

## Electronic Supplementary Information for

# Near-infrared spectroscopy of $\text{H}_3\text{O}^+\cdots\text{X}_n$ ( $\text{X} = \text{Ar}, \text{N}_2$ , and $\text{CO}$ , $n = 1\text{-}3$ ):

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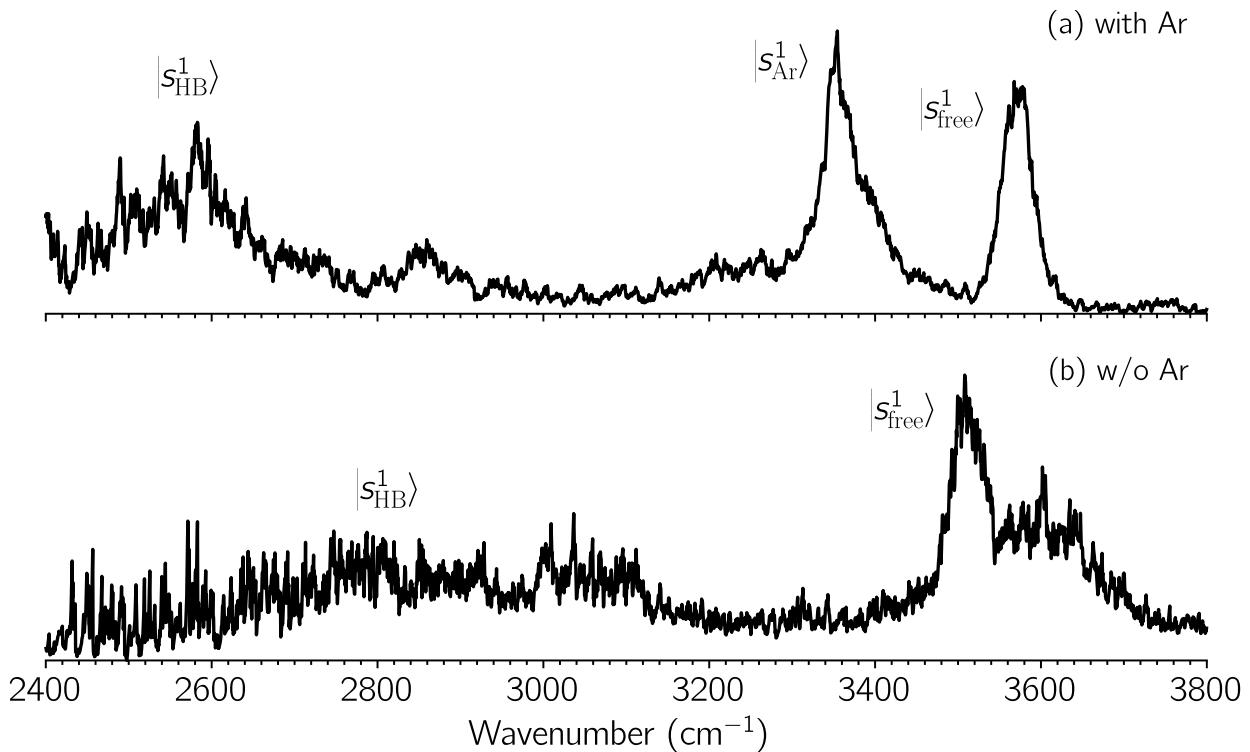
Fundamental Region.

**Table S1.** Cartesian Coordinates of  $\text{H}_3\text{O}^+\cdots\text{X}_n$  ( $\text{X} = \text{Ar}, \text{N}_2$ , and  $\text{CO}$ ,  $n = 1\text{-}3$ ) Optimized by MP2/aug-cc-pVDZ.

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**Figure S1. Infrared Spectra of Bare and Ar-Tagged  $\text{H}_3\text{O}^+\cdots\text{CO}$  in the OH Stretch Fundamental Region.** (a) Ar-tagged  $\text{H}_3\text{O}^+\cdots\text{CO}$ . (b) bare  $\text{H}_3\text{O}^+\cdots\text{CO}$ . The Ar-loss channel was monitored to measure the spectrum of the Ar-tagged cluster. The CO-loss channel was monitored in the spectrum of the bare cluster.

The CO-bound OH stretching vibrational band  $|s_{\text{HB}}^1\rangle$  is observed at  $2600 \text{ cm}^{-1}$  in the Ar-tagged cluster, while that in the bare cluster appears as a very broadened band in the  $2600 - 3200 \text{ cm}^{-1}$  region and its maximum is seen at  $\sim 2900 \text{ cm}^{-1}$ . Because the binding energy of  $\text{H}_3\text{O}^+\cdots\text{CO}$  is estimated to be  $5040 \text{ cm}^{-1}$  (at the MP2/aug-cc-pVDZ level of theory with the zero-point energy and basis set superposition error corrections), only clusters with high internal (thermal) energy can dissociate with excitation of OH-stretching fundamentals. The dissociation yield upon IR absorption in the low frequency region becomes much lower since assistance of higher internal energy is requested to dissociate. Though  $|s_{\text{HB}}^1\rangle$  in the bare cluster would be located at lower than  $2600 \text{ cm}^{-1}$ , absorption in this region was not detected due to the lack of predissociation, and only its long tail to the high frequency side was observed in the spectrum. Since the binding energy with Ar is much less,  $|s_{\text{HB}}^1\rangle$  is observed without modulation by the dissociation yield. We should also note that  $|s_{\text{HB}}^1\rangle$  would be somewhat blue-shifted from that of the bare cluster because of the anti-cooperative effect of the Ar tagging (H-bond formation with Ar).  $|s_{\text{Ar}}^1\rangle$  in the Ar-tagged cluster is the Ar-bound OH-stretching vibrational band, which shows a red shift due to the H-bond formation from the free OH stretch bands,  $|s_{\text{free}}^1\rangle$ .

**Table S1. Cartesian Coordinates of H<sub>3</sub>O<sup>+</sup>···X<sub>n</sub> (X =Ar, N<sub>2</sub>, and CO, n = 1-3) Optimized by MP2/aug-cc-pVDZ**

All the structures were optimized at MP2/aug-cc-pVDZ.

H<sub>3</sub>O<sup>+</sup>···Ar

O	-0.000000	0.010278	0.737812
H	-0.000000	0.956580	0.429174
H	-0.807049	-0.460338	0.436903
H	0.807049	-0.460338	0.436903
Ar	0.000000	2.987099	-0.123114

H<sub>3</sub>O<sup>+</sup>···Ar<sub>2</sub>

O	0.000000	-0.003497	0.740036
H	0.000000	0.928938	0.437612
H	-0.818343	-0.472551	0.433025
H	0.818343	-0.472551	0.433025
Ar	-2.603747	-1.503808	-0.129049
Ar	2.603747	-1.503808	-0.129049

H<sub>3</sub>O<sup>+</sup>···Ar<sub>3</sub>

O	1.430000	0.000000	0.000000
H	1.737403	0.000000	0.940387
H	1.737403	0.814399	-0.470194
H	1.737403	-0.814399	-0.470194
Ar	2.308733	0.000000	3.027277
Ar	2.308733	2.621698	-1.513638
Ar	2.308733	-2.621698	-1.513638

H3O<sup>+</sup>...N<sub>2</sub>

O	-1.836053	-0.000000	0.087678
H	-0.824701	-0.000000	0.003114
H	-2.236235	0.803557	-0.304432
H	-2.236235	-0.803557	-0.304432
N	0.862754	0.000000	-0.015110
N	1.992331	0.000000	0.001442

H3O<sup>+</sup>...(N<sub>2</sub>)<sub>2</sub>

O	-0.000000	-0.020285	0.647379
H	-0.000000	0.909417	0.346209
H	-0.834517	-0.493937	0.354150
H	0.834517	-0.493937	0.354150
N	-2.319600	-1.332074	-0.033601
N	2.319600	-1.332074	-0.033601
N	-3.287189	-1.873597	-0.250852
N	3.287189	-1.873597	-0.250852

H3O<sup>+</sup>...(N<sub>2</sub>)<sub>3</sub>

O	1.430000	0.000000	0.000000
H	1.724582	0.000000	0.951680
H	1.724582	0.824179	-0.475840
H	1.724582	-0.824179	-0.475840
N	2.126797	0.000000	2.700422
N	2.126797	2.338634	-1.350211
N	2.126797	-2.338634	-1.350211
N	2.343159	0.000000	3.809567
N	2.343159	3.299182	-1.904784
N	2.343159	-3.299182	-1.904784

H<sub>3</sub>O<sup>+</sup>···CO

O	0.056624	-1.888466	-0.000000
H	-0.013759	-0.839249	-0.000000
H	-0.334041	-2.293732	0.799916
H	-0.334041	-2.293732	-0.799916
C	-0.000000	0.815315	0.000000
O	0.028606	1.955319	0.000000

H<sub>3</sub>O<sup>+</sup>···(CO)<sub>2</sub>

O	0.104559	1.281489	-0.000000
H	-0.520429	2.030651	-0.000000
H	0.016368	0.730420	0.853980
H	0.016368	0.730420	-0.853980
C	-0.014729	-0.175044	2.370386
C	-0.014729	-0.175044	-2.370386
O	-0.011355	-0.750710	3.356644
O	-0.011355	-0.750710	-3.356644

H<sub>3</sub>O<sup>+</sup>···(CO)<sub>3</sub>

O	1.430000	0.000000	0.000000
H	1.719273	0.000000	0.963783
H	1.719273	0.834660	-0.481891
H	1.719273	-0.834660	-0.481891
C	2.106746	0.000000	2.757247
C	2.106746	2.387846	-1.378623
C	2.106746	-2.387846	-1.378623
O	2.318608	0.000000	3.880415
O	2.318608	3.360538	-1.940208
O	2.318608	-3.360538	-1.940208

**Table S2. Normal Modes Frequencies and Intensities of H<sub>3</sub>O<sup>+</sup>…X<sub>n</sub> Evaluated by MP2/aug-cc-pVDZ.**

H<sub>3</sub>O<sup>+</sup>…Ar

Freq	Intensity	Symmetry Representation	Assignment
150	60.5	A'	OH…Ar Intermolecular Stretching
228	5.0	A"	Hindered Rotation
313	95.1	A'	Rocking
931	328.4	A'	Umbrella
1665	71.9	A'	Anti-symmetric Bending
1671	53.3	A"	Anti-symmetric Bending
3354	956.7	A'	Hydrogen-Bonded OH Stretching
3618	374.7	A'	Symmetric Free OH Stretching
3698	416.2	A"	Anti-symmetric Free OH Stretching

H<sub>3</sub>O<sup>+</sup>…Ar<sub>2</sub>

Freq	Intensity	Symmetry Representation	Assignment
24	6.1	A'	OH…Ar Intermolecular Bending
126	31.0	A'	OH…Ar Intermolecular Stretching
155	70.4	A"	OH…Ar Intermolecular Stretching
224	76.3	A'	Rocking
281	7.9	A"	Hindered Rotation
384	70.1	A"	Rocking
948	270.2	A'	Umbrella
1666	46.2	A"	Anti-symmetric Bending
1671	35.3	A'	Anti-symmetric Bending
3393	380.4	A'	Symmetric Hydrogen-Bonded OH Stretching
3442	1591.3	A"	Anti-symmetric Hydrogen-Bonded OH Stretching
3680	417.9	A'	Free OH Stretching

$\text{H}_3\text{O}^+\cdots\text{Ar}_3$ 

Freq	Intensity	Symmetry Representation	Assignment
19	1.7	E	OH $\cdots$ Ar Intermolecular bending
19	1.7	E	OH $\cdots$ Ar Intermolecular bending
36	8.7	A <sub>1</sub>	OH $\cdots$ Ar Intermolecular Umbrella
99	11.1	A <sub>1</sub>	OH $\cdots$ Ar Intermolecular Stretching
151	55.8	E	OH $\cdots$ Ar Intermolecular Stretching
151	55.8	E	OH $\cdots$ Ar Intermolecular Stretching
339	0.0	A <sub>2</sub>	Hindered Rotation
368	69.7	E	Rocking
368	69.7	E	Rocking
962	226.4	A <sub>1</sub>	Umbrella
1669	25.1	E	Anti-symmetric bending
1669	25.1	E	Anti-symmetric bending
3419	103.2	A <sub>1</sub>	Symmetric Stretching
3492	1412.2	E	Anti-symmetric Stretching
3492	1412.2	E	Anti-symmetric Stretching

 $\text{H}_3\text{O}^+\cdots\text{N}_2$ 

Freq	Intensity	Symmetry Representation	Assignment
138	1.1	A"	N $\equiv$ N rotation
140	3.3	A'	N $\equiv$ N rotation
244	82.2	A'	OH $\cdots$ N <sub>2</sub> Intermolecular Stretching
392	2.9	A"	Hindered Rotation
499	138.3	A'	Rocking
994	288.2	A'	Umbrella
1660	38.6	A'	Anti-symmetric bending
1696	58.2	A"	Anti-symmetric bending
2173	31.9	A'	N $\equiv$ N stretching
2975	1841.8	A'	Hydrogen-Bonded OH Stretching
3635	253.2	A'	Symmetric Free OH Stretching
3725	389.1	A"	Anti-symmetric Free OH Stretching

$\text{H}_3\text{O}^{\cdot\cdot\cdot}(\text{N}_2)_2$ 

Freq	Intensity	Symmetry Representation	Assignment
34	4.9	A'	OH $\cdots$ N <sub>2</sub> Intermolecular Bonding
128	0.1	A''	N $\equiv$ N rotation
129	5.0	A'	N $\equiv$ N rotation
129	1.2	A''	N $\equiv$ N rotation
152	1.8	A'	N $\equiv$ N rotation
209	26.2	A'	OH $\cdots$ N <sub>2</sub> Intermolecular Stretching
236	104.0	A''	OH $\cdots$ N <sub>2</sub> Intermolecular Stretching
349	85.2	A'	Rocking
468	8.0	A''	Hindered Rotation
658	81.0	A''	Rocking
1009	255.7	A'	Umbrella
1674	21.2	A''	Anti-symmetric Bonding
1699	33.9	A'	Anti-symmetric Bonding
2171	38.4	A''	N $\equiv$ N stretching
2171	10.7	A'	N $\equiv$ N stretching
3170	2519.5	A''	Symmetric Hydrogen-Bonded OH Stretching
3176	660.2	A'	Anti-symmetric Hydrogen-Bonded OH Stretching
3713	334.7	A'	Free OH Stretching

 $\text{H}_3\text{O}^{\cdot\cdot\cdot}(\text{N}_2)_3$ 

Freq	Intensity	Symmetry Representation	Assignment
27	1.4	E	OH $\cdots$ N <sub>2</sub> Intermolecular Bonding
27	1.4	E	OH $\cdots$ N <sub>2</sub> Intermolecular Bonding
44	5.4	A <sub>1</sub>	OH $\cdots$ N <sub>2</sub> Intermolecular Umbrella
121	0.0	A <sub>1</sub>	N $\equiv$ N rotation
122	1.3	E	N $\equiv$ N rotation
122	1.3	E	N $\equiv$ N rotation
140	1.2	A <sub>2</sub>	N $\equiv$ N rotation
144	1.9	E	N $\equiv$ N rotation
144	1.9	E	N $\equiv$ N rotation
176	3.5	A <sub>1</sub>	OH $\cdots$ N <sub>2</sub> Intermolecular Stretching

228	72.4	E	OH···N <sub>2</sub> Intermolecular Stretching
228	72.4	E	OH···N <sub>2</sub> Intermolecular Stretching
557	0.0	A <sub>2</sub>	Hindered Rotation
618	78.3	E	Rocking
618	78.3	E	Rocking
1014	233.6	A <sub>1</sub>	Umbrella
1692	15.1	E	Anti-symmetric Bending
1692	15.1	E	Anti-symmetric Bending
2169	29.0	A <sub>1</sub>	N≡N stretching
2169	29.0	E	N≡N stretching
2170	1.5	E	N≡N stretching
3285	122.4	A <sub>1</sub>	Symmetric Stretching
3307	2070.4	E	Anti-symmetric Stretching
3307	2070.4	E	Anti-symmetric Stretching

### H<sub>3</sub>O<sup>+</sup>···CO

Freq	Intensity	Symmetry Representation	Assignment
187	0.0	A"	C≡O rotation
191	2.9	A'	C≡O rotation
277	112.4	A'	OH···CO Intermolecular Stretching
498	0.0	A"	Hindered Rotation
555	190.2	A'	Rocking
1075	179.5	A'	Umbrella
1634	15.1	A'	Anti-symmetric Bending
1687	33.5	A"	Anti-symmetric Bending
2151	3.3	A'	C≡O stretching
2338	2843.8	A'	Hydrogen-Bonded OH Stretching
3649	209.2	A'	Symmetric Free OH Stretching
3748	350.7	A"	Anti-symmetric Free OH Stretching

