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Partial Ionization Cross Sections of Organic Molecules

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Partial ionization cross sections are the absolute yields of specific ions from an electron-molecule collision. They are necessary for modeling plasmas and for determining the sensitivity of mass spectrometers, among other applications. One mass-spectrometric application is estimating the abundance of organic compounds on Mars, as sampled by the rover *Curiosity*. This is a report of semitheoretical data obtained for a collection of organic molecules identified as possible biomarkers in this exotic context.

Key words: cross section; electron ionization; gas analysis; mass spectrometry; quantum chemistry.

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1. Introduction

One of the experiments aboard the National Aeronautics and Space Administration's (NASA's) Martian rover *Curiosity* is a mass-spectrometric search for organic compounds, as possible markers of life. In this measurement, a solid sample is heated, and the evolved gases are sampled using a quadrupole mass spectrometer (QMS), which constitutes part of the remote laboratory called SAM (Sample Analysis at Mars) [1]. When an organic compound is detected, an approximate estimate of its abundance is desired. Absolute QMS ion intensities may be used to infer this abundance.

The quantitation method may be illustrated using simple equations. Ideally, the absolute intensity, I_A, of a peak in a mass spectrum will be proportional to the number density (p_A) of the gaseous analyte,

$$p_A = I_A / C \,. \tag{1}$$

The proportionality constant, C, is normally determined by calibration, using a series of known pressures of the analyte. However, this cannot be done remotely on Mars, and it is not done before launch because it is not known which molecules will be detected. To proceed anyway, note that C includes intrinsic and extrinsic effects: the partial ionization cross section (i.e., intrinsic ion yield) [2], σ_A, and the responsivity of the instrument, β. This is shown in Eq. (2). Partial ionization cross sections have units of area.

$$p_A = I_A / (\sigma_A \beta) \,. \tag{2}$$

To use carbon dioxide as an internal calibrant, we combine Eq. (2) for two gases, A and CO_2, to obtain

$$p_A = \frac{I_A}{I_{CO2}} \frac{\sigma_{CO2}}{\sigma_A} p_{CO2} \,. \tag{3}$$

Note that it has been assumed, as an approximation, that the instrument responsivity is the same for the ion representing A as for the ion representing CO_2. The QMS provides *in situ* values for the corresponding peak intensities I_A and I_{CO2}. The instrument was calibrated for CO_2 on Earth, before launch. If we believe the calibration has not drifted far, then we know p_{CO2} from I_{CO2} and Eq. (1). Partial ionization cross sections are known for CO_2 [3]. Thus, the only missing datum in Eq. (3) is σ_A, the partial ionization cross section (PICS) for the peak due to the analyte. Estimating this PICS is the focus of this report.

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2. Method

2.1 Summary of theory

PICS values, which are intrinsic molecular properties, are estimated by combining an *ab initio* total ionization cross section (TICS) with empirical ion-branching fractions, as described in detail elsewhere [4] and summarized below. All ions are assumed to be singly positive, so that the symbol *m* (mass) is used where *m/z* (mass-to-charge ratio) might be expected.

The TICS is the sum of all PICS for a given analyte and is computed here from first principles using the binary-encounter Bethe (BEB) theory developed by Yong-Ki Kim and coworkers [5–13]. However, there are no purely theoretical methods for predicting the relative intensities of fragment ions. Instead, we use standard electron-ionization mass spectra (EIMS) from the National Institute of Standards and Technology (NIST) Chemistry WebBook [14]. For each ion, the relative intensity from the experimental spectrum is denoted $I_{\mathrm{EIMS}}(m)$, where m is the ion mass. The relative intensities in ordinary EIMS reflect the relative PICS values but suffer systematic bias against low-mass fragment ions [15–20]. A correction, $w(m)$, is applied to mitigate systematic, mass-dependent measurement bias, as shown in Eq. (4) and Eq. (5). The resulting, corrected, normalized branching fractions are denoted $I_{\mathrm{corr}}(m)$. M is the molecular mass, and b is a parameter that was obtained by fitting benchmark PICS measurements, here taken as $b = 0.87$.

$$I_{\mathrm{corr}}(m) = \frac{w(m) I_{\mathrm{EIMS}}(m)}{\sum_m w(m) I_{\mathrm{EIMS}}(m)} \,. \tag{4}$$

$$w(m) = \begin{cases} 1 & \text{for } m \geq bM \\ \sqrt{b/(1-b)}\sqrt{(M-m)/m} & \text{for } m < bM \end{cases} \,. \tag{5}$$

The details and rationale for this correction are described elsewhere [4]. Briefly, the correction is based upon a rudimentary physical model that attributes mass discrimination to high kinetic-energy release during the formation of fragment ions. Low-mass ions (with a heavy coproduct) have greater velocity than high-mass ions (with a light coproduct) because of conservation of momentum. Fast ions are more likely to follow "bad" trajectories in a mass spectrometer and fail to be detected. Such mass discrimination is unimportant in analytical chemistry because the low-mass ions are seldom chemically distinctive.

The BEB calculation requires binding energies and kinetic energies for the molecular orbitals in the target molecule. These are obtained from quantum chemistry calculations. In the present work, molecular geometry optimization was done using the popular, hybrid density functional B3LYP [21, 22] using 6-31G(d) basis sets. Binding and kinetic energies for all orbitals were computed at the Hartree-Fock (HF) level using 6-311G(d,p) basis sets. For thiophenol, orbital kinetic energies for outer orbitals were recalculated using the "SDDall" effective core potential (ECP) and basis set on the sulfur center [23]. Binding energies for outer orbitals were recalculated (all-electron) using electron propagator theory [24], which includes electron correlation. Finally, the molecular thresholds for vertical single and double ionization were computed using the heavily correlated CCSD(T) theory (coupled-cluster with single and double excitations and a perturbative estimate of triples) [25] along with cc-pV(T+d)Z basis sets [26]. In-house, Python-language software was used to create the quantum chemistry input files and to parse the resulting output files. The quantum chemistry calculations were done using the Gaussian09 software [27].[1]

2.2 Experimental orbital binding energies

When experimental vertical binding energies (B) are available from published photoelectron spectroscopy (PES), they may be used instead of theoretical values. The PES values used here, along with the *ab initio* values that they replace, are listed below for all affected molecules.

[1] Certain commercial materials and equipment are identified in this paper in order to specify procedures completely. In no case does such identification imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the material or equipment identified is necessarily the best available for the purpose.

Thiophenol: For the five highest-lying orbitals, values of *B*/eV = 8.49, 9.41, 10.61, 11.61, and 12.22 [28] replaced theoretical, *ab initio* values of *B*/eV = 8.39 [CCSD(T)], 9.42 (P3 propagator theory), 10.47 (P3), 11.69 (P3), and 12.40 (P3).

o-Xylene and *m*-xylene: For the highest-lying molecular orbital, *B* = 8.56 eV [29] replaced the theoretical CCSD(T) value of 8.70 eV.

p-Xylene: For the HOMO, *B* = 8.44 eV [29] replaced the theoretical CCSD(T) value of 8.58 eV.

Styrene: For three highest orbitals, values of *B*/eV = 8.49, 9.27, and 10.55 [30] replaced the corresponding theoretical values of 8.56 [CCSD(T)], 9.22 (P3), and 10.71 (P3).

1-Hexene, 2-hexene, and 3-hexene: For the HOMOs, *B*/eV = 9.65, 9.16, and 9.14 [31] replaced the corresponding CCSD(T) values of 9.71, 9.21, and 9.20 for these three compounds, respectively.

2,3-Dimethyl-2-butene: For the highest orbitals, *B*/eV = 8.44, 10.96, and 12.71 [32] replaced the theoretical values of 8.60 [CCSD(T)], 11.09 (P3), and 12.30 (P3), respectively.

1-Heptene, 2-heptene, and 3-heptene: For the HOMOs, *B*/eV = 9.68, 9.11, and 9.05 [33] replaced the CCSD(T) values of 9.69, 9.18, and 9.14, respectively.

Benzaldehyde: The HOMO binding energy of 9.80 eV [34] replaced the CCSD(T) value of 9.71 eV.

Phenol: For the highest orbitals, *B*/eV = 8.70, 9.39, 11.59, 12.02, 12.61, and 13.44 [28] replaced the theoretical CCSD(T) value of 8.58 and the P3 values of 9.37, 11.73, 12.19, 12.76, and 13.72, respectively.

Acetophenone: For the highest orbitals, *B*/eV = 9.37, 9.55, 9.77, and 11.91 [35] replaced the CCSD(T) value of 9.38 and the P3 values of 9.59, 9.55, and 12.21, respectively.

Pyrrole: For the two highest orbitals, *B*/eV = 8.209 and 9.20 [36] replaced the CCSD(T) value of 8.26 and the P3 value of 9.05, respectively.

Pyridine: For the highest orbitals, *B*/eV = 9.60, 9.75, 10.51, and 12.61 [28] replaced the theoretical CCSD(T) value of 9.69 and the P3 values of 9.81, 10.42, and 12.93, respectively.

Benzonitrile: For the highest orbitals, *B*/eV = 9.71, 10.17, 11.84, and 12.09 [28] replaced the theoretical CCSD(T) value of 9.80 and the P3 values of 10.04, 12.29, and 12.46, respectively.

Experimental EIMS data were taken from the NIST WebBook [14] when available. These are generally "consensus" spectra that combine numerous individual measurements [37]. For 3-methyl-2-hexene, the mass spectrum was not specifically for the *E* isomer. For 2-methyl-3-hexene, the EIMS was not in the WebBook and was taken directly from the NIST mass spectral database [38]. For 2-ethyl-1-pentene, no EIMS data are available in the NIST database or in the literature, so PICS could not be computed.

3. Results

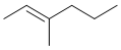
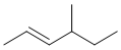
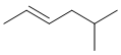
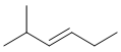
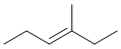
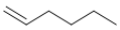
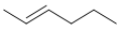
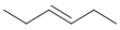
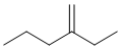
3.1 Total ionization cross sections (TICS)

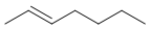
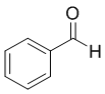
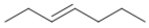
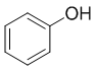
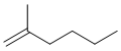
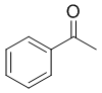
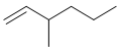
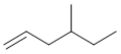
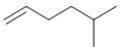
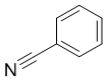
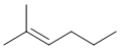
The list of molecules of interest was selected for relevance to the search for organic compounds on Mars [34]. Some of these molecules exist in multiple isomeric forms. All such isomers were considered here, except for isomers with *cis* double bonds, which were omitted because they are expected to be less stable than their *trans* counterparts. See Table 1 for the complete list of isomers studied. Also included in Table 1 are the BEB values of the TICS. Their associated standard uncertainty is about 13% [13]. In Table 1, some values were computed purely theoretically, and some were computed using available binding energies from experimental PES. In the latter situations, the differences from purely theoretical values are all less than 1%.

Molecular-orbital binding energies and kinetic energies are summarized in the data tables, one for each molecule studied. The tables are presented in the Appendix, below, and are also available, in the supplemental materials, as tab-delimited text files named "<*molecule*>.bun." The suffix "bun" derives from the symbols in the BEB equations for orbital binding energy (*B*), kinetic energy (*U*), and occupation number (*N*). Also available in the supplemental materials is a Perl-language script, "beb_tbl.pl," which reads a BUN file, applies the BEB theory, and produces a table of TICS as a function of incident electron energy. It is very similar to the script behind the NIST database [35]. For the present application, the only interesting value of the incident electron energy is 70 eV (1 eV ≈ 1.602×10^{-19} J). This is also the energy for which EIMS data are most abundant. However, the BUN files and Perl script may be used to compute

TICS at any value of the incident electron energy. For very high energies, the relativistic version of BEB [10], which is not implemented in the Perl script, would be more appropriate.

Table 1. Molecular names, structures, and TICS at 70 eV.

Name	Structure	TICS / 10^{-20} m^2	Name	Structure	TICS / 10^{-20} m^2
thiophenol		19.06	3-methyl-2-hexene		21.27
o-xylene		21.52	4-methyl-2-hexene		21.40
m-xylene		21.76	5-methyl-2-hexene		21.31
p-xylene		21.76	2-methyl-3-hexene		21.25
styrene		20.60	3-methyl-3-hexene		21.47
1-hexene		18.04	2,3-dimethyl-1-pentene		21.43
2-hexene		17.98	2,4-dimethyl-1-pentene		21.59
3-hexene		18.42	3,4-dimethyl-1-pentene		21.40
2-methyl-1-pentene		17.74	3,3-dimethyl-1-pentene		21.14
3-methyl-1-pentene		18.15	4,4-dimethyl-1-pentene		20.65
4-methyl-1-pentene		17.96	2,3-dimethyl-2-pentene		21.77
2-methyl-2-pentene		18.30	2,4-dimethyl-2-pentene		20.71
3-methyl-2-pentene		18.15	3,4-dimethyl-2-pentene		20.57
4-methyl-2-pentene		18.10	4,4-dimethyl-2-pentene		21.59
2,3-dimethyl-1-butene		17.84	2-ethyl-1-pentene		21.08
3,3-dimethyl-1-butene		17.67	3-ethyl-1-pentene		21.09
2,3-dimethyl-2-butene		18.57	3-ethyl-2-pentene		21.49
2-ethyl-1-butene		18.17	2,3,3-trimethyl-1-butene		20.97
1-heptene		21.03	2-ethyl-3-methyl-1-butene		21.23

2-heptene		21.31	benzaldehyde		17.77
3-heptene		20.45	phenol		16.46
2-methyl-1-hexene		21.24	acetophenone		21.15
3-methyl-1-hexene		21.28	pyrrole		12.43
4-methyl-1-hexene		21.37	pyridine		13.92
5-methyl-1-hexene		21.02	benzonitrile		16.78
2-methyl-2-hexene		21.44			

3.2 Partial ionization cross sections (PICS)

The estimated PICS at 70 eV are tabulated below, starting with Table 2. They are also provided in the supplemental materials, in computer-readable form. There is no table for 2-ethyl-1-pentene because the necessary EIMS data are unavailable. In addition to the PICS value for each ion, 67% and 95% uncertainty intervals are provided. Note that these intervals are not symmetric about the recommended value. The 67% uncertainty intervals are probably reliable [4]. For the strongest peak in each mass spectrum (the "base peak"), the 95% uncertainty intervals are probably also reliable, but for other peaks, the 95% intervals may be too narrow [4]. The last column in each PICS table is the uncertainty model used in the Monte Carlo determination of the uncertainty intervals: model "A" is linear in intensity, "B" is logarithmic, and "H" is a crude estimate for H^+ (m/z 1). Details of the uncertainty models are provided elsewhere [4]. A cursory look at the tables reveals that the uncertainties are much larger than would be obtained by laboratory calibration. Fortunately, the values are sufficiently precise for the Mars application, which is semiquantitative.

Table 2. Partial ionization cross sections (10^{-20} m^2) for thiophenol. TICS/10^{-20} m^2 = 19.060. *M* = 110 is base peak.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	65	0.888	[0.458, 1.455]	[0.227, 2.343]	B
17	0.023	[0.011, 0.036]	[0.006, 0.063]	B	66	2.527	[0.724, 3.357]	[0.137, 5.134]	A
18	0.158	[0.078, 0.250]	[0.040, 0.422]	B	67	0.135	[0.066, 0.213]	[0.034, 0.361]	B
26	0.072	[0.035, 0.112]	[0.018, 0.193]	B	68	0.024	[0.011, 0.037]	[0.006, 0.063]	B
27	0.191	[0.094, 0.300]	[0.049, 0.512]	B	69	0.538	[0.272, 0.869]	[0.138, 1.434]	B
28	0.186	[0.092, 0.295]	[0.047, 0.497]	B	70	0.060	[0.029, 0.094]	[0.015, 0.162]	B
32	0.062	[0.030, 0.097]	[0.016, 0.167]	B	71	0.133	[0.065, 0.209]	[0.034, 0.354]	B
33	0.046	[0.022, 0.071]	[0.012, 0.122]	B	72	0.007	[0.003, 0.011]	[0.002, 0.019]	B
34	0.015	[0.007, 0.023]	[0.004, 0.040]	B	73	0.043	[0.021, 0.067]	[0.011, 0.114]	B
36	0.029	[0.014, 0.045]	[0.007, 0.077]	B	74	0.139	[0.068, 0.218]	[0.035, 0.370]	B
37	0.209	[0.103, 0.331]	[0.053, 0.559]	B	75	0.081	[0.040, 0.127]	[0.021, 0.217]	B
38	0.301	[0.149, 0.478]	[0.076, 0.797]	B	76	0.073	[0.036, 0.115]	[0.019, 0.194]	B
39	1.171	[0.613, 1.942]	[0.301, 3.086]	B	77	0.804	[0.411, 1.309]	[0.206, 2.128]	B
40	0.079	[0.039, 0.124]	[0.020, 0.212]	B	78	0.159	[0.078, 0.251]	[0.040, 0.422]	B
44	0.086	[0.042, 0.135]	[0.022, 0.228]	B	79	0.006	[0.003, 0.010]	[0.002, 0.017]	B
45	0.695	[0.353, 1.126]	[0.177, 1.835]	B	80	0.006	[0.003, 0.009]	[0.002, 0.016]	B
46	0.012	[0.006, 0.018]	[0.003, 0.032]	B	81	0.077	[0.038, 0.121]	[0.020, 0.207]	B
47	0.035	[0.017, 0.054]	[0.009, 0.093]	B	82	0.128	[0.063, 0.203]	[0.033, 0.342]	B
48	0.011	[0.005, 0.018]	[0.003, 0.030]	B	83	0.062	[0.030, 0.098]	[0.016, 0.167]	B
49	0.067	[0.033, 0.105]	[0.017, 0.178]	B	84	0.755	[0.386, 1.230]	[0.193, 1.997]	B
50	0.590	[0.299, 0.954]	[0.150, 1.561]	B	85	0.038	[0.018, 0.059]	[0.010, 0.102]	B
51	1.020	[0.528, 1.673]	[0.260, 2.677]	B	86	0.032	[0.015, 0.049]	[0.008, 0.085]	B
52	0.095	[0.047, 0.149]	[0.024, 0.253]	B	92	0.004	[0.002, 0.007]	[0.001, 0.012]	B
53	0.041	[0.020, 0.065]	[0.011, 0.111]	B	93	0.017	[0.008, 0.027]	[0.004, 0.046]	B
54	0.131	[0.064, 0.206]	[0.033, 0.350]	B	95	0.032	[0.015, 0.049]	[0.008, 0.085]	B
55	0.209	[0.103, 0.330]	[0.053, 0.555]	B	105	0.008	[0.004, 0.012]	[0.002, 0.021]	B
56	0.020	[0.010, 0.031]	[0.005, 0.053]	B	106	0.008	[0.004, 0.012]	[0.002, 0.021]	B
57	0.144	[0.071, 0.226]	[0.037, 0.382]	B	107	0.008	[0.004, 0.012]	[0.002, 0.021]	B
58	0.254	[0.126, 0.403]	[0.065, 0.678]	B	108	0.096	[0.047, 0.151]	[0.024, 0.255]	B
59	0.065	[0.032, 0.102]	[0.017, 0.173]	B	109	0.930	[0.479, 1.522]	[0.238, 2.463]	B
60	0.027	[0.013, 0.042]	[0.007, 0.073]	B	110	3.861	[2.189, 5.066]	[1.123, 6.759]	A
61	0.081	[0.039, 0.126]	[0.021, 0.215]	B	111	0.324	[0.162, 0.517]	[0.082, 0.859]	B
62	0.105	[0.051, 0.165]	[0.027, 0.279]	B	112	0.185	[0.091, 0.292]	[0.047, 0.492]	B
63	0.198	[0.097, 0.312]	[0.051, 0.529]	B	113	0.012	[0.006, 0.018]	[0.003, 0.031]	B
64	0.034	[0.016, 0.053]	[0.009, 0.091]	B					

Table 3. Partial ionization cross sections (10^{-20} m^2) for *o*-xylene. TICS/10^{-20} m^2 = 21.518. *M* = 106, base peak is *m*/*z* 91.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.287, 0.477]	[0.216, 0.600]	H	74	0.164	[0.080, 0.258]	[0.042, 0.436]	B
15	0.097	[0.048, 0.153]	[0.025, 0.258]	B	75	0.101	[0.049, 0.158]	[0.026, 0.271]	B
26	0.092	[0.045, 0.145]	[0.024, 0.247]	B	76	0.099	[0.048, 0.156]	[0.025, 0.267]	B
27	0.494	[0.247, 0.791]	[0.126, 1.309]	B	77	1.071	[0.558, 1.776]	[0.274, 2.832]	B
29	0.021	[0.010, 0.033]	[0.005, 0.058]	B	78	0.574	[0.289, 0.925]	[0.146, 1.522]	B
37	0.090	[0.044, 0.141]	[0.023, 0.240]	B	79	0.575	[0.290, 0.925]	[0.147, 1.526]	B
38	0.246	[0.122, 0.391]	[0.063, 0.656]	B	80	0.037	[0.018, 0.059]	[0.010, 0.101]	B
39	1.342	[0.709, 2.242]	[0.344, 3.528]	B	85	0.013	[0.006, 0.020]	[0.003, 0.035]	B
40	0.135	[0.067, 0.214]	[0.034, 0.362]	B	86	0.025	[0.012, 0.040]	[0.007, 0.068]	B
41	0.182	[0.090, 0.289]	[0.047, 0.488]	B	87	0.025	[0.012, 0.039]	[0.006, 0.066]	B
43	0.016	[0.008, 0.025]	[0.004, 0.043]	B	88	0.006	[0.003, 0.009]	[0.002, 0.016]	B
45	0.015	[0.007, 0.024]	[0.004, 0.041]	B	89	0.149	[0.074, 0.237]	[0.038, 0.400]	B
49	0.071	[0.035, 0.112]	[0.018, 0.191]	B	90	0.006	[0.003, 0.009]	[0.001, 0.015]	B
50	0.708	[0.359, 1.146]	[0.180, 1.871]	B	91	5.327	[3.409, 6.599]	[2.135, 8.486]	A
51	1.499	[0.796, 2.503]	[0.387, 3.946]	B	92	0.415	[0.208, 0.666]	[0.106, 1.105]	B
52	0.602	[0.302, 0.965]	[0.153, 1.593]	B	93	0.015	[0.007, 0.024]	[0.004, 0.041]	B
53	0.341	[0.171, 0.548]	[0.087, 0.909]	B	97	0.005	[0.002, 0.008]	[0.001, 0.014]	B
54	0.026	[0.012, 0.040]	[0.007, 0.069]	B	98	0.015	[0.007, 0.024]	[0.004, 0.041]	B
55	0.013	[0.006, 0.020]	[0.003, 0.034]	B	99	0.005	[0.002, 0.008]	[0.001, 0.014]	B
60	0.011	[0.006, 0.018]	[0.003, 0.031]	B	101	0.010	[0.005, 0.016]	[0.003, 0.027]	B
61	0.101	[0.050, 0.161]	[0.026, 0.273]	B	102	0.076	[0.037, 0.119]	[0.019, 0.204]	B
62	0.265	[0.132, 0.421]	[0.068, 0.708]	B	103	0.345	[0.172, 0.549]	[0.088, 0.917]	B
63	0.683	[0.346, 1.104]	[0.175, 1.811]	B	104	0.127	[0.063, 0.201]	[0.032, 0.339]	B
64	0.117	[0.057, 0.185]	[0.030, 0.315]	B	105	1.045	[0.542, 1.718]	[0.267, 2.747]	B
65	0.813	[0.414, 1.319]	[0.207, 2.155]	B	106	2.546	[1.459, 4.362]	[0.658, 6.353]	B
66	0.092	[0.045, 0.145]	[0.024, 0.246]	B	107	0.223	[0.110, 0.352]	[0.057, 0.596]	B
67	0.010	[0.005, 0.016]	[0.003, 0.027]	B	108	0.010	[0.005, 0.016]	[0.003, 0.027]	B
73	0.026	[0.013, 0.041]	[0.007, 0.071]	B					

Table 4. Partial ionization cross sections (10^{-20} m^2) for *m*-xylene. TICS/10^{-20} m^2 = 21.758. *M* = 106, base peak is *m*/*z* 91.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	74	0.153	[0.075, 0.241]	[0.039, 0.407]	B
15	0.096	[0.047, 0.150]	[0.024, 0.255]	B	75	0.100	[0.049, 0.157]	[0.025, 0.266]	B
26	0.091	[0.044, 0.142]	[0.023, 0.243]	B	76	0.089	[0.043, 0.140]	[0.023, 0.239]	B
27	0.487	[0.243, 0.776]	[0.124, 1.288]	B	77	1.071	[0.554, 1.759]	[0.274, 2.824]	B
29	0.021	[0.010, 0.033]	[0.005, 0.056]	B	78	0.581	[0.293, 0.936]	[0.148, 1.538]	B
37	0.106	[0.052, 0.166]	[0.027, 0.284]	B	79	0.559	[0.281, 0.898]	[0.143, 1.483]	B
38	0.277	[0.137, 0.439]	[0.070, 0.735]	B	80	0.037	[0.018, 0.057]	[0.009, 0.098]	B
39	1.475	[0.779, 2.457]	[0.377, 3.851]	B	85	0.013	[0.006, 0.020]	[0.003, 0.035]	B
40	0.166	[0.082, 0.262]	[0.042, 0.443]	B	86	0.031	[0.015, 0.049]	[0.008, 0.083]	B
41	0.179	[0.088, 0.283]	[0.046, 0.479]	B	87	0.030	[0.015, 0.047]	[0.008, 0.081]	B
43	0.016	[0.008, 0.024]	[0.004, 0.042]	B	88	0.006	[0.003, 0.009]	[0.001, 0.016]	B
45	0.015	[0.007, 0.023]	[0.004, 0.040]	B	89	0.153	[0.075, 0.239]	[0.039, 0.407]	B
49	0.056	[0.027, 0.087]	[0.014, 0.149]	B	90	0.049	[0.024, 0.077]	[0.012, 0.131]	B
50	0.630	[0.317, 1.011]	[0.161, 1.674]	B	91	5.250	[3.318, 6.703]	[2.011, 8.716]	A
51	1.424	[0.748, 2.364]	[0.365, 3.727]	B	92	0.404	[0.202, 0.645]	[0.103, 1.074]	B
52	0.633	[0.317, 1.013]	[0.162, 1.686]	B	93	0.015	[0.007, 0.023]	[0.004, 0.040]	B
53	0.349	[0.174, 0.556]	[0.089, 0.928]	B	97	0.005	[0.002, 0.008]	[0.001, 0.013]	B
54	0.025	[0.012, 0.040]	[0.006, 0.068]	B	98	0.015	[0.007, 0.023]	[0.004, 0.040]	B
55	0.012	[0.006, 0.019]	[0.003, 0.033]	B	99	0.005	[0.002, 0.008]	[0.001, 0.013]	B
60	0.011	[0.005, 0.018]	[0.003, 0.031]	B	101	0.010	[0.005, 0.015]	[0.003, 0.027]	B
61	0.111	[0.054, 0.175]	[0.028, 0.297]	B	102	0.070	[0.034, 0.110]	[0.018, 0.186]	B
62	0.294	[0.146, 0.466]	[0.075, 0.786]	B	103	0.340	[0.169, 0.542]	[0.087, 0.904]	B
63	0.727	[0.368, 1.174]	[0.185, 1.915]	B	104	0.115	[0.056, 0.180]	[0.029, 0.307]	B
64	0.136	[0.067, 0.215]	[0.035, 0.363]	B	105	1.160	[0.602, 1.908]	[0.297, 3.049]	B
65	0.781	[0.396, 1.261]	[0.200, 2.065]	B	106	2.604	[0.473, 3.357]	[0.040, 5.526]	A
66	0.101	[0.049, 0.158]	[0.026, 0.270]	B	107	0.230	[0.114, 0.364]	[0.059, 0.615]	B
67	0.010	[0.005, 0.015]	[0.003, 0.027]	B	108	0.010	[0.005, 0.015]	[0.003, 0.027]	B
73	0.026	[0.013, 0.041]	[0.007, 0.070]	B					

Table 5. Partial ionization cross sections (10^{-20} m^2) for *p*-xylene. TICS/10^{-20} m^2 = 21.758. *M* = 106, base peak is *m*/*z* 91.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.289, 0.479]	[0.215, 0.600]	H	69	0.010	[0.005, 0.015]	[0.002, 0.026]	B
15	0.033	[0.016, 0.051]	[0.008, 0.088]	B	73	0.018	[0.009, 0.028]	[0.005, 0.048]	B
18	0.059	[0.029, 0.092]	[0.015, 0.157]	B	74	0.112	[0.055, 0.177]	[0.029, 0.303]	B
26	0.070	[0.034, 0.109]	[0.018, 0.185]	B	75	0.068	[0.033, 0.107]	[0.017, 0.183]	B
27	0.790	[0.403, 1.285]	[0.201, 2.087]	B	76	0.066	[0.032, 0.104]	[0.017, 0.179]	B
28	0.177	[0.087, 0.280]	[0.046, 0.475]	B	77	0.965	[0.495, 1.578]	[0.245, 2.541]	B
29	0.022	[0.010, 0.034]	[0.006, 0.058]	B	78	0.459	[0.230, 0.735]	[0.117, 1.217]	B
32	0.040	[0.020, 0.063]	[0.010, 0.109]	B	79	0.548	[0.277, 0.884]	[0.141, 1.463]	B
37	0.072	[0.035, 0.113]	[0.019, 0.194]	B	80	0.030	[0.015, 0.047]	[0.008, 0.081]	B
38	0.211	[0.104, 0.335]	[0.054, 0.566]	B	83	0.007	[0.003, 0.011]	[0.002, 0.019]	B
39	1.386	[0.735, 2.327]	[0.355, 3.642]	B	85	0.007	[0.003, 0.010]	[0.002, 0.018]	B
40	0.119	[0.059, 0.189]	[0.031, 0.320]	B	86	0.026	[0.012, 0.040]	[0.007, 0.068]	B
41	0.215	[0.107, 0.344]	[0.055, 0.581]	B	87	0.025	[0.012, 0.039]	[0.006, 0.066]	B
43	0.016	[0.008, 0.025]	[0.004, 0.043]	B	89	0.109	[0.054, 0.173]	[0.028, 0.294]	B
49	0.057	[0.028, 0.091]	[0.015, 0.155]	B	90	0.039	[0.019, 0.061]	[0.010, 0.105]	B
50	0.559	[0.281, 0.898]	[0.142, 1.479]	B	91	5.371	[3.444, 6.750]	[2.156, 8.732]	A
51	1.180	[0.613, 1.945]	[0.302, 3.109]	B	92	0.387	[0.192, 0.615]	[0.099, 1.034]	B
52	0.457	[0.229, 0.733]	[0.117, 1.218]	B	93	0.010	[0.005, 0.016]	[0.003, 0.028]	B
53	0.369	[0.183, 0.586]	[0.094, 0.977]	B	97	0.005	[0.002, 0.008]	[0.001, 0.014]	B
54	0.013	[0.006, 0.020]	[0.003, 0.035]	B	98	0.005	[0.002, 0.008]	[0.001, 0.014]	B
55	0.025	[0.012, 0.040]	[0.007, 0.069]	B	101	0.010	[0.005, 0.016]	[0.003, 0.028]	B
57	0.025	[0.012, 0.038]	[0.006, 0.066]	B	102	0.056	[0.027, 0.087]	[0.014, 0.150]	B
61	0.080	[0.039, 0.126]	[0.020, 0.215]	B	103	0.301	[0.149, 0.477]	[0.077, 0.803]	B
62	0.177	[0.088, 0.281]	[0.046, 0.477]	B	104	0.148	[0.073, 0.236]	[0.038, 0.396]	B
63	0.513	[0.257, 0.821]	[0.130, 1.352]	B	105	1.477	[0.785, 2.479]	[0.379, 3.889]	B
64	0.096	[0.047, 0.153]	[0.025, 0.262]	B	106	3.370	[1.411, 4.425]	[0.508, 6.370]	A
65	0.587	[0.297, 0.946]	[0.152, 1.568]	B	107	0.296	[0.148, 0.473]	[0.076, 0.794]	B
66	0.072	[0.035, 0.113]	[0.019, 0.194]	B	108	0.005	[0.002, 0.008]	[0.001, 0.014]	B
67	0.010	[0.005, 0.016]	[0.003, 0.027]	B					

Table 6. Partial ionization cross sections (10^{-20} m^2) for styrene. TICS/10^{-20} m^2 = 20.601. *M* = 104 is base peak.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	72	0.007	[0.003, 0.010]	[0.002, 0.018]	B
15	0.024	[0.012, 0.037]	[0.006, 0.065]	B	73	0.077	[0.038, 0.122]	[0.020, 0.208]	B
25	0.018	[0.009, 0.028]	[0.005, 0.048]	B	74	0.397	[0.199, 0.635]	[0.102, 1.057]	B
26	0.154	[0.076, 0.244]	[0.040, 0.414]	B	75	0.265	[0.133, 0.426]	[0.068, 0.707]	B
27	0.351	[0.175, 0.560]	[0.090, 0.938]	B	76	0.312	[0.155, 0.495]	[0.080, 0.831]	B
36	0.014	[0.007, 0.021]	[0.003, 0.036]	B	77	1.284	[0.667, 2.112]	[0.327, 3.359]	B
37	0.147	[0.072, 0.230]	[0.037, 0.388]	B	78	2.652	[0.676, 3.463]	[0.143, 5.550]	A
38	0.261	[0.130, 0.416]	[0.066, 0.692]	B	79	0.173	[0.085, 0.273]	[0.044, 0.462]	B
39	0.869	[0.443, 1.409]	[0.220, 2.276]	B	80	0.005	[0.003, 0.008]	[0.001, 0.015]	B
40	0.038	[0.018, 0.059]	[0.010, 0.101]	B	84	0.005	[0.002, 0.008]	[0.001, 0.013]	B
41	0.025	[0.012, 0.039]	[0.006, 0.067]	B	85	0.014	[0.007, 0.022]	[0.004, 0.037]	B
43	0.012	[0.006, 0.018]	[0.003, 0.032]	B	86	0.023	[0.011, 0.035]	[0.006, 0.061]	B
48	0.011	[0.005, 0.017]	[0.003, 0.029]	B	87	0.035	[0.017, 0.055]	[0.009, 0.094]	B
49	0.147	[0.072, 0.230]	[0.038, 0.394]	B	88	0.004	[0.002, 0.007]	[0.001, 0.011]	B
50	1.399	[0.729, 2.305]	[0.358, 3.667]	B	89	0.085	[0.042, 0.136]	[0.022, 0.230]	B
51	2.695	[0.739, 3.544]	[0.156, 5.599]	A	90	0.008	[0.004, 0.012]	[0.002, 0.021]	B
52	0.871	[0.447, 1.419]	[0.224, 2.309]	B	97	0.008	[0.004, 0.012]	[0.002, 0.021]	B
53	0.117	[0.057, 0.185]	[0.030, 0.313]	B	98	0.034	[0.017, 0.054]	[0.009, 0.093]	B
54	0.010	[0.005, 0.015]	[0.002, 0.026]	B	99	0.008	[0.004, 0.012]	[0.002, 0.021]	B
60	0.017	[0.008, 0.026]	[0.004, 0.046]	B	101	0.034	[0.017, 0.054]	[0.009, 0.093]	B
61	0.133	[0.065, 0.209]	[0.034, 0.355]	B	102	0.321	[0.160, 0.512]	[0.082, 0.859]	B
62	0.269	[0.133, 0.428]	[0.069, 0.718]	B	103	1.856	[0.998, 3.128]	[0.473, 4.806]	B
63	0.631	[0.318, 1.015]	[0.162, 1.675]	B	104	3.827	[1.959, 5.000]	[0.965, 6.961]	A
64	0.070	[0.035, 0.111]	[0.018, 0.189]	B	105	0.352	[0.175, 0.561]	[0.090, 0.943]	B
65	0.115	[0.057, 0.182]	[0.030, 0.309]	B	106	0.011	[0.006, 0.018]	[0.003, 0.031]	B
66	0.008	[0.004, 0.012]	[0.002, 0.020]	B					

