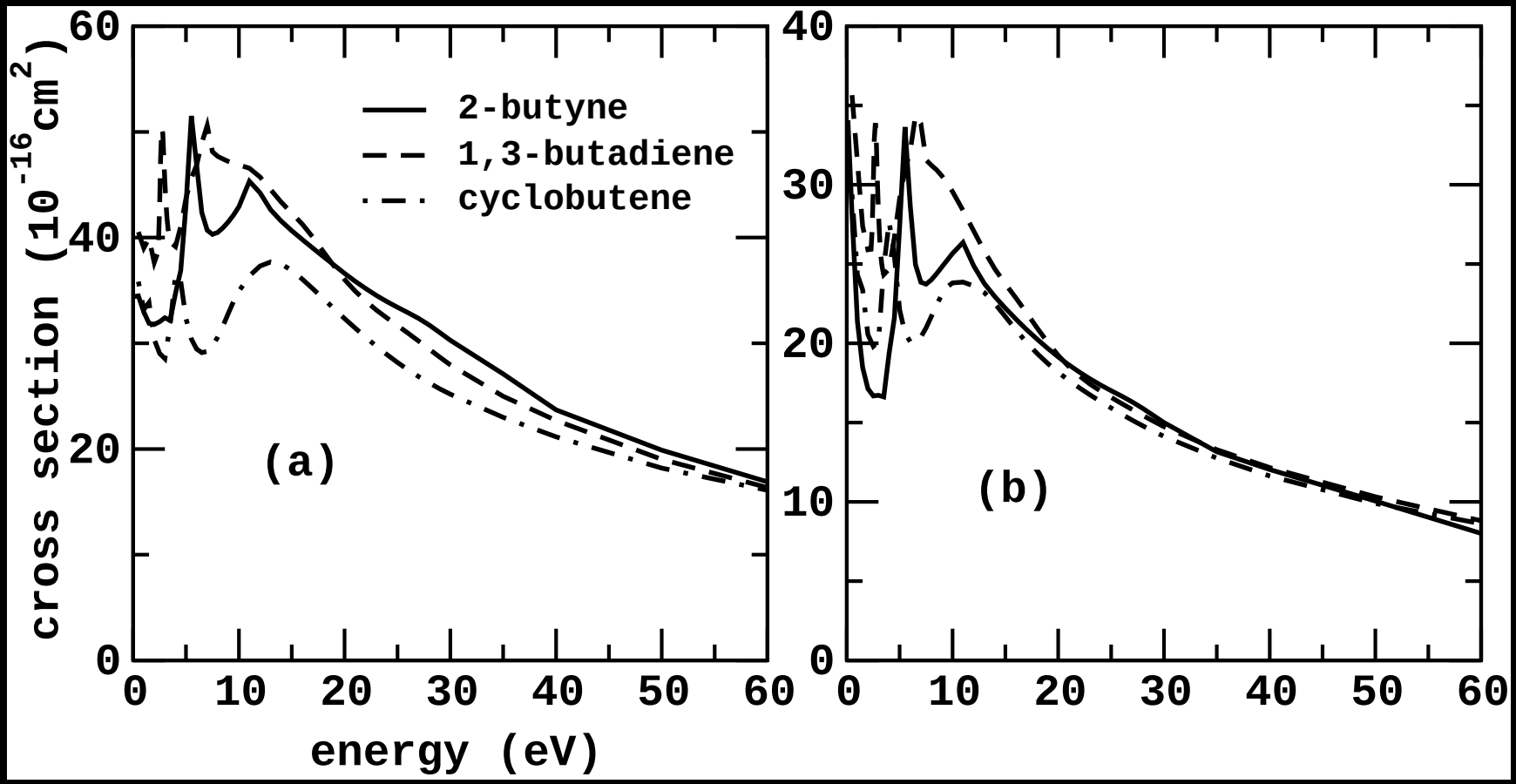
Geometrical structure of the C_4H_6 isomers: (a) trans-1,3-butadiene (C_{2h}), (b) 2-butyne (D_{3h}), and (c) cyclobutene (C_{2v}).

