Isotopic Compositions of the Elements 1989

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Isotopic Compositions of the Elements 1989

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Received June 3, 1991

The Subcommittee for Isotopic Abundance Measurements (SIAM) of the IUPAC Commission on Atomic Weights and Isotopic Abundances has carried out its biennial review of isotopic compositions, as determined by mass spectrometry and other relevant methods. The Subcommittee's critical evaluation of the published literature element by element forms the basis of the Table of Isotopic Compositions of the Elements as Determined by Mass Spectrometry 1989, which is presented in this Report. Atomic Weights calculated from the tabulated isotopic abundances are consistent with $A(E)$ values listed in the Table of Standard Atomic Weights 1989.

Key words: atomic weight; critical evaluation; elements; isotopic composition; mass spectrometry.

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1. Introduction

The "Table of Isotopic Compositions of the Elements as Determined by Mass Spectrometry 1983", published in 1984 (Ref. 1), was the culmination of a 10 year effort by the Commission on Atomic Weights and Isotopic Abundances (CAWIA) of the International Union of Pure and Applied Chemistry to assemble a set of abundances yielding atomic weights consistent with the Commission's "Table of Standard Atomic Weights 1983" (Ref. 2, 3 4).

The Commission, through its Subcommittee for Isotopic Abundance Measurements (SIAM), has continued to assemble and evaluate new data which has led to changes in the representative isotopic compositions of nine chemical elements. Also in 1984 the statistical guidelines for assigning uncertainties to the representative abundances were re-examined by the Commission's Working Party on Statistics for Atomic Weights which led to changes in the uncertainties on some representative isotopic compositions.

At the 35th IUPAC General Assembly in Lund in 1989 the Commission therefore decided to publish an updated table incorporating these changes as a companion paper to the Report on the Atomic Weights of the Elements 1989. The present paper is the result of this decision.

Membership of the Commission for the period 1987-1989 was as follows: J. R. De Laeter (Australia, Chairman); K. G. Heumann (FRG, Secretary); R. C. Barber (Canada, Associate); L. L. Barnes (USA, Associate); J. W. Césario (France, Titular); T. L. Chang (China, Titular); J. W. Gramlich (USA, Associate); H. R. Krouse (Canada, Associate); I. A. Lebedev (USSR, Associate); T. J. Murphy (USA, Associate); K. J. Rosman (Australia, Titular); M. P. Seyfried (FRG, Associate) M. Shima (Japan, Titular); K. Wade (UK, Associate); P. De Bièvre (Belgium, National Representative); R. L. Martin (Australia, National Representative); H. S. Peiser (USA, National Representative).

The Commission dedicates this report to Dr. I. Lynus Barnes who died in January, 1990. Dr. Barnes was an associate and titular member of the Commission for 14 years, Secretary of the Subcommittee on the Assessment of the Isotopic Compositions of the Elements (SIAC) from 1975 to 1983, and Chairman of the Commission's Subcommittee for Isotopic Abundance Measurements (SIAM) from 1983 to 1989.

2. General References


3. Introduction to the Table of Isotopic Compositions of the Elements as Determined by Mass Spectrometry

3.1. Introduction

The Subcommittee for Isotopic Abundance Measurements (SIAM) has examined all of the literature available to it through July 1989. The Subcommittee has evaluated these data to produce a table of recommended isotopic abundances for the elements. The table is intended to include values for normal terrestrial samples only and does not include values published for meteoritic or other extra-terrestrial materials.

Description of the contents of each of the Columns

Column 1: The elements are tabulated in ascending order of their atomic numbers.

Column 2: The names of the elements are listed using the abbreviations recommended by IUPAC.

Column 3: The mass number for each isotope is listed.

Column 4: Evaluated limits of published values: Given are the highest and lowest abundances published for each isotope from measurements which have been evaluated and accepted by the Subcommittee. The limits given include known natural variations and published data which may exceed those variations. No data are given in this Column when the absence of a range has been reliably established. The limits given do not include certain exceptional samples, these are noted with a “g” in Column 5.

