Appendix Materials for "A revised diamond-graphite transition curve"

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deposit number AM-12-001
Jan 2012 issue of American Mineralogist, pages 52-62,
DOI: http://dx.doi.org/10.2138/am.2011.3763

Figure A1. Deviations of measured graphite heat capacity from the selected values of Chase (1998). Abbreviations: CM, Cezairliyan and Miiller (1985); CR, Cezairliyan and Righini (1975, po: poco graphite; py: pyrolitic graphite); M, Macdonald (1965); WI, West and Ishihara (1965).

Figure A2. Heat capacity of graphite versus temperature. The smoothed data from Chase et al. (1998) are constrained by measurements up to 3000 K. Abbreviations: C, Chase (1998); G, Gustafson (1986); H&P, Holland and Powell (1998).

Figure A3. Deviations of graphite heat capacity functions from the selected values of Chase (1998). Abbreviations: E, Evans (1960); G, Gustafson (1986); Gl, Glusko et al. (1979); H, Hultgren et al. (1973); H&P, Holland and Powell (1998); RH, Robie and Hemingway (1995).

Figure A4. Heat capacity of diamond versus temperature. Measurements of the heat capacity are restricted to temperatures below 1073 K (Victor, 1962). Abbreviations: R&W, Reeber and Wang (1996, B_0=5560); V, Victor (1962); others as in Figure A3.

Figure A5. Deviations of diamond heat capacity functions from the smoothed values of Victor (1962). R&W, Reeber and Wang (1996, B_0=5560 or 4400); others as in Figs. A3, A4.

Figure A6. Compression of graphite versus pressure at 293 K. Abbreviations: B, Bridgeman (1945,1948); G, Gustafson,(1986); H, Hanfland et al., 1989; H&P, Holland and Powell (1998); L&D, Lynch & Drickamer (1966).

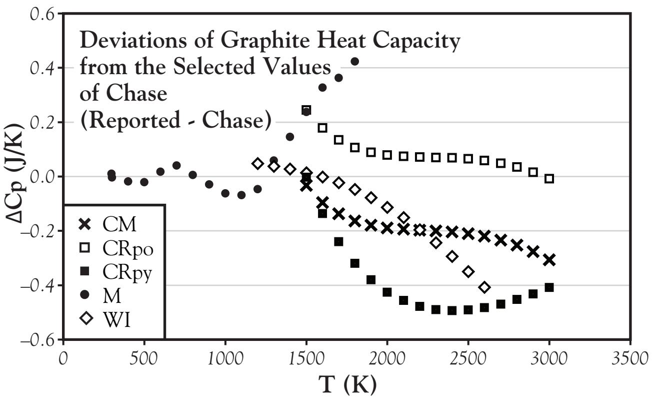
Figure A7. Compression of diamond versus pressure. Temperature was not specified but is presumed to be 293 K, as for graphite (Lynch and Drickamer, 1966). Abbreviations: D, Drickamer (1966); L&D, Lynch and Drickamer, 1966; OC03, Occelli et al., 2003.

Figure A8. Thermal expansion of graphite. Abbreviations: G, Gustafson (1986); H&P, Holland and Powell (1998); N&R, Nelson and Riley, 1945; T, Touloukian et al. (1977).

Figure A9. Thermal expansion coefficient of graphite versus temperature. Abbreviations as in Fig. A8.

Figure A10. Thermal expansion of diamond. Abbreviations: R&W, Reeber and Wang (1996), others as in Figure A8.

Figure A11. Thermal expansion coefficient of diamond versus temperature. Abbreviations as in Fig. A10, A8.