Results: C_4H_6 isomers



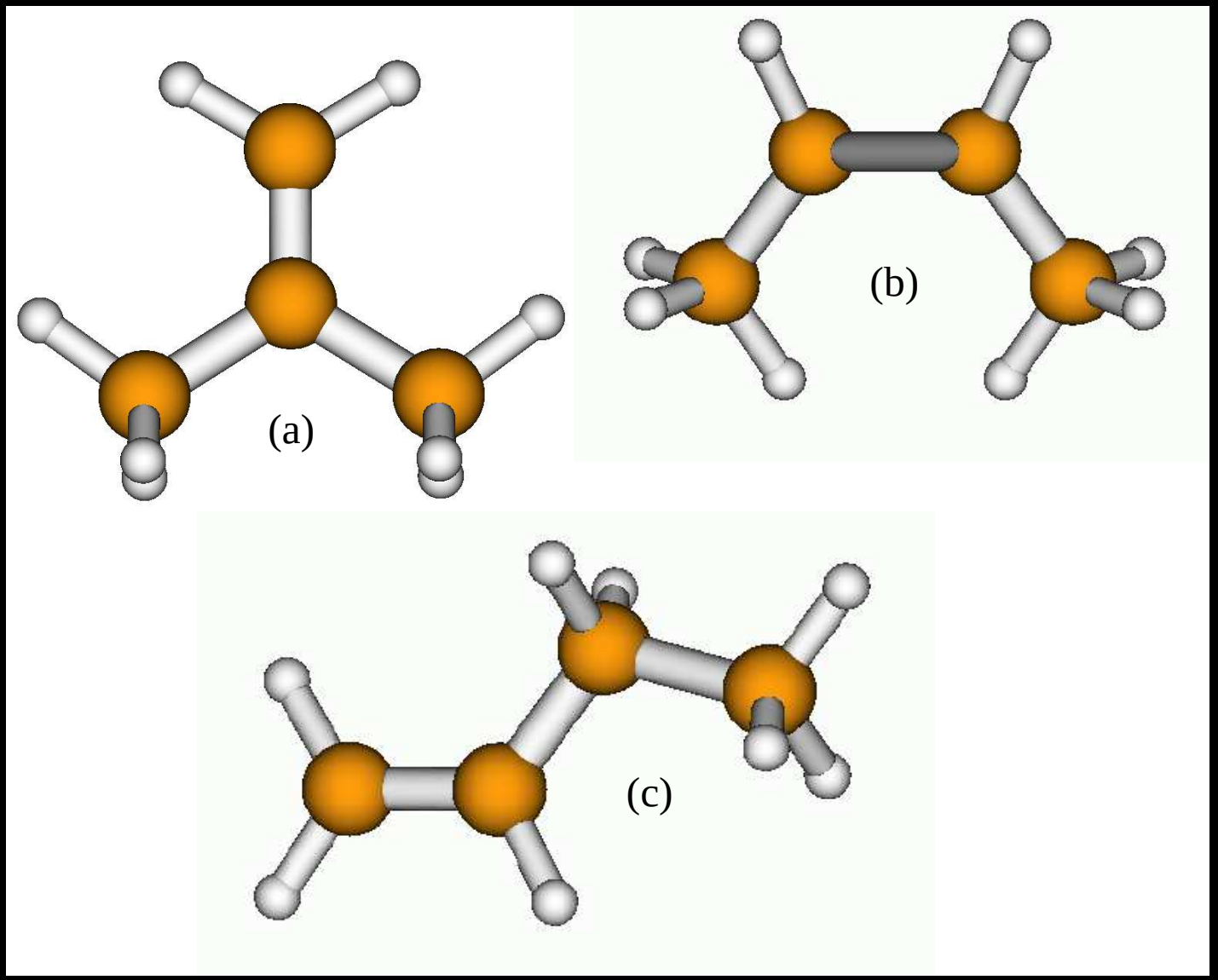
Integral cross sections for C_4H_6 isomers 2-butyne and 1,3-butadiene at the SE approximation. Solid lines, our resuls; stars, total cross sections of Szmytkowski and Kwitnewski.

Results: C_4H_6 isomers



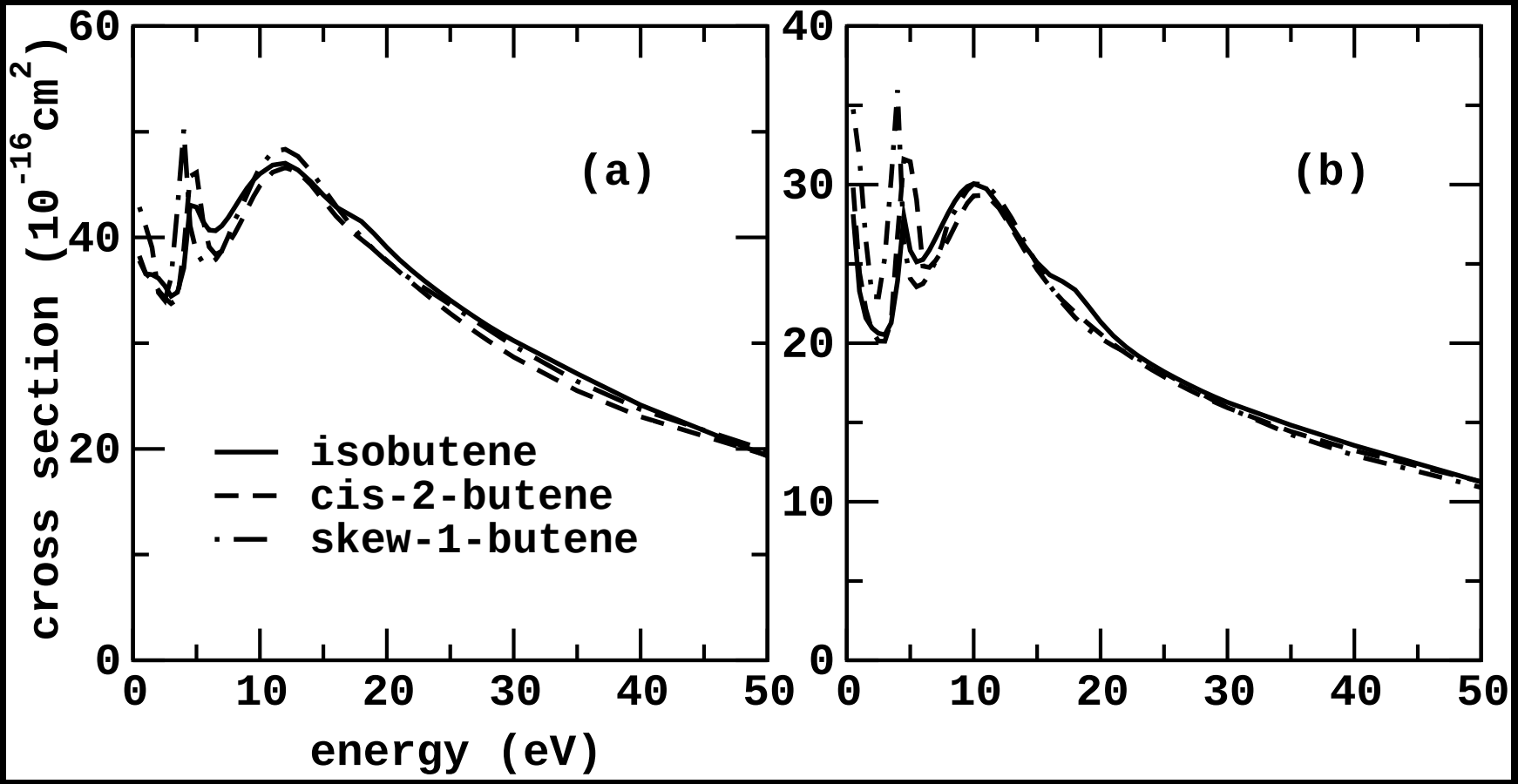
(a) Integral and (b) momentum transfer cross sections for C_4H_6 isomers at the SE approximation.