### H<sub>3</sub>O<sup>+</sup>···(CO)<sub>2</sub>

Freq	Intensity	Symmetry Representation	Assignment
39	3.8	A'	OH···CO Intermolecular Bending

168	6.4	A'	C≡O rotation
172	2.3	A"	C≡O rotation
173	1.3	A"	C≡O rotation
195	15.7	A'	C≡O rotation
245	8.8	A'	OH···CO Intermolecular Stretching
253	126.8	A"	OH···CO Intermolecular Stretching
393	92.4	A'	Rocking
579	12.8	A"	Hindered Rotation
806	64.5	A"	Rocking
1053	167.1	A'	Umbrella
1667	0.8	A"	Anti-symmetric Bending
1693	11.7	A'	Anti-symmetric Bending
2136	0.5	A'	C≡O stretching
2137	0.5	A"	C≡O stretching
2809	3538.4	A"	Symmetric Hydrogen-Bonded OH Stretching
2874	858.4	A'	Anti-symmetric Hydrogen-Bonded OH Stretching
3732	280.7	A'	Free OH Stretching

### $\text{H}_3\text{O}^{\cdot\cdot\cdot}(\text{CO})_3$

Freq	Intensity	Symmetry Representation	Assignment
31	1.0	E	OH···CO Intermolecular Bending
31	1.0	E	OH···CO Intermolecular Bending
47	3.8	A <sub>1</sub>	OH···CO Intermolecular Umbrella
160	3.6	A <sub>1</sub>	C≡O rotation
161	3.4	E	C≡O rotation
161	3.4	E	C≡O rotation
162	0.0	A <sub>2</sub>	C≡O rotation
189	18.2	E	C≡O rotation
189	18.2	E	C≡O rotation
216	0.3	A <sub>1</sub>	OH···CO Intermolecular Stretching
249	57.2	E	OH···CO Intermolecular Stretching
249	57.2	E	OH···CO Intermolecular Stretching
694	0.0	A <sub>2</sub>	Hindered Rotation
735	62.6	E	Rocking

735	62.6	E	Rocking
1040	155.3	A <sub>1</sub>	Umbrella
1690	0.5	E	Anti-symmetric Bending
1690	0.5	E	Anti-symmetric Bending
2127	0.3	A <sub>1</sub>	C≡O stretching
2129	3.5	E	C≡O stretching
2129	3.5	E	C≡O stretching
3079	2658.5	E	Anti-symmetric Stretching
3079	2658.5	E	Anti-symmetric Stretching
3096	140.4	A <sub>1</sub>	Symmetric Stretching

**Table S3. Energy and Intrinsic IR Intensities of Selected FBR Basis**

As mentioned in the main text, we expand the Hamiltonian using FBR basis function  $|T_i, b_j, s_k\rangle$ . The following tables shows the FBR basis kets in the region of  $4000 - 7000\text{cm}^{-1}$  with their zeroth-order transition energy  $\omega$  (from  $\langle T_0, b_0, s_0 |$ ). This transition energy are plotted in Fig. 4-6 as the filled- and empty-circles. The intrinsic IR Intensities  $I$ , that is, the IR intensity obtained from the transition dipole  $\langle T_0, b_0, s_0 | \hat{\mu} | T_i, b_j, s_k \rangle$ , are also listed in the tables. We call it "intrinsic" IR intensity since the intensity is not borrowed from other bright states in this picture.

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H<sub>3</sub>O<sup>+</sup> ··· Ar<sub>1</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

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$\omega$	$I$	Label	$\omega$	$I$	Label
4761.2	0.5	$ T^0, b^1, s_{\text{HB}}^1\rangle$	6372.1	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
4800.9	2.8	$ T^0, b^1, s_{\text{HB}}^1\rangle$	6382.6	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
4930.8	0.1	$ T^0, b^3, s^0\rangle$	6401.8	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
4933.8	0.0	$ T^0, b^3, s^0\rangle$	6407.0	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
4947.3	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6656.1	0.2	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
4958.1	0.0	$ T^0, b^3, s^0\rangle$	6714.4	0.4	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
4960.9	0.0	$ T^0, b^3, s^0\rangle$	6725.8	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
4987.3	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6746.8	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
5109.1	0.8	$ T^0, b^1, s_{\text{free}}^1\rangle$	6752.3	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
5127.9	0.7	$ T^0, b^1, s_{\text{free}}^1\rangle$	6763.0	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
5151.4	2.2	$ T^0, b^1, s_{\text{free}}^1\rangle$	6787.2	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
5178.1	2.5	$ T^0, b^1, s_{\text{free}}^1\rangle$	6795.8	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
5274.0	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$	6839.8	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
5292.2	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$	6876.0	2.1	$ T^0, b^0, s_{\text{free}}^2\rangle$
6164.0	2.5	$ T^0, b^0, s_{\text{HB}}^2\rangle$	6889.6	4.0	$ T^0, b^0, s_{\text{free}}^2\rangle$
			6897.9	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$

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H<sub>3</sub>O<sup>+</sup> · · · Ar<sub>2</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

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$\omega$	$I$	Label			
4837.3	2.4	$ T^0, b^1, s_{\text{HB}}^1\rangle$	6255.9	3.8	$ T^0, b^0, s_{\text{HB}}^2\rangle$
4857.0	2.0	$ T^0, b^1, s_{\text{HB}}^1\rangle$	6407.1	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
4862.6	0.1	$ T^0, b^1, s_{\text{HB}}^1\rangle$	6409.1	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
4872.1	2.2	$ T^0, b^1, s_{\text{HB}}^1\rangle$	6439.4	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
4932.0	0.1	$ T^0, b^3, s^0\rangle$	6456.5	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
4936.7	0.1	$ T^0, b^3, s^0\rangle$	6463.5	0.1	$ T^0, b^2, s_{\text{HB}}^1\rangle$
4960.0	0.0	$ T^0, b^3, s^0\rangle$	6464.9	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
4963.1	0.0	$ T^0, b^3, s^0\rangle$	6487.3	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
4982.7	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6490.1	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5002.4	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6493.5	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5006.6	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6496.6	0.2	$ T^0, b^0, s_{\text{HB}}^2\rangle$
5016.2	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6676.6	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5016.6	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6757.6	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
5034.1	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6771.4	0.1	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
5038.7	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6777.1	0.8	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
5046.3	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$	6785.5	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
5142.5	1.9	$ T^0, b^1, s_{\text{free}}^1\rangle$	6805.6	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
5182.5	1.5	$ T^0, b^1, s_{\text{free}}^1\rangle$	6919.5	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
5310.7	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$	6947.1	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
5352.6	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$	6949.6	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6253.7	0.7	$ T^0, b^0, s_{\text{HB}}^2\rangle$	6954.5	2.5	$ T^0, b^0, s_{\text{free}}^2\rangle$

$\omega$	$I$	Label	$\omega$	$I$	Label
4900.3	2.2	$ T^0, b^1, s^1\rangle$	6392.8	2.4	$ T^0, b^0, s^2\rangle$
4902.9	2.4	$ T^0, b^1, s^1\rangle$	6486.8	0.0	$ T^1, b^0, s^2\rangle$
4918.9	0.3	$ T^0, b^1, s^1\rangle$	6500.8	0.0	$ T^1, b^0, s^2\rangle$
4924.5	2.3	$ T^0, b^1, s^1\rangle$	6506.5	0.0	$ T^1, b^0, s^2\rangle$
4925.1	0.8	$ T^0, b^1, s^1\rangle$	6522.4	0.1	$ T^0, b^2, s^1\rangle$
4928.0	2.6	$ T^0, b^1, s^1\rangle$	6522.4	0.1	$ T^0, b^2, s^1\rangle$
4937.2	0.1	$ T^0, b^3, s^0\rangle$	6533.4	0.0	$ T^1, b^0, s^2\rangle$
4937.2	0.1	$ T^0, b^3, s^0\rangle$	6534.0	0.0	$ T^0, b^2, s^1\rangle$
4964.6	0.0	$ T^0, b^3, s^0\rangle$	6534.3	0.0	$ T^0, b^2, s^1\rangle$
5010.8	0.0	$ T^1, b^1, s^1\rangle$	6534.5	0.0	$ T^0, b^2, s^1\rangle$
5013.5	0.0	$ T^1, b^1, s^1\rangle$	6535.0	0.0	$ T^0, b^2, s^1\rangle$
5028.9	0.0	$ T^1, b^1, s^1\rangle$	6540.6	0.0	$ T^0, b^2, s^1\rangle$
5035.1	0.0	$ T^1, b^1, s^1\rangle$	6551.6	0.0	$ T^1, b^0, s^2\rangle$
5035.1	0.0	$ T^1, b^1, s^1\rangle$	6553.0	0.0	$ T^0, b^2, s^1\rangle$
5038.5	0.0	$ T^1, b^1, s^1\rangle$	6553.1	0.0	$ T^1, b^0, s^2\rangle$
5062.2	0.0	$ T^1, b^1, s^1\rangle$	6553.4	0.0	$ T^0, b^2, s^1\rangle$
5066.5	0.0	$ T^1, b^1, s^1\rangle$	6556.3	0.0	$ T^1, b^0, s^2\rangle$
5072.0	0.0	$ T^1, b^1, s^1\rangle$	6558.4	0.0	$ T^1, b^0, s^2\rangle$
5072.9	0.0	$ T^1, b^1, s^1\rangle$	6574.6	0.0	$ T^1, b^0, s^2\rangle$
5082.5	0.0	$ T^1, b^1, s^1\rangle$	6590.6	0.2	$ T^0, b^0, s^2\rangle$
5086.0	0.0	$ T^1, b^1, s^1\rangle$	6596.1	0.2	$ T^0, b^0, s^2\rangle$
5088.8	0.0	$ T^1, b^1, s^1\rangle$	6600.5	0.2	$ T^0, b^0, s^2\rangle$
5089.3	0.0	$ T^1, b^1, s^1\rangle$	6703.4	0.0	$ T^1, b^0, s^2\rangle$
5090.4	0.0	$ T^1, b^1, s^1\rangle$	6708.3	0.0	$ T^1, b^0, s^2\rangle$
5091.6	0.0	$ T^1, b^1, s^1\rangle$	6713.3	0.0	$ T^1, b^0, s^2\rangle$
5093.7	0.0	$ T^1, b^1, s^1\rangle$	6757.5	0.0	$ T^1, b^0, s^2\rangle$
5099.0	0.0	$ T^1, b^1, s^1\rangle$	6761.1	0.0	$ T^1, b^0, s^2\rangle$
6373.2	1.1	$ T^0, b^0, s^2\rangle$	6762.6	0.0	$ T^1, b^0, s^2\rangle$
6387.0	1.7	$ T^0, b^0, s^2\rangle$	6763.7	0.0	$ T^1, b^0, s^2\rangle$
			6766.5	0.0	$ T^1, b^0, s^2\rangle$

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H<sub>3</sub>O<sup>+</sup> ··· (N<sub>2</sub>)<sub>1</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

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$\omega$	$I$	Label
4367.1	0.7	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4378.8	4.7	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4661.8	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4676.4	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4923.8	0.0	$ T^0, b^3, s^0\rangle$
4968.9	0.0	$ T^0, b^3, s^0\rangle$
5003.2	0.0	$ T^0, b^3, s^0\rangle$
5014.5	0.0	$ T^0, b^3, s^0\rangle$
5129.2	0.5	$ T^0, b^1, s_{\text{free}}^1\rangle$
5177.7	2.3	$ T^0, b^1, s_{\text{free}}^1\rangle$
5180.0	0.6	$ T^0, b^1, s_{\text{free}}^1\rangle$
5236.1	2.4	$ T^0, b^1, s_{\text{free}}^1\rangle$
5299.5	19.2	$ T^0, b^0, s_{\text{HB}}^2\rangle$
5385.4	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5636.4	0.3	$ T^1, b^0, s_{\text{HB}}^2\rangle$

5981.5	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6001.1	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6004.6	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6267.5	0.3	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6334.9	0.3	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6561.7	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6628.4	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6738.4	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6777.5	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6795.3	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6835.9	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6841.5	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6889.0	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6926.7	2.1	$ T^0, b^0, s_{\text{free}}^2\rangle$
6942.4	4.1	$ T^0, b^0, s_{\text{free}}^2\rangle$

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H<sub>3</sub>O<sup>+</sup> ··· (N<sub>2</sub>)<sub>2</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

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$\omega$	$I$	Label
4587.0	2.7	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4588.3	3.5	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4658.0	3.6	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4671.7	0.1	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4835.3	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4838.9	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4846.2	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4846.2	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4903.9	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4917.0	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4919.9	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4929.5	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4974.7	0.0	$ T^0, b^3, s^0\rangle$
5003.7	0.0	$ T^0, b^3, s^0\rangle$
5029.9	0.0	$ T^0, b^3, s^0\rangle$
5046.7	0.0	$ T^0, b^3, s^0\rangle$
5199.9	1.5	$ T^0, b^1, s_{\text{free}}^1\rangle$
5257.0	1.6	$ T^0, b^1, s_{\text{free}}^1\rangle$
5443.4	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5451.9	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5502.7	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5507.7	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$

5641.7	3.6	$ T^0, b^0, s_{\text{HB}}^2\rangle$
5663.9	15.4	$ T^0, b^0, s_{\text{HB}}^2\rangle$
5900.2	0.1	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5910.1	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5921.4	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5932.4	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
6039.9	0.2	$ T^0, b^0, s_{\text{HB}}^2\rangle$
6219.6	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6224.6	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6225.5	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6288.8	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
6293.8	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6311.2	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6322.0	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6535.0	0.0	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6598.5	0.6	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6783.8	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6792.6	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6817.9	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6844.9	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6856.1	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6875.0	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6926.8	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$

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H<sub>3</sub>O<sup>+</sup> ··· (N<sub>2</sub>)<sub>3</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

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$\omega$	$I$	Label	$\omega$	$I$	Label
4753.2	2.8	$ T^0, b^1, s^1\rangle$	6019.7	6.3	$ T^0, b^0, s^2\rangle$
4758.8	3.2	$ T^0, b^1, s^1\rangle$	6233.2	0.0	$ T^1, b^0, s^2\rangle$
4781.2	3.6	$ T^0, b^1, s^1\rangle$	6244.2	0.0	$ T^1, b^0, s^2\rangle$
4782.4	3.2	$ T^0, b^1, s^1\rangle$	6258.1	0.0	$ T^1, b^0, s^2\rangle$
4832.0	0.4	$ T^0, b^1, s^1\rangle$	6261.1	0.0	$ T^1, b^0, s^2\rangle$
4836.9	1.1	$ T^0, b^1, s^1\rangle$	6265.4	0.0	$ T^1, b^0, s^2\rangle$
4998.1	0.0	$ T^1, b^1, s^1\rangle$	6271.1	0.3	$ T^0, b^0, s^2\rangle$
5003.2	0.0	$ T^1, b^1, s^1\rangle$	6273.1	0.0	$ T^1, b^0, s^2\rangle$
5004.2	0.0	$ T^1, b^1, s^1\rangle$	6284.8	0.2	$ T^0, b^0, s^2\rangle$
5008.2	0.0	$ T^1, b^1, s^1\rangle$	6296.5	0.0	$ T^1, b^0, s^2\rangle$
5026.8	0.0	$ T^1, b^1, s^1\rangle$	6317.3	0.0	$ T^1, b^0, s^2\rangle$
5028.5	0.0	$ T^1, b^1, s^1\rangle$	6326.9	0.0	$ T^1, b^0, s^2\rangle$
5029.7	0.1	$ T^0, b^3, s^0\rangle$	6341.6	0.2	$ T^0, b^0, s^2\rangle$
5029.8	0.1	$ T^0, b^3, s^0\rangle$	6407.3	0.1	$ T^0, b^2, s^1\rangle$
5030.7	0.0	$ T^1, b^1, s^1\rangle$	6410.8	0.1	$ T^0, b^2, s^1\rangle$
5031.2	0.0	$ T^1, b^1, s^1\rangle$	6417.5	0.0	$ T^0, b^2, s^1\rangle$
5054.2	0.0	$ T^0, b^3, s^0\rangle$	6418.1	0.0	$ T^0, b^2, s^1\rangle$
5058.1	0.0	$ T^1, b^1, s^1\rangle$	6421.1	0.0	$ T^0, b^2, s^1\rangle$
5063.7	0.0	$ T^1, b^1, s^1\rangle$	6421.6	0.0	$ T^0, b^2, s^1\rangle$
5079.1	0.0	$ T^1, b^1, s^1\rangle$	6485.7	0.0	$ T^0, b^2, s^1\rangle$
5080.5	0.0	$ T^1, b^1, s^1\rangle$	6496.5	0.0	$ T^0, b^2, s^1\rangle$
5084.7	0.0	$ T^1, b^1, s^1\rangle$	6497.4	0.0	$ T^0, b^2, s^1\rangle$
5084.8	0.0	$ T^1, b^1, s^1\rangle$	6517.6	0.0	$ T^1, b^0, s^2\rangle$
5086.2	0.0	$ T^1, b^1, s^1\rangle$	6519.7	0.0	$ T^1, b^0, s^2\rangle$
5087.3	0.0	$ T^1, b^1, s^1\rangle$	6531.8	0.0	$ T^1, b^0, s^2\rangle$
5136.8	0.0	$ T^1, b^1, s^1\rangle$	6532.9	0.0	$ T^1, b^0, s^2\rangle$
5141.8	0.0	$ T^1, b^1, s^1\rangle$	6589.3	0.0	$ T^1, b^0, s^2\rangle$
5989.2	1.6	$ T^0, b^0, s^2\rangle$	6589.7	0.0	$ T^1, b^0, s^2\rangle$
6010.1	5.2	$ T^0, b^0, s^2\rangle$	6591.2	0.0	$ T^1, b^0, s^2\rangle$