Table 7. Partial ionization cross sections (10^{-20} m^2) for 1-hexene. TICS/10^{-20} m^2 = 18.038. M = 84, base peak is m/z 56.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.214, 0.598]	H	56	2.395	[0.672, 3.116]	[0.171, 4.955]	A
15	0.065	[0.032, 0.103]	[0.017, 0.176]	B	57	0.142	[0.070, 0.225]	[0.037, 0.382]	B
26	0.106	[0.052, 0.167]	[0.027, 0.283]	B	58	0.002	[0.001, 0.004]	[0.001, 0.006]	B
27	1.584	[0.849, 2.663]	[0.405, 4.119]	B	61	0.002	[0.001, 0.003]	[0.001, 0.006]	B
28	0.277	[0.138, 0.440]	[0.071, 0.738]	B	62	0.006	[0.003, 0.009]	[0.002, 0.016]	B
29	0.867	[0.442, 1.408]	[0.220, 2.280]	B	63	0.010	[0.005, 0.015]	[0.003, 0.027]	B
30	0.018	[0.009, 0.028]	[0.005, 0.049]	B	65	0.015	[0.007, 0.023]	[0.004, 0.039]	B
37	0.031	[0.015, 0.048]	[0.008, 0.083]	B	66	0.004	[0.002, 0.005]	[0.001, 0.010]	B
38	0.089	[0.044, 0.141]	[0.023, 0.239]	B	67	0.036	[0.017, 0.056]	[0.009, 0.096]	B
39	1.124	[0.581, 1.839]	[0.287, 2.934]	B	68	0.007	[0.003, 0.010]	[0.002, 0.018]	B
40	0.216	[0.108, 0.344]	[0.055, 0.578]	B	69	0.379	[0.190, 0.607]	[0.097, 1.007]	B
41	3.299	[1.648, 4.283]	[0.810, 6.027]	A	70	0.021	[0.010, 0.033]	[0.005, 0.057]	B
42	2.445	[0.739, 3.189]	[0.196, 5.003]	A	71	0.001	[0.001, 0.002]	[0.000, 0.004]	B
43	1.945	[1.066, 3.304]	[0.500, 5.010]	B	74	0.003	[0.001, 0.004]	[0.001, 0.007]	B
44	0.064	[0.031, 0.100]	[0.016, 0.173]	B	77	0.005	[0.003, 0.008]	[0.001, 0.014]	B
49	0.006	[0.003, 0.009]	[0.001, 0.016]	B	78	0.001	[0.001, 0.002]	[0.000, 0.004]	B
50	0.056	[0.027, 0.088]	[0.014, 0.150]	B	79	0.004	[0.002, 0.006]	[0.001, 0.011]	B
51	0.079	[0.038, 0.124]	[0.020, 0.212]	B	81	0.003	[0.001, 0.004]	[0.001, 0.007]	B
52	0.032	[0.015, 0.049]	[0.008, 0.085]	B	83	0.004	[0.002, 0.006]	[0.001, 0.011]	B
53	0.176	[0.087, 0.278]	[0.045, 0.469]	B	84	0.382	[0.190, 0.609]	[0.097, 1.015]	B
54	0.131	[0.064, 0.206]	[0.034, 0.352]	B	85	0.026	[0.013, 0.041]	[0.007, 0.070]	B
55	1.579	[0.842, 2.645]	[0.403, 4.099]	B	86	0.003	[0.001, 0.004]	[0.001, 0.007]	B

Table 8. Partial ionization cross sections (10^{-20} m^2) for 2-hexene. TICS/10^{-20} m^2 = 17.975. M = 84, base peak is m/z 55.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	54	0.262	[0.130, 0.415]	[0.067, 0.699]	B
14	0.034	[0.017, 0.054]	[0.009, 0.092]	B	55	3.698	[2.062, 4.741]	[1.149, 6.470]	A
15	0.119	[0.059, 0.188]	[0.031, 0.320]	B	56	0.972	[0.499, 1.586]	[0.246, 2.543]	B
26	0.144	[0.071, 0.228]	[0.037, 0.386]	B	57	0.056	[0.027, 0.087]	[0.014, 0.150]	B
27	1.487	[0.791, 2.494]	[0.379, 3.884]	B	61	0.003	[0.002, 0.005]	[0.001, 0.008]	B
28	0.151	[0.074, 0.237]	[0.038, 0.403]	B	62	0.009	[0.004, 0.014]	[0.002, 0.024]	B
29	1.549	[0.833, 2.611]	[0.399, 4.054]	B	63	0.012	[0.006, 0.018]	[0.003, 0.032]	B
30	0.034	[0.017, 0.053]	[0.009, 0.091]	B	65	0.022	[0.011, 0.035]	[0.006, 0.060]	B
37	0.034	[0.017, 0.054]	[0.009, 0.093]	B	66	0.008	[0.004, 0.012]	[0.002, 0.022]	B
38	0.095	[0.046, 0.149]	[0.024, 0.255]	B	67	0.074	[0.036, 0.116]	[0.019, 0.200]	B
39	1.214	[0.638, 2.011]	[0.312, 3.180]	B	68	0.017	[0.008, 0.027]	[0.004, 0.047]	B
40	0.208	[0.103, 0.328]	[0.053, 0.552]	B	69	0.536	[0.270, 0.861]	[0.137, 1.417]	B
41	2.185	[0.450, 2.815]	[0.067, 4.675]	A	70	0.027	[0.013, 0.043]	[0.007, 0.074]	B
42	2.566	[0.874, 3.371]	[0.267, 5.141]	A	74	0.004	[0.002, 0.006]	[0.001, 0.011]	B
43	0.676	[0.343, 1.090]	[0.172, 1.778]	B	77	0.008	[0.004, 0.012]	[0.002, 0.021]	B
44	0.019	[0.009, 0.030]	[0.005, 0.052]	B	78	0.002	[0.001, 0.003]	[0.001, 0.005]	B
45	0.009	[0.005, 0.015]	[0.002, 0.026]	B	79	0.006	[0.003, 0.009]	[0.002, 0.016]	B
49	0.009	[0.004, 0.013]	[0.002, 0.023]	B	81	0.004	[0.002, 0.006]	[0.001, 0.011]	B
50	0.075	[0.037, 0.119]	[0.019, 0.202]	B	83	0.008	[0.004, 0.012]	[0.002, 0.021]	B
51	0.110	[0.054, 0.174]	[0.028, 0.297]	B	84	0.744	[0.378, 1.201]	[0.191, 1.972]	B
52	0.044	[0.021, 0.068]	[0.011, 0.118]	B	85	0.049	[0.024, 0.077]	[0.013, 0.132]	B
53	0.292	[0.146, 0.467]	[0.075, 0.782]	B	86	0.002	[0.001, 0.003]	[0.001, 0.005]	B

Table 9. Partial ionization cross sections (10^{-20} m^2) for 3-hexene. TICS/10^{-20} m^2 = 18.416. M = 84, base peak is m/z 55.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.216, 0.600]	H	61	0.005	[0.002, 0.007]	[0.001, 0.013]	B
26	0.114	[0.056, 0.180]	[0.029, 0.304]	B	62	0.014	[0.007, 0.022]	[0.004, 0.038]	B
27	1.154	[0.602, 1.904]	[0.293, 3.005]	B	63	0.031	[0.015, 0.048]	[0.008, 0.082]	B
28	0.158	[0.078, 0.249]	[0.040, 0.420]	B	64	0.003	[0.002, 0.005]	[0.001, 0.009]	B
29	0.903	[0.465, 1.478]	[0.232, 2.385]	B	65	0.044	[0.021, 0.068]	[0.011, 0.118]	B
30	0.018	[0.009, 0.028]	[0.005, 0.048]	B	66	0.019	[0.009, 0.030]	[0.005, 0.051]	B
37	0.045	[0.022, 0.070]	[0.012, 0.121]	B	67	0.115	[0.056, 0.180]	[0.029, 0.308]	B
38	0.125	[0.062, 0.198]	[0.032, 0.336]	B	68	0.025	[0.012, 0.039]	[0.006, 0.067]	B
39	1.416	[0.746, 2.350]	[0.362, 3.702]	B	69	0.610	[0.308, 0.985]	[0.155, 1.610]	B
40	0.229	[0.114, 0.365]	[0.058, 0.611]	B	70	0.034	[0.017, 0.053]	[0.009, 0.092]	B
41	3.539	[1.864, 4.582]	[0.973, 6.348]	A	71	0.007	[0.003, 0.010]	[0.002, 0.018]	B
42	2.850	[1.145, 3.749]	[0.419, 5.519]	A	74	0.007	[0.004, 0.011]	[0.002, 0.020]	B
43	0.597	[0.301, 0.961]	[0.151, 1.578]	B	75	0.005	[0.003, 0.008]	[0.001, 0.014]	B
44	0.021	[0.010, 0.033]	[0.005, 0.057]	B	76	0.006	[0.003, 0.009]	[0.001, 0.015]	B
49	0.012	[0.006, 0.019]	[0.003, 0.033]	B	77	0.017	[0.008, 0.027]	[0.004, 0.046]	B
50	0.106	[0.052, 0.167]	[0.027, 0.283]	B	78	0.006	[0.003, 0.009]	[0.002, 0.016]	B
51	0.156	[0.077, 0.246]	[0.040, 0.417]	B	79	0.010	[0.005, 0.015]	[0.002, 0.026]	B
52	0.059	[0.029, 0.093]	[0.015, 0.159]	B	81	0.008	[0.004, 0.012]	[0.002, 0.021]	B
53	0.287	[0.143, 0.456]	[0.074, 0.769]	B	82	0.003	[0.002, 0.005]	[0.001, 0.009]	B
54	0.171	[0.085, 0.271]	[0.044, 0.459]	B	83	0.010	[0.005, 0.015]	[0.002, 0.026]	B
55	3.444	[1.772, 4.467]	[0.893, 6.222]	A	84	0.729	[0.371, 1.181]	[0.187, 1.928]	B
56	0.803	[0.410, 1.304]	[0.206, 2.129]	B	85	0.050	[0.025, 0.079]	[0.013, 0.135]	B
57	0.051	[0.025, 0.080]	[0.013, 0.136]	B					

Table 10. Partial ionization cross sections (10^{-20} m^2) for 2-methyl-1-pentene. TICS/10^{-20} m^2 = 17.743. M = 84, base peak is m/z 56.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	54	0.088	[0.043, 0.139]	[0.023, 0.237]	B
12	0.024	[0.012, 0.037]	[0.006, 0.064]	B	55	1.108	[0.578, 1.831]	[0.283, 2.909]	B
13	0.050	[0.024, 0.078]	[0.013, 0.134]	B	56	2.279	[0.584, 2.976]	[0.118, 4.780]	A
14	0.174	[0.086, 0.276]	[0.045, 0.467]	B	57	0.108	[0.053, 0.171]	[0.028, 0.290]	B
15	0.864	[0.443, 1.406]	[0.220, 2.263]	B	58	0.004	[0.002, 0.007]	[0.001, 0.012]	B
16	0.021	[0.010, 0.033]	[0.005, 0.057]	B	61	0.007	[0.003, 0.010]	[0.002, 0.018]	B
25	0.014	[0.007, 0.022]	[0.004, 0.038]	B	62	0.011	[0.005, 0.017]	[0.003, 0.030]	B
26	0.283	[0.140, 0.450]	[0.072, 0.753]	B	63	0.017	[0.008, 0.027]	[0.004, 0.047]	B
27	2.099	[0.391, 2.702]	[0.045, 4.559]	A	64	0.003	[0.001, 0.005]	[0.001, 0.008]	B
28	0.429	[0.215, 0.688]	[0.109, 1.131]	B	65	0.022	[0.011, 0.034]	[0.006, 0.058]	B
29	1.449	[0.768, 2.416]	[0.371, 3.771]	B	66	0.010	[0.005, 0.016]	[0.003, 0.028]	B
30	0.042	[0.020, 0.065]	[0.011, 0.113]	B	67	0.069	[0.034, 0.108]	[0.018, 0.184]	B
31	0.011	[0.005, 0.017]	[0.003, 0.030]	B	68	0.012	[0.006, 0.019]	[0.003, 0.033]	B
32	0.007	[0.003, 0.011]	[0.002, 0.019]	B	69	0.607	[0.306, 0.976]	[0.154, 1.596]	B
39	1.806	[0.991, 3.079]	[0.464, 4.659]	B	70	0.034	[0.017, 0.053]	[0.009, 0.091]	B
40	0.367	[0.183, 0.586]	[0.094, 0.977]	B	71	0.005	[0.003, 0.008]	[0.001, 0.014]	B
41	2.949	[1.318, 3.869]	[0.574, 5.595]	A	74	0.003	[0.001, 0.005]	[0.001, 0.008]	B
42	1.026	[0.529, 1.679]	[0.260, 2.679]	B	77	0.004	[0.002, 0.007]	[0.001, 0.012]	B
43	0.313	[0.155, 0.498]	[0.080, 0.832]	B	79	0.003	[0.002, 0.005]	[0.001, 0.009]	B
44	0.012	[0.006, 0.019]	[0.003, 0.033]	B	81	0.002	[0.001, 0.004]	[0.001, 0.007]	B
50	0.099	[0.049, 0.155]	[0.026, 0.267]	B	83	0.006	[0.003, 0.010]	[0.002, 0.017]	B
51	0.132	[0.065, 0.209]	[0.034, 0.354]	B	84	0.402	[0.202, 0.647]	[0.104, 1.078]	B
52	0.049	[0.024, 0.077]	[0.013, 0.134]	B	85	0.027	[0.013, 0.043]	[0.007, 0.073]	B
53	0.288	[0.143, 0.458]	[0.073, 0.764]	B					

Table 11. Partial ionization cross sections (10^{-20} m^2) for 3-methyl-1-pentene. TICS/10^{-20} m^2 = 18.152. M = 84, base peak is m/z 55.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.287, 0.478]	[0.215, 0.599]	H	52	0.096	[0.047, 0.151]	[0.025, 0.258]	B
15	0.347	[0.174, 0.554]	[0.089, 0.923]	B	53	0.495	[0.248, 0.791]	[0.126, 1.314]	B
26	0.389	[0.197, 0.629]	[0.100, 1.040]	B	54	0.304	[0.153, 0.489]	[0.078, 0.812]	B
27	2.083	[1.169, 3.599]	[0.532, 5.317]	B	55	2.638	[0.949, 3.443]	[0.305, 5.181]	A
28	0.197	[0.099, 0.315]	[0.051, 0.529]	B	56	1.118	[0.582, 1.843]	[0.286, 2.932]	B
29	1.429	[0.760, 2.387]	[0.365, 3.706]	B	57	0.071	[0.035, 0.112]	[0.018, 0.192]	B
37	0.058	[0.028, 0.091]	[0.015, 0.156]	B	63	0.029	[0.014, 0.045]	[0.007, 0.077]	B
38	0.188	[0.093, 0.299]	[0.048, 0.507]	B	65	0.043	[0.021, 0.068]	[0.011, 0.117]	B
39	1.675	[0.904, 2.821]	[0.429, 4.335]	B	66	0.023	[0.011, 0.036]	[0.006, 0.062]	B
40	0.300	[0.150, 0.480]	[0.077, 0.803]	B	67	0.119	[0.059, 0.188]	[0.030, 0.318]	B
41	2.799	[1.128, 3.655]	[0.427, 5.381]	A	69	1.499	[0.800, 2.508]	[0.385, 3.892]	B
42	0.643	[0.326, 1.040]	[0.163, 1.693]	B	70	0.081	[0.039, 0.126]	[0.021, 0.217]	B
43	0.205	[0.102, 0.326]	[0.053, 0.549]	B	84	0.457	[0.231, 0.739]	[0.118, 1.225]	B
50	0.183	[0.090, 0.290]	[0.047, 0.489]	B	85	0.030	[0.014, 0.046]	[0.008, 0.080]	B
51	0.253	[0.126, 0.402]	[0.065, 0.676]	B					

Table 12. Partial ionization cross sections (10^{-20} m^2) for 4-methyl-1-pentene. TICS/10^{-20} m^2 = 17.956. M = 84, base peak is m/z 43.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.479]	[0.215, 0.599]	H	53	0.111	[0.055, 0.176]	[0.028, 0.298]	B
14	0.012	[0.006, 0.018]	[0.003, 0.031]	B	54	0.038	[0.019, 0.060]	[0.010, 0.103]	B
15	0.166	[0.083, 0.264]	[0.043, 0.444]	B	55	0.332	[0.166, 0.531]	[0.085, 0.882]	B
26	0.085	[0.042, 0.134]	[0.022, 0.228]	B	56	1.831	[1.008, 3.121]	[0.471, 4.727]	B
27	1.571	[0.846, 2.650]	[0.399, 4.064]	B	57	0.082	[0.040, 0.130]	[0.021, 0.220]	B
28	0.088	[0.043, 0.138]	[0.022, 0.235]	B	61	0.003	[0.002, 0.005]	[0.001, 0.009]	B
29	0.300	[0.150, 0.478]	[0.077, 0.798]	B	62	0.009	[0.004, 0.014]	[0.002, 0.025]	B
31	0.007	[0.003, 0.011]	[0.002, 0.018]	B	63	0.012	[0.006, 0.019]	[0.003, 0.032]	B
37	0.047	[0.023, 0.073]	[0.012, 0.127]	B	65	0.017	[0.008, 0.027]	[0.004, 0.046]	B
38	0.114	[0.056, 0.180]	[0.029, 0.304]	B	66	0.005	[0.003, 0.009]	[0.001, 0.015]	B
39	1.117	[0.581, 1.842]	[0.284, 2.920]	B	67	0.060	[0.029, 0.095]	[0.016, 0.163]	B
40	0.207	[0.102, 0.327]	[0.052, 0.545]	B	68	0.013	[0.006, 0.020]	[0.003, 0.034]	B
41	3.632	[2.002, 4.627]	[1.095, 6.310]	A	69	0.410	[0.205, 0.652]	[0.104, 1.078]	B
42	1.633	[0.881, 2.753]	[0.418, 4.225]	B	70	0.023	[0.011, 0.036]	[0.006, 0.062]	B
43	5.078	[3.437, 6.260]	[2.323, 7.981]	A	77	0.002	[0.001, 0.003]	[0.001, 0.005]	B
44	0.168	[0.082, 0.264]	[0.043, 0.447]	B	79	0.002	[0.001, 0.003]	[0.001, 0.005]	B
49	0.004	[0.002, 0.007]	[0.001, 0.012]	B	83	0.014	[0.007, 0.022]	[0.004, 0.038]	B
50	0.039	[0.019, 0.060]	[0.010, 0.104]	B	84	0.235	[0.118, 0.378]	[0.061, 0.631]	B
51	0.054	[0.026, 0.084]	[0.014, 0.145]	B	85	0.016	[0.008, 0.025]	[0.004, 0.043]	B
52	0.020	[0.010, 0.032]	[0.005, 0.055]	B					

Table 13. Partial ionization cross sections (10^{-20} m^2) for 2-methyl-2-pentene. TICS/10^{-20} m^2 = 18.300. M = 84, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	56	0.633	[0.322, 1.027]	[0.162, 1.680]	B
15	0.100	[0.049, 0.158]	[0.026, 0.269]	B	57	0.040	[0.020, 0.063]	[0.010, 0.108]	B
26	0.079	[0.038, 0.123]	[0.020, 0.211]	B	58	0.012	[0.006, 0.018]	[0.003, 0.032]	B
27	0.986	[0.512, 1.626]	[0.252, 2.600]	B	59	0.027	[0.013, 0.042]	[0.007, 0.072]	B
28	0.190	[0.094, 0.302]	[0.049, 0.507]	B	61	0.007	[0.003, 0.011]	[0.002, 0.019]	B
29	0.701	[0.359, 1.141]	[0.179, 1.854]	B	62	0.014	[0.007, 0.022]	[0.004, 0.038]	B
30	0.016	[0.008, 0.025]	[0.004, 0.042]	B	63	0.024	[0.011, 0.037]	[0.006, 0.064]	B
31	0.015	[0.007, 0.024]	[0.004, 0.041]	B	64	0.003	[0.002, 0.005]	[0.001, 0.009]	B
32	0.007	[0.004, 0.012]	[0.002, 0.020]	B	65	0.041	[0.020, 0.064]	[0.010, 0.110]	B
37	0.040	[0.019, 0.062]	[0.010, 0.106]	B	66	0.015	[0.007, 0.024]	[0.004, 0.041]	B
38	0.109	[0.053, 0.171]	[0.028, 0.291]	B	67	0.183	[0.090, 0.291]	[0.047, 0.490]	B
39	1.213	[0.643, 2.030]	[0.311, 3.180]	B	68	0.045	[0.022, 0.071]	[0.011, 0.121]	B
40	0.257	[0.127, 0.408]	[0.065, 0.680]	B	69	2.724	[1.051, 3.554]	[0.350, 5.221]	A
41	5.995	[4.327, 7.302]	[3.107, 9.076]	A	70	0.146	[0.072, 0.231]	[0.037, 0.390]	B
42	0.930	[0.482, 1.531]	[0.239, 2.453]	B	71	0.010	[0.005, 0.016]	[0.003, 0.027]	B
43	0.451	[0.227, 0.725]	[0.115, 1.198]	B	74	0.005	[0.002, 0.007]	[0.001, 0.012]	B
44	0.017	[0.008, 0.026]	[0.004, 0.045]	B	77	0.009	[0.004, 0.014]	[0.002, 0.024]	B
45	0.005	[0.003, 0.009]	[0.001, 0.015]	B	78	0.002	[0.001, 0.004]	[0.001, 0.006]	B
49	0.010	[0.005, 0.015]	[0.003, 0.027]	B	79	0.009	[0.004, 0.014]	[0.002, 0.025]	B
50	0.077	[0.038, 0.121]	[0.020, 0.205]	B	81	0.007	[0.003, 0.011]	[0.002, 0.018]	B
51	0.117	[0.058, 0.185]	[0.030, 0.312]	B	82	0.005	[0.002, 0.007]	[0.001, 0.012]	B
52	0.045	[0.022, 0.071]	[0.012, 0.123]	B	83	0.029	[0.014, 0.046]	[0.008, 0.079]	B
53	0.322	[0.161, 0.515]	[0.082, 0.861]	B	84	0.964	[0.500, 1.587]	[0.246, 2.533]	B
54	0.091	[0.045, 0.146]	[0.023, 0.245]	B	85	0.072	[0.035, 0.113]	[0.019, 0.194]	B
55	1.101	[0.575, 1.825]	[0.280, 2.893]	B	86	0.002	[0.001, 0.004]	[0.001, 0.006]	B

Table 14. Partial ionization cross sections (10^{-20} m^2) for 3-methyl-2-pentene. TICS/10^{-20} m^2 = 18.147. M = 84, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.168	[0.083, 0.265]	[0.043, 0.448]	B	54	0.154	[0.076, 0.244]	[0.040, 0.414]	B
2	0.118	[0.058, 0.186]	[0.030, 0.313]	B	55	1.477	[0.796, 2.492]	[0.378, 3.826]	B
12	0.011	[0.005, 0.017]	[0.003, 0.030]	B	56	0.693	[0.352, 1.121]	[0.177, 1.823]	B
13	0.011	[0.005, 0.017]	[0.003, 0.029]	B	57	0.035	[0.017, 0.054]	[0.009, 0.094]	B
14	0.031	[0.015, 0.049]	[0.008, 0.084]	B	58	0.003	[0.001, 0.005]	[0.001, 0.008]	B
15	0.473	[0.236, 0.754]	[0.120, 1.248]	B	61	0.003	[0.001, 0.004]	[0.001, 0.008]	B
16	0.009	[0.005, 0.015]	[0.002, 0.026]	B	62	0.005	[0.003, 0.009]	[0.001, 0.015]	B
26	0.165	[0.082, 0.262]	[0.042, 0.439]	B	63	0.016	[0.008, 0.025]	[0.004, 0.043]	B
27	2.159	[1.222, 3.694]	[0.556, 5.418]	B	64	0.003	[0.001, 0.004]	[0.001, 0.007]	B
28	0.443	[0.223, 0.711]	[0.114, 1.177]	B	65	0.037	[0.018, 0.058]	[0.010, 0.101]	B
29	1.166	[0.612, 1.934]	[0.298, 3.046]	B	66	0.019	[0.009, 0.030]	[0.005, 0.052]	B
30	0.031	[0.015, 0.048]	[0.008, 0.083]	B	67	0.148	[0.073, 0.235]	[0.038, 0.398]	B
31	0.006	[0.003, 0.009]	[0.002, 0.016]	B	68	0.031	[0.015, 0.049]	[0.008, 0.083]	B
32	0.006	[0.003, 0.009]	[0.002, 0.016]	B	69	1.712	[0.936, 2.902]	[0.441, 4.420]	B
33	0.006	[0.003, 0.009]	[0.001, 0.016]	B	70	0.090	[0.044, 0.142]	[0.023, 0.241]	B
36	0.005	[0.003, 0.008]	[0.001, 0.014]	B	71	0.002	[0.001, 0.003]	[0.001, 0.005]	B
37	0.026	[0.013, 0.040]	[0.007, 0.070]	B	72	0.002	[0.001, 0.003]	[0.000, 0.005]	B
38	0.081	[0.040, 0.127]	[0.021, 0.217]	B	74	0.002	[0.001, 0.003]	[0.000, 0.005]	B
39	1.374	[0.731, 2.293]	[0.352, 3.575]	B	75	0.002	[0.001, 0.003]	[0.000, 0.005]	B
40	0.246	[0.123, 0.392]	[0.063, 0.653]	B	77	0.009	[0.004, 0.014]	[0.002, 0.024]	B
41	4.707	[3.034, 5.822]	[1.962, 7.523]	A	78	0.002	[0.001, 0.003]	[0.000, 0.005]	B
42	0.644	[0.328, 1.043]	[0.164, 1.698]	B	79	0.007	[0.003, 0.011]	[0.002, 0.019]	B
43	0.346	[0.172, 0.552]	[0.088, 0.922]	B	80	0.002	[0.001, 0.003]	[0.000, 0.005]	B
44	0.013	[0.006, 0.021]	[0.003, 0.036]	B	81	0.007	[0.003, 0.011]	[0.002, 0.019]	B
49	0.004	[0.002, 0.006]	[0.001, 0.011]	B	82	0.002	[0.001, 0.003]	[0.000, 0.005]	B
50	0.068	[0.033, 0.107]	[0.017, 0.182]	B	83	0.018	[0.009, 0.028]	[0.005, 0.048]	B
51	0.159	[0.079, 0.252]	[0.041, 0.425]	B	84	0.674	[0.344, 1.094]	[0.173, 1.783]	B
52	0.072	[0.035, 0.113]	[0.018, 0.193]	B	85	0.043	[0.021, 0.066]	[0.011, 0.115]	B
53	0.401	[0.200, 0.639]	[0.102, 1.060]	B	86	0.002	[0.001, 0.003]	[0.000, 0.005]	B

Table 15. Partial ionization cross sections (10^{-20} m^2) for 4-methyl-2-pentene. TICS/10^{-20} m^2 = 18.095. M = 84, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	54	0.062	[0.031, 0.098]	[0.016, 0.168]	B
2	0.071	[0.035, 0.112]	[0.018, 0.192]	B	55	0.425	[0.213, 0.681]	[0.109, 1.132]	B
12	0.014	[0.007, 0.021]	[0.004, 0.037]	B	56	0.272	[0.135, 0.432]	[0.070, 0.727]	B
13	0.026	[0.013, 0.041]	[0.007, 0.070]	B	57	0.015	[0.007, 0.024]	[0.004, 0.042]	B
14	0.137	[0.068, 0.218]	[0.035, 0.368]	B	58	0.004	[0.002, 0.006]	[0.001, 0.010]	B
15	0.946	[0.493, 1.561]	[0.242, 2.487]	B	60	0.004	[0.002, 0.005]	[0.001, 0.010]	B
16	0.046	[0.022, 0.072]	[0.012, 0.125]	B	61	0.010	[0.005, 0.016]	[0.003, 0.028]	B
26	0.200	[0.098, 0.316]	[0.051, 0.537]	B	62	0.017	[0.008, 0.026]	[0.004, 0.045]	B
27	1.694	[0.935, 2.901]	[0.439, 4.400]	B	63	0.029	[0.014, 0.046]	[0.007, 0.079]	B
28	0.260	[0.128, 0.414]	[0.066, 0.698]	B	64	0.006	[0.003, 0.010]	[0.002, 0.017]	B
29	0.554	[0.279, 0.892]	[0.141, 1.468]	B	65	0.036	[0.018, 0.057]	[0.009, 0.098]	B
30	0.015	[0.007, 0.023]	[0.004, 0.040]	B	66	0.020	[0.010, 0.032]	[0.005, 0.055]	B
31	0.029	[0.014, 0.046]	[0.007, 0.079]	B	67	0.129	[0.064, 0.204]	[0.033, 0.347]	B
32	0.021	[0.010, 0.033]	[0.005, 0.057]	B	68	0.046	[0.022, 0.072]	[0.012, 0.124]	B
33	0.007	[0.003, 0.011]	[0.002, 0.019]	B	69	2.375	[0.667, 3.071]	[0.144, 4.782]	A
34	0.007	[0.003, 0.011]	[0.002, 0.019]	B	70	0.122	[0.061, 0.193]	[0.031, 0.324]	B
36	0.006	[0.003, 0.010]	[0.002, 0.017]	B	71	0.005	[0.002, 0.007]	[0.001, 0.013]	B
37	0.088	[0.043, 0.139]	[0.023, 0.235]	B	73	0.002	[0.001, 0.003]	[0.001, 0.006]	B
38	0.202	[0.100, 0.321]	[0.052, 0.541]	B	74	0.002	[0.001, 0.003]	[0.001, 0.006]	B
39	1.660	[0.910, 2.837]	[0.427, 4.322]	B	75	0.002	[0.001, 0.003]	[0.001, 0.006]	B
40	0.286	[0.142, 0.454]	[0.073, 0.760]	B	77	0.004	[0.002, 0.007]	[0.001, 0.012]	B
41	5.708	[4.048, 6.971]	[2.842, 8.702]	A	78	0.002	[0.001, 0.003]	[0.001, 0.006]	B
42	0.491	[0.247, 0.791]	[0.125, 1.295]	B	79	0.004	[0.002, 0.007]	[0.001, 0.012]	B
43	0.398	[0.200, 0.639]	[0.102, 1.062]	B	80	0.002	[0.001, 0.003]	[0.001, 0.006]	B
44	0.016	[0.008, 0.025]	[0.004, 0.043]	B	81	0.004	[0.002, 0.007]	[0.001, 0.012]	B
48	0.005	[0.002, 0.008]	[0.001, 0.013]	B	82	0.002	[0.001, 0.003]	[0.001, 0.006]	B
49	0.009	[0.005, 0.015]	[0.002, 0.025]	B	83	0.022	[0.010, 0.034]	[0.005, 0.058]	B
50	0.078	[0.038, 0.123]	[0.020, 0.210]	B	84	0.597	[0.303, 0.965]	[0.154, 1.588]	B
51	0.121	[0.060, 0.192]	[0.031, 0.326]	B	85	0.039	[0.019, 0.062]	[0.010, 0.105]	B
52	0.044	[0.021, 0.069]	[0.011, 0.119]	B	86	0.002	[0.001, 0.003]	[0.001, 0.006]	B
53	0.290	[0.144, 0.462]	[0.074, 0.771]	B					

Table 16. Partial ionization cross sections (10^{-20} m^2) for 2,3-dimethyl-1-butene. TICS/10^{-20} m^2 = 17.841. M = 84, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.216, 0.601]	H	55	0.456	[0.230, 0.735]	[0.117, 1.211]	B
15	0.119	[0.059, 0.188]	[0.031, 0.321]	B	56	0.342	[0.171, 0.547]	[0.087, 0.910]	B
26	0.062	[0.030, 0.097]	[0.016, 0.166]	B	57	0.024	[0.012, 0.037]	[0.006, 0.065]	B
27	0.853	[0.438, 1.393]	[0.218, 2.252]	B	61	0.004	[0.002, 0.007]	[0.001, 0.012]	B
28	0.078	[0.038, 0.124]	[0.020, 0.210]	B	62	0.012	[0.006, 0.019]	[0.003, 0.033]	B
29	0.342	[0.170, 0.545]	[0.087, 0.910]	B	63	0.020	[0.010, 0.031]	[0.005, 0.054]	B
37	0.047	[0.023, 0.074]	[0.012, 0.127]	B	65	0.034	[0.016, 0.053]	[0.009, 0.091]	B
38	0.121	[0.060, 0.191]	[0.031, 0.324]	B	66	0.011	[0.005, 0.017]	[0.003, 0.029]	B
39	1.284	[0.685, 2.156]	[0.329, 3.362]	B	67	0.177	[0.088, 0.283]	[0.045, 0.475]	B
40	0.260	[0.129, 0.413]	[0.067, 0.698]	B	68	0.033	[0.016, 0.052]	[0.008, 0.089]	B
41	7.082	[5.361, 8.438]	[4.059, 10.247]	A	69	3.221	[1.640, 4.177]	[0.771, 5.779]	A
42	0.615	[0.311, 0.994]	[0.157, 1.631]	B	70	0.173	[0.085, 0.274]	[0.044, 0.464]	B
43	0.465	[0.235, 0.751]	[0.119, 1.237]	B	71	0.003	[0.001, 0.005]	[0.001, 0.008]	B
44	0.013	[0.006, 0.021]	[0.003, 0.036]	B	77	0.003	[0.001, 0.004]	[0.001, 0.007]	B
49	0.006	[0.003, 0.009]	[0.002, 0.016]	B	79	0.003	[0.001, 0.004]	[0.001, 0.007]	B
50	0.062	[0.031, 0.098]	[0.016, 0.169]	B	81	0.003	[0.001, 0.004]	[0.001, 0.007]	B
51	0.100	[0.049, 0.157]	[0.026, 0.267]	B	83	0.032	[0.015, 0.050]	[0.008, 0.085]	B
52	0.038	[0.018, 0.059]	[0.010, 0.102]	B	84	0.927	[0.481, 1.529]	[0.235, 2.433]	B
53	0.296	[0.147, 0.470]	[0.075, 0.787]	B	85	0.064	[0.031, 0.100]	[0.016, 0.173]	B
54	0.056	[0.028, 0.089]	[0.015, 0.152]	B					

