FY97 Status Report on the HSV and Titanium Tritide Samples

by

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0		2/98	Initial Release

FY97 Status Report on the HSV and Titanium Tritide Samples (U)

Kirk L. Shanahan

Summary

The HSV in storage in MTF has been monitored, and the gas sampled and analyzed. The net conclusion is that no significant He evolution has occurred to date, and thus the HSV is performing as expected. The annual desorption isotherms have been recorded on a titanium tritide sample with 582 total days tritium exposure, and no significant effects have been noted. A gas sample was also taken from the test cell and analyzed.

Part 1. The Hydrogen Storage Vessel

The first loaded HSV, HSV-002, was loaded on April 3, 1996 and delivered to the MTF and installed in a monitoring manifold. Temperature and pressure data have been recorded from this apparatus since late May, 1996. Plots of that data are shown in Figures 1 and 2. Figure 3 shows a plot of the pressure data after correcting via Charles' Law ($P_1/T_1 = P_2/T_2$) to a constant 74 °C in an attempt to remove scatter arising from the temperature fluctuations.

The plot shows a slight curvature, noted through a slightly better statistical fit for a quadratic function when compared to a simple linear fit. The initial pressure inside the HSV was approximately 12 torr, and was attributed to residual inerts in the process gas. A gas sample was taken on Sept. 22, 1997, and it analyzed as 100% He3 by mass spectrometry. The maximum pressure reached, as shown in Figures 1 and 3, of approximately 22 torr, represents much less than 1% of the total helium produced by radioactive decay. Thus, it is essentially correct to say all the He decay products are being retained in the titanium tritide.

Part 2. Titanium Tritide Samples

Nine samples were originally prepared with varying tritium and deuterium loadings for use in a long term storage program. One sample has been used to collect pure tritium isotherm data on an annual basis. This sample was reexamined this year, and the 650 °C isotherms recorded are presented in Figures 4 (linear scale) and 5 (logarithmic scale). Also shown are all prior isotherms collected on the same sample (including one 600 °C isotherm on virgin data).

There does not seem to be any significant change in the isotherm characteristics after 582 days of tritium exposure. The first few months of the exposure used an initial T/M value of approximately 2, with the subsequent loading at approximately 1.5. An gas sample was taken from the test cell prior to collecting isotherm data. Analysis showed no hydrogen isotopes, small amounts of residual background gases, and predominantly ³He. This agrees with the sample taken from HSV-002.

An interesting side observation is illustrated in Figure 6. There, pressure data recorded on a 2-3 minute interval are plotted versus the simultaneously measured temperature. (The only exception was that there was a 23 minute gap between the points 31 and 32 of 36.) The P-T data correlate with a linear correlation coefficient of .999784.

At the time the data was recorded, no temperature controller was in use. A simple Variac was being used to drive the heating mantle used to heat the sample. On prior days the stability of that system was adequate, but on the day Figure 6's data was recorded there was work being done on the building's HVAC system. We suspect voltage or cooling air flow irregularities (the experiment was conducted in a flow-through air hood) due to ventilation fan switching. Subsequently a controller was added, and this greatly improved

stability. Figure 6 seems to indicate that the hydride 'breathes' rapidly at near-equilibrium conditions, since the pressure swings noted are well in excess of those expected simply from temperature induced pressure changes.

Figure 7 plots the sequence of both loading and temperature data over the entire history of the sample (note that the X axis is not absolute time). The degree of temperature control is easily observed.

The T/M plot in Figure 7 shows some additional information beyond the desorption isotherms. Namely, initial loadings are noted, as well as loadings after decay while in storage. When correlated with temperature, the sample's loading/temperature history can be noted.

Appendix

In analyzing the titanium tritide sample data, the software package-RS/1, installed on an RS/6000 UNIX computer was utilized. A complete P-T-V history of the sample was developed starting from its initial T2 loading on November 11, 1995. All operations conducted on the sample are represented in this history file to the best of our ability to reconstruct prior happenings. The file includes a few points for aborted isotherms and typical process interruptions. The data rows represent the initial, equilibrium, and final conditions normally recorded during isotherms (i.e. P_i , T_i , V_i , P_{eq} , T_{eq} , V_{eq} , P_f , T_f , V_f) and two more numbers that respectively represent the sample cell volume (V_s) and the additional system volume between the manifold's last valve and the sample's last valve (V_x). System volumes vary of course due to the differing selection of expansion volumes.

Computational results are found in the following columns. They are: N_i , the initial number of T2 moles present at the start of that step; N_{gas} , the number of T2 moles in the gas phase; N_f , the final number of T2 moles present after aliquot removal/addition and equilibration; N_{sys} , the number of moles present in the system at equilibrium; N_m , the moles of T2 in the hydride; Q/M , the calculated loading value; and Seq#, a sequence number used for plotting,

The only truly artificial data points in the history file are those that were created to represent tritium decay. These can be seen as negative P_i values. The sample's final tritium content prior to storage was used as the initial T content in a decay equation ($E = E_0 \cdot \exp\{-kt\}$), the final T content after decay calculated, and an appropriate 'negative aliquot' inserted in the history to represent decay.

The RS/1 software offers a programming language called RPL to create 'procedures' (equivalent to 'macros' or 'scripts') used to analyze data and create graphical displays. The RPL procedure used to analyze the history file is included in this appendix. Future upgrades may include direct decay calculations to remove the artificiality of the 'negative aliquots'. In that situation, the history file will have to be modified to include timestamp information. The procedure uses some standard values for the ETM volumes.