Deviations of Graphite Heat Capacity
from the Selected Values
of Chase
(Reported - Chase)
ΔCp (J/K)
T (K)
CM
CRpo
CRpy
M
WI
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000
2500
3000
3500

Fig A1

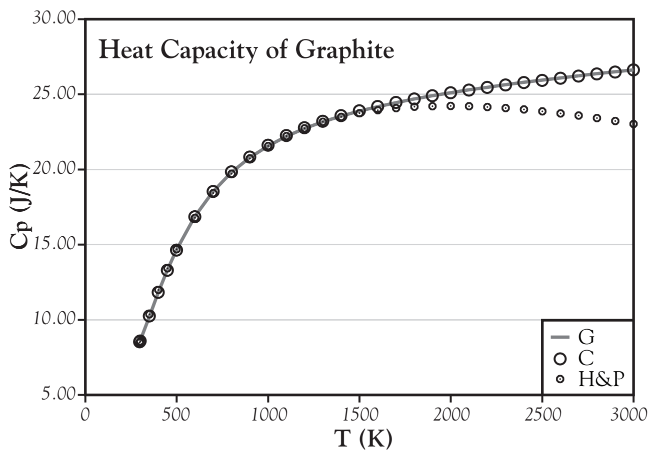
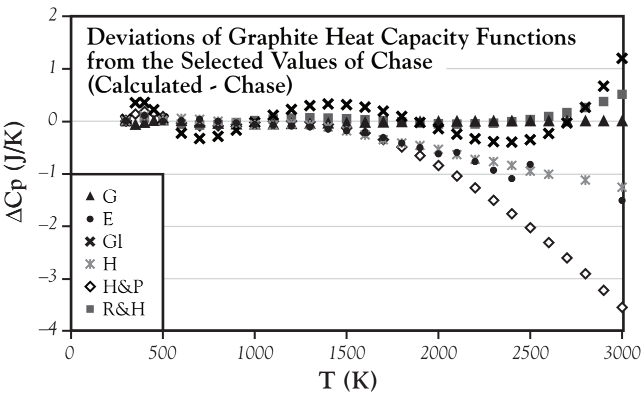
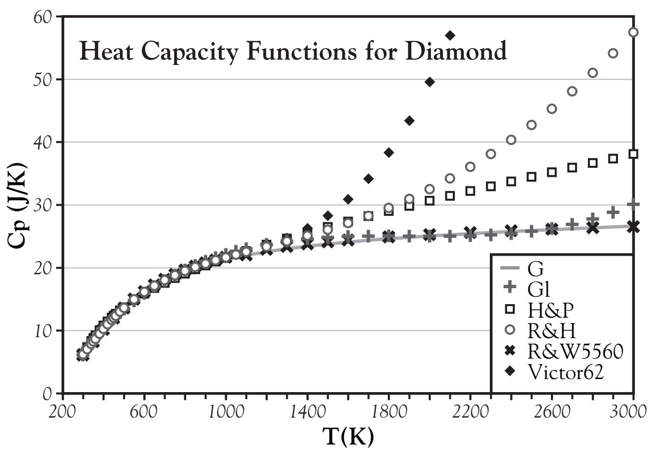

Heat Capacity of Graphite
30.00
25.00
20.00
15.00
10.00
5.00
Cp (J/K)
0
500
1000
1500
2000
2500
3000
T (K)
G
C
H&P

Fig A2



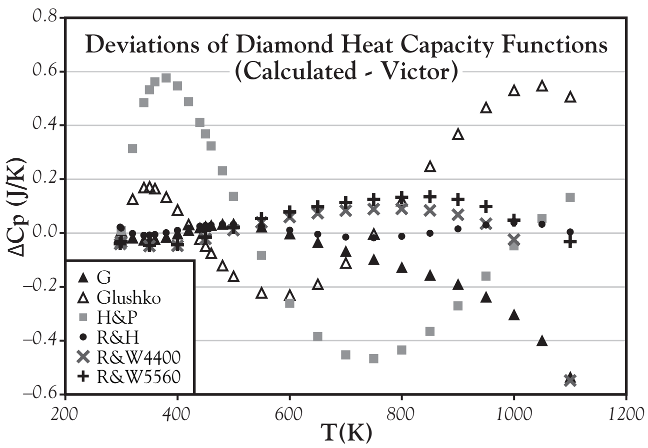
Deviations of Graphite Heat Capacity Functions
from the Selected Values of Chase
(Calculated - Chase)
ΔCp (J/K)
T (K)
G
E
Gl
H
H&P
R&H

