

Supplementary Online Material for ICARUS_2019_521, “On the Origin & Thermal Stability of KBO 2014 MU69’s and Pluto’s Ices”

Appendix : Experimental Laboratory Saturation Vapor Pressure Fits

These two tables present the best-fit parameters compiled/used by Prialnik *et al.* (2004) and Fray & Schmitt (2009) to describe the vapor pressure P_{sat} versus temperature T behavior of ices found in solar system bodies. We reproduce them here both to record the values used in making the vapor pressure versus temperature curves used in our manuscript’s analysis and as a service to the reader in making their own future analyses.

The 2-parameter fits of Prialnik *et al.* (2004; Table 1) assume ice Heats of Vaporization (ΔH_{vap} ’s) that are independent of temperature and use data collected at/near room temperature, and so are most accurate at/near room temperature and less so at low cryogenic temperatures. These parameters are most familiar to the cometary community of researchers at the time of this writing.

Table 1 – Prialnik *et al.* 2004 Empirical $P_{\text{sat}} = A \cdot \exp(-B/T)$ Parameter Values Assuming $\Delta H_{\text{vap}} = \text{Constant}$

Ice Component	Formula	A Value (10^{10} Nm^{-2})	B Value (Kelvin)
Water	H ₂ O	356.	6141.667
Carbon Monoxide	CO	0.12631	764.16
Carbon Dioxide	CO ₂	107.9	3148
Methane	CH ₄	0.597	1190.2
Propyne	C ₃ H ₄	3.417	3000
Propadine	C ₃ H ₄	2.382	2758
Ethane	C ₂ H ₆	0.459	1938
Methanol	CH ₃ OH	8.883	4632
Hydrogen Cyanide	HCN	3.8665	4024.66
Hydrogen Sulphide	H ₂ S	1.2631	2648.42
Ammonia	NH ₃	61.412	3603.6
Acetylene	C ₂ H ₂	9.831	2613.6

The more extensive compendium of laboratory measurements compounded by Fray & Schmitt (2009; Table 2), produced by an extensive search & comparison of the existing literature for laboratory data, expands the list of ices studied to encompass most of the materials expected in outer solar system icy bodies. It also includes the results of heat of vaporization and vapor pressure measurements at temperatures ranging from 10 to 300 K for the candidate ices, without assuming that ΔH_{vap} is constant with Temperature. The resulting polynomial fits of $\ln(P_{\text{sat}})$ in $1/T$ (i.e., $\ln(P_{\text{sat}}) = A_0 + \sum A_i/T^i$) were tabulated and compared to those of other works (like Huebner 2006) in their work with good results. These parameters, along with the subset used by Schaller & Brown (2007), are most familiar to the KBO/TNO community of researchers.

We recommend the use of the Fray and Schmitt 2009 values as being more completely researched and more accurate throughout the temperature range of interest for icy solar system bodies, especially at low temperatures below 50K, and this is what we have done in our analysis. On the other hand the Prialnik *et al.* 2004 formulation is much easier to use for a quick order of magnitude estimate of the P_{sat} vs Temperature behavior: the A coefficient tells one quickly the relative volatility of a species, while the B coefficient divided by 35 gives one a quick approximate temperature where P_{sat} climbs steeply from negligible to rapidly sublimating for an ice.

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Table 2 - Coefficients of the polynomials of extrapolations $\ln(P_{\text{sat}}) = A_0 + \sum_i A_i/T^i$, from Fray & Schmitt 2009