Table 17. Partial ionization cross sections (10^{-20} m^2) for 3,3-dimethyl-1-butene. TICS/10^{-20} m^2 = 17.672. *M* = 84, base peak is *m*/*z* 69.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.287, 0.477]	[0.215, 0.599]	H	54	0.061	[0.030, 0.096]	[0.016, 0.164]	B
14	0.017	[0.008, 0.026]	[0.004, 0.045]	B	55	0.376	[0.189, 0.604]	[0.096, 1.005]	B
15	0.176	[0.087, 0.279]	[0.045, 0.472]	B	56	0.387	[0.195, 0.625]	[0.099, 1.033]	B
26	0.111	[0.054, 0.175]	[0.028, 0.298]	B	57	0.392	[0.196, 0.625]	[0.100, 1.043]	B
27	1.068	[0.558, 1.770]	[0.273, 2.814]	B	58	0.015	[0.007, 0.024]	[0.004, 0.041]	B
28	0.064	[0.031, 0.101]	[0.016, 0.172]	B	61	0.009	[0.004, 0.014]	[0.002, 0.025]	B
29	0.671	[0.342, 1.092]	[0.171, 1.781]	B	62	0.013	[0.007, 0.021]	[0.003, 0.036]	B
30	0.010	[0.005, 0.016]	[0.003, 0.027]	B	63	0.022	[0.011, 0.034]	[0.006, 0.058]	B
37	0.042	[0.021, 0.067]	[0.011, 0.114]	B	65	0.028	[0.014, 0.045]	[0.007, 0.077]	B
38	0.123	[0.061, 0.195]	[0.032, 0.330]	B	66	0.008	[0.004, 0.012]	[0.002, 0.021]	B
39	1.129	[0.594, 1.878]	[0.289, 2.969]	B	67	0.136	[0.067, 0.216]	[0.035, 0.365]	B
40	0.188	[0.093, 0.299]	[0.048, 0.503]	B	68	0.029	[0.014, 0.045]	[0.007, 0.078]	B
41	6.421	[4.763, 7.714]	[3.530, 9.462]	A	69	3.501	[1.936, 4.483]	[1.023, 6.074]	A
42	0.435	[0.219, 0.700]	[0.112, 1.165]	B	70	0.205	[0.101, 0.323]	[0.052, 0.547]	B
43	0.271	[0.136, 0.436]	[0.069, 0.725]	B	71	0.006	[0.003, 0.010]	[0.002, 0.017]	B
44	0.007	[0.003, 0.011]	[0.002, 0.019]	B	77	0.003	[0.001, 0.004]	[0.001, 0.008]	B
49	0.013	[0.006, 0.020]	[0.003, 0.034]	B	79	0.003	[0.001, 0.005]	[0.001, 0.008]	B
50	0.086	[0.042, 0.135]	[0.022, 0.233]	B	83	0.012	[0.006, 0.018]	[0.003, 0.031]	B
51	0.138	[0.069, 0.220]	[0.036, 0.372]	B	84	0.656	[0.336, 1.071]	[0.168, 1.747]	B
52	0.041	[0.020, 0.065]	[0.011, 0.111]	B	85	0.043	[0.021, 0.068]	[0.011, 0.117]	B
53	0.356	[0.177, 0.566]	[0.091, 0.948]	B					

Table 18. Partial ionization cross sections (10^{-20} m^2) for 2,3-dimethyl-2-butene. TICS/10^{-20} m^2 = 18.571. *M* = 84, base peak is *m*/*z* 41.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.216, 0.600]	H	53	0.379	[0.189, 0.604]	[0.097, 1.006]	B
14	0.032	[0.016, 0.050]	[0.008, 0.086]	B	54	0.073	[0.036, 0.117]	[0.019, 0.199]	B
15	0.333	[0.165, 0.528]	[0.085, 0.888]	B	55	0.432	[0.216, 0.690]	[0.110, 1.146]	B
24	0.011	[0.005, 0.017]	[0.003, 0.030]	B	56	0.325	[0.162, 0.518]	[0.083, 0.869]	B
26	0.095	[0.047, 0.151]	[0.024, 0.255]	B	57	0.034	[0.017, 0.053]	[0.009, 0.092]	B
27	1.174	[0.617, 1.955]	[0.300, 3.078]	B	61	0.004	[0.002, 0.007]	[0.001, 0.012]	B
28	0.040	[0.019, 0.063]	[0.010, 0.108]	B	62	0.008	[0.004, 0.013]	[0.002, 0.023]	B
29	0.419	[0.209, 0.670]	[0.107, 1.118]	B	63	0.016	[0.008, 0.026]	[0.004, 0.045]	B
37	0.056	[0.027, 0.088]	[0.014, 0.152]	B	65	0.027	[0.013, 0.042]	[0.007, 0.072]	B
38	0.124	[0.061, 0.196]	[0.032, 0.332]	B	66	0.015	[0.007, 0.023]	[0.004, 0.040]	B
39	1.371	[0.734, 2.310]	[0.351, 3.585]	B	67	0.200	[0.099, 0.319]	[0.051, 0.538]	B
40	0.312	[0.156, 0.500]	[0.080, 0.835]	B	68	0.041	[0.020, 0.064]	[0.011, 0.111]	B
41	7.263	[5.489, 8.679]	[4.139, 10.552]	A	69	2.976	[1.304, 3.890]	[0.502, 5.562]	A
42	0.645	[0.329, 1.047]	[0.165, 1.707]	B	70	0.168	[0.083, 0.266]	[0.043, 0.448]	B
43	0.484	[0.244, 0.781]	[0.123, 1.282]	B	71	0.003	[0.001, 0.005]	[0.001, 0.008]	B
44	0.020	[0.010, 0.032]	[0.005, 0.055]	B	79	0.003	[0.001, 0.004]	[0.001, 0.007]	B
49	0.006	[0.003, 0.009]	[0.002, 0.016]	B	81	0.003	[0.001, 0.004]	[0.001, 0.007]	B
50	0.053	[0.026, 0.083]	[0.014, 0.143]	B	83	0.027	[0.013, 0.042]	[0.007, 0.073]	B
51	0.091	[0.045, 0.143]	[0.023, 0.244]	B	84	0.811	[0.418, 1.335]	[0.207, 2.146]	B
52	0.039	[0.019, 0.061]	[0.010, 0.105]	B	85	0.057	[0.028, 0.089]	[0.015, 0.155]	B

Table 19. Partial ionization cross sections (10^{-20} m^2) for 2-ethyl-1-butene. TICS/10^{-20} m^2 = 18.169. M = 84, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	55	1.828	[1.006, 3.119]	[0.471, 4.722]	B
12	0.008	[0.004, 0.013]	[0.002, 0.022]	B	56	0.746	[0.381, 1.213]	[0.190, 1.973]	B
13	0.008	[0.004, 0.012]	[0.002, 0.021]	B	57	0.035	[0.017, 0.054]	[0.009, 0.093]	B
14	0.053	[0.026, 0.082]	[0.013, 0.141]	B	58	0.002	[0.001, 0.004]	[0.001, 0.006]	B
15	0.498	[0.251, 0.804]	[0.126, 1.320]	B	61	0.002	[0.001, 0.003]	[0.001, 0.006]	B
16	0.014	[0.007, 0.022]	[0.004, 0.038]	B	62	0.006	[0.003, 0.009]	[0.002, 0.016]	B
25	0.005	[0.002, 0.008]	[0.001, 0.014]	B	63	0.014	[0.007, 0.021]	[0.003, 0.037]	B
26	0.211	[0.105, 0.334]	[0.054, 0.563]	B	64	0.002	[0.001, 0.003]	[0.000, 0.005]	B
27	2.417	[0.707, 3.131]	[0.170, 4.886]	A	65	0.025	[0.012, 0.040]	[0.007, 0.069]	B
28	0.471	[0.237, 0.757]	[0.120, 1.247]	B	66	0.012	[0.006, 0.019]	[0.003, 0.033]	B
29	1.597	[0.865, 2.706]	[0.407, 4.125]	B	67	0.085	[0.042, 0.134]	[0.022, 0.227]	B
30	0.036	[0.018, 0.057]	[0.009, 0.097]	B	68	0.015	[0.007, 0.023]	[0.004, 0.039]	B
31	0.004	[0.002, 0.007]	[0.001, 0.012]	B	69	1.399	[0.742, 2.336]	[0.358, 3.651]	B
32	0.004	[0.002, 0.007]	[0.001, 0.012]	B	70	0.072	[0.035, 0.113]	[0.018, 0.192]	B
33	0.004	[0.002, 0.006]	[0.001, 0.011]	B	71	0.001	[0.001, 0.002]	[0.000, 0.004]	B
36	0.004	[0.002, 0.006]	[0.001, 0.010]	B	73	0.001	[0.001, 0.002]	[0.000, 0.004]	B
37	0.030	[0.015, 0.047]	[0.008, 0.082]	B	74	0.001	[0.001, 0.002]	[0.000, 0.004]	B
38	0.111	[0.054, 0.174]	[0.029, 0.298]	B	75	0.001	[0.001, 0.002]	[0.000, 0.004]	B
39	1.415	[0.753, 2.364]	[0.364, 3.690]	B	76	0.001	[0.001, 0.002]	[0.000, 0.004]	B
40	0.261	[0.129, 0.413]	[0.066, 0.692]	B	77	0.005	[0.002, 0.008]	[0.001, 0.014]	B
41	3.438	[1.812, 4.459]	[0.927, 6.155]	A	78	0.001	[0.001, 0.002]	[0.000, 0.004]	B
42	1.055	[0.549, 1.736]	[0.270, 2.762]	B	79	0.004	[0.002, 0.006]	[0.001, 0.011]	B
43	0.325	[0.162, 0.518]	[0.084, 0.867]	B	80	0.001	[0.001, 0.002]	[0.000, 0.003]	B
44	0.013	[0.006, 0.020]	[0.003, 0.035]	B	81	0.003	[0.001, 0.004]	[0.001, 0.007]	B
49	0.006	[0.003, 0.009]	[0.001, 0.015]	B	82	0.001	[0.001, 0.002]	[0.000, 0.004]	B
50	0.083	[0.041, 0.131]	[0.021, 0.224]	B	83	0.010	[0.005, 0.016]	[0.003, 0.028]	B
51	0.160	[0.079, 0.255]	[0.041, 0.429]	B	84	0.551	[0.278, 0.886]	[0.141, 1.463]	B
52	0.074	[0.036, 0.116]	[0.019, 0.198]	B	85	0.036	[0.018, 0.057]	[0.009, 0.098]	B
53	0.391	[0.195, 0.622]	[0.100, 1.031]	B	86	0.001	[0.001, 0.002]	[0.000, 0.003]	B
54	0.210	[0.104, 0.335]	[0.054, 0.560]	B					

Table 20. Partial ionization cross sections (10^{-20} m^2) for 1-heptene. TICS/10^{-20} m^2 = 21.030. M = 98, base peak is m/z 56.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	56	2.791	[0.780, 3.647]	[0.187, 5.785]	A
15	0.083	[0.040, 0.128]	[0.021, 0.221]	B	57	0.839	[0.426, 1.354]	[0.213, 2.202]	B
26	0.107	[0.053, 0.169]	[0.028, 0.288]	B	58	0.035	[0.017, 0.054]	[0.009, 0.093]	B
27	1.343	[0.696, 2.211]	[0.340, 3.513]	B	61	0.003	[0.001, 0.004]	[0.001, 0.007]	B
28	0.249	[0.123, 0.393]	[0.063, 0.661]	B	62	0.007	[0.004, 0.011]	[0.002, 0.020]	B
29	2.779	[0.789, 3.650]	[0.180, 5.764]	A	63	0.012	[0.006, 0.019]	[0.003, 0.032]	B
30	0.058	[0.028, 0.091]	[0.015, 0.154]	B	65	0.018	[0.009, 0.029]	[0.005, 0.049]	B
36	0.004	[0.002, 0.007]	[0.001, 0.012]	B	66	0.007	[0.003, 0.010]	[0.002, 0.018]	B
37	0.021	[0.010, 0.033]	[0.005, 0.056]	B	67	0.050	[0.024, 0.078]	[0.013, 0.134]	B
38	0.073	[0.035, 0.114]	[0.019, 0.195]	B	68	0.077	[0.037, 0.120]	[0.020, 0.206]	B
39	1.209	[0.627, 1.986]	[0.309, 3.163]	B	69	0.650	[0.329, 1.050]	[0.166, 1.718]	B
40	0.190	[0.094, 0.301]	[0.048, 0.505]	B	70	0.901	[0.460, 1.463]	[0.229, 2.369]	B
41	3.679	[1.754, 4.813]	[0.800, 6.836]	A	71	0.049	[0.024, 0.077]	[0.013, 0.133]	B
42	2.043	[1.104, 3.442]	[0.525, 5.296]	B	77	0.007	[0.003, 0.011]	[0.002, 0.018]	B
43	0.579	[0.290, 0.926]	[0.147, 1.534]	B	78	0.002	[0.001, 0.003]	[0.000, 0.004]	B
44	0.018	[0.009, 0.028]	[0.005, 0.048]	B	79	0.005	[0.002, 0.007]	[0.001, 0.013]	B
49	0.003	[0.002, 0.005]	[0.001, 0.009]	B	81	0.004	[0.002, 0.007]	[0.001, 0.012]	B
50	0.047	[0.023, 0.074]	[0.012, 0.127]	B	82	0.001	[0.001, 0.002]	[0.000, 0.004]	B
51	0.071	[0.035, 0.111]	[0.018, 0.190]	B	83	0.057	[0.028, 0.091]	[0.015, 0.155]	B
52	0.030	[0.015, 0.047]	[0.008, 0.081]	B	84	0.004	[0.002, 0.006]	[0.001, 0.011]	B
53	0.193	[0.095, 0.305]	[0.049, 0.511]	B	97	0.001	[0.001, 0.002]	[0.000, 0.003]	B
54	0.221	[0.108, 0.348]	[0.056, 0.590]	B	98	0.172	[0.085, 0.272]	[0.044, 0.462]	B
55	1.926	[1.034, 3.238]	[0.494, 5.007]	B	99	0.014	[0.007, 0.021]	[0.004, 0.037]	B

Table 21. Partial ionization cross sections (10^{-20} m^2) for 2-heptene. TICS/10^{-20} m^2 = 21.308. M = 98, base peak is m/z 55.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.289, 0.479]	[0.214, 0.599]	H	62	0.015	[0.007, 0.023]	[0.004, 0.040]	B
14	0.009	[0.005, 0.015]	[0.002, 0.025]	B	63	0.023	[0.011, 0.036]	[0.006, 0.062]	B
15	0.126	[0.062, 0.199]	[0.032, 0.337]	B	64	0.003	[0.001, 0.004]	[0.001, 0.008]	B
26	0.141	[0.069, 0.221]	[0.036, 0.377]	B	65	0.035	[0.017, 0.055]	[0.009, 0.096]	B
27	1.644	[0.873, 2.753]	[0.419, 4.285]	B	66	0.016	[0.008, 0.025]	[0.004, 0.043]	B
28	0.225	[0.113, 0.361]	[0.058, 0.604]	B	67	0.131	[0.065, 0.208]	[0.034, 0.355]	B
29	1.308	[0.679, 2.151]	[0.333, 3.421]	B	68	0.092	[0.045, 0.145]	[0.024, 0.248]	B
30	0.029	[0.014, 0.046]	[0.007, 0.078]	B	69	1.203	[0.622, 1.975]	[0.307, 3.167]	B
37	0.040	[0.019, 0.062]	[0.010, 0.107]	B	70	0.412	[0.205, 0.655]	[0.104, 1.085]	B
38	0.101	[0.049, 0.158]	[0.026, 0.269]	B	71	0.026	[0.013, 0.041]	[0.007, 0.070]	B
39	1.309	[0.682, 2.165]	[0.333, 3.435]	B	72	0.002	[0.001, 0.004]	[0.001, 0.006]	B
40	0.222	[0.110, 0.353]	[0.056, 0.590]	B	74	0.002	[0.001, 0.003]	[0.001, 0.006]	B
41	3.379	[1.412, 4.450]	[0.552, 6.506]	A	77	0.014	[0.007, 0.022]	[0.004, 0.038]	B
42	0.859	[0.437, 1.395]	[0.217, 2.259]	B	78	0.004	[0.002, 0.006]	[0.001, 0.011]	B
43	0.894	[0.457, 1.456]	[0.228, 2.361]	B	79	0.015	[0.007, 0.023]	[0.004, 0.041]	B
44	0.030	[0.015, 0.047]	[0.008, 0.081]	B	80	0.002	[0.001, 0.003]	[0.000, 0.005]	B
45	0.013	[0.006, 0.020]	[0.003, 0.034]	B	81	0.021	[0.010, 0.033]	[0.005, 0.057]	B
49	0.012	[0.006, 0.018]	[0.003, 0.031]	B	82	0.005	[0.002, 0.008]	[0.001, 0.014]	B
50	0.068	[0.033, 0.106]	[0.017, 0.181]	B	83	0.069	[0.034, 0.109]	[0.018, 0.186]	B
51	0.114	[0.056, 0.180]	[0.029, 0.307]	B	84	0.005	[0.002, 0.007]	[0.001, 0.013]	B
52	0.050	[0.025, 0.079]	[0.013, 0.136]	B	85	0.002	[0.001, 0.002]	[0.000, 0.004]	B
53	0.352	[0.177, 0.567]	[0.090, 0.944]	B	95	0.001	[0.001, 0.002]	[0.000, 0.004]	B
54	0.404	[0.202, 0.647]	[0.103, 1.071]	B	96	0.001	[0.001, 0.002]	[0.000, 0.004]	B
55	3.410	[1.447, 4.500]	[0.569, 6.548]	A	97	0.006	[0.003, 0.009]	[0.002, 0.016]	B
56	3.019	[1.023, 3.981]	[0.308, 6.073]	A	98	0.647	[0.327, 1.043]	[0.166, 1.719]	B
57	0.324	[0.161, 0.514]	[0.082, 0.857]	B	99	0.054	[0.026, 0.084]	[0.014, 0.143]	B
58	0.013	[0.006, 0.020]	[0.003, 0.035]	B	100	0.001	[0.001, 0.002]	[0.000, 0.004]	B
61	0.006	[0.003, 0.009]	[0.002, 0.016]	B					

Table 22. Partial ionization cross sections (10^{-20} m^2) for 3-heptene. TICS/10^{-20} m^2 = 20.454. M = 98, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.216, 0.600]	H	60	0.003	[0.001, 0.005]	[0.001, 0.008]	B
12	0.010	[0.005, 0.016]	[0.003, 0.028]	B	61	0.006	[0.003, 0.009]	[0.002, 0.016]	B
13	0.019	[0.009, 0.030]	[0.005, 0.052]	B	62	0.014	[0.007, 0.023]	[0.004, 0.039]	B
14	0.075	[0.037, 0.117]	[0.019, 0.199]	B	63	0.028	[0.014, 0.044]	[0.007, 0.077]	B
15	0.538	[0.270, 0.863]	[0.137, 1.427]	B	64	0.006	[0.003, 0.009]	[0.001, 0.015]	B
16	0.009	[0.004, 0.013]	[0.002, 0.023]	B	65	0.041	[0.020, 0.064]	[0.010, 0.109]	B
24	0.007	[0.003, 0.010]	[0.002, 0.018]	B	66	0.019	[0.009, 0.029]	[0.005, 0.050]	B
25	0.013	[0.006, 0.020]	[0.003, 0.035]	B	67	0.129	[0.064, 0.204]	[0.033, 0.346]	B
26	0.279	[0.138, 0.442]	[0.071, 0.738]	B	68	0.078	[0.039, 0.124]	[0.020, 0.212]	B
27	2.291	[1.287, 3.933]	[0.585, 5.781]	B	69	1.378	[0.725, 2.286]	[0.351, 3.590]	B
28	0.446	[0.223, 0.712]	[0.113, 1.175]	B	70	0.303	[0.151, 0.484]	[0.077, 0.809]	B
29	1.134	[0.591, 1.871]	[0.289, 2.976]	B	71	0.014	[0.007, 0.022]	[0.004, 0.038]	B
30	0.029	[0.014, 0.045]	[0.007, 0.077]	B	73	0.002	[0.001, 0.003]	[0.001, 0.006]	B
31	0.006	[0.003, 0.009]	[0.001, 0.015]	B	75	0.002	[0.001, 0.003]	[0.001, 0.006]	B
36	0.005	[0.002, 0.008]	[0.001, 0.014]	B	76	0.002	[0.001, 0.003]	[0.001, 0.006]	B
37	0.049	[0.024, 0.077]	[0.012, 0.131]	B	77	0.014	[0.007, 0.022]	[0.004, 0.037]	B
38	0.143	[0.070, 0.225]	[0.037, 0.383]	B	78	0.004	[0.002, 0.006]	[0.001, 0.010]	B
39	1.499	[0.801, 2.519]	[0.384, 3.907]	B	79	0.013	[0.006, 0.020]	[0.003, 0.036]	B
40	0.234	[0.116, 0.371]	[0.060, 0.624]	B	80	0.002	[0.001, 0.003]	[0.000, 0.005]	B
41	4.486	[2.632, 5.643]	[1.526, 7.502]	A	81	0.016	[0.008, 0.024]	[0.004, 0.042]	B
42	0.765	[0.387, 1.234]	[0.194, 2.010]	B	82	0.002	[0.001, 0.003]	[0.000, 0.005]	B
43	0.551	[0.279, 0.889]	[0.140, 1.456]	B	83	0.052	[0.025, 0.082]	[0.013, 0.140]	B
44	0.025	[0.012, 0.040]	[0.006, 0.068]	B	84	0.003	[0.001, 0.005]	[0.001, 0.008]	B
45	0.004	[0.002, 0.006]	[0.001, 0.011]	B	85	0.001	[0.001, 0.002]	[0.000, 0.004]	B
46	0.004	[0.002, 0.006]	[0.001, 0.011]	B	86	0.001	[0.001, 0.002]	[0.000, 0.004]	B
49	0.008	[0.004, 0.012]	[0.002, 0.021]	B	87	0.001	[0.001, 0.002]	[0.000, 0.004]	B
50	0.082	[0.040, 0.129]	[0.021, 0.221]	B	89	0.001	[0.001, 0.002]	[0.000, 0.004]	B
51	0.139	[0.069, 0.220]	[0.036, 0.371]	B	91	0.001	[0.001, 0.002]	[0.000, 0.004]	B
52	0.061	[0.030, 0.095]	[0.015, 0.161]	B	95	0.001	[0.001, 0.002]	[0.000, 0.004]	B
53	0.302	[0.150, 0.481]	[0.077, 0.805]	B	96	0.001	[0.001, 0.002]	[0.000, 0.004]	B
54	0.237	[0.118, 0.378]	[0.061, 0.635]	B	97	0.001	[0.001, 0.002]	[0.000, 0.004]	B
55	1.606	[0.859, 2.695]	[0.412, 4.189]	B	98	0.411	[0.205, 0.653]	[0.105, 1.087]	B
56	2.180	[1.209, 3.709]	[0.559, 5.544]	B	99	0.032	[0.016, 0.051]	[0.008, 0.087]	B
57	0.226	[0.112, 0.360]	[0.058, 0.605]	B	100	0.001	[0.001, 0.002]	[0.000, 0.004]	B
58	0.006	[0.003, 0.010]	[0.002, 0.017]	B					

Table 23. Partial ionization cross sections (10^{-20} m^2) for 2-methyl-1-hexene. TICS/10^{-20} m^2 = 21.242. *M* = 98, base peak is *m*/*z* 56.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	55	1.214	[0.633, 2.006]	[0.310, 3.181]	B
15	0.128	[0.063, 0.201]	[0.033, 0.342]	B	56	6.722	[4.771, 8.192]	[3.378, 10.243]	A
26	0.078	[0.038, 0.123]	[0.020, 0.209]	B	57	0.691	[0.350, 1.119]	[0.175, 1.822]	B
27	1.472	[0.780, 2.458]	[0.378, 3.855]	B	58	0.026	[0.012, 0.040]	[0.007, 0.070]	B
28	0.306	[0.153, 0.489]	[0.079, 0.819]	B	62	0.006	[0.003, 0.009]	[0.002, 0.016]	B
29	1.065	[0.554, 1.757]	[0.274, 2.816]	B	63	0.012	[0.006, 0.018]	[0.003, 0.031]	B
30	0.023	[0.011, 0.036]	[0.006, 0.063]	B	65	0.017	[0.008, 0.026]	[0.004, 0.045]	B
37	0.020	[0.010, 0.031]	[0.005, 0.053]	B	66	0.005	[0.003, 0.008]	[0.001, 0.015]	B
38	0.068	[0.033, 0.108]	[0.017, 0.184]	B	67	0.079	[0.039, 0.125]	[0.020, 0.213]	B
39	1.002	[0.516, 1.641]	[0.255, 2.645]	B	68	0.031	[0.015, 0.048]	[0.008, 0.084]	B
40	0.270	[0.133, 0.427]	[0.069, 0.720]	B	69	0.498	[0.249, 0.797]	[0.127, 1.324]	B
41	4.264	[2.374, 5.461]	[1.279, 7.403]	A	70	0.608	[0.306, 0.977]	[0.156, 1.619]	B
42	0.501	[0.252, 0.805]	[0.128, 1.337]	B	71	0.043	[0.021, 0.067]	[0.011, 0.116]	B
43	1.009	[0.518, 1.647]	[0.257, 2.657]	B	77	0.008	[0.004, 0.013]	[0.002, 0.022]	B
44	0.034	[0.017, 0.054]	[0.009, 0.093]	B	79	0.011	[0.006, 0.018]	[0.003, 0.031]	B
50	0.046	[0.022, 0.071]	[0.012, 0.122]	B	81	0.014	[0.007, 0.022]	[0.004, 0.038]	B
51	0.060	[0.029, 0.093]	[0.015, 0.161]	B	83	0.036	[0.018, 0.057]	[0.009, 0.097]	B
52	0.029	[0.014, 0.046]	[0.008, 0.078]	B	84	0.006	[0.003, 0.010]	[0.002, 0.017]	B
53	0.228	[0.113, 0.363]	[0.059, 0.613]	B	98	0.093	[0.046, 0.147]	[0.024, 0.250]	B
54	0.111	[0.055, 0.176]	[0.029, 0.298]	B	99	0.009	[0.004, 0.014]	[0.002, 0.024]	B

Table 24. Partial ionization cross sections (10^{-20} m^2) for 3-methyl-1-hexene. TICS/10^{-20} m^2 = 21.178. *M* = 98, base peak is *m*/*z* 55.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.289, 0.479]	[0.216, 0.600]	H	58	0.003	[0.002, 0.005]	[0.001, 0.009]	B
14	0.010	[0.005, 0.016]	[0.003, 0.027]	B	61	0.003	[0.002, 0.005]	[0.001, 0.009]	B
15	0.107	[0.052, 0.168]	[0.027, 0.286]	B	62	0.010	[0.005, 0.015]	[0.002, 0.026]	B
26	0.117	[0.058, 0.186]	[0.030, 0.315]	B	63	0.015	[0.007, 0.024]	[0.004, 0.042]	B
27	1.564	[0.834, 2.618]	[0.402, 4.076]	B	65	0.029	[0.014, 0.046]	[0.008, 0.079]	B
28	0.118	[0.058, 0.186]	[0.030, 0.317]	B	66	0.012	[0.006, 0.018]	[0.003, 0.031]	B
29	1.224	[0.638, 2.020]	[0.313, 3.216]	B	67	0.152	[0.075, 0.241]	[0.039, 0.407]	B
30	0.025	[0.012, 0.039]	[0.006, 0.067]	B	68	0.085	[0.042, 0.134]	[0.022, 0.230]	B
37	0.027	[0.013, 0.042]	[0.007, 0.073]	B	69	2.121	[1.165, 3.606]	[0.548, 5.467]	B
38	0.067	[0.033, 0.107]	[0.017, 0.182]	B	70	1.073	[0.551, 1.750]	[0.273, 2.817]	B
39	1.084	[0.558, 1.774]	[0.276, 2.851]	B	71	0.059	[0.029, 0.092]	[0.015, 0.159]	B
40	0.170	[0.084, 0.269]	[0.044, 0.454]	B	72	0.002	[0.001, 0.004]	[0.001, 0.007]	B
41	3.539	[1.605, 4.610]	[0.697, 6.608]	A	74	0.002	[0.001, 0.004]	[0.001, 0.006]	B
42	0.648	[0.328, 1.047]	[0.166, 1.723]	B	77	0.013	[0.006, 0.020]	[0.003, 0.035]	B
43	1.006	[0.517, 1.644]	[0.256, 2.638]	B	78	0.002	[0.001, 0.003]	[0.001, 0.006]	B
44	0.041	[0.020, 0.065]	[0.011, 0.113]	B	79	0.014	[0.007, 0.022]	[0.004, 0.038]	B
49	0.008	[0.004, 0.013]	[0.002, 0.022]	B	80	0.002	[0.001, 0.003]	[0.001, 0.005]	B
50	0.065	[0.032, 0.102]	[0.017, 0.173]	B	81	0.019	[0.009, 0.029]	[0.005, 0.051]	B
51	0.107	[0.053, 0.169]	[0.027, 0.286]	B	82	0.013	[0.006, 0.020]	[0.003, 0.035]	B
52	0.047	[0.023, 0.073]	[0.012, 0.125]	B	83	0.187	[0.093, 0.299]	[0.048, 0.503]	B
53	0.337	[0.168, 0.537]	[0.086, 0.897]	B	84	0.012	[0.006, 0.018]	[0.003, 0.032]	B
54	0.307	[0.153, 0.489]	[0.078, 0.820]	B	97	0.003	[0.002, 0.005]	[0.001, 0.009]	B
55	3.676	[1.733, 4.757]	[0.795, 6.753]	A	98	0.128	[0.063, 0.203]	[0.033, 0.347]	B
56	2.329	[1.298, 3.993]	[0.599, 5.961]	B	99	0.011	[0.005, 0.017]	[0.003, 0.030]	B
57	0.183	[0.090, 0.289]	[0.047, 0.488]	B					

Table 25. Partial ionization cross sections (10^{-20} m^2) for 4-methyl-1-hexene. TICS/10^{-20} m^2 = 21.365. M = 98, base peak is m/z 57.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	57	3.779	[1.807, 4.932]	[0.845, 7.011]	A
14	0.011	[0.005, 0.017]	[0.003, 0.029]	B	58	0.170	[0.084, 0.269]	[0.044, 0.458]	B
15	0.125	[0.061, 0.195]	[0.032, 0.332]	B	59	0.004	[0.002, 0.006]	[0.001, 0.010]	B
26	0.088	[0.043, 0.139]	[0.023, 0.239]	B	60	0.004	[0.002, 0.006]	[0.001, 0.010]	B
27	0.982	[0.500, 1.590]	[0.251, 2.588]	B	61	0.003	[0.002, 0.005]	[0.001, 0.009]	B
28	0.105	[0.052, 0.166]	[0.027, 0.282]	B	62	0.007	[0.003, 0.011]	[0.002, 0.018]	B
29	3.628	[1.655, 4.751]	[0.714, 6.817]	A	63	0.010	[0.005, 0.016]	[0.003, 0.027]	B
30	0.080	[0.039, 0.124]	[0.020, 0.212]	B	64	0.003	[0.002, 0.005]	[0.001, 0.009]	B
31	0.013	[0.006, 0.020]	[0.003, 0.035]	B	65	0.022	[0.011, 0.035]	[0.006, 0.060]	B
37	0.023	[0.011, 0.036]	[0.006, 0.062]	B	66	0.009	[0.004, 0.015]	[0.002, 0.025]	B
38	0.072	[0.035, 0.114]	[0.018, 0.192]	B	67	0.088	[0.043, 0.137]	[0.022, 0.234]	B
39	0.926	[0.471, 1.499]	[0.236, 2.438]	B	68	0.032	[0.016, 0.051]	[0.008, 0.088]	B
40	0.166	[0.082, 0.264]	[0.043, 0.447]	B	69	0.309	[0.154, 0.491]	[0.079, 0.822]	B
41	4.492	[2.552, 5.763]	[1.425, 7.812]	A	70	0.400	[0.199, 0.640]	[0.102, 1.073]	B
42	0.437	[0.218, 0.696]	[0.112, 1.165]	B	71	0.025	[0.012, 0.039]	[0.006, 0.067]	B
43	0.206	[0.102, 0.325]	[0.053, 0.550]	B	73	0.003	[0.001, 0.004]	[0.001, 0.007]	B
44	0.010	[0.005, 0.015]	[0.003, 0.027]	B	77	0.009	[0.005, 0.015]	[0.002, 0.025]	B
45	0.010	[0.005, 0.015]	[0.002, 0.026]	B	78	0.002	[0.001, 0.004]	[0.001, 0.006]	B
49	0.004	[0.002, 0.007]	[0.001, 0.012]	B	79	0.009	[0.004, 0.014]	[0.002, 0.024]	B
50	0.035	[0.017, 0.055]	[0.009, 0.095]	B	81	0.012	[0.006, 0.019]	[0.003, 0.033]	B
51	0.059	[0.029, 0.094]	[0.015, 0.161]	B	82	0.004	[0.002, 0.006]	[0.001, 0.011]	B
52	0.025	[0.012, 0.039]	[0.006, 0.068]	B	83	0.026	[0.013, 0.041]	[0.007, 0.071]	B
53	0.176	[0.087, 0.278]	[0.045, 0.471]	B	84	0.002	[0.001, 0.003]	[0.000, 0.005]	B
54	0.080	[0.039, 0.126]	[0.020, 0.214]	B	97	0.007	[0.003, 0.011]	[0.002, 0.019]	B
55	0.929	[0.475, 1.509]	[0.239, 2.455]	B	98	0.083	[0.040, 0.130]	[0.021, 0.223]	B
56	3.253	[1.255, 4.288]	[0.445, 6.396]	A	99	0.009	[0.004, 0.013]	[0.002, 0.023]	B

Table 26. Partial ionization cross sections (10^{-20} m^2) for 5-methyl-1-hexene. TICS/10^{-20} m^2 = 21.018. M = 98, base peak is m/z 56.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	57	1.661	[0.881, 2.777]	[0.421, 4.307]	B
14	0.011	[0.006, 0.018]	[0.003, 0.031]	B	58	0.070	[0.034, 0.109]	[0.018, 0.187]	B
15	0.120	[0.059, 0.188]	[0.031, 0.320]	B	61	0.004	[0.002, 0.006]	[0.001, 0.010]	B
26	0.093	[0.045, 0.146]	[0.024, 0.249]	B	62	0.007	[0.003, 0.011]	[0.002, 0.019]	B
27	1.220	[0.636, 2.015]	[0.312, 3.206]	B	63	0.010	[0.005, 0.016]	[0.003, 0.028]	B
28	0.118	[0.058, 0.186]	[0.030, 0.315]	B	65	0.020	[0.010, 0.031]	[0.005, 0.054]	B
29	2.077	[1.136, 3.526]	[0.535, 5.366]	B	66	0.010	[0.005, 0.015]	[0.003, 0.026]	B
30	0.049	[0.024, 0.077]	[0.013, 0.133]	B	67	0.066	[0.032, 0.104]	[0.017, 0.179]	B
37	0.030	[0.015, 0.047]	[0.008, 0.081]	B	68	0.028	[0.014, 0.043]	[0.007, 0.075]	B
38	0.064	[0.031, 0.101]	[0.016, 0.172]	B	69	0.542	[0.272, 0.868]	[0.138, 1.434]	B
39	1.092	[0.563, 1.785]	[0.279, 2.870]	B	70	0.547	[0.274, 0.876]	[0.139, 1.454]	B
40	0.163	[0.080, 0.257]	[0.041, 0.433]	B	71	0.029	[0.014, 0.045]	[0.007, 0.077]	B
41	3.655	[1.726, 4.726]	[0.802, 6.716]	A	74	0.003	[0.001, 0.004]	[0.001, 0.007]	B
42	0.577	[0.290, 0.926]	[0.148, 1.530]	B	77	0.012	[0.006, 0.019]	[0.003, 0.033]	B
43	1.411	[0.739, 2.333]	[0.361, 3.706]	B	78	0.002	[0.001, 0.004]	[0.001, 0.006]	B
44	0.047	[0.023, 0.073]	[0.012, 0.127]	B	79	0.011	[0.006, 0.018]	[0.003, 0.031]	B
49	0.005	[0.002, 0.007]	[0.001, 0.013]	B	81	0.017	[0.008, 0.027]	[0.004, 0.046]	B
50	0.050	[0.024, 0.078]	[0.013, 0.135]	B	82	0.004	[0.002, 0.006]	[0.001, 0.011]	B
51	0.076	[0.037, 0.119]	[0.019, 0.203]	B	83	0.125	[0.062, 0.198]	[0.032, 0.336]	B
52	0.035	[0.017, 0.056]	[0.009, 0.095]	B	84	0.010	[0.005, 0.015]	[0.002, 0.026]	B
53	0.198	[0.098, 0.315]	[0.051, 0.532]	B	97	0.005	[0.003, 0.008]	[0.001, 0.015]	B
54	0.156	[0.077, 0.247]	[0.040, 0.418]	B	98	0.025	[0.012, 0.039]	[0.006, 0.068]	B
55	2.112	[1.156, 3.583]	[0.545, 5.459]	B	99	0.002	[0.001, 0.003]	[0.000, 0.005]	B
56	4.049	[2.135, 5.201]	[1.112, 7.186]	A					