Fig A3



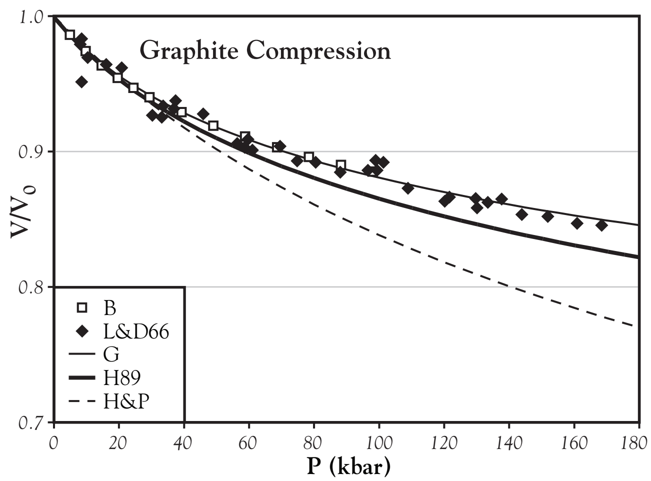
Heat Capacity Functions for Diamond
Cp (J/K)
T(K)
60
50
40
30
20
10
0
200
600
1000
1400
1800
2200
2600
3000
G
Gl
H&P
R&H
R&W5560
Victor62

Fig A4



Deviations of Diamond Heat Capacity Functions
(Calculated - Victor)
ΔCp (J/K)
T(K)
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
200
400
600
800
1000
1200
G
Glushko
H&P
R&H
R&W4400
R&W5560

Fig A5



Graphite Compression
1.0
0.9
0.8
0.7
V/V0
0
20
40
60
80
100
120
140
160
180
P (kbar)
B
L&D66
G
H89
H&P

Fig A6

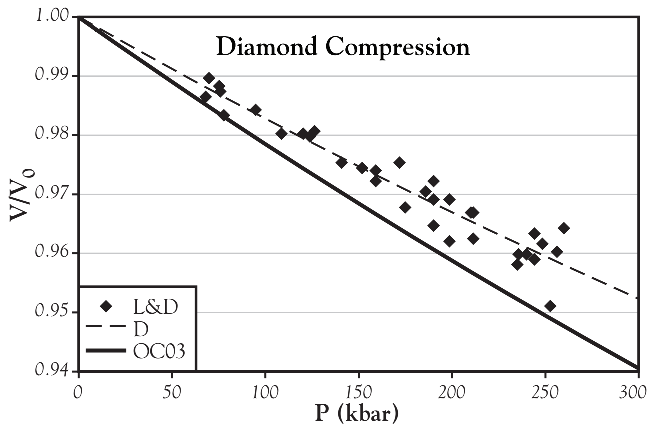

Diamond Compression
1.00
0.99
0.98
0.97
0.96
0.95
0.94
V/V0
0
50
100
150
200
250
300
P (kbar)
L&D
D
OC03

