

Supporting Information

An algebraic alternative for the accurate simulation of CO₂ Raman spectra

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1 Partition Function

Table 1: Vibrational partition function values at different temperatures for each polyad scheme.

Temperature (K)	Partition equation value ^a $E_{max}=26552.21\text{cm}^{-1}$		
	P_{212}	P_{213}	P_{214}
10	1.	1.	1.
50	1.	1.	1.
100	1.00014	1.00014	1.00014
150	1.00333	1.00333	1.00333
200	1.01672	1.01672	1.01672
250	1.04489	1.04489	1.04489
300	1.08862	1.08862	1.08862
500	1.40513	1.40512	1.40512
1000	3.19101	3.18828	3.18822
1500	6.96758	6.88528	6.88409
1743	9.83858	9.59713	9.59484
2000	13.8307	13.2299	13.2266
3000	42.209	36.1361	36.1622
Number of states ^b	3938	3389	4096

^a E_{max} is the maximum predicted energy considered to compute the vibrational partition function as a direct sum.

^b Number of predicted vibrational levels up to energy E_{max} considered in the partition sum.

2 Fit of energies

In Table 2 the parameter values of Hamiltonians (17), (18) and (19) for each polyad scheme are given. They have been obtained by fitting them to the available 178 experimental levels of energy.

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Table 2: Parameter values (cm^{-1}) from the fit of the Hamiltonian associated to each polyad.

Parameter	P_{212}	P_{213}	P_{214}
ω_1	1356.441	1356.765	1356.435
ω_2	667.22	667.225	667.268
ω_3	2381.082	2380.741	2380.604
x_{11}	1.628	1.43	1.354
x_{22}	0.338	0.303	0.421
x_{33}	-5.48	-5.142	-5.104
x_{12}	-0.636	-0.528	-0.965
x_{13}	4.002	4.055	3.985
x_{23}	-12.58	-12.591	-12.56
g_{22}	-0.158	-0.122	-0.25
$f_{g/bb}$	-36.758	-36.761	-36.714
α_1^{sb}	0.307	0.311	0.289
$\hat{V}_P^a$	-10.575	0.99	0.096
x_{113}	0.315	-0.062	-0.035
x_{133}	-0.454	0.008	0.042
x_{123}	-0.039	-0.037	-0.046
α_1^s	-0.028	-0.027	-0.016
α_2^{sb}	-0.035	-0.032	-0.022
$f_{g/bb}^{[2]}$	0.008	0.01	0.001

^a This interaction parameter is $f_{uu/gg}$ for the polyad scheme P_{212} , $f_{uu/ggg}$ for P_{213} , and $f_{uu/gggg}$ for P_{214} .

The calculated energies for each polyad scheme are given in Tables 3, 4 and 5 respectively.

Table 3: Fit of energies (in cm^{-1}) of $^{12}\text{CO}_2$ provided by the Hamiltonian (17) associated with Polyad P_{212} .

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
	P_{212}	P_{214}	P_{213}							
Symmetry Σ_g										
1	2	2	2	0, 2, 0	0.510	0, 0, 1, 1	0.510	1285.41	1285.40	0.01
2	2	2	2	1, 0, 0	0.510	0, 0, 1, 1	0.490	1388.18	1388.29	-0.11
1	4	4	4	1, 2, 0	0.501	0, 0, 2, 2	0.324	2548.37	2548.27	0.10
2	4	4	4	2, 0, 0	0.665	0, 0, 2, 2	0.335	2671.14	2671.35	-0.21
3	4	4	4	1, 2, 0	0.499	0, 0, 2, 2	0.341	2797.14	2797.20	-0.06
4	4	8	6	0, 0, 2	1.000	1, 1, 0, 0	0.516	4673.33	4673.29	0.03
1	6	6	6	1, 4, 0	0.445	1, 0, 2, 2	0.445	3792.68	3792.57	0.11
2	6	6	6	3, 0, 0	0.491	0, 0, 3, 3	0.265	3942.54	3942.73	-0.19
3	6	6	6	3, 0, 0	0.415	0, 0, 3, 3	0.296	4064.28	4064.48	-0.21
4	6	6	6	1, 4, 0	0.461	0, 0, 3, 3	0.238	4225.1	4225.06	0.04
5	6	10	8	0, 2, 2	0.566	1, 1, 1, 1	0.292	5915.21	5915.22	0.00
6	6	10	8	1, 0, 2	0.565	1, 1, 1, 1	0.225	6016.69	6016.68	0.01
1	8	8	8	2, 4, 0	0.362	1, 0, 3, 3	0.355	-	5022.46	-
2	8	8	8	3, 2, 0	0.357	0, 0, 4, 4	0.216	5197.15	5197.37	-0.22
3	8	8	8	4, 0, 0	0.570	0, 0, 4, 4	0.222	5330.6	5329.89	0.71
4	8	8	8	3, 2, 0	0.385	0, 0, 4, 4	0.275	5475.57	5475.62	-0.05
5	8	8	8	1, 6, 0	0.399	1, 0, 3, 3	0.399	-	5667.55	-
6	8	12	10	1, 2, 2	0.490	1, 1, 2, 2	0.191	7133.82	7133.79	0.03
7	8	12	10	2, 0, 2	0.659	4, 0, 0, 0	0.494	7259.75	7259.81	-0.06
8	8	12	10	1, 2, 2	0.504	3, 0, 1, 1	0.365	7377.62	7377.71	-0.09
9	8	16	12	0, 0, 4	0.998	2, 2, 0, 0	0.400	9246.93	9246.87	0.06
1	10	10	10	2, 6, 0	0.364	1, 1, 3, 3	0.177	-	6240.73	-
2	10	10	10	4, 2, 0	0.332	0, 0, 5, 5	0.165	-	6435.70	-
3	10	10	10	5, 0, 0	0.514	0, 0, 5, 5	0.180	-	6588.35	-
4	10	10	10	5, 0, 0	0.328	0, 0, 5, 5	0.230	-	6725.29	-
5	10	10	10	3, 4, 0	0.295	0, 0, 5, 5	0.239	-	6903.93	-
6	10	10	10	2, 6, 0	0.354	1, 1, 3, 3	0.170	-	7121.73	-
7	10	14	12	1, 4, 2	0.458	3, 0, 2, 2	0.332	-	8334.25	-
8	10	14	12	3, 0, 2	0.428	1, 1, 3, 3	0.150	-	8488.43	-
9	10	14	12	3, 0, 2	0.473	5, 0, 0, 0	0.316	-	8607.14	-
10	10	14	12	1, 4, 2	0.449	3, 0, 2, 2	0.324	-	8756.80	-
11	10	18	14	0, 2, 4	0.623	2, 2, 1, 1	0.249	10444.89	10444.93	-0.04
12	10	18	14	1, 0, 4	0.621	4, 1, 0, 0	0.371	10546.61	10546.55	0.07
1	12	12	12	2, 8, 0	0.325	1, 1, 4, 4	0.158	-	7449.32	-
2	12	12	12	4, 4, 0	0.285	0, 0, 6, 6	0.117	-	7660.50	-
3	12	12	12	6, 0, 0	0.340	0, 0, 6, 6	0.153	-	7834.59	-
4	12	12	12	6, 0, 0	0.486	0, 0, 6, 6	0.175	-	7973.97	-
5	12	12	12	5, 2, 0	0.334	0, 0, 6, 6	0.234	-	8138.34	-
6	12	12	12	4, 4, 0	0.292	0, 0, 6, 6	0.199	-	8345.60	-
7	12	12	12	2, 8, 0	0.352	1, 1, 4, 4	0.168	-	8585.60	-
8	12	16	14	1, 6, 2	0.379	3, 0, 3, 3	0.275	-	9520.81	-
9	12	16	14	3, 2, 2	0.375	1, 1, 4, 4	0.127	-	9698.87	-
10	12	16	14	4, 0, 2	0.575	6, 0, 0, 0	0.316	-	9833.28	-
11	12	16	14	3, 2, 2	0.377	1, 1, 4, 4	0.129	-	9969.29	-
12	12	16	14	1, 6, 2	0.379	3, 0, 3, 3	0.273	-	10150.17	-
13	12	20	16	1, 2, 4	0.470	2, 2, 2, 2	0.167	-	11619.20	-
14	12	20	16	2, 0, 4	0.632	2, 2, 2, 2	0.134	-	11749.53	-
15	12	20	16	1, 2, 4	0.498	4, 1, 1, 1	0.299	-	11860.65	-
16	12	24	18	0, 0, 6	0.996	3, 3, 0, 0	0.344	13721.14	13721.10	0.03
1	14	14	14	3, 8, 0	0.308	1, 1, 5, 5	0.129	-	8649.62	-

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Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
2	14	14	14	5, 4, 0	0.276	1, 0, 6, 6	0.206	-	8874.20	-
3	14	14	14	6, 2, 0	0.313	0, 0, 7, 7	0.125	-	9066.85	-
4	14	14	14	7, 0, 0	0.520	0, 0, 7, 7	0.137	-	9218.91	-
5	14	14	14	6, 2, 0	0.275	0, 0, 7, 7	0.194	-	9371.39	-
6	14	14	14	5, 4, 0	0.253	0, 0, 7, 7	0.223	-	9567.01	-
7	14	14	14	4, 6, 0	0.275	0, 0, 7, 7	0.162	-	9798.01	-
8	14	14	14	2, 10, 0	0.331	1, 1, 5, 5	0.158	-	10057.66	-
9	14	18	16	2, 6, 2	0.362	4, 0, 3, 3	0.271	-	10696.17	-
10	14	18	16	4, 2, 2	0.305	1, 1, 5, 5	0.098	-	10893.15	-
11	14	18	16	5, 0, 2	0.455	1, 1, 5, 5	0.101	-	11049.71	-
12	14	18	16	5, 0, 2	0.384	1, 1, 5, 5	0.111	-	11181.02	-
13	14	18	16	4, 2, 2	0.277	1, 1, 5, 5	0.112	-	11348.00	-
14	14	18	16	2, 6, 2	0.360	4, 0, 3, 3	0.271	-	11554.86	-
15	14	22	18	1, 4, 4	0.464	4, 1, 2, 2	0.278	-	12775.98	-
16	14	22	18	3, 0, 4	0.352	2, 2, 3, 3	0.127	-	12934.99	-
17	14	22	18	3, 0, 4	0.523	7, 0, 0, 0	0.258	-	13052.94	-
18	14	22	18	1, 4, 4	0.426	4, 1, 2, 2	0.257	-	13191.65	-
19	14	26	20	0, 2, 6	0.679	3, 3, 1, 1	0.234	14874.78	14874.88	-0.10
20	14	26	20	1, 0, 6	0.673	5, 2, 0, 0	0.333	14978.78	14978.43	0.35
1	16	16	16	3, 10, 0	0.292	2, 1, 5, 5	0.212	-	9842.76	-
2	16	16	16	5, 6, 0	0.238	1, 0, 7, 7	0.172	-	10078.57	-
3	16	16	16	7, 2, 0	0.276	0, 0, 8, 8	0.096	-	10286.37	-
4	16	16	16	8, 0, 0	0.426	0, 0, 8, 8	0.112	-	10455.77	-
5	16	16	16	8, 0, 0	0.384	0, 0, 8, 8	0.148	-	10603.34	-
6	16	16	16	7, 2, 0	0.292	0, 0, 8, 8	0.206	-	10786.16	-
7	16	16	16	6, 4, 0	0.257	0, 0, 8, 8	0.204	-	11007.79	-
8	16	16	16	1, 14, 0	0.230	0, 0, 8, 8	0.130	-	11259.34	-
9	16	16	16	2, 12, 0	0.301	1, 1, 6, 6	0.143	-	11536.72	-
10	16	20	18	2, 8, 2	0.336	4, 0, 4, 4	0.251	-	11862.17	-
11	16	20	18	4, 4, 2	0.295	6, 0, 2, 2	0.162	-	12074.38	-
12	16	20	18	5, 2, 2	0.280	1, 1, 6, 6	0.090	-	12251.91	-
13	16	20	18	6, 0, 2	0.508	7, 1, 0, 0	0.202	-	12390.80	-
14	16	20	18	5, 2, 2	0.329	1, 1, 6, 6	0.113	-	12543.88	-
15	16	20	18	4, 4, 2	0.297	1, 1, 6, 6	0.093	-	12739.83	-
16	16	20	18	2, 8, 2	0.349	4, 0, 4, 4	0.262	-	12968.87	-
17	16	24	20	1, 6, 4	0.400	4, 1, 3, 3	0.239	-	13919.46	-
18	16	24	20	3, 2, 4	0.373	2, 2, 4, 4	0.111	-	14101.37	-
19	16	24	20	4, 0, 4	0.545	8, 0, 0, 0	0.298	-	14239.74	-
20	16	24	20	3, 2, 4	0.348	2, 2, 4, 4	0.087	-	14367.19	-
21	16	24	20	2, 4, 4	0.360	4, 1, 3, 3	0.212	-	14536.65	-
22	16	28	22	0, 4, 6	0.471	3, 3, 2, 2	0.162	-	16004.87	-
23	16	28	22	2, 0, 6	0.582	7, 1, 0, 0	0.265	-	16140.86	-
24	16	28	22	1, 2, 6	0.478	5, 2, 1, 1	0.238	-	16246.88	-
25	16	32	24	0, 0, 8	0.993	4, 4, 0, 0	0.310	18096.36	18096.41	-0.05
1	20	20	20	4, 12, 0	0.264	2, 2, 6, 6	0.093	-	12210.91	-
2	20	20	20	7, 6, 0	0.204	1, 1, 8, 8	0.086	-	12464.24	-
3	20	20	20	8, 4, 0	0.242	1, 0, 9, 9	0.142	-	12694.74	-
4	20	20	20	9, 2, 0	0.282	0, 0, 10, 10	0.073	-	12895.74	-
5	20	20	20	10, 0, 0	0.478	5, 5, 0, 0	0.100	-	13058.45	-
6	20	20	20	10, 0, 0	0.269	0, 0, 10, 10	0.130	-	13218.69	-
7	20	20	20	9, 2, 0	0.245	0, 0, 10, 10	0.183	-	13419.52	-
8	20	20	20	8, 4, 0	0.226	0, 0, 10, 10	0.199	-	13654.67	-
9	20	20	20	7, 6, 0	0.206	0, 0, 10, 10	0.159	-	13917.13	-