Species	Polynomial Designation	A0	A1(K)	A2(K ²)	A3(K ³)	A4(K ⁴)	A5(K ⁵)	A6(K ⁶)	
H ₂ O	H ₂ O-1	- See below for special treatment of water ice vapor pressure -							
O ₂	O ₂ -1	1.541x10 ⁺¹	-1.148x10 ⁺³	3.349x10 ⁺²	6.021x10 ⁺¹	0	0	0	
	O ₂ -2	1.335x10 ⁺¹	-1.012x10 ⁺³	-2.971x10 ⁺³	2.926x10 ⁺⁴	0	0	0	
	O ₂ -3	1.018x10 ⁺¹	-8.035x10 ⁺²	-7.080x10 ⁺³	7.553x10 ⁺⁴	0	0	0	
O ₃	O ₃ -1	1.746x10 ⁺¹	-2.352x10 ⁺³	0	0	0	0	0	
CO	CO-1	1.043x10 ⁺¹	-7.213x10 ⁺²	-1.074x10 ⁺⁴	2.341x10 ⁺⁵	-2.392x10 ⁺⁶	9.478x10 ⁺⁶	0	
	CO-2	1.025x10 ⁺¹	-7.482x10 ⁺²	-5.843x10 ⁺³	3.939x10 ⁺⁴	0	0	0	
CO ₂	CO ₂ -1	1.476x10 ⁺¹	-2.571x10 ⁺³	-7.781x10 ⁺⁴	4.325x10 ⁺⁶	-1.207x10 ⁺⁸	1.350x10 ⁺⁹	0	
	CO ₂ -2	1.861x10 ⁺¹	-4.154x10 ⁺³	1.041x10 ⁺⁵	0	0	0	0	
CH ₃ OH	CH ₃ OH-1	1.918x10 ⁺¹	-5.648x10 ⁺³	0	0	0	0	0	
	CH ₃ OH-2	1.706x10 ⁺¹	-5.314x10 ⁺³	0	0	0	0	0	
HCOOH	HCOOH-1	2.189x10 ⁺¹	-7.213x10 ⁺³	0	0	0	0	0	
	HCOOH-2	2.164x10 ⁺¹	-6.942x10 ⁺³	-6.579x10 ⁺⁴	3.316x10 ⁺⁶	-6.004x10 ⁺⁷	0	0	
CH ₄	CH ₄ -1	1.051x10 ⁺¹	-1.110x10 ⁺³	-4.341x10 ⁺³	1.035x10 ⁺⁵	-7.910x10 ⁺⁵	0	0	
C ₂ H ₂	C ₂ H ₂ -1	1.340x10 ⁺¹	-2.536x10 ⁺³	0	0	0	0	0	
C ₂ H ₄	C ₂ H ₄ -1	1.540x10 ⁺¹	-2.206 10 ⁺³	-1.216x10 ⁺⁴	2.843x10 ⁺⁵	-2.203x10 ⁺⁶	0	0	
C ₂ H ₆	C ₂ H ₆ -1	1.511x10 ⁺¹	-2.207x10 ⁺³	-2.411x10 ⁺⁴	7.744x10 ⁺⁵	-1.161x10 ⁺⁷	6.763x10 ⁺⁷	0	
C ₆ H ₆	C ₆ H ₆ -1	1.735x10 ⁺¹	-5.663x10 ⁺³	0	0	0	0	0	
HCN	HCN-1	1.393x10 ⁺¹	-3.624x10 ⁺³	-1.325x10 ⁺⁵	6.314x10 ⁺⁶	-1.128x10 ⁺⁸	0	0	
HC ₃ N	HC ₃ N-1	1.301x10 ⁺¹	-4.426x10 ⁺³	0	0	0	0	0	
C ₂ N ₂	C ₂ N ₂ -1	1.653x10 ⁺¹	-4.109x10 ⁺³	0	0	0	0	0	
C ₄ N ₂	C ₄ N ₂ -1	1.909x10 ⁺¹	-6.036x10 ⁺³	0	0	0	0	0	
N ₂	N ₂ -1	1.240x10 ⁺¹	-8.074x10 ⁺²	-3.926x10 ⁺³	6.297x10 ⁺⁴	-4.633x10 ⁺⁵	1.325x10 ⁺⁶	0	
	N ₂ -2	8.514	-4.584x10 ⁺²	-1.987x10 ⁺⁴	4.800x10 ⁺⁵	-4.524x10 ⁺⁶	0	0	
NH ₃	NH ₃ -1	1.596x10 ⁺¹	-3.537x10 ⁺³	-3.310x10 ⁺⁴	1.742x10 ⁺⁶	-2.995x10 ⁺⁷	0	0	
	NO-1	1.691x10 ⁺¹	-2.016x10 ⁺³	0	0	0	0	0	
	NO-2	1.2352x10 ⁺²	-4.7607x10 ⁺⁴	7.7292x10 ⁺⁶	-6.4950x10 ⁺⁸	2.7061x10 ⁺¹⁰	-4.4739x10 ⁺¹¹	0	