Fig A7

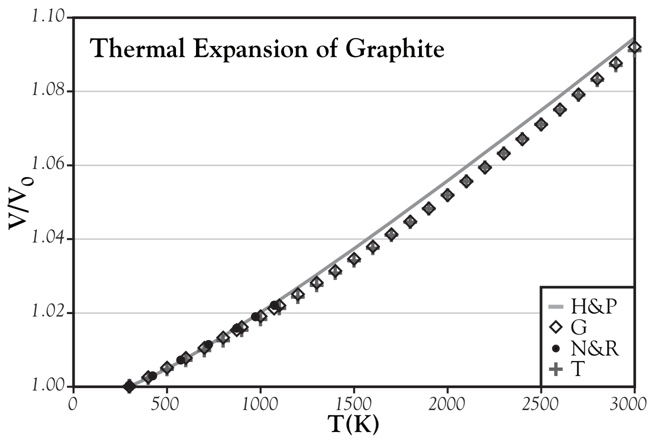
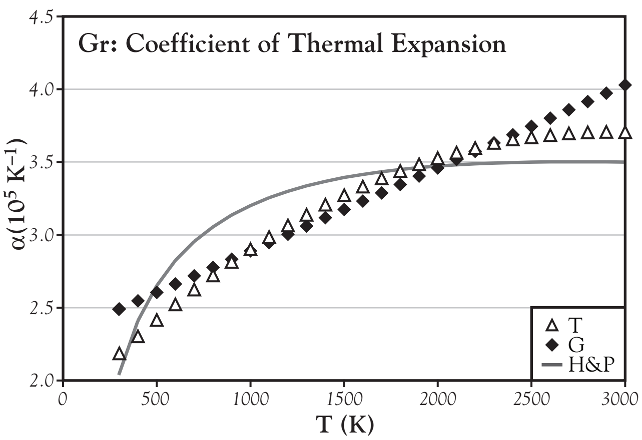
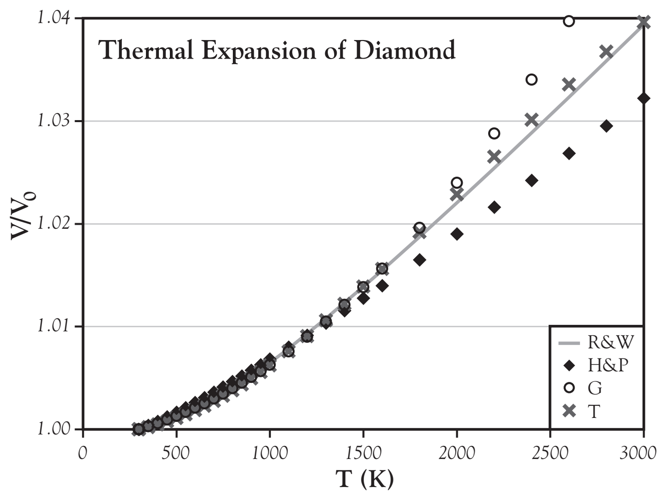

Thermal Expansion of Graphite
1.10
1.08
1.06
1.04
1.02
1.00
V/V0
0
500
1000
1500
2000
2500
3000
T(K)
H&P
G
N&R
T

Fig A8



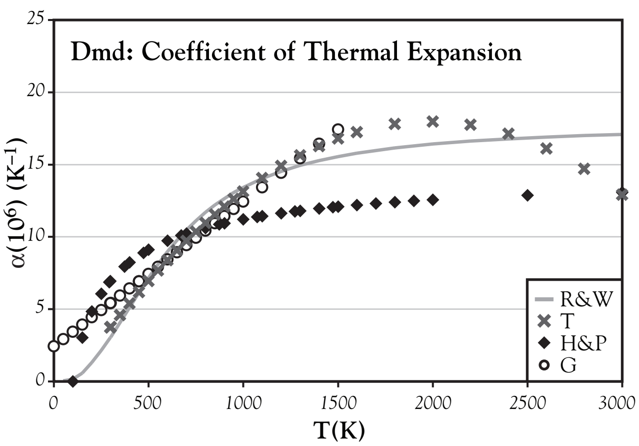
Gr: Coefficient of Thermal Expansion
4.5
4.0
3.5
3.0
2.5
2.0
α(10⁵ K⁻¹)
0
500
1000
1500
2000
2500
3000
T (K)
T
G
H&P

Fig A9



Thermal Expansion of Diamond
1.04
1.03
1.02
1.01
1.00
V/V0
0
500
1000
1500
2000
2500
3000
T (K)
R&W
H&P
G
T

Fig A10



Dmd: Coefficient of Thermal Expansion
25
20
15
10
5
0
α(10^6) (K^-1)
0
500
1000
1500
2000
2500
3000
T(K)
R&W
T
H&P
G

Fig A11

Table A1. Entropy and high temperature heat capacity of graphite.

