NASA Polynomial for the thermodynamic data base

1. 'Old' 7-coefficients form (~1993)

$$\frac{C_p^\circ}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \qquad (1o)$$

$$\frac{H^\circ}{RT} = \frac{1}{T}\int \frac{C_p^\circ}{R}\,\mathrm{d}T \qquad (2)$$

$$\frac{H^\circ}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \qquad (2o)$$

$$\frac{S^\circ}{R} = \int \frac{C_p^\circ}{RT}\,\mathrm{d}T \qquad (3)$$

$$\frac{S^\circ}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \qquad (3o)$$

Card Formatting:

header-1		
A6	1–6	'THERMO'
header-2		
3E10.0	1–30	Low, common, and high temperatures for default
card-1		
A18	1–18	Species name (must start in column 1, space delimits the name)
A6	19–24	Date
4(A2,I3)	25–44	Atomic symbols and formula
A1	45	Phase (S, L, or G for solid, liquid, or gas, respectively)
E10.0	46–55	Low temperature
E10.0	56–65	High temperature
E8.0	66–73	Common temperature (blank for default)
A2,I3	74–78	Auxiliary atomic symbols and formula
I1	80	1
card-2		
5E15.0	1–75	a_1 – a_5 for UPPER temperature interval
I1	80	2
card-3		
5E15.0	1–75	a_6 and a_7 for UPPER and a_1 – a_3 for LOWER temperature intervals
I1	80	3
card-4		
4E15.0	1–60	a_4 – a_7 for LOWER temperature interval
I1	80	4
footer		
A3	1–3	'END'

2. 'New' 9-coefficients form (1994~)

$$\frac{C_p^\circ}{R} = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4 \qquad (1n)$$

$$\frac{H^\circ}{RT} = -a_1T^{-2} + a_2T^{-1}\ln T + a_3 + a_4\frac{T}{2} + a_5\frac{T^2}{3} + a_6\frac{T^3}{4} + a_7\frac{T^4}{5} + \frac{b_1}{T} \qquad (2n)$$

$$\frac{S^\circ}{R} = -a_1\frac{T^{-2}}{2} - a_2T^{-1} + a_3\ln T + a_4T + a_5\frac{T^2}{2} + a_6\frac{T^3}{3} + a_7\frac{T^4}{4} + b_2 \qquad (3n)$$

Card Formatting:

header-1		
A6	1–6	'thermo'
header-2		
4F10.2	1–40	Temperature intervals
A10	41–50	Date
card-1		
A15	1–15	Species name (space delimits the name)
A65	16–80	Comments (data source)
card-2		
I2	1–2	Number of *T* intervals
1X	3	
A6	4–9	(optional identification code)
1X	10	
5(A2,F6.2)	11–50	Chemical formulas (atomic symbols and numbers)
I2	51–52	Phase (0 for gas and nonzero for condensed)
F13.7	53–65	Molecular weight
F15.3	66–80	Heat of formation at 298.15 K in J mol^{-1}
card-3		
2F11.3	1–22	Temperature range
I1	23	Number of coefficients for $C_p°/R$ (normally 7)
8F5.1	24–63	*T* exponents in empirical equation for $C_p°/R$
2X	64–65	
F15.3	66–80	$H°(298.15) - H°(0)$ in J mol^{-1}
card-4		
5D16.8	1–80	First five coefficients for $C_p°/R$
card-5		
2D16.8	1–32	Last two coefficients for $C_p°/R$
16X	33–48	
2D16.8	49–80	Integration constants b_1 and b_2
(cards 3–5 repeated for each temperature interval)		
footer		
A12	1–12	'END PRODUCTS'