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Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
10	20	24	22	3, 10, 2	0.295	5, 0, 5, 5	0.195	-	14171.21	-
11	20	20	20	5, 10, 0	0.225	1, 0, 9, 9	0.208	-	14203.58	-
12	20	24	22	5, 6, 2	0.246	3, 0, 7, 7	0.136	-	14406.37	-
13	20	20	20	3, 14, 0	0.285	1, 1, 8, 8	0.110	-	14511.92	-
14	20	24	22	7, 2, 2	0.241	1, 1, 8, 8	0.058	-	14615.07	-
15	20	24	22	8, 0, 2	0.348	9, 1, 0, 0	0.135	-	14787.79	-
16	20	24	22	8, 0, 2	0.416	9, 1, 0, 0	0.162	-	14931.14	-
17	20	24	22	7, 2, 2	0.292	1, 1, 8, 8	0.102	-	15101.90	-
18	20	24	22	6, 4, 2	0.257	1, 1, 8, 8	0.099	-	15312.28	-
19	20	24	22	5, 6, 2	0.233	3, 0, 7, 7	0.162	-	15552.85	-
20	20	24	22	2, 12, 2	0.288	4, 0, 6, 6	0.216	-	15819.16	-
21	20	28	24	2, 8, 4	0.341	4, 1, 5, 5	0.139	-	16176.01	-
22	20	28	24	4, 4, 4	0.289	8, 0, 2, 2	0.157	-	16390.22	-
23	20	28	24	5, 2, 4	0.298	9, 0, 1, 1	0.169	-	16572.00	-
24	20	28	24	6, 0, 4	0.484	10, 0, 0, 0	0.270	-	16713.21	-
25	20	28	24	5, 2, 4	0.296	9, 0, 1, 1	0.168	-	16855.62	-
26	20	28	24	4, 4, 4	0.288	8, 0, 2, 2	0.158	-	17039.82	-
27	20	28	24	2, 8, 4	0.338	5, 1, 4, 4	0.148	-	17257.84	-
28	20	32	26	1, 6, 6	0.417	5, 2, 3, 3	0.205	-	18218.79	-
29	20	32	26	3, 2, 6	0.350	3, 3, 4, 4	0.106	-	18405.40	-
30	20	32	26	4, 0, 6	0.477	9, 1, 0, 0	0.182	-	18549.77	-
31	20	32	26	4, 0, 6	0.295	8, 1, 1, 1	0.135	-	18670.67	-
32	20	32	26	2, 4, 6	0.367	7, 1, 2, 2	0.168	-	18828.05	-
33	20	36	28	0, 4, 8	0.524	4, 4, 2, 2	0.163	-	20291.20	-
34	20	36	28	2, 0, 8	0.511	8, 2, 0, 0	0.222	-	20434.05	-
35	20	36	28	1, 2, 8	0.440	6, 3, 1, 1	0.190	-	20537.29	-
36	20	40	30	0, 0, 10	0.989	5, 5, 0, 0	0.288	22373.15	22373.24	-0.10
1	24	24	24	5, 14, 0	0.241	3, 2, 7, 7	0.141	-	14559.11	-
2	24	24	24	8, 8, 0	0.195	2, 1, 9, 9	0.119	-	14824.94	-
3	24	24	24	9, 6, 0	0.206	1, 1, 10, 10	0.068	-	15071.31	-
4	24	24	24	11, 2, 0	0.201	1, 0, 11, 11	0.115	-	15294.04	-
5	24	24	24	12, 0, 0	0.284	6, 6, 0, 0	0.053	-	15484.26	-
6	24	24	24	12, 0, 0	0.449	6, 6, 0, 0	0.084	-	15642.83	-
7	24	24	24	11, 2, 0	0.259	0, 0, 12, 12	0.113	-	15820.99	-
8	24	24	24	11, 2, 0	0.190	0, 0, 12, 12	0.162	-	16038.76	-
9	24	24	24	10, 4, 0	0.192	0, 0, 12, 12	0.189	-	16286.63	-
10	24	28	26	4, 12, 2	0.262	5, 0, 7, 7	0.147	-	16455.69	-
11	24	24	24	9, 6, 0	0.183	0, 0, 12, 12	0.174	-	16559.43	-
12	24	28	26	6, 8, 2	0.209	4, 0, 8, 8	0.136	-	16706.83	-
13	24	24	24	7, 10, 0	0.185	0, 0, 12, 12	0.117	-	16854.49	-
14	24	28	26	8, 4, 2	0.221	3, 0, 9, 9	0.111	-	16936.18	-
15	24	28	26	9, 2, 2	0.261	10, 1, 1, 1	0.093	-	17138.06	-
16	24	24	24	6, 12, 0	0.205	1, 0, 11, 11	0.168	-	17170.01	-
17	24	28	26	10, 0, 2	0.413	11, 1, 0, 0	0.131	-	17302.62	-
18	24	28	26	10, 0, 2	0.296	1, 1, 10, 10	0.068	-	17454.63	-
19	24	24	24	3, 18, 0	0.254	2, 1, 9, 9	0.180	-	17504.70	-
20	24	28	26	9, 2, 2	0.246	1, 1, 10, 10	0.093	-	17643.61	-
21	24	28	26	8, 4, 2	0.223	1, 1, 10, 10	0.099	-	17867.76	-
22	24	28	26	7, 6, 2	0.206	1, 1, 10, 10	0.077	-	18119.36	-
23	24	28	26	5, 10, 2	0.211	3, 0, 9, 9	0.140	-	18394.84	-
24	24	32	28	3, 10, 4	0.290	7, 0, 5, 5	0.142	-	18401.68	-
25	24	32	28	5, 6, 4	0.238	9, 0, 3, 3	0.134	-	18637.39	-
26	24	28	26	3, 14, 2	0.279	5, 0, 7, 7	0.193	-	18692.07	-

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Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
27	24	32	28	6, 4, 4	0.214	10, 0, 2, 2	0.121	-	18847.94	-
28	24	32	28	8, 0, 4	0.241	12, 0, 0, 0	0.122	-	19025.18	-
29	24	32	28	8, 0, 4	0.399	12, 0, 0, 0	0.206	-	19167.35	-
30	24	32	28	7, 2, 4	0.261	2, 2, 8, 8	0.074	-	19325.91	-
31	24	32	28	6, 4, 4	0.236	2, 2, 8, 8	0.070	-	19524.67	-
32	24	32	28	5, 6, 4	0.227	4, 1, 7, 7	0.134	-	19754.24	-
33	24	32	28	3, 10, 4	0.283	7, 0, 5, 5	0.137	-	20009.60	-
34	24	36	30	2, 8, 6	0.338	7, 1, 4, 4	0.153	-	20391.23	-
35	24	36	30	4, 4, 6	0.265	3, 3, 6, 6	0.065	-	20608.69	-
36	24	36	30	5, 2, 6	0.284	3, 3, 6, 6	0.077	-	20795.64	-
37	24	36	30	6, 0, 6	0.409	12, 0, 0, 0	0.193	-	20942.20	-
38	24	36	30	5, 2, 6	0.233	3, 3, 6, 6	0.059	-	21075.51	-
39	24	36	30	4, 4, 6	0.261	5, 2, 5, 5	0.114	-	21247.09	-
40	24	36	30	2, 8, 6	0.318	7, 1, 4, 4	0.145	-	21453.76	-
41	24	40	32	1, 6, 8	0.427	6, 3, 3, 3	0.181	-	22419.10	-
42	24	40	32	0, 8, 8	0.334	4, 4, 4, 4	0.105	-	22611.38	-
43	24	40	32	4, 0, 8	0.379	11, 1, 0, 0	0.162	-	22763.45	-
44	24	40	32	4, 0, 8	0.348	11, 1, 0, 0	0.150	-	22881.05	-
45	24	40	32	2, 4, 8	0.362	8, 2, 2, 2	0.162	-	23025.60	-
46	24	44	34	0, 4, 10	0.575	5, 5, 2, 2	0.166	-	24478.63	-
47	24	44	34	2, 0, 10	0.426	5, 5, 2, 2	0.092	-	24629.31	-
48	24	44	34	2, 0, 10	0.450	9, 3, 0, 0	0.181	-	24732.75	-
49	24	48	36	0, 0, 12	0.984	6, 6, 0, 0	0.272	26552.21	26552.12	0.09
Symmetry Σ_u										
1	2	4	3	0, 0, 1	1.000	1, 0, 0, 0	1.000	2349.14	2349.13	0.01
1	4	6	5	0, 2, 1	0.538	1, 0, 1, 1	0.538	3612.84	3612.84	0.00
2	4	6	5	1, 0, 1	0.538	2, 0, 0, 0	0.538	3714.79	3714.83	-0.04
1	6	8	7	1, 2, 1	0.497	2, 0, 1, 1	0.497	4853.62	4853.57	0.05
2	6	8	7	2, 0, 1	0.664	3, 0, 0, 0	0.514	4977.83	4977.95	-0.11
3	6	8	7	1, 2, 1	0.503	2, 0, 1, 1	0.503	5099.66	5099.70	-0.04
4	6	12	9	0, 0, 3	0.999	2, 1, 0, 0	0.774	6972.58	6972.52	0.05
1	8	10	9	1, 4, 1	0.452	2, 0, 2, 2	0.452	6075.98	6075.93	0.05
2	8	10	9	3, 0, 1	0.461	1, 0, 3, 3	0.277	6227.92	6228.00	-0.09
3	8	10	9	3, 0, 1	0.445	1, 0, 3, 3	0.284	6347.85	6347.97	-0.12
4	8	10	9	1, 4, 1	0.456	2, 0, 2, 2	0.456	6503.08	6503.10	-0.02
5	8	14	11	0, 2, 3	0.594	2, 1, 1, 1	0.460	8192.55	8192.56	-0.01
6	8	14	11	1, 0, 3	0.593	3, 1, 0, 0	0.326	8293.95	8293.89	0.06
1	10	12	11	1, 6, 1	0.367	2, 0, 3, 3	0.367	7283.98	7284.13	-0.15
2	10	12	11	3, 2, 1	0.368	1, 0, 4, 4	0.231	7460.52	7460.54	-0.01
3	10	12	11	4, 0, 1	0.576	4, 1, 0, 0	0.302	7593.69	7593.75	-0.06
4	10	12	11	3, 2, 1	0.383	1, 0, 4, 4	0.262	7734.45	7734.51	-0.06
5	10	12	11	1, 6, 1	0.390	2, 0, 3, 3	0.390	7920.83	7920.94	-0.11
6	10	16	13	1, 2, 3	0.481	2, 1, 2, 2	0.305	9388.99	9388.99	0.01
7	10	16	13	2, 0, 3	0.648	5, 0, 0, 0	0.378	9516.97	9516.98	-0.02
8	10	16	13	1, 2, 3	0.503	3, 1, 1, 1	0.278	9631.35	9631.33	0.02
9	10	20	15	0, 0, 5	0.997	3, 2, 0, 0	0.665	11496.4	11496.38	0.06
1	12	14	13	2, 6, 1	0.364	3, 0, 3, 3	0.281	-	8480.91	-
2	12	14	13	4, 2, 1	0.321	2, 0, 4, 4	0.198	8676.72	8676.80	-0.08
3	12	14	13	5, 0, 1	0.489	5, 1, 0, 0	0.242	8831.48	8831.25	0.23
4	12	14	13	5, 0, 1	0.357	1, 0, 5, 5	0.222	8965.23	8965.10	0.13
5	12	14	13	3, 4, 1	0.281	1, 0, 5, 5	0.227	9137.8	9137.94	-0.14
6	12	14	13	2, 6, 1	0.358	2, 0, 4, 4	0.322	-	9350.27	-
7	12	18	15	1, 4, 3	0.462	3, 1, 2, 2	0.254	-	10567.59	-