Source		S^0(298,1) 2σ (J/mol-K)	References Cited: S & Low-T C_p	High-T C_p
Holland&Powell*	1998	5.85 none	*Robie&Hemingway95	Robie&Hemingway95
Chase (JANAF)	1998	5.74 0.21	Cox71	MacDonald65 West&Ishihara65 Cezairliyan&Righini75 **Cezairliyan&McClure77
Robie&Hemingway	1995	5.74 0.10	Cox89	Cox89
Cox et al. (CODATA)	1989	5.74 0.10	DesSorbo55 DeSorbo&Nichols58 DeSorbo&Tyler53	Chase82
Gustafson	1986	5.74 0.21	Chase82	Chase82
Chase et al. (JANAF)	1982	5.74 0.21	Cox71	McDonald65 West&Ishihara65
Berman	1979	5.72 0.02	Berman65	Berman65
Robie et al.	1978	5.74 0.01	Hultgren73	Hultgren73
Hultgren et al.	1973	5.73 0.04	DeSorbo&Nichols58 DeSorbo&Tyler53 Evans64 Jacobs&Park34 Keesome&Pearlman55 van de Hoeven&Keesom63	Evans60
Cox et al. (CODATA)	1971	5.74 0.12	DeSorbo&Tyler53	
Berman	1965	5.720 0.02	DeSorbo&Tyler53 Bergenlid54 DeSorbo&Nichols58 Bowman&Krumhansl,1958	Kelley60 Lucks60 Rasor&McClelland60
Evans	1964	5.74	none	
Evans	1960	5.74	none	none
Berman&Simon	1955	5.73 0.02	DeSorbo&Tyler53 Bergenlid54	Kelley49
DeSorbo&Tyler***	1953	5.74 0.02		

* value adjusted from that reported by reference

** Does not contain cited information

*** 298.16 K

Table A2. Entropy, enthalpy of formation, and heat capacity of diamond.

Source		$S^0(298,1)$	ΔH_f	References cited		
		J/mol-K	kJ/mol	S & Lo-T C_p	H	High-T C_p
Holland&Powell	1998	2.30	2.07 0.07	*Robie&Hemingway95	derived	Robie&Hemingway95
Robie&Hemingway	1995	2.38 0.2	1.900 0.000	Wagman82	Wagman82	Wagman82?
Gustafson	1986	2.36	1.895	from equation Hultgren73	from equation Hultgren73	 Hultgren73
Wagman et al.	1982	2.377	1.895	none	none	none
Berman	1979	2.356 0.02	1.872 0.075	Berman65	Hawtin66	
Robie et al	1978	2.38 0.01	1.895 0.042	Hultgren73	Hawtin66	Hultgren73
Hultgren et al.	1973	2.38 0.04	1.895	Evans64	Evans64	Victor62
Wagman et al.	1973	2.38 0.04	1.895	Desnoyers&Morrison58 DeSorbo53	Evans,1964	Victor62
Hawtin et al.	1966		1.872 0.074			
Berman	1965	2.356 0.02	1.895 0.084	DeSorbo53 Berman&Poulter53 Burk&Friedburg58 Desnoyers&Morrison58	Prosen44	Victor62
Evans	1964	2.377	1.897	none	none	
Berman&Simon**	1955	2.377 0.020	1.895	DeSorbo53 Berman&Poulter53	Prosen44	Kelley49
DeSorbo	1953	2.38 0.02				
Prosen et al.**	1944		1.896 0.085		Dewey&Harper38 Jessup38 Prosen&Rossini44	

* value adjusted from that reported by reference

** 298.16 K

Table A3. Coefficients of heat capacity functions.

	*a	b	c	d	e	f	g	h
Diamond								
H&P98	2.430E+01	6.272E-03	-3.774E+05	-2.734E+02				
R&H95	9.845E+01	-3.655E-02	1.217E+06	-1.659E+03	1.098E-05			
Gustafson86	2.431E+01	9.446E-04	-5.396E+06			1.566E+09	-1.332E+11	
Glushko79	-1.892E+00	4.305E-02	-2.592E+05		-2.275E-05			3.987E-09
Victor62	-7.193E+00	7.099E-02	-7.311E+05		-6.197E-05	1.239E-04		2.035E-08
Kelley49	9.121E+00	1.322E-02	-6.192E+05					
Graphite								
H&P98	5.100E+01	-4.428E-03	4.886E+05	-8.055E+02				
R&H95	6.086E+01	-1.024E-02	7.139E+05	-9.922E+02	1.669E-06			
Gustafson86	2.430E+01	9.446E-04	-5.125E+06			1.586E+09	-1.440E+11	
Glushko79	4.824E+00	2.863E-02	-3.250E+05		-1.381E-05			2.276E-09
RHF78	6.316E+01	-1.147E-02	7.481E+05	-1.032E+03	1.808E-06			

References: Glusko et al., 1979; Gustafson, 1986; Holland and Powell, 1998; Kelley, 1949; Robie and Hemingway, 1995; Robie et al, 1978, Victor, 1962.