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H<sub>3</sub>O<sup>+</sup> ··· (CO)<sub>1</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

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$\omega$	$I$	Label
4136.9	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4162.3	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4178.9	122.0	$ T^0, b^0, s_{\text{HB}}^2\rangle$
4595.5	2.5	$ T^1, b^0, s_{\text{HB}}^2\rangle$
4895.6	0.0	$ T^0, b^3, s^0\rangle$
4928.0	0.0	$ T^0, b^3, s^0\rangle$
4952.9	0.0	$ T^0, b^3, s^0\rangle$
4958.3	0.1	$ T^0, b^3, s^0\rangle$
5130.4	0.2	$ T^0, b^1, s_{\text{free}}^1\rangle$
5176.0	0.5	$ T^0, b^1, s_{\text{free}}^1\rangle$
5187.9	2.6	$ T^0, b^1, s_{\text{free}}^1\rangle$
5241.2	2.1	$ T^0, b^1, s_{\text{free}}^1\rangle$
5360.1	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5386.1	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5398.2	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$

5421.2	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5456.0	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5478.5	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5736.5	0.5	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
5820.3	0.2	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6087.2	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6169.4	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6621.6	2.1	$ T^0, b^0, s_{\text{free}}^2\rangle$
6731.7	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6779.7	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6779.7	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6815.8	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6835.0	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6878.3	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6951.4	2.2	$ T^0, b^0, s_{\text{free}}^2\rangle$
6972.3	3.9	$ T^0, b^0, s_{\text{free}}^2\rangle$

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H<sub>3</sub>O<sup>+</sup> ··· (CO)<sub>2</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

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$\omega$	$I$	Label
4206.8	3.5	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4210.1	2.2	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4341.5	6.0	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4354.6	0.0	$ T^0, b^1, s_{\text{HB}}^1\rangle$
4468.8	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4470.2	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4530.4	0.1	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4536.5	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4599.7	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4614.5	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4668.5	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4678.6	0.0	$ T^1, b^1, s_{\text{HB}}^1\rangle$
4847.7	15.5	$ T^0, b^0, s_{\text{HB}}^2\rangle$
4891.4	57.0	$ T^0, b^0, s_{\text{HB}}^2\rangle$
4945.1	0.0	$ T^0, b^3, s^0\rangle$
4968.8	0.0	$ T^0, b^3, s^0\rangle$
4992.5	0.0	$ T^0, b^3, s^0\rangle$
5007.8	0.0	$ T^0, b^3, s^0\rangle$
5125.5	1.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5169.1	0.3	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5184.8	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5211.2	1.3	$ T^0, b^1, s_{\text{free}}^1\rangle$

5228.9	0.2	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5263.1	1.5	$ T^0, b^1, s_{\text{free}}^1\rangle$
5445.0	0.4	$ T^0, b^0, s_{\text{HB}}^2\rangle$
5469.0	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5522.7	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5578.6	0.0	$ T^1, b^1, s_{\text{free}}^1\rangle$
5704.8	0.0	$ T^1, b^0, s_{\text{HB}}^2\rangle$
5823.7	0.1	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5827.4	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5827.7	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5962.2	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5977.7	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
5988.6	0.0	$ T^0, b^2, s_{\text{HB}}^1\rangle$
6193.0	0.0	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6316.3	0.7	$ T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6455.3	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6516.9	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6576.6	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6640.7	0.0	$ T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1\rangle$
6822.5	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6873.5	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6920.6	0.0	$ T^0, b^2, s_{\text{free}}^1\rangle$
6993.0	0.3	$ T^0, b^0, s_{\text{free}}^2\rangle$

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H<sub>3</sub>O<sup>+</sup> ··· (CO)<sub>3</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

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$\omega$	$I$	Label	$\omega$	$I$	Label
4508.7	2.7	$ T^0, b^1, s^1\rangle$	5515.0	15.5	$ T^0, b^0, s^2\rangle$
4514.7	3.0	$ T^0, b^1, s^1\rangle$	5769.9	0.2	$ T^1, b^0, s^2\rangle$
4536.7	3.4	$ T^0, b^1, s^1\rangle$	5770.5	0.1	$ T^1, b^0, s^2\rangle$
4540.0	3.1	$ T^0, b^1, s^1\rangle$	5798.5	0.1	$ T^1, b^0, s^2\rangle$
4636.9	1.2	$ T^0, b^1, s^1\rangle$	5798.8	0.1	$ T^1, b^0, s^2\rangle$
4640.0	1.8	$ T^0, b^1, s^1\rangle$	5809.1	0.1	$ T^1, b^0, s^2\rangle$
4798.3	0.1	$ T^1, b^1, s^1\rangle$	5810.3	0.1	$ T^1, b^0, s^2\rangle$
4798.3	0.0	$ T^1, b^1, s^1\rangle$	5818.8	0.0	$ T^1, b^0, s^2\rangle$
4804.2	0.1	$ T^1, b^1, s^1\rangle$	5842.0	0.6	$ T^0, b^0, s^2\rangle$
4804.6	0.0	$ T^1, b^1, s^1\rangle$	5847.1	0.0	$ T^1, b^0, s^2\rangle$
4824.7	0.0	$ T^1, b^1, s^1\rangle$	5857.9	0.0	$ T^1, b^0, s^2\rangle$
4828.0	0.0	$ T^1, b^1, s^1\rangle$	5858.5	0.5	$ T^0, b^0, s^2\rangle$
4828.3	0.0	$ T^1, b^1, s^1\rangle$	5966.4	0.2	$ T^0, b^0, s^2\rangle$
4831.1	0.0	$ T^1, b^1, s^1\rangle$	6131.8	0.0	$ T^1, b^0, s^2\rangle$
4848.1	0.0	$ T^1, b^1, s^1\rangle$	6134.2	0.0	$ T^1, b^0, s^2\rangle$
4854.1	0.0	$ T^1, b^1, s^1\rangle$	6148.5	0.0	$ T^1, b^0, s^2\rangle$
4876.1	0.0	$ T^1, b^1, s^1\rangle$	6150.5	0.0	$ T^1, b^0, s^2\rangle$
4879.3	0.0	$ T^1, b^1, s^1\rangle$	6150.8	0.1	$ T^0, b^2, s^1\rangle$
4926.1	0.0	$ T^1, b^1, s^1\rangle$	6155.7	0.1	$ T^0, b^2, s^1\rangle$
4927.4	0.0	$ T^1, b^1, s^1\rangle$	6160.5	0.0	$ T^0, b^2, s^1\rangle$
4928.9	0.0	$ T^1, b^1, s^1\rangle$	6160.9	0.0	$ T^0, b^2, s^1\rangle$
4930.9	0.0	$ T^1, b^1, s^1\rangle$	6165.3	0.0	$ T^0, b^2, s^1\rangle$
4975.9	0.0	$ T^1, b^1, s^1\rangle$	6166.4	0.0	$ T^0, b^2, s^1\rangle$
4979.0	0.0	$ T^1, b^1, s^1\rangle$	6183.3	0.0	$ T^1, b^0, s^2\rangle$
5000.9	0.1	$ T^0, b^3, s^0\rangle$	6199.7	0.0	$ T^1, b^0, s^2\rangle$
5000.9	0.1	$ T^0, b^3, s^0\rangle$	6257.4	0.0	$ T^1, b^0, s^2\rangle$
5024.4	0.0	$ T^0, b^3, s^0\rangle$	6257.7	0.0	$ T^1, b^0, s^2\rangle$
5475.8	1.8	$ T^0, b^0, s^2\rangle$	6279.6	0.0	$ T^0, b^2, s^1\rangle$
5504.2	15.1	$ T^0, b^0, s^2\rangle$	6290.9	0.0	$ T^0, b^2, s^1\rangle$

**Table S4. Assignment, Projection and Transition Dipole Decomposition of the Pronounced Peaks**

Here we listed all of the calculated transitions in the region of  $4000 \text{ cm}^{-1}$  -  $7000 \text{ cm}^{-1}$  whose IR intensity is larger than  $0.05 \text{ km/mol}$ . The *transition energy* ( $\omega$ , in  $\text{cm}^{-1}$ ), the *IR intensity* ( $I$ , in  $\text{km/mol}$ ), and the *components of the transition dipole* ( $\mu_x$ ,  $\mu_y$  and  $\mu_z$ ) are listed in the following tables. In order to make reasonable assignments for these transitions, for each eigenstate  $\psi_a$ , we also listed a few of large components whose contribution ( $|\langle a | T_i, b_j, s_k \rangle|^2$ , or  $|c_{ijk}|^2$ ) are more than 10%.

To analyze the actual source of the transitions, we can decompose the transition dipole moment  $\mu^{g \rightarrow f}$  between ground state  $|g\rangle$  and final state  $|f\rangle$  into contribution from its components:

$$\mu^{g \rightarrow f} = \langle g | \hat{\mu} | f \rangle = \sum_{ijk} c_{ijk} \langle g | \hat{\mu} | T_i, b_j, s_k \rangle = \sum_{ijk} \mu^{ijk}$$

in which  $\mu^{ijk}$  represents the contribution of FBR basis function  $|T_i, b_j, s_k\rangle$  to the total transition dipole moment  $\mu^{g \rightarrow f}$ . For each eigenstates, we also listed *the contribution of the FBR components to the total transition moment*, ( $\mu_x^{ijk}$ ,  $\mu_y^{ijk}$  and  $\mu_z^{ijk}$ ), in Debye); we list the first three with largest norm of its transition dipole components (though some of them have small  $|c_{ijk}|^2$ ).

In Figure 4-6, there are some discrepancies between the IR intensity of the bright states *with* and *without* mechanical anharmonicity, and a large portion of them can be explained by analyzing the following table of the transition dipole decomposition. For example, in the calculated spectrum of  $\text{H}_3\text{O}^+ \cdots \text{Ar}_2$ , the small peak located at  $6418 \text{ cm}^{-1}$  is assigned as  $|T^1, b^0, s_{\text{HB}}^2\rangle$ , and its intensity mostly comes from  $|T^0, b^0, s_{\text{HB}}^2\rangle$ , which couples to  $|T^1, b^0, s_{\text{HB}}^2\rangle$  by the CB interaction similar to the MIR region. However, although the fundamental OH-stretching  $|T^0, b^0, s_{\text{HB}}^1\rangle$  is  $\approx 3000 \text{ cm}^{-1}$  lower, it still has large contribution to the total transition dipole moment; its  $\mu^{ijk}$  is in opposite direction to the contribution from  $|T^0, b^0, s_{\text{HB}}^2\rangle$ , leading to a *destructive interference*. The interference in the transition dipole moment makes the intuitive prediction very difficult, which again highlights the importance of high-quality anharmonic vibrational analysis.











						$\langle 200 T^0, b^0, s_{\text{free}}^2 \rangle$	0.34%	-0.000	0.001	-0.000
6965.0	1.2	0.004	-0.007	-0.000		$\langle 208 T^0, b^0, s_{\text{free}}^2 \rangle$	41.20%	0.005	-0.008	0.000
						$\langle 208 T^1, b^2, s_{\text{free}}^1 \rangle$	22.61%	0.000	0.001	0.000
						$\langle 208 T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	12.49%	-0.000	0.000	0.000
						$\langle 208 T^1, b^2, s_{\text{free}}^1 \rangle$	10.54%	0.000	-0.001	0.000
						$\langle 208 T^0, b^2, s_{\text{free}}^1 \rangle$	2.70%	-0.001	0.001	-0.000
						$\langle 208 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	1.32%	0.001	-0.001	-0.000
6970.0	0.1	0.001	-0.002	-0.000		$\langle 210 T^2, b^4, s^0 \rangle$	35.69%	0.000	0.000	0.000
						$\langle 210 T^2, b^2, s_{\text{HB}}^1 \rangle$	15.80%	0.000	0.000	0.000
						$\langle 210 T^2, b^4, s^0 \rangle$	11.86%	0.000	0.000	0.000
						$\langle 210 T^0, b^0, s_{\text{free}}^2 \rangle$	3.29%	0.001	-0.002	0.000
						$\langle 210 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	-0.000	0.000	-0.000
						$\langle 210 T^1, b^2, s_{\text{free}}^1 \rangle$	1.05%	-0.000	0.000	-0.000
6972.9	1.1	-0.004	0.007	0.000		$\langle 211 T^0, b^0, s_{\text{free}}^2 \rangle$	39.00%	-0.004	0.008	-0.000
						$\langle 211 T^1, b^2, s_{\text{free}}^1 \rangle$	12.96%	0.000	0.000	0.000
						$\langle 211 T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	10.63%	-0.000	0.000	0.000
						$\langle 211 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	0.000	-0.001	0.000
						$\langle 211 T^1, b^2, s_{\text{free}}^1 \rangle$	6.83%	0.000	-0.001	0.000

$\omega$	$I$	$\mu_x$	$\mu_y$	$\mu_z$	Assignment	$ c_{ijk}^2 $	$\mu_x^{ijk}$	$\mu_y^{ijk}$	$\mu_z^{ijk}$
4813.6	0.7	-0.006	-0.004	0.000	$\langle 90 T^0, b^1, s^1 \rangle$	32.26%	-0.008	-0.002	0.000
					$\langle 90 T^0, b^3, s^0 \rangle$	15.02%	0.002	0.000	0.000
					$\langle 90 T^0, b^1, s^1 \rangle$	12.79%	0.004	-0.001	-0.000
					$\langle 90 T^0, b^3, s^0 \rangle$	11.52%	0.000	0.000	0.000
					$\langle 90 T^0, b^1, s^1 \rangle$	11.13%	-0.001	0.003	0.000
					$\langle 90 T^0, b^0, s^1 \rangle$	0.01%	-0.001	-0.003	0.000
4815.8	1.4	-0.004	0.010	-0.000	$\langle 91 T^0, b^3, s^0 \rangle$	32.88%	0.000	-0.003	0.000
					$\langle 91 T^0, b^1, s^1 \rangle$	20.42%	0.001	-0.004	-0.000
					$\langle 91 T^0, b^1, s^1 \rangle$	12.97%	-0.000	0.005	0.000
					$\langle 91 T^0, b^0, s^1 \rangle$	0.01%	0.001	0.005	-0.000
					$\langle 91 T^0, b^1, s^1 \rangle$	9.30%	-0.001	0.004	-0.000
4818.4	0.7	0.007	0.002	-0.000	$\langle 92 T^0, b^1, s^1 \rangle$	45.90%	0.009	0.002	0.000
					$\langle 92 T^0, b^3, s^0 \rangle$	20.25%	-0.002	-0.000	-0.000
					$\langle 92 T^0, b^3, s^0 \rangle$	11.72%	0.000	0.000	0.000
					$\langle 92 T^0, b^0, s^1 \rangle$	0.01%	0.004	-0.001	0.000
					$\langle 92 T^0, b^1, s^1 \rangle$	8.13%	-0.003	0.001	0.000
4904.3	4.4	0.016	-0.010	-0.000	$\langle 94 T^0, b^1, s^1 \rangle$	28.46%	0.006	-0.001	-0.000
					$\langle 94 T^0, b^1, s^1 \rangle$	15.21%	0.001	-0.006	0.000
					$\langle 94 T^0, b^1, s^1 \rangle$	14.43%	0.005	0.001	0.000
					$\langle 94 T^0, b^1, s^1 \rangle$	10.92%	0.004	0.001	-0.000
					$\langle 94 T^0, b^1, s^1 \rangle$	10.02%	0.001	-0.002	-0.000
4911.4	4.6	0.010	0.017	0.000	$\langle 95 T^0, b^1, s^1 \rangle$	21.93%	-0.001	0.007	-0.000
					$\langle 95 T^0, b^1, s^1 \rangle$	19.41%	-0.000	0.006	0.000
					$\langle 95 T^0, b^1, s^1 \rangle$	16.72%	0.006	0.002	-0.000
					$\langle 95 T^0, b^1, s^1 \rangle$	10.94%	0.004	0.001	0.000
4923.8	0.1	-0.002	-0.002	-0.000	$\langle 96 T^1, b^1, s^1 \rangle$	23.22%	0.001	0.000	0.000
					$\langle 96 T^1, b^3, s^0 \rangle$	16.95%	0.000	0.000	0.000
					$\langle 96 T^1, b^1, s^1 \rangle$	12.68%	-0.001	0.000	-0.000
					$\langle 96 T^1, b^1, s^1 \rangle$	12.14%	0.000	-0.001	-0.000
					$\langle 96 T^0, b^1, s^1 \rangle$	2.04%	-0.002	-0.001	0.000
					$\langle 96 T^0, b^0, s^1 \rangle$	0.00%	-0.000	-0.001	0.000
4925.6	0.1	-0.001	0.002	0.000	$\langle 97 T^1, b^3, s^0 \rangle$	29.79%	0.000	0.000	0.000
					$\langle 97 T^1, b^1, s^1 \rangle$	15.83%	-0.000	0.001	0.000
					$\langle 97 T^1, b^1, s^1 \rangle$	10.32%	-0.000	-0.001	0.000
					$\langle 97 T^0, b^1, s^1 \rangle$	1.26%	-0.000	0.002	0.000
					$\langle 97 T^0, b^1, s^1 \rangle$	1.00%	-0.000	0.001	-0.000
					$\langle 97 T^0, b^0, s^1 \rangle$	0.00%	0.000	0.001	-0.000
4950.1	0.1	0.001	0.003	0.000	$\langle 99 T^0, b^3, s^0 \rangle$	38.51%	-0.000	0.003	-0.000
					$\langle 99 T^0, b^1, s^1 \rangle$	25.65%	0.001	-0.004	-0.000
					$\langle 99 T^0, b^0, s^1 \rangle$	0.01%	0.001	0.003	-0.000

