Format Change Proposals

CR Lubitz and TH Trumbull
KAPL, Inc.

Cross Section Evaluation Working Group
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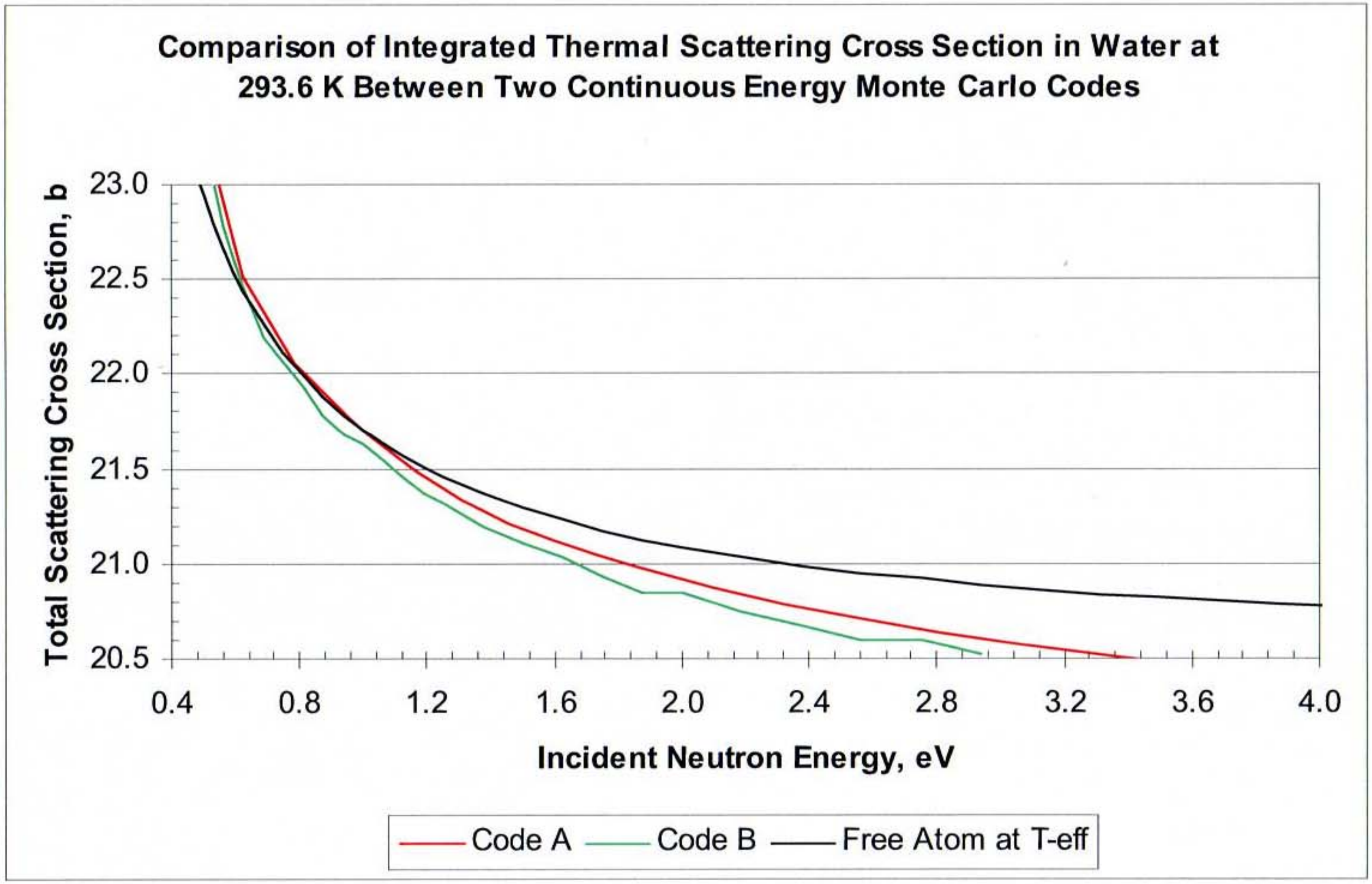
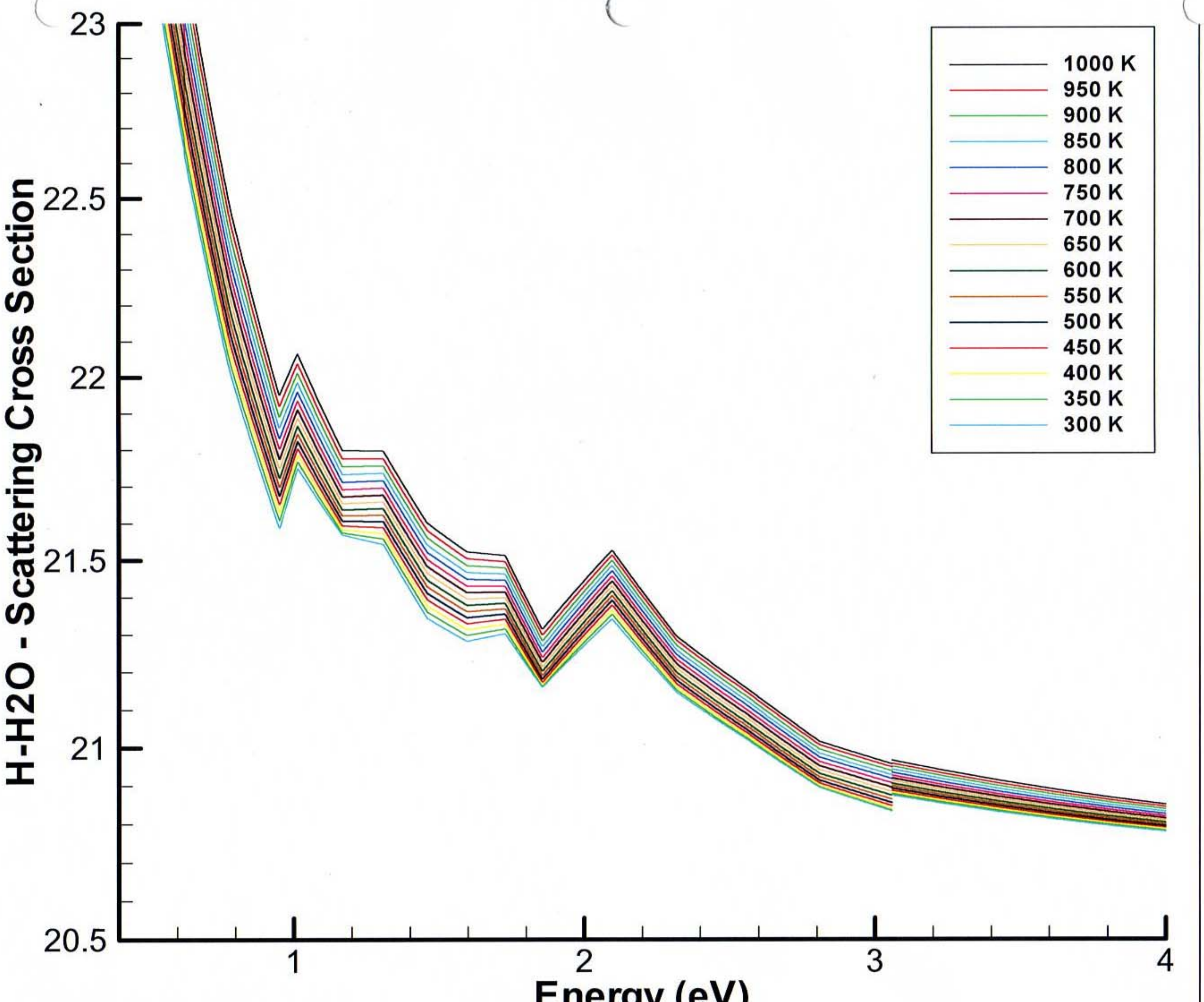
1. Explicit bound-atom cross sections for hydrogen in water

