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(NASA-TM-83953) A CALIBRATION LINE LIST FOR
807-1167 cm^{-1} FROM HIGH RESOLUTION FOURIER
SPECTROSCOPY OF THE $^{14}\text{NH}_3$ ν_2 BAND
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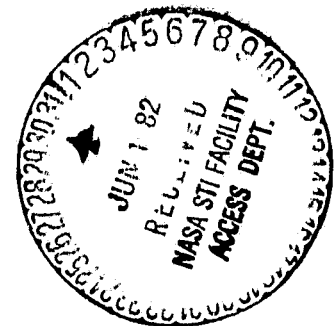


Technical Memorandum 83953

A Calibration Line List for 807-1167 cm^{-1} from High Resolution Fourier Spectroscopy of the $^{14}\text{NH}_3$ ν_2 Band

J. J. Hillman
D. E. Jennings
J. W. Brault

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National Aeronautics and
Space Administration

Goddard Space Flight Center
Greenbelt, Maryland 20771

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high resolution Fourier spectroscopy of the
 $^{14}\text{NH}_3\text{ v}_2$ band

J. J. Hillman, D. E. Jennings

NASA, Goddard Space Flight Center
Molecular Astrophysics Section
Greenbelt, Maryland 20771

and

J. W. Brault

Kitt Peak National Observatory
Tucson, AZ 85726

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high resolution Fourier spectroscopy of the $^{14}\text{NH}_3 \nu_2$ band

The ammonia 8-12 μm bands are often used for calibrating diode laser spectra, both because of the wide spectral extent of the bands and because the gas is convenient to use. However, the accuracies of available NH_3 frequencies have often been inadequate for absolute calibration of diode spectra. It is now possible to significantly improve the NH_3 transition frequencies by measuring them with respect to CO_2 standards using Fourier transform spectroscopy. Besides improving the calibration of new spectra, the results given here can be used to re-calibrate previously recorded diode laser spectra. The frequencies can also be used, of course, in the calibration of Fourier transform and grating spectra.

The accompanying line frequency list is the result of measurements of a spectrum recorded using the McMath 1-meter Fourier transform spectrometer at Kitt Peak. The spectrum included the stronger lines of NH_3 (in ν_2 and ν_4) and CO_2 (9-11 μm laser bands), and also lines of C_2H_6 in the 12 μm region. The path length for both NH_3 and CO_2 , which were contained in the same cell, was 193 meters, and the total pressure was 0.5 Torr. The resolution was 0.005 cm^{-1} . Using the well established laser frequencies for CO_2 (C. Freed, et al. 1980) an average frequency correction was determined and applied over the entire spectrum. The residuals of individual CO_2 measurements from the laser frequencies were then used to establish error estimates for the NH_3 and CO_2 measurements.

Only normal isotope ν_2 NH_3 lines which were not blended with CO_2 , C_2H_6 , or other NH_3 lines have been tabulated, since this list is intended for use as a calibration reference. The accuracy of these measurements can be judged from Figure 1, which shows the residuals of our CO_2 line frequencies from the known laser frequencies. The systematic trend in the residuals is described closely by

$$\Delta\nu = (7.92 \times 10^{-7})(996 - \nu) \quad (1)$$

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where $\Delta\nu$ and ν are in cm^{-1} . The scatter about this slope reflects the measurement precision and is limited by the intensity of the CO_2 lines as compared to the noise in the spectrum. For the NH_3 measurements the errors are estimated to be $\pm 10^{-4} \text{ cm}^{-1}$ plus the systematic error given by (1). [This estimate is conservative - the actual accuracy may be better for the stronger NH_3 lines.] This gives error bars of approximately $\pm 3 \times 10^{-4} \text{ cm}^{-1}$ near 800 and 1170 cm^{-1} , and $\pm 1 \times 10^{-4} \text{ cm}^{-1}$ near 1000 cm^{-1} .