They are:

A-manifold	92.23 cc
B-manifold	151.93 cc
C-manifold	194.19 cc
A-volume	1492.04 cc
B-volume	1471.46 cc
C-volume	403.39 cc
D-volume	398.93 cc
E-volume	101.82 cc
F-volume	98.46 cc

Figure 1. HSV-002 Pressure vs. Time

Figure 2. HSV-002 Temperature vs. Time

Figure 3. HSV-002 Adjusted Pressure with Time

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Figure 4. TiTx Desorption Isotherms (Linear Y)

Figure 5. TiTx Desorption Isotherms (Log Y)

Figure 6. Sample 'Breathing' with Temperature

Figure 7. Historical Plot of Ti-3 Sample

Master Data File for TiTx Sample Ti-3

0	33.570	1 Pi	2 Ti	3 Vi	4 Peq	5 Teq	6 Veq	7 Pf	8 Tf	9 Vf	10 Vx	11 Vs	12 Ni
1	0.000	1107.510	18.4	566.17	341.08	595.7	574.66	341.44	16.6	566.17	15.31	8.49	34.487894
2		221.260	16.7	566.17	340.70	601.7	574.66	340.59	16.4	566.17	15.31	8.49	6.930454
3		245.200	16.6	566.17	301.24	601.4	574.66	301.01	16.6	566.17	15.31	8.49	7.682969
4		200.760	17.6	566.17	249.99	599.7	574.66	250.14	17.7	566.17	15.31	8.49	6.268874
5		150.900	17.9	566.17	180.83	599.4	574.66	180.83	18.1	566.17	15.31	8.49	4.707103
6		170.600	19.0	566.17	177.35	605.3	574.66	177.48	18.6	566.17	15.31	8.49	5.301579
7		77.400	18.2	566.17	110.55	604.8	574.66	110.70	17.4	566.17	15.31	8.49	2.411893
8		10.500	17.1	566.17	58.84	604.0	574.66	58.85	17.6	566.17	15.31	8.49	0.328435
9		6.860	17.5	566.17	38.67	602.2	574.66	38.70	17.4	566.17	15.31	8.49	0.214282
10		30.120	16.4	664.63	36.51	598.7	673.12	36.51	16.6	664.63	15.31	8.49	1.108655
11		3.160	16.5	664.63	26.34	601.6	673.12	26.33	17.5	664.63	15.31	8.49	0.116273
12		0.000	18.6	664.63	22.21	609.1	673.12	22.74	18.2	664.63	15.31	8.49	0.000000
13		0.000	16.2	2136.09	12.88	606.5	2144.58	12.74	16.3	2136.09	15.31	8.49	0.000000
14		0.000	16.2	2136.09	9.82	609.2	2144.58	9.82	16.5	2136.09	15.31	8.49	0.000000
15		0.000	16.5	2136.09	4.28	583.7	2144.58	4.30	16.6	2136.09	15.31	8.49	0.000000
16		0.000	16.4	2136.09	5.15	601.4	2144.58	5.15	17.2	2136.09	15.31	8.49	0.000000
17		0.000	16.8	2136.09	4.32	604.0	2144.58	4.36	17.3	2136.09	15.31	8.49	0.000000
18		0.000	16.9	2136.09	4.56	602.9	2144.58	4.54	18.1	2136.09	15.31	8.49	0.000000
19		0.000	17.8	2136.09	4.06	603.5	2144.58	4.08	18.3	2136.09	15.31	8.49	0.000000
20		0.000	17.8	2136.09	3.62	603.9	2144.58	3.62	18.4	2136.09	15.31	8.49	0.000000
21		1098.410	20.3	558.86	134.02	148.0	567.35	133.76	20.0	558.86	8.00	8.49	33.544290
22		404.180	17.9	159.93	449.79	366.2	168.42	458.01	17.9	159.93	8.00	8.49	3.561413
23		310.410	17.9	159.93	516.19	458.8	168.42	513.80	18.0	159.93	8.00	8.49	2.735163
24		502.630	16.2	159.93	1380.60	652.8	168.42	1380.60	17.3	159.93	8.00	8.49	4.454922
25		1137.200	17.4	159.93	1217.20	650.2	168.42	1219.50	17.7	159.93	8.00	8.49	10.037629
26		968.900	18.0	159.93	1160.00	650.2	168.42	1161.40	18.8	159.93	8.00	8.49	8.534485
27		916.300	18.9	159.93	1097.00	650.3	168.42	1098.70	19.1	159.93	8.00	8.49	8.046289
28		849.100	19.1	159.93	1009.56	650.0	168.42	1010.94	18.9	159.93	8.00	8.49	7.451084
29		763.190	18.8	159.93	856.60	650.0	168.42	857.27	18.4	159.93	8.00	8.49	6.704082
30		608.140	18.4	159.93	672.55	649.9	168.42	673.00	17.8	159.93	8.00	8.49	5.349407
31		420.140	16.5	159.93	497.62	650.3	168.42	498.01	17.1	159.93	8.00	8.49	3.719938
32		295.360	17.1	159.93	372.60	650.8	168.42	372.85	17.4	159.93	8.00	8.49	2.609724
33		165.520	17.4	159.93	260.02	650.2	168.42	260.26	17.3	159.93	8.00	8.49	1.460982
34		58.510	17.3	159.93	173.06	650.3	168.42	173.17	17.1	159.93	8.00	8.49	0.516623
35		0.000	17.1	159.93	116.38	650.1	168.42	116.44	17.0	159.93	8.00	8.49	0.000000
36		0.000	15.8	258.39	78.44	650.9	266.88	78.44	16.2	258.39	8.00	8.49	0.000000
37		0.000	16.3	258.39	58.75	650.8	266.88	58.78	16.9	258.39	8.00	8.49	0.000000
38		0.000	16.5	258.39	46.97	650.4	266.88	46.98	16.8	258.39	8.00	8.49	0.000000
39		0.000	16.9	258.39	39.07	650.6	266.88	39.07	17.3	258.39	8.00	8.49	0.000000
40		0.000	16.9	258.39	33.50	650.4	266.88	33.51	17.4	258.39	8.00	8.49	0.000000