4951.6	0.2	-0.004	0.001	0.000		$\langle 100 T^0, b^3, s^0 \rangle$	38.88%	-0.003	-0.000	-0.000	
						$\langle 100 T^0, b^1, s^1 \rangle$	22.52%	0.005	-0.001	-0.000	
						$\langle 100 T^0, b^0, s^1 \rangle$	0.01%	-0.003	0.001	-0.000	
4994.3	0.1	-0.002	-0.002	0.000		$\langle 107 T^1, b^3, s^0 \rangle$	24.83%	0.000	0.000	0.000	
						$\langle 107 T^1, b^1, s^1 \rangle$	15.97%	0.000	0.000	0.000	
						$\langle 107 T^0, b^1, s^1 \rangle$	4.78%	-0.003	-0.001	0.000	
						$\langle 107 T^0, b^1, s^1 \rangle$	2.76%	0.000	-0.002	-0.000	
						$\langle 107 T^0, b^1, s^1 \rangle$	2.16%	0.002	-0.000	-0.000	
4996.9	0.3	0.000	-0.005	0.000		$\langle 108 T^1, b^1, s^1 \rangle$	18.85%	0.000	0.000	0.000	
						$\langle 108 T^1, b^3, s^0 \rangle$	14.22%	0.000	0.000	0.000	
						$\langle 108 T^0, b^0, s^1 \rangle$	0.00%	-0.001	-0.003	0.000	
						$\langle 108 T^0, b^1, s^1 \rangle$	3.09%	0.000	-0.002	-0.000	
						$\langle 108 T^0, b^1, s^1 \rangle$	6.94%	-0.001	0.002	0.000	
4999.8	0.4	0.005	-0.001	0.000		$\langle 109 T^1, b^1, s^1 \rangle$	26.35%	0.000	0.000	0.000	
						$\langle 109 T^1, b^3, s^0 \rangle$	16.30%	0.000	0.000	0.000	
						$\langle 109 T^1, b^3, s^0 \rangle$	14.53%	0.000	0.000	0.000	
						$\langle 109 T^0, b^1, s^1 \rangle$	5.46%	-0.003	0.000	0.000	
						$\langle 109 T^0, b^0, s^1 \rangle$	0.00%	0.003	-0.001	0.000	
						$\langle 109 T^0, b^1, s^1 \rangle$	3.74%	0.002	0.000	0.000	
5021.8	0.2	-0.003	0.002	-0.000		$\langle 112 T^1, b^3, s^0 \rangle$	22.61%	0.000	0.000	0.000	
						$\langle 112 T^1, b^1, s^1 \rangle$	14.14%	0.000	0.000	0.000	
						$\langle 112 T^0, b^1, s^1 \rangle$	0.92%	-0.001	-0.000	0.000	
						$\langle 112 T^0, b^1, s^1 \rangle$	0.78%	-0.000	0.001	-0.000	
						$\langle 112 T^0, b^1, s^1 \rangle$	1.26%	-0.001	0.000	0.000	
5025.9	0.1	0.002	0.003	-0.000		$\langle 113 T^1, b^1, s^1 \rangle$	14.85%	0.000	-0.001	-0.000	
						$\langle 113 T^1, b^1, s^1 \rangle$	13.06%	-0.000	-0.001	0.000	
						$\langle 113 T^1, b^1, s^1 \rangle$	11.78%	-0.001	-0.000	-0.000	
						$\langle 113 T^0, b^1, s^1 \rangle$	1.11%	-0.000	0.002	-0.000	
						$\langle 113 T^0, b^1, s^1 \rangle$	1.26%	-0.000	0.002	0.000	
						$\langle 113 T^0, b^1, s^1 \rangle$	1.07%	0.001	0.000	-0.000	
5119.1	0.1	0.000	0.002	-0.000		$\langle 132 T^1, b^3, s^0 \rangle$	26.63%	0.000	0.000	0.000	
						$\langle 132 T^1, b^1, s^1 \rangle$	20.22%	0.000	-0.000	-0.000	
						$\langle 132 T^1, b^3, s^0 \rangle$	13.28%	0.000	0.000	0.000	
						$\langle 132 T^1, b^1, s^1 \rangle$	10.60%	-0.000	0.000	0.000	
						$\langle 132 T^0, b^1, s^1 \rangle$	0.57%	-0.000	0.001	0.000	
						$\langle 132 T^0, b^1, s^1 \rangle$	0.18%	-0.000	0.001	-0.000	
5124.9	0.1	0.002	0.000	0.000		$\langle 136 T^1, b^3, s^0 \rangle$	21.85%	0.000	0.000	0.000	
						$\langle 136 T^1, b^3, s^0 \rangle$	17.05%	0.000	0.000	0.000	
						$\langle 136 T^1, b^1, s^1 \rangle$	13.34%	0.000	0.000	0.000	
						$\langle 136 T^1, b^1, s^1 \rangle$	12.32%	0.000	0.000	0.000	
						$\langle 136 T^0, b^1, s^1 \rangle$	0.47%	0.001	0.000	0.000	
						$\langle 136 T^0, b^1, s^1 \rangle$	0.23%	0.001	0.000	-0.000	
						$\langle 136 T^0, b^1, s^1 \rangle$	0.08%	-0.000	0.000	0.000	
6306.1	1.0	-0.007	0.004	-0.000		$\langle 190 T^0, b^0, s^2 \rangle$	64.60%	-0.007	0.004	-0.000	



6533.6	0.1	-0.002	-0.000	-0.000	$\langle 214 T^1, b^2, s^1 \rangle$	12.91%	0.000	0.000	0.000
					$\langle 214 T^1, b^2, s^1 \rangle$	11.41%	0.000	0.000	0.000
					$\langle 214 T^1, b^4, s^0 \rangle$	11.09%	0.000	0.000	0.000
					$\langle 214 T^0, b^0, s^1 \rangle$	0.00%	0.003	-0.001	0.000
					$\langle 214 T^0, b^0, s^2 \rangle$	2.85%	-0.002	0.000	0.000
					$\langle 214 T^0, b^2, s^1 \rangle$	1.27%	-0.001	0.000	-0.000
6537.8	0.1	0.000	0.003	0.000	$\langle 215 T^1, b^2, s^1 \rangle$	13.61%	0.000	0.001	0.000
					$\langle 215 T^1, b^0, s^2 \rangle$	10.79%	-0.000	0.001	-0.000
					$\langle 215 T^0, b^0, s^1 \rangle$	0.01%	-0.001	-0.005	0.000
					$\langle 215 T^0, b^0, s^2 \rangle$	9.06%	0.001	0.004	0.000
					$\langle 215 T^0, b^2, s^1 \rangle$	2.05%	0.000	0.002	-0.000
6562.4	0.1	-0.002	-0.001	0.000	$\langle 218 T^0, b^0, s^2 \rangle$	19.62%	-0.002	-0.003	0.000
					$\langle 218 T^2, b^0, s^2 \rangle$	12.63%	0.000	0.000	0.000
					$\langle 218 T^0, b^4, s^0 \rangle$	12.50%	0.000	0.000	0.000
					$\langle 218 T^0, b^0, s^1 \rangle$	0.00%	0.003	-0.001	0.000
					$\langle 218 T^0, b^0, s^1 \rangle$	0.00%	0.001	0.003	-0.000
6567.3	0.1	-0.001	0.002	0.000	$\langle 220 T^0, b^4, s^0 \rangle$	14.57%	0.000	0.000	0.000
					$\langle 220 T^0, b^0, s^2 \rangle$	12.97%	0.001	0.003	-0.000
					$\langle 220 T^0, b^0, s^1 \rangle$	0.01%	-0.001	-0.003	0.000
					$\langle 220 T^0, b^0, s^2 \rangle$	9.21%	-0.002	0.001	-0.000
6619.1	0.1	0.002	-0.001	-0.000	$\langle 235 T^0, b^4, s^0 \rangle$	13.90%	0.000	0.000	0.000
					$\langle 235 T^0, b^2, s^1 \rangle$	10.50%	0.000	0.000	0.000
					$\langle 235 T^0, b^2, s^1 \rangle$	3.19%	-0.002	0.000	-0.000
					$\langle 235 T^0, b^0, s^1 \rangle$	0.00%	0.002	-0.000	0.000
					$\langle 235 T^0, b^0, s^2 \rangle$	1.10%	0.001	-0.000	-0.000
6621.8	0.1	0.000	0.003	0.000	$\langle 236 T^0, b^4, s^0 \rangle$	15.69%	0.000	0.000	0.000
					$\langle 236 T^0, b^2, s^1 \rangle$	10.80%	0.000	0.000	0.000
					$\langle 236 T^0, b^0, s^2 \rangle$	2.32%	0.001	0.002	0.000
					$\langle 236 T^0, b^2, s^1 \rangle$	2.80%	-0.000	-0.002	0.000
					$\langle 236 T^0, b^0, s^1 \rangle$	0.00%	0.000	0.002	-0.000
6622.3	0.1	-0.002	-0.001	0.000	$\langle 237 T^2, b^0, s^2 \rangle$	19.48%	0.000	0.000	0.000
					$\langle 237 T^0, b^0, s^2 \rangle$	0.71%	-0.000	-0.001	-0.000
					$\langle 237 T^0, b^2, s^1 \rangle$	0.89%	0.000	0.001	-0.000
					$\langle 237 T^0, b^0, s^1 \rangle$	0.00%	-0.000	-0.001	0.000

H<sub>3</sub>O<sup>+</sup> ··· (N<sub>2</sub>)<sub>1</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

$\omega$	$I$	$\mu_x$	$\mu_y$	$\mu_z$	Assignment	$ c_{ijk}^2 $	$\mu_x^{ijk}$	$\mu_y^{ijk}$	$\mu_z^{ijk}$
4259.1	2.1	-0.000	0.000	0.014	$\langle 27 T^0, b^1, s_{\text{HB}}^1 \rangle$	74.39%	0.000	-0.000	0.006
					$\langle 27 T^1, b^1, s_{\text{HB}}^1 \rangle$	20.34%	-0.000	0.000	0.001
					$\langle 27 T^0, b^0, s_{\text{free}}^1 \rangle$	0.05%	-0.000	0.000	0.005
					$\langle 27 T^0, b^1, s^0 \rangle$	0.01%	0.000	0.000	0.001
4268.1	0.5	0.005	-0.005	0.000	$\langle 28 T^0, b^1, s_{\text{HB}}^1 \rangle$	73.01%	0.003	0.038	-0.000
					$\langle 28 T^1, b^1, s_{\text{HB}}^1 \rangle$	19.44%	0.000	0.005	-0.000
					$\langle 28 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.55%	-0.000	-0.042	-0.000
					$\langle 28 T^1, b^0, s_{\text{HB}}^1 \rangle$	0.24%	-0.000	-0.007	0.000
4607.9	0.2	-0.000	-0.000	0.005	$\langle 29 T^1, b^1, s_{\text{HB}}^1 \rangle$	54.50%	0.000	-0.000	-0.002
					$\langle 29 T^0, b^1, s_{\text{HB}}^1 \rangle$	22.87%	0.000	-0.000	0.003
					$\langle 29 T^2, b^1, s_{\text{HB}}^1 \rangle$	20.25%	-0.000	-0.000	-0.000
					$\langle 29 T^0, b^1, s^0 \rangle$	0.04%	0.000	0.000	0.003
					$\langle 29 T^0, b^0, s_{\text{free}}^1 \rangle$	0.01%	-0.000	0.000	0.002
4619.4	0.3	-0.001	-0.005	-0.000	$\langle 30 T^1, b^1, s_{\text{HB}}^1 \rangle$	53.58%	0.000	0.009	-0.000
					$\langle 30 T^0, b^1, s_{\text{HB}}^1 \rangle$	22.88%	-0.002	-0.021	0.000
					$\langle 30 T^2, b^1, s_{\text{HB}}^1 \rangle$	19.92%	0.000	0.002	-0.000
					$\langle 30 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.09%	0.000	0.017	0.000
4846.2	0.1	-0.000	-0.002	0.000	$\langle 31 T^0, b^3, s^0 \rangle$	84.75%	0.002	0.003	0.000
					$\langle 31 T^0, b^1, s^0 \rangle$	0.14%	-0.002	-0.003	-0.000
					$\langle 31 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	-0.000	-0.003	-0.000
4955.5	0.1	-0.001	-0.002	-0.000	$\langle 33 T^0, b^3, s^0 \rangle$	89.01%	-0.000	0.002	0.000
					$\langle 33 T^0, b^1, s_{\text{free}}^1 \rangle$	4.97%	-0.000	-0.003	0.000
					$\langle 33 T^0, b^1, s_{\text{HB}}^1 \rangle$	0.24%	-0.000	-0.002	0.000
4983.8	0.2	0.000	-0.000	0.004	$\langle 34 T^0, b^3, s^0 \rangle$	93.34%	-0.000	0.000	0.004
					$\langle 34 T^0, b^1, s^0 \rangle$	0.03%	-0.000	-0.000	-0.002
					$\langle 34 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	-0.000	0.000	0.001
5126.3	18.9	-0.002	-0.038	-0.000	$\langle 38 T^0, b^0, s_{\text{HB}}^2 \rangle$	62.24%	-0.002	-0.025	-0.000
					$\langle 38 T^1, b^0, s_{\text{HB}}^2 \rangle$	25.99%	-0.000	0.002	0.000
					$\langle 38 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	-0.000	-0.006	-0.000
					$\langle 38 T^1, b^0, s^0 \rangle$	0.01%	-0.000	-0.004	-0.000
5145.1	4.8	-0.004	-0.019	-0.000	$\langle 39 T^0, b^1, s_{\text{free}}^1 \rangle$	82.11%	-0.003	-0.006	0.000
					$\langle 39 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	-0.000	-0.005	-0.000
					$\langle 39 T^0, b^0, s_{\text{HB}}^2 \rangle$	1.82%	-0.000	-0.004	-0.000
5177.4	2.1	0.000	0.000	-0.013	$\langle 41 T^0, b^1, s_{\text{free}}^1 \rangle$	71.10%	-0.000	-0.000	-0.005
					$\langle 41 T^0, b^1, s_{\text{free}}^2 \rangle$	11.06%	-0.000	-0.000	0.003
					$\langle 41 T^0, b^3, s^0 \rangle$	10.31%	-0.000	0.000	-0.001
					$\langle 41 T^0, b^0, s_{\text{free}}^1 \rangle$	0.13%	0.000	-0.000	-0.008
5186.3	2.4	-0.000	0.000	-0.014	$\langle 42 T^0, b^1, s_{\text{free}}^1 \rangle$	80.01%	0.000	0.000	-0.008
					$\langle 42 T^0, b^1, s_{\text{free}}^2 \rangle$	15.87%	-0.000	-0.000	-0.002
					$\langle 42 T^0, b^0, s_{\text{free}}^1 \rangle$	0.04%	0.000	-0.000	-0.005

