

# **Negative electron transfer dissociation sequencing of 3-*O*-sulfation containing heparan sulfate oligosaccharides**

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Figure S1. NETD cleavage maps of synthetic HS tetrasulfated tetramers T3, GlcA-GlcNS-IdoA2S-GlcNS3S6S using different precursors: a,  $[M - 5H]^{5-}$ ; b,  $[M - 5H + Na]^4$

Figure S2. Mass spectrum of T3, showing the precursor distribution.

Figure S3. NETD tandem mass spectra of the  $[M - 5H]^{5-}$  precursor of synthetic HS hexamers: a, H1, GlcA-GlcNS6S-IdoA-GlcNS3S-GlcA-GlcNS6S; b, H2, GlcA-GlcNS6S-IdoA-GlcNS6S-GlcA-GlcNS6S; c, H3, GlcA-GlcNS6S-IdoA-GlcNS3S6S-GlcA-GlcNS6S.

Figure S4. NETD tandem mass spectra of the lyase resistant tetramers from HSPIM: a,  $\Delta$ HexA-GlcNAc6S-GlcA-GlcNS3S,  $[M - 3H]^{3-}$ ; b,  $\Delta$ HexA-GlcNAc6S-GlcA-GlcNS3S6S,  $[M - 4H]^4$ ; c,  $\Delta$ HexA2S-GlcNAc6S-GlcA-GlcNS3S6S,  $[M - 4H]^4$ ; d,  $\Delta$ HexA2S-GlcNS6S-GlcA-GlcNS3S6S,  $[M - 4H]^4$ .

Figure S5. Percent of sulfate retention in glycosidic fragment ions generated by NETD of native tetramer  $\Delta$ HexA2S-GlcNS6S-GlcA-GlcNS3S6S from HSPIM.

Table S1. List of assigned peaks in the NETD spectrum of T1,  $[M - 4H]^4$  (relative intensity was normalized to the total intensity in the spectrum, same below)

Table S2. List of assigned peaks in the NETD spectrum of T2,  $[M - 4H]^4$

Table S3. List of assigned peaks in the NETD spectrum of T3,  $[M - 4H]^4$

Table S4. List of assigned peaks in the NETD spectrum of T3,  $[M - 5H]^{5-}$

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Table S12. List of assigned peaks in the NETD spectrum of [1, 1, 2, 1, 5] from HSPIM,  $[M - 4H]^4$

Table S13. List of assigned peaks in the NETD spectrum of [1, 1, 2, 0, 6] from HSPIM,  $[M - 4H]^4$

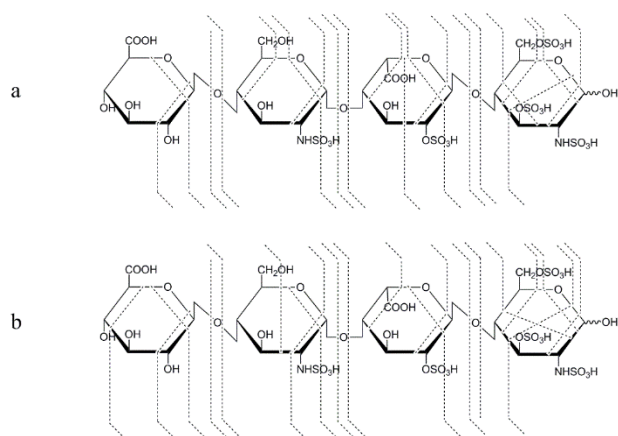


Figure S1. NETD cleavage maps of synthetic HS tetrasulfated tetramers T3, GlcA-GlcNS-IdoA2S-GlcNS3S6S using different precursors: a,  $[M - 5H]^{5-}$ ; b,  $[M - 5H + Na]^{4-}$

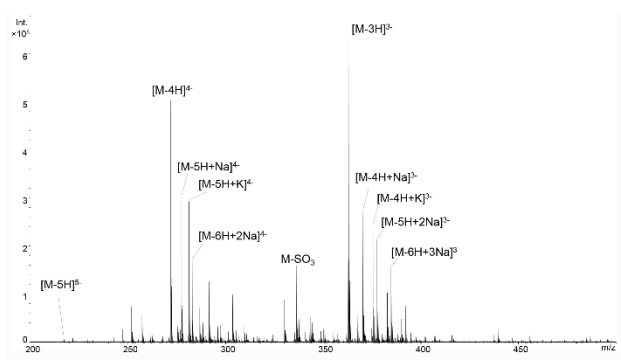


Figure S2. Mass spectrum of T3, showing the precursor distribution.

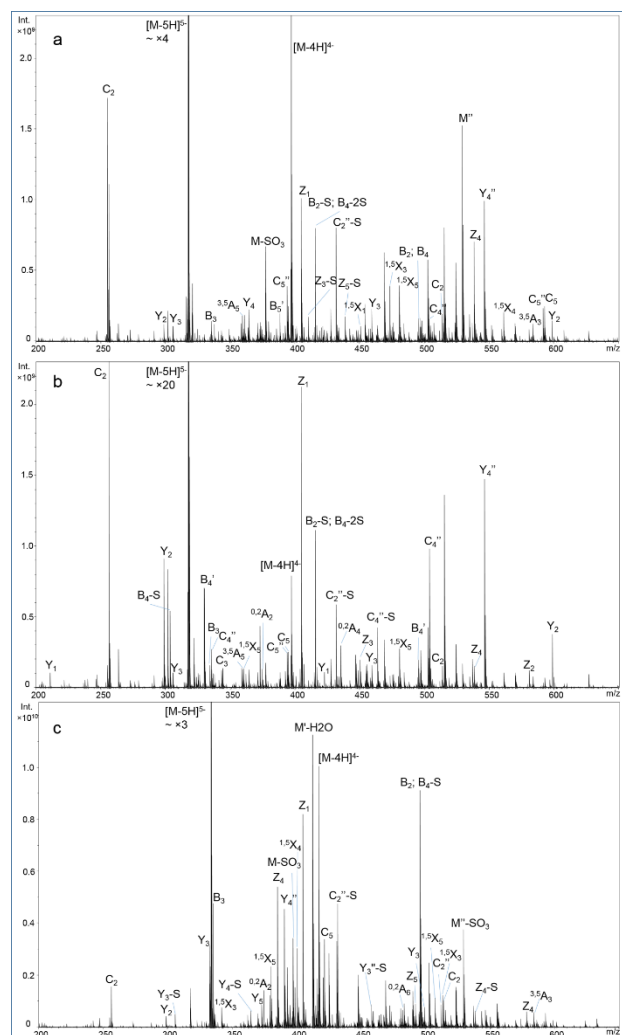


Figure S3. NETD tandem mass spectra of the  $[M - 5H]^{5-}$  precursor of synthetic HS hexamers: a, H1, GlcA-GlcNS6S-IdoA-GlcNS3S-GlcA-GlcNS6S; b, H2, GlcA-GlcNS6S-IdoA-GlcNS6S-GlcA-GlcNS6S; c, H3, GlcA-GlcNS6S-IdoA-GlcNS3S6S-GlcA-GlcNS6S.

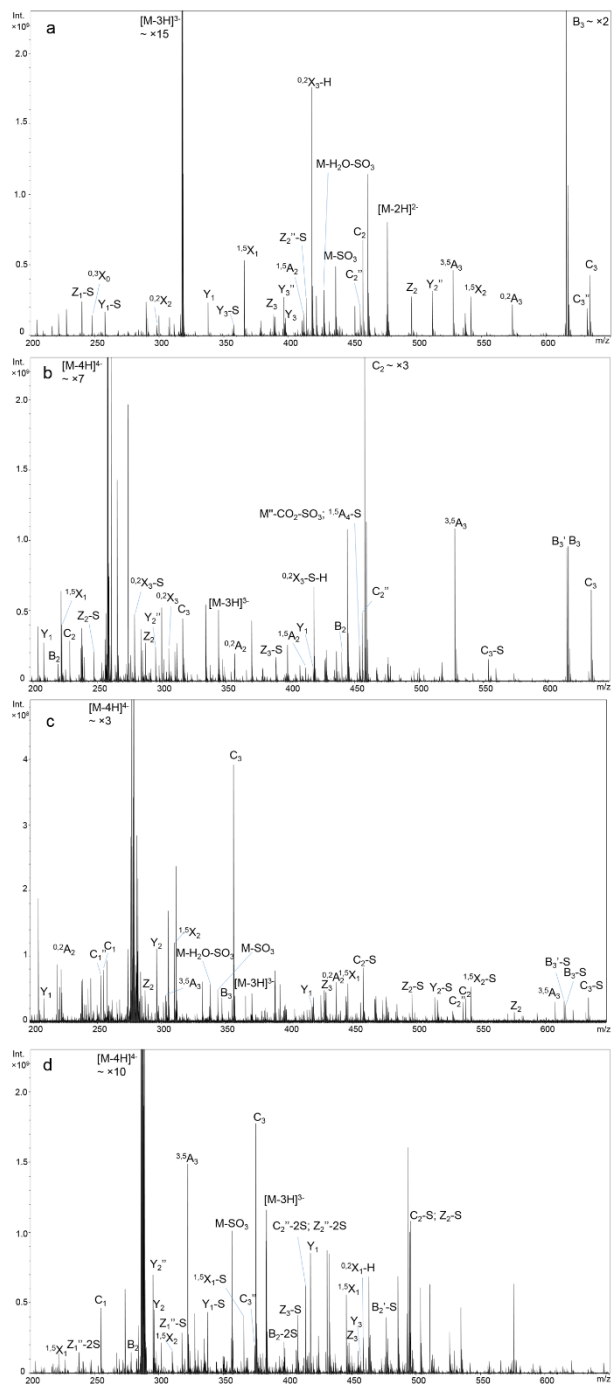


Figure S4. NETD tandem mass spectra of the lyase resistant tetramers from HSPIM: a,  $\Delta$ HexA-GlcNAc6S-GlcA-GlcNS3S,  $[M - 3H]^{3-}$ ; b,  $\Delta$ HexA-GlcNAc6S-GlcA-GlcNS3S6S,  $[M - 4H]^{4-}$ ; c,  $\Delta$ HexA2S-GlcNAc6S-GlcA-GlcNS3S6S,  $[M - 4H]^{4-}$ ; d,  $\Delta$ HexA2S-GlcNS6S-GlcA-GlcNS3S6S,  $[M - 4H]^{4-}$ .

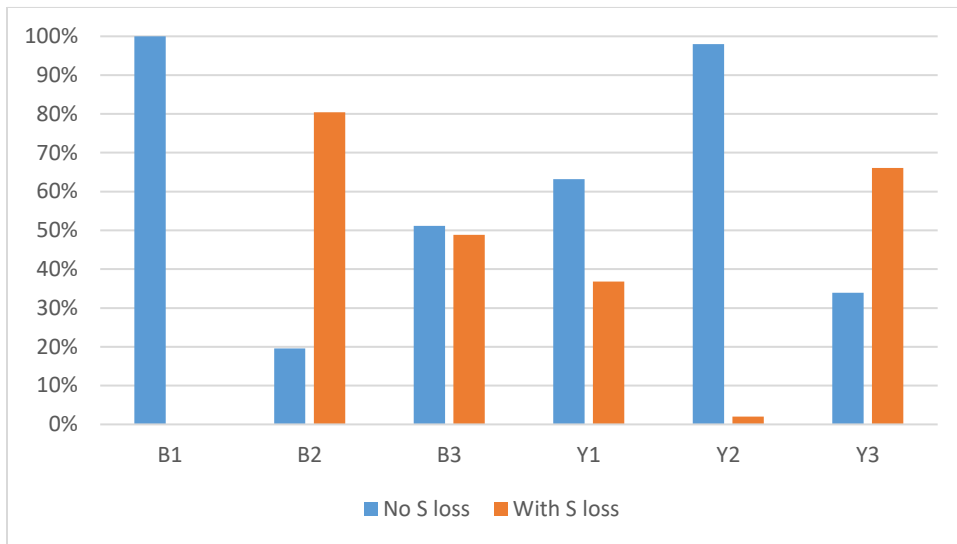


Figure S5. Percent of sulfate retention in glycosidic fragment ions generated by NETD of native tetramer  $\Delta$ HexA2S-GlcNS6S-GlcA-GlcNS3S6S from HSPIM.

Table S1. List of assigned peaks in the NETD spectrum of T1 [M - 4H]<sup>4+</sup> (relative intensity was normalized to the total intensity in the spectrum, + A = + reagent cation, same below).

m/z	Intensity	Charge	Error (ppm)	Assignment
159.4835	0.005%	-2	-3.05	Z1-S
168.4888	0.005%	-2	-2.46	Y1-S
175.0243	0.009%	-1	-2.70	B1
191.0192	0.004%	-1	-2.84	C1"
193.0349	0.105%	-1	-2.67	C1
203.9968	0.097%	-2	4.37	0,3X1-S-H
207.5209	0.007%	-2	-3.24	B2
208.4672	0.027%	-2	-2.23	Y1
216.5264	0.004%	-2	-2.10	C2
222.4646	0.035%	-2	-2.09	1,5X1
247.4995	0.150%	-2	-1.83	Z2-S
251.0090	0.421%	-3	-2.39	Y3-S
251.4673	0.004%	-2	-2.22	3,5X1-2H;1,4X1
251.5292	0.101%	-2	-1.63	3,5A3
253.3517	0.020%	-3	-1.79	0,3A4
255.4970	0.017%	-2	-1.87	Y2"-S
256.5048	0.149%	-2	-1.83	Y2-S
257.6543	0.005%	-3	-2.12	2,4X2
260.3408	0.008%	-3	-1.68	1,5X3-S
263.0403	0.005%	-1	-2.10	0,3A2-2H
263.3551	0.025%	-3	-2.04	0,2A4-S
265.5267	0.006%	-2	-1.47	2,5A3-2H
270.5023	0.079%	-2	-1.69	1,5X2-S
271.6578	0.138%	-3	-2.22	Z3
274.5319	0.012%	-2	-1.70	0,2A3
276.9896	0.077%	-3	-1.67	Y3"
277.0560	0.404%	-1	-1.79	2,5A2-2H
277.6614	0.822%	-3	-1.80	Y3
286.0233	0.010%	-1	-1.86	1,5X1-2S
286.4701	0.007%	-2	-1.75	Z2"
286.9739	0.005%	-2	-2.09	Z2'
286.9930	0.289%	-3	-2.04	1,5X3
287.4779	0.367%	-2	-1.74	Z2
289.0195	0.004%	-3	-2.26	M-H2O-CO2-SO3
290.0074	0.263%	-3	-1.76	0,2A4
291.3288	0.079%	-3	-2.21	0,2X3-H
291.5075	0.015%	-2	-1.62	1,4X2-S-2H
291.6648	0.049%	-3	-2.18	0,2X3
293.0510	0.004%	-1	-1.31	0,2A2-2H



295.0333	0.008%	-2	-1.35	B3'
295.0665	0.130%	-1	-1.92	0,2A2
295.4752	0.125%	-2	-2.22	Y2"
295.5371	0.131%	-2	-1.92	B3
296.4830	0.142%	-2	-2.14	Y2
300.9964	0.004%	-3	-2.23	0,3X3-2H
303.0111	0.005%	-3	-1.48	M"-H2O-SO3
303.5346	0.041%	-2	-1.73	C3"
303.6831	1.807%	-3	-1.17	M-H2O-SO3
304.5424	5.283%	-2	-1.79	C3
309.0146	0.016%	-3	-1.73	M"-SO3
309.3508	0.013%	-3	-0.74	M'-SO3
309.6865	0.469%	-3	-1.74	M-SO3
310.4806	1.588%	-2	-1.72	1,5X2
315.6719	0.075%	-3	-1.71	M-H2O-CO2
315.9886	0.018%	-2	-1.62	0,2X2-S-2H
316.4924	0.207%	-2	-2.07	0,2X2-S-H
317.9588	0.004%	-1	-2.26	Z1"-S
319.9746	0.014%	-1	-1.86	Z1-S
321.0036	0.025%	-3	-1.57	M"-CO2; 1,5A4
327.0259	0.006%	-2	-2.14	Z3"-2S
328.0338	0.126%	-2	-1.78	Z3-2S
329.9992	0.005%	-3	-1.93	M'-H2O
330.3352	0.026%	-3	-1.50	M-H2O
335.6668	0.016%	-3	-1.79	M"
336.0932	0.007%	-1	-1.11	B2-S
336.3388	0.733%	-3	-1.49	M
337.0391	0.017%	-2	-1.81	Y3-2S
337.9852	0.086%	-1	-1.70	Y1-S
351.0366	0.024%	-2	-1.37	1,5X3-2S
352.0881	0.015%	-1	-1.36	C2"-S
354.1036	0.008%	-1	-1.53	C2-S
356.4708	0.946%	-2	-1.94	0,2X2-H
365.9801	0.028%	-1	-1.52	1,5X1-S
367.0044	0.064%	-2	-1.50	Z3"-S
368.0123	0.065%	-2	-1.41	Z3-S
372.5335	0.004%	-2	-2.42	3,5A4
376.0096	0.010%	-2	-1.65	Y3"-S
376.7099	0.009%	-3	-1.51	M'-SO3+A
377.0175	0.078%	-2	-1.63	Y3-S
377.0452	0.006%	-3	-3.16	M-SO3+A
378.9877	0.008%	-1	-2.02	0,2X1-S-H
379.9961	0.004%	-1	-0.53	0,2X1-S