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Table 3 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
8	12	18	15	3, 0, 3	0.391	6, 0, 0, 0	0.243	10724.03	10724.07	-0.04
9	12	18	15	3, 0, 3	0.500	6, 0, 0, 0	0.312	10842.06	10842.09	-0.03
10	12	18	15	1, 4, 3	0.439	3, 1, 2, 2	0.244	10986.27	10986.28	-0.01
11	12	22	17	0, 2, 5	0.651	3, 2, 1, 1	0.434	12672.28	12672.35	-0.07
12	12	22	17	1, 0, 5	0.648	5, 1, 0, 0	0.321	12774.73	12774.70	0.03
1	14	16	15	2, 8, 1	0.331	3, 0, 4, 4	0.256	-	9668.15	-
2	14	16	15	4, 4, 1	0.292	2, 0, 5, 5	0.222	-	9879.75	-
3	14	16	15	6, 0, 1	0.305	1, 0, 6, 6	0.164	-	10055.47	-
4	14	16	15	6, 0, 1	0.502	6, 1, 0, 0	0.213	-	10194.28	-
5	14	16	15	5, 2, 1	0.334	1, 0, 6, 6	0.226	-	10352.96	-
6	14	16	15	4, 4, 1	0.296	2, 0, 5, 5	0.208	-	10554.59	-
7	14	16	15	2, 8, 1	0.351	3, 0, 4, 4	0.275	-	10789.10	-
8	14	20	17	1, 6, 3	0.390	3, 1, 3, 3	0.214	-	11732.57	-
9	14	20	17	3, 2, 3	0.377	6, 0, 1, 1	0.235	11912.44	11912.46	-0.02
10	14	20	17	4, 0, 3	0.565	7, 0, 0, 0	0.340	12048.73	12048.58	0.15
11	14	20	17	3, 2, 3	0.366	6, 0, 1, 1	0.228	12179.97	12180.13	-0.16
12	14	20	17	1, 6, 3	0.366	5, 0, 2, 2	0.206	-	12355.36	-
13	14	24	19	1, 2, 5	0.457	3, 2, 2, 2	0.296	-	13824.48	-
14	14	24	19	2, 0, 5	0.610	6, 1, 0, 0	0.303	13957.22	13957.48	-0.25
15	14	24	19	1, 2, 5	0.490	5, 1, 1, 1	0.243	14065.69	14065.80	-0.11
16	14	28	21	0, 0, 7	0.995	4, 3, 0, 0	0.600	15921.09	15921.10	-0.01
1	18	20	19	3, 10, 1	0.294	3, 0, 6, 6	0.166	-	12019.28	-
2	18	20	19	5, 6, 1	0.244	2, 0, 7, 7	0.179	-	12254.64	-
3	18	20	19	7, 2, 1	0.262	2, 0, 7, 7	0.155	-	12462.79	-
4	18	20	19	8, 0, 1	0.392	7, 2, 0, 0	0.150	-	12633.72	-
5	18	20	19	8, 0, 1	0.405	7, 2, 0, 0	0.155	-	12778.86	-
6	18	20	19	7, 2, 1	0.296	1, 0, 8, 8	0.201	-	12955.66	-
7	18	20	19	6, 4, 1	0.260	1, 0, 8, 8	0.196	-	13171.68	-
8	18	20	19	5, 6, 1	0.231	2, 0, 7, 7	0.229	-	13417.72	-
9	18	20	19	2, 12, 1	0.296	3, 0, 6, 6	0.232	-	13689.52	-
10	18	24	21	2, 8, 3	0.339	5, 0, 4, 4	0.198	-	14031.43	-
11	18	24	21	4, 4, 3	0.294	7, 0, 2, 2	0.177	-	14244.50	-
12	18	24	21	5, 2, 3	0.293	8, 0, 1, 1	0.162	-	14424.05	-
13	18	24	21	6, 0, 3	0.502	9, 0, 0, 0	0.244	-	14563.72	-
14	18	24	21	5, 2, 3	0.316	8, 0, 1, 1	0.175	-	14711.36	-
15	18	24	21	4, 4, 3	0.295	7, 0, 2, 2	0.180	-	14901.51	-
16	18	24	21	2, 8, 3	0.344	5, 0, 4, 4	0.198	-	15125.07	-
17	18	28	23	1, 6, 5	0.409	5, 1, 3, 3	0.203	-	16081.52	-
18	18	28	23	3, 2, 5	0.364	3, 2, 4, 4	0.195	-	16265.67	-
19	18	28	23	4, 0, 5	0.516	9, 0, 0, 0	0.222	-	16406.79	-
20	18	28	23	3, 2, 5	0.324	3, 2, 4, 4	0.132	-	16530.65	-
21	18	28	23	2, 4, 5	0.364	6, 1, 2, 2	0.185	-	16694.16	-
22	18	32	25	0, 4, 7	0.498	4, 3, 2, 2	0.299	-	18160.43	-
23	18	32	25	2, 0, 7	0.549	7, 2, 0, 0	0.212	-	18299.71	-
24	18	32	25	1, 2, 7	0.461	6, 2, 1, 1	0.221	-	18404.01	-
25	18	36	27	0, 0, 9	0.991	5, 4, 0, 0	0.557	20247.02	20247.10	-0.09
1	22	24	23	4, 12, 1	0.264	4, 1, 6, 6	0.139	-	14345.43	-
2	22	24	23	6, 8, 1	0.208	3, 0, 8, 8	0.139	-	14597.53	-
3	22	24	23	8, 4, 1	0.235	2, 0, 9, 9	0.147	-	14827.35	-
4	22	24	23	9, 2, 1	0.277	2, 0, 9, 9	0.122	-	15028.70	-
5	22	24	23	10, 0, 1	0.455	8, 3, 0, 0	0.147	-	15192.11	-
6	22	24	23	10, 0, 1	0.287	1, 0, 10, 10	0.131	-	15348.03	-
7	22	24	23	9, 2, 1	0.250	1, 0, 10, 10	0.181	-	15542.96	-

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Table 3 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
8	22	24	23	8, 4, 1	0.228	1, 0, 10, 10	0.194	-	15772.61	-
9	22	24	23	7, 6, 1	0.208	2, 0, 9, 9	0.153	-	16029.60	-
10	22	28	25	3, 10, 3	0.293	6, 0, 5, 5	0.182	-	16298.65	-
11	22	24	23	5, 10, 1	0.220	2, 0, 9, 9	0.204	-	16310.51	-
12	22	28	25	5, 6, 3	0.244	8, 0, 3, 3	0.134	-	16533.92	-
13	22	24	23	3, 14, 1	0.284	3, 0, 8, 8	0.178	-	16613.24	-
14	22	28	25	7, 2, 3	0.215	9, 0, 2, 2	0.103	-	16743.40	-
15	22	28	25	8, 0, 3	0.296	2, 1, 8, 8	0.106	-	16918.22	-
16	22	28	25	8, 0, 3	0.414	11, 0, 0, 0	0.151	-	17060.54	-
17	22	28	25	7, 2, 3	0.281	2, 1, 8, 8	0.148	-	17225.21	-
18	22	28	25	6, 4, 3	0.249	2, 1, 8, 8	0.140	-	17429.86	-
19	22	28	25	5, 6, 3	0.232	8, 0, 3, 3	0.133	-	17664.96	-
20	22	28	25	3, 10, 3	0.286	6, 0, 5, 5	0.180	-	17925.80	-
21	22	32	27	2, 8, 5	0.340	6, 1, 4, 4	0.168	-	18295.93	-
22	22	32	27	4, 4, 5	0.279	9, 0, 2, 2	0.119	-	18511.60	-
23	22	32	27	5, 2, 5	0.295	10, 0, 1, 1	0.147	-	18695.84	-
24	22	32	27	6, 0, 5	0.452	11, 0, 0, 0	0.248	-	18839.35	-
25	22	32	27	5, 2, 5	0.268	10, 0, 1, 1	0.133	-	18976.92	-
26	22	32	27	4, 4, 5	0.277	9, 0, 2, 2	0.118	-	19154.94	-
27	22	32	27	2, 8, 5	0.329	6, 1, 4, 4	0.170	-	19367.35	-
28	22	36	29	1, 6, 7	0.423	6, 2, 3, 3	0.202	-	20331.31	-
29	22	36	29	3, 2, 7	0.331	4, 3, 4, 4	0.194	-	20520.63	-
30	22	36	29	4, 0, 7	0.431	10, 1, 0, 0	0.196	-	20668.66	-
31	22	36	29	4, 0, 7	0.323	10, 1, 0, 0	0.149	-	20787.42	-
32	22	36	29	2, 4, 7	0.366	7, 2, 2, 2	0.149	-	20938.48	-
33	22	40	31	0, 4, 9	0.550	5, 4, 2, 2	0.307	-	22397.25	-
34	22	40	31	2, 0, 9	0.470	9, 2, 0, 0	0.182	-	22543.91	-
35	22	40	31	1, 2, 9	0.415	7, 3, 1, 1	0.189	-	22646.84	-
36	22	44	33	0, 0, 11	0.986	6, 5, 0, 0	0.526	24474.85	24474.89	-0.05
Symmetry Π_g										
1	3	5	4	0, 1, 1	1.000	1, 0, 1, 0	1.000	3004.01	3004.07	-0.05
1	5	7	6	0, 3, 1	0.520	1, 0, 2, 1	0.520	4247.71	4247.67	0.03
2	5	7	6	1, 1, 1	0.520	2, 0, 1, 0	0.520	4390.63	4390.66	-0.03
1	7	9	8	1, 3, 1	0.499	2, 0, 2, 1	0.499	5475.07	5475.00	0.08
2	7	9	8	2, 1, 1	0.598	3, 0, 1, 0	0.463	5632.77	5632.77	-0.01
3	7	9	8	1, 3, 1	0.501	2, 0, 2, 1	0.501	5790.58	5790.58	0.00
4	7	13	10	0, 1, 3	0.999	2, 1, 1, 0	0.774	7602.51	7602.57	-0.06
1	9	11	10	1, 5, 1	0.426	2, 0, 3, 2	0.426	6688.17	6688.18	-0.01
2	9	11	10	3, 1, 1	0.442	1, 0, 4, 3	0.306	6863.56	6863.55	0.01
3	9	11	10	3, 1, 1	0.417	1, 0, 4, 3	0.318	7023.67	7023.69	-0.02
4	9	11	10	1, 5, 1	0.436	2, 0, 3, 2	0.436	7203.83	7203.85	-0.03
5	9	15	12	0, 3, 3	0.561	2, 1, 2, 1	0.434	8803.27	8803.28	-0.01
6	9	15	12	1, 1, 3	0.560	2, 1, 2, 1	0.341	8944.14	8944.11	0.03
1	11	13	12	2, 5, 1	0.366	2, 0, 4, 3	0.330	-	7889.46	-
2	11	13	12	3, 3, 1	0.329	1, 0, 5, 4	0.227	8081.84	8081.91	-0.08
3	11	13	12	4, 1, 1	0.497	1, 0, 5, 4	0.272	8250.63	8250.60	0.04
4	11	13	12	3, 3, 1	0.358	1, 0, 5, 4	0.262	8425.01	8425.06	-0.05
5	11	13	12	1, 7, 1	0.363	2, 0, 4, 3	0.363	-	8628.88	-
6	11	17	14	1, 3, 3	0.490	3, 1, 2, 1	0.270	9987.37	9987.35	0.02
7	11	17	14	2, 1, 3	0.589	5, 0, 1, 0	0.344	10145.49	10145.48	0.01
8	11	17	14	1, 3, 3	0.500	3, 1, 2, 1	0.277	10297.08	10297.05	0.03
9	11	21	16	0, 1, 5	0.997	3, 2, 1, 0	0.666	12101.57	12101.62	-0.05
1	15	17	16	2, 9, 1	0.309	3, 0, 5, 4	0.239	-	10263.23	-

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Table 3 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
2	15	17	16	4, 5, 1	0.255	2, 0, 6, 5	0.225	-	10484.07	-
3	15	17	16	6, 1, 1	0.310	1, 0, 7, 6	0.173	-	10678.21	-
4	15	17	16	6, 1, 1	0.430	1, 0, 7, 6	0.212	-	10855.16	-
5	15	17	16	5, 3, 1	0.309	1, 0, 7, 6	0.231	-	11043.98	-
6	15	17	16	4, 5, 1	0.291	2, 0, 6, 5	0.220	-	11261.46	-
7	15	17	16	2, 9, 1	0.343	3, 0, 5, 4	0.269	-	11507.42	-
8	15	21	18	1, 7, 3	0.355	5, 0, 3, 2	0.204	-	12315.91	-
9	15	21	18	3, 3, 3	0.346	6, 0, 2, 1	0.216	-	12509.93	-
10	15	21	18	4, 1, 3	0.488	7, 0, 1, 0	0.295	-	12677.73	-
11	15	21	18	3, 3, 3	0.336	6, 0, 2, 1	0.209	-	12844.90	-
12	15	21	18	2, 5, 3	0.361	5, 0, 3, 2	0.210	-	13038.54	-
13	15	25	20	1, 3, 5	0.475	3, 2, 3, 2	0.256	-	14400.02	-
14	15	25	20	2, 1, 5	0.567	6, 1, 1, 0	0.282	-	14559.87	-
15	15	25	20	1, 3, 5	0.491	5, 1, 2, 1	0.243	-	14706.32	-
16	15	29	22	0, 1, 7	0.994	4, 3, 1, 0	0.601	16501.57	16501.61	-0.04
1	19	21	20	3, 11, 1	0.281	4, 0, 6, 5	0.154	-	12606.90	-
2	19	21	20	6, 5, 1	0.224	2, 0, 8, 7	0.163	-	12848.50	-
3	19	21	20	7, 3, 1	0.270	2, 0, 8, 7	0.165	-	13066.52	-
4	19	21	20	8, 1, 1	0.355	7, 2, 1, 0	0.136	-	13260.46	-
5	19	21	20	8, 1, 1	0.359	1, 0, 9, 8	0.175	-	13445.12	-
6	19	21	20	7, 3, 1	0.281	1, 0, 9, 8	0.208	-	13647.44	-
7	19	21	20	6, 5, 1	0.253	1, 0, 9, 8	0.188	-	13877.65	-
8	19	21	20	5, 7, 1	0.238	2, 0, 8, 7	0.227	-	14134.34	-
9	19	21	20	3, 11, 1	0.289	3, 0, 7, 6	0.220	-	14415.11	-
10	19	25	22	2, 9, 3	0.321	5, 0, 5, 4	0.188	-	14605.04	-
11	19	25	22	4, 5, 3	0.269	7, 0, 3, 2	0.162	-	14826.50	-
12	19	25	22	6, 1, 3	0.251	2, 1, 7, 6	0.148	-	15021.52	-
13	19	25	22	6, 1, 3	0.422	9, 0, 1, 0	0.206	-	15195.91	-
14	19	25	22	5, 3, 3	0.283	2, 1, 7, 6	0.168	-	15376.29	-
15	19	25	22	4, 5, 3	0.281	7, 0, 3, 2	0.172	-	15583.29	-
16	19	25	22	2, 9, 3	0.333	5, 0, 5, 4	0.191	-	15818.46	-
17	19	29	24	1, 7, 5	0.378	5, 1, 4, 3	0.187	-	16643.06	-
18	19	29	24	3, 3, 5	0.348	3, 2, 5, 4	0.186	-	16839.79	-
19	19	29	24	4, 1, 5	0.456	9, 0, 1, 0	0.196	-	17008.38	-
20	19	29	24	3, 3, 5	0.297	3, 2, 5, 4	0.140	-	17169.39	-
21	19	29	24	2, 5, 5	0.366	6, 1, 3, 2	0.186	-	17352.91	-
22	19	33	26	1, 3, 7	0.451	4, 3, 3, 2	0.259	-	18713.35	-
23	19	33	26	2, 1, 7	0.530	4, 3, 3, 2	0.234	-	18876.37	-
24	19	33	26	1, 3, 7	0.472	6, 2, 2, 1	0.227	-	19019.14	-
25	19	37	28	0, 1, 9	0.991	5, 4, 1, 0	0.558	20803.02	20802.98	0.04
Symmetry Π_u										
1	1	1	1	0, 1, 0	1.000	0, 0, 1, 0	1.000	667.38	667.40	-0.02
1	3	3	3	0, 3, 0	0.500	0, 0, 2, 1	0.500	1932.47	1932.38	0.09
2	3	3	3	1, 1, 0	0.500	0, 0, 2, 1	0.500	2076.86	2076.89	-0.04
1	5	5	5	1, 3, 0	0.500	0, 0, 3, 2	0.286	3181.46	3181.31	0.15
2	5	5	5	2, 1, 0	0.598	0, 0, 3, 2	0.402	3339.36	3339.39	-0.03
3	5	5	5	1, 3, 0	0.499	0, 0, 3, 2	0.312	3500.67	3500.65	0.02
4	5	9	7	0, 1, 2	1.000	1, 1, 1, 0	0.516	5315.71	5315.78	-0.06
1	7	7	7	1, 5, 0	0.417	1, 0, 3, 2	0.417	4416.15	4416.10	0.05
2	7	7	7	3, 1, 0	0.460	0, 0, 4, 3	0.297	4591.12	4591.15	-0.03
3	7	7	7	3, 1, 0	0.399	0, 0, 4, 3	0.327	4753.45	4753.49	-0.03
4	7	7	7	1, 5, 0	0.442	1, 0, 3, 2	0.442	4938.35	4938.29	0.07
5	7	11	9	0, 3, 2	0.540	1, 1, 2, 1	0.279	6537.96	6537.96	0.00

