

v.9.10.131
from 07/10/15

M.H. & H.W. requests

The screenshot shows the LISE++ software interface with two main windows:

- Top Window (Databases):** Shows a menu with "Ionization energy database" highlighted with a red box and a red arrow pointing to it from the text "Ionization energy database".
- Bottom Window (Calculations):** Shows a menu with "Calculators" highlighted with a red box. A sub-menu for "Calculators" is open, listing various calculators. "Ion Mass Calculator" is highlighted with a red box and a red arrow pointing to it from the text "Ion Mass Calculator".
- Right Panel (Ion Mass Calculator / Ionisation Energy Database):** Displays a table of ionization energies for various elements. The columns include SH, Z, Q, IsoSeq, Ground Shells, IonEnergy, and Total BE.

SH	Z	Q	IsoSeq	Ground Shells	IonEnergy	Total BE
1	92	0+	U	[Rn]93.8d7s2	0.0002	761.513
1	92	1+	Th	[Rn]93.8d7s2	0.0198	761.495
1	92	2+	Ra	[Rn]93.8d7s2	0.046	761.428
1	92	3+	Ac	[Rn]93.8d7s2	0.0367	761.476
1	92	4+	Ra	[Rn]93.8d7s2	0.116	761.553
1	92	5+	Fm	[Rn]93.8d7s2	0.099	761.333
1	92	6+	Rn	[Rg]93.8d7s2	0.101	761.244
1	92	7+	Fr	[Rg]93.8d7s2	0.116	761.142
1	92	8+	Po	[Rg]93.8d7s2	0.128	761.027
1	92	9+	Bk	[Rg]93.8d7s2	0.158	760.898
1	92	10+	Pb	[Rg]93.8d7s2	0.173	760.740
1	92	11+	Tl	[Rg]93.8d7s2	0.173	760.740
1	92	12+	Hg	[Rg]93.8d7s2	0.21	760.539
1	92	13+	Fr	[Rg]93.8d7s2	0.227	760.357
1	92	14+	Pt	[Rg]93.8d7s2	0.323	760.130
1	92	15+	Ir	[Rg]93.8d7s2	0.348	759.807
1	92	16+	Os	[Rg]93.8d7s2	0.376	759.493
1	92	17+	Re	[Rg]93.8d7s2	0.402	759.084
1	92	18+	W	[Rg]93.8d7s2	0.431	758.682
1	92	19+	Ta	[Rg]93.8d7s2	0.459	758.251
1	92	20+	Hf	[Rg]93.8d7s2	0.487	757.730
1	92	21+	Lu	[Rg]93.8d7s2	0.525	757.296
1	92	22+	Yb	[Rg]93.8d7s2	0.957	756.771
1	92	23+	Tm	[Rg]93.8d7s2	0.995	756.214
1	92	24+	Dy	[Rg]93.8d7s2	0.77	755.629
1	92	25+	Ho	[Rg]93.8d7s2	0.77	754.889
1	92	26+	Dy	[Og]94.8p4	0.8	754.129
1	92	27+	Tb	[Og]94.8p3	0.84	753.329
1	92	28+	Gd	[Og]94.8p2	0.93	752.489

Ion Mass Calculator / Ionisation Energy Database

A	Element	Z
238	u	92
<input type="button" value="Stable"/>		
<input type="button" value="Table of Nuclides"/> <input type="button" value="Z"/> <input type="button" value="N"/> 		

Atom & Ion Masses

Charge State	Ground shell configuration	Total binding energy [keV]	Mass	
			amu	GeV
Q=0 atom	[Rn].5f3.6d.7s2	761.513	238.05079	221.742896
Q = <input type="text" value="7"/>	[Hg].6p5	761.244	238.04695	221.739319
Q=Z full stripped		0.000	238.00114	221.696645

Comments

Ionization energies are taken from the NIST Atomic Spectra Database <http://www.nist.gov/pml/data/asd.cfm> with in-house extrapolation for heavy ions. Their configurations are marked by the symbol "?". The database range is $1 \leq Z \leq 110$. For heavier ions no electron binding corrections. Binding energies are determined by summing up all relevant ionization energies.