Column 5: Annotations: The letters appended in this Column have the following significance:

- g: geologically exceptional specimens are known in which the element has an isotopic composition outside the limits of reported values.
- m: modified isotopic compositions may be found in commercially available material because it has been subjected to an undisclosed or inadvertent isotopic separation. Substantial deviations from the isotopic compositions given can occur.
- r: range in isotopic composition in normal terrestrial material is responsible for part, or all, of the difference between limits of reported values.

Column 6: The best measurement from a single terrestrial source.

The values are reproduced from the original literature. The uncertainties on the last digits are given in parenthesis as reported in the original publication. As they are not reported in any uniform manner in the literature, SIAM indicates this as follows: 1, 2, 3s indicates 1, 2, 3 standard deviations, P indicates some other error as defined by the author, and se (standard deviation of the mean) indicates standard error. Where no errors are listed, none were given by the author. “C” is appended when the measurement has been calibrated and is thus believed to be “absolute” within the errors stated in the original publication. “D” is appended when the data have been corrected for fractionation by the use of the “double spike” technique.

The user is cautioned that: a) Since the data are reproduced from the literature, the sum of the isotopic abundances may not equal 100 percent; b) When a range of compositions has been established, the samples used for the best measurement may come from any part of the range; c) A “Best Measurement” is not necessarily a good one in SIAM’s opinion.

Column 7: The reference shown is that from which the data shown in column 6 was taken. The complete citation is given in Appendix A.

Column 8: Reference materials or samples which are known to be available and which relate to the best measurement are listed. An asterisk indicates the reference material used for the best measurement. Additional information is given in Appendix B.

Column 9: Representative isotopic composition.

In this Column are listed the values for the isotopic composition of the elements which, in the opinion of SIAM, will include the chemicals and/or materials most commonly
encountered in the laboratory. They may not, therefore correspond to the most abundant natural material. For example, in the case of hydrogen, the deuterium abundance quoted corresponds to that in fresh water in temperate climates rather than to ocean water. The uncertainties listed in parenthesis cover the range of probable variations of the materials as well as experimental errors. Uncertainties quoted are from one to nine in the last digit except for a few cases where rounded values would be outside of the observed range. In those cases uncertainties greater than nine have been used.

### 3.2. Warning

1. Representative isotopic composition should be used to evaluate average properties of material of unspecified natural terrestrial origin, though no actual sample having the exact composition listed may be available.

2. When precise work is undertaken, such as assessment of individual properties, samples with more precisely known isotopic abundances (such as those listed in Column 8) should be obtained or suitable measurements should be made.