380.0285	0.004%	-2	1.44	0,3A4-H
386.0396	0.005%	-1	-0.78	1,5A2-2H
386.5307	0.005%	-2	-3.09	2,5A4-S-2H
388.0547	0.005%	-1	-2.10	1,5A2
391.0151	0.051%	-2	-1.00	1,5X3-S
395.5366	0.046%	-2	-1.43	0,2A4-S
398.0233	0.005%	-2	-0.08	0,2X3-S
406.9828	0.026%	-2	-1.48	Z3"
407.9906	0.054%	-1	-1.50	0,3X1-S-H
407.9906	0.054%	-2	-1.50	Z3
413.0282	0.007%	-2	-1.03	0,3X3-S
414.0339	0.004%	-1	-2.02	B2"
415.0419	0.024%	-1	-1.65	B2'
415.9882	0.005%	-2	-1.15	Y3"
416.0500	0.151%	-1	-0.96	B2
416.9959	0.297%	-2	-1.38	Y3
417.9419	0.011%	-1	-1.64	Y1
430.9933	0.015%	-2	-1.41	1,5X3
432.0447	0.042%	-1	-1.46	C2"
433.0257	0.006%	-2	-0.81	M"-H2O-CO2-SO3
433.0530	0.006%	-1	-0.48	C2'
434.0341	0.004%	-2	0.30	M-H2O-CO2-SO3
434.0604	0.064%	-1	-1.45	C2
438.0011	0.015%	-2	-1.57	0,2X3
442.0307	0.039%	-2	-1.44	M"-CO2-SO3; 1,5A4-S
445.9371	0.004%	-1	-0.85	1,5X1
455.0204	0.013%	-2	-1.30	M"-H2O-SO3
456.0283	0.007%	-2	-1.30	M-H2O-SO3
464.0256	0.085%	-2	-1.42	M"-SO3
473.0037	0.004%	-2	-1.65	M"-H2O-CO2
482.0091	0.080%	-2	-1.45	M"-CO2; 1,5A4
496.0072	0.004%	-1	0.00	Z2-S
496.0072	0.004%	-2	0.00	M-H2O
504.0039	0.006%	-2	-1.62	M"
592.0824	0.007%	-1	-0.22	B3

Table S2. List of assigned peaks in the NETD spectrum of T2 [M - 4H]<sup>4+</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
168.4891	0.180%	-2	-0.48	Y1
175.0247	0.037%	-1	-0.46	B1
191.0196	0.046%	-1	-0.61	C1"
193.0353	0.086%	-1	-0.60	C1
207.5215	0.079%	-2	-0.60	Z2-S;B2-S
216.5267	0.050%	-2	-0.59	Y1-S
220.9998	0.219%	-3	3.46	0,3X2
233.5024	0.016%	-2	-0.65	1,5A2
238.0025	0.181%	-1	-0.65	Z1"-S
239.0098	0.033%	-1	-3.17	Z1'-S
240.0182	0.510%	-1	-0.69	Z1-S
246.4920	0.073%	-2	-0.59	Z2";B2"
246.9959	0.043%	-2	-0.71	Z2';B2'
247.4999	0.243%	-2	-0.47	Z2;B2
247.9539	0.042%	-1	-0.60	0,3X0
251.0093	0.233%	-3	-1.14	Y3-S
255.4972	0.334%	-2	-0.86	Y2";C2"
256.0131	0.089%	-1	-0.73	Y1"-S
256.5051	5.878%	-2	-0.75	Y2;C2
258.0287	0.093%	-1	-0.75	Y1-S
260.3411	0.026%	-3	-0.49	1,5X3-S
265.0131	0.011%	-3	-0.06	0,2X3-S
270.5025	0.034%	-2	-0.85	1,5X2
276.9896	0.015%	-3	-1.38	Y3"
277.6617	0.057%	-3	-0.87	Y3
279.0052	0.011%	-3	2.22	1,4A4-S-2H
286.0236	0.109%	-1	-0.81	1,5X1-S
286.9932	0.279%	-3	-1.30	1,5X3
290.0077	0.035%	-3	-0.86	0,2A4
291.5078	0.389%	-2	-0.87	3,5A3
291.6652	0.029%	-3	-0.62	0,2X3
295.5375	0.023%	-2	-0.48	B3-S
299.0320	0.043%	-1	1.22	0,2X1-S-H
300.0392	0.044%	-1	-0.94	0,2X1-S
303.6832	0.112%	-3	-0.76	M-H2O-SO3
304.5427	0.016%	-2	-0.82	C3-S
305.5052	0.032%	-2	-0.78	2,5A3-2H

309.0149	0.012%	-3	-0.57	M"-SO3
309.6867	0.309%	-3	-0.79	M-SO3
314.5106	0.017%	-2	-0.55	0,2A3
315.3364	0.018%	-3	-0.45	M'-H2O-CO2
317.9593	0.011%	-1	-0.63	Z1"
318.9671	0.014%	-1	-0.76	Z1'
319.9749	0.047%	-1	-0.85	Z1
321.0039	0.067%	-3	-0.75	M"-CO2;1,5A4
321.3401	0.028%	-3	0.12	M'-CO2
321.5183	0.054%	-2	-0.81	1,5A3
327.0263	0.015%	-2	-0.68	Z3"-2S
328.0341	0.042%	-1	-0.88	0,3X1-S-2H
328.0341	0.042%	-2	-0.88	Z3-2S
329.0181	0.050%	-1	-0.83	3,5A2
330.3355	0.023%	-3	-0.60	M-H2O
332.0030	0.058%	-2	2.45	0,3X2
334.5079	0.017%	-2	-0.98	B3"
335.0119	0.064%	-2	-0.65	B3'
335.5158	0.356%	-2	-0.63	B3
335.6672	0.020%	-3	-0.40	M"
335.9698	0.059%	-1	-0.74	Y1"
336.0031	0.046%	-3	-0.53	M'
336.3391	0.691%	-3	-0.59	M
336.9777	0.082%	-1	-0.73	Y1'
337.0394	0.015%	-2	-0.72	Y3-2S
337.9856	0.286%	-1	-0.45	Y1
343.5132	0.079%	-2	-0.89	C3"
344.5212	0.159%	-2	-0.43	C3
357.0131	0.012%	-1	-0.64	2,5A2-2H
359.0285	0.011%	-1	-1.33	2,5A2
365.9804	0.292%	-1	-0.72	1,5X1
368.0126	0.036%	-2	-0.65	Z3-S
372.5339	0.013%	-2	-1.44	3,5A4-S
375.0236	0.272%	-1	-0.80	0,2A2
376.0102	0.019%	-2	-0.20	Y3"-S
376.7102	0.025%	-3	-0.73	M'-SO3+A
377.0176	0.035%	-2	-1.14	Y3-S
377.0462	0.026%	-3	-0.66	M-SO3+A
378.9882	0.079%	-1	-0.75	0,2X1-H
379.9960	0.306%	-1	-0.68	0,2X1
380.0290	0.073%	-2	2.78	0,3A4-H

386.0398	0.062%	-1	-0.18	1,5A2-S-2H
388.0552	0.138%	-1	-0.78	1,5A2-S
391.0152	0.181%	-2	-0.77	1,5X3-S
395.5369	0.169%	-2	-0.77	0,2A4-S
397.5192	0.037%	-2	-0.56	0,2X3-H
405.5048	0.020%	-2	-0.43	2,4A4
407.9909	0.026%	-1	-0.76	0,3X1-2H
407.9909	0.026%	-2	-0.76	Z3
414.0343	0.166%	-1	-1.17	Z2"-S;B2"-S
415.0423	0.116%	-1	-0.67	Z2'-S;B2'-S
415.9882	0.032%	-2	-1.15	Y3"
416.0501	1.550%	-1	-0.70	Z2-S;B2-S
416.9962	0.033%	-2	-0.77	Y3
420.0169	0.014%	-2	-3.38	3,5X3-S-2H;1,4X3-S
423.9857	0.022%	-1	-0.95	3,5X1-2H; 1,4X1
430.9936	0.136%	-2	-0.76	1,5X3
432.0450	3.317%	-1	-0.82	Y2"-S;C2"-S
434.0607	0.497%	-1	-0.63	Y2-S;C2-S
435.5152	0.091%	-2	-0.80	0,2A4
437.4977	0.017%	-2	-0.29	0,2X3-H
438.0016	0.019%	-2	-0.39	0,2X3
442.0310	0.135%	-2	-0.77	M"-CO2-SO3;1,5A4-S
451.9973	0.117%	-2	-4.30	0,3X3-2H
452.0170	0.408%	-2	-0.90	M-H2O-2CO2
455.0207	0.034%	-2	-0.64	M"-H2O-SO3
455.5246	0.105%	-2	-0.75	M'-H2O-SO3
456.0285	0.071%	-2	-0.74	M-H2O-SO3
459.9963	0.044%	-2	-0.80	1,4A4
462.0555	0.171%	-1	-0.83	1,5X2-S
464.0259	0.125%	-2	-0.81	M"-SO3
465.0339	0.049%	-2	-0.50	M-SO3
465.9963	0.044%	-1	-0.93	1,5A2-2H
467.0050	0.013%	-1	0.98	1,5A2-H
468.0118	0.135%	-1	-1.19	1,5A2
473.0044	0.019%	-2	-0.15	M"-H2O-CO2
482.0095	0.028%	-2	-0.51	M"-CO2;1,5A4
493.9914	0.019%	-1	-0.38	Z2";B2"
494.9991	0.107%	-2	-0.72	M"-H2O
494.9991	0.107%	-1	-0.72	Z2';B2'
496.0069	1.049%	-2	-0.79	M-H2O
496.0069	1.049%	-1	-0.79	Z2;B2

504.0660	0.082%	-1	-0.93	3,5A3-S
505.0123	0.025%	-2	-0.52	M
512.0017	1.168%	-1	-0.87	Y2";C2"
514.0175	0.481%	-1	-0.61	Y2;C2
532.0610	0.019%	-1	-0.68	2,5A3-S-2H
542.0123	0.234%	-1	-0.82	1,5X2
550.0715	0.120%	-1	-0.78	0,2A3-S
554.0361	0.033%	-1	-0.71	0,2X2-S-H
564.0872	0.020%	-1	-0.78	1,5A3-S
565.0651	0.020%	-2	-0.60	M"-SO3+A
565.5683	0.022%	-2	-1.81	M'-SO3+A
584.0230	0.046%	-1	-0.49	3,5A3
590.0664	0.061%	-1	-0.74	B3"-S
591.0744	0.251%	-1	-0.45	B3'-S
592.0823	0.382%	-1	-0.44	B3-S
608.0770	0.264%	-1	-0.65	C3"-S
610.0926	0.182%	-1	-0.75	C3-S
630.0283	0.055%	-1	-0.81	0,2A3
633.9931	0.024%	-1	-0.47	0,2X2-H
655.0600	0.011%	-1	-0.63	Z3"-2S
670.0234	0.028%	-1	-0.48	B3"
671.0312	0.104%	-1	-0.43	B3'
672.0390	0.491%	-1	-0.51	B3
688.0337	0.124%	-1	-0.76	C3"
690.0498	0.042%	-1	-0.11	C3

Table S3. List of assigned peaks in the NETD spectrum of T3 [M - 4H]<sup>4+</sup>

m/z	Intensity	Charge	Error (ppm)	
191.0192	0.010%	-1	-2.85	C1''
193.0349	0.055%	-1	-2.72	C1
203.9968	0.117%	-2	4.42	0,3X1-2S-H
207.5211	0.122%	-2	-2.08	B2
208.4671	0.027%	-2	-2.56	Y1
220.9994	0.016%	-3	1.55	0,3X2-2S
222.4646	0.018%	-2	-2.42	1,5X1
223.9717	0.231%	-3	-2.55	Y2
229.3446	0.011%	-3	-2.30	C3
240.0178	0.013%	-1	-2.12	Z1-2S
247.4994	0.021%	-2	-2.27	Z2-2S
247.9539	0.001%	-1	-0.40	0,3X0
255.4969	0.013%	-2	-2.23	Y2''-2S
256.5047	0.029%	-2	-2.11	Y2-2S
268.9469	0.011%	-2	-1.97	0,2X1-H
270.5021	0.012%	-2	-2.14	1,5X2-2S
270.9869	0.032%	-3	1.53	Z3''-S
271.6578	0.090%	-3	-2.08	Z3-S
274.5318	0.090%	-2	-2.04	0,2A3
274.6726	0.013%	-3	-0.61	3,5A4
277.0558	0.264%	-1	-2.68	2,5A2-2H
277.6613	0.050%	-3	-2.02	Y3-S
283.9535	0.138%	-2	2.72	0,3X1-H
284.4560	0.007%	-2	-2.05	0,3X1
286.4700	0.009%	-2	-1.83	Z2-S
286.9737	0.007%	-2	-2.78	Z2'-S
286.9930	0.034%	-3	-2.05	1,5X3-S
287.4780	0.095%	-2	-1.50	Z2-S
290.0076	0.008%	-3	-1.26	0,2A4-S
291.3289	0.010%	-3	-2.03	0,2X3-S-H
292.4534	0.011%	-2	-2.23	3,5X1
295.0665	0.248%	-1	-2.02	0,2A2
295.4752	0.180%	-2	-2.10	Y2''-S
295.5370	0.056%	-2	-2.05	B3-S
296.4831	0.616%	-2	-2.05	Y2-S
297.6382	0.007%	-3	-1.79	Z3''
298.3102	0.132%	-3	-1.43	Z3
303.5345	0.014%	-2	-1.96	C3''-S
303.6417	0.052%	-3	-1.96	Y3''
303.9779	0.013%	-3	-1.04	Y3'

304.3137	0.795%	-3	-1.56	Y3
304.5423	0.089%	-2	-2.02	C3-S
310.4805	0.350%	-2	-1.99	1,5X2-S
313.6454	0.302%	-3	-1.38	1,5X3
315.6718	0.014%	-3	-2.16	M-H2O-CO2-SO3
316.4925	0.013%	-2	-1.59	0,2X2-2S-H
316.6597	0.013%	-3	-1.76	0,2A4
317.9589	0.033%	-1	-1.98	Z1"-S
317.9811	0.116%	-3	-1.89	0,2X3-H
318.3176	0.029%	-3	-0.25	0,2X3
318.9666	0.009%	-1	-2.26	Z1'-S
319.9745	0.025%	-1	-2.05	Z1-S
321.0035	0.026%	-3	-1.78	M"-CO2-SO3; 1,5A4-S
321.5179	0.018%	-2	-1.99	1,5A3
327.4562	0.137%	-2	-1.90	Z2
327.6486	0.011%	-3	-2.10	0,3X3-2H
328.3206	0.009%	-3	-1.93	0,3X3
329.6632	0.015%	-3	-1.88	M"-H2O-SO3
329.9993	0.015%	-3	-1.60	M'-H2O-SO3
330.3350	1.118%	-3	-2.21	M-H2O-SO3
332.0028	0.012%	-2	1.68	0,3X2-2S
334.5075	0.008%	-2	-2.17	B3"
335.4538	0.102%	-2	-1.43	Y2"
335.5154	0.112%	-2	-1.79	B3
335.6669	0.103%	-3	-1.37	M"-SO3
335.9694	0.022%	-1	-1.92	Y1"-S
336.0030	0.022%	-3	-0.95	M'-SO3
336.0929	0.021%	-1	-2.20	B2-S
336.3388	0.810%	-3	-1.31	M-SO3
336.4615	0.313%	-2	-1.82	Y2
337.9852	0.105%	-1	-1.46	Y1-S
341.6522	0.021%	-3	-1.82	M"-H2O-CO2
341.9883	0.018%	-3	-1.53	M'-H2O-CO2
342.3241	0.130%	-3	-1.76	M-H2O-CO2
343.5128	0.050%	-2	-1.93	C3"
344.5207	1.443%	-2	-1.87	C3
347.3199	0.014%	-3	-1.66	1,5A4-H
347.6558	0.155%	-3	-1.71	M"-CO2; 1,5A4
347.9918	0.050%	-3	-1.40	M'-CO2
352.0879	0.031%	-1	-1.80	C2"-S
356.4708	0.397%	-2	-1.74	0,2X2-S-H
356.6514	0.031%	-3	-1.79	M'-H2O
356.9875	0.025%	-3	-1.40	M-H2O



362.3191	0.305%	-3	-1.45	M"
362.6550	0.129%	-3	-1.69	M'
362.9909	1.417%	-3	-1.78	M
363.9644	0.008%	-1	-1.63	1,5X1-S-2H
363.9644	0.008%	-2	-1.63	2,5X2-S-2H
365.9801	0.174%	-1	-1.50	1,5X1-S
367.0044	0.017%	-2	-1.69	Z3"-2S
368.0122	0.031%	-2	-1.72	Z3-2S
377.0174	0.009%	-2	-1.93	Y3-2S
378.9879	0.009%	-1	-1.53	0,2X1-2S-H
380.0286	0.009%	-2	1.65	0,3A4-S-H
386.0395	0.009%	-1	-0.97	1,5A2-2H
391.0148	0.024%	-2	-1.77	1,5X3-2S
396.4492	0.473%	-2	-1.72	0,2X2-H
399.9311	0.007%	-1	-2.14	Z1
403.3619	0.040%	-3	-2.02	M'-SO3+A
403.6972	0.021%	-3	-3.75	M-SO3+A
405.5047	0.002%	-2	-0.74	2,4A4
406.9827	0.045%	-2	-1.69	Z3"-S
407.9904	0.081%	-1	-2.06	0,3X1-2S-2H
407.9904	0.081%	-2	-2.06	Z3-S
414.0341	0.029%	-1	-1.69	B2"
415.0419	0.034%	-1	-1.71	B2'
415.9907	0.015%	-2	4.97	Y3"-S
416.0497	0.436%	-1	-1.72	B2
416.9959	0.117%	-2	-1.37	Y3-S
417.9418	0.115%	-1	-1.74	Y1
430.9932	0.063%	-2	-1.83	1,5X3-S
432.0446	0.175%	-1	-1.71	C2"
434.0603	0.088%	-1	-1.72	C2
437.4969	0.010%	-2	-2.11	0,2X3-S-H
445.9367	0.052%	-1	-1.75	1,5X1
446.9610	0.027%	-2	-1.73	Z3"
447.9687	0.066%	-2	-2.09	Z3
453.0063	0.015%	-2	-1.61	0,3X3-S
456.9739	0.194%	-2	-2.07	Y3
461.0037	0.015%	-2	-1.79	3,5X3-S
470.9716	0.028%	-2	-1.63	1,5X3
473.0037	0.126%	-2	-1.76	M"-H2O-CO2-SO3
477.4756	0.008%	-2	-1.30	0,2X3-H
477.9794	0.014%	-2	-1.64	0,2X3
482.0088	0.119%	-2	-2.06	M"-CO2-SO3; 1,5A4-S
493.9908	0.011%	-1	-1.65	Z2"-2S