Alternatively, if the trend described by (1) is assumed to hold over the entire $800\text{--}1170 \text{ cm}^{-1}$ range, the observed frequencies can be corrected by subtracting $\Delta\nu$ as given by (1). This correction has been applied and the resulting frequencies are included in Table I. This procedure is certainly valid for the range $900\text{--}1100 \text{ cm}^{-1}$ and results in an RMS residual of the CO_2 lines of $6.5 \times 10^{-5} \text{ cm}^{-1}$. Further error analyses will be needed to decide if this procedure is strictly valid for $800\text{--}900$ and $1100\text{--}1170 \text{ cm}^{-1}$. The remaining error on the frequencies after this correction is estimated to be $\pm 1 \times 10^{-4} \text{ cm}^{-1}$.

Table I reveals the observed frequencies, corrected frequencies, transition assignments, and reference frequencies for 295 lines observed over the $800\text{--}1170 \text{ cm}^{-1}$ region. Ammonia assignments were confirmed by comparison with the analysis of S. Urban and coworkers (1990) and their notation has been used for the assignments. The notation employed for the CO_2 transitions is:

IP(J'') or IR(J'') are P- and R-branches from
 $00^0_1 - [10^0_0, 02^0_0]_{\text{I}}$; the $10.4\mu\text{m}$ band.

IIP(J'') or IIR(J'') are P- and R-branches from
 $00^0_1 - [10^0_0, 01^0_0]_{\text{II}}$; the $9.4\mu\text{m}$ band.

In the table, the CO_2 reference frequencies have been rounded off to the nearest 30 KHz.

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C. Freed, L. C. Bradley, and R. G. O'Donnell, IEEE J. Quantum Electron.
QE-16, 1195-1206 (1980).

S. Urban, V. Spirko, D. Papousek, R. S. McDowell, N. G. Hereson, S. P. Belov, L.
I. Gershstein, A. V. Maslouskij, A. F. Krupnov, J. Curtis, and K. N. Rao,
J. Mol. Spectrosc. 79 455-495 (1980).

Figure Caption:

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Figure 1 - Residuals, (observed-reference), of the CO₂ laser band line frequencies. The straight line is the result of a linear least-squares fit to these data and is given in Eq (1).

