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Tcalc

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

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96/11

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

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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/.

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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:

$$\mathbf{A} + \mathbf{b} \rightarrow \mathbf{1} + \mathbf{2} + \mathbf{3} + \ldots + \mathbf{n}$$

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

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

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
FR1 · · · 1 · 0	

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 - ${}^{27}Al(n,\alpha){}^{24}Na$
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:	0 0 0 0 0 0 1
	photon (g), neutron (n), proton (p),	
	deuteron (d), triton (t), helion (h), alpha (a)	
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,α) 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	Ν
	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	6
		(0 when there is an error)	
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=²⁷Al, Projectile=n, Product=²⁴Na

Input

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

Output

	13 0	27 1	Al	2513 93	3.143	890 M 420 M	leV leV		
	11	24	Na	2234	7.440	547 M	leV		
6									
	g	n	р	d	t	h	а	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=²⁷Al, Projectile=n, Ejectile=α

Input

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

Output

13 0	27 1	Al n	2513 93	3.143 9.565	890 M 420 M	eV eV		
11	24	Na	2234	7.440	547 M	eV		
g	n	р	d	t	h	а	Qval(MeV)	Ethr(MeV)
0	0	0	0	0	0	1	-3.132561	3.249862
	13 0 11 g 0	13 27 0 1 11 24 g n 0 0	13 27 Al 0 1 n 11 24 Na g n p 0 0 0	13 27 Al 2513 0 1 n 93 11 24 Na 2234 g n p d 0 0 0 0	13 27 Al 25133.143 0 1 n 939.565 11 24 Na 22347.440 g n p d t 0 0 0 0 0	13 27 Al 25133.143890 M 0 1 n 939.565420 M 11 24 Na 22347.440547 M g n p d t h 0 0 0 0 0 0	13 27 Al 25133.143890 MeV 0 1 n 939.565420 MeV 11 24 Na 22347.440547 MeV g n p d t h a 0 0 0 0 0 0 1	13 27 Al 25133.143890 MeV 0 1 n 939.565420 MeV 11 24 Na 22347.440547 MeV g n p d t h a Qval(MeV) 0 0 0 0 0 0 1 -3.132561

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