494.9986	0.102%	-2	-1.72	M"-H2O-SO3
496.0067	0.040%	-1	-1.04	Z2-2S
496.0067	0.040%	-2	-1.04	M-H2O-SO3
500.9820	0.009%	-2	-1.91	3,5X3
504.0038	0.405%	-2	-1.73	M"-SO3
504.0656	0.075%	-1	-1.82	3,5A3
512.0012	0.022%	-1	-1.86	Y2"-2S
512.9819	0.680%	-2	-1.99	M"-H2O-CO2
514.0166	0.014%	-1	-2.36	Y2-2S
514.9794	0.015%	-2	-1.97	2,4X3
521.9874	0.106%	-2	-1.57	M"-CO2; 1,5A4
543.9819	0.008%	-2	-2.29	M"
590.0656	0.025%	-1	-2.15	B3"-S
592.0814	0.041%	-1	-1.90	B3-S
608.0762	0.035%	-1	-1.96	C3"-S
610.0919	0.012%	-1	-1.89	C3-S
672.0380	0.029%	-1	-1.98	B3
690.0479	0.008%	-1	-2.91	C3

Table S4. List of assigned peaks in the NETD spectrum of T3 [M - 5H]<sup>5-</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
191.0196	0.030%	-1	-0.49	C1"
193.0353	0.191%	-1	-0.43	C1
206.6516	0.012%	-3	-0.48	1,5X2-S
207.4597	0.013%	-2	-0.39	Z1"
207.5215	0.017%	-2	-0.33	B2
208.4676	0.096%	-2	-0.38	Y1
215.5189	0.056%	-2	-0.41	C2"
216.5268	0.201%	-2	-0.43	C2
217.2540	0.470%	-4	-0.49	0,2A4-S
217.9687	0.040%	-3	-0.46	Z2
218.4972	0.068%	-4	-0.44	0,2X3-S
220.9996	0.065%	-3	2.57	1,4A4-S
222.4650	0.128%	-2	-0.44	1,5X1
223.9722	0.156%	-3	-0.43	Y2
228.6731	0.019%	-3	-0.51	C3"
228.9689	0.077%	-2	-0.39	0,2X1-S-H
229.3449	0.500%	-3	-0.95	C3
229.4728	0.013%	-2	-0.34	0,2X1-S
233.3038	0.820%	-3	-0.62	1,5X2
237.2433	0.018%	-4	-0.41	0,2A4
237.4703	0.020%	-2	-0.42	2,5X1
239.0104	0.014%	-1	-0.56	Z1'-2S
240.0182	0.047%	-1	-0.44	Z1-2S
246.4921	0.013%	-2	-0.37	Z2"-2S
247.2479	0.029%	-4	-0.40	M'-H2O-SO3
247.3485	0.013%	-3	-0.37	3,5A4-S-2H
247.4999	0.199%	-4	-0.47	M-H2O-SO3
247.9538	0.039%	-1	-0.81	0,3X0
249.0615	0.025%	-1	-0.39	3,5A2
251.4986	0.017%	-4	-0.45	M"-SO3
251.5295	0.503%	-2	-0.58	3,5A3
252.0025	0.619%	-4	-0.51	M-SO3
255.4973	0.016%	-2	-0.47	Y2"-2S
256.4916	0.035%	-4	-0.54	M-H2O-CO2
256.5051	0.079%	-2	-0.54	Y2-2S
258.0288	0.018%	-1	-0.49	Y1-2S
263.9640	0.054%	-3	-0.53	0,2X2-H

265.5269	0.015%	-2	-0.48	2,5A3-2H
267.2370	0.017%	-4	-0.71	M'-H2O
267.4891	0.044%	-4	-0.26	M-H2O
269.2956	0.058%	-3	-0.54	2,5X2-H
270.5026	0.040%	-2	-0.60	1,5X2-2S
271.4878	0.013%	-4	-0.59	M''
271.6582	0.210%	-3	-0.69	Z3-S
271.9916	1.104%	-4	-0.70	M
274.5322	0.047%	-2	-0.68	0,2A3
277.0563	0.094%	-1	-0.63	2,5A2-2H
277.6617	0.063%	-3	-0.68	Y3-S
280.5321	0.014%	-2	-0.68	1,5A3-S-2H
283.9539	0.089%	-2	4.11	0,3X1-H
286.0237	0.027%	-1	-0.55	1,5X1-2S
286.4704	0.016%	-2	-0.62	Z2''-S
286.9935	0.446%	-3	0.03	1,5X3-S
287.4782	0.082%	-2	-0.58	Z2-S
290.0078	0.216%	-3	-0.60	0,2A4-S
292.0107	0.264%	-2	-4.10	1,4X2-2S-H; 1,4A3-H
295.0669	0.050%	-1	-0.55	0,2A2
295.4757	0.194%	-2	-0.59	Y2''-S
295.5375	0.139%	-2	-0.54	B3-S
296.4834	0.314%	-2	-0.95	Y2-S
298.3104	0.383%	-3	-0.85	Z3
303.5348	0.378%	-2	-0.81	C3''-S
304.3140	0.241%	-3	-0.55	Y3
304.5426	0.213%	-2	-1.10	C3-S
306.0829	0.015%	-1	-0.44	1,5A2-S-2H
309.4731	0.028%	-2	-0.53	1,5X2-S-2H
310.4810	0.299%	-2	-0.57	1,5X2-S
313.6456	0.505%	-3	-0.65	1,5X3
315.0005	0.054%	-3	-0.12	M''-H2O-CO2-SO3
315.3351	0.016%	-3	-4.66	M'-H2O-CO2-SO3
315.9889	0.020%	-3	1.85	0,2A4-2H
315.9889	0.020%	-2	-0.64	0,2X2-S-2H
316.6601	0.028%	-3	-0.55	0,2A4
317.9593	0.131%	-1	-0.60	Z1''-S
317.9817	0.014%	-3	-0.25	0,2X3-H
318.3176	0.036%	-3	-0.22	0,2X3
319.9749	0.025%	-1	-0.84	Z1-S

				M''-CO2-SO3; 1,5A4-
321.0039	1.502%	-3	-0.70	S
321.3385	0.408%	-3	-4.80	M'-CO2-SO3
321.5184	0.047%	-2	-0.59	1,5A3
323.9864	0.028%	-2	-0.53	2,5X2-2S-2H
327.4566	0.024%	-2	-0.48	Z2
329.6637	0.184%	-3	-0.57	M''-H2O-SO3
330.0001	0.041%	-3	0.78	M'-H2O-SO3
330.3348	0.061%	-3	-2.73	M-H2O-SO3
334.0778	0.021%	-1	-0.54	B2''-S
335.4541	0.070%	-2	-0.56	Y2''
335.5158	0.760%	-2	-0.55	B3
335.6671	0.364%	-3	-0.69	M''-SO3
335.9699	0.099%	-1	-0.56	Y1''-S
336.0017	0.100%	-3	-4.68	M'-SO3
336.0934	0.045%	-1	-0.60	B2-S
336.4617	0.144%	-2	-1.21	Y2
337.9856	0.070%	-1	-0.42	Y1-S
341.6527	0.123%	-3	-0.55	M''-H2O-CO2
341.9872	0.032%	-3	-4.72	M'-H2O-CO2
343.5133	0.073%	-2	-0.55	C3''
344.5211	0.690%	-2	-0.62	C3
347.6562	3.995%	-3	-0.54	M''-CO2; 1,5A4
347.9907	1.081%	-3	-4.52	M'-CO2
350.4593	0.229%	-2	-0.56	1,5X2
352.0883	0.112%	-1	-0.56	C2''-S
354.1039	0.018%	-1	-0.78	C2-S
355.9673	0.020%	-2	-0.62	0,2X2-S-2H
356.4713	0.061%	-2	-0.44	0,2X2-S-H
356.9878	0.024%	-3	-0.66	M-H2O
362.3194	0.039%	-3	-0.68	M''
362.9913	0.024%	-3	-0.57	M
363.9648	0.063%	-1	-0.50	1,5X1-S-2H
363.9648	0.063%	-2	-0.50	2,5X2-S-2H
364.9724	0.024%	-1	-1.25	1,5X1-S-H
364.9724	0.024%	-2	-1.25	2,5X2-S
365.0224	0.016%	-2	-0.64	2,4A4-S-H
365.5264	0.082%	-2	-0.47	2,4A4-S
365.9804	0.236%	-1	-0.53	1,5X1-S
367.0048	0.067%	-2	-0.59	Z3''-2S
368.0126	0.022%	-2	-0.50	Z3-2S

371.5264	0.013%	-2	-0.47	3,5A4-S-2H
377.9804	0.022%	-1	-0.63	0,2X1-2S-2H
378.9881	0.012%	-1	-1.02	0,2X1-2S-H
379.5238	0.079%	-2	-0.57	0,3A4-S-2H
380.0292	0.073%	-2	3.25	0,3A4-S-H
386.0401	0.063%	-1	0.57	1,5A2-2H
388.0553	0.034%	-1	-0.57	1,5A2
391.0166	0.016%	-2	2.81	1,5X3-2S
396.4496	0.097%	-2	-0.53	0,2X2-H
405.5048	0.060%	-2	-0.56	2,4A4
406.9832	0.048%	-2	-0.52	Z3"-S
407.9910	0.059%	-2	-0.54	Z3-S
412.5126	0.027%	-2	-0.46	3,5A4
414.0346	0.047%	-1	-0.57	B2"
415.0424	0.564%	-1	-0.55	B2'
416.0504	0.244%	-1	-0.11	B2
416.9962	0.033%	-2	-0.78	Y3-S
417.9423	0.107%	-1	-0.51	Y1
424.1096	0.016%	-1	-0.23	3,5A3-S
427.0155	0.012%	-2	3.08	2,5A4-S-H
429.9859	0.017%	-2	-0.45	1,5X3-S-2H
432.0451	0.206%	-1	-0.63	C2"
434.0607	0.409%	-1	-0.61	C2
438.0018	0.020%	-2	0.04	0,2X3-S
445.9371	0.051%	-1	-0.69	1,5X1
447.9695	0.024%	-2	-0.31	Z3
451.9991	0.020%	-2	-0.30	0,3X3-S-2H
456.9747	0.022%	-2	-0.48	Y3
458.9451	0.013%	-1	-0.39	0,2X1-S-2H
459.9860	0.021%	-2	2.56	1,4A4-H
470.9721	0.022%	-2	-0.55	1,5X3
473.0043	0.105%	-2	-0.41	M"-H2O-CO2-SO3
473.5063	0.029%	-2	-4.52	M'-H2O-CO2-SO3
477.4760	0.020%	-2	-0.55	0,2X3-H
477.9802	0.019%	-2	0.12	0,2X3
481.0017	0.109%	-2	-0.55	1,5A4-S-2H
481.5044	0.037%	-2	-3.09	1,5A4-S-H
482.0096	0.124%	-2	-0.38	M"-CO2-SO3; 1,5A4-S
482.5113	0.036%	-2	-4.94	M'-CO2-SO3
491.9772	0.022%	-2	-0.92	0,3X3-2H

493.9913	0.022%	-1	-0.61	Z2"-2S
494.9994	0.020%	-1	0.05	Z2'-2S
494.9994	0.020%	-2	0.05	M"-H2O-SO3
496.0071	0.079%	-1	-0.31	Z2-2S
496.0071	0.079%	-2	-0.31	M-H2O-SO3
504.0045	0.042%	-2	-0.37	M"-SO3
504.0662	0.204%	-1	-0.59	3,5A3
504.5061	0.014%	-2	-4.95	M'-SO3
512.0020	0.021%	-1	-0.31	Y2"-2S
512.9827	0.076%	-2	-0.50	M"-H2O-CO2
514.0176	0.035%	-1	-0.38	Y2-2S
521.4840	0.026%	-2	-0.54	1,5A4-H
521.9875	0.055%	-2	-1.35	M"-CO2; 1,5A4
522.4898	0.014%	-2	-4.52	M'-CO2
539.9969	0.033%	-1	-0.42	1,5X2-2S-2H
542.0125	0.029%	-1	-0.51	1,5X2-2S
562.0716	0.021%	-1	-0.62	1,5A3-S-2H
564.0874	0.026%	-1	-0.43	1,5A3-S M"-H2O-CO2-
574.0423	0.027%	-2	-2.35	SO3+A
575.9638	0.013%	-1	-0.53	Z2-S
583.0463	0.013%	-2	-4.54	M"-CO2-SO3+A
590.0666	0.123%	-1	-0.50	B3"-S
592.0822	0.598%	-1	-0.46	B3-S
608.0771	0.148%	-1	-0.55	C3"-S
610.0930	0.032%	-1	-0.17	C3-S
644.0441	0.035%	-1	-0.44	1,5A3
672.0392	0.750%	-1	-0.27	B3
690.0497	0.017%	-1	-0.33	C3

Table S5. List of assigned peaks in the NETD spectrum of T3 [M - 5H + Na]<sup>4+</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
191.0198	0.013%	-1	0.44	C1''
193.0355	0.056%	-1	0.45	C1
207.5217	0.010%	-2	0.43	B2
219.4587	0.014%	-2	0.34	Y1+Na
229.3452	0.009%	-3	0.25	C3
231.2997	0.010%	-3	0.30	Y2+Na
238.0028	0.009%	-1	0.49	Z1''-2S
247.9542	0.002%	-1	0.60	0,3X0
255.4975	0.017%	-2	0.41	Y2''-2S
256.5053	0.012%	-2	0.14	Y2-2S
271.2916	0.009%	-3	0.40	0,2X2-H+Na
274.5324	0.001%	-2	0.18	0,2A3
277.0566	0.496%	-1	0.40	2,5A2-H
277.3249	0.009%	-3	-3.95	Y3'-S
277.6620	0.710%	-3	0.25	Y3-S
279.0720	0.016%	-1	-0.41	2,5A2
280.0047	0.020%	-3	0.98	0,3A4
283.9541	0.034%	-2	4.98	0,3X1-H
284.9894	0.024%	-3	0.54	Y3-S+Na
294.3209	0.011%	-3	0.26	1,5X3-S+Na
294.9439	0.016%	-2	0.95	0,3X1-H+Na
295.0672	0.360%	-1	0.39	0,2A2
295.4760	0.023%	-2	0.53	Y2''-S
295.5378	0.013%	-2	0.64	B3-S
296.4838	0.009%	-2	0.32	Y2-S
297.3354	0.013%	-3	0.60	0,2A4-S+Na
298.4696	0.015%	-2	0.64	Z2-S+Na
299.0384	0.020%	-1	-0.03	2,5A2-2H+Na
303.5352	0.010%	-2	0.40	C3''-S
304.5430	0.013%	-2	0.47	C3-S
304.9663	0.012%	-3	0.63	Z3''+Na
305.6383	0.272%	-3	1.00	Z3+Na
306.4670	0.181%	-2	0.47	Y2''-S+Na
307.4748	0.088%	-2	0.57	Y2-S+Na
310.4813	0.016%	-2	0.61	1,5X2
310.9697	0.036%	-3	0.41	Y3''+Na
311.3061	0.013%	-3	1.76	Y3'+Na
311.6416	0.559%	-3	0.43	Y3+Na
313.6460	0.019%	-3	0.50	1,5X3



317.9596	0.011%	-1	0.39	Z1"-S
320.9734	0.345%	-3	0.96	1,5X3+Na
321.4724	0.130%	-2	0.87	1,5X2-S+Na
323.9877	0.168%	-3	0.57	0,2A4+Na
323.9877	0.168%	-2	3.52	2,5X2-2S-2H
325.3093	0.056%	-3	0.64	0,2X3-H+Na
325.6457	0.014%	-3	2.20	0,2X3+Na
330.3050	0.016%	-3	0.63	2,5X3-2H+Na
335.4545	0.016%	-2	0.76	Y2"
335.5163	0.076%	-2	0.73	B3
337.6634	0.575%	-3	1.06	M-H2O-SO3
337.9869	0.018%	-1	3.48	Y1-S
338.4479	0.084%	-2	0.47	Z2+Na
339.9416	0.010%	-1	0.49	Z1"-S+Na
340.9495	0.012%	-1	0.73	Z1'-S+Na
341.9573	0.011%	-1	0.67	Z1-S+Na
343.6669	0.491%	-3	0.80	M-SO3
344.5215	0.078%	-2	0.63	C3
346.4455	0.100%	-2	0.69	Y2"+Na
347.4529	0.103%	-2	-0.34	Y2+Na
349.3163	0.058%	-3	0.47	M'-H2O-CO2
349.6524	0.027%	-3	0.94	M-H2O-CO2
349.9814	0.013%	-2	-4.13	3,5X2-2S-2H+Na
350.4598	0.059%	-2	0.68	1,5X2
352.0888	0.073%	-1	0.69	C2"-S
354.5047	0.010%	-2	0.80	C3"+Na
354.9839	0.194%	-3	0.62	M"-CO2; 1,5A4+Na
355.3199	0.064%	-3	0.65	M'-CO2
355.5124	0.405%	-2	0.45	C3+Na
357.9523	0.043%	-1	0.67	Y1"-S+Na
359.9681	0.016%	-1	1.27	Y1-S+Na
361.4506	1.177%	-2	0.36	1,5X2+Na
363.9797	0.012%	-3	0.75	M'-H2O
364.3157	0.018%	-3	0.94	M-H2O
366.9587	0.023%	-2	0.55	0,2X2-S-2H+Na
367.4626	0.232%	-2	0.46	0,2X2-S-H+Na
367.9645	0.034%	-2	-4.97	0,2X2-S+Na
369.6472	0.156%	-3	0.52	M"
369.9832	0.076%	-3	0.79	M'
370.3191	0.988%	-3	0.63	M
375.0241	0.015%	-3	0.18	M"-H2O-2CO2-SO3+A
377.0183	0.018%	-2	0.70	Y3-2S
379.0040	0.022%	-2	0.56	Z3-2S+Na