Results: C_4H_8 isomers



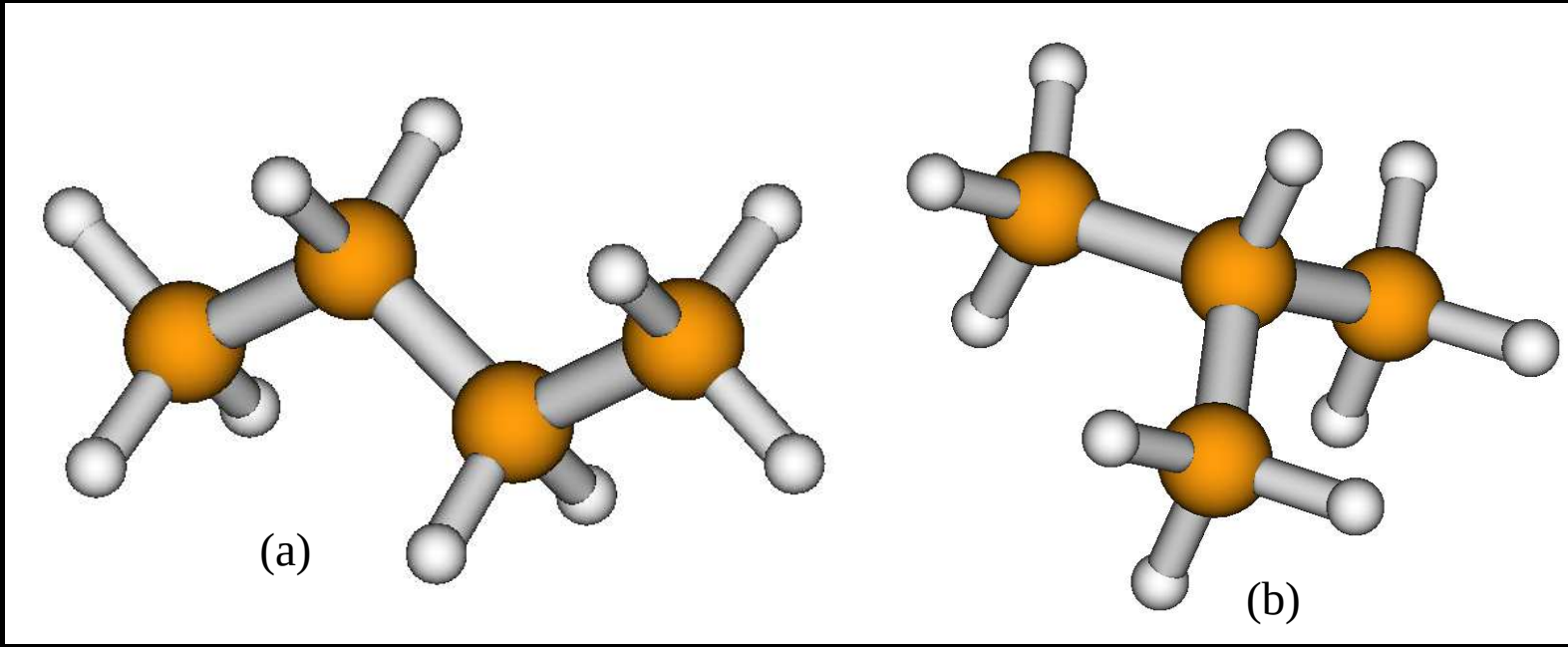
Geometrical structure of the C_4H_8 isomers: (a) isobutene (C_{2v}), (b) cis-2-butene (C_{2v}), and (c) skew-1-butene (C_s).)