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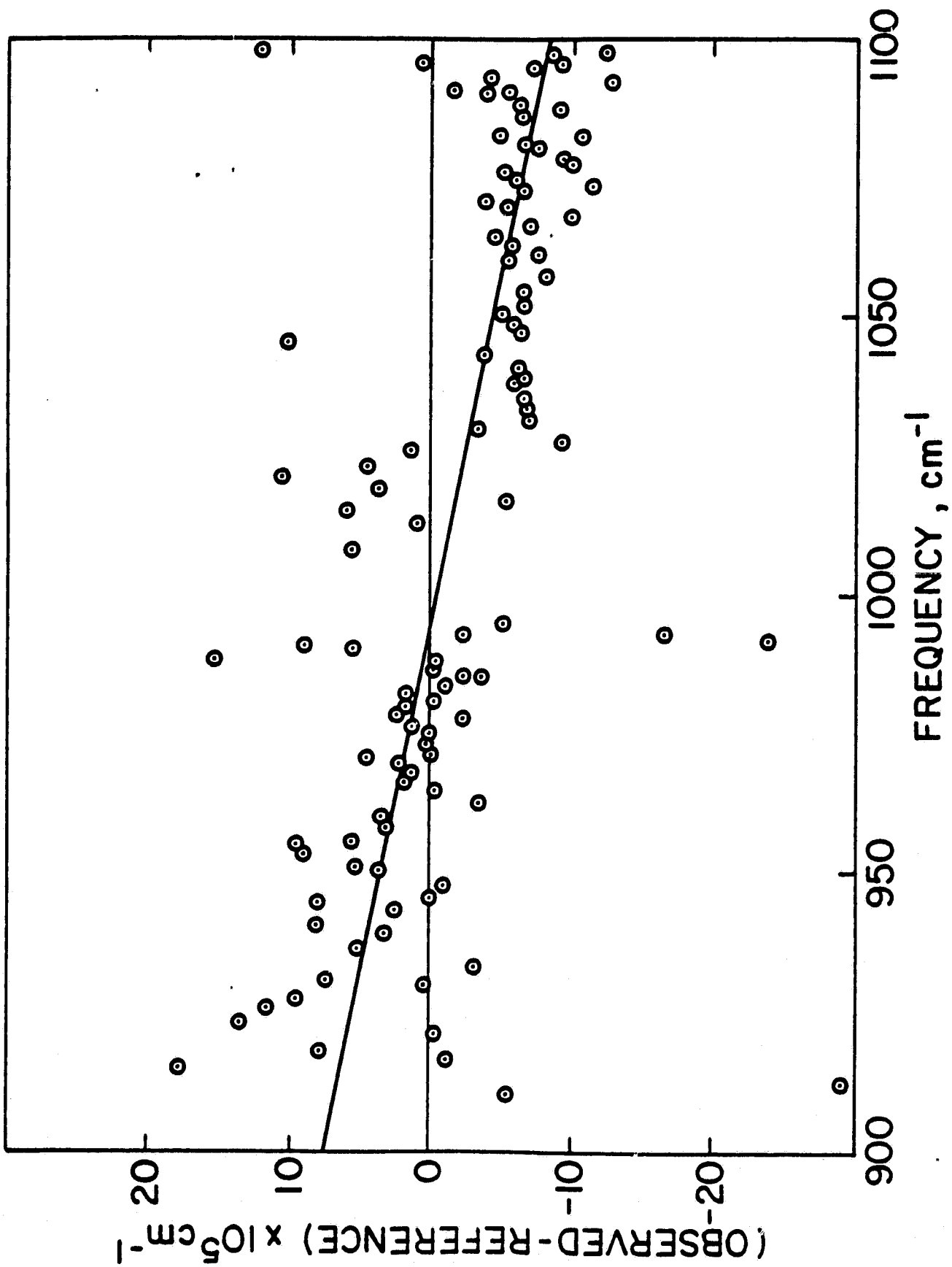


TABLE I

OBSERVED TRANSITION WAVENUMBERS

LINE	OBSERVED FREQUENCY	CORRECTED FREQUENCY	ASSIGNMENT	REFERENCE FREQUENCY
----	-----	-----	-----	-----
1	807.47115	807.47100	sP(8, 3)	
2	812.30116	812.30101	aP(6, 4)	
3	816.64962	816.64948	aP(6, 0)	
4	826.46988	826.46975	sP(7, 6)	
5	826.85562	826.85549	sP(7, 5)	
6	827.70165	827.70152	sP(7, 2)	
7	827.83365	827.83352	sP(7, 1)	
8	827.87714	827.87701	sP(7, 0)	
9	830.65292	830.65279	aP(5, 4)	
10	834.01221	834.01208	aP(5, 2)	
11	847.05252	847.05240	sP(6, 5)	
12	847.57820	847.57808	sP(6, 3)	
13	847.87626	847.87614	sP(6, 1)	
14	851.32800	851.32789	aP(4, 3)	
15	852.72478	852.72467	aP(4, 2)	
16	853.54817	853.54806	aP(4, 1)	

17	853.81817	853.81806	aP(4, 0)	
18	867.51988	867.51978	sP(5, 4)	
19	867.87286	867.87276	sP(5, 2)	
20	867.96668	867.96658	sP(5, 1)	
21	868.00149	868.00139	sP(5, 0)	
22	871.73701	871.73691	aP(3, 2)	
23	872.56721	872.56711	aP(3, 1)	
24	887.87691	887.87682	sP(4, 3)	
25	887.99914	887.99905	sP(4, 2)	
26	888.07947	888.07938	sP(4, 1)	
27	891.88196	891.88188	aP(2, 1)	
28	892.15687	892.15679	aP(2, 0)	
29	908.11244	908.11237	sP(3, 2)	
30	908.17684	908.17677	sP(3, 1)	
31	908.19928	908.19921	sP(3, 0)	
32	910.01580	910.01573	IP(54)	910.015853
33	912.23041	912.23034	IP(52)	912.230703
34	912.38650	912.38643	aQ(12,12)	
35	914.41946	914.41940	IP(50)	914.419283
36	915.66754	915.66748	aQ(11,11)	
37	916.58176	916.58170	IP(48)	916.581770
38	918.62048	918.62042	aQ(10,10)	
39	918.71841	918.71835	IP(46)	918.718331
40	920.82912	920.82906	IP(44)	920.829123
41	921.25522	921.25516	aQ(9, 9)	
42	921.81246	921.81240	aQ(11,10)	
43	922.91443	922.91437	IP(42)	922.914294