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Master Data File for TiTx Sample Ti-3

0	33.570	13 Ngas	14 Nf	15 Nsya	16 Nm	17 Q/M	18 Seq#
1	0.000	10.784577	10.698503	34.487894	23.703318	1.412173	1
2		10.779765	10.679241	30.719845	19.940080	1.187970	2
3		9.524698	9.431691	27.723573	18.198875	1.084234	3
4		7.874497	7.808114	24.560756	16.686259	0.994117	4
5		5.688215	5.636852	21.459745	15.771530	0.939621	5
6		5.569105	5.522944	21.124472	15.555367	0.926742	6
7		3.485768	3.459066	18.013421	14.527653	0.865514	7
8		1.854025	1.837633	14.882790	13.028765	0.776215	8
9		1.219320	1.209267	13.259439	12.040119	0.717314	9
10		1.353340	1.342931	13.158828	11.805488	0.703336	10
11		0.973338	0.965485	11.932170	10.958832	0.652894	11
12		0.818738	0.831842	10.966685	10.147946	0.604584	12
13		1.527882	1.507650	10.134843	8.606961	0.512777	13
14		1.164085	1.161295	8.627193	7.463108	0.444630	14
15		0.507198	0.508335	7.465897	6.958700	0.414578	15
16		0.609026	0.607561	6.957563	6.348536	0.378227	16
17		0.510696	0.514186	6.350001	5.839306	0.347888	17
18		0.537588	0.533943	5.835816	5.298227	0.315652	18
19		0.478314	0.479514	5.301873	4.823559	0.287373	19
20		0.426331	0.425305	4.822359	4.396029	0.261902	20
21		4.148119	4.089071	37.941345	33.793226	2.013299	21
22		4.106197	4.035734	37.413687	33.307490	1.984360	22
23		4.702586	4.525770	36.113117	31.410530	1.871345	23
24		12.575784	12.190223	36.042269	23.466484	1.398063	24
25		11.072579	10.752956	33.889675	22.817095	1.359374	25
26		10.512866	10.202075	31.671203	21.158337	1.260550	26
27		9.931790	9.641392	29.515417	19.583627	1.166734	27
28		9.146372	8.877350	27.325109	18.178738	1.083035	28
29		7.773772	7.540840	25.151842	17.378070	1.035333	29
30		6.115964	5.932146	22.960409	16.844446	1.003542	30
31		4.535995	4.400287	20.748201	16.212206	0.965875	31
32		3.392899	3.291004	18.957638	15.564739	0.927301	32
33		2.368567	2.298006	17.127616	14.759049	0.879300	33
34		1.577507	1.530085	15.346233	13.768725	0.820299	34
35		1.061212	1.029188	13.816147	12.754935	0.759901	35
36		1.145224	1.123246	12.786959	11.641736	0.693580	36
37		0.855693	0.839687	11.663713	10.808020	0.643909	37
38		0.684353	0.671353	10.824026	10.139672	0.604091	38
39		0.568276	0.557356	10.152673	9.584397	0.571010	39
40		0.487093	0.477875	9.595316	9.108223	0.542641	40

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Master Data File for TiTx Sample Ti-3