#### Table of isotopic compositions of the elements as determined by mass spectrometry

<table>
<thead>
<tr>
<th>Atomic Number</th>
<th>Element</th>
<th>Mass Number</th>
<th>Evaluated limits of published values (Atom %)</th>
<th>Best measurement from a single natural source (Atom %)</th>
<th>Reference (Appendix A)</th>
<th>Available reference materials (Appendix B)</th>
<th>Representative isotopic composition (Atom %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H</td>
<td>1</td>
<td>99.9918 - 99.9816</td>
<td>r,g</td>
<td>70HAG1</td>
<td>IAEA VSMOW*</td>
<td>99.984426 (5) 2s C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2</td>
<td>0.0184 - 0.0082</td>
<td>m</td>
<td>IAEA SLAP</td>
<td>C.E.A.</td>
<td>0.015574 (5)</td>
</tr>
<tr>
<td>2</td>
<td>He</td>
<td>3</td>
<td>0.0041 - 4.6×10^{-8}</td>
<td>r,g</td>
<td>88HAG1</td>
<td>Air*</td>
<td>0.0001234 (13) 2s C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4</td>
<td>100 - 99.959</td>
<td>m</td>
<td>NIST-SRM</td>
<td></td>
<td>99.9998657 (13)</td>
</tr>
<tr>
<td>3</td>
<td>Li</td>
<td>6</td>
<td>7.68 - 7.30</td>
<td>r,g</td>
<td>83HAG1</td>
<td>NIST-RS LSVEC</td>
<td>7.5 (7) P</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7</td>
<td>92.70 - 92.32</td>
<td>m</td>
<td>NIST-SRM</td>
<td></td>
<td>92.475 (29)</td>
</tr>
<tr>
<td>4</td>
<td>Be</td>
<td>9</td>
<td>-</td>
<td>100</td>
<td>63LE1I</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>5</td>
<td>B</td>
<td>10</td>
<td>20.316 - 19.098</td>
<td>r,m</td>
<td>69BIE1</td>
<td>CBNM-GEEL 011*</td>
<td>19.82 (2) C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>11</td>
<td>80.902 - 79.684</td>
<td>g</td>
<td>NIST-SRM</td>
<td></td>
<td>80.18 (2)</td>
</tr>
<tr>
<td>6</td>
<td>C</td>
<td>12</td>
<td>98.99 - 98.86</td>
<td>m</td>
<td>57CRA1</td>
<td>NIST-RS 20*</td>
<td>98.889 (3) P</td>
</tr>
<tr>
<td></td>
<td></td>
<td>13</td>
<td>1.15 - 1.01</td>
<td>m</td>
<td>NIST-SRM</td>
<td></td>
<td>1.111 (3)</td>
</tr>
<tr>
<td>7</td>
<td>N</td>
<td>14</td>
<td>99.651 - 99.622</td>
<td>r,g</td>
<td>58JUN1</td>
<td>Air*</td>
<td>99.6337 (4) C</td>
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<tr>
<td></td>
<td></td>
<td>15</td>
<td>0.378 - 0.349</td>
<td>m</td>
<td>NIST-RS NSVEC*</td>
<td></td>
<td>0.366 (4)</td>
</tr>
<tr>
<td>8</td>
<td>O</td>
<td>16</td>
<td>99.7771 - 99.7539</td>
<td>r</td>
<td>76BAE1</td>
<td>NIST-RS 20*</td>
<td>99.7628 (5) 1s</td>
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<tr>
<td></td>
<td></td>
<td>17</td>
<td>0.0407 - 0.035</td>
<td>m</td>
<td>NIST-SRM</td>
<td></td>
<td>0.0372 (4)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>18</td>
<td>0.2084 - 0.1879</td>
<td>m</td>
<td>IAEA VSMOW*, IAEA SLAP</td>
<td></td>
<td>0.20004 (5)</td>
</tr>
<tr>
<td>9</td>
<td>F</td>
<td>19</td>
<td>-</td>
<td>100</td>
<td>20AST1</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>10</td>
<td>Ne</td>
<td>20</td>
<td>90.541 - 88.47</td>
<td>r,g</td>
<td>84BOT1</td>
<td>IAEA*</td>
<td>90.484 (9) 1s C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>21</td>
<td>1.70 - 0.366</td>
<td>m</td>
<td>NIST-SRM</td>
<td></td>
<td>0.270 (4)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>22</td>
<td>9.96 - 9.20</td>
<td>m</td>
<td>NIST-SRM</td>
<td></td>
<td>9.246 (9)</td>
</tr>
<tr>
<td>11</td>
<td>Na</td>
<td>23</td>
<td>-</td>
<td>100</td>
<td>56WHI1</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>12</td>
<td>Mg</td>
<td>24</td>
<td>-</td>
<td>66CAT1</td>
<td>NIST-SRM 980*</td>
<td></td>
<td>78.992 (25) 2s C</td>
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<tr>
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<td></td>
<td>25</td>
<td>-</td>
<td>NIST-SRM 980*</td>
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<td>10.003 (9)</td>
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<td></td>
<td>26</td>
<td>-</td>
<td>NIST-SRM 980*</td>
<td></td>
<td></td>
<td>11.025 (19)</td>
</tr>
<tr>
<td>13</td>
<td>Al</td>
<td>27</td>
<td>-</td>
<td>100</td>
<td>56WHI1</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>14</td>
<td>Si</td>
<td>28</td>
<td>92.41 - 92.14</td>
<td>r</td>
<td>75BAR1</td>
<td>NIST-SRM 990*</td>
<td>92.22933 (155) 2s C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>29</td>
<td>4.73 - 4.57</td>
<td>m</td>
<td>IAEA VSMOW*, IAEA SLAP</td>
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<td>4.66982 (124)</td>
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<tr>
<td></td>
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<td>30</td>
<td>3.14 - 3.01</td>
<td>m</td>
<td>IAEA VSMOW*, IAEA SLAP</td>
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<td>3.10085 (74)</td>
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</table>