44	923.57912	923.57906	aQ(8, 8)	
45	924.07031	924.07025	aQ(10, 9)	
46	924.97410	924.97404	IP(40)	924.973985
47	925.59967	925.59961	aQ(7, 7)	
48	926.04563	926.04557	aQ(9, 8)	
49	926.88468	926.88463	aQ(11, 9)	
50	927.00842	927.00837	IP(38)	927.008325
51	927.32312	927.32307	aQ(6, 6)	
52	927.74221	927.74216	aQ(8, 7)	
53	928.23207	928.23202	sP(2, 1)	
54	928.55777	928.55772	aQ(10, 8)	
55	928.75456	928.75451	aQ(5, 5)	
56	929.01744	929.01739	IP(36)	929.017437
57	931.00151	931.00146	IP(34)	931.001434
58	931.12199	931.12194	aQ(8, 6)	
59	931.17737	931.17732	aQ(5, 4)	
60	931.33329	931.33324	aQ(2, 2)	
61	931.62785	931.62780	aQ(1, 1)	
62	931.77362	931.77357	aQ(4, 3)	
63	932.01131	932.01126	aQ(7, 5)	
64	932.09416	932.09411	aQ(3, 2)	
65	932.13630	932.13625	aQ(2, 1)	
66	932.63562	932.63557	aQ(6, 4)	
67	932.88134	932.88129	aQ(3, 1)	
68	932.96039	932.96034	IP(32)	932.960421
69	932.99245	932.99240	aQ(5, 3)	
70	933.07599	933.07594	aQ(4, 2)	

71	933.15724	933.15719	aQ(9, 6)	
72	933.82643	933.82638	aQ(8, 5)	
73	933.84221	933.84216	aQ(4, 1)	
74	934.23622	934.23617	aQ(7, 4)	
75	934.25186	934.25181	aQ(5, 2)	
76	934.37975	934.37970	aQ(6, 3)	
77	935.59242	935.59237	aQ(6, 2)	
78	935.90351	935.90346	aQ(7, 3)	
79	936.08568	936.08563	aQ(8, 4)	
80	936.80380	936.80375	IP(28)	936.803748
81	937.51585	937.51580	aQ(8, 3)	
82	938.68829	938.68824	IP(26)	938.688257
83	940.24375	940.24371	aQ(9, 2)	
84	940.54818	940.54814	IP(24)	940.548098
85	942.38336	942.38332	IP(22)	942.383336
86	944.19411	944.19407	IP(20)	944.194030
87	945.98023	945.98019	IP(18)	945.980230
88	947.74197	947.74193	IP(16)	947.741979
89	948.23207	948.23203	sP(1, 0)	
90	949.47935	949.47931	IP(14)	949.479314
91	951.19232	951.19228	IP(12)	951.192264
92	951.77628	951.77625	aR(0, 0)	
93	952.88094	952.88091	IP(10)	952.880850
94	954.54518	954.54515	IP(8)	954.545087
95	956.18504	956.18501	IP(6)	956.184982
96	957.80057	957.80054	IP(4)	957.800537
97	957.83901	957.83898	sQ(12,12)	