387.9628	0.053%	-1	0.66	1,5X1-S+Na
396.4501	0.014%	-2	0.64	0,2X2-H
402.0069	0.014%	-2	1.09	1,5X3-2S+Na
407.4412	1.050%	-2	0.93	0,2X2-H+Na
407.9430	0.163%	-2	-4.25	0,2X2+Na
410.6904	0.072%	-3	0.74	M'-SO3+A
411.0253	0.040%	-3	-1.62	M-SO3+A
414.0350	0.021%	-1	0.54	B2''
415.0429	0.024%	-1	0.71	B2'
416.0507	0.187%	-1	0.76	B2
416.9967	0.013%	-2	0.50	Y3-S
417.9429	0.030%	-1	0.81	Y1
417.9745	0.066%	-1	3.29	2,5X1-2S+Na
417.9745	0.066%	-2	0.42	Z3''-S+Na
418.4762	0.012%	-2	-4.98	Z3'-S+Na
418.9825	0.092%	-2	0.67	Z3-S+Na
423.5046	0.002%	-2	1.98	3,5A4+Na
426.9800	0.016%	-2	0.78	Y3''-S+Na
427.9878	0.102%	-2	0.75	Y3-S+Na
432.0456	0.161%	-1	0.62	C2''
434.0613	0.073%	-1	0.70	C2
439.9248	0.048%	-1	0.76	Y1+Na
441.9851	0.139%	-2	0.33	1,5X3-S+Na
445.9378	0.016%	-1	0.81	1,5X1
446.5069	0.068%	-2	0.82	0,2A4-S+Na
448.4892	0.013%	-2	0.78	0,2X3-S-H+Na
454.0275	0.011%	-1	0.39	C2''+Na
456.0432	0.009%	-1	0.67	C2+Na
457.9531	0.120%	-2	0.72	Z3''+Na
458.4566	0.036%	-2	-0.12	Z3'+Na
458.9610	0.182%	-2	0.89	Z3+Na
463.9983	0.020%	-2	0.69	0,3X3-S+Na
466.9583	0.019%	-2	0.57	Y3''+Na
467.9197	0.101%	-1	0.64	1,5X1+Na
467.9662	0.519%	-2	0.80	Y3+Na
470.9880	0.030%	-2	0.65	1,4A4+Na
471.9959	0.014%	-2	0.99	3,5X3-S+Na
475.4948	0.019%	-2	1.73	0,2A4
481.9637	0.108%	-2	0.76	1,5X3+Na
483.9949	0.036%	-2	-1.21	M''-H2O-CO2-SO3
486.4853	0.027%	-2	0.74	0,2A4+Na
488.4676	0.016%	-2	0.82	0,2X3-H+Na
488.9716	0.036%	-2	0.84	0,2X3+Na

493.0011	0.132%	-2	0.72	M''-CO2-SO3; 1,5A4-S
493.5028	0.037%	-2	-3.72	M'-CO2-SO3
495.0001	0.010%	-1	1.33	Z2'-2S
496.0077	0.018%	-1	0.99	Z2-2S
503.9771	0.012%	-2	1.33	0,3X3+Na
504.0668	0.118%	-1	0.61	3,5A3
505.9908	0.209%	-2	0.75	M''-H2O-SO3
506.4935	0.082%	-2	-1.53	M'-H2O-SO3
506.9990	0.036%	-2	1.51	M-H2O-SO3
511.9744	0.021%	-2	1.08	3,5X3+Na
514.0182	0.009%	-1	0.84	Y2-2S
514.9961	0.605%	-2	0.79	M''-SO3
515.4977	0.197%	-2	-3.71	M'-SO3
517.9895	0.023%	-1	0.53	Z2-2S+Na
523.9742	0.279%	-2	0.64	M''-H2O-CO2
524.4759	0.089%	-2	-3.54	M'-H2O-CO2
526.0487	0.011%	-1	0.54	3,5A3+Na
532.9795	0.374%	-2	0.69	M''-CO2; 1,5A4+Na
533.4811	0.119%	-2	-3.77	M'-CO2
536.0003	0.010%	-1	1.00	Y2-2S+Na
554.9745	0.021%	-2	0.71	M''
590.0673	0.034%	-1	0.79	B3''-S
592.0832	0.031%	-1	1.10	B3-S
597.9465	0.015%	-1	0.76	Z2-S+Na
608.0779	0.037%	-1	0.82	C3''-S
610.0937	0.011%	-1	0.97	C3-S
616.0358	0.014%	-2	1.61	M''-SO3+A
630.0601	0.024%	-1	1.09	C3''-S+Na
643.9520	0.013%	-1	0.74	1,5X2-S+Na
654.9680	0.010%	-1	0.79	0,2X2-2S-2H+Na
664.0112	0.014%	-1	0.77	1,5A3-2H+Na
672.0401	0.053%	-1	1.16	B3
694.0222	0.038%	-1	1.35	B3+Na
710.0171	0.015%	-1	1.22	C3''+Na

Table S6. List of assigned peaks in the NETD spectrum of T4 [M - 4H]<sup>4+</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
174.0169	0.013%	-1	-0.48	B1'
191.0196	0.026%	-1	-0.62	C1''
193.0353	0.015%	-1	-0.56	C1
208.4675	0.121%	-2	-0.51	Y1
220.9998	0.047%	-3	3.47	0,3X2-S
222.4650	0.472%	-2	-0.62	1,5X1
228.9689	0.075%	-2	-0.50	0,2X1-H
238.0025	0.120%	-1	-0.62	Z1''-2S
239.0103	0.013%	-1	-0.92	Z1'-2S
240.0182	0.031%	-1	-0.66	Z1-2S
246.4920	0.098%	-2	-0.61	B2''
246.9958	0.014%	-2	-1.03	B2'
247.4998	0.050%	-2	-0.62	B2
247.9539	0.029%	-1	-0.40	0,3X0
251.4677	0.014%	-2	-0.53	1,4X1; 3,5X1-2H
255.4973	0.548%	-2	-0.68	C2''
256.0130	0.014%	-1	-0.85	Y1''-2S
256.5051	0.937%	-2	-0.79	C2
270.5026	0.036%	-2	-0.64	1,5X2-S
284.0080	0.016%	-1	-0.61	1,5X1-2S-2H
284.0080	0.016%	-2	-0.61	2,5X2-2S-2H
286.4703	0.091%	-2	-0.79	Z2''
286.9743	0.135%	-2	-0.77	Z2'
286.9933	0.022%	-3	-0.81	1,5X3-S
287.4782	0.825%	-2	-0.60	Z2
290.5000	0.019%	-2	-0.73	3,5A3-2H
291.5078	0.557%	-2	-0.63	3,5A3
295.4757	3.011%	-2	-0.62	Y2''
296.4832	0.772%	-2	-1.57	Y2
299.5052	0.032%	-2	-0.80	0,3A3
303.9771	0.017%	-3	-3.59	Y3'
304.3140	0.075%	-3	-0.64	Y3
305.5052	0.054%	-2	-0.78	2,5A3-2H
310.4810	0.395%	-2	-0.30	1,5X2
313.6456	0.404%	-3	-0.76	1,5X3
314.5105	0.074%	-2	-0.71	0,2A3
316.4928	0.021%	-2	-0.67	0,2X2-S-H
317.9593	0.131%	-1	-0.74	Z1''-S
318.3176	0.014%	-3	-0.19	0,2X3

318.9671	0.052%	-1	-0.59	Z1'
319.9749	0.076%	-1	-0.69	Z1-S
321.5184	0.023%	-2	-0.63	1,5A3
322.9772	0.019%	-3	-0.64	2,5X3-2H
323.9864	0.023%	-2	-0.53	2,5X2-S-2H
327.6491	0.039%	-3	-0.84	0,3X3-2H
328.0103	0.013%	-1	-0.99	3,5A4-H
328.0342	0.016%	-1	-0.49	0,3X1-2S-2H
329.0182	0.138%	-1	-0.77	3,5A2
329.6635	0.015%	-3	-1.00	M"-H2O-SO3
329.9998	0.015%	-3	0.05	M'-H2O-SO3
330.3355	0.130%	-3	-0.58	M-H2O-SO3
332.9806	0.039%	-3	-0.97	1,4X3;3,5X3-2H
334.5080	0.158%	-2	-0.66	B3"
335.0117	0.160%	-2	-1.31	B3'
335.5144	0.049%	-2	-4.88	B3
335.6673	0.041%	-3	-0.14	M"-SO3
335.9698	0.099%	-1	-0.74	Y1"-S
336.0035	0.014%	-3	0.49	M'-SO3
336.3391	0.617%	-3	-0.57	M-SO3
337.9854	0.371%	-1	-0.85	Y1-S
341.6526	0.025%	-3	-0.69	M"-H2O-CO2
341.9889	0.013%	-3	0.19	M'-H2O-CO2
343.5132	0.234%	-2	-0.73	C3"
344.5210	0.424%	-2	-0.82	C3
347.6561	0.032%	-3	-0.65	M"-CO2;1,5A4
347.9924	0.020%	-3	0.30	M'-CO2
356.4710	0.187%	-2	-1.21	0,2X2-H
356.6516	0.166%	-3	-1.19	M'-H2O
357.0131	0.037%	-1	-0.61	2,5A2-2H
359.0287	0.086%	-1	-0.71	2,5A2
362.3194	0.044%	-3	-0.76	M"
362.6554	0.054%	-3	-0.40	M'
362.9913	0.773%	-3	-0.62	M
363.9648	0.019%	-1	-0.59	1,5X1-S-2H
363.9648	0.019%	-2	-0.59	2,5X2-2H
365.9804	0.438%	-1	-0.79	1,5X1-S
375.0236	0.411%	-1	-0.75	0,2A2
377.0195	0.019%	-2	3.83	Y3-2S
377.9804	0.061%	-1	-0.65	0,2X1-S-2H
378.9881	0.154%	-1	-0.84	0,2X1-S-H
379.9957	0.020%	-1	-1.67	0,2X1-S
380.0290	0.023%	-2	2.60	0,3A4-S-H

386.0399	0.029%	-1	0.08	1,5A2-S-2H
387.0473	0.012%	-1	-0.94	1,5A2-S-H
388.0553	0.015%	-1	-0.58	1,5A2-S
391.0152	0.018%	-2	-0.76	1,5X3-2S
399.9317	0.073%	-1	-0.67	Z1
403.3625	0.097%	-3	-0.67	M'-SO3+A
403.6972	0.055%	-3	-3.59	M-SO3+A
406.9831	0.071%	-2	-0.78	Z3"-S
407.9909	0.153%	-1	-0.74	0,3X1-S-2H
407.9909	0.153%	-2	-0.74	Z3-S
412.5127	0.006%	-2	-0.24	3,5A4
414.0345	0.131%	-1	-0.68	B2"-S
415.0423	0.120%	-1	-0.65	B2'-S
416.0502	1.374%	-1	-0.68	B2-S
416.9961	0.030%	-2	-0.82	Y3-S
417.9422	0.720%	-1	-0.72	Y1
423.9857	0.027%	-1	-0.99	1,4X1-S; 3,5X1-S-2H
429.9860	0.014%	-2	-0.29	1,5X3-S-2H
430.9936	0.231%	-2	-0.81	1,5X3-S
432.0450	1.895%	-1	-0.76	C2"-S
434.0608	0.457%	-1	-0.54	C2-S
435.5153	0.027%	-2	-0.68	0,2A4-S
436.9938	0.026%	-2	-0.27	0,2X3-S-2H
437.4976	0.018%	-2	-0.48	0,2X3-S-H
445.9371	0.565%	-1	-0.73	1,5X1
447.4656	0.018%	-2	-0.27	Z3'
447.9693	0.068%	-2	-0.65	Z3
451.9983	0.017%	-2	-2.08	0,3X3-S-2H
452.0171	0.117%	-2	-0.74	M-H2O-2CO2-SO3
455.9667	0.022%	-2	-0.77	Y3"
456.9746	0.034%	-2	-0.63	Y3
458.9449	0.272%	-1	-0.79	0,2X1-H
459.9866	0.067%	-2	3.86	1,4A4-H
459.9964	0.067%	-2	-0.65	1,4A4
462.0557	0.013%	-1	-0.42	1,5X2-2S
465.9965	0.033%	-1	-0.39	1,5A2-2H
467.0042	0.119%	-1	-0.58	1,5A2-H
468.0128	0.023%	-1	0.96	1,5A2
470.9720	0.082%	-2	-0.67	1,5X3
475.4939	0.004%	-2	-0.21	0,2A4
481.0017	0.023%	-2	-0.49	1,5A4-S-2H
482.0095	0.083%	-2	-0.71	M"-CO2-SO3;1,5A4-S

492.9835	0.031%	-2	-4.04	0,3X3
493.9913	0.113%	-1	-0.60	B2"
494.9992	1.194%	-1	-0.45	B2'
494.9992	1.194%	-2	-0.45	M"-H2O-SO3
496.0077	0.397%	-1	0.85	B2
496.0077	0.397%	-2	0.85	M-H2O-SO3
502.0506	0.026%	-1	-0.39	3,5A3-S-2H
504.0045	0.584%	-2	-0.47	M"-SO3
504.0661	0.135%	-1	-0.80	3,5A3-S
505.0125	0.059%	-2	-0.02	M-SO3
512.0018	0.566%	-1	-0.79	C2"
514.0175	0.768%	-1	-0.66	C2
520.0610	0.017%	-1	-0.76	0,3A3-S
522.9942	0.014%	-2	-3.49	M-CO2
539.9970	0.014%	-1	-0.10	1,5X2-S-2H
542.0124	0.092%	-1	-0.68	1,5X2-S
550.0717	0.026%	-1	-0.47	0,2A3-S
553.0283	0.038%	-1	-0.69	0,2X2-2S-2H
562.0716	0.012%	-1	-0.57	1,5A3-S-2H
569.0227	0.014%	-1	-1.57	2,5X2-2S-2H
574.9558	0.027%	-1	-0.69	Z2'
575.9639	0.065%	-1	-0.36	Z2
584.0229	0.119%	-1	-0.66	3,5A3
590.0666	0.093%	-1	-0.52	B3"-S
591.0745	0.277%	-1	-0.29	B3'-S
591.9586	0.025%	-1	-0.62	Y2"
592.0827	0.193%	-1	0.22	B3-S
593.9742	0.030%	-1	-0.67	Y2
605.0434	0.016%	-2	-0.79	M"-SO3+A
605.5469	0.031%	-2	-1.43	M'-SO3+A
606.0493	0.012%	-2	-3.85	M-SO3+A
608.0770	0.116%	-1	-0.65	C3"-S
610.0927	0.050%	-1	-0.58	C3-S
621.9689	0.039%	-1	-1.00	1,5X2
630.0286	0.017%	-1	-0.22	0,2A3
633.9929	0.015%	-1	-0.69	0,2X2-S-H
648.9805	0.016%	-1	0.12	2,5X2-S-2H
670.0235	0.056%	-1	-0.31	B3"
671.0312	0.195%	-1	-0.48	B3'
672.0391	0.372%	-1	-0.38	B3
688.0340	0.045%	-1	-0.41	C3"
690.0496	0.142%	-1	-0.41	C3

Table S7. List of assigned peaks in the NETD spectrum of H1 [M - 5H]<sup>5-</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
191.0190	0.024%	-1	-3.87	C1"
193.0346	0.016%	-1	-3.92	C1
202.0278	0.023%	-2	-3.65	Z1
211.0330	0.014%	-2	-3.91	Y1
246.9953	0.049%	-2	-3.30	B2'
246.9953	0.049%	-4	-3.30	B4"
247.4992	0.079%	-2	-3.29	B2
247.4992	0.079%	-4	-3.29	B4
255.4966	0.166%	-2	-3.33	C2"
256.5044	1.554%	-2	-3.29	C2
279.3718	0.049%	-3	-3.18	Y3-S
291.5071	0.078%	-2	-3.11	3,5A3
291.5071	0.078%	-4	-3.11	B5
298.0411	0.021%	-2	-2.96	Y2"
299.0487	0.138%	-2	-3.72	Y2
303.6825	0.032%	-3	-3.04	B4-S
306.0240	0.122%	-3	-3.07	Y3
309.0141	0.015%	-3	-3.18	C4"-S
312.0084	0.023%	-4	4.36	C5"-S
314.5098	0.015%	-2	-3.03	0,2A3
315.3556	0.047%	-3	-3.02	1,5X3
323.0909	0.062%	-1	-3.08	Z1"-S
324.0987	0.017%	-1	-2.96	Z1'-S
325.1065	0.093%	-1	-3.04	Z1-S
329.0174	0.025%	-1	-2.94	3,5A2
329.9988	0.026%	-3	-3.02	B4'
330.3349	0.048%	-3	-2.67	B4
333.0211	0.013%	-3	-3.29	3,5A5-S;1,4A5-S-2H
334.5072	0.031%	-2	-3.07	B3"
335.0111	0.054%	-2	-3.06	B3'
335.5152	0.171%	-2	-2.58	B3
335.6664	0.107%	-3	-3.06	C4"
338.0490	0.135%	-3	-3.05	Y4-S
341.1014	0.074%	-1	-2.99	Y1"-S
343.1171	0.047%	-1	-2.94	Y1-S
343.5124	0.081%	-2	-3.02	C3"
344.0345	0.022%	-4	1.66	0,2X5-S