$M_i(A,Z,Q) = M_A(A,Z) - Q^* Me + TBE(0) - TBE(Q)$

IselSeq -- Isoelectronic sequence
 Ground Shells -- Ground-state electronic shells
 Ioniz.Energy -- Ionization energy [keV]
 Total BE -- Total binding energy [keV]

Designations used in the ground shell lists:

- [Ne] = 1s²2s²2p⁶
- [Ar] = [Ne].3s²3p⁶
- [Kr] = [Ar].3d¹⁰4s²4p⁶
- [Cd] = [Kr].4d¹⁰5s²
- [Xe] = [Cd].5p⁶
- [Hg] = [Xe].4f¹⁴5d¹⁰6s²
- [Rn] = [Hg].6p⁶

"U" --- Z = 92 --- Uranium

Shl.	Z	Q	IsoelSeq	Ground Shells	Ioniz.Energy	Total BE
7	92	0+	U	[Rn].5f3.6d.7s2	0.0062	761.513
7	92	1+	Pa	[Rn].5f3.7s2	0.0116	761.507
5	92	2+	Th	[Rn].5f4	0.0198	761.495
5	92	3+	Ac	[Rn].5f3	0.0367	761.476
5	92	4+	Ra	[Rn].5f2	0.046	761.439
5	92	5+	Fr	[Rn].5f	0.06	761.393
6	92	6+	Rn	[Hg].6p6	0.089	761.333
6	92	7+	At	[Hg].6p5	0.101	761.244
6	92	8+	Po	[Hg].6p4	0.116	761.143
6	92	9+	Bi	[Hg].6p3	0.129	761.027
6	92	10+	Pb	[Hg].6p2	0.158	760.898
6	92	11+	Tl	[Hg].6p	0.173	760.740
6	92	12+	Hg	[Xe].4f14.5d10.6s2	0.21	760.567
6	92	13+	Au	[Xe].4f14.5d10.6s	0.227	760.357
5	92	14+	Pt	[Xe].4f14.5d10	0.323	760.130
5	92	15+	Ir	[Xe].4f14.5d9	0.348	759.807
5	92	16+	Os	[Xe].4f14.5d8	0.375	759.459
5	92	17+	Re	[Xe].4f14.5d7	0.402	759.084
5	92	18+	W	[Xe].4f14.5d6	0.431	758.682
5	92	19+	Ta	[Xe].4f14.5d5	0.458	758.251
5	92	20+	Hf	[Xe].4f14.5d4	0.497	757.793
5	92	21+	Lu	[Xe].4f14.5d3	0.525	757.296
5	92	22+	Yb	[Xe].4f14.5d2	0.557	756.771
5	92	23+	Tm	[Xe].4f14.5d	0.585	756.214
4	92	24+	Er	[Xe].4f14	0.73	755.629
5	92	25+	Ho	[Cd].4f14.5p5	0.77	754.899
5	92	26+	Dy	[Cd].4f14.5p4	0.8	754.129
5	92	27+	Tb	[Cd].4f14.5p3	0.84	753.329
5	92	28+	Gd	[Cd].4f14.5p2	0.93	752.489

You can enter Q manually in the cell or click by mouse in the table

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- Ion mass Calculator
- Ionization Energy Database
- Ion mass corrections on electron binding energy

v.9.8.114

238.0508	amu
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Physical calculator

v.9.8.117

A	Element	Z	Q		
238	U	92	92		
<input type="button" value="Table of Nuclides"/>					
<input type="button" value="Stable"/>		<input type="button" value="Z"/>			
<input type="button" value="N"/>		<input type="button" value=""/>			
Ion mass = 238.0003 amu					
Energy	99.9999	MeV/u	Energy	100	AMeV
Brho	3.8232	Tm	TKE	23800	MeV
Erho	492.983	MJ/C	Velocity	12.8769	cm/ns
P	105447	MeV/c	Beta	0.4295284	
p_trnspt	1.146168	GeV/c	Gamma	1.107354	

Physical calculator

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A	Element	Z	Q		
238	U	92	92		
<input type="button" value="Table of Nuclides"/>					
<input type="button" value="Stable"/>		<input type="button" value="Z"/>			
<input type="button" value="N"/>		<input type="button" value=""/>			
Ion mass = 238.0011 amu					
Energy	99.9995	MeV/u	Energy	100	AMeV
Brho	3.82321	Tm	TKE	23800	MeV
Erho	492.983	MJ/C	Velocity	12.8769	cm/ns
P	105448	MeV/c	Beta	0.4295277	
p_trnspt	1.14617	GeV/c	Gamma	1.107354	

The “Production mechanism” dialog

The Check box to take into account electron binding energies for ion mass calculation in the code. For debug and comparison purpose. It is recommended to use.

Note: the Ionization energy database (Ion mass calculator) is always taking into account electron binding energies in spite of the production mechanism settings