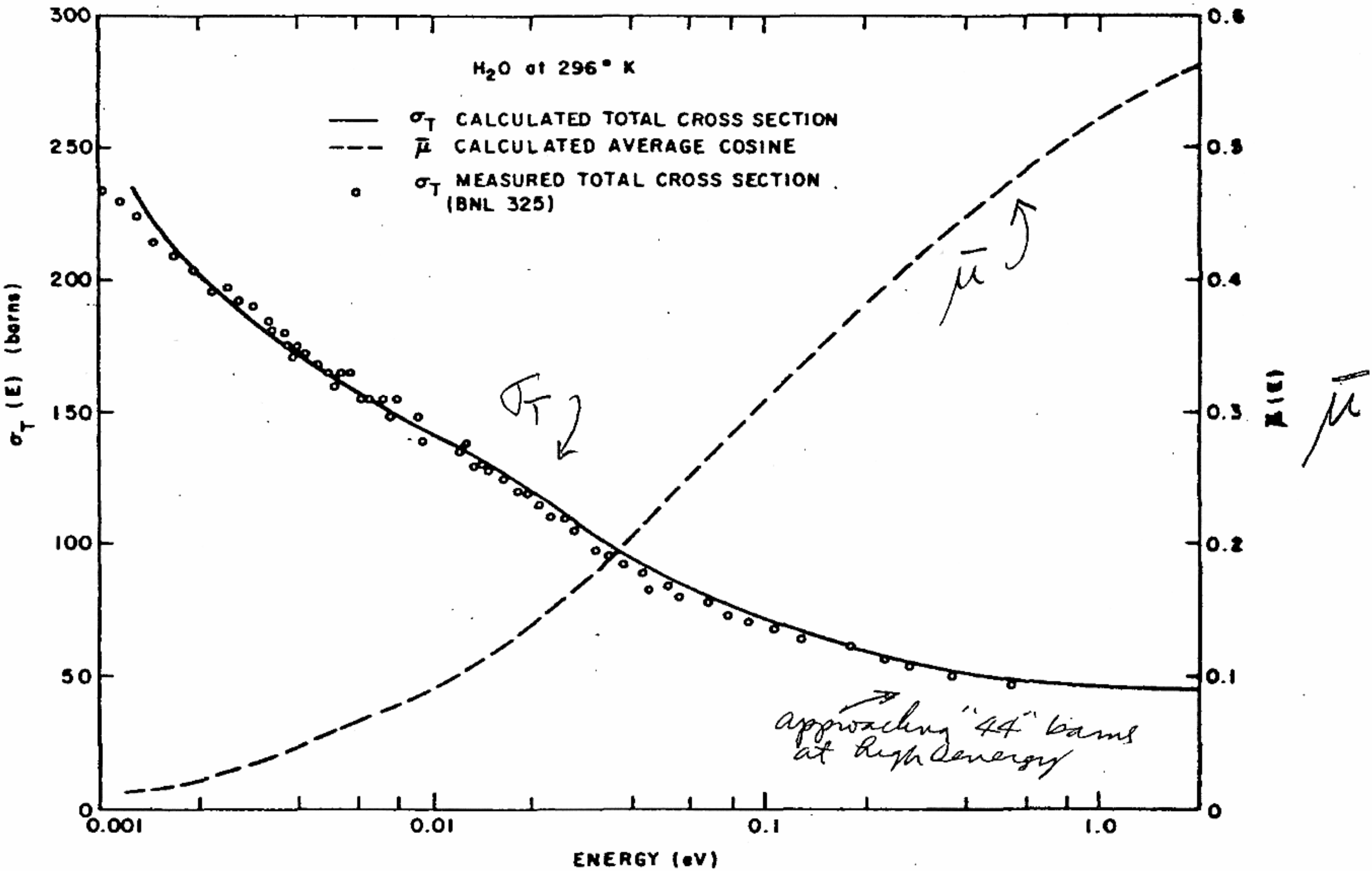
- Cross section of H-H2O not specified by CSEWG, in either energy or temperature.
- Reconstructed by a difficult integration over $\sigma(E,E',\theta)$ in α,β space.
- The ENDF Manual says "Computer precision can be a real problem" and "temperature interpolation of $S(\alpha,\beta)$ is unreliable". Those are true statements.
- Specifying the cross sections solves many of the problems.