Results: C_4H_8 isomers



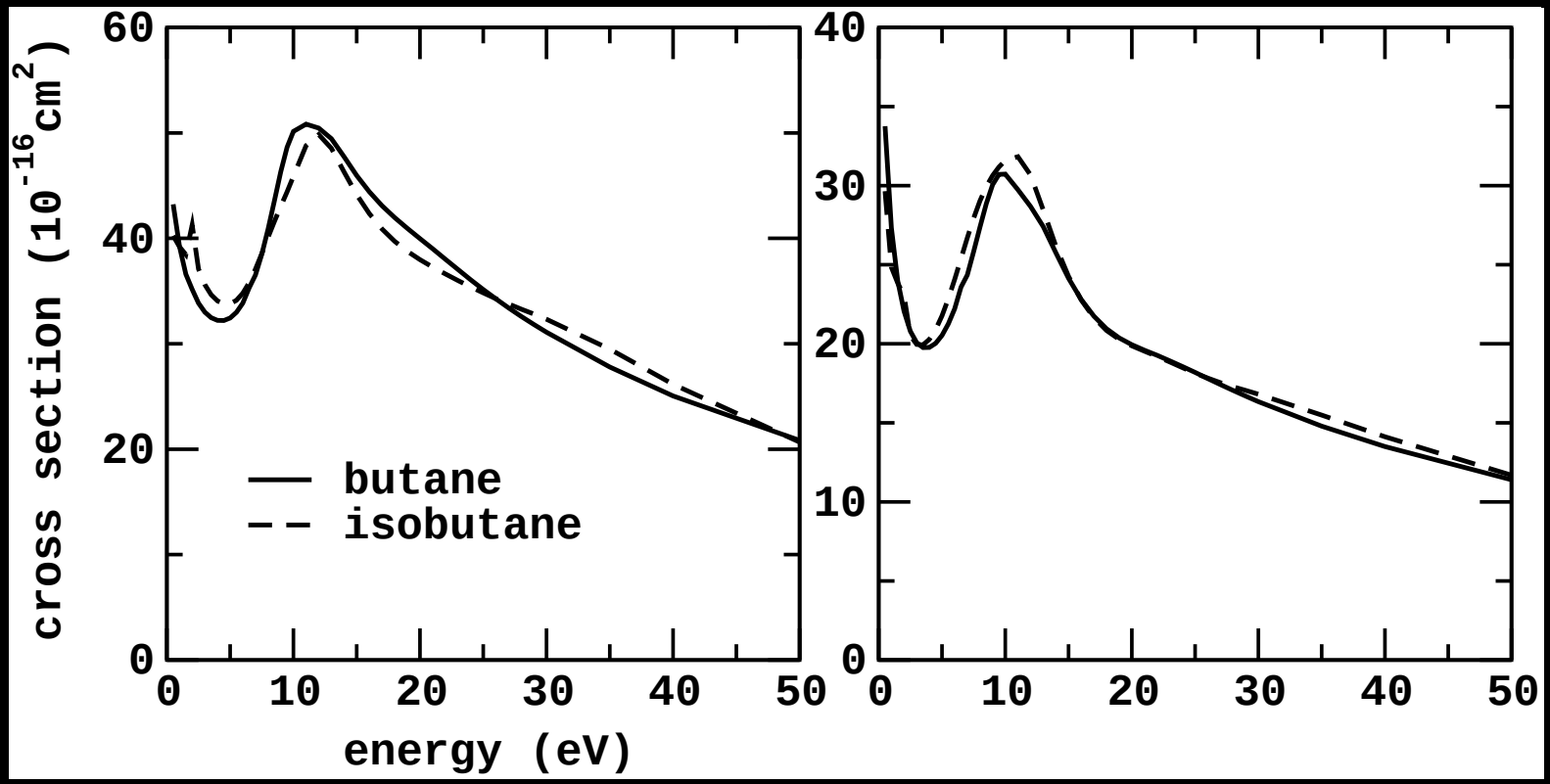
(a) Integral and (b) momentum transfer cross sections for C_4H_8 isomers at the SE approximation.