Table 27. Partial ionization cross sections (10^{-20} m^2) for 2-methyl-2-hexene. TICS/10^{-20} m^2 = 21.435. *M* = 98, base peak is *m*/*z* 69.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.287, 0.477]	[0.216, 0.600]	H	57	0.094	[0.046, 0.148]	[0.024, 0.253]	B
12	0.026	[0.013, 0.041]	[0.007, 0.070]	B	58	0.004	[0.002, 0.006]	[0.001, 0.011]	B
13	0.025	[0.012, 0.038]	[0.006, 0.066]	B	60	0.004	[0.002, 0.006]	[0.001, 0.010]	B
14	0.094	[0.046, 0.148]	[0.024, 0.253]	B	61	0.008	[0.004, 0.012]	[0.002, 0.020]	B
15	0.828	[0.420, 1.342]	[0.212, 2.196]	B	62	0.018	[0.009, 0.028]	[0.005, 0.049]	B
16	0.033	[0.016, 0.051]	[0.008, 0.088]	B	63	0.032	[0.016, 0.051]	[0.008, 0.088]	B
24	0.008	[0.004, 0.013]	[0.002, 0.023]	B	64	0.007	[0.003, 0.011]	[0.002, 0.019]	B
25	0.016	[0.008, 0.026]	[0.004, 0.044]	B	65	0.048	[0.023, 0.075]	[0.012, 0.129]	B
26	0.305	[0.151, 0.485]	[0.078, 0.813]	B	66	0.020	[0.010, 0.032]	[0.005, 0.054]	B
27	2.502	[1.414, 4.312]	[0.646, 6.373]	B	67	0.164	[0.081, 0.259]	[0.042, 0.439]	B
28	0.411	[0.205, 0.656]	[0.105, 1.091]	B	68	0.128	[0.063, 0.202]	[0.033, 0.344]	B
29	0.989	[0.509, 1.615]	[0.254, 2.620]	B	69	3.122	[1.132, 4.068]	[0.367, 6.083]	A
30	0.022	[0.011, 0.034]	[0.006, 0.059]	B	70	0.211	[0.105, 0.336]	[0.054, 0.563]	B
31	0.007	[0.003, 0.011]	[0.002, 0.019]	B	71	0.006	[0.003, 0.009]	[0.002, 0.016]	B
32	0.007	[0.003, 0.011]	[0.002, 0.019]	B	73	0.003	[0.001, 0.004]	[0.001, 0.008]	B
36	0.006	[0.003, 0.010]	[0.002, 0.017]	B	74	0.005	[0.003, 0.008]	[0.001, 0.015]	B
37	0.062	[0.030, 0.097]	[0.016, 0.166]	B	75	0.003	[0.001, 0.004]	[0.001, 0.007]	B
38	0.169	[0.083, 0.267]	[0.043, 0.455]	B	76	0.003	[0.001, 0.004]	[0.001, 0.007]	B
39	1.744	[0.940, 2.952]	[0.446, 4.542]	B	77	0.023	[0.011, 0.035]	[0.006, 0.061]	B
40	0.284	[0.142, 0.454]	[0.073, 0.760]	B	78	0.005	[0.002, 0.008]	[0.001, 0.013]	B
41	4.985	[3.060, 6.302]	[1.847, 8.293]	A	79	0.019	[0.009, 0.029]	[0.005, 0.051]	B
42	0.295	[0.147, 0.470]	[0.076, 0.791]	B	80	0.005	[0.002, 0.007]	[0.001, 0.012]	B
43	0.415	[0.206, 0.658]	[0.106, 1.109]	B	81	0.031	[0.015, 0.049]	[0.008, 0.084]	B
44	0.016	[0.008, 0.025]	[0.004, 0.043]	B	82	0.011	[0.005, 0.017]	[0.003, 0.029]	B
45	0.005	[0.003, 0.008]	[0.001, 0.014]	B	83	0.158	[0.078, 0.250]	[0.040, 0.423]	B
46	0.005	[0.002, 0.008]	[0.001, 0.014]	B	84	0.010	[0.005, 0.015]	[0.003, 0.026]	B
47	0.005	[0.002, 0.008]	[0.001, 0.014]	B	85	0.002	[0.001, 0.003]	[0.000, 0.005]	B
48	0.005	[0.002, 0.008]	[0.001, 0.013]	B	91	0.002	[0.001, 0.003]	[0.000, 0.005]	B
49	0.010	[0.005, 0.015]	[0.002, 0.026]	B	92	0.002	[0.001, 0.003]	[0.000, 0.005]	B
50	0.118	[0.058, 0.184]	[0.030, 0.315]	B	93	0.002	[0.001, 0.003]	[0.000, 0.005]	B
51	0.199	[0.099, 0.316]	[0.051, 0.530]	B	95	0.002	[0.001, 0.003]	[0.000, 0.005]	B
52	0.082	[0.040, 0.129]	[0.021, 0.221]	B	96	0.002	[0.001, 0.003]	[0.000, 0.005]	B
53	0.458	[0.229, 0.730]	[0.117, 1.213]	B	97	0.004	[0.002, 0.006]	[0.001, 0.010]	B
54	0.122	[0.060, 0.193]	[0.031, 0.326]	B	98	0.466	[0.234, 0.748]	[0.119, 1.234]	B
55	1.027	[0.524, 1.664]	[0.263, 2.707]	B	99	0.035	[0.017, 0.055]	[0.009, 0.096]	B
56	1.094	[0.566, 1.802]	[0.279, 2.881]	B	100	0.002	[0.001, 0.003]	[0.000, 0.005]	B

Table 28. Partial ionization cross sections (10^{-20} m^2) for 3-methyl-2-hexene. TICS/10^{-20} m^2 = 21.270. M = 98, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.287, 0.477]	[0.216, 0.600]	H	61	0.016	[0.008, 0.025]	[0.004, 0.044]	B
25	0.060	[0.030, 0.095]	[0.016, 0.163]	B	62	0.016	[0.008, 0.025]	[0.004, 0.043]	B
26	0.290	[0.143, 0.459]	[0.074, 0.773]	B	63	0.033	[0.016, 0.053]	[0.009, 0.090]	B
27	1.635	[0.873, 2.746]	[0.418, 4.260]	B	65	0.068	[0.033, 0.108]	[0.018, 0.185]	B
28	0.495	[0.247, 0.789]	[0.125, 1.306]	B	66	0.031	[0.015, 0.049]	[0.008, 0.084]	B
29	1.212	[0.627, 1.989]	[0.310, 3.190]	B	67	0.225	[0.111, 0.357]	[0.057, 0.599]	B
30	0.044	[0.021, 0.068]	[0.011, 0.117]	B	68	0.061	[0.030, 0.096]	[0.016, 0.165]	B
31	0.045	[0.022, 0.071]	[0.012, 0.122]	B	69	2.525	[0.472, 3.194]	[0.050, 5.304]	A
33	0.021	[0.010, 0.033]	[0.005, 0.057]	B	70	0.773	[0.392, 1.246]	[0.197, 2.034]	B
34	0.015	[0.007, 0.024]	[0.004, 0.041]	B	71	0.043	[0.021, 0.067]	[0.011, 0.114]	B
36	0.050	[0.025, 0.079]	[0.013, 0.136]	B	73	0.011	[0.005, 0.017]	[0.003, 0.030]	B
37	0.055	[0.027, 0.086]	[0.014, 0.147]	B	74	0.006	[0.003, 0.010]	[0.002, 0.017]	B
38	0.181	[0.089, 0.285]	[0.046, 0.483]	B	75	0.008	[0.004, 0.013]	[0.002, 0.022]	B
39	1.443	[0.762, 2.412]	[0.368, 3.793]	B	76	0.009	[0.005, 0.015]	[0.002, 0.025]	B
40	0.221	[0.110, 0.351]	[0.057, 0.590]	B	77	0.025	[0.012, 0.040]	[0.007, 0.069]	B
41	5.689	[3.788, 7.107]	[2.483, 9.108]	A	78	0.022	[0.011, 0.035]	[0.006, 0.060]	B
42	0.467	[0.235, 0.749]	[0.120, 1.242]	B	79	0.025	[0.012, 0.038]	[0.006, 0.066]	B
43	0.397	[0.199, 0.638]	[0.102, 1.062]	B	80	0.008	[0.004, 0.013]	[0.002, 0.022]	B
44	0.041	[0.020, 0.064]	[0.010, 0.110]	B	81	0.024	[0.012, 0.038]	[0.006, 0.065]	B
45	0.020	[0.010, 0.032]	[0.005, 0.055]	B	82	0.020	[0.010, 0.031]	[0.005, 0.053]	B
46	0.022	[0.010, 0.034]	[0.006, 0.058]	B	83	0.224	[0.110, 0.353]	[0.057, 0.596]	B
47	0.011	[0.005, 0.017]	[0.003, 0.030]	B	84	0.020	[0.010, 0.031]	[0.005, 0.053]	B
48	0.022	[0.011, 0.034]	[0.006, 0.059]	B	85	0.003	[0.001, 0.004]	[0.001, 0.008]	B
50	0.102	[0.050, 0.162]	[0.026, 0.274]	B	86	0.007	[0.003, 0.010]	[0.002, 0.018]	B
51	0.159	[0.079, 0.254]	[0.041, 0.429]	B	88	0.005	[0.002, 0.007]	[0.001, 0.013]	B
52	0.077	[0.038, 0.122]	[0.020, 0.207]	B	90	0.005	[0.002, 0.008]	[0.001, 0.014]	B
53	0.320	[0.159, 0.510]	[0.082, 0.850]	B	91	0.011	[0.005, 0.017]	[0.003, 0.029]	B
54	0.087	[0.043, 0.138]	[0.023, 0.236]	B	92	0.009	[0.004, 0.013]	[0.002, 0.023]	B
55	2.245	[1.258, 3.877]	[0.580, 5.789]	B	93	0.008	[0.004, 0.012]	[0.002, 0.022]	B
56	0.836	[0.426, 1.356]	[0.212, 2.200]	B	94	0.004	[0.002, 0.006]	[0.001, 0.011]	B
57	0.108	[0.053, 0.170]	[0.028, 0.292]	B	95	0.004	[0.002, 0.006]	[0.001, 0.011]	B
58	0.012	[0.006, 0.019]	[0.003, 0.034]	B	96	0.003	[0.002, 0.005]	[0.001, 0.009]	B
59	0.007	[0.003, 0.010]	[0.002, 0.018]	B	98	0.203	[0.100, 0.322]	[0.052, 0.548]	B
60	0.007	[0.004, 0.011]	[0.002, 0.020]	B	99	0.018	[0.009, 0.029]	[0.005, 0.050]	B

Table 29. Partial ionization cross sections (10^{-20} m^2) for 4-methyl-2-hexene. TICS/10^{-20} m^2 = 21.403. M = 98, base peak is m/z 69.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	53	0.455	[0.228, 0.729]	[0.116, 1.209]	B
14	0.200	[0.099, 0.317]	[0.051, 0.534]	B	55	1.863	[1.010, 3.162]	[0.478, 4.851]	B
15	0.370	[0.186, 0.594]	[0.095, 0.991]	B	56	0.571	[0.288, 0.918]	[0.145, 1.509]	B
26	0.227	[0.113, 0.364]	[0.058, 0.604]	B	57	0.075	[0.037, 0.118]	[0.019, 0.202]	B
27	1.550	[0.823, 2.598]	[0.395, 4.057]	B	63	0.057	[0.028, 0.091]	[0.015, 0.156]	B
28	1.081	[0.557, 1.767]	[0.278, 2.863]	B	65	0.104	[0.051, 0.163]	[0.027, 0.278]	B
29	0.966	[0.495, 1.576]	[0.246, 2.540]	B	66	0.048	[0.023, 0.075]	[0.012, 0.130]	B
32	0.227	[0.112, 0.360]	[0.058, 0.609]	B	67	0.338	[0.169, 0.539]	[0.087, 0.904]	B
38	0.185	[0.092, 0.296]	[0.048, 0.498]	B	69	3.677	[1.734, 4.770]	[0.774, 6.738]	A
39	1.792	[0.965, 3.029]	[0.458, 4.663]	B	70	0.495	[0.247, 0.789]	[0.126, 1.304]	B
41	4.949	[3.010, 6.235]	[1.839, 8.251]	A	77	0.035	[0.017, 0.054]	[0.009, 0.093]	B
42	0.312	[0.155, 0.496]	[0.080, 0.833]	B	79	0.034	[0.017, 0.053]	[0.009, 0.092]	B
43	0.194	[0.096, 0.308]	[0.050, 0.519]	B	83	0.258	[0.127, 0.408]	[0.066, 0.692]	B
50	0.108	[0.053, 0.170]	[0.028, 0.289]	B	98	0.497	[0.249, 0.795]	[0.127, 1.323]	B
51	0.199	[0.098, 0.314]	[0.051, 0.536]	B	99	0.043	[0.021, 0.068]	[0.011, 0.116]	B
52	0.090	[0.044, 0.142]	[0.023, 0.243]	B					

Table 30. Partial ionization cross sections (10^{-20} m^2) for 5-methyl-2-hexene. TICS/10^{-20} m^2 = 21.309. M = 98, base peak is m/z 56.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	59	0.003	[0.001, 0.004]	[0.001, 0.008]	B
12	0.009	[0.004, 0.014]	[0.002, 0.025]	B	60	0.003	[0.001, 0.004]	[0.001, 0.007]	B
13	0.026	[0.013, 0.041]	[0.007, 0.071]	B	61	0.005	[0.003, 0.008]	[0.001, 0.014]	B
14	0.075	[0.037, 0.118]	[0.019, 0.202]	B	62	0.010	[0.005, 0.016]	[0.003, 0.028]	B
15	0.684	[0.346, 1.102]	[0.174, 1.809]	B	63	0.023	[0.011, 0.036]	[0.006, 0.061]	B
16	0.031	[0.015, 0.048]	[0.008, 0.083]	B	64	0.002	[0.001, 0.004]	[0.001, 0.007]	B
19	0.007	[0.003, 0.011]	[0.002, 0.019]	B	65	0.034	[0.017, 0.053]	[0.009, 0.092]	B
20	0.007	[0.003, 0.010]	[0.002, 0.018]	B	66	0.017	[0.008, 0.026]	[0.004, 0.045]	B
24	0.006	[0.003, 0.009]	[0.002, 0.016]	B	67	0.093	[0.046, 0.146]	[0.024, 0.250]	B
25	0.006	[0.003, 0.009]	[0.002, 0.016]	B	68	0.029	[0.014, 0.046]	[0.008, 0.080]	B
26	0.205	[0.102, 0.326]	[0.053, 0.550]	B	69	0.432	[0.217, 0.690]	[0.111, 1.144]	B
27	2.400	[1.329, 4.102]	[0.616, 6.158]	B	70	0.309	[0.153, 0.489]	[0.079, 0.826]	B
28	0.400	[0.198, 0.633]	[0.102, 1.063]	B	71	0.017	[0.008, 0.026]	[0.004, 0.046]	B
29	1.186	[0.616, 1.951]	[0.302, 3.099]	B	72	0.002	[0.001, 0.003]	[0.001, 0.005]	B
30	0.026	[0.013, 0.040]	[0.007, 0.070]	B	73	0.002	[0.001, 0.003]	[0.001, 0.005]	B
31	0.005	[0.002, 0.008]	[0.001, 0.014]	B	74	0.004	[0.002, 0.006]	[0.001, 0.011]	B
36	0.004	[0.002, 0.007]	[0.001, 0.012]	B	75	0.002	[0.001, 0.003]	[0.000, 0.005]	B
37	0.039	[0.019, 0.062]	[0.010, 0.106]	B	76	0.002	[0.001, 0.003]	[0.000, 0.005]	B
38	0.120	[0.059, 0.191]	[0.031, 0.324]	B	77	0.021	[0.010, 0.033]	[0.005, 0.057]	B
39	1.379	[0.724, 2.284]	[0.352, 3.593]	B	78	0.003	[0.002, 0.005]	[0.001, 0.009]	B
40	0.210	[0.104, 0.333]	[0.054, 0.561]	B	79	0.015	[0.007, 0.023]	[0.004, 0.041]	B
41	2.507	[1.403, 4.315]	[0.645, 6.423]	B	80	0.002	[0.001, 0.003]	[0.000, 0.004]	B
42	0.280	[0.139, 0.443]	[0.072, 0.752]	B	81	0.023	[0.011, 0.037]	[0.006, 0.063]	B
43	3.050	[1.047, 3.971]	[0.335, 6.064]	A	82	0.005	[0.002, 0.007]	[0.001, 0.012]	B
44	0.098	[0.049, 0.155]	[0.025, 0.263]	B	83	0.097	[0.048, 0.153]	[0.025, 0.261]	B
45	0.004	[0.002, 0.006]	[0.001, 0.010]	B	84	0.006	[0.003, 0.009]	[0.001, 0.015]	B
46	0.004	[0.002, 0.006]	[0.001, 0.010]	B	85	0.001	[0.001, 0.002]	[0.000, 0.004]	B
47	0.004	[0.002, 0.006]	[0.001, 0.010]	B	86	0.001	[0.001, 0.002]	[0.000, 0.004]	B
48	0.003	[0.002, 0.005]	[0.001, 0.009]	B	87	0.001	[0.001, 0.002]	[0.000, 0.004]	B
49	0.007	[0.003, 0.011]	[0.002, 0.018]	B	89	0.001	[0.001, 0.002]	[0.000, 0.004]	B
50	0.104	[0.051, 0.164]	[0.027, 0.278]	B	91	0.001	[0.001, 0.002]	[0.000, 0.004]	B
51	0.161	[0.080, 0.256]	[0.041, 0.431]	B	92	0.001	[0.001, 0.002]	[0.000, 0.004]	B
52	0.067	[0.033, 0.106]	[0.017, 0.181]	B	93	0.001	[0.001, 0.002]	[0.000, 0.004]	B
53	0.287	[0.144, 0.460]	[0.074, 0.772]	B	95	0.001	[0.001, 0.002]	[0.000, 0.004]	B
54	0.416	[0.207, 0.663]	[0.107, 1.106]	B	96	0.001	[0.001, 0.002]	[0.000, 0.004]	B
55	2.481	[1.383, 4.248]	[0.640, 6.347]	B	97	0.011	[0.005, 0.016]	[0.003, 0.028]	B
56	2.957	[0.935, 3.838]	[0.269, 5.950]	A	98	0.186	[0.092, 0.295]	[0.048, 0.498]	B
57	0.258	[0.128, 0.410]	[0.066, 0.691]	B	99	0.015	[0.007, 0.023]	[0.004, 0.039]	B
58	0.009	[0.004, 0.013]	[0.002, 0.023]	B	100	0.001	[0.001, 0.002]	[0.000, 0.004]	B

Table 31. Partial ionization cross sections (10^{-20} m^2) for 2-methyl-3-hexene. TICS/10^{-20} m^2 = 21.250. M = 98, base peak is m/z 69.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	53	0.485	[0.242, 0.773]	[0.124, 1.288]	B
14	0.550	[0.275, 0.879]	[0.140, 1.453]	B	55	2.728	[0.688, 3.579]	[0.123, 5.696]	A
15	0.833	[0.425, 1.352]	[0.212, 2.192]	B	56	1.214	[0.628, 1.984]	[0.311, 3.187]	B
16	0.190	[0.094, 0.301]	[0.049, 0.510]	B	57	0.098	[0.048, 0.154]	[0.025, 0.263]	B
26	0.233	[0.116, 0.371]	[0.060, 0.623]	B	63	0.060	[0.029, 0.094]	[0.015, 0.160]	B
27	0.586	[0.294, 0.938]	[0.149, 1.551]	B	65	0.137	[0.067, 0.215]	[0.035, 0.368]	B
28	1.402	[0.737, 2.326]	[0.359, 3.671]	B	66	0.061	[0.030, 0.095]	[0.016, 0.164]	B
29	0.827	[0.421, 1.341]	[0.211, 2.178]	B	67	0.358	[0.178, 0.569]	[0.092, 0.954]	B
38	0.203	[0.099, 0.319]	[0.052, 0.540]	B	69	2.270	[1.256, 3.876]	[0.580, 5.780]	B
39	2.104	[1.146, 3.560]	[0.539, 5.416]	B	70	0.228	[0.113, 0.361]	[0.058, 0.607]	B
40	0.384	[0.191, 0.611]	[0.098, 1.019]	B	77	0.066	[0.032, 0.103]	[0.017, 0.177]	B
41	3.609	[1.650, 4.751]	[0.703, 6.766]	A	79	0.050	[0.024, 0.077]	[0.013, 0.134]	B
42	0.291	[0.144, 0.463]	[0.074, 0.776]	B	81	0.040	[0.020, 0.063]	[0.010, 0.108]	B
43	0.571	[0.287, 0.915]	[0.146, 1.512]	B	83	0.243	[0.119, 0.382]	[0.062, 0.649]	B
50	0.175	[0.086, 0.277]	[0.045, 0.469]	B	98	0.416	[0.208, 0.666]	[0.106, 1.108]	B
51	0.289	[0.144, 0.459]	[0.074, 0.770]	B	99	0.035	[0.017, 0.055]	[0.009, 0.095]	B
52	0.112	[0.055, 0.176]	[0.029, 0.301]	B					

Table 32. Partial ionization cross sections (10^{-20} m^2) for 3-methyl-3-hexene. TICS/10^{-20} m^2 = 21.467. *M* = 98, base peak is *m*/*z* 69.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.216, 0.600]	H	57	0.051	[0.025, 0.081]	[0.013, 0.139]	B
12	0.022	[0.010, 0.034]	[0.006, 0.058]	B	58	0.003	[0.002, 0.005]	[0.001, 0.009]	B
13	0.031	[0.015, 0.048]	[0.008, 0.083]	B	60	0.003	[0.002, 0.005]	[0.001, 0.009]	B
14	0.138	[0.068, 0.217]	[0.035, 0.370]	B	61	0.013	[0.006, 0.019]	[0.003, 0.034]	B
15	1.111	[0.577, 1.826]	[0.284, 2.909]	B	62	0.025	[0.012, 0.039]	[0.006, 0.067]	B
16	0.037	[0.018, 0.057]	[0.009, 0.098]	B	63	0.045	[0.022, 0.071]	[0.012, 0.122]	B
24	0.007	[0.003, 0.011]	[0.002, 0.019]	B	64	0.009	[0.004, 0.014]	[0.002, 0.024]	B
25	0.014	[0.007, 0.022]	[0.004, 0.037]	B	65	0.069	[0.034, 0.109]	[0.018, 0.186]	B
26	0.255	[0.125, 0.402]	[0.065, 0.681]	B	66	0.031	[0.015, 0.048]	[0.008, 0.083]	B
27	2.298	[1.269, 3.918]	[0.589, 5.880]	B	67	0.223	[0.111, 0.355]	[0.057, 0.595]	B
28	0.428	[0.214, 0.686]	[0.109, 1.141]	B	68	0.088	[0.043, 0.138]	[0.022, 0.236]	B
29	1.078	[0.556, 1.763]	[0.277, 2.843]	B	69	2.615	[0.544, 3.329]	[0.078, 5.485]	A
30	0.024	[0.012, 0.038]	[0.006, 0.065]	B	70	0.306	[0.152, 0.487]	[0.078, 0.815]	B
31	0.006	[0.003, 0.009]	[0.002, 0.016]	B	71	0.010	[0.005, 0.016]	[0.003, 0.027]	B
32	0.012	[0.006, 0.018]	[0.003, 0.031]	B	73	0.002	[0.001, 0.004]	[0.001, 0.006]	B
36	0.005	[0.003, 0.008]	[0.001, 0.014]	B	74	0.005	[0.002, 0.007]	[0.001, 0.012]	B
37	0.062	[0.030, 0.098]	[0.016, 0.167]	B	75	0.002	[0.001, 0.003]	[0.001, 0.006]	B
38	0.182	[0.090, 0.288]	[0.047, 0.487]	B	76	0.002	[0.001, 0.003]	[0.001, 0.006]	B
39	1.787	[0.962, 3.022]	[0.457, 4.656]	B	77	0.027	[0.013, 0.043]	[0.007, 0.074]	B
40	0.292	[0.146, 0.467]	[0.075, 0.779]	B	78	0.006	[0.003, 0.010]	[0.002, 0.017]	B
41	4.241	[2.292, 5.455]	[1.225, 7.477]	A	79	0.026	[0.012, 0.040]	[0.007, 0.069]	B
42	0.322	[0.160, 0.511]	[0.082, 0.853]	B	80	0.004	[0.002, 0.006]	[0.001, 0.010]	B
43	0.356	[0.177, 0.567]	[0.091, 0.948]	B	81	0.037	[0.018, 0.058]	[0.010, 0.100]	B
44	0.013	[0.006, 0.021]	[0.003, 0.036]	B	82	0.011	[0.005, 0.017]	[0.003, 0.029]	B
45	0.004	[0.002, 0.007]	[0.001, 0.012]	B	83	0.244	[0.120, 0.385]	[0.062, 0.649]	B
46	0.004	[0.002, 0.007]	[0.001, 0.012]	B	84	0.015	[0.007, 0.023]	[0.004, 0.040]	B
47	0.004	[0.002, 0.006]	[0.001, 0.011]	B	85	0.002	[0.001, 0.002]	[0.000, 0.004]	B
48	0.004	[0.002, 0.006]	[0.001, 0.011]	B	91	0.002	[0.001, 0.002]	[0.000, 0.004]	B
49	0.012	[0.006, 0.019]	[0.003, 0.033]	B	93	0.002	[0.001, 0.002]	[0.000, 0.004]	B
50	0.126	[0.062, 0.199]	[0.033, 0.341]	B	95	0.002	[0.001, 0.002]	[0.000, 0.004]	B
51	0.225	[0.112, 0.359]	[0.058, 0.604]	B	96	0.002	[0.001, 0.002]	[0.000, 0.004]	B
52	0.087	[0.043, 0.138]	[0.023, 0.236]	B	97	0.003	[0.002, 0.005]	[0.001, 0.008]	B
53	0.435	[0.218, 0.698]	[0.111, 1.153]	B	98	0.453	[0.226, 0.721]	[0.116, 1.204]	B
54	0.106	[0.052, 0.166]	[0.027, 0.282]	B	99	0.034	[0.017, 0.054]	[0.009, 0.093]	B
55	2.310	[1.282, 3.961]	[0.597, 5.972]	B	100	0.002	[0.001, 0.002]	[0.000, 0.004]	B
56	0.657	[0.330, 1.053]	[0.168, 1.737]	B					

Table 33. Partial ionization cross sections (10^{-20} m^2) for 2,3-dimethyl-1-pentene. TICS/10^{-20} m^2 = 21.425. *M* = 98, base peak is *m*/*z* 41.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.216, 0.600]	H	53	0.464	[0.233, 0.744]	[0.119, 1.235]	B
15	0.411	[0.206, 0.658]	[0.105, 1.093]	B	54	0.021	[0.010, 0.033]	[0.005, 0.057]	B
18	0.052	[0.026, 0.082]	[0.013, 0.140]	B	55	2.146	[1.184, 3.652]	[0.550, 5.479]	B
26	0.210	[0.104, 0.333]	[0.054, 0.563]	B	56	0.596	[0.299, 0.955]	[0.152, 1.577]	B
27	1.822	[0.978, 3.054]	[0.467, 4.724]	B	57	0.073	[0.036, 0.114]	[0.019, 0.196]	B
28	0.107	[0.053, 0.170]	[0.028, 0.290]	B	62	0.024	[0.012, 0.038]	[0.006, 0.065]	B
29	1.114	[0.578, 1.828]	[0.285, 2.920]	B	63	0.037	[0.018, 0.058]	[0.009, 0.099]	B
30	0.035	[0.017, 0.054]	[0.009, 0.093]	B	65	0.085	[0.041, 0.133]	[0.022, 0.227]	B
37	0.070	[0.034, 0.110]	[0.018, 0.187]	B	67	0.295	[0.147, 0.469]	[0.075, 0.785]	B
38	0.196	[0.098, 0.313]	[0.050, 0.527]	B	69	2.500	[1.413, 4.299]	[0.638, 6.280]	B
39	2.110	[1.160, 3.590]	[0.541, 5.411]	B	70	0.925	[0.473, 1.507]	[0.236, 2.440]	B
40	0.424	[0.211, 0.675]	[0.108, 1.123]	B	71	0.049	[0.024, 0.076]	[0.012, 0.131]	B
41	5.307	[3.359, 6.594]	[2.119, 8.568]	A	77	0.027	[0.013, 0.043]	[0.007, 0.073]	B
42	0.419	[0.209, 0.669]	[0.106, 1.106]	B	79	0.027	[0.013, 0.042]	[0.007, 0.073]	B
43	0.314	[0.156, 0.499]	[0.080, 0.831]	B	81	0.025	[0.012, 0.040]	[0.006, 0.068]	B
44	0.026	[0.013, 0.041]	[0.007, 0.070]	B	83	0.431	[0.214, 0.685]	[0.110, 1.142]	B
50	0.126	[0.062, 0.199]	[0.032, 0.338]	B	84	0.028	[0.014, 0.045]	[0.007, 0.076]	B
51	0.213	[0.106, 0.340]	[0.055, 0.569]	B	98	0.213	[0.106, 0.338]	[0.054, 0.568]	B
52	0.086	[0.042, 0.134]	[0.022, 0.230]	B	99	0.018	[0.009, 0.028]	[0.005, 0.048]	B

Table 34. Partial ionization cross sections (10^{-20} m^2) for 2,4-dimethyl-1-pentene. TICS/10^{-20} m^2 = 21.589. *M* = 98, base peak is *m/z* 56.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	55	1.331	[0.694, 2.199]	[0.338, 3.478]	B
15	0.528	[0.264, 0.844]	[0.134, 1.396]	B	56	4.461	[2.518, 5.762]	[1.386, 7.820]	A
26	0.167	[0.082, 0.262]	[0.043, 0.445]	B	57	0.398	[0.198, 0.633]	[0.101, 1.055]	B
27	1.826	[0.975, 3.067]	[0.468, 4.768]	B	63	0.032	[0.016, 0.051]	[0.008, 0.088]	B
28	0.195	[0.097, 0.311]	[0.050, 0.524]	B	65	0.059	[0.029, 0.094]	[0.015, 0.160]	B
29	0.826	[0.420, 1.336]	[0.211, 2.172]	B	66	0.026	[0.013, 0.041]	[0.007, 0.071]	B
37	0.061	[0.030, 0.096]	[0.016, 0.164]	B	67	0.142	[0.071, 0.226]	[0.036, 0.381]	B
38	0.232	[0.115, 0.368]	[0.059, 0.618]	B	68	0.029	[0.014, 0.046]	[0.007, 0.078]	B
39	2.167	[1.176, 3.662]	[0.554, 5.587]	B	69	0.083	[0.041, 0.131]	[0.021, 0.223]	B
40	0.519	[0.262, 0.836]	[0.133, 1.376]	B	70	0.444	[0.223, 0.711]	[0.113, 1.177]	B
41	3.364	[1.347, 4.419]	[0.512, 6.527]	A	71	0.023	[0.011, 0.036]	[0.006, 0.063]	B
42	0.338	[0.168, 0.538]	[0.086, 0.902]	B	77	0.030	[0.015, 0.047]	[0.008, 0.082]	B
43	2.648	[0.565, 3.420]	[0.090, 5.652]	A	79	0.027	[0.013, 0.043]	[0.007, 0.074]	B
44	0.094	[0.046, 0.148]	[0.024, 0.253]	B	81	0.017	[0.008, 0.026]	[0.004, 0.045]	B
50	0.116	[0.057, 0.183]	[0.030, 0.311]	B	83	0.189	[0.094, 0.300]	[0.048, 0.507]	B
51	0.179	[0.088, 0.284]	[0.046, 0.481]	B	84	0.013	[0.006, 0.020]	[0.003, 0.034]	B
52	0.071	[0.035, 0.111]	[0.018, 0.191]	B	98	0.192	[0.095, 0.304]	[0.049, 0.514]	B
53	0.305	[0.151, 0.483]	[0.078, 0.811]	B	99	0.013	[0.006, 0.020]	[0.003, 0.036]	B
54	0.043	[0.021, 0.067]	[0.011, 0.115]	B					

Table 35. Partial ionization cross sections (10^{-20} m^2) for 3,4-dimethyl-1-pentene. TICS/10^{-20} m^2 = 21.402. *M* = 98, base peak is *m/z* 56.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.289, 0.479]	[0.214, 0.599]	H	58	0.005	[0.002, 0.008]	[0.001, 0.013]	B
12	0.016	[0.008, 0.025]	[0.004, 0.043]	B	60	0.002	[0.001, 0.004]	[0.001, 0.006]	B
13	0.030	[0.015, 0.047]	[0.008, 0.081]	B	61	0.005	[0.002, 0.007]	[0.001, 0.012]	B
14	0.123	[0.061, 0.196]	[0.031, 0.332]	B	62	0.011	[0.005, 0.017]	[0.003, 0.030]	B
15	0.897	[0.454, 1.438]	[0.229, 2.350]	B	63	0.024	[0.012, 0.038]	[0.006, 0.065]	B
16	0.040	[0.020, 0.063]	[0.010, 0.108]	B	64	0.004	[0.002, 0.007]	[0.001, 0.012]	B
25	0.010	[0.005, 0.016]	[0.003, 0.027]	B	65	0.038	[0.018, 0.059]	[0.010, 0.103]	B
26	0.246	[0.122, 0.389]	[0.063, 0.653]	B	66	0.019	[0.009, 0.029]	[0.005, 0.050]	B
27	2.793	[0.758, 3.625]	[0.171, 5.774]	A	67	0.102	[0.050, 0.161]	[0.026, 0.277]	B
28	0.528	[0.266, 0.847]	[0.134, 1.392]	B	68	0.024	[0.011, 0.037]	[0.006, 0.064]	B
29	1.217	[0.632, 2.001]	[0.312, 3.196]	B	69	0.188	[0.093, 0.296]	[0.048, 0.500]	B
30	0.027	[0.013, 0.042]	[0.007, 0.072]	B	70	1.108	[0.567, 1.803]	[0.283, 2.922]	B
31	0.004	[0.002, 0.007]	[0.001, 0.012]	B	71	0.064	[0.031, 0.100]	[0.016, 0.171]	B
32	0.004	[0.002, 0.007]	[0.001, 0.012]	B	72	0.002	[0.001, 0.003]	[0.000, 0.005]	B
36	0.004	[0.002, 0.006]	[0.001, 0.010]	B	73	0.002	[0.001, 0.003]	[0.000, 0.005]	B
37	0.049	[0.024, 0.077]	[0.013, 0.133]	B	74	0.003	[0.002, 0.005]	[0.001, 0.009]	B
38	0.145	[0.071, 0.228]	[0.037, 0.387]	B	75	0.002	[0.001, 0.003]	[0.000, 0.004]	B
39	1.545	[0.813, 2.556]	[0.399, 4.044]	B	76	0.002	[0.001, 0.002]	[0.000, 0.004]	B
40	0.239	[0.119, 0.381]	[0.061, 0.637]	B	77	0.014	[0.007, 0.022]	[0.004, 0.037]	B
41	2.526	[1.412, 4.328]	[0.653, 6.463]	B	78	0.003	[0.001, 0.005]	[0.001, 0.008]	B
42	0.321	[0.160, 0.512]	[0.083, 0.859]	B	79	0.012	[0.006, 0.018]	[0.003, 0.031]	B
43	2.470	[1.377, 4.234]	[0.639, 6.328]	B	80	0.003	[0.001, 0.004]	[0.001, 0.008]	B
44	0.078	[0.038, 0.123]	[0.020, 0.211]	B	81	0.014	[0.007, 0.021]	[0.003, 0.037]	B
45	0.003	[0.002, 0.005]	[0.001, 0.009]	B	82	0.003	[0.001, 0.004]	[0.001, 0.007]	B
46	0.003	[0.002, 0.005]	[0.001, 0.009]	B	83	0.151	[0.074, 0.238]	[0.039, 0.403]	B
49	0.012	[0.006, 0.018]	[0.003, 0.032]	B	84	0.010	[0.005, 0.015]	[0.002, 0.026]	B
50	0.104	[0.051, 0.165]	[0.027, 0.279]	B	85	0.001	[0.001, 0.002]	[0.000, 0.003]	B
51	0.165	[0.082, 0.261]	[0.042, 0.442]	B	91	0.001	[0.001, 0.002]	[0.000, 0.003]	B
52	0.061	[0.030, 0.096]	[0.016, 0.164]	B	95	0.001	[0.001, 0.002]	[0.000, 0.003]	B
53	0.321	[0.159, 0.510]	[0.082, 0.860]	B	96	0.001	[0.001, 0.002]	[0.000, 0.003]	B
54	0.325	[0.160, 0.513]	[0.083, 0.864]	B	97	0.006	[0.003, 0.009]	[0.001, 0.015]	B
55	2.155	[1.171, 3.653]	[0.550, 5.550]	B	98	0.009	[0.004, 0.014]	[0.002, 0.025]	B
56	2.556	[0.489, 3.255]	[0.064, 5.483]	A	99	0.001	[0.001, 0.002]	[0.000, 0.003]	B
57	0.153	[0.075, 0.240]	[0.039, 0.408]	B					