Table of isotopic compositions of the elements as determined by mass spectrometry — Continued

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<thead>
<tr>
<th>Atomic Number</th>
<th>Mass Number</th>
<th>Element</th>
<th>Evaluated limits of published values (Atom %)</th>
<th>Best measurement from a single natural source (Atom %)</th>
<th>Reference (Appendix A)</th>
<th>Available reference materials (Appendix B)</th>
<th>Representative isotopic composition (Atom %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>31</td>
<td>P</td>
<td></td>
<td>100</td>
<td>63LEI1</td>
<td></td>
<td></td>
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<tr>
<td>16</td>
<td>32</td>
<td>S</td>
<td>95.253 – 94.638</td>
<td>95.018 (4)</td>
<td>50MAC1</td>
<td>IAEA</td>
<td>95.02 (9)</td>
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<tr>
<td></td>
<td>33</td>
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<td>0.780 – 0.731</td>
<td>0.750 (7)</td>
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<td>C.E.A.</td>
<td>0.75 (4)</td>
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<td>4.562 – 4.001</td>
<td>4.215 (4)</td>
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<td>4.21 (8)</td>
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<td>36</td>
<td></td>
<td>0.0199 – 0.0153</td>
<td>0.017 (2)</td>
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<td>0.02 (1)</td>
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<tr>
<td>17</td>
<td>35</td>
<td>Cl</td>
<td>75.872 – 75.72</td>
<td>75.771 (45)</td>
<td>62SHI1</td>
<td>NIST-SRM 975*</td>
<td>75.77 (7)</td>
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<td>37</td>
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<td>24.28 – 24.128</td>
<td>24.229 (45)</td>
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<td>24.23 (7)</td>
</tr>
<tr>
<td>18</td>
<td>36</td>
<td>Ar</td>
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<td>0.3365 (6)</td>
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<td>Air*</td>
<td>0.337 (3)</td>
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<td></td>
<td>38</td>
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<td>0.0632 (1)</td>
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<td>0.063 (1)</td>
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<td>99.600 (3)</td>
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<td>(for air only)</td>
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<tr>
<td>19</td>
<td>39</td>
<td>K</td>
<td></td>
<td>93.25811 (292)</td>
<td>75GAR1</td>
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<td>93.2581 (44)</td>
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<td>96.98213 – 96.88</td>
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<td>72MOO1</td>
<td>NIST-SRM 915*</td>
<td>96.941 (18)</td>
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<td>0.6562 – 0.640</td>
<td>0.647 (3)</td>
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<td>0.647 (9)</td>
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<td>43</td>
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<td>0.1457 – 0.1312</td>
<td>0.135 (2)</td>
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<td>0.135 (6)</td>
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<td>44</td>
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<td>2.066 (4)</td>
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<td>2.086 (12)</td>
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<td>0.0046 – 0.00313</td>
<td>0.004 (1)</td>
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<td>0.004 (3)</td>
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<td>48</td>
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<td>0.200 – 0.179</td>
<td>0.187 (1)</td>
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<td>0.187 (4)</td>
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<tr>
<td>21</td>
<td>45</td>
<td>Sc</td>
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<td>50LEL1</td>
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<tr>
<td>22</td>
<td>46</td>
<td>Ti</td>
<td></td>
<td>8.0124 (1)</td>
<td>81NIE1</td>
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<td>8.0 (1)</td>
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<td>49</td>
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<td>5.4964 (3)</td>
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<td>5.5 (1)</td>
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<td></td>
<td>50</td>
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<td>5.3458 (3)</td>
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<td>5.4 (1)</td>
</tr>
<tr>
<td>23</td>
<td>50</td>
<td>V</td>
<td></td>
<td>0.2497 (6)</td>
<td>66FLE1</td>
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<td>0.250 (2)</td>
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<td>99.7503 (6)</td>
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<td>4.345 (13)</td>
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<td>52</td>
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<td>83.789 (18)</td>
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<td>53</td>
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<td>9.5006 (110)</td>
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<td>9.501 (17)</td>
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<td>Mn</td>
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<td>26</td>
<td>54</td>
<td>Fe</td>
<td>6.04 – 5.77</td>
<td>5.81</td>
<td>47VAL1</td>
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<td>5.8 (1)</td>
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<td>56</td>
<td></td>
<td>91.79 – 91.52</td>
<td>91.75</td>
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<td></td>
<td>91.72 (30)</td>
</tr>
<tr>
<td></td>
<td>57</td>
<td></td>
<td>2.25 – 2.11</td>
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<td>2.2 (1)</td>
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<td>77BRO1</td>
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<td>U</td>
<td>234</td>
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<td>0.7202 - 0.7198</td>
<td>0.7200 (1)</td>
<td>76COW1</td>
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<td>99.2752 - 99.2739</td>
<td>99.2745 (10)</td>
<td>99.2745 (60)</td>
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* Available hydrogen gases vary from 0.0032% to 0.0184% D.

