J. Phys. B: At. Mol. Opt. Phys. **38** (2005) 1077–1079 doi:10.1088/0953-4075/38/7/C01

Corrigendum

Corrections to the following three papers pertaining to electron impact ionization efficiency curves calculated using the BEB model for molecules containing third and fourth row atoms

Absolute electron impact ionization cross sections for CH_3X, where X = H, F, Cl, Br, and I
Claire Vallance *et al* 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 2465–2475

Absolute electron-impact ionization cross sections for a range of C_1 to C_5 chlorocarbons
James E Hudson *et al* 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 3025–3039

Absolute electron impact ionization cross-sections for CO, CO_2, OCS and CS_2
James E Hudson *et al* 2004 *J. Phys. B: At. Mol. Opt. Phys.* **37** 445–455

We have recently re-examined some published binary-encounter–Bethe [1–3] (BEB) calculations on the electron impact ionization cross sections for halogenated hydrocarbons [4–6] and sulfur-containing molecules [7]. The calculations were carried out primarily to support our experimental data. However, our implementation of the BEB model, while returning cross sections in very good agreement with experiment for a wide range of species, systematically returned ionization cross sections that were too low compared with experiment for molecules containing third and fourth row atoms. It now appears that this discrepancy was the result of a fault in the code used to analyse Mulliken population data output from electronic structure calculations. Mulliken populations are used in BEB calculations to determine a set of correction factors for the orbital kinetic energy of molecular orbitals dominated by contributions from atomic orbitals with principal quantum number $n > 2$. The coding error leads to an underestimation of the contribution from such orbitals, yielding erroneously low values of the kinetic energy correction factor for a few molecular orbitals. Unfortunately, in a number of cases, this has a significant effect on the calculated ionization efficiency curves.

Corrected ionization efficiency curve data are presented in table 1. The new curves are in greatly improved agreement with previously published experimental data [4–7]. We would like to apologize to Y K Kim and M E Rudd, the developers of BEB theory, for unfair criticism of the performance of their model for molecules containing third and fourth row atoms. Note that the comments in this corrigendum apply only to the BEB calculations presented in [4–7], and in no way invalidate the other results and conclusions of these papers.

References

[1] Kim Y K and Rudd M E 1994 *Phys. Rev.* A **50** 3954
[2] Hwang W, Kim Y K and Rudd M E 1996 *J. Chem. Phys.* **104** 2956
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Table 1. Corrected BEB electron impact ionization efficiency curves for halogen- and sulfur-containing molecules.

E (eV)	10	12	14	16	18	20	30	40	50	60	70	80	90	100	120	140	160	180	200	220	240	260	280	300
CS_2	0.00	0.00	0.00	0.00	0.00	0.00	2.1	4.2	5.6	6.5	7.1	7.5	7.7	7.9	8.0	7.9	7.8	7.6	7.4	7.2	7.0	6.8	6.6	6.5
OCS	0.00	0.00	0.00	0.00	0.00	0.00	0.5	1.3	2.1	2.8	3.3	3.7	4.1	4.3	4.6	4.8	4.9	4.9	4.9	4.9	4.8	4.7	4.7	4.6
SF_6	0.00	0.00	0.00	0.00	0.00	0.08	2.0	3.6	4.8	5.6	6.2	6.6	6.9	7.1	7.3	7.3	7.3	7.2	7.0	6.9	6.7	6.5	6.4	6.2
Br_2	0.00	0.34	1.46	2.91	4.17	5.21	8.2	9.3	9.6	9.6	9.4	9.1	8.8	8.5	7.9	7.5	7.0	6.6	6.3	6.0	5.7	5.4	5.2	5.0
CH_3Cl	0.00	0.01	0.62	1.28	1.93	2.57	4.7	5.7	6.2	6.3	6.3	6.3	6.2	6.0	5.7	5.4	5.1	4.9	4.6	4.4	4.2	4.0	3.9	3.7
CH_2Cl_2	0.00	0.00	0.72	1.76	2.78	3.70	6.8	8.2	8.9	9.1	9.1	9.0	8.8	8.6	8.1	7.7	7.3	6.9	6.5	6.2	5.9	5.7	5.4	5.2
$CHCl_3$	0.00	0.00	0.51	1.87	3.18	4.41	8.4	10.3	11.2	11.5	11.5	11.4	11.2	10.9	10.3	9.8	9.2	8.8	8.3	7.9	7.5	7.2	6.9	6.6
CCl_4	0.00	0.00	0.55	2.15	3.75	5.29	10.3	12.7	13.7	14.1	14.1	14.0	13.7	13.4	12.7	12.0	11.3	10.7	10.2	9.7	9.2	8.8	8.4	8.1
CF_2Cl_2	0.00	0.00	0.08	0.81	1.61	2.40	5.5	7.3	8.2	8.7	8.9	9.0	9.0	8.9	8.6	8.3	8.0	7.7	7.3	7.1	6.8	6.5	6.3	6.1
CH_2Br_2	0.00	0.71	2.32	3.81	5.12	6.25	9.6	11.0	11.4	11.4	11.3	11.0	10.7	10.4	9.8	9.3	8.8	8.4	7.9	7.6	7.2	6.9	6.7	6.4
$CHBr_3$	0.00	0.70	2.96	5.02	6.85	8.39	12.9	14.7	15.3	15.3	15.0	14.6	14.2	13.9	13.1	12.3	11.7	11.1	10.5	10.0	9.6	9.2	8.8	8.5
CF_3Br	0.00	0.00	0.55	1.18	1.75	2.31	4.7	6.2	7.0	7.4	7.7	7.8	7.8	7.8	7.7	7.5	7.3	7.0	6.8	6.6	6.4	6.2	6.0	5.8
CF_2Br_2	0.00	0.06	1.19	2.46	3.60	4.61	8.1	9.9	10.7	11.1	11.1	11.1	11.0	10.8	10.4	10.0	9.6	9.2	8.8	8.5	8.2	7.9	7.6	7.3
$C_2F_4Br_2$	0.00	0.02	1.13	2.33	3.41	4.50	8.9	11.5	12.9	13.6	14.0	14.2	14.2	14.1	13.8	13.5	13.0	12.6	12.1	11.7	11.3	10.9	10.6	10.2
C_2Cl_6	0.00	0.00	0.64	3.13	5.59	7.89	15.5	19.2	20.9	21.5	21.6	21.3	20.9	20.4	19.4	18.3	17.3	16.4	15.6	14.9	14.2	13.6	13.0	12.5
C_2H_5Cl	0.00	0.10	0.79	1.59	2.45	3.30	6.2	7.7	8.4	8.7	8.7	8.7	8.5	8.4	8.0	7.6	7.2	6.8	6.5	6.2	5.9	5.7	5.4	5.2
CH_2ClCCl_3	0.00	0.00	0.82	2.71	4.55	6.25	11.9	14.7	16.0	16.4	16.5	16.3	16.0	15.6	14.8	14.0	13.3	12.6	12.0	11.4	10.9	10.4	10.0	9.6
CH_2ClCH_2Cl	0.00	0.00	0.92	2.10	3.30	4.42	8.2	10.1	10.9	11.2	11.3	11.2	11.0	10.7	10.2	9.7	9.2	8.7	8.3	7.9	7.5	7.2	6.9	6.7
$CH_2ClCHCl_2$	0.00	0.00	0.94	2.51	4.03	5.44	10.2	12.5	13.5	13.9	13.9	13.8	13.5	13.2	12.6	11.9	11.3	10.7	10.2	9.7	9.2	8.8	8.5	8.1
CH_3CCl_3	0.00	0.00	0.72	2.08	3.44	4.79	9.3	11.7	12.8	13.3	13.4	13.3	13.1	12.9	12.3	11.7	11.1	10.5	10.0	9.5	9.1	8.7	8.4	8.0
$CHCl_2CCl_3$	0.00	0.00	0.67	2.86	5.01	7.01	13.6	16.9	18.3	18.9	18.9	18.7	18.4	18.0	17.1	16.1	15.3	14.5	13.8	13.1	12.5	11.9	11.5	11.0
$CHCl_2CH_3$	0.00	0.00	0.87	2.06	3.26	4.41	8.3	10.2	11.1	11.4	11.5	11.3	11.2	10.9	10.4	9.8	9.3	8.8	8.4	8.0	7.6	7.3	7.0	6.7