Table 36. Partial ionization cross sections (10^{-20} m^2) for 3,3-dimethyl-1-pentene. TICS/10^{-20} m^2 = 21.137. M = 98, base peak is m/z 69.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	56	0.633	[0.318, 1.015]	[0.162, 1.675]	B
12	0.025	[0.012, 0.038]	[0.006, 0.067]	B	57	0.058	[0.029, 0.092]	[0.015, 0.157]	B
13	0.047	[0.023, 0.074]	[0.012, 0.127]	B	58	0.004	[0.002, 0.006]	[0.001, 0.010]	B
14	0.169	[0.083, 0.267]	[0.043, 0.453]	B	60	0.004	[0.002, 0.006]	[0.001, 0.010]	B
15	0.941	[0.482, 1.535]	[0.240, 2.490]	B	61	0.007	[0.003, 0.011]	[0.002, 0.019]	B
16	0.021	[0.010, 0.032]	[0.005, 0.056]	B	62	0.017	[0.009, 0.027]	[0.004, 0.047]	B
24	0.008	[0.004, 0.012]	[0.002, 0.022]	B	63	0.031	[0.015, 0.048]	[0.008, 0.083]	B
25	0.016	[0.008, 0.024]	[0.004, 0.042]	B	64	0.003	[0.002, 0.005]	[0.001, 0.009]	B
26	0.313	[0.155, 0.495]	[0.080, 0.832]	B	65	0.052	[0.026, 0.082]	[0.014, 0.142]	B
27	2.593	[0.541, 3.356]	[0.079, 5.526]	A	66	0.026	[0.012, 0.040]	[0.007, 0.069]	B
28	0.334	[0.168, 0.536]	[0.086, 0.894]	B	67	0.181	[0.090, 0.288]	[0.047, 0.489]	B
29	1.049	[0.537, 1.708]	[0.266, 2.745]	B	68	0.119	[0.059, 0.188]	[0.030, 0.318]	B
30	0.021	[0.010, 0.033]	[0.005, 0.056]	B	69	2.976	[0.984, 3.919]	[0.284, 5.989]	A
31	0.007	[0.003, 0.010]	[0.002, 0.018]	B	70	0.346	[0.173, 0.552]	[0.088, 0.919]	B
32	0.007	[0.003, 0.010]	[0.002, 0.018]	B	71	0.082	[0.040, 0.128]	[0.021, 0.220]	B
36	0.006	[0.003, 0.009]	[0.002, 0.016]	B	72	0.006	[0.003, 0.009]	[0.001, 0.015]	B
37	0.053	[0.026, 0.083]	[0.014, 0.142]	B	73	0.003	[0.001, 0.004]	[0.001, 0.007]	B
38	0.150	[0.074, 0.237]	[0.038, 0.400]	B	74	0.003	[0.001, 0.004]	[0.001, 0.007]	B
39	1.628	[0.864, 2.725]	[0.414, 4.238]	B	75	0.003	[0.001, 0.004]	[0.001, 0.007]	B
40	0.243	[0.121, 0.387]	[0.062, 0.652]	B	77	0.012	[0.006, 0.019]	[0.003, 0.032]	B
41	4.388	[2.479, 5.655]	[1.369, 7.660]	A	78	0.002	[0.001, 0.004]	[0.001, 0.006]	B
42	0.270	[0.135, 0.432]	[0.070, 0.727]	B	79	0.011	[0.005, 0.018]	[0.003, 0.030]	B
43	0.644	[0.327, 1.041]	[0.165, 1.704]	B	80	0.002	[0.001, 0.003]	[0.001, 0.006]	B
44	0.020	[0.010, 0.032]	[0.005, 0.055]	B	81	0.015	[0.007, 0.023]	[0.004, 0.040]	B
45	0.005	[0.002, 0.008]	[0.001, 0.014]	B	82	0.004	[0.002, 0.006]	[0.001, 0.011]	B
46	0.005	[0.002, 0.008]	[0.001, 0.013]	B	83	0.322	[0.160, 0.511]	[0.082, 0.858]	B
48	0.005	[0.002, 0.007]	[0.001, 0.013]	B	84	0.021	[0.010, 0.032]	[0.005, 0.055]	B
49	0.014	[0.007, 0.022]	[0.004, 0.037]	B	85	0.002	[0.001, 0.003]	[0.000, 0.005]	B
50	0.126	[0.062, 0.199]	[0.032, 0.337]	B	91	0.002	[0.001, 0.003]	[0.000, 0.005]	B
51	0.207	[0.103, 0.330]	[0.053, 0.556]	B	95	0.002	[0.001, 0.003]	[0.000, 0.005]	B
52	0.078	[0.038, 0.123]	[0.020, 0.209]	B	97	0.002	[0.001, 0.003]	[0.000, 0.005]	B
53	0.462	[0.231, 0.737]	[0.118, 1.224]	B	98	0.160	[0.079, 0.254]	[0.041, 0.433]	B
54	0.120	[0.059, 0.189]	[0.031, 0.320]	B	99	0.012	[0.006, 0.019]	[0.003, 0.034]	B
55	1.642	[0.874, 2.753]	[0.420, 4.282]	B	100	0.002	[0.001, 0.003]	[0.000, 0.005]	B

Table 37. Partial ionization cross sections (10^{-20} m^2) for 4,4-dimethyl-1-pentene. TICS/10^{-20} m^2 = 20.652. M = 98, base peak is m/z 57.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	58	0.315	[0.156, 0.499]	[0.081, 0.842]	B
15	0.152	[0.075, 0.242]	[0.039, 0.410]	B	59	0.039	[0.019, 0.062]	[0.010, 0.107]	B
26	0.067	[0.033, 0.106]	[0.017, 0.179]	B	62	0.006	[0.003, 0.010]	[0.002, 0.017]	B
27	0.773	[0.391, 1.239]	[0.197, 2.021]	B	63	0.018	[0.009, 0.028]	[0.005, 0.049]	B
28	0.051	[0.025, 0.081]	[0.013, 0.139]	B	65	0.035	[0.017, 0.054]	[0.009, 0.093]	B
29	2.508	[0.502, 3.241]	[0.066, 5.367]	A	66	0.011	[0.005, 0.018]	[0.003, 0.030]	B
30	0.049	[0.024, 0.077]	[0.013, 0.132]	B	67	0.099	[0.048, 0.155]	[0.025, 0.265]	B
31	0.012	[0.006, 0.019]	[0.003, 0.032]	B	68	0.016	[0.008, 0.025]	[0.004, 0.044]	B
37	0.021	[0.010, 0.033]	[0.005, 0.056]	B	69	0.031	[0.015, 0.049]	[0.008, 0.084]	B
38	0.081	[0.040, 0.128]	[0.021, 0.218]	B	70	0.138	[0.068, 0.217]	[0.036, 0.368]	B
39	1.094	[0.568, 1.801]	[0.280, 2.876]	B	71	0.020	[0.010, 0.031]	[0.005, 0.054]	B
40	0.165	[0.081, 0.259]	[0.042, 0.439]	B	77	0.013	[0.006, 0.020]	[0.003, 0.034]	B
41	3.711	[1.842, 4.857]	[0.863, 6.802]	A	79	0.012	[0.006, 0.019]	[0.003, 0.032]	B
42	0.186	[0.091, 0.292]	[0.047, 0.496]	B	81	0.037	[0.018, 0.057]	[0.009, 0.098]	B
43	0.264	[0.132, 0.424]	[0.068, 0.709]	B	82	0.018	[0.009, 0.028]	[0.005, 0.049]	B
44	0.009	[0.004, 0.014]	[0.002, 0.024]	B	83	0.523	[0.263, 0.840]	[0.134, 1.392]	B
50	0.048	[0.023, 0.075]	[0.012, 0.128]	B	84	0.036	[0.018, 0.057]	[0.009, 0.097]	B
51	0.070	[0.034, 0.110]	[0.018, 0.186]	B	85	0.003	[0.002, 0.005]	[0.001, 0.009]	B
52	0.023	[0.011, 0.036]	[0.006, 0.062]	B	95	0.006	[0.003, 0.010]	[0.002, 0.017]	B
53	0.156	[0.077, 0.248]	[0.040, 0.420]	B	96	0.003	[0.002, 0.005]	[0.001, 0.008]	B
54	0.029	[0.014, 0.046]	[0.007, 0.079]	B	97	0.009	[0.005, 0.015]	[0.002, 0.025]	B
55	2.053	[1.117, 3.487]	[0.522, 5.293]	B	98	0.034	[0.017, 0.054]	[0.009, 0.093]	B
56	0.434	[0.217, 0.695]	[0.110, 1.150]	B	99	0.013	[0.006, 0.020]	[0.003, 0.034]	B
57	6.862	[4.915, 8.340]	[3.541, 10.421]	A					

Table 38. Partial ionization cross sections (10^{-20} m^2) for 2,3-dimethyl-2-pentene. TICS/10^{-20} m^2 = 21.773. M = 98, base peak is m/z 55.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.289, 0.479]	[0.215, 0.599]	H	61	0.004	[0.002, 0.006]	[0.001, 0.011]	B
14	0.026	[0.013, 0.041]	[0.007, 0.070]	B	62	0.012	[0.006, 0.019]	[0.003, 0.033]	B
15	0.274	[0.136, 0.434]	[0.070, 0.729]	B	63	0.024	[0.012, 0.037]	[0.006, 0.064]	B
26	0.080	[0.039, 0.125]	[0.020, 0.213]	B	64	0.004	[0.002, 0.006]	[0.001, 0.011]	B
27	1.217	[0.634, 2.006]	[0.311, 3.195]	B	65	0.064	[0.031, 0.101]	[0.016, 0.173]	B
28	0.076	[0.037, 0.119]	[0.019, 0.204]	B	66	0.026	[0.013, 0.041]	[0.007, 0.070]	B
29	1.051	[0.547, 1.738]	[0.269, 2.771]	B	67	0.264	[0.131, 0.420]	[0.068, 0.707]	B
30	0.024	[0.012, 0.038]	[0.006, 0.065]	B	68	0.056	[0.028, 0.088]	[0.014, 0.151]	B
31	0.101	[0.050, 0.160]	[0.026, 0.272]	B	69	0.728	[0.370, 1.180]	[0.186, 1.928]	B
36	0.014	[0.007, 0.022]	[0.004, 0.038]	B	70	0.151	[0.075, 0.240]	[0.039, 0.410]	B
37	0.034	[0.017, 0.054]	[0.009, 0.092]	B	71	0.033	[0.016, 0.051]	[0.008, 0.088]	B
38	0.073	[0.036, 0.115]	[0.019, 0.197]	B	72	0.006	[0.003, 0.010]	[0.002, 0.017]	B
39	1.172	[0.608, 1.930]	[0.299, 3.080]	B	73	0.003	[0.002, 0.005]	[0.001, 0.008]	B
40	0.217	[0.108, 0.345]	[0.056, 0.583]	B	74	0.006	[0.003, 0.009]	[0.002, 0.016]	B
41	4.101	[2.152, 5.299]	[1.072, 7.273]	A	77	0.025	[0.012, 0.039]	[0.006, 0.067]	B
42	0.313	[0.157, 0.503]	[0.081, 0.843]	B	78	0.005	[0.003, 0.008]	[0.001, 0.015]	B
43	1.138	[0.587, 1.862]	[0.291, 2.995]	B	79	0.039	[0.019, 0.061]	[0.010, 0.105]	B
44	0.035	[0.017, 0.055]	[0.009, 0.095]	B	80	0.005	[0.002, 0.008]	[0.001, 0.014]	B
45	0.052	[0.025, 0.081]	[0.013, 0.140]	B	81	0.102	[0.050, 0.161]	[0.026, 0.273]	B
46	0.006	[0.003, 0.009]	[0.001, 0.015]	B	82	0.021	[0.010, 0.033]	[0.005, 0.058]	B
49	0.005	[0.003, 0.008]	[0.001, 0.014]	B	83	1.877	[1.021, 3.195]	[0.483, 4.907]	B
50	0.067	[0.033, 0.106]	[0.017, 0.182]	B	84	0.124	[0.060, 0.194]	[0.031, 0.329]	B
51	0.127	[0.063, 0.202]	[0.033, 0.344]	B	85	0.100	[0.049, 0.158]	[0.026, 0.269]	B
52	0.060	[0.029, 0.093]	[0.015, 0.159]	B	86	0.006	[0.003, 0.010]	[0.002, 0.017]	B
53	0.373	[0.186, 0.594]	[0.095, 0.993]	B	91	0.002	[0.001, 0.003]	[0.001, 0.006]	B
54	0.110	[0.054, 0.174]	[0.028, 0.295]	B	95	0.006	[0.003, 0.010]	[0.002, 0.017]	B
55	4.710	[2.764, 5.993]	[1.580, 7.983]	A	96	0.014	[0.007, 0.022]	[0.004, 0.039]	B
56	0.632	[0.318, 1.014]	[0.161, 1.672]	B	97	0.019	[0.009, 0.029]	[0.005, 0.050]	B
57	0.207	[0.102, 0.326]	[0.053, 0.550]	B	98	0.778	[0.394, 1.256]	[0.198, 2.051]	B
58	0.079	[0.039, 0.124]	[0.020, 0.210]	B	99	0.084	[0.041, 0.133]	[0.022, 0.228]	B
59	0.385	[0.192, 0.614]	[0.099, 1.022]	B	100	0.008	[0.004, 0.013]	[0.002, 0.022]	B
60	0.013	[0.006, 0.020]	[0.003, 0.034]	B					

Table 39. Partial ionization cross sections (10^{-20} m^2) for 2,4-dimethyl-2-pentene. TICS/10^{-20} m^2 = 20.712. M = 98, base peak is m/z 55.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.216, 0.600]	H	54	0.087	[0.043, 0.138]	[0.023, 0.237]	B
15	0.152	[0.074, 0.239]	[0.039, 0.408]	B	55	5.707	[3.827, 7.111]	[2.557, 9.127]	A
26	0.054	[0.026, 0.085]	[0.014, 0.145]	B	56	0.475	[0.237, 0.759]	[0.121, 1.259]	B
27	1.361	[0.710, 2.246]	[0.347, 3.565]	B	57	0.109	[0.054, 0.172]	[0.028, 0.292]	B
28	0.204	[0.101, 0.323]	[0.052, 0.546]	B	65	0.092	[0.045, 0.144]	[0.023, 0.245]	B
29	1.046	[0.538, 1.708]	[0.266, 2.734]	B	67	0.307	[0.154, 0.491]	[0.079, 0.819]	B
38	0.081	[0.040, 0.127]	[0.021, 0.217]	B	69	0.146	[0.073, 0.233]	[0.038, 0.396]	B
39	1.350	[0.703, 2.223]	[0.345, 3.534]	B	70	0.033	[0.016, 0.051]	[0.008, 0.088]	B
40	0.233	[0.116, 0.372]	[0.060, 0.626]	B	77	0.034	[0.016, 0.052]	[0.009, 0.090]	B
41	2.968	[1.022, 3.911]	[0.317, 5.939]	A	79	0.047	[0.023, 0.075]	[0.012, 0.129]	B
42	0.186	[0.092, 0.296]	[0.047, 0.497]	B	81	0.044	[0.022, 0.069]	[0.011, 0.120]	B
43	1.533	[0.811, 2.563]	[0.391, 4.009]	B	82	0.043	[0.021, 0.067]	[0.011, 0.114]	B
44	0.072	[0.035, 0.112]	[0.018, 0.191]	B	83	2.538	[0.534, 3.288]	[0.073, 5.407]	A
50	0.063	[0.031, 0.099]	[0.016, 0.170]	B	84	0.145	[0.072, 0.230]	[0.037, 0.389]	B
51	0.155	[0.076, 0.244]	[0.040, 0.414]	B	97	0.012	[0.006, 0.019]	[0.003, 0.034]	B
52	0.061	[0.030, 0.096]	[0.016, 0.164]	B	98	0.624	[0.315, 1.004]	[0.160, 1.653]	B
53	0.297	[0.147, 0.471]	[0.076, 0.792]	B	99	0.050	[0.024, 0.078]	[0.013, 0.134]	B

Table 40. Partial ionization cross sections (10^{-20} m^2) for 3,4-dimethyl-2-pentene. TICS/10^{-20} m^2 = 20.574. M = 98, base peak is m/z 83.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.289, 0.479]	[0.215, 0.599]	H	61	0.014	[0.007, 0.021]	[0.003, 0.036]	B
14	0.028	[0.014, 0.045]	[0.007, 0.077]	B	62	0.022	[0.011, 0.034]	[0.006, 0.060]	B
15	0.284	[0.142, 0.456]	[0.073, 0.765]	B	63	0.043	[0.021, 0.067]	[0.011, 0.115]	B
16	0.013	[0.006, 0.020]	[0.003, 0.035]	B	64	0.008	[0.004, 0.013]	[0.002, 0.023]	B
26	0.124	[0.061, 0.195]	[0.032, 0.330]	B	65	0.090	[0.044, 0.142]	[0.023, 0.243]	B
27	1.378	[0.718, 2.282]	[0.350, 3.616]	B	66	0.032	[0.016, 0.050]	[0.008, 0.087]	B
28	0.145	[0.072, 0.230]	[0.038, 0.392]	B	67	0.354	[0.177, 0.565]	[0.091, 0.943]	B
29	0.856	[0.436, 1.389]	[0.218, 2.258]	B	68	0.053	[0.026, 0.084]	[0.014, 0.145]	B
30	0.017	[0.008, 0.027]	[0.004, 0.047]	B	69	0.446	[0.223, 0.713]	[0.114, 1.188]	B
36	0.015	[0.007, 0.024]	[0.004, 0.041]	B	70	0.164	[0.081, 0.260]	[0.042, 0.440]	B
37	0.037	[0.018, 0.058]	[0.010, 0.101]	B	71	0.039	[0.019, 0.061]	[0.010, 0.104]	B
38	0.108	[0.053, 0.171]	[0.028, 0.291]	B	72	0.007	[0.003, 0.011]	[0.002, 0.019]	B
39	1.330	[0.696, 2.202]	[0.339, 3.476]	B	74	0.010	[0.005, 0.015]	[0.003, 0.027]	B
40	0.194	[0.096, 0.308]	[0.050, 0.521]	B	75	0.003	[0.002, 0.005]	[0.001, 0.009]	B
41	2.837	[0.890, 3.730]	[0.237, 5.741]	A	77	0.036	[0.017, 0.056]	[0.009, 0.097]	B
42	0.253	[0.125, 0.400]	[0.065, 0.676]	B	78	0.006	[0.003, 0.009]	[0.002, 0.016]	B
43	1.053	[0.544, 1.729]	[0.269, 2.778]	B	79	0.042	[0.021, 0.066]	[0.011, 0.114]	B
44	0.032	[0.016, 0.050]	[0.008, 0.087]	B	80	0.008	[0.004, 0.013]	[0.002, 0.022]	B
45	0.013	[0.006, 0.020]	[0.003, 0.034]	B	81	0.087	[0.043, 0.137]	[0.022, 0.235]	B
49	0.017	[0.008, 0.027]	[0.004, 0.047]	B	82	0.046	[0.022, 0.072]	[0.012, 0.124]	B
50	0.130	[0.064, 0.205]	[0.033, 0.349]	B	83	2.459	[0.467, 3.174]	[0.054, 5.286]	A
51	0.222	[0.111, 0.354]	[0.057, 0.597]	B	84	0.149	[0.073, 0.235]	[0.038, 0.399]	B
52	0.087	[0.042, 0.136]	[0.022, 0.233]	B	85	0.007	[0.003, 0.011]	[0.002, 0.018]	B
53	0.463	[0.232, 0.743]	[0.119, 1.240]	B	86	0.004	[0.002, 0.007]	[0.001, 0.012]	B
54	0.146	[0.072, 0.229]	[0.037, 0.387]	B	95	0.002	[0.001, 0.003]	[0.001, 0.006]	B
55	4.773	[2.908, 6.077]	[1.757, 8.049]	A	96	0.004	[0.002, 0.007]	[0.001, 0.012]	B
56	0.460	[0.232, 0.741]	[0.119, 1.232]	B	97	0.020	[0.010, 0.032]	[0.005, 0.055]	B
57	0.073	[0.036, 0.114]	[0.019, 0.197]	B	98	0.843	[0.429, 1.367]	[0.216, 2.233]	B
58	0.005	[0.002, 0.008]	[0.001, 0.013]	B	99	0.067	[0.033, 0.105]	[0.017, 0.181]	B
59	0.009	[0.005, 0.015]	[0.002, 0.026]	B	100	0.002	[0.001, 0.003]	[0.001, 0.006]	B

Table 41. Partial ionization cross sections (10^{-20} m^2) for 4,4-dimethyl-2-pentene. TICS/10^{-20} m^2 = 21.590. M = 98, base peak is m/z 83.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.307	[0.152, 0.487]	[0.079, 0.819]	B	57	0.203	[0.100, 0.320]	[0.052, 0.542]	B
2	0.108	[0.053, 0.170]	[0.028, 0.288]	B	58	0.009	[0.004, 0.013]	[0.002, 0.023]	B
12	0.014	[0.007, 0.022]	[0.004, 0.037]	B	60	0.004	[0.002, 0.006]	[0.001, 0.011]	B
13	0.027	[0.013, 0.042]	[0.007, 0.072]	B	61	0.008	[0.004, 0.013]	[0.002, 0.022]	B
14	0.102	[0.050, 0.160]	[0.026, 0.272]	B	62	0.016	[0.008, 0.025]	[0.004, 0.043]	B
15	1.151	[0.593, 1.878]	[0.293, 3.000]	B	63	0.039	[0.019, 0.061]	[0.010, 0.105]	B
16	0.059	[0.029, 0.092]	[0.015, 0.158]	B	64	0.008	[0.004, 0.012]	[0.002, 0.020]	B
25	0.009	[0.004, 0.014]	[0.002, 0.024]	B	65	0.067	[0.033, 0.104]	[0.017, 0.178]	B
26	0.164	[0.081, 0.261]	[0.042, 0.442]	B	66	0.033	[0.016, 0.051]	[0.008, 0.088]	B
27	1.907	[1.031, 3.229]	[0.491, 4.992]	B	67	0.216	[0.108, 0.345]	[0.056, 0.578]	B
28	0.263	[0.131, 0.418]	[0.068, 0.701]	B	68	0.038	[0.019, 0.059]	[0.010, 0.102]	B
29	1.268	[0.659, 2.083]	[0.324, 3.322]	B	69	0.226	[0.112, 0.359]	[0.058, 0.605]	B
30	0.023	[0.011, 0.037]	[0.006, 0.063]	B	70	0.079	[0.039, 0.124]	[0.020, 0.212]	B
31	0.008	[0.004, 0.012]	[0.002, 0.021]	B	71	0.006	[0.003, 0.010]	[0.002, 0.017]	B
32	0.007	[0.004, 0.012]	[0.002, 0.020]	B	73	0.003	[0.001, 0.005]	[0.001, 0.008]	B
33	0.007	[0.004, 0.011]	[0.002, 0.020]	B	74	0.006	[0.003, 0.009]	[0.002, 0.016]	B
37	0.080	[0.039, 0.126]	[0.020, 0.215]	B	75	0.003	[0.001, 0.004]	[0.001, 0.008]	B
38	0.170	[0.084, 0.267]	[0.044, 0.453]	B	76	0.003	[0.001, 0.004]	[0.001, 0.008]	B
39	1.901	[1.028, 3.212]	[0.489, 4.936]	B	77	0.022	[0.011, 0.034]	[0.006, 0.058]	B
40	0.300	[0.149, 0.478]	[0.077, 0.804]	B	78	0.005	[0.003, 0.008]	[0.001, 0.014]	B
41	3.417	[1.386, 4.453]	[0.535, 6.529]	A	79	0.020	[0.010, 0.032]	[0.005, 0.055]	B
42	0.228	[0.113, 0.363]	[0.058, 0.612]	B	80	0.002	[0.001, 0.004]	[0.001, 0.007]	B
43	0.977	[0.500, 1.594]	[0.248, 2.578]	B	81	0.031	[0.015, 0.048]	[0.008, 0.083]	B
44	0.035	[0.017, 0.054]	[0.009, 0.093]	B	82	0.032	[0.016, 0.050]	[0.008, 0.086]	B
45	0.006	[0.003, 0.009]	[0.001, 0.015]	B	83	2.210	[1.217, 3.783]	[0.564, 5.693]	B
46	0.006	[0.003, 0.009]	[0.001, 0.015]	B	84	0.138	[0.069, 0.220]	[0.035, 0.371]	B
47	0.005	[0.003, 0.008]	[0.001, 0.015]	B	85	0.004	[0.002, 0.006]	[0.001, 0.011]	B
49	0.010	[0.005, 0.016]	[0.003, 0.028]	B	91	0.002	[0.001, 0.003]	[0.001, 0.005]	B
50	0.092	[0.045, 0.144]	[0.024, 0.247]	B	93	0.002	[0.001, 0.003]	[0.001, 0.005]	B
51	0.170	[0.085, 0.270]	[0.044, 0.455]	B	95	0.002	[0.001, 0.003]	[0.001, 0.005]	B
52	0.064	[0.031, 0.100]	[0.016, 0.171]	B	96	0.002	[0.001, 0.003]	[0.001, 0.005]	B
53	0.326	[0.162, 0.520]	[0.084, 0.873]	B	97	0.002	[0.001, 0.003]	[0.001, 0.005]	B
54	0.075	[0.037, 0.118]	[0.019, 0.199]	B	98	0.547	[0.274, 0.877]	[0.139, 1.446]	B
55	3.915	[1.909, 5.083]	[0.900, 7.139]	A	99	0.040	[0.020, 0.063]	[0.010, 0.109]	B
56	0.361	[0.180, 0.574]	[0.092, 0.958]	B	100	0.002	[0.001, 0.003]	[0.001, 0.005]	B

Table 42. Partial ionization cross sections (10^{-20} m^2) for 3-ethyl-1-pentene. TICS/10^{-20} m^2 = 21.088. M = 98, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	56	0.776	[0.394, 1.256]	[0.199, 2.055]	B
12	0.012	[0.006, 0.019]	[0.003, 0.032]	B	57	0.095	[0.047, 0.150]	[0.025, 0.257]	B
13	0.035	[0.017, 0.054]	[0.009, 0.093]	B	58	0.004	[0.002, 0.006]	[0.001, 0.010]	B
14	0.099	[0.049, 0.156]	[0.025, 0.264]	B	60	0.004	[0.002, 0.006]	[0.001, 0.010]	B
15	0.466	[0.233, 0.745]	[0.119, 1.243]	B	61	0.011	[0.005, 0.016]	[0.003, 0.028]	B
16	0.010	[0.005, 0.016]	[0.003, 0.027]	B	62	0.021	[0.010, 0.032]	[0.005, 0.055]	B
24	0.008	[0.004, 0.012]	[0.002, 0.021]	B	63	0.030	[0.015, 0.047]	[0.008, 0.082]	B
25	0.023	[0.011, 0.036]	[0.006, 0.063]	B	64	0.003	[0.002, 0.005]	[0.001, 0.009]	B
26	0.404	[0.203, 0.649]	[0.103, 1.075]	B	65	0.048	[0.024, 0.075]	[0.012, 0.129]	B
27	2.695	[0.685, 3.467]	[0.136, 5.510]	A	66	0.022	[0.011, 0.034]	[0.006, 0.059]	B
28	0.413	[0.205, 0.655]	[0.105, 1.092]	B	67	0.193	[0.096, 0.308]	[0.050, 0.518]	B
29	1.125	[0.581, 1.842]	[0.290, 2.970]	B	68	0.072	[0.035, 0.113]	[0.018, 0.194]	B
30	0.027	[0.013, 0.042]	[0.007, 0.073]	B	69	2.284	[1.277, 3.921]	[0.591, 5.870]	B
31	0.013	[0.006, 0.021]	[0.003, 0.036]	B	70	0.610	[0.307, 0.978]	[0.155, 1.604]	B
32	0.006	[0.003, 0.010]	[0.002, 0.018]	B	71	0.031	[0.015, 0.048]	[0.008, 0.082]	B
36	0.006	[0.003, 0.009]	[0.002, 0.016]	B	72	0.003	[0.001, 0.004]	[0.001, 0.007]	B
37	0.058	[0.028, 0.091]	[0.015, 0.155]	B	74	0.003	[0.001, 0.004]	[0.001, 0.007]	B
38	0.164	[0.081, 0.259]	[0.042, 0.441]	B	75	0.002	[0.001, 0.004]	[0.001, 0.007]	B
39	1.762	[0.951, 2.982]	[0.451, 4.582]	B	77	0.007	[0.003, 0.011]	[0.002, 0.019]	B
40	0.266	[0.132, 0.421]	[0.068, 0.710]	B	78	0.002	[0.001, 0.004]	[0.001, 0.006]	B
41	5.306	[3.411, 6.652]	[2.168, 8.626]	A	79	0.007	[0.003, 0.010]	[0.002, 0.018]	B
42	0.635	[0.319, 1.019]	[0.162, 1.677]	B	80	0.002	[0.001, 0.003]	[0.001, 0.006]	B
43	0.296	[0.146, 0.467]	[0.076, 0.786]	B	81	0.008	[0.004, 0.013]	[0.002, 0.022]	B
44	0.015	[0.007, 0.023]	[0.004, 0.040]	B	82	0.002	[0.001, 0.003]	[0.001, 0.005]	B
49	0.009	[0.004, 0.014]	[0.002, 0.024]	B	83	0.159	[0.079, 0.253]	[0.041, 0.427]	B
50	0.088	[0.043, 0.139]	[0.023, 0.238]	B	84	0.009	[0.004, 0.014]	[0.002, 0.025]	B
51	0.151	[0.074, 0.239]	[0.039, 0.405]	B	91	0.002	[0.001, 0.003]	[0.000, 0.005]	B
52	0.063	[0.031, 0.100]	[0.016, 0.171]	B	97	0.002	[0.001, 0.003]	[0.000, 0.005]	B
53	0.386	[0.192, 0.616]	[0.099, 1.029]	B	98	0.287	[0.142, 0.454]	[0.073, 0.764]	B
54	0.179	[0.088, 0.281]	[0.046, 0.477]	B	99	0.021	[0.010, 0.033]	[0.005, 0.057]	B
55	1.247	[0.653, 2.071]	[0.318, 3.269]	B	100	0.002	[0.001, 0.003]	[0.000, 0.005]	B

Table 43. Partial ionization cross sections (10^{-20} m^2) for 3-ethyl-2-pentene. TICS/10^{-20} m^2 = 21.487. M = 98, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	60	0.003	[0.001, 0.004]	[0.001, 0.008]	B
12	0.010	[0.005, 0.015]	[0.002, 0.026]	B	61	0.014	[0.007, 0.022]	[0.004, 0.038]	B
13	0.028	[0.014, 0.043]	[0.007, 0.075]	B	62	0.030	[0.015, 0.047]	[0.008, 0.081]	B
14	0.106	[0.052, 0.168]	[0.027, 0.284]	B	63	0.051	[0.025, 0.080]	[0.013, 0.139]	B
15	0.865	[0.441, 1.403]	[0.220, 2.273]	B	64	0.008	[0.004, 0.012]	[0.002, 0.021]	B
16	0.033	[0.016, 0.051]	[0.008, 0.088]	B	65	0.072	[0.035, 0.112]	[0.018, 0.192]	B
24	0.006	[0.003, 0.010]	[0.002, 0.017]	B	66	0.033	[0.016, 0.051]	[0.008, 0.088]	B
25	0.018	[0.009, 0.029]	[0.005, 0.050]	B	67	0.248	[0.123, 0.393]	[0.064, 0.664]	B
26	0.294	[0.146, 0.468]	[0.075, 0.786]	B	68	0.108	[0.053, 0.171]	[0.028, 0.292]	B
27	2.239	[1.249, 3.858]	[0.576, 5.758]	B	69	2.181	[1.207, 3.729]	[0.563, 5.603]	B
28	0.337	[0.168, 0.536]	[0.086, 0.899]	B	70	0.392	[0.196, 0.626]	[0.100, 1.044]	B
29	1.029	[0.529, 1.681]	[0.262, 2.702]	B	71	0.018	[0.009, 0.028]	[0.005, 0.048]	B
30	0.022	[0.011, 0.034]	[0.006, 0.058]	B	73	0.002	[0.001, 0.003]	[0.001, 0.006]	B
31	0.011	[0.005, 0.016]	[0.003, 0.029]	B	74	0.004	[0.002, 0.006]	[0.001, 0.011]	B
32	0.005	[0.002, 0.008]	[0.001, 0.014]	B	75	0.002	[0.001, 0.003]	[0.001, 0.005]	B
36	0.005	[0.002, 0.007]	[0.001, 0.013]	B	76	0.002	[0.001, 0.003]	[0.000, 0.005]	B
37	0.051	[0.025, 0.080]	[0.013, 0.137]	B	77	0.021	[0.010, 0.032]	[0.005, 0.056]	B
38	0.154	[0.076, 0.242]	[0.039, 0.411]	B	78	0.005	[0.003, 0.008]	[0.001, 0.015]	B
39	1.694	[0.903, 2.841]	[0.435, 4.431]	B	79	0.021	[0.010, 0.033]	[0.005, 0.057]	B
40	0.291	[0.145, 0.466]	[0.075, 0.781]	B	80	0.003	[0.002, 0.005]	[0.001, 0.009]	B
41	4.247	[2.319, 5.487]	[1.222, 7.482]	A	81	0.028	[0.014, 0.044]	[0.007, 0.076]	B
42	0.433	[0.216, 0.691]	[0.110, 1.144]	B	82	0.006	[0.003, 0.010]	[0.002, 0.017]	B
43	0.383	[0.192, 0.611]	[0.098, 1.016]	B	83	0.261	[0.129, 0.415]	[0.066, 0.695]	B
44	0.012	[0.006, 0.019]	[0.003, 0.032]	B	84	0.018	[0.009, 0.028]	[0.005, 0.047]	B
45	0.004	[0.002, 0.006]	[0.001, 0.011]	B	85	0.001	[0.001, 0.002]	[0.000, 0.004]	B
46	0.004	[0.002, 0.006]	[0.001, 0.010]	B	86	0.001	[0.001, 0.002]	[0.000, 0.004]	B
49	0.011	[0.005, 0.017]	[0.003, 0.029]	B	89	0.001	[0.001, 0.002]	[0.000, 0.004]	B
50	0.116	[0.057, 0.183]	[0.030, 0.312]	B	91	0.001	[0.001, 0.002]	[0.000, 0.004]	B
51	0.215	[0.106, 0.341]	[0.055, 0.573]	B	93	0.001	[0.001, 0.002]	[0.000, 0.004]	B
52	0.091	[0.045, 0.144]	[0.023, 0.246]	B	95	0.001	[0.001, 0.002]	[0.000, 0.004]	B
53	0.465	[0.233, 0.744]	[0.119, 1.239]	B	96	0.001	[0.001, 0.002]	[0.000, 0.004]	B
54	0.137	[0.067, 0.216]	[0.035, 0.365]	B	97	0.003	[0.001, 0.004]	[0.001, 0.008]	B
55	2.745	[0.702, 3.529]	[0.144, 5.629]	A	98	0.534	[0.270, 0.863]	[0.137, 1.417]	B
56	0.827	[0.423, 1.348]	[0.211, 2.187]	B	99	0.042	[0.020, 0.065]	[0.011, 0.112]	B
57	0.082	[0.040, 0.129]	[0.021, 0.221]	B	100	0.001	[0.001, 0.002]	[0.000, 0.004]	B