5243.2	4.2	-0.002	-0.018	0.000	$\langle 45 T^0, b^1, s_{\text{free}}^1 \rangle$	88.86%	-0.001	-0.012	0.000
					$\langle 45 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	-0.000	-0.005	-0.000
					$\langle 45 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.13%	-0.000	-0.001	-0.000
5569.9	1.6	-0.001	-0.011	0.000	$\langle 54 T^1, b^0, s_{\text{HB}}^2 \rangle$	39.55%	0.000	-0.003	-0.000
					$\langle 54 T^0, b^0, s_{\text{HB}}^2 \rangle$	30.86%	-0.001	-0.018	-0.000
					$\langle 54 T^2, b^0, s_{\text{HB}}^2 \rangle$	26.18%	-0.000	-0.004	-0.000
					$\langle 54 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.05%	0.000	0.012	0.000
5843.5	0.3	-0.000	-0.004	0.000	$\langle 59 T^0, b^2, s_{\text{HB}}^1 \rangle$	51.19%	0.000	0.006	-0.000
					$\langle 59 T^0, b^2, s_{\text{HB}}^1 \rangle$	19.35%	0.000	0.006	-0.000
					$\langle 59 T^1, b^2, s_{\text{HB}}^1 \rangle$	15.33%	0.000	0.000	0.000
					$\langle 59 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.07%	-0.000	-0.015	-0.000
5866.0	0.1	-0.000	0.002	0.000	$\langle 61 T^0, b^2, s_{\text{HB}}^1 \rangle$	48.72%	0.000	0.009	-0.000
					$\langle 61 T^0, b^2, s_{\text{HB}}^1 \rangle$	20.40%	-0.000	-0.004	0.000
					$\langle 61 T^1, b^2, s_{\text{HB}}^1 \rangle$	13.53%	-0.000	0.002	-0.000
					$\langle 61 T^0, b^1, s_{\text{HB}}^1 \rangle$	0.71%	-0.000	-0.004	0.000
6199.2	0.2	0.002	0.003	-0.000	$\langle 63 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	39.42%	0.002	-0.003	0.000
					$\langle 63 T^1, b^2, s_{\text{HB}}^1 \rangle$	17.43%	0.000	0.000	0.000
					$\langle 63 T^1, b^2, s_{\text{HB}}^1 \rangle$	12.82%	-0.000	0.002	-0.000
					$\langle 63 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.02%	0.000	0.008	0.000
					$\langle 63 T^0, b^2, s_{\text{HB}}^1 \rangle$	7.33%	-0.000	-0.002	0.000
6201.1	0.1	-0.002	-0.001	-0.000	$\langle 64 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	37.52%	-0.002	0.003	-0.000
					$\langle 64 T^1, b^2, s_{\text{HB}}^1 \rangle$	18.96%	0.000	0.000	0.000
					$\langle 64 T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	11.68%	-0.000	0.001	0.000
					$\langle 64 T^0, b^2, s_{\text{HB}}^1 \rangle$	10.13%	-0.000	-0.003	0.000
					$\langle 64 T^0, b^2, s_{\text{HB}}^1 \rangle$	4.93%	-0.000	-0.003	0.000
6258.9	0.2	-0.000	-0.000	-0.003	$\langle 67 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	76.13%	0.000	0.000	-0.004
					$\langle 67 T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	17.53%	0.000	0.000	0.000
					$\langle 67 T^0, b^1, s^0 \rangle$	0.00%	0.000	0.000	0.001
					$\langle 67 T^1, b^0, s_{\text{free}}^1 \rangle$	0.01%	0.000	-0.000	-0.000
6683.0	0.1	0.000	0.000	-0.003	$\langle 78 T^0, b^1, s_{\text{HB}}^2 \rangle$	61.57%	-0.000	-0.000	0.000
					$\langle 78 T^1, b^1, s_{\text{HB}}^2 \rangle$	26.35%	-0.000	-0.000	0.001
					$\langle 78 T^0, b^1, s^0 \rangle$	0.03%	-0.000	-0.000	-0.002
					$\langle 78 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	0.000	-0.000	-0.001
6749.2	0.2	0.001	0.003	-0.000	$\langle 81 T^0, b^1, s_{\text{HB}}^2 \rangle$	33.04%	0.001	-0.001	-0.000
					$\langle 81 T^0, b^2, s_{\text{free}}^1 \rangle$	29.88%	0.001	0.003	0.000
					$\langle 81 T^1, b^1, s_{\text{HB}}^2 \rangle$	13.82%	0.000	-0.002	0.000
					$\langle 81 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	0.000	0.004	0.000
					$\langle 81 T^0, b^0, s_{\text{free}}^1 \rangle$	0.03%	-0.001	-0.002	-0.000
6755.5	0.1	-0.000	-0.000	-0.003	$\langle 82 T^0, b^2, s_{\text{free}}^1 \rangle$	57.71%	0.000	0.000	-0.004
					$\langle 82 T^1, b^4, s^0 \rangle$	25.77%	0.000	0.000	0.000
					$\langle 82 T^0, b^0, s_{\text{free}}^1 \rangle$	0.05%	-0.000	0.000	0.005
					$\langle 82 T^0, b^0, s_{\text{free}}^2 \rangle$	4.32%	-0.000	-0.000	-0.004
6794.1	0.1	-0.000	0.000	-0.002	$\langle 84 T^0, b^2, s_{\text{free}}^1 \rangle$	78.04%	0.000	0.000	-0.001
					$\langle 84 T^0, b^0, s_{\text{free}}^2 \rangle$	3.38%	-0.000	-0.000	-0.003

					$\langle 84 T^0, b^2, s_{\text{free}}^1 \rangle$	3.86%	-0.000	-0.000	0.001
					$\langle 84 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	-0.000	0.000	0.001
6949.8	1.9	0.004	0.010	-0.000	$\langle 92 T^0, b^0, s_{\text{free}}^2 \rangle$	88.48%	0.005	0.012	0.000
					$\langle 92 T^0, b^2, s_{\text{free}}^1 \rangle$	5.19%	-0.000	-0.001	-0.000
					$\langle 92 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	-0.001	-0.001	-0.000
6964.1	3.6	-0.000	-0.000	-0.014	$\langle 93 T^0, b^0, s_{\text{free}}^2 \rangle$	89.13%	-0.000	-0.000	-0.016
					$\langle 93 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	-0.000	0.000	0.001
					$\langle 93 T^0, b^2, s_{\text{free}}^1 \rangle$	3.63%	-0.000	-0.000	0.001

H<sub>3</sub>O<sup>+</sup> ··· (N<sub>2</sub>)<sub>2</sub>, CCSD/aTZ 2MR // MP2/aDZ 4MR

$\omega$	$I$	$\mu_x$	$\mu_y$	$\mu_z$	Assignment	$ c_{ijk}^2 $	$\mu_x^{ijk}$	$\mu_y^{ijk}$	$\mu_z^{ijk}$
4523.1	1.1	-0.000	0.000	0.010	$\langle 54 T^0, b^1, s_{\text{HB}}^1 \rangle$	80.63%	-0.000	-0.000	0.030
					$\langle 54 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.05%	0.000	0.000	-0.014
					$\langle 54 T^0, b^1, s_{\text{HB}}^1 \rangle$	5.04%	0.000	-0.000	-0.005
4526.3	2.1	-0.008	0.011	-0.000	$\langle 55 T^0, b^1, s_{\text{HB}}^1 \rangle$	83.15%	-0.004	0.015	-0.000
					$\langle 55 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.05%	-0.000	-0.007	-0.000
					$\langle 55 T^0, b^0, s_{\text{free}}^1 \rangle$	0.06%	-0.002	0.004	-0.000
4598.0	0.2	-0.000	0.000	0.004	$\langle 56 T^0, b^1, s_{\text{HB}}^1 \rangle$	73.57%	-0.000	0.000	0.020
					$\langle 56 T^1, b^1, s_{\text{HB}}^1 \rangle$	15.20%	0.000	-0.000	0.001
					$\langle 56 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.12%	0.000	0.000	-0.022
					$\langle 56 T^0, b^1, s_{\text{HB}}^1 \rangle$	5.05%	-0.000	-0.000	0.008
4601.8	1.0	0.001	-0.009	0.000	$\langle 57 T^0, b^1, s_{\text{HB}}^1 \rangle$	72.42%	0.000	0.006	0.000
					$\langle 57 T^1, b^1, s_{\text{HB}}^1 \rangle$	15.74%	0.000	0.000	-0.000
					$\langle 57 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.22%	-0.000	-0.015	-0.000
					$\langle 57 T^0, b^1, s_{\text{HB}}^1 \rangle$	3.61%	-0.001	0.003	-0.000
4777.9	0.1	-0.000	0.000	-0.003	$\langle 58 T^1, b^1, s_{\text{HB}}^1 \rangle$	49.91%	-0.000	-0.000	0.006
					$\langle 58 T^1, b^1, s_{\text{HB}}^1 \rangle$	13.81%	0.000	-0.000	0.001
					$\langle 58 T^1, b^1, s_{\text{HB}}^1 \rangle$	12.52%	0.000	0.000	-0.001
					$\langle 58 T^0, b^1, s_{\text{HB}}^1 \rangle$	1.31%	0.000	0.000	-0.004
					$\langle 58 T^0, b^1, s_{\text{HB}}^1 \rangle$	2.01%	0.000	-0.000	-0.003
4798.5	0.2	0.001	-0.004	0.000	$\langle 61 T^1, b^1, s_{\text{HB}}^1 \rangle$	46.31%	-0.000	-0.000	0.000
					$\langle 61 T^1, b^1, s_{\text{HB}}^1 \rangle$	27.76%	-0.000	0.001	-0.000
					$\langle 61 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	-0.000	-0.004	-0.000
					$\langle 61 T^0, b^1, s_{\text{HB}}^1 \rangle$	9.48%	0.000	0.002	0.000
					$\langle 61 T^0, b^1, s^0 \rangle$	0.04%	0.001	-0.002	-0.000
4853.0	0.1	0.001	-0.003	-0.000	$\langle 62 T^1, b^1, s_{\text{HB}}^1 \rangle$	51.41%	-0.000	0.001	-0.000
					$\langle 62 T^1, b^1, s_{\text{HB}}^1 \rangle$	15.81%	-0.000	-0.001	0.000
					$\langle 62 T^2, b^1, s_{\text{HB}}^1 \rangle$	12.68%	0.000	0.000	0.000
					$\langle 62 T^0, b^1, s_{\text{HB}}^1 \rangle$	5.86%	0.001	-0.004	0.000
					$\langle 62 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	0.000	0.001	0.000
4857.1	0.1	-0.000	0.000	-0.003	$\langle 63 T^1, b^1, s_{\text{HB}}^1 \rangle$	44.00%	-0.000	-0.000	0.001
					$\langle 63 T^1, b^1, s_{\text{HB}}^1 \rangle$	29.08%	-0.000	0.000	-0.001
					$\langle 63 T^2, b^1, s_{\text{HB}}^1 \rangle$	10.56%	-0.000	0.000	0.001
					$\langle 63 T^0, b^1, s_{\text{HB}}^1 \rangle$	4.50%	0.000	0.000	-0.007
					$\langle 63 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	-0.000	-0.000	0.002
4880.3	0.3	0.000	-0.000	0.005	$\langle 64 T^1, b^1, s_{\text{HB}}^1 \rangle$	42.33%	-0.000	0.000	-0.002
					$\langle 64 T^1, b^1, s_{\text{HB}}^1 \rangle$	15.55%	0.000	0.000	-0.001
					$\langle 64 T^0, b^1, s_{\text{HB}}^1 \rangle$	3.84%	-0.000	-0.000	0.007
					$\langle 64 T^0, b^1, s_{\text{HB}}^1 \rangle$	5.91%	-0.000	0.000	0.006
					$\langle 64 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	0.000	0.000	-0.005
4919.8	0.1	-0.000	-0.000	0.003	$\langle 66 T^0, b^3, s^0 \rangle$	88.65%	-0.000	0.000	-0.004



						$\langle 103 T^0, b^1, s_{\text{free}}^1 \rangle$	0.63%	-0.000	0.001	-0.000
5513.8	14.9	0.000	-0.000	-0.033		$\langle 105 T^0, b^0, s_{\text{HB}}^2 \rangle$	58.95%	0.000	-0.000	-0.024
						$\langle 105 T^1, b^0, s_{\text{HB}}^2 \rangle$	22.46%	-0.000	0.000	0.005
						$\langle 105 T^1, b^0, s^0 \rangle$	0.02%	0.000	0.000	-0.005
						$\langle 105 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	0.000	0.000	-0.005
5515.0	0.1	0.000	-0.002	-0.000		$\langle 106 T^2, b^3, s^0 \rangle$	89.12%	-0.000	0.000	-0.000
						$\langle 106 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.99%	0.000	-0.001	-0.000
						$\langle 106 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	-0.000	-0.000	-0.000
						$\langle 106 T^1, b^0, s_{\text{HB}}^2 \rangle$	0.19%	0.000	0.000	0.000
5522.8	0.1	0.000	-0.000	-0.002		$\langle 107 T^2, b^3, s^0 \rangle$	83.74%	0.000	0.000	0.000
						$\langle 107 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.31%	0.000	-0.000	-0.002
						$\langle 107 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	0.000	0.000	-0.000
						$\langle 107 T^1, b^0, s_{\text{HB}}^2 \rangle$	0.09%	-0.000	0.000	0.000
5524.5	0.2	0.000	-0.000	-0.004		$\langle 108 T^2, b^3, s^0 \rangle$	82.18%	0.000	0.000	0.000
						$\langle 108 T^0, b^0, s_{\text{HB}}^2 \rangle$	1.04%	0.000	-0.000	-0.003
						$\langle 108 T^1, b^0, s_{\text{HB}}^2 \rangle$	0.36%	-0.000	0.000	0.001
						$\langle 108 T^1, b^0, s^0 \rangle$	0.00%	0.000	0.000	-0.000
5759.2	0.1	-0.000	0.002	-0.000		$\langle 115 T^1, b^0, s_{\text{HB}}^2 \rangle$	47.39%	-0.000	-0.001	0.000
						$\langle 115 T^1, b^0, s_{\text{HB}}^2 \rangle$	23.09%	0.000	0.002	0.000
						$\langle 115 T^1, b^0, s^0 \rangle$	0.01%	-0.000	0.002	-0.000
						$\langle 115 T^0, b^0, s_{\text{HB}}^2 \rangle$	1.60%	-0.000	0.002	0.000
5772.7	0.9	-0.000	0.000	0.008		$\langle 117 T^1, b^0, s_{\text{HB}}^2 \rangle$	48.30%	-0.000	0.000	0.002
						$\langle 117 T^1, b^0, s_{\text{HB}}^2 \rangle$	25.01%	-0.000	0.000	0.006
						$\langle 117 T^0, b^0, s_{\text{HB}}^2 \rangle$	3.54%	-0.000	0.000	0.006
						$\langle 117 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	0.000	0.000	-0.005
5887.8	0.2	0.001	-0.004	-0.000		$\langle 118 T^0, b^0, s_{\text{HB}}^2 \rangle$	26.17%	0.001	-0.007	-0.000
						$\langle 118 T^1, b^0, s_{\text{HB}}^2 \rangle$	22.27%	-0.000	-0.001	0.000
						$\langle 118 T^1, b^0, s_{\text{HB}}^2 \rangle$	22.20%	-0.000	-0.002	-0.000
						$\langle 118 T^2, b^0, s_{\text{HB}}^2 \rangle$	13.41%	-0.000	-0.000	0.000
						$\langle 118 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.02%	0.000	0.005	0.000
5896.9	1.5	0.000	-0.000	0.010		$\langle 119 T^0, b^0, s_{\text{HB}}^2 \rangle$	28.94%	-0.000	0.000	0.017
						$\langle 119 T^1, b^0, s_{\text{HB}}^2 \rangle$	22.73%	0.000	-0.000	-0.001
						$\langle 119 T^1, b^0, s_{\text{HB}}^2 \rangle$	21.93%	-0.000	0.000	0.005
						$\langle 119 T^2, b^0, s_{\text{HB}}^2 \rangle$	12.50%	-0.000	-0.000	0.002
						$\langle 119 T^2, b^0, s_{\text{HB}}^2 \rangle$	10.77%	-0.000	-0.000	0.002
						$\langle 119 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.04%	0.000	0.000	-0.013
6001.7	0.3	-0.001	-0.004	-0.000		$\langle 120 T^0, b^0, s_{\text{HB}}^2 \rangle$	78.45%	-0.001	-0.007	0.000
						$\langle 120 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.02%	0.000	0.005	0.000
						$\langle 120 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.99%	0.000	-0.001	-0.000
6122.5	0.3	-0.000	0.000	-0.005		$\langle 123 T^0, b^2, s_{\text{HB}}^1 \rangle$	50.12%	-0.000	-0.000	0.009
						$\langle 123 T^0, b^2, s_{\text{HB}}^1 \rangle$	24.80%	-0.000	-0.000	0.005
						$\langle 123 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.08%	0.000	0.000	-0.017
6137.1	0.1	-0.001	0.002	0.000		$\langle 124 T^0, b^2, s_{\text{HB}}^1 \rangle$	64.55%	-0.000	0.000	-0.000
						$\langle 124 T^0, b^2, s_{\text{HB}}^1 \rangle$	12.11%	0.000	-0.002	-0.000
						$\langle 124 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.03%	0.000	0.005	0.000