* Enriched 3Li is a commercial source of lithium.

* The reference reported a calibrated O/H ratio on VSMOW, the O was derived from a measurement on air.

* Due to 115In contamination the 115Sn abundance reported by 84ROS1 was adjusted using data from 84ROS1.

* Representative isotopic composition is for most but not all commercial samples.

* The 234U abundance is from 69SM11, 235U and 238U are from 76COW1.

* Indicates the reference material used for the best measurement.
Appendix A: References


57COL1 W. T. Leland, Phys. Rev. 77, 634 (1950). The Isotopic Composition of Scandium, Gadolinium, and Dysprosium.


ISOTOPIC COMPOSITIONS OF THE ELEMENTS 1989 1337


Appendix B: Sources of Reference Materials

I.A.E.A.

Samples such as VSMOW, SLAP, and GISP may be obtained from:

International Atomic Energy Agency
Sec. of Isotope Hydrology
P. O. Box 100
1400 Vienna, Austria

Dr. Robert D. Vocke, Jr.
National Institute of Standards and Technology
A23 Physics Building
Gaithersburg, MD 20899 U.S.A.

NIST-SRM's

NIST Standard Reference Materials may be purchased through:

Office of Standard Reference Materials
National Institute of Standards and Technology
B-311, Chemistry Building
Gaithersburg, MD 20899 U.S.A.

CBNM-GEEFL

Reference Materials may be obtained through:

Dr. Paul De Bièvre
Central Bureau for Nuclear Measurements
Commission of the European Communities
B-2440 Geel, Belgium

NBS-RS (Reference Samples)

Samples may be obtained through:

Dr. Robert D. Vocke, Jr. (Address above)
NOTE: Samples of N and Li previously available from Professor H. J. Svec have been sent to NIST for distribution.

C.E.A.

Standards may be obtained through:

Dr. 1. Césarès
Centre d'Etudes Nucléaires de Saclay
B.P. no 2 - 91990 Gif-sur-Yvette France

NBL

Standards may be obtained through:

U.S. Department of Energy
New Brunswick Laboratory
9800 S. Cass Ave.
Argonne IL 60439

Errata

Erratum: Cross Sections and Swarm Coefficients for H+, H2+, H3+, H, H2, and H− in H2 for Energies from 0.1 eV to 10 keV


A.V. Phelps

Joint Institute for Laboratory Astrophysics, University of Colorado and National Institute of Standards and Technology, Boulder, CO 80309-0440

Semrad and Golser1 have pointed out that in our comparison of stopping powers for H atoms in H2 calculated in Ref. 2 from cross sections and from conventional stopping power expressions we have omitted two important contributions to the stopping power at high energies. They also point out that our evaluation of the energy required for excitation requires modification to take into account the effect of Lyman β emission on the analysis and the fact that much of the excitation of H atoms is by projectile excitation rather than by dissociative excitation.2 These corrections have been made in Fig. 1 and Table 1 of this erratum which should replace Fig. 2 and Table 2 of the original paper. The notation of the figure and table is the same as in the original article, except for that of the additional curve discussed below.

