Supplemental HNO3 Pseudo-linelist

This HNO3 linelist is intended to supplement HITRAN, which extends only to 1770 cm-1 and therefore misses the nu1 fundamental, plus dozens of overtone and combinations bands.

This supplemental linelist covers:
2600-2670 cm-1 2nu3
3506-3595 cm-1 nu1
4004-4007 cm-1 nu1+nu9 (Q-branch only)
These are the three most noticeable missing HNO3 bands in MkIV balloon spectra.

The linelist was derived by fitting MkIV balloon spectra and PNNL lab spectra. This is described with figures in:
http://mark4sun/report/HNO3_Spectroscopy_Evaluation.pdf

Description.
Generated fake HNO3 linelists to cover the nu1 band centered at 3551 cm-1 and the 2nu3 band centered at 2645 cm-1, both of which are missing from HITRAN. I did this by exploiting the similarity of the nu1 and nu2 bands. I first generated the following list of the positions of the manifolds in the nu1, nu2, and nu3 bands

j	f_nu1	f_nu2	f_2nu3
-51	3529.17	1686.26	0.00
-50	3529.61	1686.75	0.00
-49	3530.03	1687.22	0.00
-48	3530.45	1687.71	0.00
-47	3530.89	1688.20	0.00
-46	3531.31	1688.68	0.00
-45	3531.74	1689.15	0.00
-44	3532.16	1689.63	0.00
-43	3532.58	1690.12	0.00
-42	3533.01	1690.60	0.00
-41	3533.43	1691.06	0.00
-40	3533.86	1691.55	0.00
-39	3534.30	1692.02	0.00
-38	3534.72	1692.49	0.00
-37	3535.14	1692.97	0.00
-36	3535.57	1693.43	0.00
-35	3535.99	1693.90	0.00
-34	3536.42	1694.36	0.00
-33	3536.84	1694.83	0.00
-32	3537.26	1695.29	0.00
-31	3537.69	1695.76	0.00
-30	3538.11	1696.21	0.00
-29	3538.54	1696.66	0.00
-28	3538.97	1697.12	0.00
-27	3539.39	1697.59	0.00
-26	3539.81	1698.03	0.00
-25	3540.225	1698.48	0.00
-24	3540.65	1698.95	2634.52
-23	3541.07	1699.39	2634.99
-22	3541.50	1699.84	2635.46
-21	3541.92	1700.29	2635.89
-20	3542.34	1700.73	2636.35
-19	3542.76	1701.18	2636.80

-18	3543.17	1701.62	2637.255
-17	3543.58	1702.06	2637.70
-16	3544.00	1702.51	2638.155
-15	3544.40	1702.94	2638.60
-14	3544.82	1703.38	2639.04
-13	3545.26	1703.81	2639.495
-12	3545.68	1704.24	2639.93
-11	3546.11	1704.69	2640.375
-10	3546.52	1705.11	2640.81
-9	3546.94	1705.54	2641.24
-8	3547.38	1705.97	2641.675
-7	3547.80	1706.39	2642.11
-6	3548.22	1706.82	2642.53
-5	3548.65	1707.25	2642.96
-4	3549.07	1707.68	2643.38
-3	3549.49	1708.10	2643.80
-2	3549.91	1708.52	2644.22
-1	3550.33	1708.96	2644.65
0	3550.74	1709.40	2645.07
1	3551.16	1709.82	2645.49
2	3551.58	1710.23	2645.90
3	3551.99	1710.64	2646.31
4	3552.41	1711.04	2646.71
5	3552.83	1711.45	2647.12
6	3553.24	1711.85	2647.53
7	3553.66	1712.25	2647.93
8	3554.08	1712.65	2648.33
9	3554.50	1713.06	2648.725
10	3554.91	1713.46	2649.125
11	3555.32	1713.87	2649.52
12	3555.73	1714.28	2649.91
13	3556.14	1714.67	2650.30
14	3556.55	1715.07	2650.69
15	3556.96	1715.47	2651.075
16	3557.39	1715.87	2651.46
17	3557.79	1716.26	2651.85
18	3558.24	1716.65	2652.23
19	3558.64	1717.04	2652.61
20	3559.04	1717.43	2653.01
21	3559.44	1717.82	2653.38
22	3559.89	1718.21	2653.77
23	3560.29	1718.60	2654.175
24	3560.72	1718.98	0.00
25	3561.13	1719.37	0.00
26	3561.55	1719.75	0.00
27	3561.98	1720.12	0.00
28	3562.38	1720.51	0.00
29	3562.78	1720.89	0.00
30	3563.20	1721.27	0.00
31	3563.61	1721.63	0.00
32	3564.02	1722.01	0.00
33	3564.43	1722.39	0.00
34	3564.84	1722.76	0.00
35	3565.25	1723.12	0.00
36	3565.66	1723.49	0.00
37	3566.07	1723.86	0.00
38	3566.48	1724.23	0.00
39	3566.89	1724.58	0.00
40	3567.31	1724.94	0.00

41	3567.72	1725.30	0.00
42	3568.12	1725.65	0.00
43	3568.53	1726.01	0.00
44	3568.94	1726.37	0.00
45	3569.35	1726.72	0.00
46	3569.76	1727.07	0.00
47	3570.17	1727.41	0.00
48	3570.57	1727.77	0.00
49	3570.97	1728.11	0.00
50	3571.37	1728.46	0.00
51	3571.78	1728.81	0.00
52	3572.18	1729.16	0.00
53	3572.58	1729.50	0.00
54	3572.99	1729.84	0.00

I then wrote a fortran program (linelist/f77/hno3.f) that fitted a polynomial to the nu1 and 2nu3 frequencies as functions of the nu2 manifold frequencies, .e.g.

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f_nu1-3550.7 = a0+a1*(f_nu2-1709.5)+a2*(f_nu2-1709.5)^2+a3*(f_nu2-1709.5)^3
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It turned out that a 4'th order polynomial produced a fit with a rms deviation of 0.014 cm-1. Higher order polynomials failed to improve significantly upon this.

The coefficients of the chosen polynomial were
a0 = 0.162455291
a1 = 1.00235796
a2 = 0.00362555636
a3 = 2.84212583E-05

Note that the a1 coefficient is very close to 1.0, indicating that the average spacing of the manifolds is very similar in the nu1 and nu2 bands.

I then used the polynomial to transform the frequencies of the nu2 HNO3 linelist into a nu1 linelist. At the same time, I scaled the strengths by a factor 0.20. I then had to do some massaging because the nu1 manifolds were wider than their nu2 counterparts and because the nu1 Q-branch is relatively stronger and has a different shape. This involved moving individual HNO3 lines which were producing bumps in the residuals to nearby frequencies where there were dips in the residuals.

Also kludged a HNO3 pseudo-linelist for the nu1+nu9 Q-branch at 4006.5 cm-1.