98	959.39178	959.39175	IP(2)	959.391745
99	959.40637	959.40634	sQ(11,11)	
100	959.65262	959.65259	sQ(11,10)	
101	960.01991	960.01988	sQ(11, 9)	
102	960.85220	960.85217	sQ(10,10)	
103	961.08575	961.08572	sQ(10, 9)	
104	961.41030	961.41027	sQ(10, 8)	
105	961.73284	961.73281	IR(0)	961.732874
106	962.17146	962.17143	sQ(9, 9)	
107	962.38829	962.38826	sQ(9, 8)	
108	962.66974	962.66971	sQ(9, 7)	
109	962.97354	962.97351	sQ(9, 6)	
110	963.36269	963.36266	sQ(8, 8)	
111	963.55847	963.55844	sQ(8, 7)	
112	963.79617	963.79614	sQ(8, 6)	
113	964.04121	964.04118	sQ(8, 5)	
114	964.42405	964.42403	sQ(7, 7)	
115	964.46759	964.46757	sQ(8, 3)	
116	964.59572	964.59570	sQ(7, 6)	
117	964.76898	964.76896	IR(4)	964.768982
118	964.79064	964.79062	sQ(7, 5)	
119	964.97946	964.97944	sQ(7, 4)	
120	965.13759	965.13757	sQ(7, 3)	
121	965.35394	965.35392	sQ(6, 6)	
122	965.49944	965.49942	sQ(6, 5)	
123	965.65196	965.65194	sQ(6, 4)	
124	965.79130	965.79128	sQ(6, 3)	

125	965.89959	965 .89957	sQ(6, 2)	
126	966.15118	966.15116	sQ(5, 5)	
127	966.25038	966.25036	IR(6)	966.250361
128	966.26923	966.26921	sQ(5, 4)	
129	966.37989	966.37987	sQ(5, 3)	
130	966.47359	966.47357	sQ(5, 2)	
131	966.81475	966.81473	sQ(4, 4)	
132	966.90516	966.90514	sQ(4, 3)	
133	966.98085	966.98083	sQ(4, 2)	
134	967.03073	967.03071	sQ(4, 1)	
135	967.34637	967.34635	sQ(3, 3)	
136	967.40679	967.40677	sQ(3, 2)	
137	967.44925	967.44923	sQ(3, 1)	
138	967.70725	967.70723	IR(8)	967.707233
139	967.73858	967.73856	sQ(2, 2)	
140	967.77443	967.77441	sQ(2, 1)	
141	967.99787	967.99785	sQ(1, 1)	
142	969.13957	969.13955	IR(10)	969.139547
143	970.54729	970.54727	IR(12)	970.547244
144	971.88211	971.88209	aR(1, 1)	
145	971.93026	971.93024	IR(14)	971.930258
146	973.28852	973.28850	IR(16)	973.288517
147	974.62194	974.62192	IR(18)	974.621939
148	975.93045	975.93043	IR(20)	975.930439
149	977.21390	977.21389	IR(22)	977.213922
150	978.47231	978.47230	IR(24)	978.472286
151	979.70544	979.70543	IR(26)	979.705421

152	980.91321	980.91320	IR(28)	980.913211
153	982.09555	982.09554	IR(30)	982.095531
154	983.25224	983.25223	IR(32)	983.252249
155	984.38319	984.38318	IR(34)	984.383226
156	985.48829	985.48828	IR(36)	985.488312
157	986.56735	986.56734	IR(38)	986.567352
158	987.62018	987.62017	IR(40)	987.620181
159	988.64678	988.64677	IR(42)	988.646626
160	989.64656	989.64656	IR(44)	989.646506
161	990.61972	990.61972	IR(46)	990.619630
162	991.56556	991.56556	IR(48)	991.565798
163	991.69048	991.69048	aR(2, 2)	
164	992.45027	992.45027	aR(2, 1)	
165	992.48478	992.48478	IR(50)	992.484803
166	992.69874	992.69874	aR(2, 0)	
167	993.37626	993.37626	IR(52)	993.376427
168	994.24039	994.24039	IR(54)	994.240442
169	1007.77136	1007.77137	IIP(58)	1007.771302
170	1011.20358	1011.20359	aR(3, 3)	
171	1012.29178	1012.29179	IIP(54)	1012.291767
172	1012.44511	1012.44512	aR(3, 2)	
173	1013.17552	1013.17553	aR(3, 1)	
174	1014.51795	1014.51796	IIP(52)	1014.517888
175	1016.72089	1016.72091	IIP(50)	1016.720942
176	1018.90073	1018.90075	IIP(48)	1018.900693
177	1021.05702	1021.05704	IIP(46)	1021.056912
178	1023.18942	1023.18944	IIP(44)	1023.189375