Results: C_4H_{10} isomers



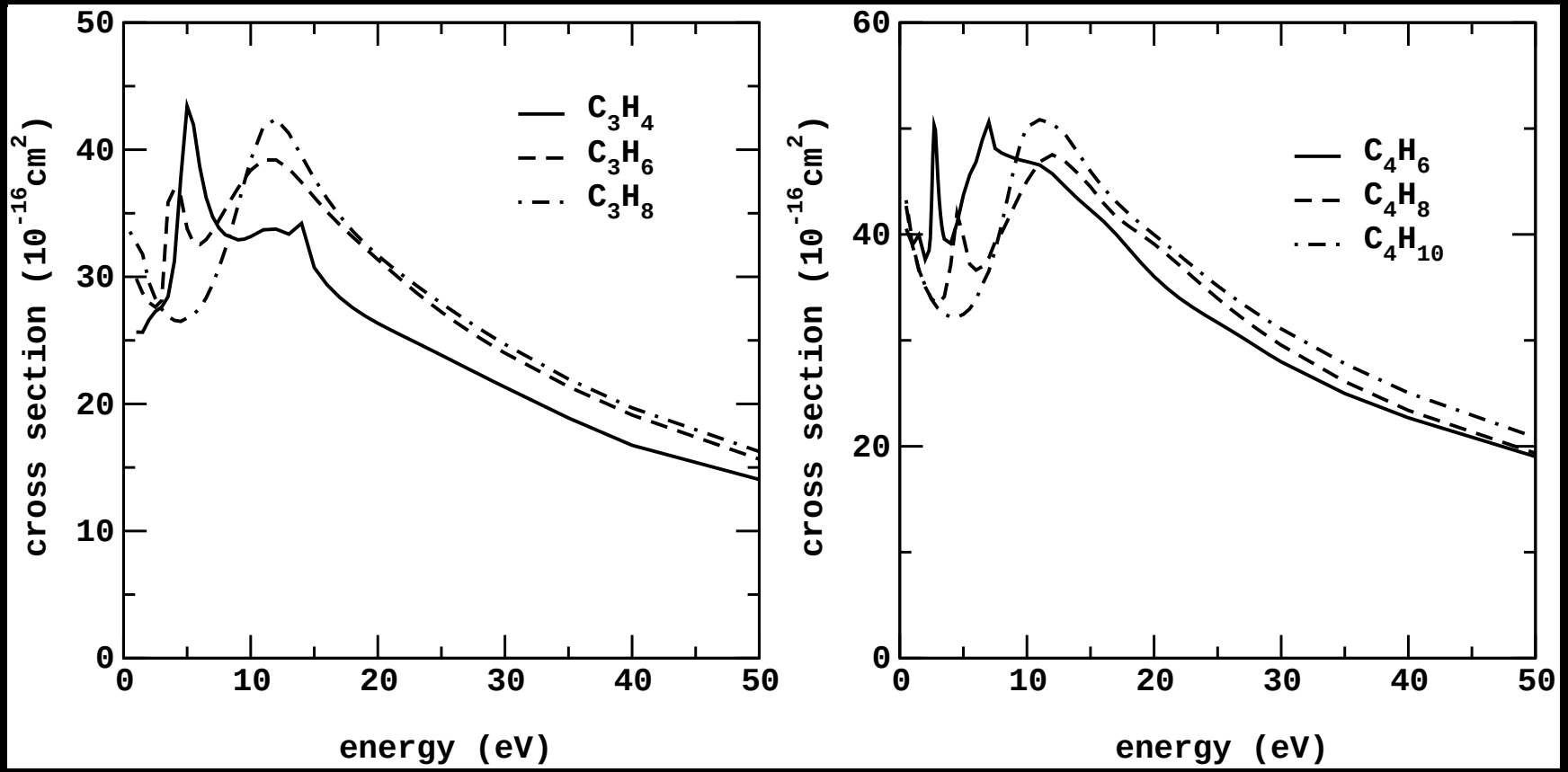
Geometrical structure of the C_4H_{10} isomers: (a) butane (C_{2h}), (b) isobutane (C_{3v}).

Results: C_4H_{10} isomers



Integral (left panel) and momentum transfer (right panel) cross sections for C_4H_{10} isomers at the SE approximation.

Results: Isocarbons.



Comparison of the integral cross sections for left panel: C_3H_4 (propyne), C_3H_6 (propene), and C_3H_8 (propane); right panel: C_4H_6 (1,3-butadiene), C_4H_8 (trans-2-butene), and C_4H_{10} (butane).