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0	33.570	1 Pi	2 Ti	3 Vi	4 Peq	5 Teq	6 Veq	7 Pf	8 Tf	9 Vf	10 Vx	11 Vs	12 Ni
41		0.000	16.9	258.39	29.35	650.4	266.88	29.36	17.5	258.39	8.00	8.49	0.000000
42		0.000	16.4	2128.78	15.80	650.5	2137.27	15.81	16.5	2128.78	8.00	8.49	0.000000
43		0.000	16.5	2128.78	10.18	650.3	2137.27	10.19	16.6	2128.78	8.00	8.49	0.000000
44		0.000	16.6	2128.78	7.59	650.0	2137.27	7.63	16.3	2128.78	8.00	8.49	0.000000
45		0.000	16.4	2128.78	6.31	650.7	2137.27	6.35	16.9	2128.78	8.00	8.49	0.000000
46		0.000	16.9	2128.78	5.30	650.9	2137.27	5.38	17.5	2128.78	8.00	8.49	0.000000
47		0.000	17.7	2128.78	4.52	650.8	2137.27	4.57	18.0	2128.78	8.00	8.49	0.000000
48	1149.100	17.9	503.62	532.76	17.9	512.11	532.76	17.9	503.62	8.00	8.49	31.884411	
49	532.760	17.9	100.23	532.76	17.9	108.72	532.76	17.9	100.23	8.00	8.49	2.942029	
50	0.000	17.9	100.23	0.00	16.7	108.72	0.00	16.7	100.23	8.00	8.49	0.000000	
51	0.000	17.9	100.23	0.00	16.7	108.72	26.50	17.9	100.23	8.00	8.49	0.000000	
52	0.000	17.9	100.23	0.00	16.7	108.72	0.00	16.7	100.23	8.00	8.49	0.000000	
53	422.050	16.7	503.62	39.57	16.7	512.11	39.57	16.7	503.62	8.00	8.49	11.759227	
54	0.000	16.7	503.62	0.00	16.7	512.11	0.00	16.7	503.62	8.00	8.49	0.000000	
55	-83.875	20.0	100.23	0.00	20.0	108.72	0.00	20.0	100.23	8.00	8.49	-0.459860	
56	421.110	19.7	159.93	461.26	509.6	168.42	461.25	20.4	159.93	8.00	8.49	3.687784	
57	465.920	19.7	159.93	1183.31	649.8	168.42	1184.54	21.6	159.93	8.00	8.49	4.080198	
58	839.970	21.7	159.93	1074.21	649.8	168.42	1074.93	22.1	159.93	8.00	8.49	7.305968	
59	775.970	22.0	159.93	990.08	649.8	168.42	991.02	22.0	159.93	8.00	8.49	6.742443	
60	696.480	22.2	159.93	877.23	650.2	168.42	877.93	22.5	159.93	8.00	8.49	6.047652	
61	579.260	22.5	159.93	620.20	650.0	168.42	671.14	22.4	159.93	8.00	8.49	5.024708	
62	381.770	22.3	159.93	472.62	649.8	168.42	472.63	22.3	159.93	8.00	8.49	3.313851	
63	274.360	19.0	159.93	353.37	649.9	168.42	353.59	18.9	159.93	8.00	8.49	2.408408	
64	158.840	18.9	159.93	250.88	649.9	168.42	251.23	19.2	159.93	8.00	8.49	1.394819	
65	59.900	19.6	159.93	169.00	649.8	168.42	169.13	19.8	159.93	8.00	8.49	0.524741	
66	69.270	19.7	159.93	134.04	649.4	168.42	134.43	19.4	159.93	8.00	8.49	0.606618	
67	37.330	19.4	159.93	106.74	649.5	168.42	106.80	18.2	159.93	8.00	8.49	0.327245	
68	17.530	18.1	159.93	85.22	649.3	168.42	85.28	18.1	159.93	8.00	8.49	0.154359	
69	14.330	18.1	159.93	71.21	649.3	168.42	71.26	18.3	159.93	8.00	8.49	0.126181	
70	16.100	18.3	159.93	61.83	649.3	168.42	61.91	18.5	159.93	8.00	8.49	0.141670	
71	15.860	20.1	159.93	58.08	649.8	168.42	58.14	20.1	159.93	8.00	8.49	0.138701	
72	17.800	20.3	159.93	50.60	649.5	168.42	50.66	20.2	159.93	8.00	8.49	0.155561	
73	13.730	18.6	159.93	30.70	649.4	168.42	30.70	19.0	159.93	8.00	8.49	0.120691	
74	16.410	19.2	1631.39	24.20	649.2	1639.88	24.22	19.8	1631.39	8.00	8.49	1.468414	
75	17.090	19.6	1631.39	21.24	649.3	1639.88	21.25	20.3	1631.39	8.00	8.49	1.527173	
76	17.550	20.3	1631.39	19.80	649.0	1639.88	19.81	20.4	1631.39	8.00	8.49	1.564538	
77	2.700	20.2	1631.39	13.85	648.7	1639.88	13.85	20.6	1631.39	8.00	8.49	0.240780	
78	2.410	20.4	1631.39	10.53	648.2	1639.88	10.53	20.8	1631.39	8.00	8.49	0.214772	
79	2.240	20.4	1631.39	8.68	647.3	1639.88	8.75	20.6	1631.39	8.00	8.49	0.199622	
80	0.000	18.4	1631.39	7.52	648.5	1639.88	7.54	18.8	1631.39	8.00	8.49	0.000000	