					$\langle 124 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.51%	-0.000	0.001	0.000
6149.4	0.1	0.000	0.000	-0.003	$\langle 125 T^0, b^2, s_{\text{HB}}^1 \rangle$	53.66%	-0.000	-0.000	0.008
					$\langle 125 T^0, b^2, s_{\text{HB}}^1 \rangle$	29.26%	0.000	0.000	-0.007
					$\langle 125 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.15%	0.000	-0.000	-0.001
6557.8	0.4	-0.004	0.004	-0.000	$\langle 150 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	77.14%	-0.005	0.003	-0.000
					$\langle 150 T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	12.30%	0.000	-0.000	0.000
					$\langle 150 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	0.000	0.002	0.000
					$\langle 150 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	0.001	-0.001	0.000
6763.1	0.1	-0.001	0.001	-0.000	$\langle 167 T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	66.87%	-0.000	0.001	-0.000
					$\langle 167 T^0, b^0, s_{\text{free}}^1 \rangle$	0.02%	0.001	-0.002	0.000
					$\langle 167 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	9.37%	-0.002	0.001	-0.000
6819.9	0.1	-0.001	0.002	-0.000	$\langle 174 T^0, b^2, s_{\text{free}}^1 \rangle$	56.31%	-0.002	0.004	-0.000
					$\langle 174 T^1, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	21.47%	0.000	0.000	-0.000
					$\langle 174 T^0, b^4, s^0 \rangle$	10.52%	0.000	0.000	0.000
					$\langle 174 T^0, b^0, s_{\text{free}}^1 \rangle$	0.05%	0.002	-0.004	0.000
					$\langle 174 T^0, b^0, s_{\text{free}}^2 \rangle$	3.52%	-0.001	0.003	-0.000

$\omega$	$I$	$\mu_x$	$\mu_y$	$\mu_z$	Assignment	$ c_{ijk}^2 $	$\mu_x^{ijk}$	$\mu_y^{ijk}$	$\mu_z^{ijk}$
4716.3	4.8	-0.000	-0.020	-0.000	$\langle 91 T^0, b^1, s^1 \rangle$	40.03%	-0.001	-0.011	-0.001
					$\langle 91 T^0, b^1, s^1 \rangle$	36.54%	-0.001	-0.011	0.001
					$\langle 91 T^0, b^1, s^1 \rangle$	10.67%	-0.001	0.003	0.000
4719.9	4.5	0.020	-0.000	-0.000	$\langle 92 T^0, b^1, s^1 \rangle$	44.24%	0.012	-0.001	-0.000
					$\langle 92 T^0, b^1, s^1 \rangle$	33.58%	0.009	-0.001	0.000
					$\langle 92 T^0, b^1, s^1 \rangle$	8.31%	-0.004	-0.000	-0.000
4746.6	0.1	-0.000	0.000	0.003	$\langle 93 T^0, b^1, s^1 \rangle$	45.75%	0.001	0.013	-0.001
					$\langle 93 T^0, b^1, s^1 \rangle$	40.16%	-0.001	-0.011	-0.001
					$\langle 93 T^0, b^0, s^1 \rangle$	0.11%	-0.000	0.002	0.004
4792.9	0.2	-0.000	-0.004	0.000	$\langle 94 T^0, b^1, s^1 \rangle$	71.68%	0.001	-0.009	-0.000
					$\langle 94 T^0, b^0, s^1 \rangle$	0.05%	0.000	0.012	-0.000
					$\langle 94 T^0, b^1, s^1 \rangle$	7.52%	-0.001	-0.005	-0.000
4799.3	0.5	-0.007	0.000	-0.000	$\langle 95 T^0, b^1, s^1 \rangle$	74.70%	-0.013	-0.001	-0.000
					$\langle 95 T^0, b^0, s^1 \rangle$	0.05%	0.012	-0.000	0.000
					$\langle 95 T^0, b^1, s^1 \rangle$	7.18%	-0.005	0.000	0.000
4936.0	0.1	0.000	-0.003	-0.000	$\langle 96 T^1, b^1, s^1 \rangle$	48.03%	0.000	0.002	0.000
					$\langle 96 T^1, b^1, s^1 \rangle$	20.19%	0.001	0.000	-0.000
					$\langle 96 T^0, b^0, s^1 \rangle$	0.01%	-0.000	-0.005	0.000
					$\langle 96 T^0, b^1, s^1 \rangle$	0.52%	-0.000	-0.001	0.000
4937.7	0.1	-0.003	-0.000	0.000	$\langle 97 T^1, b^1, s^1 \rangle$	38.02%	0.002	-0.000	0.000
					$\langle 97 T^1, b^1, s^1 \rangle$	27.92%	0.000	-0.001	0.000
					$\langle 97 T^0, b^0, s^1 \rangle$	0.01%	-0.005	0.000	-0.000
					$\langle 97 T^0, b^1, s^1 \rangle$	1.22%	-0.002	0.000	-0.000
4997.4	0.2	-0.004	-0.000	-0.000	$\langle 102 T^1, b^1, s^1 \rangle$	35.30%	-0.001	-0.001	0.000
					$\langle 102 T^1, b^1, s^1 \rangle$	21.27%	0.001	0.000	-0.000
					$\langle 102 T^0, b^1, s^1 \rangle$	1.49%	-0.002	0.000	0.000
					$\langle 102 T^0, b^1, s^1 \rangle$	0.95%	-0.001	-0.000	-0.000
					$\langle 102 T^0, b^1, s^1 \rangle$	0.54%	-0.001	0.000	-0.000
4998.5	0.1	0.002	0.000	-0.000	$\langle 103 T^1, b^1, s^1 \rangle$	38.79%	-0.001	0.000	-0.000
					$\langle 103 T^1, b^1, s^1 \rangle$	33.24%	0.001	-0.000	-0.000
					$\langle 103 T^0, b^1, s^1 \rangle$	1.17%	0.002	-0.000	0.000
4998.6	0.3	0.000	-0.005	0.000	$\langle 104 T^1, b^1, s^1 \rangle$	32.51%	-0.000	0.001	-0.000
					$\langle 104 T^1, b^1, s^1 \rangle$	30.95%	0.001	-0.001	0.000
					$\langle 104 T^0, b^1, s^1 \rangle$	1.98%	-0.000	-0.003	0.000
					$\langle 104 T^0, b^1, s^1 \rangle$	1.20%	-0.000	-0.002	-0.000
5017.2	0.3	-0.005	-0.000	-0.000	$\langle 105 T^0, b^3, s^0 \rangle$	67.81%	-0.004	-0.000	-0.000
					$\langle 105 T^0, b^1, s^1 \rangle$	9.32%	0.004	0.000	0.000
					$\langle 105 T^0, b^0, s^1 \rangle$	0.00%	-0.002	0.000	-0.000
5018.8	0.3	-0.000	0.005	0.000	$\langle 106 T^0, b^3, s^0 \rangle$	66.66%	-0.000	0.004	0.000
					$\langle 106 T^0, b^1, s^1 \rangle$	11.37%	0.001	-0.003	-0.000

						$\langle 106 T^0, b^0, s^1 \rangle$	0.00%	0.000	0.002	-0.000
5045.1	0.1	-0.003	-0.000	0.000		$\langle 111 T^1, b^1, s^1 \rangle$	45.47%	-0.000	-0.000	-0.000
						$\langle 111 T^0, b^3, s^0 \rangle$	18.77%	0.000	0.000	0.000
						$\langle 111 T^0, b^1, s^1 \rangle$	3.69%	-0.003	0.000	0.000
						$\langle 111 T^0, b^1, s^1 \rangle$	0.26%	0.001	-0.000	0.000
						$\langle 111 T^1, b^0, s^1 \rangle$	0.03%	-0.000	-0.000	0.000
5045.4	0.3	0.000	-0.004	-0.000		$\langle 112 T^1, b^1, s^1 \rangle$	33.28%	0.000	-0.000	-0.000
						$\langle 112 T^1, b^1, s^1 \rangle$	27.38%	0.000	0.000	0.000
						$\langle 112 T^0, b^1, s^1 \rangle$	2.46%	-0.000	-0.003	0.000
						$\langle 112 T^0, b^1, s^1 \rangle$	0.41%	-0.000	-0.001	-0.000
						$\langle 112 T^1, b^0, s^1 \rangle$	0.02%	0.000	-0.000	0.000
5049.7	0.1	-0.003	-0.000	0.000		$\langle 113 T^1, b^1, s^1 \rangle$	61.08%	-0.000	0.000	0.000
						$\langle 113 T^0, b^1, s^1 \rangle$	1.10%	-0.002	0.000	-0.000
						$\langle 113 T^0, b^1, s^1 \rangle$	0.87%	-0.001	-0.000	-0.000
						$\langle 113 T^0, b^1, s^1 \rangle$	0.32%	-0.001	0.000	0.000
5892.0	2.3	0.000	-0.012	0.002		$\langle 190 T^0, b^0, s^2 \rangle$	72.44%	0.000	-0.009	0.001
						$\langle 190 T^1, b^0, s^2 \rangle$	11.05%	0.001	0.002	-0.000
						$\langle 190 T^1, b^0, s^0 \rangle$	0.00%	-0.001	-0.002	0.000
5910.5	4.4	-0.000	-0.017	-0.001		$\langle 191 T^0, b^0, s^2 \rangle$	71.22%	-0.000	-0.016	-0.001
						$\langle 191 T^1, b^0, s^2 \rangle$	11.96%	-0.000	0.001	0.000
						$\langle 191 T^1, b^0, s^0 \rangle$	0.01%	-0.001	-0.003	0.000
						$\langle 191 T^1, b^0, s^2 \rangle$	6.06%	0.001	0.002	-0.000
5917.6	6.2	0.020	-0.000	-0.000		$\langle 192 T^0, b^0, s^2 \rangle$	71.02%	0.018	-0.000	-0.000
						$\langle 192 T^1, b^0, s^2 \rangle$	11.92%	-0.002	0.000	0.000
						$\langle 192 T^1, b^0, s^0 \rangle$	0.01%	0.004	-0.001	0.000
6194.2	0.2	-0.000	0.004	0.000		$\langle 196 T^1, b^0, s^2 \rangle$	27.24%	0.000	0.000	0.000
						$\langle 196 T^1, b^0, s^2 \rangle$	20.04%	0.001	0.003	-0.000
						$\langle 196 T^0, b^0, s^2 \rangle$	10.85%	-0.000	0.004	-0.000
						$\langle 196 T^0, b^0, s^1 \rangle$	0.01%	-0.000	-0.006	0.000
6209.9	0.1	0.000	0.003	-0.000		$\langle 197 T^1, b^0, s^2 \rangle$	19.90%	0.000	0.000	0.000
						$\langle 197 T^1, b^0, s^2 \rangle$	18.75%	-0.000	0.001	0.000
						$\langle 197 T^0, b^0, s^2 \rangle$	11.93%	0.000	0.007	0.000
						$\langle 197 T^0, b^0, s^1 \rangle$	0.01%	-0.000	-0.005	0.000
						$\langle 197 T^1, b^0, s^2 \rangle$	5.38%	0.000	0.002	-0.000
6210.5	0.1	-0.003	0.000	-0.000		$\langle 198 T^0, b^0, s^2 \rangle$	21.63%	0.004	-0.000	0.000
						$\langle 198 T^1, b^0, s^2 \rangle$	14.68%	-0.002	0.000	0.000
						$\langle 198 T^1, b^0, s^2 \rangle$	13.03%	-0.001	0.000	-0.000
						$\langle 198 T^0, b^0, s^2 \rangle$	12.13%	-0.008	0.000	0.000
						$\langle 198 T^0, b^0, s^1 \rangle$	0.01%	0.006	-0.000	0.000
6230.1	0.5	-0.006	0.000	-0.000		$\langle 199 T^0, b^0, s^2 \rangle$	51.99%	-0.007	0.000	-0.000
						$\langle 199 T^1, b^0, s^2 \rangle$	12.89%	-0.001	0.000	-0.000
						$\langle 199 T^0, b^0, s^1 \rangle$	0.03%	0.009	-0.000	0.000
						$\langle 199 T^0, b^0, s^2 \rangle$	3.43%	-0.004	0.000	0.000
6242.1	0.2	0.000	0.004	0.000		$\langle 201 T^0, b^0, s^2 \rangle$	55.86%	0.000	0.007	-0.000
						$\langle 201 T^1, b^0, s^2 \rangle$	16.48%	0.000	0.001	-0.000

					$\langle 201 T^0, b^0, s^1 \rangle$	0.01%	-0.000	-0.005	0.000
					$\langle 201 T^0, b^2, s^1 \rangle$	1.14%	0.000	0.002	-0.000
6253.3	0.2	0.000	0.004	-0.001	$\langle 202 T^1, b^0, s^2 \rangle$	37.31%	-0.000	-0.001	0.000
					$\langle 202 T^0, b^0, s^2 \rangle$	14.70%	0.000	0.004	-0.000
					$\langle 202 T^1, b^0, s^2 \rangle$	11.18%	-0.000	0.001	0.000
					$\langle 202 T^0, b^0, s^1 \rangle$	0.03%	-0.000	-0.009	0.000
					$\langle 202 T^0, b^0, s^2 \rangle$	8.87%	0.000	0.006	0.000
6258.1	0.1	0.003	-0.000	0.000	$\langle 203 T^1, b^0, s^2 \rangle$	54.62%	-0.001	0.000	-0.000
					$\langle 203 T^0, b^0, s^1 \rangle$	0.02%	-0.009	0.000	-0.000
					$\langle 203 T^0, b^0, s^2 \rangle$	8.59%	0.006	-0.000	-0.000
					$\langle 203 T^0, b^2, s^1 \rangle$	1.69%	0.002	-0.000	0.000
6298.2	0.2	0.000	-0.003	-0.002	$\langle 204 T^0, b^0, s^2 \rangle$	63.25%	0.000	-0.001	-0.004
					$\langle 204 T^0, b^0, s^1 \rangle$	0.01%	-0.000	-0.006	0.000
					$\langle 204 T^0, b^2, s^1 \rangle$	7.67%	0.000	0.004	-0.000
6303.2	0.4	-0.000	-0.005	0.001	$\langle 205 T^0, b^2, s^1 \rangle$	43.17%	0.000	0.009	-0.000
					$\langle 205 T^0, b^2, s^1 \rangle$	12.59%	0.000	0.000	-0.000
					$\langle 205 T^0, b^2, s^1 \rangle$	12.03%	0.000	0.000	0.000
					$\langle 205 T^0, b^0, s^2 \rangle$	10.42%	-0.000	0.000	0.002
					$\langle 205 T^0, b^0, s^1 \rangle$	0.05%	-0.000	-0.012	0.000
					$\langle 205 T^0, b^0, s^2 \rangle$	1.19%	-0.000	-0.002	-0.000
6306.3	0.5	-0.006	-0.000	0.000	$\langle 206 T^0, b^2, s^1 \rangle$	50.29%	0.010	-0.000	0.000
					$\langle 206 T^0, b^2, s^1 \rangle$	17.35%	0.000	0.000	0.000
					$\langle 206 T^0, b^0, s^1 \rangle$	0.05%	-0.013	0.000	-0.000
					$\langle 206 T^0, b^0, s^2 \rangle$	2.45%	-0.003	0.000	0.000

