https://doi.org/10.61092/iaea.725g-0hgn
IAEA-NDS-0246

INTERNATIONAL ATOMIC ENERGY AGENCY

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Tcalc

A tool for calculation of reaction Q-values and threshold energies

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March 2024

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96/11

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Abstract

Tcalc calculates reaction Q-values and threshold energies for a given projectile and target with the mass table prepared by the Atomic Mass Data Center (AMDC). The users can additionally specify the combination of the outgoing particles and/or the residual nuclide. The package is available on request from the authors. Its web interface is also available at http://www.jcprg.org/tcalc/.

March 2024

1. Introduction

Tcalc calculates reaction Q-values and threshold energies for a given projectile particle or nuclide and target nuclide. The ejectile particle combination and residual nuclide are optional. Consider the case where a projectile with laboratory energy E_b and mass m_b interacts with the target nuclide with mass m_A at rest to produce particles 1 to n:

$$A + b \rightarrow 1 + 2 + 3 + \ldots + n$$

Tcalc calculates the reaction Q-values Q and threshold energies $E_{b,\mathrm{thr}}$ by

$$Q = (m_A + m_b) - \sum_{i=1}^{n} m_i$$

$$E_{b,\mathrm{thr}} = \left[\left(\sum_{i=1}^{n} m_i\right)^2 - (m_A + m_b)^2\right] \Big/ 2m_A$$

with the light velocity c=1 and the Q-values, threshold energy and masses in keV.

2. Input specification

2.1. Mass table (mass.mas.txt)

Columns	Description
10-14	Atomic number
15-19	Mass number
21-23	Elemental symbol
29-43	Mass excess

This is the format adopted in AME2020 file (mass_1.mas20).

Note: If the AME file is renamed to mass.mas.txt and used, the head lines must be commented out by # at the first column of each header line.

2.2. Standard input

Lines	Description	Example - ^{27}Al(n,α)^{24}Na
1	Target atomic and mass numbers	`2 3`
2	Projectile atomic and mass numbers	`0 1`
3*	Residual nuclide	`11 24`
4*	Number of outgoing particles: photon (g), neutron (n), proton (p), deuteron (d), triton (t), helion (h), alpha (a)	`0 0 0 0 0 0 1`

*One of these lines is optional, but must be filled by zeros (`0`) if not specified.

Note: Integers on the same line must be separated by one or more space.

3. Output specification

Lines	Columns	Description	Example - $^{27}Al(n,\alpha)^{24}Na$
1	1-5	Target atomic number	13
	6-10	Target mass number	27
	11-15	Target elemental symbol	Al
	16-30	Target mass (MeV)	25133.143890
	32-34	Target mass unit	MeV
2	1-5	Projectile atomic number	0
	6-10	Projectile mass number	1
	11-15	Projectile elemental symbol	N
	16-30	Projectile mass (MeV)	939.565420
	32-34	Projectile mass unit	MeV
3	1-5	Product atomic number	11
	6-10	Product mass number	24
	11-15	Product elemental symbol	Na
	16-30	Product mass (MeV)	22347.440547
	32-34	Product mass unit	MeV
4	1-5	Number of channels n (0 when there is an error)	6
5	1-40	Error message	
6	1-65	Header line	
7	1-5	Number of outgoing photon in channel 1	0
	6-10	Number of outgoing neutron in channel 1	0
	11-15	Number of outgoing proton in channel 1	0
	16-20	Number of outgoing deuteron in channel 1	0
	21-25	Number of outgoing triton in channel 1	0
	26-30	Number of outgoing helion in channel 1	0
	31-35	Number of outgoing alpha in channel 1	1
8	1-5	Number of outgoing photon in channel 2	0
…	…	…	…
7+n	1-65	Footer line	

4. Input/Output Examples

4.1. Target=^{27}Al, Projectile=n, Product=^{24}Na

Input

```
13 27
 0  1
11 24
 0  0  0  0  0  0  0
```

Output

```
   13   27   Al   25133.143890 MeV
    0    1    n     939.565420 MeV
   11   24   Na   22347.440547 MeV
6

    g    n    p    d    t    h    a      Qval(MeV)      Ethr(MeV)
    0    0    0    0    0    0    1      -3.132561       3.249862
    0    0    1    0    1    0    0     -22.946427      23.814720
    0    1    0    0    0    1    0     -23.710182      24.607736
    0    0    0    2    0    0    0     -26.979091      28.002144
    0    1    1    1    0    0    0     -29.203657      30.312359
    0    2    2    0    0    0    0     -31.428223      32.622771
-----------------------------------------------------------------
```

4.2. Target=^{27}Al, Projectile=n, Ejectile=α

Input

```
13 27
 0  1
 0  0
 0  0  0  0  0  0  1
```

Output

```
   13   27   Al   25133.143890 MeV
    0    1    n     939.565420 MeV
   11   24   Na   22347.440547 MeV
1

    g    n    p    d    t    h    a      Qval(MeV)      Ethr(MeV)
    0    0    0    0    0    0    1      -3.132561       3.249862
-----------------------------------------------------------------
```

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