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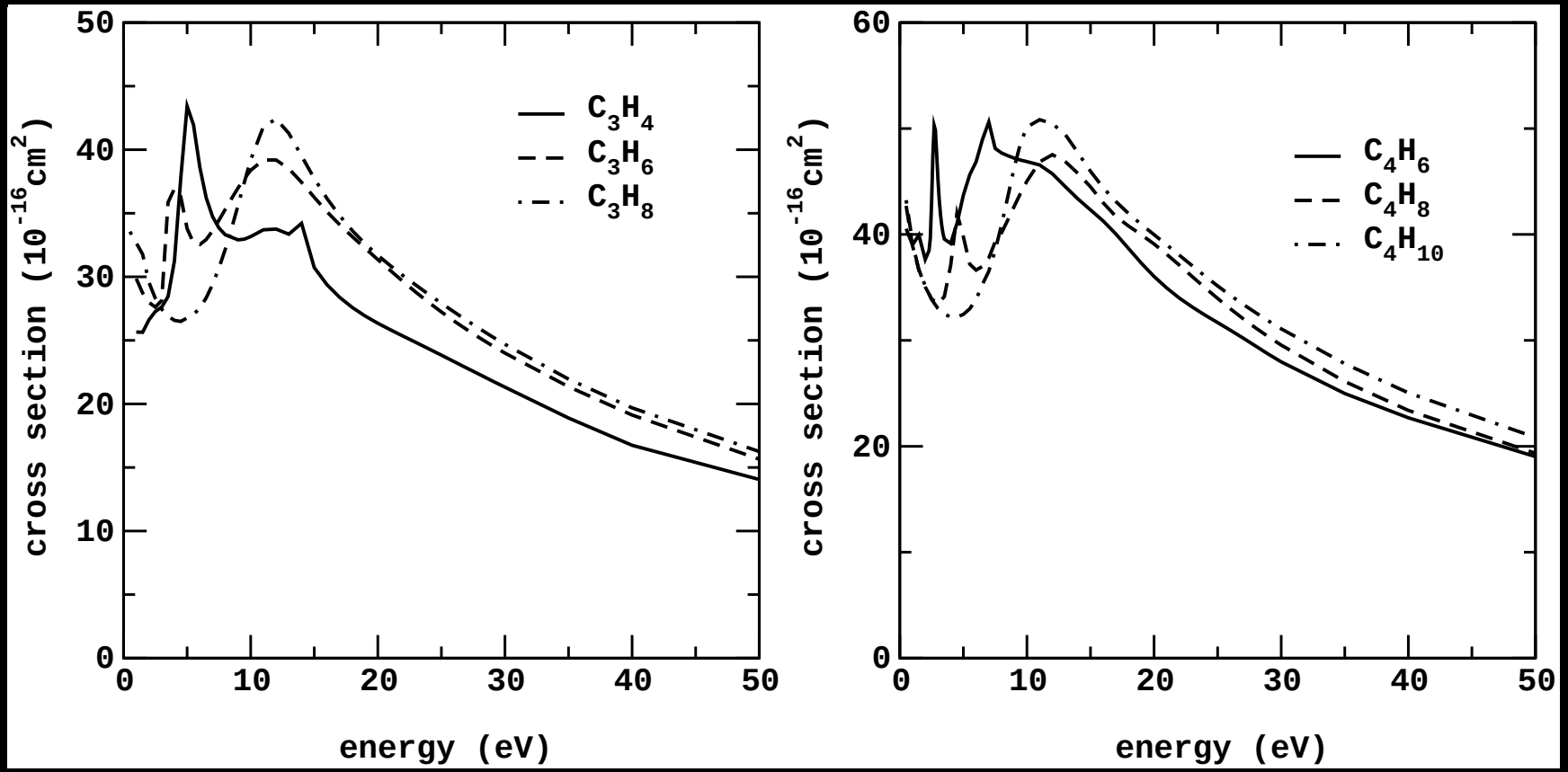