344.5202	0.036%	-2	-3.11	C3
353.5195	0.020%	-4	-3.02	Y5
358.6977	0.142%	-3	-3.02	Z4
359.6733	0.226%	-3	-3.03	3,5A5
360.5182	0.096%	-4	-3.01	1,5X5
362.3598	0.026%	-3	-2.85	B5-S
364.0293	0.106%	-3	-3.07	Y4"
364.7012	0.278%	-3	-2.95	Y4
367.6913	0.027%	-3	-3.05	C5"-S
368.0282	0.019%	-3	-0.45	C5'-S
368.3632	0.018%	-3	-3.24	C5-S
370.5779	0.019%	-2	-2.93	Z3-2S
371.1119	0.044%	-1	-2.96	1,5X1-S
371.5006	0.147%	-4	-2.98	M'-RE-H2O
372.5314	0.013%	-4	-3.75	M"-H2O-SO3
372.7836	0.024%	-4	-2.98	M'-H2O-SO3
373.0356	0.094%	-4	-2.87	M-H2O-SO3
374.0328	0.121%	-3	-3.00	1,5X4
375.0227	0.092%	-1	-3.05	0,2A2
375.7512	0.050%	-4	-2.97	M"-RE
377.0343	0.046%	-4	-3.09	M"-SO3
377.2859	0.023%	-4	-3.99	M'-SO3
377.5382	0.824%	-4	-2.94	M-SO3
379.6803	0.022%	-3	-3.01	1,5A5
381.5234	0.064%	-4	-2.99	M"-H2O-CO2
386.0261	0.097%	-4	-2.81	M"-CO2
386.0384	0.046%	-1	-3.69	1,5A2-S-2H
388.0544	0.039%	-1	-2.96	1,5A2-S
388.6762	0.238%	-3	-2.48	B5'
392.5209	0.021%	-4	-2.87	M"-H2O
392.7728	0.123%	-4	-2.88	M'-H2O
394.3434	0.481%	-3	-3.41	C5"
395.0150	0.310%	-3	-4.02	C5
397.0235	0.386%	-4	-2.80	M"
397.2754	0.611%	-4	-3.06	M'
397.5274	2.864%	-4	-2.98	M
400.0261	0.017%	-4	-0.62	M'-RE-H2O-2CO2+A
401.3096	0.014%	-4	0.50	M'-H2O-2CO2-SO3+A
401.5615	0.116%	-4	0.45	M-H2O-2CO2-SO3+A
404.0553	0.035%	-1	-2.94	Z1'
404.6929	0.022%	-3	-3.13	0,2X4-H

405.0631	1.331%	-1	-3.05	Z1
409.5483	0.029%	-2	-3.06	Z3"-S
410.5563	0.205%	-2	-2.56	Z3-S
412.3873	0.020%	-3	-2.73	Z5-2S
414.0336	0.044%	-1	-2.96	B2"-S
414.5240	0.021%	-2	-3.03	0,3X2
415.0414	0.065%	-1	-3.02	B2'-S
415.0414	0.065%	-2	-3.02	B4"-2S
416.0490	1.013%	-1	-3.51	B2-S
416.0490	1.013%	-2	-3.51	B4-2S
418.5537	0.028%	-2	-2.75	Y3"-S
419.5614	0.082%	-2	-2.99	Y3-S
423.0736	0.089%	-1	-3.04	Y1
424.0466	0.033%	-2	-3.02	C4"-2S
425.0577	0.078%	-2	4.60	C4-2S
427.7223	0.032%	-3	-2.94	1,5X5-2S
427.8057	0.273%	-4	-2.98	M'-SO3+A
432.0440	1.045%	-1	-3.02	C2"-S
432.0440	1.045%	-4	-0.12	M"-H2O-CO2+A
433.5588	0.078%	-2	-3.08	1,5X3-S
434.0597	0.108%	-1	-3.06	C2-S
435.5143	0.020%	-2	-2.97	0,2A4
438.7037	0.014%	-3	-2.44	Z5'-S
439.0391	0.211%	-3	-3.50	Z5-S
440.3430	0.027%	-3	-2.91	3,5A6
444.3709	0.016%	-3	-3.15	Y5"-S
447.7948	0.084%	-4	-2.98	M'+A
450.3465	0.014%	-3	-3.01	2,5A6
450.5344	0.050%	-2	-3.04	Z3
451.0684	0.117%	-1	-3.06	1,5X1
454.3744	0.311%	-3	-3.04	1,5X5-S
455.0197	0.041%	-2	-2.82	B4"-S
455.5238	0.036%	-2	-2.41	B4'-S
455.6780	0.037%	-3	-3.26	0,2A6
456.0277	0.038%	-2	-2.48	B4-S
458.5318	0.019%	-2	-3.13	Y3"
458.7104	0.095%	-3	-3.02	0,2X5-S-H
459.5399	0.278%	-2	-2.59	Y3
463.7060	0.035%	-3	-3.05	2,5X5-S-2H
464.0249	0.128%	-2	-3.03	C4"-S
465.0323	0.023%	-2	-3.82	C4-S

465.6916	0.023%	-3	-2.80	Z5
468.3779	0.024%	-3	-3.03	0,3X5-S-2H
468.6817	0.033%	-3	-3.02	M"-RE-H2O-SO3
469.3537	0.785%	-3	-2.65	M-RE-H2O-SO3
471.0233	0.023%	-3	-2.77	Y5"
471.3589	0.014%	-3	-3.51	Y5'
471.6950	0.044%	-3	-2.99	Y5
473.5369	0.479%	-2	-3.44	1,5X3
473.7095	0.018%	-3	-3.17	1,4X5-S;3,5X5-S-2H
474.6852	0.044%	-3	-3.00	M"-RE-SO3
476.0709	0.031%	-1	-1.47	2,4A3-S
477.0642	0.039%	-2	-0.08	2,4X3-S-H
480.0409	0.052%	-2	-3.18	0,2X3-H
480.5452	0.041%	-2	-2.32	0,2X3
481.0268	0.490%	-3	-2.65	1,5X5
482.3813	0.032%	-3	-3.18	M"-H2O-CO2-SO3
483.0535	0.028%	-3	-2.69	M-H2O-CO2-SO3
485.6984	0.021%	-3	-3.30	0,2X5
488.3849	0.068%	-3	-3.00	M"-CO2-SO3
490.3583	0.014%	-3	-3.00	2,5X5-2H
494.9979	0.072%	-1	-3.14	B2'
494.9979	0.072%	-2	-3.14	B4"
495.0300	0.019%	-3	-3.37	0,3X5-2H
495.5019	0.041%	-2	-2.94	B4'
495.6697	0.018%	-3	-3.18	M'-RE-H2O
495.7023	0.016%	-3	-2.47	0,3X5
496.0055	0.193%	-1	-3.55	B2
496.0055	0.193%	-2	-3.55	B4
496.0055	0.193%	-3	-3.55	M-RE-H2O
497.0445	0.114%	-3	-3.29	M"-H2O-SO3
498.5718	0.167%	-2	-3.26	Z4-S
500.0353	0.041%	-2	-3.07	3,5A5-S
500.3617	0.051%	-3	-3.13	3,5X5-2H;1,4X5
501.1380	0.055%	-1	-3.19	Z2-S
503.0483	0.715%	-3	-2.80	M-2H-SO3
504.0033	0.186%	-2	-2.72	C4"
505.0106	0.127%	-2	-3.84	C4
506.5693	0.073%	-2	-3.09	Y4"-S
507.5771	0.147%	-2	-3.16	Y4-S
509.0336	0.042%	-3	-3.04	M"-H2O-CO2
509.0730	0.016%	-1	-4.37	1,4X1;3,5X1-2H

512.0006	0.083%	-1	-3.15	C2"
514.0164	0.229%	-1	-2.83	C2
515.0369	0.145%	-3	-3.36	M"-CO2
519.1484	0.106%	-1	-3.32	Y2-S M"-H2O-3CO2-
520.4158	0.013%	-3	0.10	SO3+A
521.5744	0.069%	-2	-3.29	1,5X4-S
523.6967	0.075%	-3	-3.21	M"-H2O
529.7002	1.851%	-3	-3.37	M"
535.0792	0.224%	-2	-4.53	2,5X4-2S-2H
535.0792	0.224%	-3	0.33	M"-H2O-2CO2-SO3+A
535.4138	0.111%	-3	-2.20	M'-H2O-2CO2-SO3+A
537.5422	0.034%	-2	-3.28	Z4"
538.0459	0.021%	-2	-3.67	Z4'
538.5498	0.870%	-2	-3.71	Z4
540.0135	0.090%	-2	-3.31	3,5A5
543.0351	0.037%	-2	-3.52	B5"-S
543.5389	0.017%	-2	-3.73	B5'-S
546.5476	1.223%	-2	-2.99	Y4"
547.1432	0.034%	-1	-3.40	1,5X2-S
548.0556	0.111%	-1	-1.28	0,2A3-S-2H
552.0405	0.126%	-2	-3.43	C5"-S
553.0482	0.095%	-2	-3.65	C5-S
561.5529	0.243%	-2	-3.00	1,5X4
567.0605	0.015%	-2	-3.55	0,2X4-S-2H
567.5645	0.016%	-2	-3.45	0,2X4-S-H
570.0239	0.050%	-2	-3.46	1,5A5
570.4072	0.144%	-3	-3.29	M"-SO3+A
581.0944	0.089%	-1	-3.43	Z2
583.0135	0.031%	-1	-3.46	3,5A3-H
583.0135	0.031%	-2	-3.46	B5"
583.5174	0.033%	-2	-3.47	B5'
584.0214	0.140%	-1	-3.27	3,5A3
584.0214	0.140%	-2	-3.27	B5
590.0648	0.021%	-2	-0.82	3,5X4-S-2H
590.0648	0.021%	-1	-3.50	B3"-S
591.0729	0.034%	-2	-0.38	3,5X4-S
591.0729	0.034%	-1	-3.04	B3'-S
592.0187	0.287%	-2	-3.47	C5"
592.0809	0.050%	-1	-2.76	B3-S
593.0265	0.296%	-2	-3.43	C5

597.0592	0.022%	-3	-3.57	M"+A
597.0894	0.031%	-1	-3.14	Y2"
597.3945	0.027%	-3	-4.64	M'+A
599.1049	0.166%	-1	-3.47	Y2
608.0753	0.083%	-1	-3.58	C3"-S
619.0844	0.015%	-2	-3.02	Z5-2S
620.0317	0.019%	-2	-3.40	3,5A6-S-2H
627.0997	0.077%	-1	-3.53	1,5X2
639.1236	0.014%	-1	-3.25	0,2X2-S-H
642.0869	0.017%	-2	-3.17	1,5X5-2S
670.0217	0.016%	-1	-3.02	B3"
671.0293	0.045%	-1	-3.31	B3'
672.0372	0.067%	-1	-3.24	B3
682.0649	0.023%	-2	-3.57	1,5X5-S
688.0317	0.105%	-1	-3.70	C3"
688.5685	0.013%	-2	-4.04	0,2X5-S-H
690.0475	0.031%	-1	-3.50	C3
704.5333	0.024%	-2	-4.05	M-RE-H2O-SO3
724.1519	0.029%	-1	4.56	1,5A4-3S-H
740.1468	0.023%	-1	-3.68	Z3"-2S
742.1627	0.014%	-1	-3.35	Z3-2S
755.0753	0.024%	-2	-3.77	M"-SO3
795.0531	0.021%	-2	-4.39	M"
820.1027	0.014%	-1	-4.47	Z3"-S
822.1189	0.015%	-1	-3.83	Z3-S
831.0892	0.015%	-1	-3.93	B4"-2S
838.1136	0.017%	-1	-3.97	Y3"-S

Table S8. List of assigned peaks in the NETD spectrum of H2 [M - 5H]<sup>5-</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
167.6859	0.006%	-3	-4.05	1,4A3-H
191.0197	0.009%	-1	-0.15	C1"
193.0354	0.012%	-1	-0.11	C1
207.5215	0.006%	-2	-0.25	B2-S
207.5215	0.006%	-4	-0.25	B4-2S
211.0338	0.054%	-2	-0.22	Y1
246.4921	0.030%	-2	-0.26	B2"
247.4999	0.046%	-2	-0.36	B2
247.4999	0.046%	-4	-0.36	B4
255.4974	0.091%	-2	-0.25	C2"
256.0132	0.031%	-1	-0.29	C1"-S
256.5052	1.506%	-2	-0.34	C2
273.2749	0.009%	-4	-0.20	Y4
277.0066	0.010%	-2	0.03	2,4A3-H
277.0066	0.010%	-4	0.03	2,5A5
279.3726	0.023%	-3	-0.39	Y3-S
290.0079	0.013%	-3	-0.25	0,2A4
291.5079	0.044%	-2	-0.34	3,5A3
291.5079	0.044%	-4	-0.34	B5
298.0419	0.034%	-2	-0.26	Y2"
299.0498	0.551%	-2	-0.23	Y2
303.6834	0.323%	-3	-0.36	B4-S
305.5053	0.007%	-2	-0.52	2,5A3-2H
306.0248	0.054%	-3	-0.34	Y3
309.0151	0.006%	-3	0.03	C4"-S
314.5107	0.017%	-2	-0.21	0,2A3
317.0150	0.012%	-4	-2.98	2,5A6-S-2H
319.0595	0.008%	-2	0.83	0,2X2-S-H
319.6925	0.006%	-3	-0.11	0,2X3-H
323.0181	0.007%	-3	-1.74	2,4A5-S-2H
323.0918	0.019%	-1	-0.29	Z1"-S
325.1075	0.010%	-1	-0.09	Z1-S
329.0183	0.013%	-1	-0.36	3,5A2
329.6638	0.013%	-3	-0.08	B4"
329.9998	0.417%	-3	-0.12	B4'
330.3361	0.404%	-3	0.99	B4
333.0221	0.006%	-3	-0.01	3,5A5-S
334.5081	0.090%	-2	-0.18	B3"
335.0119	0.027%	-2	-0.76	B3'

335.5159	0.133%	-2	-0.24	B3
335.6673	0.158%	-3	-0.25	C4"
336.0019	0.038%	-3	-4.36	C4'
336.3379	0.037%	-3	-3.93	C4
337.0042	0.006%	-4	-2.76	2,5A6-2H
337.0401	0.051%	-2	1.21	C3-2S
338.0500	0.048%	-3	-0.17	Y4-S
343.1180	0.012%	-1	-0.29	Y1-S
343.5134	0.063%	-2	-0.24	C3"
344.5214	0.074%	-2	0.27	C3
353.5205	0.009%	-4	-0.21	Y5
357.0134	0.007%	-1	0.18	2,5A2-2H
359.0374	0.074%	-2	-0.47	0,2X2-H
359.6744	0.068%	-3	-0.12	3,5A5
360.0088	0.021%	-3	-4.21	1,4A5-H
360.5192	0.070%	-4	-0.16	1,5X5
362.3608	0.050%	-3	-0.18	B5-S
364.0303	0.008%	-3	-0.35	Y4"
364.7022	0.067%	-3	-0.18	Y4
367.6924	0.008%	-3	-0.31	C5"-S
368.3642	0.014%	-3	-0.34	C5-S
369.0061	0.007%	-3	0.10	2,5A5-2H
371.5016	0.055%	-4	-0.19	M'-RE-H2O
371.7524	0.025%	-4	-3.21	M-RE-H2O
373.0366	0.252%	-4	-0.21	M-H2O-SO3
374.0334	0.009%	-3	-1.55	1,5X4
375.0100	0.021%	-3	1.05	0,2A5
375.0237	0.074%	-1	-0.38	0,2A2
377.0354	0.007%	-4	0.03	M"-SO3
377.2873	0.007%	-4	-0.25	M'-SO3
377.5392	0.096%	-4	-0.43	M-SO3
379.3455	0.020%	-3	-0.17	1,5A5-H
379.6813	0.009%	-3	-0.48	1,5A5
381.5244	0.005%	-4	-0.31	M"-H2O-CO2
381.7764	0.011%	-4	-0.21	M'-H2O-CO2
386.0273	0.013%	-4	0.31	M"-CO2
386.0398	0.015%	-1	-0.13	1,5A2-S-2H
386.2788	0.013%	-4	-0.82	M'-CO2
388.0555	0.030%	-1	-0.05	1,5A2-S
388.3411	0.008%	-3	-0.22	B5"
388.6771	0.055%	-3	-0.17	B5'
389.0128	0.031%	-3	-0.65	B5
392.5219	0.008%	-4	-0.33	M"-H2O

392.7738	0.060%	-4	-0.32	M'-H2O
393.0248	0.027%	-4	-2.92	M-H2O
394.3448	0.139%	-3	0.23	C5''
394.6792	0.045%	-3	-3.86	C5'
395.0168	0.141%	-3	0.34	C5
395.5371	0.027%	-4	-0.33	M'-RE-CO2-SO3+A
397.0245	0.036%	-4	-0.35	M''
397.2766	0.126%	-4	0.04	M'
397.5285	0.456%	-4	-0.14	M
400.0272	0.008%	-4	2.32	M'-RE-H2O-2CO2+A
403.0486	0.020%	-1	-0.21	Z1''
404.0564	0.068%	-1	-0.15	Z1'
405.0642	1.248%	-1	-0.17	Z1
409.5494	0.007%	-2	-0.25	Z3''-S
410.5573	0.023%	-2	-0.10	Z3-S
412.5129	0.011%	-2	0.11	3,5A4
414.0347	0.019%	-1	-0.26	B2''-S
415.0426	0.056%	-1	-0.09	B2'-S
415.0426	0.056%	-2	-0.09	B4''-2S
416.0504	0.642%	-1	-0.07	B2-S
416.0504	0.642%	-2	-0.07	B4-2S
418.5549	0.006%	-2	0.05	Y3''-S
419.5626	0.015%	-2	-0.09	Y3-S
421.0590	0.006%	-1	-0.45	Y1''
423.0748	0.058%	-1	-0.11	Y1
424.0478	0.013%	-2	-0.29	C4''-2S
426.5103	0.008%	-2	-0.01	2,5A4-2H
427.5181	0.017%	-2	-0.11	2,5A4
427.8069	0.113%	-4	-0.12	M'-SO3+A
428.0578	0.074%	-4	-2.56	M-SO3+A
432.0453	0.339%	-1	-0.16	C2''-S
432.0453	0.339%	-4	2.74	M''-H2O-CO2+A
433.5601	0.008%	-2	-0.02	1,5X3-S
434.0609	0.040%	-1	-0.24	C2-S
435.5155	0.167%	-2	-0.13	0,2A4
440.3443	0.007%	-3	0.05	3,5A6
447.7960	0.034%	-4	-0.27	M'+A
448.0467	0.024%	-4	-3.16	M+A
450.0315	0.006%	-2	-0.77	Z3'
450.5356	0.107%	-2	-0.42	Z3
451.0697	0.058%	-1	-0.20	1,5X1
454.3757	0.024%	-3	-0.18	1,5X5-S
455.0208	0.082%	-2	-0.44	B4''-S