The first correction results from the transformation into the center-of-mass frame, from the change in mass of the projectile caused by electron transfer, and from the transformation back to the laboratory frame.4 In general, the fractional energy loss by the projectile is \( m/(M + m) \), where \( m \) is the electron mass and \( M \) is the target mass. With H2 as the target, this energy loss by the projectile is 2.7 eV at a projectile energy of 10 keV. Note that this energy appears as a recoil of the H2+ for small angle scattering of the projectile, whereas the recoil indicated in Fig. 1 by the curve labeled RECOIL is the result of large angle scattering of the projectile.

The second correction results from the inadvertent omission of the contribution to the energy loss resulting from the difference in ionization potentials of the H and H2 during charge transfer. In the corrected calculation of Fig. 1 and Table 1, it is assumed that all of the electrons are captured into the ground state for which the difference between the ionization potentials of H2+ and H+ is 1.8 eV. The additional energy loss caused by electron capture into excited states is considered under excitation.

These two corrections are associated with the charge transfer process and have been combined into a single loss function shown in Fig. (1) by the dotted line labeled CHARGE TRANS. and listed in Table 1 under the heading \( L_\text{elexc} \).

Semrad and Golser1 also point out that the discussion in Ref. 2 is not clear as to details of the contribution of the excitation H atoms to \( n \geq 3 \) levels to the electronic excitation loss function \( L_\text{elexc} \). In the present recalculation of \( L_\text{elexc} \) we have included terms representing the energy loss caused by dissociative excitation of the target and by projectile excitation using the respective cross sections.2 For target dissociative excitation we have added 3 eV for the average energy of the fragments and so raised the energy loss per collision to 19.6 eV. For the projectile excitation energy loss,3 we have used an excitation energy of 15.2. For both terms the cross sections are multiplied by a factor2 of 2.1 to allow for the excitation of the higher levels of atomic H and by a factor1 of 1.33 to allow for the Lyman β not included in the experimental cross sections.3 Note that the increase in the calculated stopping power relative to the values of Ref. 2 resulting from this improved analysis of electronic excitation varies from \(< 1\% \) at 1 keV to 2.4% at 10 keV.

In summary, the addition of the energy losses caused by charge transfer in H+ + H2 collisions omitted from the original analysis of energy loss data raises the stopping power calculated from known collision processes to 50–65% of conventional stopping power theory.5 The question remains as to whether or not the uncertainties associated with the energy loss caused by ionization, the unknown excitation of radiating states of H2, the unknown dissociation of H2 to ground state H atoms, and/or errors in the cross sections can account for the remaining discrepancy.6

The author wishes to thank M. Inokuti for helpful discussions and comments on the text and D. Semrad and R. Golser for permission to cite their constructive criticism.

References

1D. Semrad and R. Golser (private communication to M. Inokuti).
Table 1. Revised energy and momentum loss functions for H⁺ + H₂ tabulated by process (Loss in units of 10⁻²⁰ eV m²)

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<th>Lab. ion energy (eV)</th>
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<th>Lₑ(ion)</th>
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FIG. 1. Energy loss $L_e$ and momentum loss $L_m$ coefficients for $H^+$ in $H_2$ versus $H^+$ laboratory energy. The solid curves show the total loss coefficients defined by Eqs. (1) and (3) of Ref. 2 from 0.1 eV to 10 keV. The dashed curves show the contributions resulting from elastic recoil (RECOIL), rotational excitation (ROT.), vibrational excitation (VIB.), electronic excitation (ELECT. EXCIT.), ionization (ION.), and charge transfer (CHARGE TRANS.). The short solid curve shows the recommended stopping power results of Andersen and Ziegler, while the chain curve is the sum of the various excitation, ionization, and charge transfer curves, but does not include the recoil loss due to large angle scattering of the $H^+$ ion. The loss coefficients for $H^+$ in $H_2$ are listed in Table 2.