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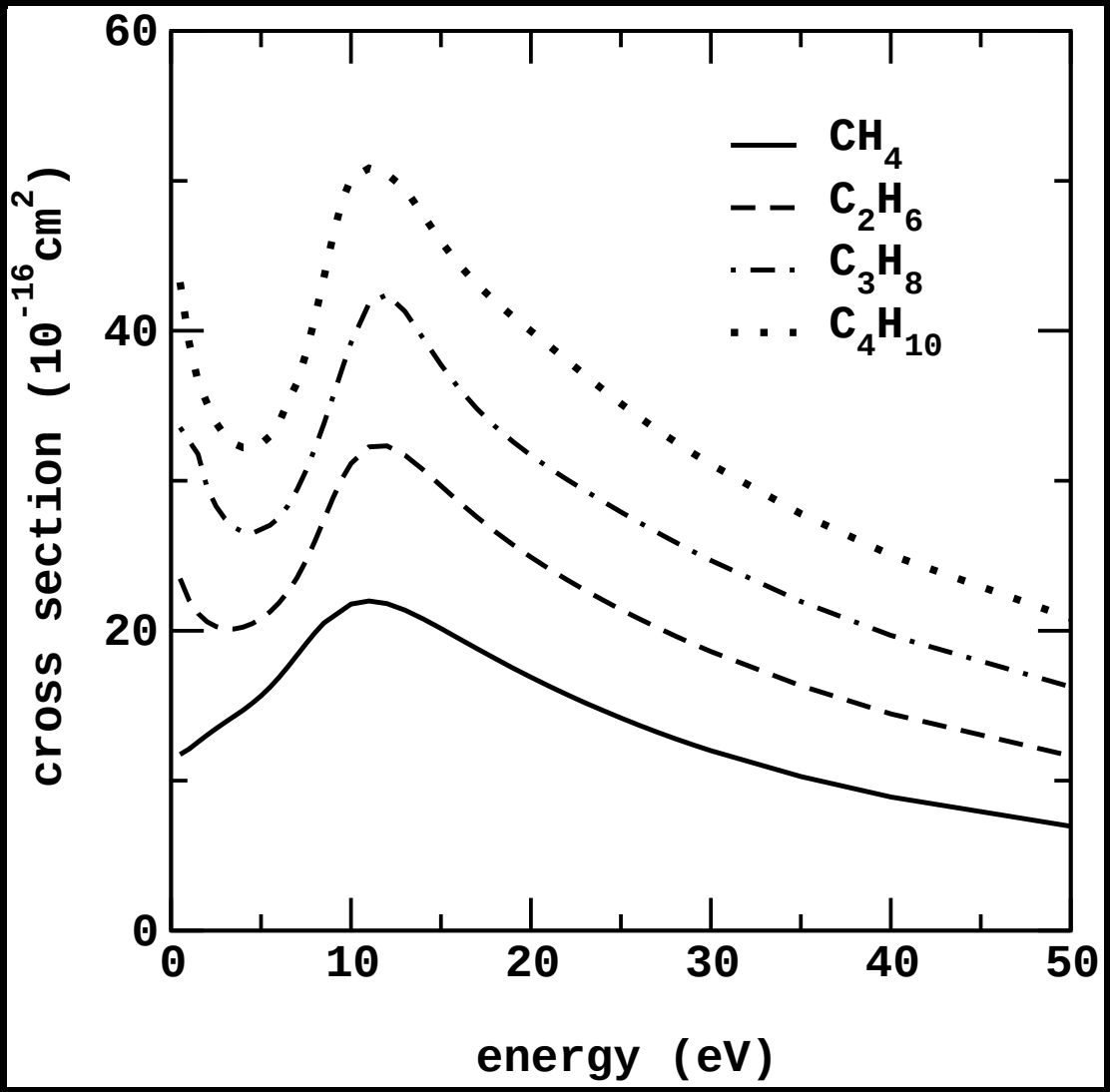
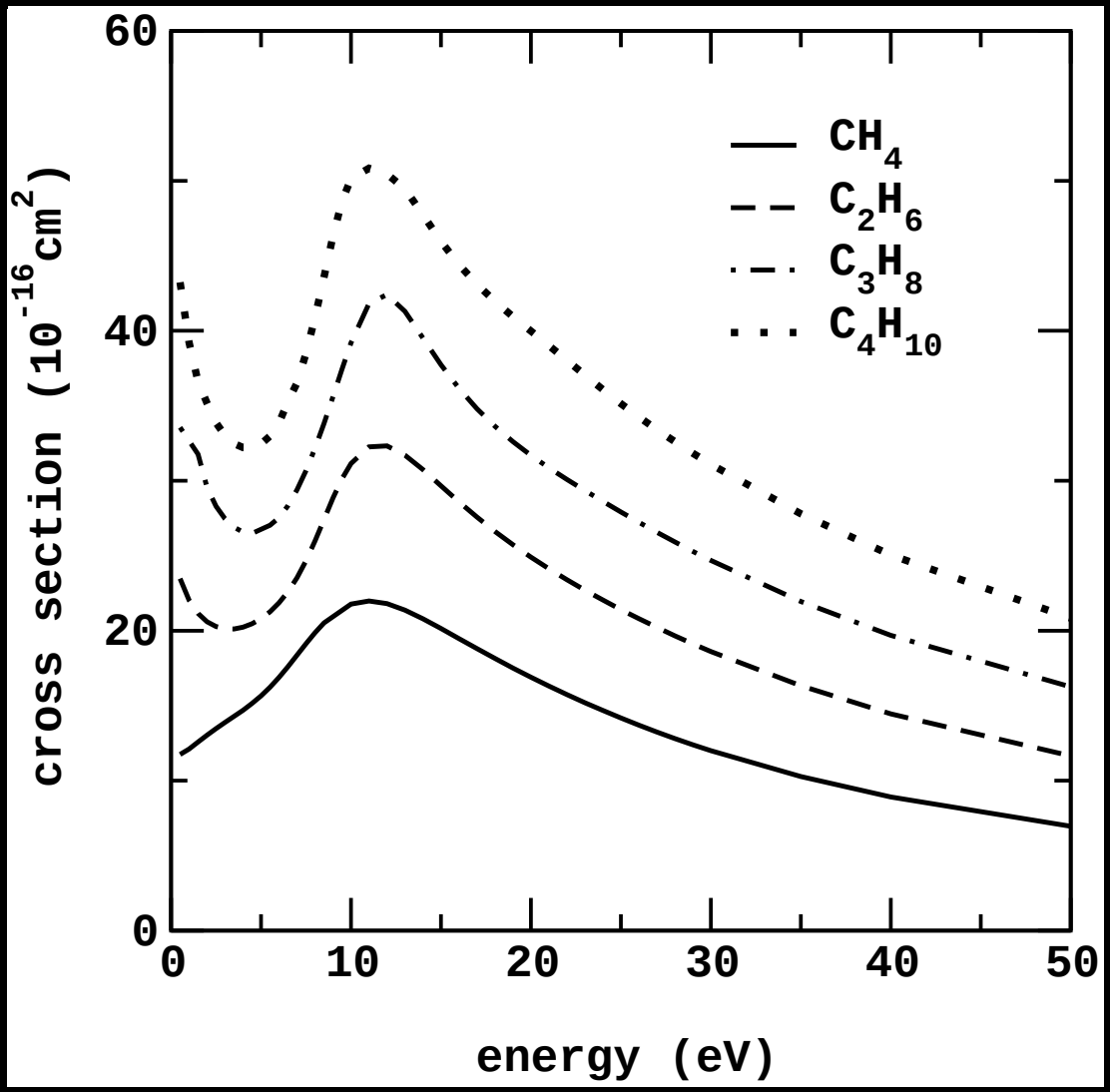
[For the comparison of C_3H_4, C_3H_6 and C_3H_8 we observe the same behavior reported by Szmytkowski and Kwitnewski, JPB **35**, 3781 (2002)]

Results: Alkanes.