Master Data File for TiTx Sample Ti-3

0 33.570 13 Ngas 14 Nf 15 Nsys 16 Nm 17 Q/M 18 Seq#

41	0.426606	0.418549	9.117441	8.690835	0.517774	41
42	1.866510	1.863264	8.698892	6.832382	0.407053	42
43	1.202185	1.200513	6.835628	5.633444	0.335624	43
44	0.897253	0.899843	5.635116	4.737863	0.282268	44
45	0.744395	0.747338	4.735272	3.990877	0.237764	45
46	0.623955	0.631870	3.987934	3.363980	0.200416	46
47	0.531214	0.535816	3.356064	2.824850	0.168296	47
48	15.031852	14.782646	34.704660	19.672808	1.172047	48
49	3.191234	2.942029	22.864042	19.672808	1.172047	49
50	0.000000	0.000000	19.922013	19.922013	1.186894	50
51	0.000000	0.146339	19.922013	19.922013	1.186894	51
52	0.000000	0.000000	19.775674	19.775674	1.178175	52
53	1.121092	1.102506	31.534901	30.413809	1.811964	53
54	0.000000	0.000000	30.432395	30.432395	1.813071	54
55	0.000000	0.000000	29.972535	29.972535	1.785674	55
56	4.164942	4.029670	33.660319	29.495377	1.757246	56
57	10.623266	10.306497	33.710848	23.087582	1.375489	57
58	9.627638	9.336959	30.710320	21.082682	1.256043	58
59	8.876598	8.611024	28.115805	19.239207	1.146214	59
60	7.851632	7.615478	25.552433	17.700802	1.054561	60
61	5.552961	5.823677	22.961663	17.408702	1.037158	61
62	4.233031	4.102536	20.451837	16.218806	0.966268	62
63	3.201451	3.104974	18.757708	15.556257	0.926795	63
64	2.270605	2.203858	17.047554	14.776949	0.880366	64
65	1.526444	1.480616	15.368437	13.841993	0.824664	65
66	1.212322	1.178450	14.494439	13.282117	0.791309	66
67	0.969345	0.940094	13.643234	12.673889	0.755072	67
68	0.774179	0.750925	12.857498	12.083320	0.719888	68
69	0.646466	0.627042	12.232755	11.586289	0.690276	69
70	0.560930	0.544395	11.747382	11.186452	0.666455	70
71	0.524059	0.508455	11.341689	10.817629	0.644482	71
72	0.456414	0.442888	10.988795	10.532381	0.627488	72
73	0.278042	0.269493	10.666598	10.388556	0.618919	73
74	2.167777	2.162836	11.865519	9.697742	0.577762	74
75	1.899389	1.894383	11.229855	9.330467	0.555881	75
76	1.770014	1.765409	10.900010	9.129995	0.543938	76
77	1.237274	1.233431	9.375381	8.138106	0.484844	77
78	0.940047	0.937126	8.356722	7.416675	0.441863	78
79	0.775419	0.779243	7.619218	6.843799	0.407733	79
80	0.675929	0.675625	6.839975	6.164046	0.367235	80

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Master Data File for TiTx Sample Ti-3

0	33.570	1 Pi	2 Ti	3 Vi	4 Peq	5 Teq	6 Veq	7 Pf	8 Tf	9 Vf	10 Vx	11 Vs	12 Ni
81		0.000	19.6	2128.78	6.08	649.0	2137.27	6.04	20.7	2128.78	8.00	8.49	0.000000
82		0.000	20.4	2128.78	5.10	648.7	2137.27	5.17	21.2	2128.78	8.00	8.49	0.000000
83		0.000	21.0	2128.78	4.60	648.9	2137.27	4.60	20.8	2128.78	8.00	8.49	0.000000
84		1101.440	20.2	558.86	305.00	138.0	567.35	304.08	20.9	558.86	8.00	8.49	33.648290
85		0.000	20.0	558.86	0.00	20.0	567.35	0.00	20.0	558.86	8.00	8.49	0.000000
86		-244.120	20.0	159.93	0.00	20.0	168.42	0.00	20.0	159.93	8.00	8.49	-2.135643
87		0.200	19.0	159.93	817.60	647.3	168.42	818.40	19.0	159.93	8.00	8.49	0.001756
88		684.000	19.0	159.93	728.00	651.0	168.42	729.00	19.0	159.93	8.00	8.49	6.004341
89		629.400	19.1	159.93	661.10	653.0	168.42	661.90	19.0	159.93	8.00	8.49	5.523157
90		562.000	18.9	159.93	592.40	653.5	168.42	593.40	18.9	159.93	8.00	8.49	4.935081
91		489.800	19.0	159.93	518.50	652.1	168.42	518.60	19.0	159.93	8.00	8.49	4.299600
92		420.900	17.9	159.93	465.40	656.1	168.42	466.70	18.2	159.93	8.00	8.49	3.708741
93		368.000	18.2	159.93	392.60	650.8	168.42	392.80	18.3	159.93	8.00	8.49	3.239276
94		293.200	18.4	159.93	338.40	652.3	168.42	338.70	18.3	159.93	8.00	8.49	2.579087
95		238.400	18.4	159.93	285.80	652.9	168.42	286.00	18.1	159.93	8.00	8.49	2.097048
96		186.700	18.1	159.93	237.60	652.9	168.42	237.70	17.9	159.93	8.00	8.49	1.643969
97		138.500	17.8	159.93	193.70	652.5	168.42	193.90	17.6	159.93	8.00	8.49	1.220806
98		93.000	17.5	159.93	152.00	650.2	168.42	152.00	17.3	159.93	8.00	8.49	0.820593
99		9.700	17.5	159.93	106.90	648.9	168.42	107.10	17.5	159.93	8.00	8.49	0.085589
100		9.800	17.7	159.93	85.10	649.1	168.42	85.20	17.7	159.93	8.00	8.49	0.086412
101		0.000	16.2	159.93	72.20	651.6	168.42	72.20	16.2	159.93	8.00	8.49	0.000000
102		0.000	16.2	159.93	60.50	651.6	168.42	60.60	16.3	159.93	8.00	8.49	0.000000
103		0.000	16.2	159.93	50.10	648.5	168.42	50.10	16.7	159.93	8.00	8.49	0.000000
104		0.000	17.8	1631.39	25.60	651.1	1639.88	25.60	18.0	1631.39	8.00	8.49	0.000000
105		0.000	17.8	1631.39	15.30	649.9	1639.88	15.40	17.9	1631.39	8.00	8.49	0.000000
106		0.000	18.2	1631.39	10.70	648.2	1639.88	10.70	18.2	1631.39	8.00	8.49	0.000000
107		0.000	17.6	2128.78	9.80	653.0	2137.27	9.90	18.6	2128.78	8.00	8.49	0.000000
108		0.000	19.0	2128.78	7.40	653.6	2137.27	7.40	19.5	2128.78	8.00	8.49	0.000000
109		0.000	18.3	2128.78	6.20	652.4	2137.27	6.20	17.9	2128.78	8.00	8.49	0.000000
110		0.000	17.7	2128.78	5.60	649.4	2137.27	5.70	17.9	2128.78	8.00	8.49	0.000000
111		0.000	18.9	2128.78	6.65	653.5	2137.27	6.59	20.3	2128.78	8.00	8.49	0.000000
112		0.000	20.6	2128.78	4.59	652.5	2137.27	4.58	20.6	2128.78	8.00	8.49	0.000000
113		0.000	20.8	2128.78	3.30	652.5	2137.27	3.31	20.6	2128.78	8.00	8.49	0.000000
114		0.000	19.3	2128.78	2.68	653.6	2137.27	2.67	19.8	2128.78	8.00	8.49	0.000000
115		4003.200	19.1	159.93	1379.30	649.0	168.42	1380.80	20.4	159.93	8.00	8.49	35.129173
116		1131.200	20.4	159.93	1342.10	652.9	168.42	1338.90	20.4	159.93	8.00	8.49	9.882628
117		1024.400	20.5	159.93	1147.70	648.6	168.42	1148.90	20.7	159.93	8.00	8.49	8.946532
118		1002.100	18.7	159.93	1194.80	651.6	168.42	1195.20	19.2	159.93	8.00	8.49	8.805753
119		919.900	19.3	159.93	1086.90	652.9	168.42	1087.30	20.3	159.93	8.00	8.49	8.066853
120		849.400	20.5	159.93	907.70	651.2	168.42	907.80	20.7	159.93	8.00	8.49	7.418181