455.5243	0.052%	-2	-1.29	B4'-S
455.6795	0.088%	-3	0.13	0,2A6
456.0284	0.065%	-2	-1.06	B4-S
458.5332	0.035%	-2	-0.13	Y3"
459.0372	0.022%	-2	0.16	Y3'
459.5410	0.087%	-2	-0.16	Y3
459.6894	0.011%	-3	4.41	1,5A6-S-H
464.0263	0.241%	-2	-0.10	C4"-S
464.0775	0.019%	-1	-0.19	0,2X1-H
464.5279	0.060%	-2	-4.91	C4'-S
465.6929	0.020%	-3	-0.15	Z5
468.6831	0.024%	-3	0.02	M"-RE-H2O-SO3
469.0177	0.011%	-3	-2.86	M'-RE-H2O-SO3
469.3550	0.189%	-3	0.04	M-RE-H2O-SO3
471.6965	0.017%	-3	0.17	Y5
472.0119	0.009%	-3	-0.87	M"-RE-2CO2
473.5385	0.043%	-2	-0.12	1,5X3
476.0723	0.015%	-1	1.51	2,4A3-S
477.0619	0.006%	-2	-4.90	2,4X3-S-H
480.0423	0.041%	-2	-0.24	0,2X3-H
480.0423	0.041%	-3	-4.60	M'-H2O-3CO2
480.5450	0.013%	-2	-2.79	0,2X3
481.0281	0.155%	-3	-0.04	1,5X5
482.3827	0.007%	-3	-0.36	M"-H2O-CO2-SO3
488.3864	0.017%	-3	0.01	M"-CO2-SO3
488.7210	0.008%	-3	-2.71	M'-H2O-SO3
493.9917	0.012%	-1	0.16	B2"
494.5436	0.008%	-2	-0.31	0,3X3-2H
494.9995	0.036%	-1	0.09	B2'
494.9995	0.036%	-2	0.09	B4"
495.0314	0.008%	-3	-0.35	0,3X5-2H
495.3354	0.007%	-3	0.01	M"-RE-H2O
495.5033	0.108%	-2	-0.03	B4'
495.6705	0.006%	-3	-1.56	M'-RE-H2O
496.0071	0.071%	-1	-0.28	B2
496.0071	0.071%	-2	-0.28	B4
496.0071	0.071%	-3	-0.28	M-RE-H2O
497.0461	0.053%	-3	-0.13	M"-H2O-SO3
498.5734	0.025%	-2	0.01	Z4-S
500.0368	0.008%	-2	-0.12	3,5A5-S
500.3632	0.008%	-3	-0.09	1,4X5
501.1396	0.007%	-1	0.10	Z2-S
502.5413	0.006%	-2	0.11	1,4X3;3,5X3-2H

503.0495	0.237%	-3	-0.41	M''-SO3
503.3841	0.115%	-3	-2.90	M'-SO3
504.0047	0.554%	-2	-0.02	C4''
504.5065	0.151%	-2	-4.30	C4'
506.5708	0.028%	-2	-0.07	Y4''-S
507.0723	0.008%	-2	-4.81	Y4'-S
507.5794	0.007%	-2	1.36	Y4-S
509.0348	0.008%	-3	-0.74	M''-H2O-CO2
512.0021	0.022%	-1	-0.09	C2''
514.0179	0.083%	-1	0.11	C2
515.0381	0.016%	-3	-1.18	M''-CO2
515.3732	0.008%	-3	-2.74	M'-CO2
517.1346	0.015%	-1	0.12	Y2''-S
517.5468	0.010%	-2	0.50	2,4X3
519.1500	0.035%	-1	-0.20	Y2-S
521.5759	0.011%	-2	-0.45	1,5X4-S
523.6985	0.018%	-3	0.19	M''-H2O
524.0335	0.008%	-3	-1.59	M'-H2O
529.7019	0.091%	-3	0.02	M''
530.0365	0.049%	-3	-2.57	M'
537.5442	0.008%	-2	0.33	Z4''
538.0476	0.009%	-2	-0.49	Z4'
538.5519	0.082%	-2	0.17	Z4
540.0152	0.012%	-2	-0.22	3,5A5
543.0371	0.011%	-2	0.01	B5''-S
543.5403	0.007%	-2	-1.27	B5'-S
544.0450	0.018%	-2	0.28	B5-S
546.5492	0.838%	-2	-0.11	Y4''
547.0510	0.287%	-2	-4.05	Y4'
547.1452	0.009%	-1	0.29	1,5X2-S
552.0423	0.021%	-2	-0.10	C5''-S
552.5435	0.008%	-2	-4.94	C5'-S
553.0504	0.022%	-2	0.35	C5-S
561.5546	0.055%	-2	0.01	1,5X4
570.4090	0.054%	-3	-0.10	M''-SO3+A
570.7437	0.043%	-3	-2.30	M'-SO3+A
580.0888	0.010%	-1	0.35	Z2'
581.0965	0.063%	-1	0.14	Z2
583.5192	0.008%	-2	-0.28	B5'
584.0233	0.039%	-1	-0.03	3,5A3
584.0233	0.039%	-2	-0.03	B5
591.0746	0.005%	-2	2.47	3,5X4-S
591.0746	0.005%	-1	-0.20	B3'-S

592.0205	0.013%	-2	-0.34	C5"
592.0826	0.015%	-1	0.21	B3-S
593.0288	0.034%	-2	0.31	C5
597.0610	0.010%	-3	-0.52	M"+A
597.0913	0.027%	-1	-0.04	Y2"
597.3963	0.012%	-3	-1.75	M'+A
599.1070	0.209%	-1	0.09	Y2
608.0775	0.011%	-1	0.11	C3"-S
610.0932	0.014%	-1	0.16	C3-S
627.1019	0.048%	-1	0.10	1,5X2
638.1178	0.006%	-1	-0.10	0,2X2-S-2H
671.0316	0.014%	-1	0.11	B3'
672.0394	0.017%	-1	0.08	B3
688.0344	0.014%	-1	0.15	C3"
690.0504	0.018%	-1	0.74	C3
704.0327	0.008%	-2	0.66	M'-RE-H2O-SO3
704.5359	0.018%	-2	-0.23	M-RE-H2O-SO3
719.0832	0.006%	-1	1.03	0,2X2-H

Table S9. List of assigned peaks in the NETD spectrum of H3 [M - 5H]<sup>5-</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
132.5113	0.021%	-4	-3.77	2,5A3-S-H
167.6862	0.014%	-3	-2.25	1,4A3-S-H
193.0356	0.013%	-1	0.94	C1
246.4925	0.020%	-2	1.17	B2"
247.5002	0.069%	-2	0.72	B2
247.5002	0.069%	-4	0.72	B4-S
255.4977	0.073%	-2	0.97	C2"
256.5055	0.377%	-2	0.91	C2
291.5083	0.021%	-2	0.83	3,5A3
291.5083	0.021%	-4	0.83	B5-S
293.2644	0.015%	-4	0.92	Y4
299.0503	0.087%	-2	1.45	Y2
306.0252	0.102%	-3	0.96	Y3-S
314.5112	0.010%	-2	1.59	0,2A3
323.0923	0.052%	-1	1.39	Z1"-S
325.1079	0.013%	-1	1.26	Z1-S
329.0188	0.035%	-1	1.27	3,5A2
330.0002	0.027%	-3	1.23	B4'-S
330.3363	0.039%	-3	1.66	B4-S
332.0058	0.022%	-3	1.26	Y3"
332.6779	0.748%	-3	1.99	Y3
334.5087	0.099%	-4	3.79	3,5X4-2H
334.5087	0.099%	-2	1.44	B3"
335.0599	0.111%	-2	-1.43	1,4X2-S
335.5165	1.166%	-2	1.54	B3
335.6681	0.026%	-3	2.03	C4"-S
336.0941	0.061%	-1	1.50	B2-2S
336.3399	0.046%	-3	1.94	C4-S
337.0036	0.034%	-4	-4.69	2,5A6-S-2H
338.0506	0.017%	-3	1.51	Y4-2S
342.0094	0.163%	-3	1.57	1,5X3
343.1185	0.027%	-1	1.41	Y1-S
343.5140	0.023%	-2	1.51	C3"
344.5218	0.022%	-2	1.51	C3
346.3453	0.023%	-3	1.40	0,2X3-H
356.6525	0.022%	-3	1.22	B4'
356.9888	0.030%	-3	2.09	B4

358.6995	0.018%	-3	1.92	Z4-S
359.0296	0.041%	-1	1.84	2,5A2
359.6751	0.027%	-3	1.93	3,5A5-S
360.5199	0.018%	-4	1.82	1,5X5-S
362.3203	0.097%	-3	1.88	C4"
362.6549	0.027%	-3	-1.97	C4'
362.9916	0.055%	-3	0.20	C4
364.0311	0.014%	-4	-3.11	M"-3CO2-SO3
364.0311	0.014%	-3	1.92	Y4"-S
364.7030	0.134%	-3	1.77	Y4-S
368.7557	0.013%	-4	1.45	Z5'
371.0230	0.024%	-4	3.00	0,3X5-S-2H
371.5022	0.024%	-4	1.58	M'-RE-H2O-SO3
373.2583	0.015%	-4	1.35	Y5'
373.5105	0.076%	-4	2.10	Y5
373.5373	0.046%	-2	-4.60	0,3X2-S-2H
374.0344	0.020%	-3	1.10	1,5X4-S
375.0246	0.331%	-1	1.92	0,2A2
380.5090	0.558%	-4	1.51	1,5X5
384.0131	0.019%	-4	1.79	0,2X5
384.6798	0.083%	-3	1.61	Z4"
385.0159	0.072%	-3	2.04	Z4'
385.3519	1.277%	-3	2.12	Z4
386.0403	0.018%	-1	1.22	1,5A2-S-2H
386.3273	0.165%	-3	1.51	3,5A5
386.6618	0.054%	-3	-2.17	1,4X4-S-H
387.5080	0.026%	-4	2.23	2,5X5-2H
387.7588	0.014%	-4	-0.92	2,5X5-H
388.6778	0.015%	-3	1.68	B5'-S
389.0139	0.038%	-3	1.99	B5-S
390.6833	1.086%	-3	1.46	Y4"
391.0178	0.365%	-3	-2.25	Y4'
391.2626	0.028%	-4	-1.20	0,3X5-H
391.3548	0.399%	-3	0.48	Y4
391.4917	0.128%	-4	2.22	M'-RE-H2O
391.7426	0.065%	-4	-0.47	M-RE-H2O
392.5226	0.036%	-4	1.66	M"-H2O-SO3
392.7744	0.049%	-4	1.03	M'-H2O-SO3
393.0265	0.540%	-4	1.42	M-H2O-SO3
394.3455	0.076%	-3	1.86	C5"-S
394.6799	0.025%	-3	-1.99	C5'-S

395.0112	0.207%	-4	3.45	1,4X5;3,5X5-2H
395.2616	0.093%	-4	-0.44	3,5X5-H
395.7423	0.031%	-4	1.87	M"-RE
395.9929	0.015%	-3	-3.35	2,5A5-H
395.9929	0.015%	-1	4.40	2,5X1
395.9929	0.015%	-4	-1.41	M'-RE
397.0253	0.134%	-4	1.64	M"-SO3
397.2767	0.107%	-4	0.18	M'-SO3
397.5292	0.808%	-4	1.65	M-SO3
400.0156	0.017%	-3	3.24	1,5X4-2H
400.0280	0.043%	-4	4.27	M'-RE-H2O-2CO2-SO3+A
400.6868	0.716%	-3	1.48	1,5X4
401.5145	0.034%	-4	1.94	M"-H2O-CO2
401.6625	0.019%	-3	1.64	0,2A5
401.7661	0.042%	-4	1.10	M'-H2O-CO2
402.0169	0.027%	-4	-1.95	M-H2O-CO2
402.2610	0.025%	-4	1.17	2,4X5-H
402.5118	0.014%	-4	-1.71	2,4X5
403.0493	0.040%	-1	1.64	Z1"
404.0573	0.054%	-1	2.02	Z1'
404.6949	0.031%	-3	1.93	0,2X4-S-H
405.0651	1.967%	-1	1.95	Z1
406.0170	0.050%	-4	1.61	M"-CO2
406.2691	0.111%	-4	1.86	M'-CO2
406.3344	0.025%	-3	1.65	1,5A5
406.5201	0.053%	-4	-0.53	M-CO2
407.9918	0.038%	-1	1.48	0,3X1-2H
407.9918	0.038%	-2	1.48	B3-S
409.5504	0.012%	-2	2.12	Z3"-2S
410.0267	0.016%	-3	2.26	2,5X4-S-H
410.5581	0.024%	-2	1.79	Z3-2S
412.5112	0.047%	-2	-3.83	3,5A4
412.5112	0.047%	-4	0.13	M"-H2O
412.7637	2.684%	-4	1.41	M'-H2O
413.0145	1.513%	-4	-1.47	M-H2O
414.0354	0.048%	-1	1.47	B2"-S
414.5256	0.016%	-2	0.96	0,3X2
414.9943	0.017%	-3	1.90	B5"
415.0434	0.042%	-1	1.89	B2'-S
415.0434	0.042%	-2	1.89	B4"-3S
415.3302	0.100%	-3	1.90	B5'

415.6659	0.070%	-3	1.35	B5
416.0512	0.437%	-1	1.95	B2-S
417.0148	0.291%	-4	2.33	M''
417.2664	0.555%	-4	1.38	M'
417.5183	2.396%	-4	1.21	M
419.5635	0.020%	-2	1.96	Y3-2S
420.9977	0.440%	-3	1.69	C5''
421.3323	0.161%	-3	-1.47	C5'
421.5526	0.024%	-4	4.92	M-H2O-2CO2-SO3+A
421.6695	0.781%	-3	1.53	C5
423.0758	0.093%	-1	2.24	Y1
431.3474	0.786%	-3	2.24	0,2X4-H
431.6821	0.300%	-3	-0.60	0,2X4
432.0461	1.131%	-1	1.72	C2''-S
432.0461	1.131%	-4	4.62	M''-H2O-CO2-SO3+A
433.5611	0.013%	-2	2.19	1,5X3-2S
434.0617	0.118%	-1	1.73	C2-S
435.5165	0.029%	-2	2.20	0,2A4-S
435.5165	0.029%	-4	2.10	M'-RE-CO2+A
436.6790	0.075%	-3	2.03	2,5X4-H
437.0138	0.027%	-3	-0.45	2,5X4
439.0415	0.017%	-3	2.01	Z5-2S
440.3452	0.013%	-3	2.15	3,5A6-S
447.5441	0.026%	-4	-0.26	M''-SO3+A
447.7970	0.474%	-4	1.89	M'-SO3+A
448.0478	0.356%	-4	-0.76	M-SO3+A
449.5288	0.035%	-2	1.84	B3''-S
450.0327	0.078%	-2	1.78	Z3'-S
450.5367	0.076%	-2	2.02	Z3-S
451.0705	0.070%	-1	1.60	1,5X1
454.3766	0.037%	-3	1.77	1,5X5-2S
455.6801	0.058%	-3	1.37	0,2A6-S
456.0303	0.022%	-2	3.14	B4-2S
458.5341	0.194%	-2	1.96	Y3''-S
459.0360	0.048%	-2	-2.54	Y3'-S
459.5418	0.132%	-2	1.52	Y3-S
464.0273	0.055%	-2	2.05	C4''-2S
464.5283	0.015%	-2	-4.14	C4'-2S
465.0206	0.030%	-3	-0.93	Z5''-S
465.3574	0.014%	-3	0.91	Z5'-S
465.6940	0.106%	-3	2.28	Z5-S

466.9971	0.008%	-3	1.07	3,5A6
467.7863	0.098%	-4	1.95	M'+A
468.0371	0.080%	-4	-0.42	M+A
471.0259	0.015%	-3	2.77	Y5"-S
471.6978	0.031%	-3	2.89	Y5-S
473.5395	0.129%	-2	2.12	1,5X3-S
475.4950	0.005%	-2	2.10	0,2A4
477.0005	0.023%	-3	0.84	2,5A6
477.9976	0.017%	-3	-0.41	M"-RE-H2O-3CO2
479.5397	0.016%	-2	2.44	0,2X3-S-2H
480.0434	0.060%	-2	2.05	0,2X3-S-H
480.0434	0.060%	-3	-2.31	M'-H2O-3CO2-SO3
480.5459	0.018%	-2	-0.95	0,2X3-S
481.0293	0.160%	-3	2.60	1,5X5-S
482.3329	0.140%	-3	2.44	0,2A6
483.9997	0.094%	-3	-3.26	M"-RE-3CO2
485.3647	0.025%	-3	1.33	0,2X5-S-H
485.6998	0.013%	-3	-0.44	0,2X5-S
486.6773	0.015%	-3	3.51	1,5A6-S
492.3465	0.197%	-3	2.64	Z5
495.0005	0.107%	-1	2.10	B2'
495.0005	0.107%	-2	2.10	B4"-S
495.3364	0.129%	-3	2.14	M"-RE-H2O-SO3
495.5034	0.037%	-2	0.18	B4'-S
495.6711	0.052%	-3	-0.49	M'-RE-H2O-SO3
496.0082	2.129%	-1	1.86	B2
496.0082	2.129%	-2	1.86	B4-S
496.0082	2.129%	-3	1.86	M-RE-H2O-SO3
497.6782	0.041%	-3	2.69	Y5"
498.0135	0.016%	-3	1.35	Y5'
498.3499	0.077%	-3	2.26	Y5
498.5126	0.039%	-2	1.85	Y3"
498.5745	0.021%	-2	2.21	Z4-2S
499.0159	0.050%	-2	0.68	Y3'
499.5205	0.167%	-2	2.01	Y3
500.3642	0.017%	-3	1.95	1,4X5-S; 3,5X5-2H
504.0059	0.094%	-2	2.38	C4"-S
504.0670	0.028%	-1	1.00	3,5A3-S
504.5075	0.026%	-2	-2.28	C4'-S
505.0147	0.018%	-2	4.22	C4-S
507.6814	0.254%	-3	1.95	1,5X5