Table 44. Partial ionization cross sections (10^{-20} m^2) for 2,3,3-trimethyl-1-butene. TICS/10^{-20} m^2 = 20.973. *M* = 98, base peak is *m*/*z* 83.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	61	0.004	[0.002, 0.007]	[0.001, 0.012]	B
14	0.042	[0.021, 0.066]	[0.011, 0.114]	B	62	0.013	[0.006, 0.021]	[0.003, 0.036]	B
15	0.338	[0.168, 0.539]	[0.086, 0.899]	B	63	0.021	[0.010, 0.034]	[0.006, 0.058]	B
16	0.013	[0.006, 0.020]	[0.003, 0.035]	B	64	0.004	[0.002, 0.006]	[0.001, 0.011]	B
26	0.067	[0.033, 0.106]	[0.017, 0.181]	B	65	0.057	[0.028, 0.090]	[0.015, 0.153]	B
27	0.906	[0.463, 1.471]	[0.231, 2.383]	B	66	0.024	[0.012, 0.038]	[0.006, 0.065]	B
28	0.064	[0.031, 0.099]	[0.016, 0.171]	B	67	0.219	[0.109, 0.349]	[0.056, 0.588]	B
29	1.378	[0.723, 2.290]	[0.353, 3.620]	B	68	0.034	[0.017, 0.054]	[0.009, 0.093]	B
30	0.026	[0.013, 0.041]	[0.007, 0.070]	B	69	0.220	[0.109, 0.348]	[0.056, 0.585]	B
31	0.017	[0.008, 0.026]	[0.004, 0.046]	B	70	0.036	[0.018, 0.057]	[0.009, 0.098]	B
36	0.015	[0.007, 0.024]	[0.004, 0.041]	B	71	0.014	[0.007, 0.022]	[0.004, 0.038]	B
37	0.030	[0.014, 0.046]	[0.008, 0.080]	B	72	0.003	[0.002, 0.005]	[0.001, 0.009]	B
38	0.108	[0.053, 0.171]	[0.028, 0.291]	B	73	0.003	[0.002, 0.005]	[0.001, 0.009]	B
39	1.404	[0.737, 2.329]	[0.358, 3.673]	B	74	0.007	[0.003, 0.010]	[0.002, 0.018]	B
40	0.228	[0.114, 0.364]	[0.059, 0.613]	B	75	0.019	[0.009, 0.030]	[0.005, 0.051]	B
41	3.889	[1.986, 5.026]	[0.972, 6.963]	A	77	0.018	[0.009, 0.028]	[0.005, 0.049]	B
42	0.252	[0.125, 0.401]	[0.064, 0.673]	B	78	0.006	[0.003, 0.009]	[0.002, 0.016]	B
43	0.919	[0.472, 1.500]	[0.235, 2.423]	B	79	0.025	[0.012, 0.040]	[0.006, 0.068]	B
44	0.038	[0.019, 0.060]	[0.010, 0.104]	B	80	0.005	[0.003, 0.008]	[0.001, 0.015]	B
45	0.019	[0.009, 0.029]	[0.005, 0.051]	B	81	0.047	[0.023, 0.074]	[0.012, 0.128]	B
49	0.006	[0.003, 0.009]	[0.001, 0.016]	B	82	0.020	[0.010, 0.032]	[0.005, 0.055]	B
50	0.056	[0.027, 0.088]	[0.014, 0.150]	B	83	2.451	[1.395, 4.263]	[0.633, 6.271]	B
51	0.099	[0.049, 0.156]	[0.026, 0.267]	B	84	0.186	[0.092, 0.294]	[0.047, 0.495]	B
52	0.043	[0.021, 0.068]	[0.011, 0.117]	B	85	0.025	[0.012, 0.039]	[0.006, 0.066]	B
53	0.265	[0.132, 0.422]	[0.068, 0.710]	B	86	0.002	[0.001, 0.003]	[0.001, 0.006]	B
54	0.067	[0.033, 0.106]	[0.017, 0.180]	B	91	0.002	[0.001, 0.003]	[0.001, 0.006]	B
55	4.380	[2.483, 5.579]	[1.391, 7.533]	A	95	0.002	[0.001, 0.003]	[0.001, 0.006]	B
56	0.799	[0.408, 1.300]	[0.204, 2.115]	B	96	0.007	[0.003, 0.010]	[0.002, 0.018]	B
57	0.885	[0.450, 1.430]	[0.225, 2.321]	B	97	0.007	[0.003, 0.010]	[0.002, 0.018]	B
58	0.062	[0.030, 0.097]	[0.016, 0.166]	B	98	0.410	[0.205, 0.657]	[0.105, 1.094]	B
59	0.206	[0.101, 0.326]	[0.052, 0.549]	B	99	0.044	[0.022, 0.070]	[0.011, 0.120]	B
60	0.009	[0.004, 0.014]	[0.002, 0.025]	B	100	0.002	[0.001, 0.003]	[0.001, 0.006]	B

Table 45. Partial ionization cross sections (10^{-20} m^2) for 2-ethyl-3-methyl-1-butene. TICS/10^{-20} m^2 = 21.226. M = 98, base peak is m/z 41.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	58	0.003	[0.001, 0.004]	[0.001, 0.007]	B
12	0.017	[0.008, 0.026]	[0.004, 0.046]	B	60	0.002	[0.001, 0.004]	[0.001, 0.007]	B
13	0.032	[0.016, 0.050]	[0.008, 0.086]	B	61	0.007	[0.004, 0.011]	[0.002, 0.020]	B
14	0.146	[0.072, 0.230]	[0.038, 0.395]	B	62	0.019	[0.009, 0.030]	[0.005, 0.051]	B
15	1.131	[0.585, 1.854]	[0.289, 2.968]	B	63	0.035	[0.017, 0.054]	[0.009, 0.094]	B
16	0.043	[0.021, 0.067]	[0.011, 0.114]	B	64	0.005	[0.002, 0.007]	[0.001, 0.012]	B
24	0.006	[0.003, 0.009]	[0.001, 0.015]	B	65	0.060	[0.029, 0.095]	[0.015, 0.162]	B
25	0.005	[0.003, 0.008]	[0.001, 0.015]	B	66	0.026	[0.013, 0.041]	[0.007, 0.071]	B
26	0.209	[0.104, 0.332]	[0.054, 0.560]	B	67	0.214	[0.107, 0.342]	[0.055, 0.573]	B
27	2.488	[1.399, 4.249]	[0.643, 6.283]	B	68	0.098	[0.048, 0.154]	[0.025, 0.261]	B
28	0.373	[0.186, 0.595]	[0.095, 0.997]	B	69	2.028	[1.105, 3.420]	[0.522, 5.200]	B
29	0.970	[0.499, 1.588]	[0.247, 2.553]	B	70	0.191	[0.094, 0.303]	[0.049, 0.513]	B
30	0.019	[0.009, 0.030]	[0.005, 0.051]	B	71	0.008	[0.004, 0.012]	[0.002, 0.021]	B
31	0.005	[0.002, 0.007]	[0.001, 0.013]	B	72	0.002	[0.001, 0.003]	[0.000, 0.005]	B
32	0.005	[0.002, 0.007]	[0.001, 0.012]	B	73	0.002	[0.001, 0.003]	[0.000, 0.005]	B
36	0.004	[0.002, 0.006]	[0.001, 0.011]	B	74	0.004	[0.002, 0.006]	[0.001, 0.010]	B
37	0.044	[0.022, 0.070]	[0.011, 0.120]	B	75	0.002	[0.001, 0.003]	[0.000, 0.005]	B
38	0.142	[0.070, 0.222]	[0.036, 0.375]	B	76	0.002	[0.001, 0.003]	[0.000, 0.005]	B
39	1.601	[0.852, 2.679]	[0.409, 4.161]	B	77	0.018	[0.009, 0.028]	[0.005, 0.049]	B
40	0.258	[0.127, 0.407]	[0.066, 0.686]	B	78	0.005	[0.002, 0.007]	[0.001, 0.013]	B
41	3.703	[1.760, 4.756]	[0.798, 6.688]	A	79	0.020	[0.010, 0.031]	[0.005, 0.054]	B
42	0.276	[0.137, 0.439]	[0.071, 0.734]	B	80	0.003	[0.001, 0.005]	[0.001, 0.008]	B
43	0.846	[0.431, 1.365]	[0.217, 2.226]	B	81	0.024	[0.012, 0.038]	[0.006, 0.066]	B
44	0.028	[0.014, 0.044]	[0.007, 0.075]	B	82	0.004	[0.002, 0.006]	[0.001, 0.011]	B
45	0.003	[0.002, 0.005]	[0.001, 0.009]	B	83	0.556	[0.279, 0.893]	[0.141, 1.474]	B
46	0.003	[0.002, 0.005]	[0.001, 0.009]	B	84	0.035	[0.017, 0.054]	[0.009, 0.093]	B
47	0.003	[0.002, 0.005]	[0.001, 0.009]	B	85	0.001	[0.001, 0.002]	[0.000, 0.003]	B
48	0.003	[0.002, 0.005]	[0.001, 0.009]	B	86	0.001	[0.001, 0.002]	[0.000, 0.003]	B
49	0.016	[0.008, 0.025]	[0.004, 0.043]	B	91	0.001	[0.001, 0.002]	[0.000, 0.003]	B
50	0.154	[0.076, 0.244]	[0.040, 0.414]	B	92	0.001	[0.001, 0.002]	[0.000, 0.003]	B
51	0.245	[0.122, 0.390]	[0.063, 0.654]	B	93	0.001	[0.001, 0.002]	[0.000, 0.003]	B
52	0.103	[0.050, 0.160]	[0.027, 0.274]	B	95	0.001	[0.001, 0.002]	[0.000, 0.003]	B
53	0.458	[0.229, 0.730]	[0.117, 1.214]	B	96	0.001	[0.001, 0.002]	[0.000, 0.003]	B
54	0.142	[0.069, 0.222]	[0.036, 0.377]	B	97	0.005	[0.002, 0.008]	[0.001, 0.013]	B
55	2.427	[1.365, 4.142]	[0.632, 6.144]	B	98	0.367	[0.183, 0.585]	[0.094, 0.976]	B
56	1.040	[0.536, 1.700]	[0.266, 2.728]	B	99	0.028	[0.014, 0.044]	[0.007, 0.075]	B
57	0.096	[0.047, 0.151]	[0.025, 0.255]	B	100	0.001	[0.001, 0.002]	[0.000, 0.003]	B

Table 46. Partial ionization cross sections (10^{-20} m^2) for benzaldehyde. TICS/10^{-20} m^2 = 17.773. *M* = 106, base peak is *m*/*z* 77.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.599]	H	53	0.143	[0.070, 0.225]	[0.036, 0.380]	B
17	0.022	[0.011, 0.035]	[0.006, 0.060]	B	60	0.037	[0.018, 0.058]	[0.009, 0.099]	B
18	0.046	[0.023, 0.072]	[0.012, 0.124]	B	61	0.089	[0.044, 0.141]	[0.023, 0.241]	B
25	0.049	[0.024, 0.077]	[0.013, 0.132]	B	62	0.120	[0.059, 0.189]	[0.031, 0.321]	B
26	0.217	[0.107, 0.344]	[0.056, 0.580]	B	63	0.139	[0.068, 0.220]	[0.036, 0.372]	B
27	0.400	[0.200, 0.640]	[0.102, 1.067]	B	73	0.110	[0.054, 0.174]	[0.028, 0.295]	B
28	0.071	[0.035, 0.112]	[0.018, 0.191]	B	74	0.350	[0.175, 0.561]	[0.089, 0.929]	B
29	0.450	[0.225, 0.719]	[0.116, 1.200]	B	75	0.154	[0.076, 0.244]	[0.039, 0.413]	B
36	0.046	[0.023, 0.073]	[0.012, 0.124]	B	76	0.026	[0.013, 0.041]	[0.007, 0.071]	B
37	0.364	[0.182, 0.582]	[0.092, 0.967]	B	77	3.342	[1.724, 4.303]	[0.884, 5.982]	A
38	0.444	[0.223, 0.711]	[0.113, 1.174]	B	78	0.536	[0.272, 0.867]	[0.137, 1.427]	B
39	0.525	[0.264, 0.843]	[0.134, 1.394]	B	79	0.034	[0.017, 0.054]	[0.009, 0.092]	B
40	0.035	[0.017, 0.055]	[0.009, 0.094]	B	85	0.013	[0.006, 0.020]	[0.003, 0.035]	B
43	0.036	[0.018, 0.057]	[0.009, 0.098]	B	86	0.016	[0.008, 0.025]	[0.004, 0.044]	B
49	0.273	[0.135, 0.434]	[0.069, 0.727]	B	105	1.873	[1.032, 3.190]	[0.480, 4.798]	B
50	1.709	[0.935, 2.912]	[0.437, 4.411]	B	106	1.969	[1.098, 3.380]	[0.508, 5.063]	B
51	2.802	[1.171, 3.651]	[0.467, 5.331]	A	107	0.160	[0.079, 0.252]	[0.041, 0.426]	B
52	0.772	[0.394, 1.252]	[0.198, 2.042]	B					

Table 47. Partial ionization cross sections (10^{-20} m^2) for phenol. TICS/10^{-20} m^2 = 16.457. *M* = 94 is base peak.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.287, 0.477]	[0.215, 0.599]	H	51	0.359	[0.181, 0.578]	[0.092, 0.951]	B
12	0.022	[0.011, 0.034]	[0.006, 0.059]	B	52	0.065	[0.032, 0.102]	[0.017, 0.175]	B
13	0.028	[0.014, 0.044]	[0.007, 0.076]	B	53	0.234	[0.116, 0.372]	[0.060, 0.627]	B
14	0.018	[0.009, 0.028]	[0.005, 0.049]	B	54	0.007	[0.003, 0.011]	[0.002, 0.019]	B
15	0.074	[0.036, 0.116]	[0.019, 0.199]	B	55	0.506	[0.254, 0.813]	[0.129, 1.343]	B
17	0.006	[0.003, 0.010]	[0.002, 0.017]	B	56	0.019	[0.009, 0.030]	[0.005, 0.052]	B
19	0.021	[0.010, 0.033]	[0.005, 0.056]	B	60	0.039	[0.019, 0.062]	[0.010, 0.106]	B
24	0.013	[0.006, 0.020]	[0.003, 0.035]	B	61	0.159	[0.079, 0.254]	[0.041, 0.428]	B
25	0.078	[0.038, 0.123]	[0.020, 0.209]	B	62	0.234	[0.117, 0.374]	[0.060, 0.625]	B
26	0.337	[0.168, 0.538]	[0.086, 0.901]	B	63	0.378	[0.188, 0.602]	[0.096, 1.004]	B
27	0.435	[0.219, 0.697]	[0.112, 1.157]	B	64	0.141	[0.070, 0.223]	[0.036, 0.378]	B
29	0.276	[0.137, 0.438]	[0.071, 0.735]	B	65	1.338	[0.720, 2.262]	[0.343, 3.496]	B
30	0.012	[0.006, 0.019]	[0.003, 0.032]	B	66	1.898	[1.077, 3.291]	[0.491, 4.859]	B
31	0.070	[0.034, 0.110]	[0.018, 0.187]	B	67	0.130	[0.064, 0.207]	[0.034, 0.351]	B
36	0.065	[0.032, 0.102]	[0.017, 0.175]	B	68	0.051	[0.025, 0.080]	[0.013, 0.136]	B
37	0.491	[0.248, 0.791]	[0.125, 1.298]	B	72	0.005	[0.002, 0.007]	[0.001, 0.012]	B
38	0.849	[0.438, 1.393]	[0.215, 2.229]	B	73	0.038	[0.019, 0.060]	[0.010, 0.102]	B
39	2.176	[0.632, 2.825]	[0.147, 4.388]	A	74	0.084	[0.041, 0.133]	[0.021, 0.225]	B
40	1.005	[0.526, 1.665]	[0.257, 2.643]	B	75	0.040	[0.019, 0.062]	[0.010, 0.108]	B
41	0.082	[0.040, 0.130]	[0.021, 0.222]	B	76	0.028	[0.014, 0.044]	[0.007, 0.076]	B
42	0.098	[0.048, 0.155]	[0.025, 0.262]	B	77	0.029	[0.014, 0.046]	[0.008, 0.079]	B
43	0.052	[0.025, 0.081]	[0.013, 0.140]	B	79	0.035	[0.017, 0.054]	[0.009, 0.094]	B
45	0.009	[0.004, 0.013]	[0.002, 0.023]	B	91	0.003	[0.001, 0.005]	[0.001, 0.008]	B
46	0.067	[0.033, 0.106]	[0.017, 0.179]	B	94	2.910	[1.421, 3.788]	[0.676, 5.320]	A
47	0.286	[0.143, 0.455]	[0.073, 0.758]	B	95	0.198	[0.098, 0.315]	[0.051, 0.530]	B
49	0.101	[0.049, 0.158]	[0.026, 0.271]	B	96	0.011	[0.005, 0.017]	[0.003, 0.030]	B
50	0.446	[0.224, 0.716]	[0.114, 1.181]	B					

Table 48. Partial ionization cross sections (10^{-20} m^2) for acetophenone. TICS/10^{-20} m^2 = 21.152. *M* = 120, base peak is *m*/*z* 105.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.215, 0.600]	H	65	0.162	[0.080, 0.257]	[0.041, 0.433]	B
26	0.139	[0.069, 0.221]	[0.036, 0.375]	B	66	0.013	[0.006, 0.021]	[0.003, 0.036]	B
27	0.504	[0.253, 0.806]	[0.128, 1.326]	B	72	0.006	[0.003, 0.009]	[0.002, 0.016]	B
28	0.107	[0.052, 0.167]	[0.027, 0.286]	B	73	0.070	[0.035, 0.111]	[0.018, 0.190]	B
29	0.052	[0.025, 0.081]	[0.013, 0.140]	B	74	0.313	[0.156, 0.498]	[0.080, 0.836]	B
36	0.011	[0.005, 0.018]	[0.003, 0.030]	B	75	0.165	[0.081, 0.261]	[0.042, 0.442]	B
37	0.219	[0.108, 0.346]	[0.056, 0.587]	B	76	0.257	[0.127, 0.408]	[0.066, 0.688]	B
38	0.496	[0.249, 0.796]	[0.127, 1.314]	B	77	4.775	[2.870, 6.093]	[1.704, 8.107]	A
39	0.784	[0.398, 1.270]	[0.199, 2.066]	B	78	0.453	[0.226, 0.725]	[0.116, 1.208]	B
40	0.042	[0.020, 0.066]	[0.011, 0.113]	B	79	0.016	[0.008, 0.025]	[0.004, 0.043]	B
41	0.072	[0.035, 0.112]	[0.018, 0.193]	B	85	0.009	[0.005, 0.015]	[0.002, 0.026]	B
42	0.200	[0.098, 0.314]	[0.051, 0.533]	B	86	0.014	[0.007, 0.022]	[0.004, 0.037]	B
43	1.772	[0.946, 2.982]	[0.449, 4.604]	B	87	0.009	[0.004, 0.014]	[0.002, 0.024]	B
44	0.048	[0.024, 0.076]	[0.012, 0.129]	B	89	0.043	[0.021, 0.067]	[0.011, 0.116]	B
45	0.019	[0.009, 0.030]	[0.005, 0.051]	B	90	0.008	[0.004, 0.013]	[0.002, 0.023]	B
48	0.009	[0.004, 0.014]	[0.002, 0.024]	B	91	0.074	[0.036, 0.117]	[0.019, 0.199]	B
49	0.150	[0.074, 0.238]	[0.038, 0.401]	B	92	0.004	[0.002, 0.006]	[0.001, 0.011]	B
50	1.471	[0.768, 2.432]	[0.374, 3.847]	B	98	0.003	[0.002, 0.005]	[0.001, 0.009]	B
51	3.244	[1.289, 4.288]	[0.465, 6.317]	A	102	0.003	[0.001, 0.005]	[0.001, 0.008]	B
52	0.344	[0.171, 0.548]	[0.088, 0.914]	B	103	0.006	[0.003, 0.009]	[0.002, 0.016]	B
53	0.123	[0.061, 0.197]	[0.032, 0.334]	B	105	2.845	[0.839, 3.732]	[0.207, 5.822]	A
60	0.015	[0.007, 0.023]	[0.004, 0.039]	B	106	0.207	[0.102, 0.328]	[0.053, 0.555]	B
61	0.093	[0.046, 0.148]	[0.024, 0.253]	B	107	0.011	[0.005, 0.018]	[0.003, 0.031]	B
62	0.163	[0.080, 0.258]	[0.042, 0.437]	B	120	0.868	[0.442, 1.408]	[0.221, 2.288]	B
63	0.223	[0.110, 0.354]	[0.057, 0.598]	B	121	0.071	[0.035, 0.112]	[0.018, 0.190]	B
64	0.041	[0.020, 0.065]	[0.011, 0.112]	B	122	0.003	[0.001, 0.004]	[0.001, 0.008]	B

Table 49. Partial ionization cross sections (10^{-20} m^2) for pyrrole. TICS/10^{-20} m^2 = 12.426. *M* = 67 is base peak.

m/*z*	PICS	67% interval	95% interval	unc. model	*m*/*z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.288, 0.478]	[0.216, 0.601]	H	38	0.790	[0.410, 1.296]	[0.202, 2.065]	B
2	0.023	[0.011, 0.035]	[0.006, 0.061]	B	39	2.077	[0.941, 2.717]	[0.412, 3.924]	A
12	0.122	[0.061, 0.194]	[0.032, 0.329]	B	40	1.598	[0.419, 2.082]	[0.096, 3.362]	A
13	0.127	[0.063, 0.202]	[0.033, 0.341]	B	41	1.814	[0.661, 2.391]	[0.227, 3.629]	A
14	0.142	[0.070, 0.224]	[0.036, 0.379]	B	42	0.044	[0.022, 0.070]	[0.011, 0.120]	B
15	0.032	[0.016, 0.050]	[0.008, 0.086]	B	48	0.004	[0.002, 0.006]	[0.001, 0.011]	B
16	0.003	[0.001, 0.004]	[0.001, 0.007]	B	49	0.014	[0.007, 0.021]	[0.003, 0.037]	B
24	0.036	[0.017, 0.056]	[0.009, 0.097]	B	50	0.023	[0.011, 0.036]	[0.006, 0.061]	B
25	0.113	[0.056, 0.181]	[0.029, 0.305]	B	51	0.024	[0.012, 0.038]	[0.006, 0.066]	B
26	0.258	[0.129, 0.413]	[0.066, 0.688]	B	52	0.051	[0.025, 0.080]	[0.013, 0.137]	B
27	0.199	[0.099, 0.315]	[0.051, 0.532]	B	53	0.002	[0.001, 0.003]	[0.000, 0.005]	B
28	2.172	[1.037, 2.826]	[0.493, 4.038]	A	62	0.010	[0.005, 0.015]	[0.002, 0.026]	B
29	0.032	[0.016, 0.051]	[0.008, 0.087]	B	63	0.016	[0.008, 0.024]	[0.004, 0.042]	B
30	0.005	[0.002, 0.008]	[0.001, 0.013]	B	64	0.016	[0.008, 0.026]	[0.004, 0.044]	B
31	0.001	[0.000, 0.001]	[0.000, 0.002]	B	65	0.013	[0.006, 0.020]	[0.003, 0.035]	B
32	0.023	[0.011, 0.037]	[0.006, 0.063]	B	66	0.110	[0.054, 0.174]	[0.028, 0.295]	B
33	0.009	[0.004, 0.014]	[0.002, 0.024]	B	67	1.397	[0.758, 2.357]	[0.355, 3.575]	B
34	0.012	[0.006, 0.019]	[0.003, 0.033]	B	68	0.066	[0.033, 0.105]	[0.017, 0.177]	B
36	0.096	[0.047, 0.152]	[0.025, 0.259]	B	69	0.001	[0.000, 0.001]	[0.000, 0.002]	B
37	0.553	[0.284, 0.902]	[0.141, 1.450]	B					

Table 50. Partial ionization cross sections (10^{-20} m^2) for pyridine. TICS/10^{-20} m^2 = 13.915. *M* = 79 is base peak.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.289, 0.479]	[0.215, 0.600]	H	52	3.877	[2.613, 4.772]	[1.761, 6.092]	A
25	0.056	[0.028, 0.089]	[0.015, 0.153]	B	53	0.410	[0.208, 0.664]	[0.104, 1.083]	B
26	0.643	[0.330, 1.050]	[0.164, 1.694]	B	54	0.013	[0.006, 0.021]	[0.003, 0.035]	B
27	0.185	[0.092, 0.294]	[0.047, 0.495]	B	62	0.005	[0.002, 0.008]	[0.001, 0.014]	B
28	0.052	[0.025, 0.082]	[0.013, 0.141]	B	63	0.005	[0.002, 0.008]	[0.001, 0.013]	B
36	0.011	[0.005, 0.017]	[0.003, 0.028]	B	64	0.014	[0.007, 0.022]	[0.004, 0.038]	B
37	0.142	[0.071, 0.227]	[0.036, 0.381]	B	74	0.007	[0.004, 0.012]	[0.002, 0.020]	B
38	0.179	[0.089, 0.284]	[0.046, 0.479]	B	75	0.059	[0.029, 0.093]	[0.015, 0.158]	B
39	0.583	[0.298, 0.948]	[0.148, 1.530]	B	76	0.044	[0.022, 0.070]	[0.011, 0.119]	B
40	0.047	[0.023, 0.074]	[0.012, 0.127]	B	77	0.011	[0.005, 0.017]	[0.003, 0.030]	B
48	0.023	[0.011, 0.036]	[0.006, 0.062]	B	78	0.419	[0.211, 0.674]	[0.106, 1.105]	B
49	0.195	[0.096, 0.309]	[0.050, 0.518]	B	79	3.714	[2.460, 4.601]	[1.618, 5.907]	A
50	0.995	[0.526, 1.659]	[0.252, 2.582]	B	80	0.234	[0.116, 0.371]	[0.060, 0.623]	B
51	1.587	[0.893, 2.734]	[0.406, 4.039]	B	81	0.004	[0.002, 0.006]	[0.001, 0.010]	B

Table 51. Partial ionization cross sections (10^{-20} m^2) for benzonitrile. TICS/10^{-20} m^2 = 16.783. *M* = 103 is base peak.

m/z	PICS	67% interval	95% interval	unc. model	*m/z*	PICS	67% interval	95% interval	unc. model
1	0.400	[0.289, 0.479]	[0.215, 0.599]	H	72	0.015	[0.007, 0.024]	[0.004, 0.041]	B
25	0.020	[0.010, 0.032]	[0.005, 0.055]	B	73	0.118	[0.059, 0.189]	[0.030, 0.319]	B
26	0.238	[0.119, 0.380]	[0.061, 0.635]	B	74	0.354	[0.177, 0.567]	[0.090, 0.938]	B
27	0.174	[0.087, 0.278]	[0.045, 0.468]	B	75	0.691	[0.352, 1.122]	[0.175, 1.812]	B
36	0.047	[0.023, 0.074]	[0.012, 0.127]	B	76	2.571	[1.030, 3.407]	[0.374, 5.004]	A
37	0.416	[0.210, 0.671]	[0.106, 1.103]	B	77	0.395	[0.197, 0.631]	[0.100, 1.044]	B
38	0.392	[0.198, 0.631]	[0.101, 1.043]	B	78	0.020	[0.009, 0.030]	[0.005, 0.053]	B
39	0.591	[0.299, 0.952]	[0.151, 1.566]	B	84	0.005	[0.003, 0.009]	[0.001, 0.015]	B
40	0.043	[0.021, 0.068]	[0.011, 0.117]	B	85	0.011	[0.005, 0.017]	[0.003, 0.029]	B
43	0.014	[0.007, 0.021]	[0.003, 0.037]	B	86	0.015	[0.007, 0.024]	[0.004, 0.042]	B
48	0.049	[0.024, 0.078]	[0.013, 0.134]	B	87	0.015	[0.007, 0.023]	[0.004, 0.040]	B
49	0.327	[0.163, 0.523]	[0.084, 0.875]	B	88	0.033	[0.016, 0.052]	[0.009, 0.090]	B
50	2.031	[0.424, 2.637]	[0.052, 4.321]	A	89	0.005	[0.002, 0.007]	[0.001, 0.012]	B
51	1.200	[0.634, 2.009]	[0.304, 3.130]	B	98	0.009	[0.004, 0.014]	[0.002, 0.024]	B
52	0.628	[0.320, 1.020]	[0.161, 1.670]	B	99	0.058	[0.028, 0.091]	[0.015, 0.156]	B
53	0.078	[0.038, 0.123]	[0.020, 0.211]	B	100	0.022	[0.011, 0.035]	[0.006, 0.060]	B
60	0.039	[0.019, 0.061]	[0.010, 0.105]	B	101	0.013	[0.006, 0.021]	[0.003, 0.036]	B
61	0.144	[0.070, 0.226]	[0.037, 0.385]	B	102	0.085	[0.042, 0.134]	[0.022, 0.229]	B
62	0.150	[0.074, 0.238]	[0.038, 0.401]	B	103	4.458	[2.941, 5.581]	[1.924, 7.191]	A
63	0.312	[0.157, 0.502]	[0.080, 0.833]	B	104	0.401	[0.200, 0.641]	[0.102, 1.066]	B
64	0.162	[0.080, 0.258]	[0.042, 0.435]	B	105	0.013	[0.007, 0.021]	[0.003, 0.036]	B
65	0.018	[0.009, 0.028]	[0.005, 0.048]	B					

4. Appendix

Table A1. Molecular orbital data for thiophenol. Double-ionization threshold = 22.50 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	2502.6	3297.09	2	Yes	
2	307.01	436.08	2	Yes	
3	306.03	435.81	2	Yes	
4	306.0	435.87	2	Yes	
5	305.99	436.15	2	Yes	
6	305.94	436.08	2	Yes	
7	305.82	436.04	2	Yes	
8	244.12	509.17	2	Yes	
9	181.05	477.93	2	Yes	
10	181.02	478.6	2	Yes	
11	180.97	479.58	2	Yes	
12	31.77	38.1	2	Yes	
13	28.81	32.04	2	Yes	
14	27.93	42.13	2	Yes	B from P3
15	25.78	27.65	2	Yes	B from P3
16	18.99	38.3	2	No	B from P2
17	22.08	37.18	2	No	
18	17.11	26.2	2	No	B from P3
19	15.75	33.87	2	No	B from P3
20	15.43	36.34	2	No	B from P3
21	14.6	32.08	2	No	B from P3
22	14.31	30.9	2	No	B from P3
23	13.02	30.1	2	No	B from P3
24	12.69	23.11	2	No	B from P3
25	12.22	37.18	2	No	B from expt
26	11.61	28.65	2	No	B from expt
27	10.61	21.39	2	No	B from expt
28	9.41	28.19	2	No	B from expt
29	8.49	26.99	2	No	B from expt

Table A2. Molecular orbital data for *o*-xylene. Double-ionization threshold = 23.14 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.78	435.83	2	Yes	
2	305.74	436.16	2	Yes	
3	305.53	435.71	2	Yes	
4	305.51	435.9	2	Yes	
5	305.49	436.1	2	Yes	
6	305.47	436.27	2	Yes	
7	305.43	436.01	2	Yes	
8	305.43	436.01	2	Yes	
9	31.39	38.85	2	Yes	B from P3
10	28.54	39.32	2	Yes	B from P3
11	28.07	39.92	2	Yes	
12	25.75	38.92	2	Yes	B from P3
13	20.96	38.0	2	No	B from P2
14	18.35	37.27	2	No	B from P2
15	19.23	39.16	2	No	B from P3
16	16.44	27.52	2	No	B from P3
17	15.61	33.88	2	No	B from P3
18	15.05	34.9	2	No	B from P3
19	14.6	23.53	2	No	B from P3
20	13.97	32.63	2	No	B from P3
21	13.62	34.84	2	No	B from P3
22	13.75	26.56	2	No	B from P3
23	13.4	29.58	2	No	B from P3
24	13.27	32.69	2	No	B from P3
25	11.74	38.11	2	No	B from P3
26	11.7	24.91	2	No	B from P3
27	11.68	39.96	2	No	B from P3
28	8.88	28.49	2	No	B from P3
29	8.56	29.4	2	No	B from expt

Table A3. Molecular orbital data for *m*-xylene. Double-ionization threshold = 23.11 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.83	435.99	2	Yes	
2	305.83	436.01	2	Yes	
3	305.61	435.94	2	Yes	
4	305.42	436.01	2	Yes	
5	305.42	436.01	2	Yes	
6	305.39	435.99	2	Yes	
7	305.39	436.04	2	Yes	
8	305.38	436.01	2	Yes	
9	31.37	38.96	2	Yes	
10	28.68	39.17	2	Yes	
11	27.92	40.35	2	Yes	
12	25.52	37.34	2	Yes	B from P3
13	25.16	39.23	2	Yes	
14	18.39	37.64	2	No	B from P2
15	18.59	39.19	2	No	B from P3
16	16.5	27.33	2	No	B from P3
17	15.53	34.53	2	No	B from P3
18	14.98	34.56	2	No	B from P3
19	14.28	24.31	2	No	B from P3
20	13.89	33.32	2	No	B from P3
21	14.16	25.43	2	No	B from P3
22	13.63	34.3	2	No	B from P3
23	13.68	28.77	2	No	B from P3
24	13.0	32.43	2	No	B from P3
25	11.73	39.84	2	No	B from P3
26	11.73	38.14	2	No	B from P3
27	11.6	25.61	2	No	B from P3
28	8.86	28.55	2	No	B from P3
29	8.56	29.44	2	No	B from expt

Table A4. Molecular orbital data for *p*-xylene. Double-ionization threshold = 23.11 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.74	435.97	2	Yes	
2	305.74	435.97	2	Yes	
3	305.51	435.8	2	Yes	
4	305.51	435.86	2	Yes	
5	305.48	436.16	2	Yes	
6	305.48	436.21	2	Yes	
7	305.4	436.02	2	Yes	
8	305.4	436.01	2	Yes	
9	31.33	38.97	2	Yes	B from P3
10	28.83	39.17	2	Yes	
11	27.44	41.92	2	Yes	
12	26.43	36.02	2	Yes	B from P3
13	24.15	39.48	2	Yes	B from P3
14	26.71	37.61	2	Yes	B from P3
15	18.62	37.42	2	No	B from P3
16	16.2	29.34	2	No	B from P3
17	15.55	34.25	2	No	B from P3
18	15.15	34.12	2	No	B from P3
19	14.04	32.48	2	No	B from P3
20	14.21	24.38	2	No	B from P3
21	14.17	25.2	2	No	B from P3
22	13.82	27.8	2	No	B from P3
23	13.36	36.63	2	No	B from P3
24	12.94	32.2	2	No	B from P3
25	11.75	40.59	2	No	B from P3
26	11.71	37.22	2	No	B from P3
27	11.58	25.68	2	No	B from P3
28	8.99	28.05	2	No	B from P3
29	8.44	29.94	2	No	B from expt