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Master Data File for TiTx Sample Ti-3

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0	33.570	13 Ngas	14 Nf	15 Nsys	16 Nm	17 Q/M	18 Seq#
81		0.707994	0.701661	6.164349	5.456355	0.325073	81
82		0.592869	0.599574	5.462689	4.869820	0.290129	82
83		0.535471	0.534196	4.863115	4.327643	0.257828	83
84		9.412901	9.267336	37.977209	28.564308	1.701776	84
85		0.000000	0.000000	28.709873	28.709873	1.710448	85
86		0.000000	0.000000	26.574230	26.574230	1.583213	86
87		7.404957	7.184142	26.575986	19.171028	1.142152	87
88		6.593201	6.399364	25.396185	18.802984	1.120225	88
89		5.987191	5.810341	24.519978	18.532787	1.104128	89
90		5.366808	5.210813	23.644718	18.277910	1.088943	90
91		4.695791	4.552414	22.733505	18.037714	1.074633	91
92		4.226180	4.108071	21.889831	17.663651	1.052347	92
93		3.564085	3.456389	21.021036	17.456952	1.040033	93
94		3.072001	2.980343	20.143735	17.071734	1.017083	94
95		2.596246	2.518345	19.260440	16.664194	0.992803	95
96		2.159860	2.094482	18.386063	16.226204	0.966709	96
97		1.762601	1.710304	17.512386	15.749785	0.938325	97
98		1.384594	1.342108	16.622676	15.238082	0.907839	98
99		0.973120	0.945005	15.366157	14.393037	0.857494	99
100		0.774143	0.751252	14.507563	13.733420	0.818196	100
101		0.660149	0.639925	13.756311	13.096162	0.780230	101
102		0.552983	0.536926	13.116386	12.563404	0.748490	102
103		0.457313	0.443281	12.579460	12.122147	0.722201	103
104		2.307345	2.300203	12.136179	9.828834	0.585572	104
105		1.379474	1.384191	9.835976	8.456502	0.503813	105
106		0.963739	0.960753	8.451785	7.488045	0.446115	106
107		1.149379	1.158351	7.491032	6.341652	0.377817	107
108		0.865231	0.863176	6.332680	5.467449	0.325734	108
109		0.728906	0.727177	5.469504	4.740598	0.282431	109
110		0.658368	0.668534	4.742328	4.083959	0.243310	110
111		0.775421	0.766597	4.073794	3.298373	0.196507	111
112		0.534669	0.532235	3.307197	2.772527	0.165179	112
113		0.384403	0.384650	2.774961	2.390559	0.142422	113
114		0.313033	0.311124	2.390311	2.077278	0.123758	114
115		12.433016	12.063237	37.208359	24.775343	1.476041	115
116		12.097204	11.697181	35.027751	22.930547	1.366133	116
117		10.334956	10.027015	32.277102	21.942146	1.307247	117
118		10.813421	10.484619	31.055840	20.242419	1.205983	118
119		9.800230	9.502337	28.638074	18.837845	1.122302	119
120		8.173551	7.922817	26.553918	18.380367	1.095047	120

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Master Data File for TiTx Sample Ti-3