509.0363	0.023%	-3	2.33	M"-H2O-CO2-SO3
509.3710	0.013%	-3	-0.24	M'-H2O-CO2-SO3
512.0035	0.194%	-1	2.56	C2"
513.5180	0.274%	-2	2.16	1,5X3
514.0192	0.232%	-1	2.66	C2
515.0396	0.043%	-2	-4.96	2,5A4-2S
515.0396	0.043%	-3	1.81	M"-CO2-SO3
515.3742	0.024%	-3	-0.70	M'-CO2-SO3
517.0129	0.012%	-3	1.66	2,5X5-2H
519.1513	0.023%	-1	2.23	Y2-S
520.0219	0.095%	-2	2.11	0,2X3-H
520.5253	0.052%	-2	0.97	0,2X3
523.6998	0.349%	-3	2.58	M"-H2O-SO3
524.0351	0.312%	-3	1.39	M'-H2O-SO3
527.0166	0.031%	-3	2.05	1,4X5;3,5X5-2H
527.3514	0.015%	-3	-0.19	3,5X5-H
529.7032	0.868%	-3	2.36	M"-SO3
530.0373	0.459%	-3	-1.08	M'-SO3
535.0284	0.026%	-2	4.32	0,3X3-H
535.0826	0.013%	-2	1.93	2,5X4-3S-2H
535.5311	0.024%	-2	1.96	0,3X3
535.6887	0.016%	-3	2.37	M"-H2O-CO2
537.5452	0.028%	-2	2.22	Z4"-S
538.0485	0.017%	-2	1.15	Z4'-S
538.5531	0.134%	-2	2.35	Z4-S
541.6921	0.014%	-3	2.23	M"-CO2
543.0382	0.015%	-2	2.11	B5"-2S
543.9843	0.053%	-2	2.25	C4"
544.4861	0.017%	-2	-1.65	C4'
546.5504	0.140%	-2	2.01	Y4"-S
547.0523	0.050%	-2	-1.55	Y4'-S
547.5593	0.019%	-2	3.99	Y4-S
548.0332	0.032%	-3	3.11	M"-RE-H2O-CO2-SO3+A
550.3518	0.079%	-3	2.05	M"-H2O
550.6866	0.045%	-3	-0.10	M'-H2O
552.0434	0.012%	-2	1.90	C5"-2S
553.0517	0.020%	-2	2.78	C5-2S
556.0305	0.073%	-1	3.84	2,4A3
556.3557	0.124%	-3	2.66	M"
556.6900	0.075%	-3	-0.25	M'
557.0200	0.038%	-2	-1.89	2,4X3-H

561.5559	0.035%	-2	2.34	1,5X4-S
577.5237	0.013%	-2	2.29	Z4"
578.0274	0.031%	-2	1.85	Z4'
578.5316	0.128%	-2	2.31	Z4
581.0978	0.025%	-1	2.39	Z2
583.0166	0.019%	-1	2.01	3,5A3-H
583.0166	0.019%	-2	2.01	B5"-S
583.5201	0.014%	-2	1.17	B5'-S
584.0246	0.119%	-1	2.28	3,5A3
584.0246	0.119%	-2	2.28	B5-S
586.5290	0.053%	-2	2.21	Y4"
587.0325	0.034%	-2	1.46	Y4'
587.5371	0.021%	-2	2.66	Y4
590.0682	0.017%	-2	4.95	3,5X4-2S-2H
590.0682	0.017%	-1	2.28	B3"-S
591.0763	0.022%	-1	2.66	B3'-S
592.0222	0.041%	-2	2.53	C5"-S
592.0841	0.027%	-1	2.71	B3-S
593.0302	0.114%	-2	2.74	C5-S
597.0628	0.027%	-3	2.40	M"-SO3+A
597.3977	0.026%	-3	0.64	M'-SO3+A
597.7316	0.013%	-3	-2.66	M-SO3+A
599.1084	0.050%	-1	2.40	Y2
601.5343	0.036%	-2	2.29	1,5X4
607.0424	0.016%	-2	2.33	0,2X4-S-2H
615.0400	0.014%	-2	2.63	2,5X4-S-2H
624.0032	0.048%	-2	2.33	B5
627.1034	0.014%	-1	2.38	1,5X2
633.0086	0.063%	-2	2.60	C5

Table S10. List of assigned peaks in the NETD spectrum of [1, 1, 2, 1, 3] from HSPIM, [M - 3H]<sup>3-</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
157.0144	0.006%	-1	0.78	B1
168.4893	3.544%	-2	0.47	Y1
175.0249	0.020%	-1	0.57	C1
219.5217	0.004%	-2	0.53	B2
228.5270	0.007%	-2	0.67	C2
239.0106	0.017%	-1	0.45	Z1'-S
240.0185	0.276%	-1	0.55	Z1-S
247.5000	0.007%	-2	0.10	Z2
247.9542	0.147%	-1	0.81	0,3X0
256.0134	0.017%	-1	0.50	Y1''-S
257.0212	0.003%	-1	0.59	Y1'-S
258.0290	0.192%	-1	0.49	Y1-S
286.0240	0.027%	-1	0.54	1,5X1-S
286.4708	0.010%	-2	0.82	Z2''
298.0241	0.076%	-1	0.90	0,2X1-S-2H
298.0241	0.076%	-2	0.90	0,2X2
300.0396	0.156%	-1	0.30	0,2X1-S
307.5379	0.060%	-2	1.03	B3
311.0082	0.004%	-1	1.29	3,5A2
315.0267	0.024%	-1	0.55	2,5X1-S-H
316.5431	0.042%	-2	0.56	C3
319.9754	0.018%	-1	0.77	Z1
328.0346	0.026%	-1	0.61	0,3X1-S-2H
328.0346	0.026%	-2	0.61	2,4X2-S
337.9859	0.258%	-1	0.60	Y1
339.0030	0.009%	-1	0.63	2,5A2-2H
349.0400	0.012%	-2	0.81	Z3-S
350.1093	0.004%	-1	0.19	1,5A2-S
357.0136	0.041%	-1	0.71	0,2A2
357.0378	0.004%	-2	1.83	Y3''-S
357.5414	0.011%	-2	1.03	Y3'-S
358.0452	0.079%	-2	0.78	Y3-S
365.9809	0.609%	-1	0.77	1,5X1
372.0428	0.015%	-2	1.00	1,5X3-S
376.0888	0.004%	-1	0.65	C2''-S
378.0428	0.010%	-2	0.99	0,2X3-S-2H
378.1046	0.013%	-1	1.07	C2-S

378.5465	0.051%	-2	0.42	0,2X3-S-H
378.9888	0.053%	-1	0.89	0,2X1-H
379.0505	0.112%	-2	0.68	0,2X3-S
384.0610	0.005%	-2	1.15	M-H2O-2CO2-SO3
386.0403	0.023%	-2	1.01	2,5X3-S-2H
388.0106	0.021%	-2	0.88	Z3"
388.5148	0.009%	-2	1.52	Z3'
389.0186	0.156%	-2	1.32	Z3
393.9763	0.004%	-1	1.99	2,5X1-2H
397.0161	0.291%	-2	1.46	Y3"
397.5192	0.112%	-2	-0.57	Y3'
398.0240	0.128%	-2	1.51	Y3
405.5520	0.007%	-2	0.95	M'-H2O-CO2-SO3
407.5375	0.038%	-2	0.92	0,2A4
410.0401	0.003%	-1	0.51	1,5A2-2H
412.0213	0.113%	-2	1.05	1,5X3
412.0561	0.167%	-1	1.33	1,5A2
414.0352	0.291%	-1	1.10	Z2"-S
414.5574	0.012%	-2	1.30	M'-CO2-SO3
416.0506	0.048%	-1	0.44	Z2-S
418.0213	0.028%	-2	1.05	0,2X3-2H
418.5254	1.935%	-2	1.53	0,2X3-H
426.0188	0.010%	-2	1.24	2,5X3-2H
427.0434	0.007%	-2	1.85	M"-H2O-SO3
427.5470	0.041%	-2	1.09	M'-H2O-SO3
428.0511	0.343%	-2	1.62	M-H2O-SO3
432.0188	0.103%	-2	1.19	1,4A4
432.0458	0.014%	-1	1.08	Y2"-S
436.0484	0.036%	-2	1.14	M"-SO3
436.5526	0.023%	-2	1.84	M'-SO3
437.0564	0.531%	-2	1.67	M-SO3
439.0432	0.038%	-1	1.29	B2'
440.0511	0.064%	-1	1.42	B2
445.0266	0.003%	-2	1.17	M"-H2O-CO2
445.5304	0.011%	-2	0.88	M'-H2O-CO2
453.0215	0.024%	-2	-4.51	1,5A4-2H
453.5281	0.007%	-2	1.39	1,5A4-H
454.0315	0.011%	-2	0.33	M"-CO2;1,5A4
454.5359	0.038%	-2	1.39	M'-CO2
455.0380	0.017%	-2	-2.73	M-CO2
456.0459	0.223%	-1	1.31	C2"

457.0537	0.070%	-1	1.24	C2'
458.0616	0.750%	-1	1.31	C2
467.5257	0.056%	-2	1.71	M'-H2O
468.0296	0.013%	-2	1.54	M-H2O
476.0271	0.020%	-2	1.58	M''
476.5310	0.152%	-2	1.73	M-H
477.0350	0.861%	-2	1.89	M
493.9924	0.020%	-1	1.61	Z2''
495.0005	0.008%	-1	2.11	Z2'
496.0079	0.298%	-1	1.41	Z2
500.0723	0.019%	-1	1.40	2,4A3
512.0032	0.334%	-1	1.96	Y2''
514.0184	0.017%	-1	1.21	Y2
516.0912	0.004%	-1	1.71	0,2X2-S-H
528.0675	0.491%	-1	2.02	3,5A3
536.1267	0.051%	-1	1.77	B3-S
537.5918	0.165%	-2	1.68	M-H-SO3+A
538.0938	0.078%	-2	-1.94	M-SO3+A
542.0137	0.291%	-1	1.76	1,5X2
554.1374	0.020%	-1	2.03	C3-S
572.0580	0.003%	-1	2.94	0,2A3-2H
574.0731	0.229%	-1	1.98	0,2A3
577.5706	0.022%	-2	2.14	M'+A
578.0734	0.014%	-2	0.21	M+A
588.0889	0.007%	-1	2.20	1,5A3
596.0484	0.010%	-1	2.19	0,2X2-H
614.0685	0.007%	-1	2.68	B3''
615.0760	0.085%	-1	2.12	B3'
616.0840	5.220%	-1	2.43	B3
619.1311	0.015%	-1	2.01	Z3-2S
632.0788	0.199%	-1	2.20	C3''
634.0946	0.455%	-1	2.34	C3
698.0811	0.005%	-1	3.36	Z3'-S
699.0884	0.035%	-1	2.60	Z3-S
715.0839	0.005%	-1	3.34	Y3''-S
718.1162	0.015%	-1	2.83	2,5A4-S-2H
736.1268	0.183%	-1	2.79	0,2A4-S
757.0947	0.030%	-1	3.37	0,2X3-S-2H
758.1018	0.017%	-1	2.41	0,2X3-S-H
811.1015	0.008%	-1	-1.43	M''-H2O-CO2-SO3
816.0846	0.042%	-1	3.65	0,2A4

828.1088	0.011%	-1	4.07	1,5A4-S-H
829.1155	0.006%	-1	2.70	M"-CO2-SO3;1,5A4-S
838.0608	0.003%	-1	4.85	0,2X3-H
856.1040	0.019%	-1	4.31	M'-H2O-SO3
857.1078	0.006%	-1	-0.34	M-H2O-SO3
873.1069	0.012%	-1	4.45	M"-SO3

Table S11. List of assigned peaks in the NETD spectrum of [1, 1, 2, 1, 4] from HSPIM, [M - 4H]<sup>4+</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
129.0193	0.019%	-2	-0.34	2,5A2-S-2H
138.6426	0.011%	-3	-0.47	Y1
157.0142	0.065%	-1	-0.43	B1
159.4839	0.047%	-2	-0.39	Z1-S
168.4892	0.098%	-2	-0.41	Y1-S
175.0247	0.640%	-1	-0.57	C1
178.0024	0.017%	-2	-3.36	0,2A2
197.3199	0.017%	-3	-0.49	Y2
199.4623	0.013%	-2	-0.44	Z1
208.4675	0.306%	-2	-0.71	Y1
219.5215	0.118%	-2	-0.49	B2
222.4650	0.455%	-2	-0.58	1,5X1
228.5267	0.318%	-2	-0.75	C2
228.9689	0.043%	-2	-0.48	0,2X1-H
238.0026	0.084%	-1	-0.43	Z1''-2S
239.0103	0.017%	-1	-0.74	Z1'-2S
240.0182	0.183%	-1	-0.48	Z1-2S
247.4999	0.224%	-2	-0.53	Z2-S
247.9539	0.013%	-1	-0.60	0,3X0
255.4973	0.015%	-2	-0.53	Y2''-S
256.0131	0.030%	-1	-0.61	Y1''-2S
256.5051	0.095%	-2	-0.54	Y2-S
258.0287	0.233%	-1	-0.72	Y1-2S
259.0096	0.070%	-3	0.04	Z3-S
265.0130	0.061%	-3	-0.54	Y3-S
270.5026	0.036%	-2	-0.58	1,5X2-S
271.3555	0.020%	-3	-0.68	0,2A4-S
274.3446	0.016%	-3	-0.66	1,5X3-S
277.5269	0.058%	-2	-0.63	2,5A3-2H
279.0163	0.509%	-3	-1.18	0,2X3-S
286.4704	0.028%	-2	-0.63	Z2''
286.5322	0.041%	-2	-0.66	0,2A3
287.4781	0.294%	-2	-0.89	Z2
290.9934	0.056%	-3	-0.63	Y3''
291.3296	0.029%	-3	0.42	Y3'
291.6653	0.082%	-3	-0.40	Y3
295.4756	0.262%	-2	-0.84	Y2''
296.6840	0.013%	-3	-0.80	M'-H2O-CO2-SO3
298.0078	0.106%	-3	-0.64	0,2A4

298.0243	0.064%	-1	1.66	0,2X1-2S-2H
298.0243	0.064%	-2	1.66	0,2X2-S
300.0393	0.571%	-1	-0.56	0,2X1-2S
300.9968	0.018%	-3	-0.77	1,5X3
302.6875	0.011%	-3	-0.84	M'-CO2-SO3
305.3328	0.016%	-3	-0.53	0,2X3-H
305.6688	0.244%	-3	-0.38	0,2X3
307.0336	0.026%	-2	-0.39	B3'
307.5375	0.062%	-2	-0.49	B3
310.4811	0.212%	-2	-0.18	1,5X2
311.6833	0.287%	-3	-0.61	M-H2O-SO3
315.5349	0.014%	-2	-0.61	C3"
316.5427	0.480%	-2	-0.56	C3
317.0149	0.011%	-3	-0.60	M"-SO3
317.3512	0.009%	-3	0.52	M'-SO3
317.6868	0.171%	-3	-0.56	M-SO3
317.9593	0.019%	-1	-0.61	Z1"-S
318.9671	0.015%	-1	-0.68	Z2'-S
319.9750	0.057%	-1	-0.60	Z1-S
323.3364	0.042%	-3	-0.52	M'-H2O-CO2
328.0342	0.042%	-2	-0.53	2,4X2-2S
329.3399	0.011%	-3	-0.48	M'-CO2
335.9699	0.013%	-1	-0.45	Y1"-S
337.9856	0.109%	-1	-0.48	Y1-S
337.9995	0.096%	-3	-0.77	M'-H2O
339.0027	0.017%	-1	-0.24	2,5A2-2H
343.6671	0.016%	-3	-0.71	M"
344.0032	0.043%	-3	-0.38	M'
344.3393	0.533%	-3	0.03	M
345.4955	0.038%	-2	-0.70	2,5X2-H
348.5356	0.010%	-2	-0.46	Z3'-2S
349.0395	0.097%	-2	-0.52	Z3-2S
357.0132	0.202%	-1	-0.39	0,2A2
357.0371	0.013%	-2	-0.16	Y3"-2S
358.0448	0.017%	-2	-0.46	Y3-2S
365.9805	0.073%	-1	-0.51	1,5X1-S
377.9804	0.027%	-1	-0.51	0,2X1-S-2H
378.1040	0.029%	-1	-0.52	C2-S
378.9883	0.076%	-1	-0.52	0,2X1-S-H
384.7103	0.023%	-3	-0.44	M'-SO3+A
385.0457	0.013%	-3	-1.78	M-SO3+A
389.0179	0.177%	-2	-0.40	Z3-S
397.0153	0.050%	-2	-0.50	Y3"-S