*$Cp = a + bT + cT^{-2} + dT^{-0.5} + eT^{2} + fT^{-3} + gT^{-4} + hT^{3}$ (J/K).

Table A4. Molar volume, bulk modulus and thermal expansion of graphite.

		V(298,1) 2σ (cm^3)	B_0* (kbar)	n**	References cited V	B_0	α***
Holland&Powell	1998	5.30 none	390	4	Robie& Hemingway95	Birch66	Skinner66
Robie&Hemingway	1995	5.298 0.001			Robie67 (?)		
Hanfland et al.	1989	5.287 0.003	338 3	8.9 0.1			
Gustafson	1986	5.297 none	333	12	Berman&Simon55	Lynch&Drickamer66	Nelson&Riley45 Bacon50 Touloukian77
Berman	1979	5.299 0.001	337	12.2	Berman65	Drickamer et al.66	Berman65
Robie et al.	1978	5.298 0.001			Robie67 (?)		
Robie et al.	1967	5.2982 0.0009			Nelson&Riley45		
Drickamer et al.	1966		337	12.2		Lynch&Drickamer66	
Lynch&Drickamer	1966						
Birch	1966		333			Richards15	
Skinner	1966						Nelson&Riley45
Berman	1965	5.299	379		Berman&Simon55 Implied	Bridgman45,48	Nelson&Riley45 Bacon50
Berman&Simon	1955	5.299			Nelson&Riley45 Bacon50	Bridgman45,48	Nelson&Riley45 Bacon50
Nelson&Riley	1945	not reported					

* Initial bulk modulus.

**Pressure derivative of bulk modulus.

***Coefficient of thermal expansion.

Table A5. Molar volume bulk modulus, and thermal expansion of diamond.

Reference		**V(298,1) 2σ**	**B_0***	**n****	**References Cited**		
		cm3	kbar		V	B_0	α***
Occelli et al.	2003	3.4170	4460	3.2			
		0.0008	10				
Holland&Powell	1998	3.42	5800	4	Robie&Hemingway95	Birch66?	Skinner,66
Reeber&Wang	1996	3.4166			calculated using	Table IV	
		0.0003			cell volume	Equation	
					Tu32		
					Straumanis&Aka51		
					Thewlis&Davey56		
					Skinner57		
					Hom75		
Robie&Hemingway	1995	3.417			Robie67?		
		0.001					
Gustafson	1986	3.416	5882	5	from equation	Lynch&Drickamer66	Touloukian77
					Berman&Simon55		
Berman	1979	3.4165	4400		Berman65	McSkimin&Bond57	Berman65
					Mykolajewycz65	McSkimin&Andreatch72	Wright66
						McSkimin et al.72	Slack&Bartram75
						Grimsditch&Ramdas75	
Robie et al.	1978	3.417			Robie67?		
		0.001					
Robie et al.	1967	3.4166			Parrish60		
		0.0003			Mykolajewycz64		
					Skinner57		
Drickamer et al.	1966		5560	4		Lynch&Drickamer66	
Lynch&Drickamer	1966		6250				
Birch	1966		5556			Adams21,23	
			#4425			McSkimin&Bond57	
			#5747			Bhagavantam& Bhimasenachar44	
Skinner	1966						Mauer&Bolz57a

						Skinner57
Berman	1965	3.4165	5448	Straumanis&Aka51 Thewlis&Davey56	Bridgman45? No value reported	Thewlis&Davey56 Skinner57 Kaiser&Bond59 Parrish60
Mauer&Bolz	1957					only supplement found
Skinner	1957	3.4168 0.0001				
Berman&Simon	1955	3.4165	not reported	Straumanis&Aka51 Bearden38 Tu32	Bridgeman45	Thewlis&Davey56?

*Initial bulk modulus

** Pressure derivative of bulk modulus

***Coefficient of thermal expansion

#Calculated from elastic constants