An Example of Differing Results





H-H2O - Scattering Cross Section
Energy (eV)
23
22.5
22
21.5
21
20.5
1
2
3
4
1000 K
950 K
900 K
850 K
800 K
750 K
700 K
650 K
600 K
550 K
500 K
450 K
400 K
350 K
300 K



H2O at 296° K
σT CALCULATED TOTAL CROSS SECTION
μ̄ CALCULATED AVERAGE COSINE
σT MEASURED TOTAL CROSS SECTION (BNL 325)
σT (E) (barns)
μ̄ (E)
ENERGY (eV)
0.001
0.01
0.1
1.0
300
250
200
150
100
50
0
0.6
0.5
0.4
0.3
0.2
0.1
0
σT
μ̄
approaching "44" barns at high energy

5. INTEGRAL DATA

TABULATION OF ENERGY IN EV (E), THE TOTAL CROSS SECTION IN BARNS (SIGTOT) AND THE AVERAGE COSINE OF THE SCATTERING ANGLE (MUBAR).

DATA FOR H2O AT 296 DEGREES K.

	E	SIGTOT	MUBAR		E	SIGTOT	MUBAR
1	.00025	446.61971	-.00062	37	.22400	58.70315	.39348
2	.00075	282.53653	.00300	38	.24800	57.47408	.40517
3	.00125	235.44726	.01043	39	.27200	56.36451	.41506
4	.00175	211.74469	.01803	40	.29600	55.31012	.42290
5	.00225	197.61657	.02566	41	.32500	54.23526	.43161
6	.00275	187.82400	.03261	42	.35500	53.22526	.43916
7	.00325	180.28262	.03899	43	.38500	52.31221	.44591
8	.00375	174.26069	.04444	44	.41500	51.47195	.45179
9	.00450	167.82642	.05282	45	.44500	50.71632	.45715
10	.00550	160.71212	.06131	46	.47500	50.06524	.46199
11	.00650	155.49000	.06921	47	.50500	49.51662	.46655
12	.00750	150.82354	.07573	48	.53500	49.05239	.47094
13	.00850	146.91556	.08100	49	.56500	48.66251	.47526
14	.00950	143.49759	.08727	50	.59500	48.33092	.47953
15	.01100	139.45900	.09716	51	.62500	48.04959	.48369
16	.01300	134.57830	.10883	52	.65500	47.80850	.48774
17	.01500	130.06634	.11841	53	.68500	47.60161	.49161
18	.01700	125.98003	.12736	54	.71500	47.42690	.49522
19	.01900	122.25222	.13588	55	.74500	47.27436	.49870
20	.02100	118.81882	.14404	56	.77500	47.13997	.50197
21	.02500	112.66597	.15921	57	.80500	47.01971	.50507
22	.02900	107.04419	.17109	58	.85500	46.84422	.50992
23	.03600	99.47064	.19467	59	.90500	46.69502	.51431
24	.04400	92.58750	.21742	60	.95500	46.56007	.51831
25	.05300	86.63676	.23902	61	1.00500	46.43735	.52199
26	.06500	81.00226	.26240	62	1.10500	46.21047	.52849
27	.07700	76.98061	.28097	63	1.20500	46.00821	.53404
28	.08900	73.96602	.29640	64	1.30500	45.82845	.53893
29	.10100	71.53633	.30968 33.89	65	1.40500	45.67310	.54336
30	.11300	69.47619	.32143	66	1.50500	45.54009	.54743
31	.12500	67.68473	.33177	67	1.60500	45.42736	.55109
32	.13700	66.05334	.34024	68	1.70500	45.32688	.55445
33	.15200	64.35290	.35069	69	1.80500	45.23461	.55750
34	.16800	62.76767	.36123	70	1.90500	45.13252	.56038
35	.18400	61.37622	.37122	71	2.00500	44.19259	.55834
36	.20000	60.17616	.38052				

Proposed Addition to File 7

7.5 Total Scattering Cross Section $\sigma_n(E',T)$

This section specifies the total scattering cross section as a function of the neutron incident energy and the temperature of the moderator. The upper limit of 20 eV is considered to be above the energy where chemical binding and target motion are significant. Users have the option of using this reliably-interpolable representation or values reconstructed by integration over $S(\alpha,\beta,T)$.

7.5.1. Formats for Total Scattering $\sigma_n(E',T)$

NT Total number of temperatures given.

The structure of a section is

[MAT, 7, 3 / ZA, AWR, 0, 0, 0, 0] HEAD
[MAT, 7, 3 / 0.0, 0.0, 0, 0, NR, NT/ T_{int}] TAB2
[MAT, 7, 3 / T_1, 0, 0, 0, NR, NP/ E'_{int} /$\sigma_n(E',T_1)$] TAB1
[MAT, 7, 3 / T_2, 0, 0, 0, NR, NP/ E'_{int} /$\sigma_n(E',T_2)$] TAB1

< continue with TAB1 records for $T_3,T_4,\ldots T_{NT}$ >

[MAT, 7, 3 / T_{NT}, 0, 0, 0, NR, NP/ E'_{int} /$\sigma_n(E',T_{NT})$] TAB1

7.5.2. Procedures for Total Scattering $\sigma_n(E',T)$

There are no procedures. The caveats of Section 7.4 still apply to the calculation of the secondary energy and angle from $S(\alpha,\beta,T)$, but are irrelevant to these tabulated total scattering cross sections. Any thermal (non-threshhold) reactions other than scattering must be added to these values to obtain the total cross section.