Table A5. Molecular orbital data for styrene. Double-ionization threshold = 22.65 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	306.03	435.95	2	Yes	
2	305.88	436.0	2	Yes	
3	305.79	435.72	2	Yes	
4	305.78	435.81	2	Yes	
5	305.76	436.02	2	Yes	
6	305.74	436.15	2	Yes	
7	305.73	436.3	2	Yes	
8	305.53	436.03	2	Yes	
9	31.63	39.26	2	Yes	B from P3
10	29.19	40.76	2	Yes	
11	27.65	42.02	2	Yes	B from P3
12	26.99	42.77	2	Yes	
13	23.25	38.53	2	Yes	B from P3
14	18.71	38.56	2	No	B from P2
15	18.36	35.56	2	No	B from P3
16	16.96	27.14	2	No	B from P3
17	15.84	32.73	2	No	B from P3
18	15.37	36.41	2	No	B from P3
19	14.8	32.45	2	No	B from P3
20	14.31	32.76	2	No	B from P3
21	14.09	37.31	2	No	B from P3
22	12.92	33.48	2	No	B from P3
23	12.48	23.56	2	No	B from P3
24	12.12	38.58	2	No	B from P3
25	11.96	36.84	2	No	B from P3
26	10.55	26.01	2	No	B from expt
27	9.27	28.1	2	No	B from expt
28	8.49	29.4	2	No	B from expt

Table A6. Molecular orbital data for 1-hexene. Double-ionization threshold = 25.22 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.6	435.98	2	Yes	
2	305.46	436.04	2	Yes	
3	305.34	435.96	2	Yes	
4	305.33	436.16	2	Yes	
5	305.24	436.02	2	Yes	
6	305.15	436.03	2	Yes	
7	29.69	35.88	2	Yes	B from P3
8	28.37	37.54	2	Yes	
9	26.3	37.58	2	Yes	
10	20.54	37.0	2	No	B from P2
11	21.59	32.57	2	No	B from P3
12	18.33	32.15	2	No	B from P3
13	16.12	24.25	2	No	B from P3
14	15.38	25.9	2	No	B from P3
15	14.71	30.17	2	No	B from P3
16	14.52	28.11	2	No	B from P3
17	13.84	29.7	2	No	B from P3
18	13.29	30.34	2	No	B from P3
19	12.65	29.56	2	No	B from P3
20	12.21	29.93	2	No	B from P3
21	11.8	33.07	2	No	B from P3
22	11.62	28.28	2	No	B from P3
23	11.36	35.64	2	No	B from P3
24	9.65	28.55	2	No	B from expt

Table A7. Molecular orbital data for 2-hexene. Double-ionization threshold = 25.23 eV from P3/cc-pVTZ (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.41	435.89	2	Yes	
2	305.37	435.99	2	Yes	
3	305.31	436.09	2	Yes	
4	305.31	436.12	2	Yes	
5	305.3	436.06	2	Yes	
6	305.13	436.03	2	Yes	
7	29.63	37.08	2	Yes	
8	28.27	36.51	2	Yes	B from P3
9	22.56	36.12	2	No	B from P2
10	24.33	38.14	2	No	B from P3
11	19.42	34.29	2	No	B from P3
12	18.04	30.3	2	No	B from P3
13	15.71	24.7	2	No	B from P3
14	15.22	28.9	2	No	B from P3
15	14.53	29.23	2	No	B from P3
16	14.16	26.5	2	No	B from P3
17	14.01	26.93	2	No	B from P3
18	13.31	31.47	2	No	B from P3
19	13.02	28.7	2	No	B from P3
20	12.37	31.8	2	No	B from P3
21	11.95	30.99	2	No	B from P3
22	11.66	28.82	2	No	B from P3
23	11.43	36.2	2	No	B from P3
24	9.16	29.63	2	No	B from expt

Table A8. Molecular orbital data for 3-hexene. Double-ionization threshold = 25.08 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.44	436.01	2	Yes	
2	305.44	436.03	2	Yes	
3	305.36	435.81	2	Yes	
4	305.32	436.26	2	Yes	
5	305.17	436.04	2	Yes	
6	305.17	436.04	2	Yes	
7	29.66	37.51	2	Yes	B from P3
8	28.22	35.22	2	Yes	
9	26.3	37.99	2	Yes	
10	25.76	35.89	2	Yes	B from P3
11	19.41	36.31	2	No	B from P2
12	18.05	29.59	2	No	B from P3
13	15.59	26.84	2	No	B from P3
14	15.43	26.21	2	No	B from P3
15	14.63	27.09	2	No	B from P3
16	14.37	26.84	2	No	B from P3
17	13.42	31.68	2	No	B from P3
18	13.22	29.56	2	No	B from P3
19	12.63	32.37	2	No	B from P3
20	12.68	29.14	2	No	B from P3
21	12.04	29.39	2	No	B from P3
22	11.96	29.69	2	No	B from P3
23	11.33	35.03	2	No	B from P3
24	9.14	29.95	2	No	B from expt

Table A9. Molecular orbital data for 2-methyl-1-pentene. Double-ionization threshold = 26.35 eV P3/cc-pVTZ (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.75	436.03	2	Yes	
2	305.41	436.01	2	Yes	
3	305.38	436.09	2	Yes	
4	305.32	436.01	2	Yes	
5	305.18	436.03	2	Yes	
6	305.0	436.0	2	Yes	
7	29.93	36.81	2	Yes	
8	28.11	36.55	2	Yes	
9	25.41	35.78	2	No	B from P3
10	25.02	37.38	2	No	B from P3
11	19.64	34.03	2	No	B from P3
12	17.44	33.95	2	No	B from P3
13	15.84	24.09	2	No	B from P3
14	15.38	27.1	2	No	B from P3
15	14.58	29.35	2	No	B from P3
16	14.47	25.56	2	No	B from P3
17	14.06	26.92	2	No	B from P3
18	13.21	30.09	2	No	B from P3
19	12.95	28.88	2	No	B from P3
20	12.59	33.68	2	No	B from P3
21	11.99	31.38	2	No	B from P3
22	11.68	29.48	2	No	B from P3
23	11.36	36.33	2	No	B from P3
24	9.31	28.95	2	No	B from CCSD(T)

Table A10. Molecular orbital data for 3-methyl-1-pentene. Double-ionization threshold = 25.68 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.63	436.04	2	Yes	
2	305.55	436.01	2	Yes	
3	305.35	436.06	2	Yes	
4	305.24	436.03	2	Yes	
5	305.16	436.03	2	Yes	
6	305.16	436.02	2	Yes	
7	29.97	35.84	2	Yes	B from P3
8	27.78	38.22	2	Yes	B from P3
9	26.41	36.77	2	Yes	
10	21.12	35.1	2	No	B from P3
11	19.24	35.82	2	No	B from P3
12	18.25	30.0	2	No	B from P3
13	15.75	26.77	2	No	B from P3
14	15.32	27.26	2	No	B from P3
15	14.92	28.04	2	No	B from P3
16	14.39	27.03	2	No	B from P3
17	13.51	29.69	2	No	B from P3
18	13.43	28.15	2	No	B from P3
19	13.01	29.93	2	No	B from P3
20	12.54	30.63	2	No	B from P3
21	11.61	31.31	2	No	B from P3
22	11.5	30.73	2	No	B from P3
23	11.27	35.87	2	No	B from P3
24	9.68	29.01	2	No	B from CCSD(T)

Table A11. Molecular orbital data for 4-methyl-1-pentene. Double-ionization threshold = 25.46 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.59	435.98	2	Yes	
2	305.58	436.08	2	Yes	
3	305.42	436.06	2	Yes	
4	305.26	436.03	2	Yes	
5	305.13	436.02	2	Yes	
6	305.13	436.02	2	Yes	
7	29.89	35.43	2	Yes	B from P3
8	28.2	38.86	2	Yes	B from P3
9	22.09	34.64	2	No	B from P2
10	21.54	37.47	2	No	B from P2
11	18.98	34.59	2	No	B from P3
12	18.15	31.57	2	No	B from P3
13	16.08	25.01	2	No	B from P3
14	15.12	27.34	2	No	B from P3
15	14.79	29.99	2	No	B from P3
16	14.65	26.49	2	No	B from P3
17	13.5	29.3	2	No	B from P3
18	13.31	28.37	2	No	B from P3
19	13.16	29.13	2	No	B from P3
20	12.45	30.06	2	No	B from P3
21	11.66	33.18	2	No	B from P3
22	11.5	31.05	2	No	B from P3
23	11.31	35.12	2	No	B from P3
24	9.69	28.56	2	No	B from CCSD(T)

Table A12. Molecular orbital data for 2-methyl-2-pentene. Double-ionization threshold = 24.54 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.6	436.02	2	Yes	
2	305.37	436.03	2	Yes	
3	305.27	436.01	2	Yes	
4	305.23	436.02	2	Yes	
5	305.15	436.04	2	Yes	
6	305.13	436.04	2	Yes	
7	29.85	37.63	2	Yes	B from P3
8	27.96	35.53	2	Yes	B from P3
9	25.54	34.98	2	Yes	B from P3
10	21.53	37.44	2	No	B from P2
11	20.8	36.22	2	No	B from P3
12	17.11	32.62	2	No	B from P3
13	15.69	26.69	2	No	B from P3
14	15.03	27.29	2	No	B from P3
15	14.66	24.63	2	No	B from P3
16	14.31	26.9	2	No	B from P3
17	13.67	28.45	2	No	B from P3
18	13.34	26.95	2	No	B from P3
19	12.86	30.62	2	No	B from P3
20	12.64	31.75	2	No	B from P3
21	12.46	32.2	2	No	B from P3
22	11.92	31.24	2	No	B from P3
23	11.23	35.32	2	No	B from P3
24	8.88	29.93	2	No	B from CCSD(T)

Table A13. Molecular orbital data for 3-methyl-2-pentene. Double-ionization threshold = 24.60 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.52	435.99	2	Yes	
2	305.37	436.06	2	Yes	
3	305.25	436.01	2	Yes	
4	305.24	435.95	2	Yes	
5	305.21	436.12	2	Yes	
6	305.14	436.03	2	Yes	
7	29.9	37.36	2	Yes	
8	27.61	35.82	2	Yes	B from P3
9	26.26	36.03	2	Yes	B from P3
10	24.51	35.9	2	No	B from P3
11	21.45	36.51	2	No	B from P3
12	17.03	33.1	2	No	B from P3
13	15.77	25.93	2	No	B from P3
14	15.19	25.84	2	No	B from P3
15	14.38	26.17	2	No	B from P3
16	13.82	30.28	2	No	B from P3
17	13.88	26.65	2	No	B from P3
18	13.63	27.39	2	No	B from P3
19	13.16	28.97	2	No	B from P3
20	12.56	31.78	2	No	B from P3
21	12.37	31.61	2	No	B from P3
22	11.86	30.99	2	No	B from P3
23	11.18	36.05	2	No	B from P3
24	8.88	29.98	2	No	B from CCSD(T)

Table A14. Molecular orbital data for 4-methyl-2-pentene. Double-ionization threshold = 25.05 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.59	436.07	2	Yes	
2	305.42	435.92	2	Yes	
3	305.31	436.03	2	Yes	
4	305.28	436.09	2	Yes	
5	305.11	436.02	2	Yes	
6	305.11	436.03	2	Yes	
7	29.81	36.78	2	Yes	B from P3
8	28.11	36.98	2	Yes	B from P3
9	22.21	34.78	2	No	B from P3
10	21.7	37.49	2	No	B from P2
11	18.86	37.07	2	No	B from P2
12	18.06	29.09	2	No	B from P3
13	15.65	26.92	2	No	B from P3
14	15.04	28.4	2	No	B from P3
15	14.2	25.79	2	No	B from P3
16	13.95	30.8	2	No	B from P3
17	13.83	27.05	2	No	B from P3
18	13.86	28.38	2	No	B from P3
19	13.36	26.83	2	No	B from P3
20	12.5	30.75	2	No	B from P3
21	11.92	32.64	2	No	B from P3
22	11.62	32.0	2	No	B from P3
23	11.3	34.56	2	No	B from P3
24	9.21	30.0	2	No	B from CCSD(T)

Table A15. Molecular orbital data for 2,3-dimethyl-1-butene. Double-ionization threshold = 25.59 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.71	436.01	2	Yes	
2	305.65	436.11	2	Yes	
3	305.31	436.01	2	Yes	
4	305.17	436.02	2	Yes	
5	305.17	436.03	2	Yes	
6	305.0	436.0	2	Yes	
7	30.12	36.46	2	Yes	B from P3
8	27.73	37.43	2	Yes	B from P3
9	25.33	36.46	2	No	
10	22.85	34.73	2	No	B from P3
11	19.69	35.48	2	No	B from P3
12	17.29	33.35	2	No	B from P3
13	15.77	26.64	2	No	B from P3
14	15.22	27.18	2	No	B from P3
15	14.52	25.14	2	No	B from P3
16	14.27	27.73	2	No	B from P3
17	13.86	27.1	2	No	B from P3
18	13.65	29.0	2	No	B from P3
19	13.17	27.86	2	No	B from P3
20	12.73	31.6	2	No	B from P3
21	11.94	32.92	2	No	B from P3
22	11.59	33.25	2	No	B from P3
23	11.23	34.76	2	No	B from P3
24	9.31	29.2	2	No	B from CCSD(T)

Table A16. Molecular orbital data for 3,3-dimethyl-1-butene. Double-ionization threshold = 25.96 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.9	436.11	2	Yes	
2	305.54	435.99	2	Yes	
3	305.21	436.02	2	Yes	
4	305.17	436.02	2	Yes	
5	305.17	436.03	2	Yes	
6	305.11	436.01	2	Yes	
7	30.71	35.62	2	Yes	B from P3
8	27.3	39.93	2	Yes	B from P3
9	25.36	34.39	2	No	
10	22.27	34.58	2	No	B from P3
11	22.26	35.56	2	No	
12	17.39	33.46	2	No	B from P3
13	15.79	25.63	2	No	B from P3
14	15.36	29.41	2	No	B from P3
15	14.9	25.8	2	No	B from P3
16	14.43	26.86	2	No	B from P3
17	13.56	26.61	2	No	B from P3
18	13.23	29.38	2	No	B from P3
19	13.17	29.21	2	No	B from P3
20	12.83	28.37	2	No	B from P3
21	11.71	33.04	2	No	B from P3
22	11.44	35.48	2	No	B from P3
23	11.3	34.22	2	No	B from P3
24	9.69	28.64	2	No	B from CCSD(T)

Table A17. Molecular orbital data for 2,3-dimethyl-2-butene. Double-ionization threshold = 24.00 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.5	435.83	2	Yes	
2	305.46	436.26	2	Yes	
3	305.17	436.0	2	Yes	
4	305.17	436.01	2	Yes	
5	305.17	436.03	2	Yes	
6	305.17	436.03	2	Yes	
7	30.0	37.55	2	Yes	
8	27.17	35.61	2	Yes	B from P3
9	25.72	33.83	2	Yes	
10	24.88	36.35	2	Yes	
11	23.23	38.21	2	No	
12	16.35	35.9	2	No	B from P3
13	15.77	26.2	2	No	B from P3
14	14.87	23.11	2	No	B from P3
15	14.69	27.75	2	No	B from P3
16	14.24	24.44	2	No	B from P3
17	13.35	28.45	2	No	B from P3
18	13.24	26.83	2	No	B from P3
19	13.12	27.29	2	No	B from P3
20	12.84	30.96	2	No	B from P3
21	12.65	30.5	2	No	B from P3
22	12.71	35.74	2	No	B from expt
23	10.96	37.74	2	No	B from expt
24	8.44	29.93	2	No	B from expt

Table A18. Molecular orbital data for 2-ethyl-1-butene. Double-ionization threshold = 25.74 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.68	436.02	2	Yes	
2	305.46	436.03	2	Yes	
3	305.46	436.06	2	Yes	
4	305.22	436.03	2	Yes	
5	305.22	436.03	2	Yes	
6	305.01	436.0	2	Yes	
7	30.03	36.84	2	Yes	B from P3
8	27.61	35.47	2	Yes	
9	26.6	38.0	2	Yes	
10	20.48	36.59	2	No	B from P3
11	20.55	33.76	2	No	B from P3
12	17.3	33.7	2	No	B from P3
13	15.77	25.67	2	No	B from P3
14	15.62	25.01	2	No	B from P3
15	14.42	28.69	2	No	B from P3
16	14.22	27.41	2	No	B from P3
17	14.26	26.87	2	No	B from P3
18	12.98	29.95	2	No	B from P3
19	12.97	29.3	2	No	B from P3
20	12.47	34.22	2	No	B from P3
21	12.24	29.07	2	No	B from P3
22	11.77	31.86	2	No	B from P3
23	11.24	34.59	2	No	B from P3
24	9.3	29.27	2	No	B from CCSD(T)

Table A19. Molecular orbital data for 1-heptene. Double-ionization threshold = 24.47 eV from P3 (to triplet or singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.6	435.98	2	Yes	
2	305.45	436.04	2	Yes	
3	305.33	436.04	2	Yes	
4	305.3	436.0	2	Yes	
5	305.27	436.13	2	Yes	
6	305.23	436.02	2	Yes	
7	305.13	436.03	2	Yes	
8	29.74	35.48	2	Yes	B from P3
9	28.74	36.97	2	Yes	
10	27.11	37.52	2	Yes	B from P3
11	24.38	37.37	2	No	B from P3
12	19.98	36.69	2	No	B from P3
13	19.19	31.09	2	No	B from P3
14	18.3	32.24	2	No	B from P3
15	16.18	23.53	2	No	B from P3
16	15.54	25.7	2	No	B from P3
17	14.88	29.17	2	No	B from P3
18	14.57	27.05	2	No	B from P3
19	14.1	29.36	2	No	B from P3
20	13.76	31.42	2	No	B from P3
21	13.06	29.64	2	No	B from P3
22	12.67	30.38	2	No	B from P3
23	12.25	31.57	2	No	B from P3
24	11.9	29.31	2	No	B from P3
25	11.56	31.61	2	No	B from P3
26	11.52	27.94	2	No	B from P3
27	11.13	38.04	2	No	B from P3
28	9.68	28.63	2	No	B from expt

Table A20. Molecular orbital data for 2-heptene. Double-ionization threshold = 24.37 eV from CCSD(T)/cc-pVTZ (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.41	435.88	2	Yes	
2	305.36	436.0	2	Yes	
3	305.31	436.13	2	Yes	
4	305.3	436.06	2	Yes	
5	305.28	436.0	2	Yes	
6	305.25	436.12	2	Yes	
7	305.11	436.03	2	Yes	
8	29.7	36.49	2	Yes	B from P3
9	28.67	36.7	2	Yes	
10	26.99	35.83	2	Yes	
11	21.64	37.4	2	No	B from P2
12	20.04	37.85	2	No	B from P2
13	19.18	32.18	2	No	B from P3
14	18.0	30.55	2	No	B from P3
15	15.9	23.57	2	No	B from P3
16	15.04	29.72	2	No	B from P3
17	14.8	28.8	2	No	B from P3
18	14.53	26.79	2	No	B from P3
19	14.1	25.38	2	No	B from P3
20	13.68	28.44	2	No	B from P3
21	13.26	32.65	2	No	B from P3
22	12.84	30.21	2	No	B from P3
23	12.39	30.12	2	No	B from P3
24	12.02	30.37	2	No	B from P3
25	11.69	32.94	2	No	B from P3
26	11.52	28.24	2	No	B from P3
27	11.18	36.8	2	No	B from P3
28	9.11	29.75	2	No	B from expt

Table A21. Molecular orbital data for 3-heptene. Double-ionization threshold = 24.98 eV from P3 (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.43	436.02	2	Yes	
2	305.37	435.91	2	Yes	
3	305.36	435.89	2	Yes	
4	305.32	436.1	2	Yes	
5	305.31	436.26	2	Yes	
6	305.16	436.04	2	Yes	
7	305.13	436.03	2	Yes	
8	29.73	37.05	2	No	
9	28.62	35.29	2	No	B from P3
10	27.04	37.13	2	No	
11	24.95	37.23	2	No	B from P3
12	20.25	36.43	2	No	B from P3
13	19.3	34.27	2	No	B from P3
14	18.02	29.72	2	No	B from P3
15	15.77	24.85	2	No	B from P3
16	15.41	27.09	2	No	B from P3
17	14.84	27.31	2	No	B from P3
18	14.56	27.53	2	No	B from P3
19	13.89	28.44	2	No	B from P3
20	13.54	27.87	2	No	B from P3
21	13.04	32.87	2	No	B from P3
22	12.65	30.21	2	No	B from P3
23	12.49	31.32	2	No	B from P3
24	11.97	30.09	2	No	B from P3
25	11.93	30.63	2	No	B from P3
26	11.66	28.65	2	No	B from P3
27	11.2	36.62	2	No	B from P3
28	9.05	30.15	2	No	B from expt

Table A22. Molecular orbital data for 2-methyl-1-hexene. Double-ionization threshold = 24.64 eV from P3 (to singlet or triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.74	436.03	2	Yes	
2	305.41	436.03	2	Yes	
3	305.33	435.98	2	Yes	
4	305.32	436.01	2	Yes	
5	305.31	436.14	2	Yes	
6	305.15	436.03	2	Yes	
7	305.0	436.0	2	Yes	
8	29.98	36.45	2	Yes	
9	28.67	36.29	2	Yes	
10	26.42	36.37	2	Yes	
11	25.31	36.73	2	Yes	
12	23.59	36.67	2	No	
13	19.29	32.36	2	No	B from P3
14	17.38	34.49	2	No	B from P3
15	16.01	23.21	2	No	B from P3
16	15.25	27.22	2	No	B from P3
17	14.94	27.85	2	No	B from P3
18	14.73	26.08	2	No	B from P3
19	14.05	26.31	2	No	B from P3
20	13.68	29.21	2	No	B from P3
21	13.33	31.0	2	No	B from P3
22	12.86	30.64	2	No	B from P3
23	12.39	30.75	2	No	B from P3
24	12.09	31.77	2	No	B from P3
25	11.75	32.91	2	No	B from P3
26	11.54	28.56	2	No	B from P3
27	11.14	36.87	2	No	B from P3
28	9.28	29.05	2	No	B from CCSD(T)

Table A23. Molecular orbital data for 3-methyl-1-hexene. Double-ionization threshold = 25.10 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.63	436.05	2	Yes	
2	305.55	436.01	2	Yes	
3	305.31	436.0	2	Yes	
4	305.28	436.11	2	Yes	
5	305.23	436.03	2	Yes	
6	305.16	436.02	2	Yes	
7	305.14	436.03	2	Yes	
8	30.03	35.55	2	Yes	B from P3
9	28.38	36.73	2	Yes	
10	26.91	38.33	2	Yes	B from P3
11	21.76	35.54	2	No	B from P2
12	19.95	35.86	2	No	B from P2
13	19.01	34.01	2	No	B from P3
14	18.22	30.34	2	No	B from P3
15	15.88	25.75	2	No	B from P3
16	15.31	26.05	2	No	B from P3
17	15.07	28.97	2	No	B from P3
18	14.58	27.85	2	No	B from P3
19	14.09	27.26	2	No	B from P3
20	13.51	29.22	2	No	B from P3
21	13.31	28.42	2	No	B from P3
22	12.84	31.82	2	No	B from P3
23	12.38	30.59	2	No	B from P3
24	11.96	30.51	2	No	B from P3
25	11.48	31.53	2	No	B from P3
26	11.42	30.81	2	No	B from P3
27	11.05	36.31	2	No	B from P3
28	9.64	29.16	2	No	B from CCSD(T)

Table A24. Molecular orbital data for 4-methyl-1-hexene. Double-ionization threshold = 24.87 eV from P3 (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.61	435.98	2	Yes	
2	305.53	436.08	2	Yes	
3	305.41	436.06	2	Yes	
4	305.29	436.05	2	Yes	
5	305.25	436.03	2	Yes	
6	305.13	436.03	2	Yes	
7	304.98	436.02	2	Yes	
8	30.0	35.04	2	Yes	
9	28.46	38.26	2	Yes	
10	26.71	36.75	2	Yes	B from P3
11	25.89	36.05	2	Yes	B from P3
12	20.6	35.79	2	No	B from P3
13	18.56	34.09	2	No	B from P3
14	18.3	30.74	2	No	B from P3
15	15.77	26.42	2	No	B from P3
16	15.4	26.08	2	No	B from P3
17	15.16	25.2	2	No	B from P3
18	14.67	29.57	2	No	B from P3
19	13.95	29.37	2	No	B from P3
20	13.54	29.51	2	No	B from P3
21	13.29	28.23	2	No	B from P3
22	12.74	30.07	2	No	B from P3
23	12.34	29.92	2	No	B from P3
24	12.09	30.38	2	No	B from P3
25	11.41	33.92	2	No	B from P3
26	11.35	30.48	2	No	B from P3
27	11.03	36.12	2	No	B from P3
28	9.66	28.62	2	No	B from CCSD(T)

Table A25. Molecular orbital data for 5-methyl-1-hexene. Double-ionization threshold = 24.71 eV from P3 (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.59	435.98	2	Yes	
2	305.53	436.08	2	Yes	
3	305.42	436.03	2	Yes	
4	305.31	436.08	2	Yes	
5	305.22	436.02	2	Yes	
6	305.11	436.02	2	Yes	
7	305.1	436.02	2	Yes	
8	29.9	34.91	2	Yes	B from P3
9	28.73	37.98	2	Yes	
10	26.39	38.2	2	Yes	
11	22.58	34.61	2	No	B from OVGF
12	23.67	35.69	2	No	B from P3
13	18.44	34.04	2	No	B from P3
14	18.17	31.99	2	No	B from P3
15	15.93	24.91	2	No	B from P3
16	15.55	26.68	2	No	B from P3
17	14.83	27.16	2	No	B from P3
18	14.79	26.47	2	No	B from P3
19	14.08	30.78	2	No	B from P3
20	13.66	28.37	2	No	B from P3
21	13.17	28.32	2	No	B from P3
22	12.93	30.0	2	No	B from P3
23	12.34	30.59	2	No	B from P3
24	12.09	30.64	2	No	B from P3
25	11.36	33.1	2	No	B from P3
26	11.28	32.17	2	No	B from P3
27	11.11	35.35	2	No	B from P3
28	9.66	28.64	2	No	B from CCSD(T)

Table A26. Molecular orbital data for 2-methyl-2-hexene. Double-ionization threshold = 24.10 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.6	436.02	2	Yes	
2	305.31	435.98	2	Yes	
3	305.28	436.1	2	Yes	
4	305.27	436.01	2	Yes	
5	305.23	436.02	2	Yes	
6	305.14	436.04	2	Yes	
7	305.11	436.03	2	Yes	
8	29.9	37.29	2	Yes	B from P3
9	28.56	35.5	2	Yes	B from P3
10	26.23	36.46	2	Yes	B from P3
11	25.48	34.92	2	Yes	
12	23.84	38.18	2	No	B from P3
13	19.34	33.89	2	No	B from P3
14	17.08	32.92	2	No	B from P3
15	15.83	25.32	2	No	B from P3
16	14.96	28.76	2	No	B from P3
17	14.87	26.29	2	No	B from P3
18	14.66	23.93	2	No	B from P3
19	13.99	27.6	2	No	B from P3
20	13.25	29.67	2	No	B from P3
21	13.32	27.07	2	No	B from P3
22	13.09	30.57	2	No	B from P3
23	12.71	30.51	2	No	B from P3
24	12.14	34.15	2	No	B from P3
25	11.87	31.22	2	No	B from P3
26	11.56	30.28	2	No	B from P3
27	11.14	36.2	2	No	B from P3
28	8.83	30.12	2	No	B from CCSD(T)

Table A27. Molecular orbital data for 3-methyl-2-hexene. Double-ionization threshold = 24.16 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.52	436.0	2	Yes	
2	305.3	435.98	2	Yes	
3	305.28	436.13	2	Yes	
4	305.24	436.0	2	Yes	
5	305.24	435.96	2	Yes	
6	305.21	436.12	2	Yes	
7	305.12	436.03	2	Yes	
8	29.97	36.94	2	Yes	B from P3
9	28.27	35.95	2	Yes	
10	26.18	35.99	2	Yes	B from P3
11	21.81	35.38	2	No	B from P2
12	23.81	37.7	2	No	B from P3
13	19.36	34.15	2	No	B from P3
14	17.01	33.23	2	No	B from P3
15	15.8	25.36	2	No	B from P3
16	15.45	25.58	2	No	B from P3
17	14.39	28.44	2	No	B from P3
18	14.39	25.63	2	No	B from P3
19	13.9	27.69	2	No	B from P3
20	13.75	27.08	2	No	B from P3
21	13.25	29.54	2	No	B from P3
22	13.02	30.87	2	No	B from P3
23	12.78	29.44	2	No	B from P3
24	12.18	33.34	2	No	B from P3
25	11.86	31.42	2	No	B from P3
26	11.55	29.48	2	No	B from P3
27	11.06	37.46	2	No	B from P3
28	8.82	30.16	2	No	B from CCSD(T)

Table A28. Molecular orbital data for 4-methyl-2-hexene. Double-ionization threshold = 24.79 eV from P3 (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.54	436.07	2	Yes	
2	305.41	435.92	2	Yes	
3	305.3	436.03	2	Yes	
4	305.27	436.09	2	Yes	
5	305.27	436.06	2	Yes	
6	305.11	436.03	2	Yes	
7	305.08	436.03	2	Yes	
8	29.96	36.2	2	Yes	
9	28.37	37.15	2	Yes	
10	26.7	35.68	2	Yes	B from P3
11	25.16	36.81	2	Yes	
12	23.51	35.95	2	No	B from P3
13	18.78	35.96	2	No	B from P3
14	18.04	29.08	2	No	B from P3
15	15.57	27.02	2	No	B from P3
16	15.41	26.01	2	No	B from P3
17	14.58	27.64	2	No	B from P3
18	14.11	29.54	2	No	B from P3
19	14.04	26.26	2	No	B from P3
20	13.76	27.69	2	No	B from P3
21	13.33	28.75	2	No	B from P3
22	13.1	30.46	2	No	B from P3
23	12.55	29.57	2	No	B from P3
24	12.32	31.45	2	No	B from P3
25	11.48	31.3	2	No	B from P3
26	11.37	30.87	2	No	B from P3
27	11.08	37.15	2	No	B from P3
28	9.15	30.2	2	No	B from CCSD(T)

Table A29. Molecular orbital data for 5-methyl-2-hexene. Double-ionization threshold = 24.79 eV from P3 (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.5	436.08	2	Yes	
2	305.42	435.89	2	Yes	
3	305.34	435.97	2	Yes	
4	305.32	436.16	2	Yes	
5	305.31	436.07	2	Yes	
6	305.07	436.02	2	Yes	
7	304.96	436.02	2	Yes	
8	29.88	35.89	2	Yes	
9	28.66	37.57	2	Yes	
10	26.09	36.21	2	Yes	B from P3
11	25.15	34.66	2	Yes	
12	23.36	38.23	2	No	B from P3
13	20.86	34.5	2	No	B from P3
14	18.03	29.88	2	No	B from P3
15	15.61	26.32	2	No	B from P3
16	15.05	28.47	2	No	B from P3
17	14.8	27.06	2	No	B from P3
18	14.55	27.44	2	No	B from P3
19	14.09	25.44	2	No	B from P3
20	13.68	30.54	2	No	B from P3
21	13.3	27.1	2	No	B from P3
22	12.94	29.05	2	No	B from P3
23	12.56	30.66	2	No	B from P3
24	12.04	31.23	2	No	B from P3
25	11.6	33.84	2	No	B from P3
26	11.35	30.4	2	No	B from P3
27	11.2	36.53	2	No	B from P3
28	9.17	29.75	2	No	B from CCSD(T)

Table A30. Molecular orbital data for 2-methyl-3-hexene. Double-ionization threshold = 24.66 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.59	436.07	2	Yes	
2	305.44	436.02	2	Yes	
3	305.35	435.86	2	Yes	
4	305.29	436.19	2	Yes	
5	305.17	436.04	2	Yes	
6	305.11	436.03	2	Yes	
7	305.11	436.03	2	Yes	
8	29.92	36.78	2	Yes	B from P3
9	28.62	35.56	2	Yes	B from P3
10	26.48	38.36	2	Yes	B from P3
11	25.18	34.78	2	Yes	
12	23.16	36.14	2	No	B from P3
13	21.41	36.59	2	No	
14	18.05	28.72	2	No	B from P3
15	15.78	26.51	2	No	B from P3
16	15.19	27.66	2	No	B from P3
17	14.7	26.12	2	No	B from P3
18	14.47	26.92	2	No	B from P3
19	13.95	27.71	2	No	B from P3
20	13.35	27.03	2	No	B from P3
21	13.15	30.2	2	No	B from P3
22	13.09	32.08	2	No	B from P3
23	12.61	30.0	2	No	B from P3
24	11.96	30.49	2	No	B from P3
25	11.9	31.8	2	No	B from P3
26	11.59	30.81	2	No	B from P3
27	11.09	35.95	2	No	B from P3
28	9.14	30.52	2	No	B from CCSD(T)

Table A31. Molecular orbital data for 3-methyl-3-hexene. Double-ionization threshold = 24.17 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.54	436.0	2	Yes	
2	305.37	436.03	2	Yes	
3	305.37	436.06	2	Yes	
4	305.25	436.01	2	Yes	
5	305.15	436.04	2	Yes	
6	305.14	436.03	2	Yes	
7	305.13	436.04	2	Yes	
8	29.98	37.18	2	Yes	
9	28.23	35.16	2	Yes	B from P3
10	26.74	36.44	2	Yes	B from P3
11	25.14	36.68	2	Yes	B from P3
12	23.26	35.04	2	No	B from P3
13	19.55	36.26	2	No	B from P3
14	17.07	32.2	2	No	B from P3
15	15.85	25.74	2	No	B from P3
16	15.29	25.56	2	No	B from P3
17	14.6	26.25	2	No	B from P3
18	14.28	27.71	2	No	B from P3
19	14.21	26.28	2	No	B from P3
20	13.47	27.68	2	No	B from P3
21	13.12	31.11	2	No	B from P3
22	12.75	31.47	2	No	B from P3
23	12.51	32.02	2	No	B from P3
24	12.49	30.21	2	No	B from P3
25	11.94	29.52	2	No	B from P3
26	11.74	31.63	2	No	B from P3
27	10.98	36.18	2	No	B from P3
28	8.81	30.49	2	No	B from CCSD(T)

Table A32. Molecular orbital data for 2,3-dimethyl-1-pentene. Double-ionization threshold = 24.89 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.7	436.02	2	Yes	
2	305.59	436.09	2	Yes	
3	305.32	436.06	2	Yes	
4	305.3	436.01	2	Yes	
5	305.16	436.03	2	Yes	
6	305.14	436.02	2	Yes	
7	304.98	436.0	2	Yes	
8	30.22	36.01	2	Yes	
9	28.17	37.05	2	Yes	
10	26.44	35.97	2	Yes	B from P3
11	25.31	36.44	2	Yes	
12	20.7	34.94	2	No	B from P2
13	19.13	34.91	2	No	B from P3
14	17.3	32.92	2	No	B from P3
15	15.66	26.81	2	No	B from P3
16	15.5	25.51	2	No	B from P3
17	14.66	27.63	2	No	B from P3
18	14.51	26.36	2	No	B from P3
19	14.2	26.24	2	No	B from P3
20	13.58	28.73	2	No	B from P3
21	13.31	27.85	2	No	B from P3
22	13.01	30.63	2	No	B from P3
23	12.68	30.99	2	No	B from P3
24	12.47	31.5	2	No	B from P3
25	11.49	32.08	2	No	B from P3
26	11.34	31.96	2	No	B from P3
27	11.04	36.83	2	No	B from P3
28	9.25	29.37	2	No	B from CCSD(T)