$\omega$	$I$	$\mu_x$	$\mu_y$	$\mu_z$	Assignment	$ c_{ijk}^2 $	$\mu_x^{ijk}$	$\mu_y^{ijk}$	$\mu_z^{ijk}$
4028.7	0.3	-0.000	0.000	-0.005	$\langle 29   T^0, b^1, s_{\text{HB}}^1 \rangle$	34.22%	0.000	0.000	-0.002
					$\langle 29   T^2, b^1, s_{\text{HB}}^1 \rangle$	27.21%	-0.000	-0.000	0.001
					$\langle 29   T^1, b^1, s_{\text{HB}}^1 \rangle$	25.99%	-0.000	-0.000	0.001
					$\langle 29   T^0, b^0, s_{\text{free}}^1 \rangle$	0.26%	0.000	0.000	-0.010
					$\langle 29   T^1, b^0, s_{\text{free}}^1 \rangle$	1.56%	0.000	0.000	0.008
4422.5	8.4	0.002	0.027	-0.000	$\langle 32   T^0, b^0, s_{\text{HB}}^2 \rangle$	31.25%	0.003	0.046	-0.000
					$\langle 32   T^2, b^0, s_{\text{HB}}^2 \rangle$	27.53%	0.000	0.003	0.000
					$\langle 32   T^1, b^0, s_{\text{HB}}^2 \rangle$	23.06%	-0.001	-0.010	0.000
					$\langle 32   T^0, b^0, s_{\text{HB}}^1 \rangle$	0.28%	-0.001	-0.038	0.000
					$\langle 32   T^0, b^1, s_{\text{HB}}^1 \rangle$	3.48%	0.001	0.022	-0.000
4679.2	0.1	-0.000	0.002	0.000	$\langle 34   T^2, b^1, s_{\text{HB}}^1 \rangle$	55.36%	-0.000	-0.017	-0.000
					$\langle 34   T^1, b^1, s_{\text{HB}}^1 \rangle$	27.20%	0.000	0.028	0.000
					$\langle 34   T^1, b^0, s_{\text{HB}}^1 \rangle$	0.95%	-0.001	-0.030	0.000
					$\langle 34   T^0, b^1, s_{\text{HB}}^1 \rangle$	2.57%	-0.000	-0.019	0.000
4691.5	0.2	0.000	-0.004	-0.000	$\langle 35   T^0, b^3, s^0 \rangle$	45.88%	0.001	-0.002	0.000
					$\langle 35   T^1, b^3, s^0 \rangle$	13.20%	0.000	0.000	0.000
					$\langle 35   T^0, b^1, s_{\text{HB}}^1 \rangle$	2.95%	0.001	0.020	-0.000
					$\langle 35   T^1, b^1, s_{\text{HB}}^1 \rangle$	4.09%	0.000	0.011	0.000
					$\langle 35   T^0, b^2, s_{\text{HB}}^1 \rangle$	5.56%	-0.000	-0.008	-0.000
4748.2	0.1	0.000	-0.000	-0.003	$\langle 36   T^0, b^3, s^0 \rangle$	41.92%	0.000	-0.000	0.002
					$\langle 36   T^1, b^3, s^0 \rangle$	13.15%	0.000	-0.000	0.000
					$\langle 36   T^0, b^0, s_{\text{free}}^1 \rangle$	0.02%	0.000	0.000	-0.003
					$\langle 36   T^0, b^1, s^0 \rangle$	0.04%	-0.000	0.000	-0.002
4904.3	0.1	-0.000	0.000	-0.003	$\langle 38   T^0, b^3, s^0 \rangle$	76.17%	0.000	0.000	-0.003
					$\langle 38   T^1, b^3, s^0 \rangle$	15.43%	-0.000	-0.000	-0.001
					$\langle 38   T^0, b^1, s^0 \rangle$	0.03%	0.000	-0.000	0.002
					$\langle 38   T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	0.000	0.000	-0.001
4930.6	0.2	-0.001	0.004	-0.000	$\langle 39   T^0, b^3, s^0 \rangle$	29.38%	0.001	-0.001	0.000
					$\langle 39   T^0, b^2, s_{\text{HB}}^1 \rangle$	19.61%	0.000	0.014	0.000
					$\langle 39   T^0, b^1, s_{\text{HB}}^1 \rangle$	2.11%	-0.000	-0.017	0.000
					$\langle 39   T^0, b^0, s_{\text{HB}}^2 \rangle$	1.45%	0.001	0.010	-0.000
5022.3	0.7	-0.001	-0.008	-0.000	$\langle 41   T^0, b^2, s_{\text{HB}}^1 \rangle$	32.34%	0.000	0.007	-0.000
					$\langle 41   T^0, b^3, s^0 \rangle$	30.32%	0.000	0.000	0.000
					$\langle 41   T^1, b^2, s_{\text{HB}}^1 \rangle$	20.12%	0.000	0.003	-0.000
					$\langle 41   T^0, b^0, s_{\text{HB}}^1 \rangle$	0.02%	-0.000	-0.010	0.000
					$\langle 41   T^1, b^0, s_{\text{HB}}^1 \rangle$	0.03%	-0.000	-0.005	0.000
5123.6	1.4	-0.002	-0.010	-0.000	$\langle 43   T^0, b^1, s_{\text{free}}^1 \rangle$	72.09%	-0.004	-0.010	0.000
					$\langle 43   T^0, b^0, s_{\text{free}}^1 \rangle$	0.34%	0.004	0.007	-0.000
					$\langle 43   T^0, b^1, s_{\text{HB}}^1 \rangle$	0.19%	0.000	0.005	-0.000
5152.4	0.5	-0.000	-0.000	0.006	$\langle 44   T^1, b^3, s^0 \rangle$	43.45%	-0.000	0.000	-0.001

						$\langle 44 T^0, b^3, s^0 \rangle$	15.54%	0.000	-0.000	0.001
						$\langle 44 T^2, b^3, s^0 \rangle$	11.67%	0.000	0.000	0.000
						$\langle 44 T^0, b^0, s_{\text{free}}^1 \rangle$	0.08%	-0.000	-0.000	0.006
						$\langle 44 T^1, b^0, s_{\text{free}}^1 \rangle$	0.08%	0.000	0.000	0.002
5162.0	3.6	-0.000	-0.000	0.017		$\langle 45 T^0, b^1, s_{\text{free}}^1 \rangle$	67.52%	0.000	-0.000	-0.001
						$\langle 45 T^1, b^3, s^0 \rangle$	12.93%	0.000	-0.000	0.000
						$\langle 45 T^0, b^0, s_{\text{free}}^1 \rangle$	0.61%	-0.000	-0.000	0.016
						$\langle 45 T^1, b^0, s_{\text{free}}^1 \rangle$	0.07%	0.000	0.000	0.002
5183.2	0.9	0.000	0.000	-0.008		$\langle 46 T^0, b^1, s_{\text{free}}^1 \rangle$	81.75%	0.000	0.000	-0.006
						$\langle 46 T^0, b^0, s_{\text{free}}^1 \rangle$	0.02%	0.000	0.000	-0.003
						$\langle 46 T^0, b^1, s^0 \rangle$	0.01%	0.000	-0.000	0.001
5206.4	0.2	-0.000	-0.003	-0.000		$\langle 47 T^1, b^3, s^0 \rangle$	57.80%	0.000	0.000	0.000
						$\langle 47 T^2, b^3, s^0 \rangle$	14.30%	0.000	0.000	0.000
						$\langle 47 T^0, b^3, s^0 \rangle$	13.59%	0.000	0.000	0.000
						$\langle 47 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	-0.000	-0.005	0.000
						$\langle 47 T^0, b^2, s_{\text{HB}}^1 \rangle$	4.13%	0.000	0.003	-0.000
						$\langle 47 T^1, b^0, s_{\text{HB}}^1 \rangle$	0.00%	-0.000	-0.001	0.000
5250.0	2.4	-0.002	-0.013	-0.000		$\langle 49 T^0, b^1, s_{\text{free}}^1 \rangle$	75.69%	-0.001	-0.010	0.000
						$\langle 49 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	-0.000	-0.007	0.000
						$\langle 49 T^1, b^0, s_{\text{HB}}^1 \rangle$	0.03%	0.000	0.005	-0.000
5255.9	0.3	-0.001	-0.005	-0.000		$\langle 50 T^2, b^0, s_{\text{HB}}^2 \rangle$	47.49%	0.000	0.004	0.000
						$\langle 50 T^1, b^0, s_{\text{HB}}^2 \rangle$	29.41%	0.001	0.011	-0.000
						$\langle 50 T^1, b^0, s_{\text{HB}}^1 \rangle$	0.23%	-0.000	-0.015	0.000
						$\langle 50 T^0, b^0, s_{\text{HB}}^2 \rangle$	3.07%	-0.001	-0.015	0.000
						$\langle 50 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.03%	0.000	0.013	-0.000
5392.4	0.3	-0.002	-0.004	0.000		$\langle 52 T^1, b^1, s_{\text{free}}^1 \rangle$	44.10%	0.001	0.002	0.000
						$\langle 52 T^0, b^1, s_{\text{free}}^1 \rangle$	11.36%	-0.002	-0.004	0.000
						$\langle 52 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	11.10%	-0.001	0.002	0.000
						$\langle 52 T^0, b^1, s_{\text{HB}}^1 \rangle$	0.39%	-0.000	-0.007	0.000
						$\langle 52 T^0, b^2, s_{\text{HB}}^1 \rangle$	4.46%	0.000	0.007	0.000
5432.2	1.0	-0.001	-0.008	-0.000		$\langle 53 T^0, b^1, s_{\text{HB}}^2 \rangle$	20.73%	0.000	-0.003	-0.000
						$\langle 53 T^1, b^1, s_{\text{HB}}^2 \rangle$	11.83%	0.000	-0.007	-0.000
						$\langle 53 T^2, b^3, s^0 \rangle$	10.53%	0.000	0.000	0.000
						$\langle 53 T^0, b^0, s_{\text{HB}}^2 \rangle$	1.95%	-0.001	-0.012	0.000
						$\langle 53 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	0.000	0.008	-0.000
						$\langle 53 T^0, b^2, s_{\text{HB}}^1 \rangle$	5.46%	0.000	0.007	0.000
5528.7	0.2	0.002	0.003	-0.000		$\langle 59 T^0, b^2, s_{\text{HB}}^1 \rangle$	15.90%	0.000	0.013	0.000
						$\langle 59 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	14.02%	0.001	-0.002	-0.000
						$\langle 59 T^0, b^1, s_{\text{HB}}^1 \rangle$	1.47%	-0.000	-0.014	0.000
						$\langle 59 T^1, b^1, s_{\text{HB}}^1 \rangle$	0.69%	0.000	0.004	0.000
5560.5	0.1	0.003	-0.001	-0.000		$\langle 61 T^0, b^0, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	18.09%	0.001	-0.003	-0.000
						$\langle 61 T^1, b^1, s_{\text{free}}^1 \rangle$	12.37%	0.000	0.000	0.000
						$\langle 61 T^1, b^2, s_{\text{HB}}^1 \rangle$	12.26%	-0.000	0.007	-0.000
						$\langle 61 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.03%	0.000	0.012	-0.000
						$\langle 61 T^0, b^0, s_{\text{HB}}^2 \rangle$	1.43%	-0.001	-0.010	0.000

6225.3	3.2	0.001	0.014	-0.000		$\langle 74 T^0, b^0, s_{\text{free}}^2 \rangle$	48.23%	0.001	0.005	-0.000
						$\langle 74 T^1, b^0, s_{\text{free}}^2 \rangle$	31.96%	0.001	0.011	-0.000
						$\langle 74 T^1, b^0, s^0 \rangle$	0.01%	0.000	0.004	0.000
6330.9	0.1	0.000	0.002	-0.000		$\langle 80 T^0, b^4, s^0 \rangle$	20.48%	0.000	0.000	0.000
						$\langle 80 T^0, b^3, s_{\text{HB}}^1 \rangle$	15.44%	0.000	0.000	0.000
						$\langle 80 T^1, b^3, s_{\text{HB}}^1 \rangle$	11.30%	0.000	0.000	0.000
						$\langle 80 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	0.000	0.002	-0.000
						$\langle 80 T^0, b^2, s_{\text{HB}}^1 \rangle$	3.06%	-0.000	-0.002	0.000
						$\langle 80 T^0, b^1, s_{\text{HB}}^1 \rangle$	0.03%	-0.000	-0.002	0.000
6698.3	0.1	-0.000	-0.000	-0.002		$\langle 91 T^0, b^2, s_{\text{free}}^1 \rangle$	61.17%	0.000	-0.000	-0.003
						$\langle 91 T^1, b^2, s_{\text{free}}^1 \rangle$	12.07%	0.000	-0.000	-0.001
						$\langle 91 T^0, b^0, s_{\text{free}}^1 \rangle$	0.04%	-0.000	-0.000	0.004
						$\langle 91 T^0, b^0, s_{\text{free}}^2 \rangle$	1.37%	-0.000	-0.000	-0.002
6891.4	0.1	0.000	0.002	-0.000		$\langle 103 T^0, b^2, s_{\text{HB}}^2 \rangle$	18.50%	0.000	0.000	0.000
						$\langle 103 T^1, b^4, s^0 \rangle$	17.33%	0.000	0.000	0.000
						$\langle 103 T^1, b^2, s_{\text{HB}}^2 \rangle$	11.23%	0.000	0.001	-0.000
						$\langle 103 T^0, b^3, s_{\text{HB}}^1 \rangle$	11.16%	0.000	0.000	0.000
						$\langle 103 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.04%	0.000	0.002	-0.000
						$\langle 103 T^1, b^0, s_{\text{free}}^2 \rangle$	0.50%	-0.000	-0.001	0.000
						$\langle 103 T^0, b^1, s_{\text{HB}}^1 \rangle$	0.01%	0.000	0.001	-0.000
6912.5	0.3	0.001	0.004	-0.000		$\langle 104 T^0, b^1, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	22.74%	0.000	0.000	0.000
						$\langle 104 T^0, b^0, s_{\text{free}}^2 \rangle$	12.79%	0.002	0.004	0.000
						$\langle 104 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	-0.000	-0.004	0.000
						$\langle 104 T^0, b^1, s_{\text{HB}}^1 \rangle$	0.03%	0.000	0.002	-0.000
6933.6	0.4	0.000	0.000	0.005		$\langle 105 T^0, b^1, s_{\text{HB}}^1 s_{\text{free}}^1 \rangle$	11.17%	0.000	0.000	0.000
						$\langle 105 T^0, b^0, s_{\text{free}}^2 \rangle$	10.37%	0.000	0.000	0.005
						$\langle 105 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	0.000	0.000	-0.001
						$\langle 105 T^0, b^2, s_{\text{free}}^1 \rangle$	3.44%	-0.000	0.000	0.001
6975.8	0.2	0.000	0.000	-0.003		$\langle 106 T^1, b^2, s_{\text{free}}^1 \rangle$	19.31%	-0.000	0.000	0.001
						$\langle 106 T^0, b^0, s_{\text{free}}^2 \rangle$	8.58%	-0.000	-0.000	-0.004
						$\langle 106 T^0, b^2, s_{\text{free}}^1 \rangle$	9.79%	0.000	-0.000	-0.001
						$\langle 106 T^0, b^0, s_{\text{free}}^1 \rangle$	0.00%	-0.000	-0.000	0.001
6986.1	1.6	0.003	0.009	-0.000		$\langle 107 T^0, b^0, s_{\text{free}}^2 \rangle$	66.57%	0.004	0.009	0.000
						$\langle 107 T^1, b^0, s_{\text{free}}^2 \rangle$	7.50%	0.001	0.002	0.000
						$\langle 107 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	0.000	0.002	-0.000
6996.8	1.7	0.000	0.000	0.010		$\langle 108 T^0, b^0, s_{\text{free}}^2 \rangle$	46.30%	0.000	0.000	0.010
						$\langle 108 T^0, b^2, s_{\text{free}}^1 \rangle$	7.37%	0.000	-0.000	-0.001
						$\langle 108 T^1, b^0, s_{\text{free}}^2 \rangle$	3.07%	0.000	0.000	0.001
6999.9	0.1	-0.001	-0.002	-0.000		$\langle 109 T^1, b^2, s_{\text{free}}^1 \rangle$	29.94%	0.000	0.003	-0.000
						$\langle 109 T^0, b^2, s_{\text{HB}}^2 \rangle$	9.15%	-0.000	0.003	-0.000
						$\langle 109 T^0, b^0, s_{\text{free}}^2 \rangle$	6.62%	-0.001	-0.003	-0.000