179	1025.29788	1025.29790	IIP(42)	1025.297865
180	1027.03293	1027.03295	sR(2, 2)	
181	1027.04693	1027.04695	sR(2, 1)	
182	1027.38208	1027.38211	IIP(40)	1027.382171
183	1029.44206	1029.44209	IIP(38)	1029.442092
184	1030.42233	1030.42236	aR(4, 4)	
185	1031.47736	1031.47739	IIP(36)	1031.477430
186	1032.13104	1032.13107	aR(4, 3)	
187	1033.31572	1033.31575	aR(4, 2)	
188	1033.48793	1033.48796	IIP(34)	1033.487999
189	1034.01276	1034.01279	aR(4, 1)	
190	1034.24483	1034.24486	aR(4, 0)	
191	1035.47355	1035.47358	IIP(32)	1035.473616
192	1037.43405	1037.43408	IIP(30)	1037.434110
193	1039.36925	1039.36928	IIP(28)	1039.369315
194	1041.27901	1041.27905	IIP(26)	1041.279074
195	1043.16320	1043.16324	IIP(24)	1043.163239
196	1045.02177	1045.02181	IIP(22)	1045.021670
197	1046.37459	1046.37463	sR(3, 3)	
198	1046.38808	1046.38812	sR(3, 2)	
199	1046.85417	1046.85421	IIP(20)	1046.854234
200	1048.66075	1048.66079	IIP(18)	1048.660810
201	1049.34636	1049.34640	aR(5, 5)	
202	1050.44123	1050.44127	IIP(16)	1050.441282
203	1051.51193	1051.51197	aR(5, 4)	
204	1052.19548	1052.19552	IIP(14)	1052.195545
205	1053.13041	1053.13046	aR(5, 3)	

206	1053.92342	1053.92347	IIP(12)	1053.923503
207	1054.25268	1054.25273	aR(5, 2)	
208	1054.91256	1054.91261	aR(5, 1)	
209	1057.30008	1057.30013	IIP(8)	1057.300161
210	1058.94866	1058.94871	IIP(6)	1058.948714
211	1060.57059	1060.57064	IIP(4)	1060.570666
212	1062.16591	1062.16596	IIP(2)	1062.165965
213	1064.50881	1064.50886	IIR(0)	1064.508853
214	1065.58138	1065.58144	sR(4, 2)	
215	1065.59424	1065.59430	sR(4, 1)	
216	1066.03729	1066.03735	IIR(2)	1066.037360
217	1067.53901	1067.53907	IIR(4)	1067.539110
218	1067.97433	1067.97439	aR(6, 6)	
219	1069.01404	1069.01410	IIR(6)	1069.014093
220	1070.46227	1070.46233	IIR(8)	1070.462308
221	1070.59095	1070.59101	aR(6, 5)	
222	1071.88370	1071.88376	IIR(10)	1071.883766
223	1072.62742	1072.62748	aR(6, 4)	
224	1073.27837	1073.27843	IIR(12)	1073.278484
225	1074.14922	1074.14928	aR(6, 3)	
226	1074.64643	1074.64649	IIR(14)	1074.646490
227	1075.20312	1075.20318	aR(6, 2)	
228	1075.82287	1075.82293	aR(6, 1)	
229	1075.98777	1075.98783	IIR(16)	1075.987820
230	1076.03304	1076.03310	aR(6, 0)	
231	1077.30242	1077.30248	IIR(18)	1077.302520
232	1078.59055	1078.59062	IIR(20)	1078.590644