N ₂ O	N ₂ O-1	1.622x10 ⁺¹	-2.971x10 ⁺³	0	0	0	0	0	
	N ₂ O-2	6.5664	-1.2711x10 ⁺³	-6.6835x10 ⁺⁵	4.4959x10 ⁺⁷	-1.0967x10 ⁺⁹	0	0	
H ₂ S	H ₂ S-1	1.298x10 ⁺¹	-2.707x10 ⁺³	0	0	0	0	0	
	H ₂ S-2	8.933	-7.260x10 ⁺²	-3.504x10 ⁺⁵	2.724x10 ⁺⁷	-8.582x10 ⁺⁸	0	0	
SO ₂	SO ₂ -1	1.560x10 ⁺¹	-3.5.08x10 ⁺³	-9.401x10 ⁺⁴	4.152x10 ⁺⁶	-6.946x10 ⁺⁷	0	0	
	AsH ₃ -1	1.176x10 ⁺¹	-2.382x10 ⁺³	0	0	0	0	0	
Ne	Ne-1	9.886	-2.699x10 ⁺²	1.283x10 ⁺²	-1.624x10 ⁺²	0	0	0	
	Ne-2	1.061x10 ⁺¹	-3.086x10 ⁺²	9.860x10 ⁺²	-9.069x10 ⁺³	3.514x10 ⁺⁴	0	0	
Ar	Ar-1	1.069x10 ⁺¹	-8.932x10 ⁺²	-3.567x10 ⁺³	6.574x10 ⁺⁴	-4.280x10 ⁺⁵	0	0	
Kr	Kr-1	1.077x10 ⁺¹	-1.223x10 ⁺³	-8.903x10 ⁺³	2.635x10 ⁺⁵	-4.260x10 ⁺⁶	3.575x10 ⁺⁷	-s1.210x10 ⁺⁸	
Xe	Xe-1	1.098x10 ⁺¹	-1.737x10 ⁺³	-1.332x10 ⁺⁴	4.349x10 ⁺⁵	-7.027x10 ⁺⁶	4.447x10 ⁺⁷	0	

The special case of Water (H₂O). As a unique case due to its prevalence, its highly hydrogen bonded nature, and its phase changes at relatively high temperatures (for ices), water ice has been studied most extensively by many researchers over the last century and thus modeled differently in the literature. For water in “Astrophysical

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Applications" Fray & Schmitt 2009 recommend the special (i.e., different than the $\ln(P_{\text{sat}}) = A_0 + \sum A_i T^i$ of Table 2) treatment presented by Feistel and Wagner (2007):

$$\ln(P_{\text{subl}}(T)/P_{\text{triple}}) = 3/2 \ln(T/T_{\text{triple}}) + (1 - T_{\text{triple}}/T) \eta(T/T_{\text{triple}})$$

where

P_{triple} = Pressure of Triple Point = $(6.116577 \pm 0.0001) \times 10^{-3}$ bar

T_{triple} = Temperature of Triple Point = 273.16 K

and

$$\eta(T/T_{\text{triple}}) = \sum e_i (T/T_{\text{triple}})^i$$

with

i	e_i
0	20.9969665107897
1	3.72437478271362
2	-13.9205483215524
3	29.6988765013566
4	-40.1972392635944
5	29.7880481050215
6	-9.13050963547721

Appendix References

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