						$\langle 78 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.23%	0.000	-0.002	0.000
						$\langle 78 T^1, b^0, s_{\text{HB}}^2 \rangle$	2.23%	-0.000	-0.001	-0.000
						$\langle 78 T^1, b^0, s_{\text{HB}}^1 \rangle$	0.05%	0.000	0.001	0.000
4956.8	0.6	0.000	-0.000	0.007		$\langle 79 T^0, b^3, s^0 \rangle$	72.46%	-0.000	0.000	-0.001
						$\langle 79 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.91%	-0.000	-0.000	0.006
						$\langle 79 T^0, b^1, s_{\text{HB}}^1 \rangle$	0.49%	-0.000	0.000	-0.004
						$\langle 79 T^1, b^0, s_{\text{HB}}^2 \rangle$	2.31%	0.000	-0.000	0.002
4959.8	3.5	0.000	-0.000	0.017		$\langle 80 T^1, b^0, s_{\text{HB}}^2 \rangle$	30.34%	0.000	-0.000	0.004
						$\langle 80 T^0, b^3, s^0 \rangle$	20.75%	0.000	0.000	0.000
						$\langle 80 T^2, b^1, s_{\text{HB}}^1 \rangle$	12.32%	-0.000	-0.000	-0.001
						$\langle 80 T^0, b^0, s_{\text{HB}}^2 \rangle$	2.98%	-0.000	-0.000	0.010
						$\langle 80 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	-0.000	-0.000	-0.005
						$\langle 80 T^1, b^0, s_{\text{HB}}^2 \rangle$	7.93%	0.000	-0.000	0.004
4977.7	0.2	-0.001	0.004	-0.000		$\langle 82 T^2, b^1, s_{\text{HB}}^1 \rangle$	52.90%	0.000	0.000	0.000
						$\langle 82 T^0, b^0, s_{\text{HB}}^2 \rangle$	1.74%	-0.000	0.004	-0.000
						$\langle 82 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	-0.000	-0.002	-0.000
						$\langle 82 T^0, b^1, s_{\text{HB}}^1 \rangle$	0.48%	-0.000	0.001	0.000
4993.8	0.3	-0.000	0.000	-0.005		$\langle 83 T^2, b^1, s_{\text{HB}}^1 \rangle$	40.48%	-0.000	-0.000	-0.001
						$\langle 83 T^2, b^1, s_{\text{HB}}^1 \rangle$	33.64%	0.000	0.000	0.000
						$\langle 83 T^0, b^0, s_{\text{HB}}^2 \rangle$	0.62%	0.000	0.000	-0.005
						$\langle 83 T^1, b^1, s_{\text{HB}}^1 \rangle$	5.07%	0.000	-0.000	0.003
						$\langle 83 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	0.000	0.000	0.003
5019.4	1.1	0.000	-0.000	0.010		$\langle 84 T^2, b^1, s_{\text{HB}}^1 \rangle$	42.82%	0.000	0.000	0.000
						$\langle 84 T^2, b^1, s_{\text{HB}}^1 \rangle$	20.81%	0.000	0.000	0.001
						$\langle 84 T^0, b^0, s_{\text{HB}}^2 \rangle$	2.34%	-0.000	-0.000	0.009
						$\langle 84 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	-0.000	-0.000	-0.006
						$\langle 84 T^1, b^1, s_{\text{HB}}^1 \rangle$	4.00%	-0.000	0.000	-0.003
5037.8	0.3	0.000	-0.005	-0.000		$\langle 85 T^2, b^1, s_{\text{HB}}^1 \rangle$	64.58%	0.000	-0.001	0.000
						$\langle 85 T^1, b^1, s_{\text{HB}}^1 \rangle$	12.07%	-0.000	0.001	-0.000
						$\langle 85 T^0, b^0, s_{\text{HB}}^2 \rangle$	3.34%	0.000	-0.006	0.000
						$\langle 85 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.01%	0.000	0.004	0.000
5096.4	1.7	0.001	-0.012	0.000		$\langle 86 T^0, b^0, s_{\text{HB}}^2 \rangle$	28.47%	0.001	-0.017	0.000
						$\langle 86 T^1, b^0, s_{\text{HB}}^2 \rangle$	19.50%	0.000	0.001	-0.000
						$\langle 86 T^2, b^0, s_{\text{HB}}^2 \rangle$	13.12%	-0.000	-0.000	-0.000
						$\langle 86 T^1, b^0, s_{\text{HB}}^2 \rangle$	11.56%	-0.000	-0.002	-0.000
						$\langle 86 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.03%	0.000	0.006	0.000
5115.7	9.2	0.000	-0.000	-0.027		$\langle 87 T^0, b^0, s_{\text{HB}}^2 \rangle$	33.99%	0.000	0.000	-0.034
						$\langle 87 T^1, b^0, s_{\text{HB}}^2 \rangle$	16.07%	0.000	-0.000	0.003
						$\langle 87 T^1, b^0, s_{\text{HB}}^2 \rangle$	13.67%	-0.000	0.000	-0.006
						$\langle 87 T^2, b^0, s_{\text{HB}}^2 \rangle$	13.44%	-0.000	0.000	-0.003
						$\langle 87 T^2, b^0, s_{\text{HB}}^2 \rangle$	11.65%	-0.000	-0.000	-0.004
						$\langle 87 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.05%	0.000	0.000	0.017
5214.6	1.4	0.000	-0.000	0.010		$\langle 92 T^1, b^3, s^0 \rangle$	51.49%	0.000	0.000	0.000
						$\langle 92 T^0, b^1, s_{\text{free}}^1 \rangle$	40.58%	0.000	-0.000	0.004
						$\langle 92 T^0, b^0, s_{\text{HB}}^1 \rangle$	0.00%	0.000	0.000	0.004







						$\langle 110 T^0, b^1, s^1 \rangle$	1.87%	0.000	0.003	0.000
						$\langle 110 T^0, b^0, s^1 \rangle$	0.00%	0.000	-0.002	0.000
						$\langle 110 T^0, b^1, s^1 \rangle$	0.44%	0.000	0.001	-0.000
4967.3	0.2	0.003	0.000	-0.000		$\langle 114 T^0, b^3, s^0 \rangle$	94.30%	0.003	-0.000	-0.000
						$\langle 114 T^0, b^1, s^1 \rangle$	1.08%	-0.002	-0.000	-0.000
						$\langle 114 T^0, b^1, s^1 \rangle$	0.39%	0.001	-0.000	-0.000
4968.1	0.2	0.000	-0.003	0.000		$\langle 115 T^0, b^3, s^0 \rangle$	94.19%	-0.000	-0.003	0.000
						$\langle 115 T^0, b^1, s^1 \rangle$	1.27%	-0.000	0.002	0.000
						$\langle 115 T^0, b^1, s^1 \rangle$	0.40%	-0.000	-0.001	-0.000
5339.2	1.8	-0.000	-0.011	0.005		$\langle 165 T^0, b^0, s^2 \rangle$	53.47%	-0.000	-0.007	0.003
						$\langle 165 T^1, b^3, s^0 \rangle$	19.57%	0.000	0.000	0.000
						$\langle 165 T^0, b^0, s^1 \rangle$	0.00%	0.000	-0.002	0.000
						$\langle 165 T^1, b^0, s^2 \rangle$	3.77%	-0.000	0.001	-0.000
5340.0	0.6	0.000	0.006	-0.003		$\langle 166 T^1, b^3, s^0 \rangle$	71.60%	0.000	0.000	0.000
						$\langle 166 T^0, b^0, s^2 \rangle$	14.92%	0.000	0.004	-0.002
						$\langle 166 T^0, b^0, s^1 \rangle$	0.00%	-0.000	0.001	-0.000
						$\langle 166 T^1, b^0, s^2 \rangle$	1.15%	0.000	-0.001	0.000
5357.2	15.1	-0.001	0.034	0.002		$\langle 167 T^0, b^0, s^2 \rangle$	64.63%	-0.000	0.026	0.001
						$\langle 167 T^1, b^0, s^2 \rangle$	14.00%	0.001	-0.003	0.000
						$\langle 167 T^1, b^0, s^2 \rangle$	11.41%	-0.000	-0.001	-0.000
						$\langle 167 T^0, b^0, s^1 \rangle$	0.01%	-0.000	0.006	-0.000
						$\langle 167 T^1, b^0, s^0 \rangle$	0.02%	-0.001	0.003	-0.000
5363.7	15.9	-0.034	-0.001	-0.000		$\langle 168 T^0, b^0, s^2 \rangle$	63.80%	-0.026	-0.000	-0.000
						$\langle 168 T^1, b^0, s^2 \rangle$	11.46%	0.001	-0.000	0.000
						$\langle 168 T^0, b^0, s^1 \rangle$	0.01%	-0.007	-0.000	0.000
						$\langle 168 T^1, b^0, s^0 \rangle$	0.02%	-0.004	-0.001	0.000
5663.0	0.1	-0.003	-0.000	-0.000		$\langle 191 T^1, b^0, s^2 \rangle$	52.72%	-0.004	-0.001	0.000
						$\langle 191 T^2, b^0, s^2 \rangle$	13.33%	0.000	0.000	0.000
						$\langle 191 T^1, b^0, s^2 \rangle$	12.88%	0.002	-0.000	0.000
						$\langle 191 T^1, b^0, s^0 \rangle$	0.01%	0.003	0.001	-0.000
						$\langle 191 T^0, b^0, s^2 \rangle$	2.02%	-0.002	-0.000	0.000
5673.7	0.1	-0.000	0.003	-0.000		$\langle 192 T^1, b^0, s^2 \rangle$	30.25%	-0.001	-0.000	0.001
						$\langle 192 T^1, b^0, s^2 \rangle$	25.39%	-0.001	0.004	-0.000
						$\langle 192 T^1, b^0, s^2 \rangle$	16.76%	-0.000	-0.001	-0.001
						$\langle 192 T^1, b^0, s^0 \rangle$	0.01%	0.001	-0.003	0.000
						$\langle 192 T^0, b^0, s^2 \rangle$	0.24%	-0.000	0.002	0.000
5703.2	0.3	-0.000	-0.004	0.001		$\langle 196 T^1, b^0, s^2 \rangle$	52.06%	-0.000	-0.000	0.001
						$\langle 196 T^1, b^0, s^2 \rangle$	10.21%	-0.000	-0.000	0.000
						$\langle 196 T^0, b^0, s^1 \rangle$	0.00%	-0.000	0.004	-0.000
						$\langle 196 T^0, b^0, s^2 \rangle$	1.02%	0.000	-0.003	-0.000
						$\langle 196 T^0, b^0, s^2 \rangle$	6.58%	-0.000	-0.003	0.001
5716.8	1.3	0.000	-0.010	-0.000		$\langle 197 T^1, b^0, s^2 \rangle$	24.78%	0.000	-0.001	-0.000
						$\langle 197 T^0, b^0, s^2 \rangle$	15.64%	0.000	-0.013	-0.000
						$\langle 197 T^1, b^0, s^2 \rangle$	14.28%	0.001	-0.003	0.000
						$\langle 197 T^0, b^0, s^1 \rangle$	0.02%	-0.000	0.009	-0.000

5723.5	1.4	0.010	0.000	0.000		$\langle 198 T^1, b^0, s^2 \rangle$	26.03%	0.001	0.000	0.000
						$\langle 198 T^0, b^0, s^2 \rangle$	18.43%	0.014	0.000	0.000
						$\langle 198 T^1, b^0, s^2 \rangle$	11.35%	0.001	-0.000	0.000
						$\langle 198 T^0, b^0, s^1 \rangle$	0.02%	-0.009	-0.000	0.000
						$\langle 198 T^0, b^0, s^2 \rangle$	2.85%	-0.002	-0.000	0.000
5743.8	0.4	0.000	-0.005	-0.000		$\langle 200 T^1, b^0, s^2 \rangle$	41.46%	-0.000	0.001	0.000
						$\langle 200 T^0, b^0, s^2 \rangle$	13.66%	0.000	-0.012	-0.000
						$\langle 200 T^1, b^0, s^2 \rangle$	10.76%	-0.000	-0.001	-0.000
						$\langle 200 T^0, b^0, s^1 \rangle$	0.01%	-0.000	0.006	-0.000
						$\langle 200 T^1, b^0, s^2 \rangle$	4.39%	0.000	-0.002	0.000
5749.8	0.3	0.005	0.000	0.000		$\langle 201 T^1, b^0, s^2 \rangle$	50.61%	-0.002	-0.000	-0.000
						$\langle 201 T^0, b^0, s^2 \rangle$	11.57%	0.011	0.000	0.000
						$\langle 201 T^0, b^0, s^1 \rangle$	0.01%	-0.007	-0.000	0.000
						$\langle 201 T^0, b^0, s^2 \rangle$	3.59%	-0.002	-0.000	0.000
5811.4	1.1	-0.009	-0.000	0.000		$\langle 202 T^0, b^0, s^2 \rangle$	81.35%	-0.010	-0.000	0.000
						$\langle 202 T^0, b^0, s^1 \rangle$	0.02%	0.008	0.000	-0.000
						$\langle 202 T^0, b^0, s^2 \rangle$	2.00%	-0.005	-0.000	-0.000
5828.6	0.8	0.000	-0.007	0.000		$\langle 203 T^0, b^0, s^2 \rangle$	85.32%	0.000	-0.010	0.000
						$\langle 203 T^0, b^0, s^1 \rangle$	0.01%	-0.000	0.007	-0.000
						$\langle 203 T^0, b^0, s^2 \rangle$	0.86%	0.000	-0.003	-0.000
5915.9	0.2	-0.000	-0.001	-0.003		$\langle 204 T^0, b^0, s^2 \rangle$	75.29%	-0.000	-0.001	-0.005
						$\langle 204 T^0, b^0, s^1 \rangle$	0.02%	0.000	0.001	0.002
						$\langle 204 T^0, b^0, s^2 \rangle$	0.05%	0.000	-0.001	-0.000
6028.9	0.3	-0.000	0.004	-0.000		$\langle 205 T^0, b^2, s^1 \rangle$	51.87%	0.000	-0.013	0.000
						$\langle 205 T^0, b^2, s^1 \rangle$	16.73%	-0.000	-0.001	0.000
						$\langle 205 T^0, b^2, s^1 \rangle$	13.61%	-0.000	-0.000	-0.000
						$\langle 205 T^0, b^0, s^1 \rangle$	0.08%	-0.000	0.018	-0.000
						$\langle 205 T^0, b^0, s^2 \rangle$	0.11%	-0.000	0.001	0.000
6034.0	0.3	-0.004	-0.000	0.000		$\langle 206 T^0, b^2, s^1 \rangle$	47.94%	0.012	0.000	0.000
						$\langle 206 T^0, b^2, s^1 \rangle$	24.58%	0.001	-0.000	0.000
						$\langle 206 T^0, b^0, s^1 \rangle$	0.08%	-0.017	-0.000	0.000
						$\langle 206 T^0, b^0, s^2 \rangle$	0.12%	-0.001	-0.000	-0.000
6890.9	0.1	-0.002	-0.000	-0.000		$\langle 336 T^0, b^1, s^2 \rangle$	39.18%	-0.000	0.000	0.000
						$\langle 336 T^0, b^1, s^2 \rangle$	17.44%	-0.000	0.000	-0.000
						$\langle 336 T^1, b^1, s^2 \rangle$	4.05%	-0.001	-0.000	-0.000
						$\langle 336 T^0, b^1, s^0 \rangle$	0.04%	-0.001	-0.000	0.000
						$\langle 336 T^0, b^0, s^2 \rangle$	0.02%	-0.000	-0.000	-0.000
6892.2	0.1	0.000	-0.002	-0.000		$\langle 337 T^0, b^1, s^2 \rangle$	21.36%	0.000	0.000	0.000
						$\langle 337 T^0, b^1, s^2 \rangle$	19.31%	-0.000	-0.000	-0.000
						$\langle 337 T^0, b^1, s^2 \rangle$	16.12%	-0.000	-0.000	0.000
						$\langle 337 T^1, b^1, s^2 \rangle$	11.12%	0.000	0.000	0.000
						$\langle 337 T^0, b^0, s^1 \rangle$	0.00%	0.000	-0.001	0.000
						$\langle 337 T^0, b^1, s^0 \rangle$	0.04%	0.000	-0.001	0.000
6987.1	0.1	0.000	0.003	-0.000		$\langle 361 T^0, b^1, s^2 \rangle$	37.20%	0.000	0.000	0.000

$\langle 361   T^0, b^1, s^2 \rangle$	<b>24.45%</b>	0.000	0.001	0.000
$\langle 361   T^1, b^1, s^2 \rangle$	<b>14.60%</b>	-0.000	-0.001	0.000
$\langle 361   T^0, b^0, s^1 \rangle$	<b>0.01%</b>	-0.000	0.005	-0.000
$\langle 361   T^0, b^0, s^2 \rangle$	<b>0.27%</b>	0.000	-0.002	-0.000
$\langle 361   T^1, b^1, s^2 \rangle$	<b>7.02%</b>	0.000	-0.001	0.000