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Table 3 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
6	7	11	9	1, 1, 2	0.540	1, 1, 2, 1	0.238	6679.71	6679.71	0.00
1	9	9	9	2, 5, 0	0.371	1, 1, 3, 2	0.180	-	5638.86	-
2	9	9	9	3, 3, 0	0.316	0, 0, 5, 4	0.215	5830.80	5830.90	-0.10
3	9	9	9	4, 1, 0	0.493	0, 0, 5, 4	0.271	6000.53	6000.58	-0.05
4	9	9	9	3, 3, 0	0.363	0, 0, 5, 4	0.273	6179.04	6179.02	0.02
5	9	9	9	1, 7, 0	0.373	1, 0, 4, 3	0.373	6388.08	6387.99	0.09
6	9	13	11	1, 3, 2	0.496	3, 0, 2, 1	0.360	7743.7	7743.66	0.04
7	9	13	11	2, 1, 2	0.595	4, 0, 1, 0	0.446	7901.47	7901.45	0.02
8	9	13	11	1, 3, 2	0.502	3, 0, 2, 1	0.363	8056.03	8056.01	0.01
9	9	17	13	0, 1, 4	0.998	2, 2, 1, 0	0.400	9864.85	9864.51	0.35
1	11	11	11	2, 7, 0	0.353	1, 1, 4, 3	0.171	-	6851.41	-
2	11	11	11	4, 3, 0	0.331	0, 0, 6, 5	0.151	-	7058.87	-
3	11	11	11	5, 1, 0	0.450	0, 0, 6, 5	0.214	7240.00	7240.02	-0.02
4	11	11	11	5, 1, 0	0.324	0, 0, 6, 5	0.254	-	7416.24	-
5	11	11	11	4, 3, 0	0.274	0, 0, 6, 5	0.226	7616.63	7616.66	-0.03
6	11	11	11	2, 7, 0	0.356	1, 1, 4, 3	0.171	7847.82	7847.92	-0.10
7	11	15	13	1, 5, 2	0.434	3, 0, 3, 2	0.315	-	8935.28	-
8	11	15	13	3, 1, 2	0.421	1, 1, 4, 3	0.163	-	9111.23	-
9	11	15	13	3, 1, 2	0.435	1, 1, 4, 3	0.160	-	9269.51	-
10	11	15	13	1, 5, 2	0.428	3, 0, 3, 2	0.309	-	9445.13	-
11	11	19	15	0, 3, 4	0.582	2, 2, 2, 1	0.233	-	11043.68	-
12	11	19	15	1, 1, 4	0.580	4, 1, 1, 0	0.347	-	11183.94	-
1	13	13	13	3, 7, 0	0.303	1, 1, 5, 4	0.146	-	8055.22	-
2	13	13	13	5, 3, 0	0.256	1, 0, 6, 5	0.222	-	8276.12	-
3	13	13	13	6, 1, 0	0.332	0, 0, 7, 6	0.164	-	8470.27	-
4	13	13	13	6, 1, 0	0.422	0, 0, 7, 6	0.210	-	8649.08	-
5	13	13	13	5, 3, 0	0.313	0, 0, 7, 6	0.239	-	8842.38	-
6	13	13	13	4, 5, 0	0.291	0, 0, 7, 6	0.184	-	9065.15	-
7	13	13	13	2, 9, 0	0.345	1, 1, 5, 4	0.165	-	9316.56	-
8	13	17	15	2, 5, 2	0.359	4, 0, 3, 2	0.268	-	10115.12	-
9	13	17	15	3, 3, 2	0.340	1, 1, 5, 4	0.123	-	10308.23	-
10	13	17	15	4, 1, 2	0.496	1, 1, 5, 4	0.141	-	10476.27	-
11	13	17	15	3, 3, 2	0.349	1, 1, 5, 4	0.130	-	10646.97	-
12	13	17	15	2, 5, 2	0.356	4, 0, 3, 2	0.268	-	10845.69	-
13	13	21	17	1, 3, 4	0.483	4, 1, 2, 1	0.289	-	12206.12	-
14	13	21	17	2, 1, 4	0.580	2, 2, 3, 2	0.160	-	12364.94	-
15	13	21	17	1, 3, 4	0.497	4, 1, 2, 1	0.299	-	12513.79	-
16	13	25	19	0, 1, 6	0.996	3, 3, 1, 0	0.344	14313.92	14313.97	-0.05
1	17	17	17	3, 11, 0	0.277	2, 1, 6, 5	0.201	-	10441.07	-
2	17	17	17	6, 5, 0	0.234	1, 1, 7, 6	0.088	-	10683.42	-
3	17	17	17	7, 3, 0	0.278	0, 0, 9, 8	0.087	-	10901.80	-
4	17	17	17	8, 1, 0	0.376	0, 0, 9, 8	0.128	-	11096.36	-
5	17	17	17	8, 1, 0	0.350	0, 0, 9, 8	0.173	-	11283.88	-
6	17	17	17	7, 3, 0	0.283	0, 0, 9, 8	0.212	-	11491.07	-
7	17	17	17	6, 5, 0	0.254	0, 0, 9, 8	0.196	-	11726.62	-
8	17	17	17	5, 7, 0	0.236	0, 0, 9, 8	0.118	-	11988.78	-
9	17	17	17	3, 11, 0	0.287	1, 1, 7, 6	0.136	-	12275.11	-
10	17	21	19	2, 9, 2	0.316	4, 0, 5, 4	0.236	-	12446.48	-
11	17	21	19	4, 5, 2	0.264	3, 0, 6, 5	0.164	-	12667.49	-
12	17	21	19	6, 1, 2	0.282	1, 1, 7, 6	0.093	-	12861.91	-
13	17	21	19	6, 1, 2	0.430	1, 1, 7, 6	0.110	-	13037.37	-
14	17	21	19	5, 3, 2	0.299	1, 1, 7, 6	0.117	-	13221.87	-
15	17	21	19	4, 5, 2	0.288	1, 1, 7, 6	0.087	-	13434.11	-

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Table 3 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
16	17	21	19	2, 9, 2	0.339	4, 0, 5, 4	0.255	-	13674.66	-
17	17	25	21	1, 7, 4	0.366	4, 1, 4, 3	0.219	-	14491.87	-
18	17	25	21	3, 3, 4	0.350	2, 2, 5, 4	0.106	-	14687.10	-
19	17	25	21	4, 1, 4	0.475	8, 0, 1, 0	0.260	-	14855.07	-
20	17	25	21	3, 3, 4	0.319	2, 2, 5, 4	0.091	-	15018.99	-
21	17	25	21	2, 5, 4	0.364	4, 1, 4, 3	0.196	-	15207.57	-
22	17	29	23	1, 3, 6	0.464	3, 3, 3, 2	0.140	-	16569.08	-
23	17	29	23	2, 1, 6	0.550	3, 3, 3, 2	0.136	-	16730.33	-
24	17	29	23	1, 3, 6	0.483	5, 2, 2, 1	0.242	-	16874.74	-
25	17	33	25	0, 1, 8	0.993	4, 4, 1, 0	0.311	18664.57	18664.59	-0.01
Symmetry Δ_g										
1	2	2	2	0, 2, 0	1.000	0, 0, 2, 0	1.000	1335.13	1335.16	-0.02
1	4	4	4	1, 2, 0	0.505	0, 0, 3, 1	0.495	2585.02	2584.89	0.13
2	4	4	4	0, 4, 0	0.505	0, 0, 3, 1	0.505	2760.73	2760.69	0.03
1	6	6	6	1, 4, 0	0.500	0, 0, 4, 2	0.269	3822.01	3821.86	0.15
2	6	6	6	2, 2, 0	0.569	0, 0, 4, 2	0.430	4007.91	4007.83	0.08
3	6	6	6	1, 4, 0	0.499	0, 0, 4, 2	0.301	4197.36	4197.25	0.11
4	6	10	8	0, 2, 2	1.000	1, 1, 2, 0	0.517	5958.51	5958.62	-0.11
1	8	8	8	1, 6, 0	0.401	1, 0, 4, 2	0.401	-	5047.34	-
2	8	8	8	3, 2, 0	0.445	0, 0, 5, 3	0.312	5245.28	5245.44	-0.16
3	8	8	8	3, 2, 0	0.387	0, 0, 5, 3	0.344	5436.5	5437.13	-0.63
4	8	8	8	1, 6, 0	0.432	1, 0, 4, 2	0.432	5644.9	5644.70	0.20
5	8	12	10	0, 4, 2	0.527	1, 1, 3, 1	0.272	7166.02	7166.01	0.02
6	8	12	10	1, 2, 2	0.527	1, 1, 3, 1	0.245	7338.16	7338.15	0.01
1	10	10	10	2, 6, 0	0.374	1, 1, 4, 2	0.181	-	6262.68	-
2	10	10	10	3, 4, 0	0.292	0, 0, 6, 4	0.215	-	6473.23	-
3	10	10	10	4, 2, 0	0.459	0, 0, 6, 4	0.295	-	6670.56	-
4	10	10	10	3, 4, 0	0.348	0, 0, 6, 4	0.275	-	6875.05	-
5	10	10	10	1, 8, 0	0.356	1, 0, 5, 3	0.356	-	7102.09	-
6	10	14	12	1, 4, 2	0.497	3, 0, 3, 1	0.361	-	8360.38	-
7	10	14	12	2, 2, 2	0.568	1, 1, 4, 2	0.222	-	8544.35	-
8	10	14	12	1, 4, 2	0.501	3, 0, 3, 1	0.362	-	8727.27	-
9	10	18	14	0, 2, 4	0.998	2, 2, 2, 0	0.400	10482.43	10482.50	-0.07
1	14	14	14	3, 8, 0	0.309	1, 1, 6, 4	0.137	-	8667.88	-
2	14	14	14	5, 4, 0	0.268	1, 0, 7, 5	0.223	-	8900.92	-
3	14	14	14	6, 2, 0	0.324	0, 0, 8, 6	0.170	-	9115.05	-
4	14	14	14	6, 2, 0	0.391	0, 0, 8, 6	0.230	-	9321.46	-
5	14	14	14	5, 4, 0	0.297	0, 0, 8, 6	0.245	-	9538.67	-
6	14	14	14	4, 6, 0	0.285	0, 0, 8, 6	0.175	-	9778.10	-
7	14	14	14	2, 10, 0	0.338	1, 1, 6, 4	0.161	-	10042.01	-
8	14	18	16	2, 6, 2	0.366	4, 0, 4, 2	0.274	-	10716.13	-
9	14	18	16	3, 4, 2	0.315	1, 1, 6, 4	0.122	-	10925.99	-
10	14	18	16	4, 2, 2	0.460	1, 1, 6, 4	0.153	-	11120.04	-
11	14	18	16	3, 4, 2	0.333	1, 1, 6, 4	0.133	-	11317.20	-
12	14	18	16	2, 6, 2	0.361	4, 0, 4, 2	0.271	-	11534.54	-
13	14	22	18	1, 4, 4	0.489	4, 1, 3, 1	0.293	-	12799.22	-
14	14	22	18	2, 2, 4	0.557	2, 2, 4, 2	0.172	-	12982.42	-
15	14	22	18	1, 4, 4	0.497	4, 1, 3, 1	0.299	-	13159.75	-
16	14	26	20	0, 2, 6	0.996	3, 3, 2, 0	0.344	14907.22	14907.19	0.03
Symmetry Δ_u										
1	4	6	5	0, 2, 1	1.000	1, 0, 2, 0	1.000	3659.27	3659.36	-0.09
1	6	8	7	0, 4, 1	0.511	1, 0, 3, 1	0.511	4887.97	4887.93	0.03
2	6	8	7	1, 2, 1	0.511	2, 0, 2, 0	0.511	5061.78	5061.77	0.01