Table A33. Molecular orbital data for 2,4-dimethyl-1-pentene. Double-ionization threshold = 23.04 eV from P3 (to singlet or triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.76	436.03	2	Yes	
2	305.56	436.08	2	Yes	
3	305.38	436.05	2	Yes	
4	305.34	436.01	2	Yes	
5	305.12	436.02	2	Yes	
6	305.02	436.0	2	Yes	
7	305.0	436.02	2	Yes	
8	30.13	35.91	2	Yes	
9	28.63	37.32	2	Yes	B from P3
10	25.42	35.73	2	Yes	
11	26.0	34.69	2	Yes	B from P3
12	25.01	37.41	2	Yes	B from P3
13	18.77	34.33	2	No	B from P3
14	17.4	33.29	2	No	B from P3
15	15.74	26.22	2	No	B from P3
16	15.27	26.26	2	No	B from P3
17	14.94	25.76	2	No	B from P3
18	14.59	28.49	2	No	B from P3
19	14.07	27.04	2	No	B from P3
20	13.78	27.57	2	No	B from P3
21	13.35	27.02	2	No	B from P3
22	12.88	29.73	2	No	B from P3
23	12.63	31.02	2	No	B from P3
24	12.12	32.7	2	No	B from P3
25	11.61	33.68	2	No	B from P3
26	11.38	30.84	2	No	B from P3
27	11.17	36.72	2	No	B from P3
28	9.27	29.02	2	No	B from CCSD(T)

Table A34. Molecular orbital data for 3,4-dimethyl-1-pentene. Double-ionization threshold = 25.24 eV from EPT (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.6	436.03	2	Yes	
2	305.53	436.01	2	Yes	
3	305.53	436.12	2	Yes	
4	305.24	436.03	2	Yes	
5	305.14	436.02	2	Yes	
6	305.1	436.02	2	Yes	
7	305.09	436.02	2	Yes	
8	30.17	35.15	2	Yes	
9	28.2	38.16	2	Yes	
10	26.59	37.29	2	Yes	B from P3
11	25.24	34.58	2	Yes	
12	20.77	35.27	2	No	B from P3
13	18.81	34.97	2	No	B from P3
14	17.83	31.44	2	No	B from P3
15	15.95	25.05	2	No	B from P3
16	15.19	29.64	2	No	B from P3
17	15.01	26.29	2	No	B from P3
18	14.7	27.15	2	No	B from P3
19	13.84	26.71	2	No	B from P3
20	13.44	27.51	2	No	B from P3
21	13.24	30.26	2	No	B from P3
22	13.01	29.21	2	No	B from P3
23	12.82	30.57	2	No	B from P3
24	12.18	30.62	2	No	B from P3
25	11.22	33.56	2	No	B from P3
26	11.24	31.91	2	No	B from P3
27	11.04	36.09	2	No	B from P3
28	9.62	29.11	2	No	B from CCSD(T)

Table A35. Molecular orbital data for 3,3-dimethyl-1-pentene. Double-ionization threshold = 24.60 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.86	436.12	2	Yes	
2	305.52	435.99	2	Yes	
3	305.34	436.06	2	Yes	
4	305.19	436.02	2	Yes	
5	305.14	436.03	2	Yes	
6	305.13	436.02	2	Yes	
7	305.08	436.01	2	Yes	
8	30.39	35.24	2	Yes	
9	27.76	38.19	2	Yes	B from P3
10	26.69	37.28	2	Yes	B from P3
11	25.34	34.33	2	Yes	B from P3
12	23.77	34.12	2	No	
13	21.57	35.96	2	No	
14	17.33	33.11	2	No	B from P3
15	15.89	24.85	2	No	B from P3
16	15.44	26.78	2	No	B from P3
17	14.93	27.83	2	No	B from P3
18	14.84	26.67	2	No	B from P3
19	13.71	27.8	2	No	B from P3
20	13.4	28.83	2	No	B from P3
21	13.33	28.26	2	No	B from P3
22	13.06	28.23	2	No	B from P3
23	12.72	31.08	2	No	B from P3
24	12.18	30.04	2	No	B from P3
25	11.36	33.01	2	No	B from P3
26	11.15	34.69	2	No	B from P3
27	11.13	35.41	2	No	B from P3
28	9.62	28.87	2	No	B from CCSD(T)

Table A36. Molecular orbital data for 4,4-dimethyl-1-pentene. Double-ionization threshold = 25.17 eV from EPT (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.79	436.13	2	Yes	
2	305.6	435.98	2	Yes	
3	305.41	436.06	2	Yes	
4	305.26	436.03	2	Yes	
5	305.1	436.02	2	Yes	
6	305.09	436.02	2	Yes	
7	304.98	436.01	2	Yes	
8	30.28	34.75	2	Yes	B from P3
9	28.41	39.32	2	Yes	
10	24.86	34.45	2	No	B from P3
11	25.24	34.5	2	No	B from P3
12	25.07	37.32	2	No	
13	18.55	34.48	2	No	B from P3
14	17.62	33.13	2	No	B from P3
15	15.8	26.47	2	No	B from P3
16	15.28	25.05	2	No	B from P3
17	15.04	27.74	2	No	B from P3
18	14.75	27.72	2	No	B from P3
19	14.12	28.25	2	No	B from P3
20	13.59	27.4	2	No	B from P3
21	13.21	28.73	2	No	B from P3
22	12.75	28.31	2	No	B from P3
23	12.62	29.6	2	No	B from P3
24	12.21	30.46	2	No	B from P3
25	11.47	33.59	2	No	B from P3
26	11.23	34.59	2	No	B from P3
27	11.07	36.0	2	No	B from P3
28	9.63	28.73	2	No	B from CCSD(T)

Table A37. Molecular orbital data for 2,3-dimethyl-2-pentene. Double-ionization threshold = 23.57 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.45	435.9	2	Yes	
2	305.38	436.15	2	Yes	
3	305.31	436.06	2	Yes	
4	305.17	436.01	2	Yes	
5	305.17	436.02	2	Yes	
6	305.17	436.02	2	Yes	
7	305.13	436.04	2	Yes	
8	30.11	37.11	2	Yes	
9	27.91	35.56	2	Yes	B from P3
10	26.52	35.26	2	Yes	
11	25.31	35.29	2	Yes	B from P3
12	24.44	36.89	2	Yes	B from P3
13	22.46	36.25	2	No	
14	16.34	34.65	2	No	B from P3
15	15.88	25.42	2	No	B from P3
16	15.01	26.46	2	No	B from P3
17	14.67	24.22	2	No	B from P3
18	14.13	26.93	2	No	B from P3
19	13.99	27.24	2	No	B from P3
20	13.56	27.11	2	No	B from P3
21	13.16	27.83	2	No	B from P3
22	13.06	29.11	2	No	B from P3
23	12.6	30.78	2	No	B from P3
24	12.55	31.57	2	No	B from P3
25	12.27	33.35	2	No	B from P3
26	11.76	31.51	2	No	B from P3
27	10.84	37.52	2	No	B from P3
28	8.5	30.75	2	No	B from CCSD(T)

Table A38. Molecular orbital data for 2,4-dimethyl-2-pentene. Double-ionization threshold = 28.98 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.61	436.02	2	Yes	
2	305.53	436.07	2	Yes	
3	305.28	436.01	2	Yes	
4	305.24	436.02	2	Yes	
5	305.11	436.03	2	Yes	
6	305.07	436.02	2	Yes	
7	305.07	436.04	2	Yes	
8	30.05	36.96	2	Yes	B from P3
9	28.5	36.0	2	No	B from P3
10	24.84	34.98	2	No	B from P3
11	22.14	34.77	2	No	B from P3
12	25.0	37.87	2	No	B from P3
13	19.09	36.37	2	No	B from P3
14	17.21	31.0	2	No	B from P3
15	15.65	28.35	2	No	B from P3
16	14.95	27.47	2	No	B from P3
17	14.69	23.84	2	No	B from P3
18	14.38	27.0	2	No	B from P3
19	13.81	27.7	2	No	B from P3
20	13.64	28.71	2	No	B from P3
21	13.32	26.9	2	No	B from P3
22	13.29	26.87	2	No	B from P3
23	12.77	31.01	2	No	B from P3
24	12.29	33.33	2	No	B from P3
25	11.84	32.72	2	No	B from P3
26	11.53	33.41	2	No	B from P3
27	11.0	35.1	2	No	B from P3
28	8.83	30.47	2	No	B from CCSD(T)

Table A39. Molecular orbital data for 3,4-dimethyl-2-pentene. Double-ionization threshold = 29.07 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.54	436.05	2	Yes	
2	305.49	436.04	2	Yes	
3	305.24	435.95	2	Yes	
4	305.22	436.01	2	Yes	
5	305.21	436.11	2	Yes	
6	305.08	436.02	2	Yes	
7	305.08	436.03	2	Yes	
8	30.13	36.55	2	Yes	B from P3
9	28.06	36.46	2	No	
10	27.69	36.13	2	No	B from P3
11	21.95	34.7	2	No	B from P2
12	24.48	35.98	2	No	B from P3
13	21.57	36.92	2	No	B from P3
14	17.0	32.24	2	No	B from P3
15	15.97	25.13	2	No	B from P3
16	14.93	27.69	2	No	B from P3
17	14.48	24.7	2	No	B from P3
18	13.92	29.4	2	No	B from P3
19	13.74	30.4	2	No	B from P3
20	13.86	25.45	2	No	B from P3
21	13.74	27.3	2	No	B from P3
22	13.1	29.02	2	No	B from P3
23	13.03	27.92	2	No	B from P3
24	12.24	32.06	2	No	B from P3
25	11.8	33.0	2	No	B from P3
26	11.44	32.89	2	No	B from P3
27	10.94	36.42	2	No	B from P3
28	8.82	30.41	2	No	B from CCSD(T)

Table A40. Molecular orbital data for 4,4-dimethyl-2-pentene. Double-ionization threshold = 24.71 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.82	436.12	2	Yes	
2	305.38	435.9	2	Yes	
3	305.29	436.03	2	Yes	
4	305.26	436.11	2	Yes	
5	305.09	436.02	2	Yes	
6	305.09	436.03	2	Yes	
7	305.06	436.01	2	Yes	
8	30.27	35.81	2	Yes	B from P3
9	28.31	37.75	2	Yes	B from P3
10	25.29	34.33	2	Yes	
11	25.21	34.57	2	Yes	
12	25.11	37.65	2	Yes	
13	21.33	36.18	2	No	B from P3
14	17.33	31.54	2	No	B from P3
15	15.7	26.81	2	No	B from P3
16	15.06	28.15	2	No	B from P3
17	14.81	25.68	2	No	B from P3
18	14.0	28.91	2	No	B from P3
19	14.07	25.17	2	No	B from P3
20	13.79	29.17	2	No	B from P3
21	13.44	26.71	2	No	B from P3
22	13.04	29.15	2	No	B from P3
23	12.73	28.35	2	No	B from P3
24	12.44	30.69	2	No	B from P3
25	11.57	33.18	2	No	B from P3
26	11.29	35.62	2	No	B from P3
27	11.11	35.45	2	No	B from P3
28	9.16	29.87	2	No	B from CCSD(T)

Table A41. Molecular orbital data for 2-ethyl-1-pentene. Double-ionization threshold = 25.29 eV from EPT (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.68	436.02	2	Yes	
2	305.46	436.05	2	Yes	
3	305.39	436.0	2	Yes	
4	305.36	436.1	2	Yes	
5	305.21	436.04	2	Yes	
6	305.17	436.03	2	Yes	
7	305.01	436.0	2	Yes	
8	30.06	36.53	2	Yes	
9	28.32	35.51	2	Yes	B from P3
10	26.92	37.36	2	Yes	
11	21.53	36.92	2	No	B from P2
12	23.11	35.17	2	No	B from P3
13	19.62	33.85	2	No	B from P3
14	17.3	33.48	2	No	B from P3
15	15.93	24.26	2	No	B from P3
16	15.56	25.78	2	No	B from P3
17	14.84	26.95	2	No	B from P3
18	14.45	27.47	2	No	B from P3
19	13.97	27.64	2	No	B from P3
20	13.84	29.81	2	No	B from P3
21	13.16	28.58	2	No	B from P3
22	12.78	30.42	2	No	B from P3
23	12.38	33.49	2	No	B from P3
24	12.09	29.29	2	No	B from P3
25	11.93	32.22	2	No	B from P3
26	11.54	30.61	2	No	B from P3
27	11.13	35.69	2	No	B from P3
28	9.22	29.68	2	No	B from CCSD(T)

Table A42. Molecular orbital data for 3-ethyl-1-pentene. Double-ionization threshold = 25.28 eV from P3 (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.57	436.03	2	Yes	
2	305.52	436.02	2	Yes	
3	305.32	436.05	2	Yes	
4	305.32	436.06	2	Yes	
5	305.23	436.03	2	Yes	
6	305.15	436.03	2	Yes	
7	305.13	436.03	2	Yes	
8	30.07	35.37	2	Yes	B from P3
9	27.81	38.82	2	Yes	
10	27.49	35.54	2	Yes	B from P3
11	21.53	37.03	2	No	B from P2
12	20.44	33.23	2	No	B from P3
13	21.52	35.79	2	No	B from P3
14	17.9	31.11	2	No	B from P3
15	15.93	25.25	2	No	B from P3
16	15.44	26.63	2	No	B from P3
17	15.08	26.3	2	No	B from P3
18	14.23	30.49	2	No	B from P3
19	14.02	27.46	2	No	B from P3
20	13.96	27.96	2	No	B from P3
21	12.94	31.25	2	No	B from P3
22	12.78	29.7	2	No	B from P3
23	12.59	28.44	2	No	B from P3
24	12.23	31.31	2	No	B from P3
25	11.35	31.79	2	No	B from P3
26	11.2	32.71	2	No	B from P3
27	11.03	35.34	2	No	B from P3
28	9.62	29.07	2	No	B from CCSD(T)

Table A43. Molecular orbital data for 3-ethyl-2-pentene. Double-ionization threshold = 24.20 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.45	435.95	2	Yes	
2	305.38	436.06	2	Yes	
3	305.36	436.07	2	Yes	
4	305.24	435.96	2	Yes	
5	305.21	436.11	2	Yes	
6	305.17	436.04	2	Yes	
7	305.12	436.04	2	Yes	
8	30.04	36.88	2	Yes	B from P3
9	27.58	35.32	2	Yes	B from P3
10	27.47	36.3	2	Yes	
11	25.09	37.14	2	Yes	
12	23.05	34.02	2	No	
13	19.58	36.58	2	No	B from P2
14	16.91	32.66	2	No	B from P3
15	15.93	24.93	2	No	B from P3
16	15.25	26.51	2	No	B from P3
17	14.48	26.72	2	No	B from P3
18	14.28	26.92	2	No	B from P3
19	13.97	27.5	2	No	B from P3
20	13.74	28.54	2	No	B from P3
21	13.25	28.65	2	No	B from P3
22	12.82	30.23	2	No	B from P3
23	12.44	32.62	2	No	B from P3
24	12.44	31.43	2	No	B from P3
25	12.09	29.07	2	No	B from P3
26	11.64	32.18	2	No	B from P3
27	10.92	35.76	2	No	B from P3
28	8.78	30.78	2	No	B from CCSD(T)

Table A44. Molecular orbital data for 2,3,3-trimethyl-1-butene. Double-ionization threshold = 25.18 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.92	436.13	2	Yes	
2	305.72	436.05	2	Yes	
3	305.27	436.01	2	Yes	
4	305.14	436.02	2	Yes	
5	305.14	436.02	2	Yes	
6	305.06	436.01	2	Yes	
7	304.96	435.99	2	Yes	
8	30.47	35.59	2	Yes	B from P3
9	28.0	37.93	2	Yes	
10	25.69	34.22	2	Yes	B from P3
11	21.93	34.49	2	No	B from P2
12	24.75	37.39	2	No	B from P3
13	21.83	35.01	2	No	B from P3
14	16.73	35.42	2	No	B from P3
15	15.93	25.45	2	No	B from P3
16	15.05	27.61	2	No	B from P3
17	14.87	25.79	2	No	B from P3
18	14.29	26.69	2	No	B from P3
19	14.36	25.09	2	No	B from P3
20	13.73	27.64	2	No	B from P3
21	13.15	27.89	2	No	B from P3
22	13.03	30.78	2	No	B from P3
23	12.72	29.06	2	No	B from P3
24	12.64	30.0	2	No	B from P3
25	11.58	33.42	2	No	B from P3
26	11.26	36.06	2	No	B from P3
27	11.06	36.12	2	No	B from P3
28	9.28	29.0	2	No	B from CCSD(T)

Table A45. Molecular orbital data for 2-ethyl-3-methyl-1-butene. Double-ionization threshold = 25.21 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	305.66	435.96	2	Yes	
2	305.64	436.16	2	Yes	
3	305.45	436.05	2	Yes	
4	305.21	436.03	2	Yes	
5	305.18	436.02	2	Yes	
6	305.12	436.03	2	Yes	
7	305.0	436.0	2	Yes	
8	30.19	36.21	2	Yes	
9	28.07	35.91	2	Yes	B from P3
10	26.75	37.89	2	Yes	B from P3
11	22.02	34.61	2	No	B from P2
12	20.45	35.77	2	No	B from P3
13	19.62	34.97	2	No	B from P3
14	17.24	32.18	2	No	B from P3
15	15.85	25.96	2	No	B from P3
16	15.34	27.02	2	No	B from P3
17	14.52	27.04	2	No	B from P3
18	14.38	27.76	2	No	B from P3
19	14.13	27.04	2	No	B from P3
20	13.76	27.57	2	No	B from P3
21	13.41	27.02	2	No	B from P3
22	12.92	29.13	2	No	B from P3
23	12.7	32.0	2	No	B from P3
24	11.91	31.06	2	No	B from P3
25	11.89	32.74	2	No	B from P3
26	11.53	34.52	2	No	B from P3
27	10.93	34.41	2	No	B from P3
28	9.21	29.82	2	No	B from CCSD(T)

Table A46. Molecular orbital data for benzaldehyde. Double-ionization threshold = 24.12 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	559.21	794.65	2	Yes	
2	308.48	436.17	2	Yes	
3	306.45	435.95	2	Yes	
4	306.38	435.96	2	Yes	
5	306.26	435.85	2	Yes	
6	306.21	436.07	2	Yes	
7	306.18	436.03	2	Yes	
8	306.13	436.06	2	Yes	
9	37.9	72.05	2	Yes	B from P3
10	31.97	39.85	2	Yes	
11	28.66	43.11	2	Yes	
12	28.22	42.39	2	Yes	B from P3
13	20.32	43.42	2	No	B from P2
14	20.18	38.48	2	No	B from P3
15	19.06	41.49	2	No	B from P3
16	17.5	30.14	2	No	B from P3
17	16.42	38.79	2	No	B from P3
18	15.77	47.6	2	No	B from P3
19	15.07	37.39	2	No	B from P3
20	14.87	48.74	2	No	B from P3
21	14.84	32.75	2	No	B from P3
22	13.8	34.99	2	No	B from P3
23	13.0	40.64	2	No	B from P3
24	12.6	38.08	2	No	B from P3
25	12.49	34.29	2	No	B from P3
26	9.9	57.18	2	No	B from P3
27	9.76	29.08	2	No	B from P3
28	9.8	30.46	2	No	B from expt

Table A47. Molecular orbital data for phenol. Double-ionization threshold = 23.50 eV from CCSD(T)/cc-pV(T+d)Z (to singlet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	560.12	794.57	2	Yes	
2	307.63	436.12	2	Yes	
3	305.96	435.97	2	Yes	
4	305.89	435.97	2	Yes	
5	305.73	435.98	2	Yes	
6	305.55	435.97	2	Yes	
7	305.53	436.0	2	Yes	
8	38.31	69.03	2	Yes	
9	31.3	40.79	2	Yes	
10	27.85	42.11	2	Yes	
11	27.18	45.78	2	Yes	B from P3
12	20.28	39.74	2	No	B from P3
13	22.47	43.11	2	No	
14	18.05	39.72	2	No	B from P3
15	16.7	34.83	2	No	B from P3
16	15.83	42.58	2	No	B from P3
17	14.97	36.91	2	No	B from P3
18	14.53	32.83	2	No	B from P3
19	13.93	47.84	2	No	B from P3
20	13.44	51.94	2	No	B from expt
21	12.61	39.77	2	No	B from expt
22	12.02	40.14	2	No	B from expt
23	11.59	32.63	2	No	B from expt
24	9.39	28.19	2	No	B from expt
25	8.7	34.75	2	No	B from expt

Table A48. Molecular orbital data for acetophenone. Double-ionization threshold = 23.42 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	558.9	794.64	2	Yes	
2	308.5	436.2	2	Yes	
3	306.29	435.94	2	Yes	
4	306.22	435.95	2	Yes	
5	306.14	435.94	2	Yes	
6	306.05	435.98	2	Yes	
7	306.05	436.04	2	Yes	
8	305.98	436.09	2	Yes	
9	305.78	435.98	2	Yes	
10	37.73	70.99	2	Yes	B from P3
11	31.8	39.85	2	Yes	B from P3
12	28.7	42.26	2	Yes	B from P3
13	28.05	42.27	2	Yes	B from P3
14	27.16	39.17	2	Yes	B from P3
15	23.6	41.5	2	Yes	
16	23.07	38.93	2	No	B from P3
17	18.32	40.69	2	No	B from P3
18	17.19	35.05	2	No	B from P3
19	15.8	40.18	2	No	B from P3
20	15.64	44.26	2	No	B from P3
21	15.3	33.19	2	No	B from P3
22	15.19	27.91	2	No	B from P3
23	14.68	32.4	2	No	B from P3
24	14.38	49.11	2	No	B from P3
25	13.81	31.69	2	No	B from P3
26	12.96	28.72	2	No	B from P3
27	12.73	41.19	2	No	B from P3
28	12.38	38.56	2	No	B from P3
29	11.91	39.29	2	No	B from expt
30	9.77	59.06	2	No	B from expt
31	9.55	29.18	2	No	B from expt
32	9.37	30.03	2	No	B from expt

Table A49. Molecular orbital data for pyrrole. Double-ionization threshold = 23.93 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	424.51	601.93	2	Yes	
2	306.12	436.02	2	Yes	
3	306.12	436.03	2	Yes	
4	304.95	435.82	2	Yes	
5	304.92	436.13	2	Yes	
6	35.12	48.63	2	Yes	
7	27.81	44.2	2	Yes	B from P3
8	26.61	43.75	2	Yes	
9	21.59	39.46	2	No	
10	20.88	39.08	2	No	
11	20.04	30.84	2	No	
12	14.71	38.1	2	No	B from P3
13	14.5	37.92	2	No	B from P3
14	13.42	31.97	2	No	B from P3
15	13.57	36.46	2	No	B from P3
16	13.08	36.94	2	No	B from P3
17	9.2	34.46	2	No	B from expt
18	8.209	30.04	2	No	B from expt

Table A50. Molecular orbital data for pyridine. Double-ionization threshold = 25.53 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	423.46	602.12	2	Yes	
2	306.81	436.05	2	Yes	
3	306.81	436.05	2	Yes	
4	306.42	435.98	2	Yes	
5	305.94	435.96	2	Yes	
6	305.94	435.99	2	Yes	
7	34.29	48.54	2	Yes	
8	29.83	44.8	2	Yes	B from P3
9	28.19	43.43	2	Yes	B from P3
10	20.43	41.7	2	No	B from P3
11	23.35	41.83	2	No	B from P3
12	17.55	27.02	2	No	B from P3
13	16.12	42.38	2	No	B from P3
14	16.03	34.39	2	No	B from P3
15	14.74	32.85	2	No	B from P3
16	14.02	37.15	2	No	B from P3
17	13.3	27.41	2	No	B from P3
18	12.61	38.65	2	No	B from expt
19	9.75	49.56	2	No	B from expt
20	10.51	32.07	2	No	B from expt
21	9.6	28.57	2	No	B from expt

Table A51. Molecular orbital data for benzonitrile. Double-ionization threshold = 25.29 eV from CCSD(T)/cc-pV(T+d)Z (to triplet dication).

MO	B/eV	U/eV	N	DblIon	Remarks
1	423.77	602.28	2	Yes	
2	307.28	435.95	2	Yes	
3	306.91	435.83	2	Yes	
4	306.76	435.98	2	Yes	
5	306.76	436.01	2	Yes	
6	306.62	435.93	2	Yes	
7	306.47	436.0	2	Yes	
8	306.47	436.08	2	Yes	
9	33.38	56.44	2	Yes	B from P3
10	32.22	42.82	2	Yes	
11	28.97	43.58	2	Yes	
12	28.56	42.34	2	Yes	
13	24.22	42.1	2	No	
14	23.42	38.66	2	No	B from P3
15	18.61	33.24	2	No	B from P3
16	17.05	35.26	2	No	B from P3
17	16.1	38.88	2	No	B from P3
18	15.6	35.09	2	No	B from P3
19	15.19	32.32	2	No	B from P3
20	13.33	50.61	2	No	B from P3
21	13.71	25.63	2	No	B from P3
22	13.07	42.33	2	No	B from P3
23	13.17	37.05	2	No	B from P3
24	12.09	32.52	2	No	B from expt
25	11.84	38.55	2	No	B from expt
26	10.17	28.22	2	No	B from expt
27	9.71	31.62	2	No	B from expt

Supplemental Materials

- Text files, named "<*molecule*>.bun," containing molecular orbital data needed for computing TICS (51 files). These are the same data shown in the Appendix, but in computer-readable form.
- Perl script "beb_tbl.pl" that takes a BUN file as input for computing TICS.
- Text files, named "<*molecule*>_estPICS.txt," containing the PICS results in computer-readable form (50 files). These are the same data shown in Tables 2 to 51, but in computer-readable form.

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5. References

[1] Mahaffy PR, Webster CR, Cabane M, Conrad PG, Coll P, Atreya SK, Arvey R, Barciniak M, Benna M, Bleacher L, Brinckerhoff WB, Eigenbrode JL, Carignan D, Cascia M, Chalmers RA, Dworkin JP, Errigo T, Everson P, Franz H, Farley R, Feng S, Frazier G, Freissinet C, Glavin DP, Harpold DN, Hawk D, Holmes V, Johnson CS, Jones A, Jordan P, Kellogg J, Lewis J, Lyness E, Malespin CA, Martin DK, Maurer J, McAdam AC, McLennan D, Nolan TJ, Noriega M, Pavlov AA, Prats B, Raaen E, Sheinman O, Sheppard D, Smith J, Stern JC, Tan F, Trainer M, Ming DW, Morris RV, Jones J, Gundersen C, Steele A, Wray J, Botta O, Leshin LA, Owen T, Battel S, Jakosky BM, Manning H, Squyres S, Navarro-Gonzalez R, McKay CP, Raulin F, Sternberg R, Buch A, Sorensen P, Kline-Schoder R, Coscia D, Szopa C, Teinturier S, Baffes C, Feldman J, Flesch G, Forouhar S, Garcia R, Keymeulen D, Woodward S, Block BP, Arnett K, Miller R, Edmonson C, Gorevan S, Mumm E (2012) The Sample Analysis at Mars Investigation and Instrument Suite. *Space Science Reviews* 170(1–4):401–478. https://doi.org/10.1007/s11214-012-9879-z

[2] Nasser E (1971) *Fundamentals of Gaseous Ionization and Plasma Electronics* (Wiley-Interscience, New York).

[3] Tian CC, Vidal CR (1998) Electron impact dissociative ionization of CO_2: Measurements with a focusing time-of-flight mass spectrometer. *Journal of Chemical Physics* 108(3):927–936. https://doi.org/10.1063/1.475456

[4] Irikura KK (2016) Semi-empirical estimation of ion-specific cross sections in electron ionization of molecules. *Journal of Chemical Physics* 145(22):224102. https://doi.org/10.1063/1.4971242

[5] Kim Y-K, Rudd ME (1994) Binary-encounter-dipole model for electron-impact ionization. *Physical Review A* 50(5):3954–3967. https://link.aps.org/doi/10.1103/PhysRevA.50.3954

[6] Hwang W, Kim Y-K, Rudd ME (1996) New model for electron-impact ionization cross sections of molecules. *Journal of Chemical Physics* 104(8):2956–2966. https://doi.org/10.1063/1.471116

[7] Kim Y-K, Rudd ME (1999) Theory for ionization of molecules by electrons. *Comments on Atomic and Molecular Physics* 34(3–6):309–320.

[8] Huo WM, Kim Y-K (2000) Use of relativistic effective core potentials in the calculation of total electron-impact ionization cross-sections. *Chemical Physics Letters* 319(5–6):576–586. https://doi.org/10.1016/S0009-2614(00)00150-0

[9] Kim Y-K, Irikura KK, Ali MA (2000) Electron-impact total ionization cross sections of molecular ions. *Journal of Research of the National Institute of Standards and Technology* 105(2):285–291. https://doi.org/10.6028/jres.105.032

[10] Kim Y-K, Santos JP, Parente F (2000) Extension of the binary-encounter-dipole model to relativistic incident electrons. *Physical Review A* 62(5):052710. https://link.aps.org/doi/10.1103/PhysRevA.62.052710

[11] Kim Y-K, Irikura KK, Rudd ME, Zucker DS, Zucker MA, Coursey JS, Olsen KJ, Wiersma GG (2001) *Electron-Impact Ionization Cross Section Database*. Available at http://physics.nist.gov/ionxsec.

[12] Scott GE, Irikura KK (2005) Electron-impact ionization cross-sections of molecules containing heavy elements ($Z > 10$). *Journal of Chemical Theory and Computation* 1:1153–1161. https://doi.org/10.1021/ct050077j

[13] Scott GE, Irikura KK (2005) Performance of binary-encounter Bethe (BEB) theory for electron-impact ionization cross-sections of molecules containing heavy elements ($Z > 10$). *Surface and Interface Analsis* 37:973–977. https://doi.org/10.1002/sia.2091

[14] Linstrom PJ, Mallard WG (2016) NIST Chemistry WebBook. *NIST Standard Reference Database Number 69* (National Institute of Standards and Technology, Gaithersburg, MD). Available at http://webbook.nist.gov/chemistry/

[15] Di Palma TM, Apicella B, Armenante M, Velotta R, Wang X, Spinelli N (2004) Dissociative electron impact ionization of methyl tert-butyl ether: Total ionization cross-section and kinetic energy distributions. *Chemica Physics Letters* 400(1–3):191–195. https://doi.org/10.1016/j.cplatt.2004.10.106

[16] Feil S, Bacher A, Zangerl M, Schustereder W, Gluch K, Scheier P (2004) Discrimination effects for ions with initial kinetic energy produced by electron ionization of C_2H_2 in a Nier-type ion source. *International Jorunal of Mass Spectrometry* 233(1–3):325–333. https://doi.org/10.1016/j.ijms.2004.01.013

[17] Gluch G, Feil S, Scheier P, Schustereder W, Tepnual T, Feketeova L, Mair C, Matt-Leubner S, Stamatovic A, Märk TD (2005) Partial and differential electron impact ionization cross-sections for small hydrocarbon molecules. *Nuclear Fusion Research: Understanding Plasma-Surface Interactions*, Springer Series in Chemical Physics, Vol. 78, eds Clark REH, Reiter DH (Springer, Heidelberg, Germany), pp 437–456. https://doi.org/10.1007/3-540-27362-X_20

[18] Christophorou LG, Olthoff JK (2004) *Fundamental Electron Interactions with Plasma Processing Gases* (Kluwer Academic/Plenum, New York), p 776.

[19] Tian CC, Vidal CR (1998) Cross sections of the electron impact dissociative ionization of CO, CH_4 and C_2H_2. *Journal of Physics B–Atomic, Molecular, and Optical Physics* 31(4):895–909. https://doi.org/10.1088/0953-4075/31/4/031

[20] Pandey A, Bapat B (2014) Effect of transmission losses on measured parameters in multi-ion coincidence momentum spectrometers. *International Journal of Mass Spectrometry* 361:23–27. https://doi.org/10.1016/j.ijms.2014.01.022

[21] Lee C, Yang W, Parr RG (1988) Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Physical Review B* 37:785–789. https://doi.org/10.1103/PhysRevB.37.785

[22] Becke AD (1993) Density-functional thermochemistry. III. The role of exact exchange. *J Chemical Physics* 98(7):5648–5652. https://doi.org/10.1063/1.464913

[23] Bergner A, Dolg M, Küchle W, Stoll H, Preuß H (1993) *Ab initio* energy-adjusted pseudopotentials for elements of groups 13–17. *Molecular Physics* 80(6):1431–1441. https://doi.org/10.1080/00268979300103121

[24] Ortiz JV (1996) Partial third-order quasiparticle theory: Comparisons for closed-shell ionization energies and an application to the Borazine photoelectron spectrum. *Journal of Chemical Physics* 104(19):7599–7605. https://doi.org/10.1063/1.471468

[25] Raghavachari K, Trucks GW, Pople JA, Head-Gordon M (1989) A fifth-order perturbation comparison of electron correlation theories. *Chemical Physics Letters* 157(6):479–483. https://doi.org/10.1016/S0009-2614(89)87395-6

[26] Wilson AK, Dunning TH, Jr. (2003) SO_2 revisited: Impact of tight *d* augmented correlation consistent basis sets on structure and energetics. *Journal of Chemical Physics* 119(22):11712–11714. https://doi.org/10.1063/1.1624591

[27] Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Jr., Peralta JE, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, Fox DJ (2013) Gaussian 09 (Gaussian, Inc., Wallingford, CT), vers. D.01. Available at http://gaussian.com/glossary/g09/
[28] Kimura K, Katsumata S, Achiba Y, Yamazaki T, Iwata S (1981) *Handbook of HeI Photoelectron Spectra of Fundamental Organic Molecules* (Japan Scientific Societies, Tokyo).
[29] Howell JO, Goncalves JM, Amatore C, Klasinc L, Wightman RM, Kochi JK (1984) Electron transfer from aromatic hydrocarbons and their p-complexes with metals. Comparison of the standard oxidation potentials and vertical ionization potentials. *Journal of the American Chemical Society* 106(14):3968–3976. https://doi.org/10.1021/ja00326a014
[30] Kobayashi T, Arai T, Sakuragi H, Tokumaru K, Utsunomiya C (1981) A new method for conformational analysis by photoelectron spectroscopy with application to alkyl-substituted styrenes. *Bulletin of the Chemical Society of Japan* 54(6):1658–1661. https://doi.org/10.1246/bcsj.54.1658
[31] Krause DA, Taylor JW, Fenske RF (1978) An analysis of the effects of alkyl substituents on the ionization potentials of n-alkenes. *Journal of the American Chemical Society* 100(3):718–723. https://doi.org/10.1021/ja00471a009
[32] Mintz DM, Kuppermann A (1979) Photoelectron spectroscopy of ethylene, isobutylene, trimethylethylene, and tetramethylethylene at variable angle. *Journal of Chemical Physsics* 71(8):3499–3513. https://doi.org/10.1063/1.438739
[33] Ashmore FS, Burgess AR (1978) Photoelectron spectra of the unbranched C_5-C_7 alkenes, aldehydes and ketones. *Journal of the Chemical Society, Faraday Transactions 2–Molecular and Chemical Physics* 74(0):734–742. https://doi.org/10.1039/f29787400734
[34] Baker AD, May DP, Turner DW (1968) Molecular photoelectron spectroscopy. 7. Vertical ionisation potentials of benzene and some of its monosubstituted and 1,4-disubstituted derivatives. *Journal of the Chemical Society B–Physical Organic* (1):22–34. https://doi.org/10.1039/j29680000022
[35] Kobayashi T, Nagakura S (1974) Photoelectron spectra of substituted benzenes. *Bulletin of the Chemical Society of Japan* 47(10):2563–2572. https://doi.org/10.1246/bcsj.47.2563
[36] Derrick PJ, Åsbrink L, Edqvist O, Jonsson B-Ö, Lindholm E (1971) Rydberg series in small molecules: XII. Photoelectron spectroscopy and electronic structure of pyrrole. *International Journal of Mass Spectrometry and Ion Physics* 6(3):191–202. https://doi.org/10.1016/0020-7381(71)80003-7
[37] Ausloos P, Clifton CL, Lias SG, Mikaya AI, Stein SE, Tchekhovskoi DV, Sparkman OD, Zaikin V, Zhu D (1999) The critical evaluation of a comprehensive mass spectral library. *Journal of the American Society for Mass Spectrometry* 10(4):287–299. https://doi.org/10.1016/S1044-0305(98)00159-7
[38] Anonymous ed (2014) *NIST/EPA/NIH Mass Spectral Library* (National Institute of Standards and Technology, Gaithersburg, MD). Available at http://chemdata.nist.gov/

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