Amy Barr
2/18/2010

Dunite ANEOS in CTH with parameters suitable for molecular ANEOS in CTH 9.1. This EOS matches that used by Canup SPH simulations of the moon-forming impact. It is implemented in CTH 9.1 as DUNITE_MOL.

Number	Value	Description
V1	3	Nel; number of elements in material (H,O)
V2	4	EOS; EoS Type; Solid-gas with electronic terms and detailed treatment of liquid/vapor region
V3	3.32 g/cm^3	ρ_o; reference density
V4	0.	reference temperature defaults to 298 K.
V5	0	p_o, reference pressure
V6	-6.6e5 cm/s	S_o, from shock-particle velocity relation, $u_s=S_o+S_1u_p$ Neg sign required.
V7	0.82	Γ_o, reference Gruneisen coefficient
V8	0.057 eV	Reference Debye temperature
V9	0.86	S_1 from linear shock-particle velocity relation, $u_s=S_o+S_1u_p$
V10	2	3 times the limiting value of Γ at large compressions
V11	1.3e11 erg/g	E_{sep}, Zero-T separation energy
V12	0.19 eV	T_m, the melting temperature
V13	1.97e11	parameter c_{53}, for low density modification to move the critical point
V14	0.8	parameter c_{54}, for low density modification to move the critical point
V15	0	H_0, thermal conductivity parameter; 0 if not included
V16	0	c_{41}, thermal conductivity parameter; 0 if not included
V17	0.0	Lowest allowed solid density; defaults to $0.9\rho_o$
V18	4.65	Density at onset of high-pressure phase transition (hppt)
V19	4.9	Density at completion of hppt
V20	6.6e11 dyn/cm^2	Pressure at center of hppt
V21	3.5e12 dyn/cm^2	dP/dη at end of hppt
V22	1.3e13 dyn/cm^2	d^{2}P/dη^2 at end of hppt
V23	0	H_{fus}, heat of fusion (not used)
V24	0	Density of liquid at the melting point (not used)
V25 ...	0	Parameters V25 through V32 not used in this type of EOS,
...V32	0	so type a whole row of zeroes
V33	1	Flag for ionization model. 0=Saha; 1=Thomas-Fermi
V34	0	E_{shift}, shift energy for reactive chemistry modeling.
V35	0	S_{shift}, shift entropy for reactive chemistry modeling.
V36^m	2	Number of atoms in molecular clusters (Melosh 2007)
V37^m	8.0 eV	Bond energy
V38^m	0	Rotational degrees of freedom
V39^m	1.5e-8 cm	Bond length
V40^m	0	Vibrational degrees of freedom
V41^m	0.1723 eV	=2000 K, Vibrational Debye temperature (probably not used)
V42^m	1	Flags use of Lennard-Jones (in this case, Mie) potential
V43^m	1.27	Exponent in Mie potential (P_{cold}), should be 1.25 but CTH barfs
V44-V48	0	Not used

Z	f
8.	0.571
12.	0.286
14.	0.143