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Table 3 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
1	8	10	9	1, 4, 1	0.499	2, 0, 3, 1	0.499	6103.68	6103.61	0.08
2	8	10	9	2, 2, 1	0.569	3, 0, 2, 0	0.441	6288.49	6288.44	0.06
3	8	10	9	1, 4, 1	0.501	2, 0, 3, 1	0.501	6474.53	6474.50	0.03
4	8	14	11	0, 2, 3	0.999	2, 1, 2, 0	0.774	8232.88	8232.98	-0.10
1	10	12	11	1, 6, 1	0.409	2, 0, 4, 2	0.409	7307.67	7307.77	-0.10
2	10	12	11	3, 2, 1	0.432	1, 0, 5, 3	0.320	7505.25	7505.21	0.04
3	10	12	11	3, 2, 1	0.401	1, 0, 5, 3	0.336	7694.40	7694.38	0.02
4	10	12	11	1, 6, 1	0.426	2, 0, 4, 2	0.426	7897.55	7897.62	-0.07
5	10	16	13	0, 4, 3	0.545	2, 1, 3, 1	0.421	9419.12	9419.16	-0.04
6	10	16	13	1, 2, 3	0.544	2, 1, 3, 1	0.354	9589.82	9589.89	-0.07
1	12	14	13	2, 6, 1	0.371	2, 0, 5, 3	0.306	-	8501.85	-
2	12	14	13	3, 4, 1	0.304	1, 0, 6, 4	0.226	-	8711.92	-
3	12	14	13	4, 2, 1	0.462	1, 0, 6, 4	0.296	-	8907.46	-
4	12	14	13	3, 4, 1	0.342	1, 0, 6, 4	0.265	-	9108.18	-
5	12	14	13	2, 6, 1	0.356	2, 0, 5, 3	0.347	-	9330.32	-
6	12	18	15	1, 4, 3	0.494	3, 1, 3, 1	0.272	-	10592.24	-
7	12	18	15	2, 2, 3	0.563	2, 1, 4, 2	0.333	10776.11	10775.66	0.46
8	12	18	15	1, 4, 3	0.500	3, 1, 3, 1	0.278	-	10955.66	-
9	12	22	17	0, 2, 5	0.997	3, 2, 2, 0	0.666	12707.19	12707.22	-0.03
1	16	18	17	3, 8, 1	0.305	3, 0, 6, 4	0.225	-	10864.76	-
2	16	18	17	5, 4, 1	0.257	2, 0, 7, 5	0.226	-	11097.14	-
3	16	18	17	6, 2, 1	0.307	1, 0, 8, 6	0.178	-	11310.23	-
4	16	18	17	6, 2, 1	0.396	1, 0, 8, 6	0.231	-	11514.16	-
5	16	18	17	5, 4, 1	0.290	1, 0, 8, 6	0.238	-	11727.19	-
6	16	18	17	4, 6, 1	0.283	2, 0, 7, 5	0.228	-	11961.59	-
7	16	18	17	2, 10, 1	0.335	3, 0, 6, 4	0.263	-	12220.13	-
8	16	22	19	2, 6, 3	0.359	5, 0, 4, 2	0.209	-	12905.60	-
9	16	22	19	3, 4, 3	0.324	6, 0, 3, 1	0.202	-	13115.54	-
10	16	22	19	4, 2, 3	0.454	7, 0, 2, 0	0.274	-	13308.44	-
11	16	22	19	3, 4, 3	0.320	6, 0, 3, 1	0.199	-	13502.25	-
12	16	22	19	2, 6, 3	0.364	5, 0, 4, 2	0.211	-	13714.87	-
13	16	26	21	1, 4, 5	0.482	5, 1, 3, 1	0.239	-	14981.39	-
14	16	26	21	2, 2, 5	0.547	3, 2, 4, 2	0.284	-	15164.69	-
15	16	26	21	1, 4, 5	0.493	5, 1, 3, 1	0.244	-	15339.65	-
16	16	30	23	0, 2, 7	0.994	4, 3, 2, 0	0.602	17082.59	17082.48	0.11
Symmetry Φ_g										
1	5	7	6	0, 3, 1	1.000	1, 0, 3, 0	1.000	4314.91	4315.01	-0.09
1	7	9	8	0, 5, 1	0.505	1, 0, 4, 1	0.505	5531.30	5531.23	0.07
2	7	9	8	1, 3, 1	0.505	2, 0, 3, 0	0.505	5730.61	5730.56	0.04
1	9	11	10	1, 5, 1	0.500	2, 0, 4, 1	0.500	6736.76	6736.73	0.03
2	9	11	10	2, 3, 1	0.553	1, 0, 5, 2	0.446	6944.73	6944.62	0.12
3	9	11	10	1, 5, 1	0.500	2, 0, 4, 1	0.500	7154.63	7154.46	0.17
4	9	15	12	0, 3, 3	0.999	2, 1, 3, 0	0.775	8863.68	8863.75	-0.07
1	13	15	14	2, 7, 1	0.373	2, 0, 6, 3	0.289	-	9119.67	-
2	13	15	14	3, 5, 1	0.287	1, 0, 7, 4	0.224	-	9346.75	-
3	13	15	14	4, 3, 1	0.442	1, 0, 7, 4	0.311	-	9564.57	-
4	13	15	14	3, 5, 1	0.332	1, 0, 7, 4	0.268	-	9787.32	-
5	13	15	14	2, 7, 1	0.360	2, 0, 6, 3	0.336	-	10026.99	-
6	13	19	16	1, 5, 3	0.496	3, 1, 4, 1	0.273	-	11201.35	-
7	13	19	16	2, 3, 3	0.549	2, 1, 5, 2	0.345	-	11406.63	-
8	13	19	16	1, 5, 3	0.500	3, 1, 4, 1	0.278	-	11610.30	-
9	13	23	18	0, 3, 5	0.997	3, 2, 3, 0	0.667	13313.28	13313.18	0.10
Symmetry Φ_u										

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Table 3 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
1	3	3	3	0, 3, 0	1.000	0, 0, 3, 0	1.000	2003.25	2003.27	-0.03
1	5	5	5	1, 3, 0	0.509	0, 0, 4, 1	0.491	3240.62	3240.48	0.14
2	5	5	5	0, 5, 0	0.509	0, 0, 4, 1	0.509	3442.22	3442.13	0.09
1	7	7	7	1, 5, 0	0.500	0, 0, 5, 2	0.258	4467.12	4467.05	0.06
2	7	7	7	2, 3, 0	0.552	0, 0, 5, 2	0.446	4676.79	4676.66	0.13
3	7	7	7	1, 5, 0	0.499	0, 0, 5, 2	0.296	4890.1	4889.91	0.19
4	7	11	9	0, 3, 2	1.000	1, 1, 3, 0	0.517	6601.71	6601.82	-0.11
1	9	9	9	1, 7, 0	0.390	1, 0, 5, 2	0.390	-	5683.95	-
2	9	9	9	3, 3, 0	0.436	0, 0, 6, 3	0.320	-	5902.73	-
3	9	9	9	3, 3, 0	0.379	0, 0, 6, 3	0.355	-	6118.40	-
4	9	9	9	1, 7, 0	0.426	1, 0, 5, 2	0.426	6346.71	6346.55	0.15
5	9	13	11	0, 5, 2	0.519	1, 1, 4, 1	0.268	-	7797.04	-
6	9	13	11	1, 3, 2	0.519	1, 1, 4, 1	0.250	-	7994.32	-
1	11	11	11	2, 7, 0	0.375	1, 1, 5, 2	0.182	-	6892.16	-
2	11	11	11	4, 3, 0	0.290	0, 0, 7, 4	0.215	-	7120.41	-
3	11	11	11	4, 3, 0	0.440	0, 0, 7, 4	0.310	-	7340.53	-
4	11	11	11	3, 5, 0	0.338	0, 0, 7, 4	0.278	-	7567.05	-
5	11	11	11	2, 7, 0	0.355	1, 0, 6, 3	0.345	-	7811.48	-
6	11	15	13	1, 5, 2	0.498	3, 0, 4, 1	0.361	-	8981.48	-
7	11	15	13	2, 3, 2	0.552	1, 1, 5, 2	0.231	-	9187.91	-
8	11	15	13	1, 5, 2	0.501	3, 0, 4, 1	0.362	-	9394.56	-
9	11	19	15	0, 3, 4	0.998	2, 2, 3, 0	0.401	11100.85	11100.86	0.00
Symmetry Γ_g										
1	4	4	4	0, 4, 0	1.000	0, 0, 4, 0	1.000	2671.14	2671.75	-0.60
1	6	6	6	1, 4, 0	0.513	0, 0, 5, 1	0.487	3898.33	3898.20	0.13
2	6	6	6	0, 6, 0	0.513	0, 0, 5, 1	0.513	4122.27	4122.14	0.13
1	8	8	8	1, 6, 0	0.499	0, 0, 6, 2	0.250	5115.3	5115.57	-0.27
2	8	8	8	2, 4, 0	0.542	0, 0, 6, 2	0.456	5345.6	5345.86	-0.26
3	8	8	8	1, 6, 0	0.499	0, 0, 6, 2	0.294	-	5579.95	-
4	8	12	10	0, 4, 2	1.000	1, 1, 4, 0	0.517	-	7245.38	-
Symmetry Γ_u										
1	6	8	7	0, 4, 1	1.000	1, 0, 4, 0	1.000	4970.93	4971.02	-0.09
1	8	10	9	1, 4, 1	0.500	2, 0, 4, 0	0.500	6176.65	6176.64	0.01
2	8	10	9	0, 6, 1	0.500	1, 0, 5, 1	0.500	6398.07	6397.97	0.11
Symmetry H_g										
1	7	9	8	0, 5, 1	1.000	1, 0, 5, 0	1.000	5627.25	5627.38	-0.13
1	9	11	10	1, 5, 1	0.504	2, 0, 5, 0	0.504	-	6823.66	-
2	9	11	10	0, 7, 1	0.504	1, 0, 6, 1	0.504	7064.51	7064.46	0.06
Symmetry H_u										
1	5	5	5	0, 5, 0	1.000	0, 0, 5, 0	1.000	3340.72	3340.58	0.14
1	7	7	7	1, 5, 0	0.516	0, 0, 6, 1	0.484	4557.59	4557.56	0.03
2	7	7	7	0, 7, 0	0.516	0, 0, 6, 1	0.516	4801.36	4801.24	0.12
Symmetry I_g										
1	6	6	6	0, 6, 0	1.000	0, 0, 6, 0	1.000	4009.67	4009.77	-0.10
1	8	8	8	1, 6, 0	0.518	0, 0, 7, 1	0.482	5218.7	5218.27	0.43
2	8	8	8	0, 8, 0	0.518	0, 0, 7, 1	0.518	-	5479.70	-
Symmetry I_u										
1	8	10	9	0, 6, 1	1.000	1, 0, 6, 0	1.000	6283.98	6284.11	-0.13
Symmetry J_u										
1	7	7	7	0, 7, 0	1.000	0, 0, 7, 0	1.000	4679.15	4679.32	-0.17

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Table 3 – Continued from previous page

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
	P_{212}	P_{214}	P_{213}							

[a] The column labeled state indicates the state position from lower to higher energy inside the polyad for a given symmetry. The second column, labeled Polyad, indicates the polyad to which the state belongs. [b] The third and fourth columns, with headings normal state and coefficient, assign normal-mode labels ($\nu_1\nu_2\nu_3$) the state according to the square value of the largest contribution in this basis. [c] The fifth and sixth columns, with headings local state and coefficient, assign local-mode labels ($v_1v_2n_+n_-$) the state and its squared maximum component in the local basis is shown. [d] Experimental vibrational energies are taken from Ref.[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

Table 4: Fit of energies (in cm^{-1}) of $^{12}\text{CO}_2$ provided by the Hamiltonian (18) associated with Polyad P_{213} .