Comparison of the integral cross sections for alkanes: CH_4, C_2H_6, C_3H_8, C_4H_{10}.

Results: Alkanes.



Comparison of the integral cross sections for alkanes: CH_4, C_2H_6, C_3H_8, C_4H_{10}.
[Winstead *et al.*, JCP **94** , 5455 (1991) - we added C_4H_{10}]

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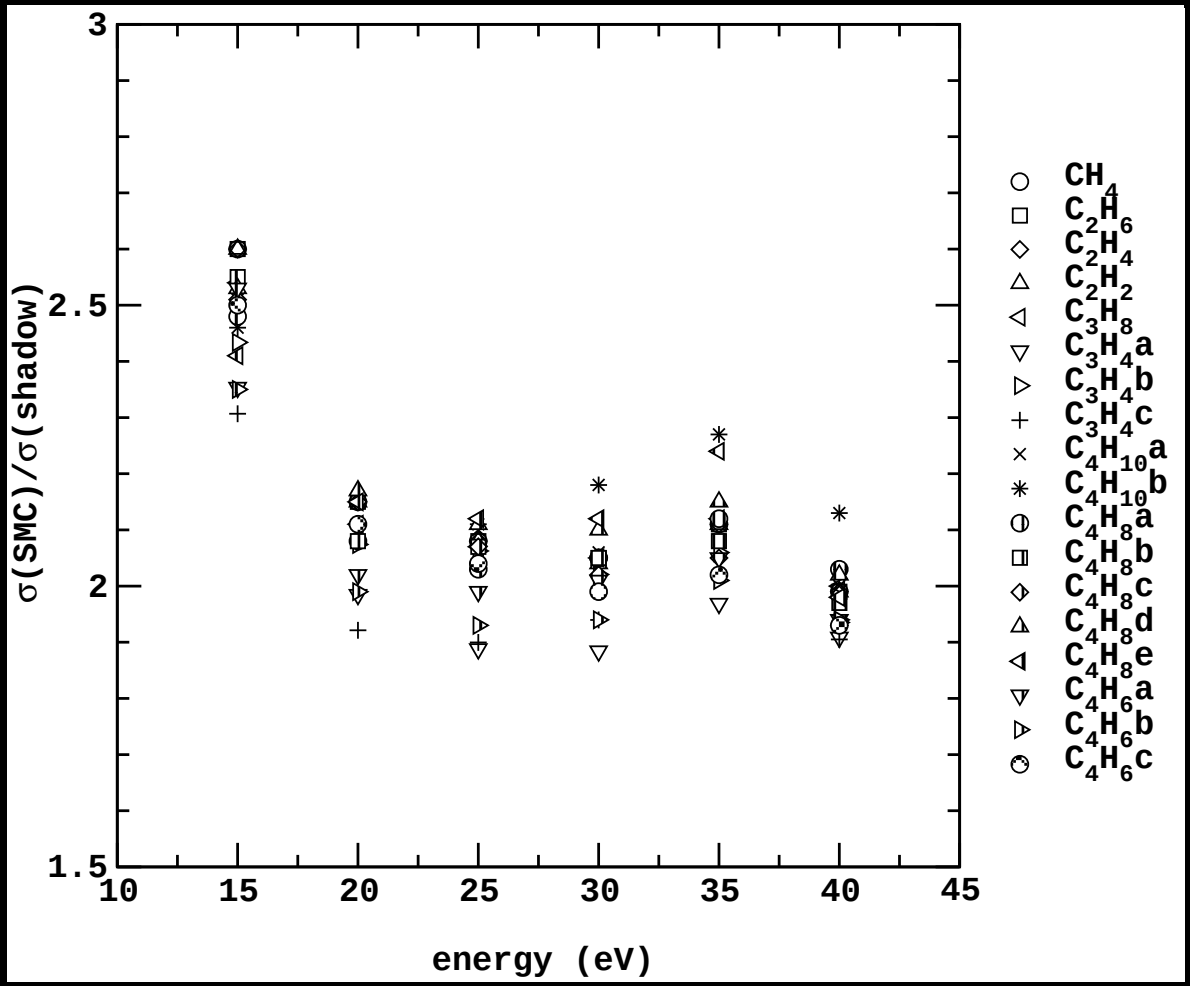
- This model provides an “scaling law” for the hydrocarbon cross sections.

Shadow model - Results



Cross section ratios: CH_4, C_2H_6, C_2H_4, C_2H_2, propane (C_3H_8), cyclopropene (C_3H_4a), propyne (C_3H_4b), allene (C_3H_4c), butane (C_4H_{10}a), isobutane (C_4H_{10}b), syn-1-butene (C_4H_8a), skew-1-butene (C_4H_8b), trans-2-butene (C_4H_8c), isobutene (C_4H_8d), cis-2-butene (C_4H_8e), 2-butyne (C_4H_6a), 1,3-butadiene (C_4H_6b), cyclobutene (C_4H_6c).

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