A Possible Addition to File 7

7.6 Legendre Moments $B_\ell(E,E',T)$

This section specifies the angular distribution of thermally-scattered neutrons as a function of the neutron's incident and exit energy and the temperature of the moderator. The upper limit of 20 eV is considered to be above the energy where chemical binding and target motion are significant. Users have the option of using this reliably-interpolable representation or values reconstructed by integration over $S(\alpha,\beta,T)$.

7.6.1. Formats for Legendre Moments $B_\ell(E,E',T)$

NT Total number of temperatures given.

The structure of a section is

```
[MAT, 7, 5 /  ZA, AWR,   0,   0,   0,   0] HEAD
[MAT, 7, 5 / 0.0, 0.0,   0,   0,  NR, NT/ Tint ] TAB3
[MAT, 7, 5 /  T1,    0,   0, 0,   0,   0/ Bℓ(E,E',T)] TAB2
[MAT, 7, 5 /  T2,    0,   0,   0, 0.   0/ Bℓ(E,E',T)] TAB2
              ------------------------------
              < continue with TAB2 records for T3,T4,...TNT >
              ------------------------------
[MAT, 7, 3 /  TNT, 0,   0,   0,  NR,  NP/  Bℓ(E,E',T)] TAB2
```

7.6.2. Procedures for Legendre Moments $B_\ell(E,E',T)$

There are no procedures. The caveats of Section 7.4 still apply to the calculation of the secondary energy and angle from $S(\alpha,\beta,T)$, but are irrelevant to these tabulated total scattering cross sections. Any thermal (non-threshhold) reactions other than scattering may be assumed isotropic..

2. Consistent Total Cross Sections for Selected Materials

- Description of the issue:
  - Gerry Hale's R-Matrix analyses of H1 and other light elements give capture and scattering cross sections which add up exactly to the total cross section.
  - For ENDF, he fits the cross sections with loglog-interpolated curves. The pieces then do not add up between the tabulated points.
  - NJOY linearizes the ENDF cross sections and reconstructs the total.

2. Consistent Total Cross Sections for Selected Materials (cont.)

- The effect of these procedures:
  - Monte Carlo codes using the "survival-probability" algorithm sample the total xsec to determine the mfp to the next collision site.
  - There the neutron is down-weighted using the non-absorption probability, σ_S / σ_T.
  - The *implicit absorption* probability is therefore incorrect by the difference between $\sigma_T - \sigma_S$ and the correct σ_C
  - Distingushing 20.3326 from 20.3320 requires great care.

2. Consistent Total Cross Sections for Selected Materials (cont.)

- The proposed format change: (really just a procedural change)
  - For materials of special importance, like hydrogen, supply the actual R-Matrix results, either as the standard ENDF file, or on a special-purpose file where interested users can access it.
  - A suggested format is linear-interpolation, to preserve the between-point additivity, with a maximum between-point error of either 0.01% or 0.00001, whichever is larger.

3. Explicit Unresolved Resonance Region Dilute Averages

- In File 2, LSSF=1 materials have explicit dilute average cross sections given in File 3, while LSSF=0 materials have zeros.
- NJOY users get the LSSF=0 values from RECONR, but it would be convenient to have them visible in the ENDF file itself.

3. Explicit Unresolved Resonance Region Dilute Averages (cont.)

- The proposal is to convert all LSSF=0 materials to LSSF=1 and replace their zeros with either:
  - Values supplied by the evaluator, or
  - Values backfitted from RECONR
- The physics of LSSF=1 is inherently superior to LSSF=0 and this could encourage evaluators to record their best estimate of what these cross sections actually are.

4. Machine-Readable Resonance Integrals and 2200 m/s Cross Sections

- The proposed format change:
  - Add explicit resonance integrals and 2200 m/s cross sections in the first two (currently empty) fields of the dictionary in File 1.
  - It would facilitate our checking procedures and reduce ambiguity.