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
	P_{213}	P_{214}	P_{212}							
Symmetry Σ_g										
1	2	2	2	0, 2, 0	0.512	0, 0, 1, 1	0.512	1285.41	1285.41	0.00
2	2	2	2	1, 0, 0	0.512	0, 0, 1, 1	0.488	1388.18	1388.31	-0.12
1	4	4	4	1, 2, 0	0.499	0, 0, 2, 2	0.327	2548.37	2548.28	0.09
2	4	4	4	2, 0, 0	0.665	0, 0, 2, 2	0.335	2671.14	2671.38	-0.24
3	4	4	4	1, 2, 0	0.500	0, 0, 2, 2	0.338	2797.14	2797.20	-0.07
1	6	6	6	1, 4, 0	0.445	1, 0, 2, 2	0.445	3792.68	3792.62	0.06
2	6	6	6	3, 0, 0	0.489	0, 0, 3, 3	0.266	3942.54	3942.76	-0.22
3	6	6	6	3, 0, 0	0.418	0, 0, 3, 3	0.295	4064.28	4064.49	-0.22
4	6	6	6	1, 4, 0	0.461	0, 0, 3, 3	0.235	4225.10	4225.05	0.04
5	6	8	4	0, 0, 2	1.000	1, 1, 0, 0	0.500	4673.33	4673.29	0.03
1	8	8	8	2, 4, 0	0.360	1, 1, 2, 2	0.180	0.00	5022.62	-
2	8	8	8	3, 2, 0	0.358	0, 0, 4, 4	0.219	5197.15	5197.42	-0.27
3	8	8	8	4, 0, 0	0.571	0, 0, 4, 4	0.223	5330.60	5329.92	0.68
4	8	8	8	3, 2, 0	0.385	0, 0, 4, 4	0.273	5475.57	5475.59	-0.03
5	8	8	8	1, 6, 0	0.398	1, 0, 3, 3	0.398	0.00	5667.56	-
6	8	10	6	0, 2, 2	0.568	1, 1, 1, 1	0.284	5915.21	5915.23	-0.02
7	8	10	6	1, 0, 2	0.568	1, 1, 1, 1	0.216	6016.69	6016.70	-0.01
1	10	10	10	2, 6, 0	0.364	1, 1, 3, 3	0.182	0.00	6241.09	-
2	10	10	10	4, 2, 0	0.331	0, 0, 5, 5	0.168	0.00	6435.84	-
3	10	10	10	5, 0, 0	0.513	0, 0, 5, 5	0.182	0.00	6588.44	-
4	10	10	10	5, 0, 0	0.331	0, 0, 5, 5	0.229	0.00	6725.30	-
5	10	10	10	3, 4, 0	0.293	0, 0, 5, 5	0.236	0.00	6903.89	-
6	10	10	10	2, 6, 0	0.356	1, 1, 3, 3	0.178	0.00	7121.79	-
7	10	12	8	1, 2, 2	0.489	1, 1, 2, 2	0.186	7133.82	7133.79	0.03
8	10	12	8	2, 0, 2	0.660	4, 0, 0, 0	0.495	7259.75	7259.81	-0.07
9	10	12	8	1, 2, 2	0.506	3, 0, 1, 1	0.379	7377.62	7377.73	-0.11
1	12	12	12	2, 8, 0	0.327	1, 1, 4, 4	0.163	0.00	7450.00	-
2	12	12	12	4, 4, 0	0.287	0, 0, 6, 6	0.120	0.00	7660.83	-
3	12	12	12	6, 0, 0	0.338	0, 0, 6, 6	0.156	0.00	7834.78	-
4	12	12	12	6, 0, 0	0.490	0, 0, 6, 6	0.176	0.00	7974.08	-
5	12	12	12	5, 2, 0	0.335	0, 0, 6, 6	0.233	0.00	8138.33	-
6	12	14	10	1, 4, 2	0.458	3, 0, 2, 2	0.344	0.00	8334.23	-
7	12	12	12	4, 4, 0	0.294	0, 0, 6, 6	0.195	0.00	8345.58	-
8	12	14	10	3, 0, 2	0.429	1, 1, 3, 3	0.146	0.00	8488.37	-
9	12	12	12	2, 8, 0	0.352	1, 1, 4, 4	0.176	0.00	8585.74	-
10	12	14	10	3, 0, 2	0.478	5, 0, 0, 0	0.299	0.00	8607.17	-
11	12	14	10	1, 4, 2	0.448	3, 0, 2, 2	0.336	0.00	8756.87	-
12	12	16	8	0, 0, 4	1.000	2, 2, 0, 0	0.375	9246.93	9246.88	0.06
1	14	14	14	3, 8, 0	0.306	1, 1, 5, 5	0.135	0.00	8650.77	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
2	14	14	14	5, 4, 0	0.275	1, 0, 6, 6	0.207	0.00	8874.83	-
3	14	14	14	6, 2, 0	0.314	0, 0, 7, 7	0.128	0.00	9067.22	-
4	14	14	14	7, 0, 0	0.522	4, 3, 0, 0	0.286	0.00	9219.18	-
5	14	14	14	6, 2, 0	0.274	0, 0, 7, 7	0.194	0.00	9371.49	-
6	14	16	12	1, 6, 2	0.381	3, 0, 3, 3	0.285	0.00	9520.81	-
7	14	14	14	5, 4, 0	0.251	0, 0, 7, 7	0.221	0.00	9567.00	-
8	14	16	12	3, 2, 2	0.377	1, 1, 4, 4	0.124	0.00	9698.79	-
9	14	14	14	4, 6, 0	0.275	0, 0, 7, 7	0.158	0.00	9798.03	-
10	14	16	12	4, 0, 2	0.582	6, 0, 0, 0	0.273	0.00	9833.30	-
11	14	16	12	3, 2, 2	0.379	1, 1, 4, 4	0.122	0.00	9969.39	-
12	14	14	14	2, 10, 0	0.330	1, 1, 5, 5	0.165	0.00	10057.94	-
13	14	16	12	1, 6, 2	0.376	3, 0, 3, 3	0.282	0.00	10150.41	-
14	14	18	10	0, 2, 4	0.626	2, 2, 1, 1	0.235	10444.89	10445.04	-0.15
15	14	18	10	1, 0, 4	0.626	4, 1, 0, 0	0.352	10546.61	10546.58	0.03
1	18	18	18	4, 10, 0	0.267	2, 2, 5, 5	0.100	0.00	11032.23	-
2	18	18	18	6, 6, 0	0.241	1, 1, 7, 7	0.092	0.00	11276.63	-
3	18	18	18	7, 4, 0	0.240	1, 0, 8, 8	0.159	0.00	11496.23	-
4	18	18	18	9, 0, 0	0.283	0, 0, 9, 9	0.096	0.00	11682.36	-
5	18	18	18	9, 0, 0	0.484	5, 4, 0, 0	0.238	0.00	11833.85	-
6	18	20	16	2, 8, 2	0.337	4, 0, 4, 4	0.253	0.00	11862.42	-
7	18	18	18	8, 2, 0	0.291	0, 0, 9, 9	0.171	0.00	12003.65	-
8	18	20	16	4, 4, 2	0.299	3, 0, 5, 5	0.165	0.00	12074.48	-
9	18	18	18	7, 4, 0	0.241	0, 0, 9, 9	0.204	0.00	12215.09	-
10	18	20	16	5, 2, 2	0.288	1, 1, 6, 6	0.089	0.00	12252.11	-
11	18	20	16	6, 0, 2	0.523	7, 1, 0, 0	0.229	0.00	12391.21	-
12	18	18	18	6, 6, 0	0.234	0, 0, 9, 9	0.177	0.00	12458.48	-
13	18	20	16	5, 2, 2	0.335	1, 1, 6, 6	0.108	0.00	12544.41	-
14	18	18	18	5, 8, 0	0.232	1, 0, 8, 8	0.215	0.00	12728.12	-
15	18	20	16	4, 4, 2	0.289	1, 1, 6, 6	0.084	0.00	12740.91	-
16	18	22	14	1, 4, 4	0.465	4, 1, 2, 2	0.262	0.00	12776.13	-
17	18	22	14	3, 0, 4	0.358	2, 2, 3, 3	0.119	0.00	12934.90	-
18	18	20	16	2, 8, 2	0.348	4, 0, 4, 4	0.261	0.00	12969.31	-
19	18	18	18	3, 12, 0	0.290	1, 1, 7, 7	0.130	0.00	13023.03	-
20	18	22	14	3, 0, 4	0.538	7, 0, 0, 0	0.294	0.00	13052.92	-
21	18	22	14	1, 4, 4	0.427	4, 1, 2, 2	0.240	0.00	13191.54	-
22	18	24	12	0, 0, 6	1.000	3, 3, 0, 0	0.312	13721.14	13721.10	0.04
1	20	20	20	4, 12, 0	0.264	2, 2, 6, 6	0.099	0.00	12214.57	-
2	20	20	20	6, 8, 0	0.207	1, 1, 8, 8	0.089	0.00	12466.78	-
3	20	20	20	8, 4, 0	0.242	1, 0, 9, 9	0.144	0.00	12696.48	-
4	20	20	20	9, 2, 0	0.284	0, 0, 10, 10	0.076	0.00	12897.00	-
5	20	22	18	3, 8, 2	0.299	4, 0, 5, 5	0.216	0.00	13020.71	-
6	20	20	20	10, 0, 0	0.482	5, 5, 0, 0	0.119	0.00	13059.47	-
7	20	20	20	10, 0, 0	0.275	0, 0, 10, 10	0.132	0.00	13219.39	-
8	20	22	18	5, 4, 2	0.261	3, 0, 6, 6	0.163	0.00	13245.28	-
9	20	20	20	9, 2, 0	0.250	0, 0, 10, 10	0.183	0.00	13419.89	-
10	20	22	18	6, 2, 2	0.313	1, 1, 7, 7	0.075	0.00	13440.17	-
11	20	22	18	7, 0, 2	0.496	8, 1, 0, 0	0.194	0.00	13595.29	-
12	20	20	20	8, 4, 0	0.230	0, 0, 10, 10	0.196	0.00	13654.87	-
13	20	22	18	7, 0, 2	0.303	1, 1, 7, 7	0.093	0.00	13739.28	-
14	20	20	20	7, 6, 0	0.200	0, 0, 10, 10	0.148	0.00	13917.09	-
15	20	24	16	1, 6, 4	0.395	4, 1, 3, 3	0.222	0.00	13919.49	-
16	20	22	18	6, 2, 2	0.229	1, 1, 7, 7	0.097	0.00	13923.47	-
17	20	24	16	3, 2, 4	0.381	2, 2, 4, 4	0.105	0.00	14101.20	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
18	20	22	18	4, 6, 2	0.263	3, 0, 6, 6	0.171	0.00	14143.09	-
19	20	20	20	5, 10, 0	0.223	1, 0, 9, 9	0.204	0.00	14204.30	-
20	20	24	16	4, 0, 4	0.568	8, 0, 0, 0	0.311	0.00	14239.69	-
21	20	24	16	3, 2, 4	0.352	7, 0, 1, 1	0.193	0.00	14367.05	-
22	20	22	18	2, 10, 2	0.319	4, 0, 5, 5	0.239	0.00	14391.93	-
23	20	20	20	3, 14, 0	0.285	1, 1, 8, 8	0.113	0.00	14513.53	-
24	20	24	16	2, 4, 4	0.367	4, 1, 3, 3	0.196	0.00	14536.71	-
25	20	26	14	0, 2, 6	0.684	3, 3, 1, 1	0.214	14874.78	14875.08	-0.31
26	20	26	14	1, 0, 6	0.684	5, 2, 0, 0	0.288	14978.78	14978.36	0.42
1	24	24	24	5, 14, 0	0.241	2, 2, 8, 8	0.076	0.00	14565.64	-
2	24	24	24	8, 8, 0	0.194	1, 1, 10, 10	0.062	0.00	14829.83	-
3	24	24	24	9, 6, 0	0.208	1, 1, 10, 10	0.069	0.00	15074.93	-
4	24	24	24	10, 4, 0	0.206	1, 0, 11, 11	0.117	0.00	15296.73	-
5	24	26	22	3, 12, 2	0.268	5, 0, 6, 6	0.168	0.00	15317.87	-
6	24	24	24	12, 0, 0	0.284	6, 6, 0, 0	0.064	0.00	15486.41	-
7	24	26	22	6, 6, 2	0.232	4, 0, 7, 7	0.134	0.00	15561.54	-
8	24	24	24	12, 0, 0	0.457	6, 6, 0, 0	0.103	0.00	15644.60	-
9	24	26	22	7, 4, 2	0.250	3, 0, 8, 8	0.122	0.00	15781.65	-
10	24	24	24	11, 2, 0	0.258	0, 0, 12, 12	0.116	0.00	15822.25	-
11	24	26	22	8, 2, 2	0.273	1, 1, 9, 9	0.057	0.00	15970.81	-
12	24	24	24	11, 2, 0	0.196	0, 0, 12, 12	0.164	0.00	16039.51	-
13	24	26	22	9, 0, 2	0.494	9, 2, 0, 0	0.174	0.00	16122.82	-
14	24	28	20	2, 8, 4	0.345	6, 0, 4, 4	0.162	0.00	16176.09	-
15	24	26	22	8, 2, 2	0.244	1, 1, 9, 9	0.081	0.00	16281.62	-
16	24	24	24	10, 4, 0	0.186	0, 0, 12, 12	0.181	0.00	16287.32	-
17	24	28	20	4, 4, 4	0.302	8, 0, 2, 2	0.165	0.00	16390.14	-
18	24	26	22	7, 4, 2	0.217	1, 1, 9, 9	0.096	0.00	16482.02	-
19	24	24	24	9, 6, 0	0.187	0, 0, 12, 12	0.168	0.00	16559.68	-
20	24	28	20	5, 2, 4	0.319	9, 0, 1, 1	0.157	0.00	16572.17	-
21	24	28	20	6, 0, 4	0.310	10, 0, 0, 0	0.127	0.00	16712.13	-
22	24	28	20	6, 0, 4	0.223	10, 0, 0, 0	0.091	0.00	16716.41	-
23	24	24	24	7, 10, 0	0.177	0, 0, 12, 12	0.108	0.00	16854.82	-
24	24	28	20	5, 2, 4	0.308	9, 0, 1, 1	0.151	0.00	16856.36	-
25	24	26	22	5, 8, 2	0.238	3, 0, 8, 8	0.158	0.00	16973.63	-