Table 1. (Continued.)

E (eV)	10	12	14	16	18	20	30	40	50	60	70	80	90	100	120	140	160	180	200	220	240	260	280	300
$CHCl_2CHCl_2$	0.00	0.00	0.85	2.77	4.61	6.32	12.0	14.8	16.0	16.5	16.5	16.3	16.0	15.7	14.9	14.1	13.3	12.6	12.0	11.4	10.9	10.4	10.0	9.6
C_2Cl_4	0.00	0.09	0.58	2.14	3.75	5.28	10.5	13.1	14.3	14.8	14.9	14.8	14.6	14.3	13.6	13.0	12.3	11.7	11.1	10.6	10.1	9.7	9.3	8.9
cis-CHClCHCl	0.00	0.12	0.45	1.00	1.64	2.25	4.8	6.4	7.3	7.8	8.1	8.2	8.3	8.2	8.0	7.8	7.5	7.2	6.9	6.6	6.4	6.2	5.9	5.7
trans-CHClCHCl	0.00	0.12	0.43	0.99	1.59	2.23	4.8	6.3	7.3	7.8	8.1	8.2	8.2	8.2	8.0	7.7	7.4	7.2	6.9	6.6	6.4	6.1	5.9	5.7
$CHClCCl_2$	0.00	0.12	0.61	1.91	3.23	4.47	8.7	10.8	11.9	12.3	12.4	12.3	12.2	11.9	11.4	10.8	10.3	9.8	9.3	8.9	8.5	8.1	7.8	7.5
1-C_3H_7Cl	0.00	0.07	0.62	1.47	2.43	3.39	6.9	8.9	9.9	10.4	10.5	10.6	10.5	10.3	9.9	9.5	9.0	8.6	8.2	7.9	7.5	7.2	6.9	6.7
1-C_4H_9Cl	0.00	0.08	0.76	1.80	2.98	4.15	8.5	11.0	12.2	12.8	13.1	13.1	13.0	12.8	12.3	11.7	11.2	10.7	10.2	9.7	9.3	8.9	8.6	8.3
2-C_3H_7Cl	0.00	0.20	0.96	1.95	3.03	4.10	7.8	9.8	10.7	11.1	11.2	11.1	11.0	10.8	10.3	9.8	9.3	8.8	8.4	8.0	7.7	7.3	7.0	6.8
2-C_4H_9Cl	0.00	0.20	1.04	2.23	3.54	4.82	9.4	11.8	13.0	13.5	13.7	13.6	13.4	13.2	12.6	12.0	11.4	10.9	10.3	9.9	9.4	9.0	8.7	8.3