233	1079.85218	1079.85225	IIR(22)	1079.852255
234	1081.08736	1081.08743	IIR(24)	1081.087426
235	1082.29613	1082.29620	IIR(26)	1082.296237
236	1083.47873	1083.47880	IIR(28)	1083.478778
237	1084.58158	1084.58165	sR(5, 4)	
238	1084.59365	1084.59372	sR(5, 3)	
239	1084.60958	1084.60965	sR(5, 2)	
240	1085.76538	1085.76545	IIR(32)	1085.765445
241	1086.30383	1086.30390	aR(7, 7)	
242	1086.86970	1086.86977	IIR(34)	1086.869791
243	1087.94824	1087.94831	IIR(36)	1087.948306
244	1089.00108	1089.00115	IIR(38)	1089.001119
245	1089.36989	1089.36996	aR(7, 6)	
246	1090.02831	1090.02838	IIR(40)	1090.028367
247	1091.03018	1091.03026	IIR(42)	1091.030196
248	1091.81176	1091.81184	aR(7, 5)	
249	1092.00663	1092.00671	IIR(44)	1092.006758
250	1092.95817	1092.95825	IIR(46)	1092.958211
251	1093.71135	1093.71143	aR(7, 4)	
252	1093.88465	1093.88473	IIR(48)	1093.884721
253	1094.78647	1094.78655	IIR(50)	1094.786462
254	1095.12927	1095.12935	aR(7, 3)	
255	1095.66352	1095.66360	IIR(52)	1095.663612
256	1096.11272	1096.11280	aR(7, 2)	
257	1096.51627	1096.51635	IIR(54)	1096.516356
258	1096.68969	1096.68977	aR(7, 1)	
259	1097.34476	1097.34484	IIR(56)	1097.344886

260	1098.14952	1098.14960	IIR(58)	1098.149398
261	1104.33222	1104.33231	aR(8, 8)	
262	1107.84947	1107.84956	aR(8, 7)	
263	1110.68896	1110.68905	aR(8, 6)	
264	1112.94921	1112.94930	aR(8, 5)	
265	1114.70659	1114.70668	aR(8, 4)	
266	1116.01958	1116.01968	aR(8, 3)	
267	1116.92689	1116.92699	aR(8, 2)	
268	1117.45857	1117.45867	aR(8, 1)	
269	1117.64778	1117.64788	aR(8, 0)	
270	1122.05523	1122.05533	aR(9, 9)	
271	1122.09397	1122.09407	sR(7, 5)	
272	1122.10365	1122.10375	sR(7, 4)	
273	1122.11782	1122.11792	sR(7, 6)	
274	1122.13281	1122.13291	sR(7, 3)	
275	1122.16004	1122.16014	sR(7, 2)	
276	1122.20348	1122.20358	sR(7, 7)	
277	1126.02943	1126.02953	aR(9, 8)	
278	1129.26163	1129.26174	aR(9, 7)	
279	1131.86948	1131.86959	aR(9, 6)	
280	1133.94455	1133.94466	aR(9, 5)	
281	1135.55636	1135.55647	aR(9, 4)	
282	1136.75729	1136.75740	aR(9, 3)	
283	1137.59202	1137.59213	aR(9, 2)	
284	1138.07735	1138.07746	aR(9, 1)	
285	1140.60344	1140.60355	sR(8, 4)	
286	1140.67889	1140.67900	sR(8, 2)	

287	1140.69947	1140.69958	sR(8, 1)
288	1143.90793	1143.90805	aR(10, 9)
289	1147.53216	1147.53228	aR(10, 8)
290	1150.47819	1150.47831	aR(10, 7)
291	1152.85274	1152.85286	aR(10, 6)
292	1156.20774	1156.20787	aR(10, 4)
293	1157.30433	1157.30446	aR(10, 3)
294	1158.66723	1158.66736	aR(10, 0)
295	1165.50226	1165.50239	aR(11, 9)