26	24	28	20	4, 4, 4	0.298	8, 0, 2, 2	0.163	0.00	17040.87	-
27	24	30	18	1, 4, 6	0.466	3, 3, 3, 3	0.099	0.00	17118.47	-
28	24	24	24	6, 12, 0	0.206	1, 1, 10, 10	0.090	0.00	17171.03	-
29	24	28	20	2, 8, 4	0.166	4, 0, 7, 7	0.101	0.00	17247.29	-
30	24	28	20	2, 8, 4	0.175	5, 0, 6, 6	0.086	0.00	17268.02	-
31	24	30	18	2, 2, 6	0.370	3, 3, 3, 3	0.106	0.00	17282.39	-
32	24	30	18	3, 0, 6	0.587	9, 0, 0, 0	0.193	0.00	17401.99	-
33	24	24	24	3, 18, 0	0.251	2, 1, 9, 9	0.188	0.00	17507.58	-
34	24	30	18	1, 4, 6	0.394	5, 2, 2, 2	0.166	0.00	17529.75	-
35	24	32	16	0, 0, 8	1.000	4, 4, 0, 0	0.273	18096.36	18096.38	-0.02
1	30	30	30	7, 16, 0	0.209	3, 3, 9, 9	0.065	0.00	18064.73	-
2	30	30	30	9, 12, 0	0.172	2, 2, 11, 11	0.055	0.00	18339.82	-
3	30	30	30	11, 8, 0	0.181	2, 1, 12, 12	0.094	0.00	18599.31	-
4	30	32	28	5, 14, 2	0.240	6, 1, 7, 7	0.101	0.00	18726.05	-
5	30	30	30	13, 4, 0	0.176	1, 1, 13, 13	0.055	0.00	18840.59	-
6	30	32	28	7, 10, 2	0.190	4, 0, 10, 10	0.103	0.00	18987.84	-
7	30	30	30	14, 2, 0	0.217	7, 7, 1, 1	0.046	0.00	19058.96	-
8	30	32	28	9, 6, 2	0.202	4, 0, 10, 10	0.098	0.00	19230.74	-
9	30	30	30	15, 0, 0	0.314	8, 7, 0, 0	0.123	0.00	19245.40	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
10	30	30	30	15, 0, 0	0.407	8, 7, 0, 0	0.160	0.00	19406.36	-
11	30	32	28	10, 4, 2	0.212	3, 0, 11, 11	0.094	0.00	19453.12	-
12	30	34	26	3, 12, 4	0.278	7, 0, 6, 6	0.152	0.00	19506.23	-
13	30	30	30	14, 2, 0	0.242	0, 0, 15, 15	0.072	0.00	19594.72	-
14	30	32	28	11, 2, 2	0.233	3, 0, 11, 11	0.073	0.00	19645.06	-
15	30	34	26	6, 6, 4	0.214	9, 0, 4, 4	0.100	0.00	19750.39	-
16	30	32	28	12, 0, 2	0.417	11, 3, 0, 0	0.127	0.00	19801.05	-
17	30	30	30	14, 2, 0	0.169	0, 0, 15, 15	0.108	0.00	19821.33	-
18	30	32	28	11, 2, 2	0.206	1, 1, 12, 12	0.050	0.00	19968.69	-
19	30	34	26	7, 4, 4	0.220	4, 1, 8, 8	0.075	0.00	19972.71	-
20	30	30	30	13, 4, 0	0.187	0, 0, 15, 15	0.153	0.00	20072.74	-
21	30	34	26	8, 2, 4	0.267	2, 2, 9, 9	0.050	0.00	20165.29	-
22	30	32	28	11, 2, 2	0.194	1, 1, 12, 12	0.081	0.00	20176.18	-
23	30	34	26	9, 0, 4	0.466	12, 1, 0, 0	0.156	0.00	20321.09	-
24	30	30	30	12, 6, 0	0.174	0, 0, 15, 15	0.172	0.00	20347.63	-
25	30	36	24	2, 8, 6	0.347	7, 1, 4, 4	0.152	0.00	20390.93	-
26	30	32	28	10, 4, 2	0.190	1, 1, 12, 12	0.086	0.00	20414.24	-
27	30	34	26	9, 0, 4	0.266	2, 2, 9, 9	0.059	0.00	20470.32	-
28	30	36	24	4, 4, 6	0.292	3, 3, 6, 6	0.061	0.00	20607.54	-
29	30	30	30	0, 30, 0	0.140	0, 0, 15, 15	0.140	0.00	20641.13	-
30	30	34	26	8, 2, 4	0.226	2, 2, 9, 9	0.066	0.00	20657.96	-
31	30	32	28	9, 6, 2	0.151	1, 1, 12, 12	0.064	0.00	20680.05	-
32	30	36	24	5, 2, 6	0.326	11, 0, 1, 1	0.147	0.00	20794.31	-
33	30	34	26	7, 4, 4	0.202	2, 2, 9, 9	0.051	0.00	20878.98	-
34	30	36	24	6, 0, 6	0.500	12, 0, 0, 0	0.226	0.00	20941.40	-
35	30	32	28	8, 8, 2	0.115	0, 0, 15, 15	0.049	0.00	20945.52	-
36	30	30	30	10, 10, 0	0.114	0, 0, 15, 15	0.072	0.00	20976.98	-
37	30	36	24	6, 0, 6	0.277	12, 0, 0, 0	0.125	0.00	21074.34	-
38	30	34	26	5, 8, 4	0.229	9, 0, 4, 4	0.113	0.00	21126.77	-
39	30	36	24	4, 4, 6	0.281	10, 0, 2, 2	0.115	0.00	21246.31	-
40	30	32	28	6, 12, 2	0.181	4, 0, 10, 10	0.118	0.00	21258.38	-
41	30	30	30	9, 12, 0	0.147	1, 0, 14, 14	0.146	0.00	21305.24	-
42	30	38	22	1, 4, 8	0.459	4, 4, 3, 3	0.099	0.00	21361.57	-
43	30	34	26	3, 12, 4	0.264	7, 0, 6, 6	0.145	0.00	21393.52	-
44	30	36	24	2, 8, 6	0.303	7, 1, 4, 4	0.133	0.00	21456.21	-
45	30	38	22	2, 2, 8	0.417	4, 4, 3, 3	0.097	0.00	21530.83	-
46	30	32	28	4, 16, 2	0.244	5, 0, 9, 9	0.144	0.00	21589.04	-
47	30	38	22	3, 0, 8	0.614	10, 1, 0, 0	0.225	0.00	21654.54	-
48	30	30	30	7, 16, 0	0.179	1, 1, 13, 13	0.086	0.00	21655.00	-
49	30	38	22	2, 2, 8	0.398	7, 2, 2, 2	0.137	0.00	21772.32	-
50	30	30	30	4, 22, 0	0.237	2, 2, 11, 11	0.089	0.00	22021.86	-
51	30	40	20	0, 0, 10	0.999	5, 5, 0, 0	0.246	22373.15	22373.21	-0.06
1	36	36	36	8, 20, 0	0.194	4, 4, 10, 10	0.053	0.00	21537.57	-
2	36	36	36	11, 14, 0	0.157	3, 3, 12, 12	0.039	0.00	21817.21	-
3	36	36	36	13, 10, 0	0.155	2, 2, 14, 14	0.042	0.00	22083.47	-
4	36	38	34	6, 18, 2	0.210	7, 1, 9, 9	0.092	0.00	22101.22	-
5	36	36	36	15, 6, 0	0.162	2, 1, 15, 15	0.074	0.00	22334.83	-
6	36	38	34	9, 12, 2	0.173	5, 0, 12, 12	0.071	0.00	22372.26	-
7	36	36	36	16, 4, 0	0.190	1, 1, 16, 16	0.039	0.00	22568.06	-
8	36	38	34	11, 8, 2	0.173	5, 0, 12, 12	0.077	0.00	22628.12	-
9	36	36	36	17, 2, 0	0.233	9, 8, 1, 1	0.086	0.00	22777.14	-
10	36	40	32	5, 14, 4	0.235	8, 0, 8, 8	0.125	0.00	22791.33	-
11	36	38	34	12, 6, 2	0.173	4, 0, 13, 13	0.085	0.00	22866.48	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
12	36	36	36	18, 0, 0	0.392	9, 9, 0, 0	0.073	0.00	22953.35	-
13	36	40	32	7, 10, 4	0.197	7, 0, 9, 9	0.082	0.00	23051.88	-
14	36	38	34	14, 2, 2	0.175	3, 0, 14, 14	0.063	0.00	23083.36	-
15	36	36	36	18, 0, 0	0.298	9, 9, 0, 0	0.055	0.00	23122.29	-
16	36	38	34	15, 0, 2	0.232	13, 4, 0, 0	0.063	0.00	23268.20	-
17	36	40	32	9, 6, 4	0.171	4, 1, 11, 11	0.066	0.00	23297.42	-
18	36	36	36	17, 2, 0	0.244	1, 0, 17, 17	0.091	0.00	23324.77	-
19	36	38	34	15, 0, 2	0.388	13, 4, 0, 0	0.106	0.00	23428.36	-
20	36	40	32	10, 4, 4	0.200	4, 1, 11, 11	0.074	0.00	23519.14	-
21	36	36	36	16, 4, 0	0.165	0, 0, 18, 18	0.068	0.00	23557.78	-
22	36	42	30	3, 12, 6	0.284	7, 1, 7, 7	0.096	0.00	23596.83	-
23	36	38	34	14, 2, 2	0.176	1, 1, 15, 15	0.040	0.00	23607.86	-
24	36	40	32	11, 2, 4	0.223	2, 2, 12, 12	0.032	0.00	23715.11	-
25	36	38	34	14, 2, 2	0.107	0, 0, 18, 18	0.062	0.00	23807.15	-
26	36	36	36	16, 4, 0	0.114	0, 0, 18, 18	0.043	0.00	23831.20	-
27	36	42	30	5, 8, 6	0.222	11, 0, 4, 4	0.100	0.00	23842.34	-
28	36	40	32	12, 0, 4	0.406	14, 2, 0, 0	0.108	0.00	23877.12	-
29	36	40	32	12, 0, 4	0.209	2, 2, 12, 12	0.043	0.00	24028.86	-
30	36	38	34	13, 4, 2	0.155	1, 1, 15, 15	0.057	0.00	24060.32	-
31	36	42	30	7, 4, 6	0.226	13, 0, 2, 2	0.095	0.00	24066.64	-
32	36	36	36	15, 6, 0	0.166	0, 0, 18, 18	0.118	0.00	24105.67	-
33	36	40	32	11, 2, 4	0.204	2, 2, 12, 12	0.060	0.00	24226.37	-
34	36	42	30	8, 2, 6	0.268	14, 0, 1, 1	0.098	0.00	24264.45	-
35	36	38	34	12, 6, 2	0.161	1, 1, 15, 15	0.076	0.00	24322.99	-
36	36	36	36	14, 8, 0	0.161	0, 0, 18, 18	0.153	0.00	24404.19	-
37	36	42	30	9, 0, 6	0.396	15, 0, 0, 0	0.121	0.00	24426.37	-
38	36	40	32	10, 4, 4	0.175	2, 2, 12, 12	0.060	0.00	24455.19	-
39	36	44	28	2, 8, 8	0.344	7, 2, 5, 5	0.117	0.00	24507.02	-
40	36	42	30	9, 0, 6	0.331	15, 0, 0, 0	0.101	0.00	24568.19	-
41	36	38	34	11, 8, 2	0.143	1, 1, 15, 15	0.067	0.00	24605.79	-
42	36	40	32	9, 6, 4	0.138	2, 2, 12, 12	0.040	0.00	24707.24	-
43	36	36	36	13, 10, 0	0.133	0, 0, 18, 18	0.129	0.00	24725.10	-
44	36	44	28	4, 4, 8	0.269	4, 4, 6, 6	0.060	0.00	24726.43	-
45	36	42	30	8, 2, 6	0.232	3, 3, 9, 9	0.047	0.00	24742.55	-
46	36	38	34	10, 10, 2	0.117	1, 1, 15, 15	0.042	0.00	24905.45	-
47	36	44	28	5, 2, 8	0.298	4, 4, 6, 6	0.066	0.00	24918.11	-
48	36	42	30	7, 4, 6	0.214	13, 0, 2, 2	0.090	0.00	24951.13	-
49	36	40	32	8, 8, 4	0.127	4, 1, 11, 11	0.068	0.00	24989.23	-
50	36	36	36	12, 12, 0	0.151	0, 0, 18, 18	0.123	0.00	25058.43	-
51	36	44	28	6, 0, 8	0.437	14, 0, 0, 0	0.160	0.00	25072.61	-
52	36	42	30	5, 8, 6	0.179	11, 0, 4, 4	0.081	0.00	25181.58	-
53	36	44	28	6, 0, 8	0.321	14, 0, 0, 0	0.118	0.00	25202.43	-
54	36	38	34	1, 28, 2	0.092	3, 0, 14, 14	0.069	0.00	25224.26	-
55	36	40	32	6, 12, 4	0.104	6, 0, 10, 10	0.047	0.00	25292.55	-
56	36	44	28	4, 4, 8	0.247	7, 2, 5, 5	0.087	0.00	25357.99	-
57	36	36	36	11, 14, 0	0.153	0, 0, 18, 18	0.078	0.00	25409.41	-
58	36	42	30	3, 12, 6	0.257	10, 0, 5, 5	0.088	0.00	25439.01	-
59	36	46	26	1, 4, 10	0.445	5, 5, 3, 3	0.102	0.00	25505.85	-
60	36	44	28	2, 8, 8	0.231	10, 1, 3, 3	0.084	0.00	25553.48	-
61	36	40	32	4, 16, 4	0.103	8, 0, 8, 8	0.056	0.00	25562.05	-
62	36	38	34	7, 16, 2	0.104	4, 0, 13, 13	0.075	0.00	25617.53	-
63	36	46	26	2, 2, 10	0.443	5, 5, 3, 3	0.090	0.00	25680.72	-
64	36	36	36	10, 16, 0	0.147	1, 1, 16, 16	0.071	0.00	25775.86	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