397.5197	0.033%	-2	0.51	Y3'-S
398.0233	0.164%	-2	-0.05	Y3-S
407.5370	0.107%	-2	-0.38	0,2A4-S
410.0397	0.020%	-1	-0.49	1,5A2-2H
412.0553	0.090%	-1	-0.51	1,5A2
414.0346	0.044%	-1	-0.45	Z2''-2S
415.9269	0.015%	-1	0.11	Y1''
416.0503	0.028%	-1	-0.34	Z2-2S
417.9424	0.085%	-1	-0.44	Y1
418.0207	0.019%	-2	-0.38	0,2X3-S-2H
418.5246	0.705%	-2	-0.41	0,2X3-S-H
426.0183	0.015%	-2	0.08	2,5X3-S-2H
428.9963	0.037%	-2	-0.53	Z3
432.0181	0.015%	-2	-0.35	1,4A4
436.9937	0.013%	-2	-0.45	Y3''
438.0016	0.062%	-2	-0.41	Y3
438.0346	0.054%	-1	-0.53	B2''
439.0428	0.016%	-1	0.48	B2'
440.0502	0.213%	-1	-0.49	B2
445.9373	0.101%	-1	-0.36	1,5X1
447.5152	0.021%	-2	-0.79	0,2A4
453.0237	0.017%	-2	0.37	1,5A4-S-2H
454.0310	0.255%	-2	-0.94	M''-CO2-SO3; 1,5A4-S
456.0452	0.497%	-1	-0.31	C2''
458.0607	7.199%	-1	-0.71	C2
458.5029	0.244%	-2	-0.56	0,2X3-H
458.9450	0.068%	-1	-0.61	0,2X1-H
462.0549	0.016%	-1	-2.15	1,5X2-2S
467.0207	0.071%	-2	-0.70	M''-H2O-SO3
467.5247	0.090%	-2	-0.48	M'-H2O-SO3
468.0283	0.047%	-2	-1.14	M-H2O-SO3
476.0261	0.117%	-2	-0.51	M''-SO3
477.0342	0.021%	-2	0.10	M-SO3
485.0043	0.039%	-2	-0.47	M''-H2O-CO2
485.5061	0.012%	-2	-4.88	M'-H2O-CO2
493.9917	0.024%	-1	0.20	Z2''-S
494.0095	0.042%	-2	-0.57	M''-CO2;1,5A4
496.0070	0.067%	-1	-0.51	Z2-S
499.0635	0.052%	-1	-0.44	2,4A3-H
500.0716	0.089%	-1	0.02	2,4A3
514.0177	0.012%	-1	-0.31	Y2-S
518.0819	0.131%	-1	-0.47	2,4A4-S
526.0503	0.011%	-1	-0.91	3,5A3-2H

528.0662	1.123%	-1	-0.52	3,5A3
536.1254	0.020%	-1	-0.61	B3-S
542.0125	0.049%	-1	-0.34	1,5X2-S
552.1205	0.011%	-1	-0.14	C3"-S
554.1360	0.152%	-1	-0.49	C3-S
556.0613	0.033%	-1	-0.21	2,5A3-2H
574.0717	0.050%	-1	-0.40	0,2A3
577.5689	0.013%	-2	-0.75	M'-SO3+A
588.0876	0.018%	-1	0.06	1,5A3
614.0668	0.027%	-1	-0.18	B3"
615.0745	0.968%	-1	-0.30	B3'
616.0826	0.984%	-1	0.17	B3
621.9699	0.011%	-1	0.51	1,5X2
632.0774	0.063%	-1	-0.07	C3"
634.0930	0.664%	-1	-0.21	C3

Table S12. List of assigned peaks in the NETD spectrum of [1, 1, 2, 1, 5] from HSPIM, [M - 4H]<sup>4+</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
175.0248	0.015%	-1	-0.09	C1-S
199.4621	0.017%	-2	-1.26	Z1
208.4675	0.120%	-2	-0.67	Y1
217.9813	0.035%	-2	-0.57	0,2A2
220.9916	0.179%	-3	2.26	1,4X2-S-H
222.4650	0.151%	-2	-0.59	1,5X1
236.9709	0.039%	-1	-0.69	B1
238.0025	0.212%	-1	-0.65	Z1"-2S
240.0182	0.086%	-1	-0.69	Z1-2S
246.0618	0.017%	-1	-0.63	1,4A2-S
246.4921	0.032%	-2	-0.37	Z2"-S
247.4998	0.045%	-2	-0.70	Z2-S
247.9536	0.009%	-1	-1.61	0,3X0 1,4X1; 3,5X1-
251.4677	0.045%	-2	-0.57	2H
252.9658	0.267%	-1	-0.57	C1"
254.9816	0.283%	-1	-0.22	C1
256.0131	0.034%	-1	-0.69	Y1"-2S
256.5050	0.040%	-2	-0.93	Y2-S
258.0288	0.056%	-1	-0.57	Y1-2S
258.9959	0.032%	-2	-0.74	B2'
267.4972	0.114%	-2	-0.75	C2"
268.5051	0.045%	-2	-0.76	C2
277.5269	0.031%	-2	-0.44	2,5A3-S-H
284.0078	0.018%	-1	-1.27	1,5X1-2S-2H
285.0158	0.133%	-1	-0.75	1,5X1-2S-H
286.0235	0.016%	-1	-0.98	1,5X1-2S
286.4703	0.043%	-2	-0.90	Z2"
287.4782	0.162%	-2	-0.81	Z2
287.6760	0.021%	-3	-1.37	1,4A4-S
291.6653	0.023%	-3	-0.58	Y3
295.4755	0.043%	-2	-1.13	Y2"
296.4834	0.413%	-2	-0.87	Y2
300.0391	0.020%	-1	-1.36	0,2X1-2S
303.5078	0.135%	-2	-0.81	3,5A3
305.3328	0.017%	-3	-0.73	0,2X3-S-H
310.4810	0.435%	-2	-0.35	1,5X2
314.3286	0.019%	-3	-0.38	1,4A4
315.0262	0.018%	-1	-1.01	2,5X1-2S-H

316.5425	0.021%	-2	-1.31	C3-S
317.9594	0.022%	-1	-0.23	Z1"-S
319.9748	0.038%	-1	-0.98	Z1-S
326.5105	0.033%	-2	-0.70	0,2A3
328.0341	0.039%	-2	-0.83	2,4X2-2S
331.9848	0.019%	-3	-1.46	0,2X3-H
337.4981	0.027%	-2	-0.56	0,2X2-H
337.6635	0.016%	-3	-1.10	M"-H2O-SO3
337.9855	0.077%	-1	-0.75	Y1-S
338.3355	0.194%	-3	-0.68	M-H2O-SO3
343.6671	0.032%	-3	-0.71	M"-SO3
344.3388	0.173%	-3	-1.33	M-SO3
347.0117	0.016%	-2	-1.25	B3'
347.5158	0.123%	-2	-0.73	B3
353.4991	0.015%	-2	-1.06	1,4X2-S
355.5132	0.114%	-2	-0.81	C3"
356.5210	1.462%	-2	-0.82	C3
365.9804	0.133%	-1	-0.73	1,5X1-S
368.0123	0.022%	-2	-1.23	2,4X2-S
370.3194	0.034%	-3	-0.78	M"
370.6554	0.033%	-3	-0.58	M'
370.9913	0.146%	-3	-0.70	M
378.9879	0.024%	-1	-1.44	0,2X1-S-H;
388.0100	0.045%	-2	-0.57	Z3"-S
388.5142	0.041%	-2	0.15	Z3'-S
389.0180	0.276%	-2	-0.32	Z3-S
392.0290	0.064%	-2	2.60	0,3A4-S-H
397.0150	0.090%	-2	-1.29	Y3"-S
398.0232	0.047%	-2	-0.44	Y3-S
407.9908	0.029%	-1	-1.02	0,3X1-S-2H
407.9908	0.029%	-2	-1.02	2,4X2
410.0396	0.034%	-1	-0.76	1,5A2-S-2H
411.3624	0.050%	-3	-0.80	M'-SO3+A
411.6971	0.028%	-3	-3.76	M-SO3+A
412.0551	0.021%	-1	-0.98	1,5A2-S
414.0345	0.058%	-1	-0.62	Z2"-2S
415.0427	0.017%	-1	0.21	Z2'-2S
416.0502	0.059%	-1	-0.45	Z2-2S
417.9422	0.077%	-1	-0.76	Y1
428.4921	0.161%	-2	-1.08	Z3'
428.9963	0.151%	-2	-0.45	Z3
432.0449	0.038%	-1	-0.96	Y2"-2S
434.0605	0.031%	-1	-1.16	Y2-2S

436.9698	0.209%	-1	-0.77	0,2A2
436.9935	0.045%	-2	-1.09	Y3"
438.0013	0.030%	-2	-0.98	Y3
438.0345	0.030%	-1	-0.69	B2"-S
439.0424	0.035%	-1	-0.43	B2'-S
440.0501	0.054%	-1	-0.72	B2-S
445.9371	0.199%	-1	-0.76	1,5X1
456.0450	0.097%	-1	-0.74	C2"-S
457.0532	0.033%	-1	0.03	C2'-S
458.0607	0.293%	-1	-0.66	C2-S
458.5029	0.055%	-2	-0.49	0,2X3-H
458.9448	0.043%	-1	-1.01	0,2X1-H
462.0559	0.024%	-1	0.03	1,5X2-2S
465.9974	0.015%	-2	1.46	2,5X3-S-2H
493.9910	0.043%	-1	-1.14	Z2"-S
494.9993	0.019%	-2	-0.18	2,4X3-S-H
494.9993	0.019%	-1	-0.18	Z2'-S
496.0070	0.142%	-1	-0.54	Z2-S
500.0712	0.017%	-1	-0.77	2,4A3-S
506.9991	0.026%	-2	-0.63	M"-H2O-SO3
508.0076	0.015%	-2	0.71	M-H2O-SO3
512.0014	0.031%	-1	-1.42	Y2"-S
514.0175	0.126%	-1	-0.67	Y2-S
516.0044	0.110%	-2	-0.56	M"-SO3
518.9987	0.023%	-1	-1.34	B2'
520.0083	0.015%	-1	2.07	B2
528.0662	0.050%	-1	-0.57	3,5A3-S
536.0017	0.102%	-1	-0.79	C2"
538.0175	0.119%	-1	-0.64	C2
542.0124	0.181%	-1	-0.60	1,5X2-S
575.9636	0.047%	-1	-0.87	Z2
593.9743	0.042%	-1	-0.49	Y2
608.0230	0.102%	-1	-0.48	3,5A3
615.0744	0.106%	-1	-0.47	B3'-S
616.0822	0.085%	-1	-0.48	B3-S
621.9694	0.055%	-1	-0.30	1,5X2
632.0772	0.044%	-1	-0.42	C3"-S
634.0928	0.124%	-1	-0.50	C3-S
695.0312	0.112%	-1	-0.39	B3'
696.0390	0.070%	-1	-0.52	B3
712.0331	0.016%	-1	-1.68	C3"
714.0500	0.023%	-1	0.20	C3

Table S13. List of assigned peaks in the NETD spectrum of [1, 1, 2, 0, 6] from HSPIM, [M - 4H]<sup>4+</sup>

m/z	Intensity	Charge	Error (ppm)	Assignment
198.4540	0.182%	-2	-2.70	Z1''
208.4671	0.018%	-2	-2.58	Y1
217.9809	0.029%	-2	-2.59	0,2A2
222.4645	0.066%	-2	-2.62	1,5X1
236.9705	0.019%	-1	-2.53	B1
238.0021	0.070%	-1	-2.61	Z1''-2S
238.4941	0.022%	-2	-2.58	B2-S
240.0177	0.013%	-1	-2.58	Z1-2S
246.4915	0.034%	-2	-2.61	C2''-S; Z2''-S
247.4993	0.042%	-2	-2.85	C2-S; Z2-S
247.9535	0.003%	-1	-2.02	0,3X0
252.9653	0.023%	-1	-2.75	C1''
254.9809	0.248%	-1	-2.84	C1
264.4750	0.014%	-2	-2.58	1,5A2
277.9685	0.038%	-2	-2.68	B2'
278.4723	0.069%	-2	-2.76	B2
282.5020	0.037%	-2	-2.65	3,5A3-S
286.0231	0.030%	-1	-2.60	1,5X1-2S
286.4698	1.986%	-2	-2.85	C2''; Z2;
286.9739	1.021%	-2	-2.15	C2'; Z2'
287.4775	16.690%	-2	-3.00	C2;Z2
295.4750	0.376%	-2	-2.81	Y2''
296.4827	0.242%	-2	-3.43	Y2
300.0386	0.011%	-1	-2.92	0,2X1-2S
307.9787	0.010%	-2	-3.51	2,4A3-H
310.4803	0.074%	-2	-2.77	1,5X2
311.0069	0.015%	-1	-2.90	3,5A2-S
313.6452	0.002%	-3	-1.91	1,5X3
317.9585	0.150%	-1	-3.16	Z1''-S
317.9809	0.023%	-3	-2.81	0,2X3-S-H
318.9664	0.026%	-1	-3.08	Z1'-S
319.9742	0.047%	-1	-2.99	Z1-S
322.4801	0.794%	-2	-3.29	3,5A3
326.5098	0.014%	-2	-2.84	B3-S
331.4854	0.019%	-2	-3.15	1,4X2-S-2H
334.5072	0.018%	-2	-3.09	C3''-S
335.5150	0.066%	-2	-2.97	C3-S
335.9692	0.040%	-1	-2.60	Y1''-S
336.4775	0.035%	-2	-3.20	2,5A3-2H

337.9847	0.227%	-1	-3.15	Y1-S
344.6329	0.035%	-3	-3.15	0,2X3-H
344.9691	0.007%	-3	-2.32	0,2X3
344.9798	0.036%	-2	-0.34	0,2A3-S-H
345.4828	0.012%	-2	-3.05	0,2A3
350.3115	0.028%	-3	-3.07	M"-H2O-SO3
350.6480	0.036%	-3	-1.59	M'-H2O-SO3
350.9834	0.054%	-3	-3.00	M-H2O-SO3
351.9866	0.019%	-2	-3.44	1,5A3-H
356.3148	0.125%	-3	-3.81	M"-SO3
356.4702	0.105%	-2	-3.45	0,2X2-H
356.6509	0.046%	-3	-3.28	M'-SO3
356.9868	0.537%	-3	-3.44	M-SO3
357.0121	0.098%	-1	-3.30	0,2A2-S
363.9638	0.039%	-1	-3.30	1,5X1-S-2H
363.9638	0.039%	-2	-3.30	2,5X2-2H
365.4800	0.015%	-2	-3.67	B3"
365.9793	0.201%	-1	-3.71	1,5X1-S
368.0280	0.010%	-1	-3.56	1,5A2-2S-2H
368.3039	0.041%	-3	-3.33	M"-CO2; 1,5A4
368.6399	0.050%	-3	-3.11	M'-CO2
370.0437	0.010%	-1	-3.36	1,5A2-2S
374.4852	0.094%	-2	-3.73	C3"
375.4931	0.937%	-2	-3.66	C3
376.9642	0.037%	-3	-1.70	M"-H2O
377.2995	0.052%	-3	-3.46	M'-H2O
377.9792	0.021%	-1	-3.70	0,2X1-S-2H
378.9871	0.065%	-1	-3.72	0,2X1-S-H
382.9670	0.051%	-3	-3.77	M"
383.3029	0.488%	-3	-3.71	M'
383.6390	0.588%	-3	-3.30	M
390.9631	0.036%	-1	-4.00	3,5A2
396.0227	0.043%	-1	-3.76	B2"-2S
397.0304	0.036%	-1	-4.11	B2'-2S
397.9148	0.024%	-1	-3.74	Z1"
398.0382	0.084%	-1	-4.26	B2-2S
399.9305	0.020%	-1	-3.79	Z1
402.4981	0.010%	-2	-4.10	3,5A4-S-2H
405.9739	0.010%	-1	-4.03	1,4A2
406.9817	0.080%	-2	-4.02	Z3"-S
407.9895	0.207%	-2	-4.14	Z3-S
410.4955	0.013%	-2	-4.05	0,3A4-S-2H
414.0330	0.317%	-1	-4.25	C2"-2S; Z2"-2S

415.9869	0.056%	-2	-4.24	Y3"-S
416.0487	0.053%	-1	-4.07	C2-2S;Z2-2S
416.9947	0.068%	-2	-4.29	Y3-S
417.9408	0.440%	-1	-4.08	Y1
420.9734	0.011%	-1	-4.23	2,5A2
424.0104	0.134%	-3	-2.67	M'-SO3+A
432.0435	0.013%	-1	-4.25	Y2"-2S
435.9605	0.012%	-1	-4.26	0,2A2-H
436.9683	0.063%	-1	-4.30	0,2A2
443.4840	0.002%	-2	-4.28	3,5A4
445.9356	0.278%	-1	-4.25	1,5X1
447.4637	0.014%	-2	-4.44	Z3'
447.9675	0.106%	-2	-4.80	Z3
447.9840	0.069%	-1	-4.75	1,5A2-S-2H
448.9923	0.035%	-1	-3.76	1,5A2-S-H
449.9998	0.058%	-1	-4.40	1,5A2-S
455.9650	0.024%	-2	-4.63	Y3"
456.9727	0.040%	-2	-4.85	Y3
458.9431	0.121%	-1	-4.69	0,2X1-H
475.9789	0.054%	-1	-4.59	B2"-S
476.9865	0.199%	-1	-4.97	B2'-S
477.4739	0.071%	-2	-4.89	0,2X3-S-H
486.0535	0.015%	-1	-4.93	3,5A3-2S
487.9459	0.013%	-1	-4.35	0,3X1-2H
494.9970	0.522%	-1	-4.86	C2'-S; Z2'-S
496.0049	0.544%	-1	-4.74	C2-S; Z2-S
506.4646	0.004%	-2	-4.94	0,2A4