0	33.570	1 Pi	2 Ti	3 Vi	4 Peq	5 Teq	6 Veq	7 Pf	8 Tf	9 Vf	10 Vx	11 Vs	12 Ni
121		707.700	20.8	159.93	755.00	650.0	168.42	745.00	21.0	159.93	8.00	8.49	6.174345
122		545.000	20.9	159.93	623.60	654.4	168.42	624.10	21.2	159.93	8.00	8.49	4.753248
123		424.400	20.8	159.93	485.00	650.5	168.42	485.20	21.0	159.93	8.00	8.49	3.702688
124		285.300	21.1	159.93	363.70	650.5	168.42	364.00	21.5	159.93	8.00	8.49	2.486569
125		164.200	21.6	159.93	258.90	650.3	168.42	259.10	21.7	159.93	8.00	8.49	1.428678
126		59.300	21.9	159.93	173.30	649.9	168.42	173.40	21.9	159.93	8.00	8.49	0.515435
127		0.000	21.6	159.93	117.70	650.0	168.42	117.80	22.0	159.93	8.00	8.49	0.000000
128		2373.200	21.1	159.93	1409.50	650.9	168.42	1409.50	18.8	159.93	8.00	8.49	20.683928
129		1209.200	18.8	159.93	1289.50	649.9	168.42	1290.50	18.6	159.93	8.00	8.49	10.621964
130		1107.600	17.9	159.93	1228.70	650.2	168.42	1229.90	17.7	159.93	8.00	8.49	9.759566
131		1030.600	17.7	159.93	1134.20	650.0	168.42	1135.20	18.1	159.93	8.00	8.49	9.087328
132		935.600	18.0	159.93	999.50	650.1	168.42	1000.30	18.4	159.93	8.00	8.49	8.241164
133		800.300	18.4	159.93	846.20	650.0	168.42	846.80	18.7	159.93	8.00	8.49	7.039712
134		620.400	18.7	159.93	679.40	649.6	168.42	679.70	18.2	159.93	8.00	8.49	5.451641
135		479.700	17.9	159.93	541.80	649.5	168.42	542.30	17.7	159.93	8.00	8.49	4.226854
136		350.200	16.7	159.93	450.40	649.5	168.42	451.20	19.0	159.93	8.00	8.49	3.098546
137		251.200	19.7	159.93	331.40	649.5	168.42	331.60	21.0	159.93	8.00	8.49	2.199832
138		131.500	20.1	159.93	231.30	649.4	168.42	231.40	17.6	159.93	8.00	8.49	1.150013
139		30.200	16.7	159.93	148.30	647.9	168.42	148.60	17.9	159.93	8.00	8.49	0.267208
140		1105.400	19.2	159.93	88.20	20.0	168.42	88.20	17.9	159.93	8.00	8.49	9.696869
141		0.000	20.0	159.93	0.00	20.0	168.42	0.00	20.0	159.93	8.00	8.49	0.000000
142		401.000	18.8	160.13	42.20	21.6	168.62	42.20	21.6	160.13	8.20	8.49	3.526905
143		0.000	20.0	160.13	0.00	20.0	168.62	0.00	20.0	160.13	8.20	8.49	0.000000

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Master Data File for TiTx Sample Ti-3

0	33.570	13 Ngas	14 Nf	15 Nsys	16 Nm	17 Q/M	18 Seq#
121		6.791754	6.495350	24.805446	18.013692	1.073202	121
122		5.605687	5.437575	23.063344	17.457656	1.040075	122
123		4.362892	4.230260	21.328456	16.965563	1.010757	123
124		3.266221	3.168182	19.584764	16.318543	0.972210	124
125		2.323504	2.253624	17.845261	15.521757	0.924740	125
126		1.554247	1.507192	16.107072	14.552825	0.867014	126
127		1.055241	1.023570	14.599880	13.544639	0.806949	127
128		12.773945	12.381457	34.260238	21.486293	1.280089	128
129		11.694471	11.343898	32.500745	20.806273	1.239575	129
130		11.177192	10.844659	30.916413	19.739221	1.176004	130
131		10.303535	9.995893	29.159083	18.855548	1.123357	131
132		9.070602	8.798981	27.404354	18.333752	1.092270	132
133		7.671573	7.441086	25.645085	17.973513	1.070808	133
134		6.169874	5.982978	23.655641	17.485767	1.041750	134
135		4.928662	4.781737	21.899517	16.970855	1.011073	135
136		4.079154	3.960758	20.216326	16.137172	0.961404	136
137		2.981191	2.891085	18.455400	15.474209	0.921907	137
138		2.104815	2.041074	16.714329	14.609513	0.870391	138
139		1.348164	1.309382	14.940462	13.592298	0.809788	139
140		0.818253	0.777170	23.327949	22.509696	1.341060	140
141		0.000000	0.000000	22.550779	22.550779	1.343508	141
142		0.387127	0.367635	26.077684	25.690557	1.530566	142
143		0.000000	0.000000	25.710049	25.710049	1.531728	143

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RPL procedure ISOTHERM2

```
procedure;
/* Procedure ISOTHERM */
/* Version 0.0 */
/* Author: Kirk L. Shanahan */
/* Version History */
/* Created 10/7/97 */
/* Purpose: Takes an input data file holding absorbtion/desorbtion */
/* data, and calculates the isotherm data, and then makes */
/* the data graph. */

/* Data file structure: */
/* row 1 has the millimoles metal followed by the initial Q/M */
/* rows 2 thru n are the isotherm data in the following order: */
/* Pi Ti Vi Peq Teq Veq Pf Tf Vf Vsamp Vexcess */
/* pressures are in torr, temps in degrees C */
/* 'volumes' are a 1 to 4 letter code which is: */
/* 1st letter is A or B and means A or B manifold */
/* 2nd thru 4th letters are the additional volumes present */
/* (a,b,c,d,e,f) (these can be caps or lowercase) */
/* The procedure reads the data file via EZ_READFILE, so it needs to */
/* have entries for all slots in the data file. */

dirstring="/afs/srtc.srs.gov/u1/t8385/";

tblname = gettext("Where is the data stored (filename w/o extension)?",
, true);

filename = dirstring CAT tblname CAT ".dat";
call $ez_readfile(filename,tblname,,,,,TRUE);

if lastcol(tblname) > 11 then goto tblerror;

row 0 col 0 of table(tblname) = row 1 col 1;
row 2 col 0 of table(tblname) = row 1 col 2;
delete row 1 of table(tblname);
/* move the mmoles metal into the 0,0 cell and the init Q/M into 1,0 */

row 0 col 1 of table(tblname) = 'Pi' ;
row 0 col 2 of table(tblname) = 'Ti' ;
row 0 col 3 of table(tblname) = 'Vi' ;
row 0 col 4 of table(tblname) = 'Peq' ;
row 0 col 5 of table(tblname) = 'Teq' ;
row 0 col 6 of table(tblname) = 'Veq' ;
row 0 col 7 of table(tblname) = 'Pf' ;
row 0 col 8 of table(tblname) = 'Tf' ;
row 0 col 9 of table(tblname) = 'Vf' ;
row 0 col 10 of table(tblname) = 'Vx' ;
row 0 col 11 of table(tblname) = 'Vs' ;
row 0 col 12 of table(tblname) = 'Ni' ;
row 0 col 13 of table(tblname) = 'Ngas' ;
row 0 col 14 of table(tblname) = 'Nf' ;
row 0 col 15 of table(tblname) = 'Nsys';
```

```

row 0 col 16 of table(tblname) = 'Nm' ;
row 0 col 17 of table(tblname) = 'Q/M' ;

lr = lastrow(tblname);
/* Translate Vol Codes to numerical values. */

if tableexists("temper") then delete table temper;

do j = 3 to 9 by 3;
do i = 1 to lr;

x= row i col j of table(tblname);

if tableexists("temper") then col 1 of temper = empty;
else
  allocate table("temper") 1 col by 4 rows;

do k = 1 to chars(x);
  if k=1 then
    {
      if caps(ext(1,1,x))='A' then z= 'Aman';
      if caps(ext(1,1,x))='B' then z= 'Bman';
    }
  else
    z= ext(k,k,x);

  row k col 1 of temper = row z col 1 of table('@etm_volumes') ;

end;

row i col j of table(tblname) = SUM of rows 1 to (k-1) of temper;

end;
end;

/* Calculations */

do i= 1 to lr;
/* Correct volumes */
row i col 3 of table(tblname) = row i col 3 of table(tblname) +
  row i col 10 of table(tblname);
row i col 6 of table(tblname) = row i col 6 of table(tblname) +
  row i col 11 + row i col 10 ;
row i col 9 of table(tblname) = row i col 9 of table(tblname) +
  row i col 10 ;
/* Calc mmoles (.0160356 is 1/R in correct units) */
row i col 12 of table(tblname) = .0160356 * row i col 3 * row i col 1 /
  (273.15 + row i col 2);
row i col 14 of table(tblname) = .0160356 * row i col 7 * row i col 9 /
  (273.15 + row i col 8);
/* This eqn corrects Neq for the temperature of the sample cell */
row i col 13 of table(tblname) = .0160356 * (row i col 9-5) * row i col 4 /
  (273.15 + row i col 8) +
  .0160356 * 5 * row i col 4 /

```



```

(273.15 + row i col 5);

if i= 1 then
/* 1st row just needs to add mmoles in sample cell + that in manifold */
row i col 15 of table(tblname) = (.5* row 1 col 0 * row 0 col 0) +
row i col 12;
else
/* every other row then corrects for aliquots */
row i col 15 of table(tblname) = row (i-1) col 15 -
( row (i-1) col 14 - row i col 12 );

/* Calc millimoles in metal (as Q2), then calc Q/M */
row i col 16 of table(tblname) = row i col 15 - row i col 13;
row i col 17 of table(tblname) = 2* row i col 16 / row 0 col 0;

end;

grphname = tblname CAT "_iso";
make graph graph(grphname) from col 17 of table(tblname) vs
col 4 of table(tblname);

label of x axis of graph graph(grphname) = 'Q/M' ;
label of y axis of graph graph(grphname) = 'P (torr)' ;
orientation of y axis of graph graph(grphname) = 'VERTICAL' ;
size of Y axis of graph graph(grphname) = 'Large' ;
size of x axis of graph graph(grphname) = 'Large' ;
graphtitlesize of graph graph(grphname) = 'LARGE' ;
symbol of curve 1 of graph graph(grphname) = 'fcircle';
label of curve 1 of graph graph(grphname) = empty;
connected of curve 1 of graph graph(grphname) = 'c' ;

call $save_dismods('graph',grphname,'box',false);

dis graph(grphname);

goto doquit;

tblerror:

type "ERROR! Wrong number of columns in table";

doquit:
type "Procedure ISOTHERM complete.";
/*if tableexists("temper") then delete temper;
*/end;

```