65	36	46	26	3, 0, 10	0.610	11, 2, 0, 0	0.177	0.00	25810.56	-
66	36	46	26	2, 2, 10	0.418	10, 2, 1, 1	0.138	0.00	25920.23	-
67	36	38	34	4, 22, 2	0.228	6, 0, 11, 11	0.107	0.00	25952.39	-
68	36	36	36	8, 20, 0	0.167	1, 1, 16, 16	0.070	0.00	26156.99	-
69	36	48	24	0, 0, 12	0.999	6, 6, 0, 0	0.225	26552.21	26552.15	0.06
70	36	36	36	5, 26, 0	0.221	2, 2, 14, 14	0.071	0.00	26552.19	-
Symmetry Σ_u										
1	3	4	2	0, 0, 1	1.000	1, 0, 0, 0	1.000	2349.14	2349.13	0.01
1	5	6	4	0, 2, 1	0.539	1, 0, 1, 1	0.539	3612.84	3612.83	0.01
2	5	6	4	1, 0, 1	0.539	2, 0, 0, 0	0.539	3714.79	3714.84	-0.05
1	7	8	6	1, 2, 1	0.495	2, 0, 1, 1	0.495	4853.62	4853.54	0.08
2	7	8	6	2, 0, 1	0.664	3, 0, 0, 0	0.498	4977.84	4977.94	-0.10
3	7	8	6	1, 2, 1	0.504	2, 0, 1, 1	0.504	5099.66	5099.71	-0.05
1	9	10	8	1, 4, 1	0.452	2, 0, 2, 2	0.452	6075.98	6075.90	0.08
2	9	10	8	3, 0, 1	0.461	1, 0, 3, 3	0.279	6227.92	6227.94	-0.02
3	9	10	8	3, 0, 1	0.448	1, 0, 3, 3	0.283	6347.85	6347.96	-0.11
4	9	10	8	1, 4, 1	0.456	2, 0, 2, 2	0.456	6503.08	6503.14	-0.06
5	9	12	6	0, 0, 3	1.000	2, 1, 0, 0	0.750	6972.58	6972.53	0.05
1	11	12	10	1, 6, 1	0.369	2, 0, 3, 3	0.369	7283.98	7284.15	-0.17
2	11	12	10	3, 2, 1	0.369	1, 0, 4, 4	0.233	7460.52	7460.46	0.06
3	11	12	10	4, 0, 1	0.579	4, 1, 0, 0	0.326	7593.69	7593.71	-0.02
4	11	12	10	3, 2, 1	0.384	1, 0, 4, 4	0.260	7734.45	7734.53	-0.08
5	11	12	10	1, 6, 1	0.388	2, 0, 3, 3	0.388	7920.83	7921.07	-0.23
6	11	14	8	0, 2, 3	0.597	2, 1, 1, 1	0.448	8192.55	8192.63	-0.08
7	11	14	8	1, 0, 3	0.597	2, 1, 1, 1	0.302	8293.95	8293.93	0.02
1	13	14	12	2, 6, 1	0.363	2, 0, 4, 4	0.278	0.00	8481.06	-
2	13	14	12	4, 2, 1	0.320	2, 0, 4, 4	0.196	8676.72	8676.77	-0.05
3	13	14	12	5, 0, 1	0.491	5, 1, 0, 0	0.245	8831.48	8831.23	0.26
4	13	14	12	5, 0, 1	0.362	1, 0, 5, 5	0.222	8965.23	8965.14	0.09
5	13	14	12	3, 4, 1	0.279	1, 0, 5, 5	0.224	9137.80	9138.06	-0.26
6	13	14	12	2, 6, 1	0.360	2, 0, 4, 4	0.318	0.00	9350.57	-
7	13	16	10	1, 2, 3	0.481	2, 1, 2, 2	0.298	9388.99	9389.05	-0.06
8	13	16	10	2, 0, 3	0.652	5, 0, 0, 0	0.407	9516.97	9517.02	-0.05
9	13	16	10	1, 2, 3	0.505	4, 0, 1, 1	0.252	9631.35	9631.33	0.02
1	15	16	14	2, 8, 1	0.332	3, 0, 4, 4	0.249	0.00	9668.54	-
2	15	16	14	4, 4, 1	0.294	2, 0, 5, 5	0.221	0.00	9879.87	-
3	15	16	14	6, 0, 1	0.306	1, 0, 6, 6	0.166	0.00	10055.54	-
4	15	16	14	6, 0, 1	0.509	5, 2, 0, 0	0.215	0.00	10194.42	-
5	15	16	14	5, 2, 1	0.337	1, 0, 6, 6	0.225	0.00	10353.15	-
6	15	16	14	4, 4, 1	0.299	2, 0, 5, 5	0.211	0.00	10554.89	-
7	15	18	12	1, 4, 3	0.462	4, 0, 2, 2	0.231	0.00	10567.64	-
8	15	18	12	3, 0, 3	0.394	6, 0, 0, 0	0.247	10724.03	10724.03	0.00
9	15	16	14	2, 8, 1	0.352	3, 0, 4, 4	0.264	0.00	10789.64	-
10	15	18	12	3, 0, 3	0.509	6, 0, 0, 0	0.318	10842.06	10842.14	-0.08
11	15	18	12	1, 4, 3	0.439	4, 0, 2, 2	0.219	10986.27	10986.31	-0.04
12	15	20	10	0, 0, 5	1.000	3, 2, 0, 0	0.625	11496.44	11496.38	0.06
1	17	18	16	3, 8, 1	0.303	3, 0, 5, 5	0.209	0.00	10848.01	-
2	17	18	16	5, 4, 1	0.269	2, 0, 6, 6	0.212	0.00	11072.20	-
3	17	18	16	6, 2, 1	0.316	1, 0, 7, 7	0.139	0.00	11265.71	-
4	17	18	16	7, 0, 1	0.513	6, 2, 0, 0	0.225	0.00	11418.96	-
5	17	18	16	7, 0, 1	0.272	1, 0, 7, 7	0.191	0.00	11566.95	-
6	17	20	14	1, 6, 3	0.392	5, 0, 2, 2	0.207	0.00	11732.61	-
7	17	18	16	5, 4, 1	0.238	1, 0, 7, 7	0.212	0.00	11756.76	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
8	17	20	14	3, 2, 3	0.381	6, 0, 1, 1	0.238	11912.44	11912.37	0.07
9	17	18	16	4, 6, 1	0.270	2, 0, 6, 6	0.229	0.00	11982.39	-
10	17	20	14	4, 0, 3	0.579	7, 0, 0, 0	0.316	12048.73	12048.64	0.09
11	17	20	14	3, 2, 3	0.370	6, 0, 1, 1	0.231	12179.97	12180.23	-0.26
12	17	18	16	2, 10, 1	0.326	3, 0, 5, 5	0.245	0.00	12236.84	-
13	17	20	14	1, 6, 3	0.363	5, 0, 2, 2	0.224	0.00	12355.60	-
14	17	22	12	0, 2, 5	0.656	3, 2, 1, 1	0.410	12672.28	12672.51	-0.23
15	17	22	12	1, 0, 5	0.655	5, 1, 0, 0	0.328	12774.73	12774.71	0.03
1	19	20	18	3, 10, 1	0.295	3, 0, 6, 6	0.164	0.00	12020.58	-
2	19	20	18	5, 6, 1	0.247	2, 0, 7, 7	0.182	0.00	12255.48	-
3	19	20	18	7, 2, 1	0.263	2, 0, 7, 7	0.154	0.00	12463.42	-
4	19	20	18	8, 0, 1	0.397	7, 2, 0, 0	0.155	0.00	12634.36	-
5	19	20	18	8, 0, 1	0.416	7, 2, 0, 0	0.163	0.00	12779.55	-
6	19	22	16	2, 6, 3	0.359	5, 0, 3, 3	0.224	0.00	12886.66	-
7	19	20	18	7, 2, 1	0.302	1, 0, 8, 8	0.201	0.00	12956.34	-
8	19	22	16	4, 2, 3	0.291	7, 0, 1, 1	0.159	0.00	13084.81	-
9	19	20	18	6, 4, 1	0.264	1, 0, 8, 8	0.192	0.00	13172.45	-
10	19	22	16	5, 0, 3	0.428	8, 0, 0, 0	0.187	0.00	13243.97	-
11	19	22	16	5, 0, 3	0.428	8, 0, 0, 0	0.187	0.00	13373.54	-
12	19	20	18	5, 6, 1	0.236	2, 0, 7, 7	0.229	0.00	13418.77	-
13	19	22	16	4, 2, 3	0.299	7, 0, 1, 1	0.163	0.00	13534.69	-
14	19	20	18	2, 12, 1	0.289	3, 0, 6, 6	0.217	0.00	13690.47	-
15	19	22	16	2, 6, 3	0.359	5, 0, 3, 3	0.225	0.00	13736.68	-
16	19	24	14	1, 2, 5	0.458	3, 2, 2, 2	0.281	0.00	13824.71	-
17	19	24	14	2, 0, 5	0.620	6, 1, 0, 0	0.262	13957.22	13957.42	-0.20
18	19	24	14	1, 2, 5	0.494	5, 1, 1, 1	0.247	14065.69	14065.60	0.10
1	21	22	20	4, 10, 1	0.264	4, 1, 5, 5	0.148	0.00	13187.16	-
2	21	22	20	6, 6, 1	0.238	2, 0, 8, 8	0.144	0.00	13431.02	-
3	21	22	20	7, 4, 1	0.247	2, 0, 8, 8	0.161	0.00	13650.70	-
4	21	22	20	8, 2, 1	0.260	1, 0, 9, 9	0.104	0.00	13838.14	-
5	21	22	20	9, 0, 1	0.493	7, 3, 0, 0	0.185	0.00	13989.50	-
6	21	24	18	2, 8, 3	0.342	5, 0, 4, 4	0.214	0.00	14031.61	-
7	21	22	20	8, 2, 1	0.281	1, 0, 9, 9	0.170	0.00	14153.94	-
8	21	24	18	4, 4, 3	0.302	7, 0, 2, 2	0.165	0.00	14244.58	-
9	21	22	20	7, 4, 1	0.232	1, 0, 9, 9	0.199	0.00	14359.82	-
10	21	24	18	5, 2, 3	0.306	2, 1, 6, 6	0.142	0.00	14424.35	-
11	21	24	18	6, 0, 3	0.531	9, 0, 0, 0	0.174	0.00	14564.34	-
12	21	22	20	6, 6, 1	0.228	1, 0, 9, 9	0.168	0.00	14597.94	-
13	21	24	18	5, 2, 3	0.328	2, 1, 6, 6	0.153	0.00	14712.12	-
14	21	22	20	5, 8, 1	0.240	2, 0, 8, 8	0.217	0.00	14862.26	-
15	21	24	18	4, 4, 3	0.298	7, 0, 2, 2	0.163	0.00	14902.68	-
16	21	26	16	1, 4, 5	0.466	5, 1, 2, 2	0.233	0.00	14959.73	-
17	21	26	16	2, 2, 5	0.318	3, 2, 3, 3	0.196	0.00	15120.80	-
18	21	24	18	2, 8, 3	0.305	5, 0, 4, 4	0.191	0.00	15124.01	-
19	21	22	20	3, 12, 1	0.273	3, 0, 7, 7	0.177	0.00	15153.40	-
20	21	26	16	3, 0, 5	0.565	8, 0, 0, 0	0.247	0.00	15239.53	-
21	21	26	16	1, 4, 5	0.412	5, 1, 2, 2	0.206	0.00	15372.65	-
22	21	28	14	0, 0, 7	1.000	4, 3, 0, 0	0.547	15921.09	15921.07	0.01
1	27	28	26	5, 14, 1	0.241	5, 1, 7, 7	0.120	0.00	16657.63	-
2	27	28	26	8, 8, 1	0.188	3, 0, 10, 10	0.097	0.00	16920.38	-
3	27	28	26	9, 6, 1	0.209	3, 0, 10, 10	0.104	0.00	17164.41	-
4	27	28	26	10, 4, 1	0.213	2, 0, 11, 11	0.121	0.00	17385.77	-
5	27	30	24	3, 12, 3	0.274	6, 0, 6, 6	0.171	0.00	17424.25	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
6	27	28	26	12, 0, 1	0.255	2, 0, 11, 11	0.099	0.00	17576.19	-
7	27	30	24	6, 6, 3	0.224	5, 0, 7, 7	0.109	0.00	17668.04	-
8	27	28	26	12, 0, 1	0.462	9, 4, 0, 0	0.155	0.00	17733.63	-
9	27	30	24	7, 4, 3	0.248	9, 1, 2, 2	0.093	0.00	17888.79	-
10	27	28	26	11, 2, 1	0.241	1, 0, 12, 12	0.119	0.00	17906.10	-
11	27	30	24	8, 2, 3	0.279	10, 1, 1, 1	0.102	0.00	18079.97	-
12	27	28	26	11, 2, 1	0.203	1, 0, 12, 12	0.164	0.00	18117.91	-
13	27	30	24	9, 0, 3	0.485	11, 1, 0, 0	0.156	0.00	18233.45	-
14	27	32	22	2, 8, 5	0.347	6, 1, 4, 4	0.146	0.00	18295.86	-
15	27	28	26	10, 4, 1	0.201	1, 0, 12, 12	0.182	0.00	18360.09	-
16	27	30	24	8, 2, 3	0.240	2, 1, 9, 9	0.121	0.00	18387.49	-
17	27	32	22	4, 4, 5	0.298	9, 0, 2, 2	0.147	0.00	18511.13	-
18	27	30	24	8, 2, 3	0.215	2, 1, 9, 9	0.139	0.00	18581.43	-
19	27	28	26	9, 6, 1	0.190	1, 0, 12, 12	0.161	0.00	18627.57	-
20	27	32	22	5, 2, 5	0.326	10, 0, 1, 1	0.160	0.00	18695.50	-
21	27	30	24	6, 6, 3	0.204	2, 1, 9, 9	0.110	0.00	18808.25	-
22	27	32	22	6, 0, 5	0.521	11, 0, 0, 0	0.235	0.00	18839.76	-
23	27	28	26	1, 22, 1	0.174	2, 0, 11, 11	0.174	0.00	18917.47	-
24	27	32	22	5, 2, 5	0.293	10, 0, 1, 1	0.144	0.00	18977.07	-
25	27	30	24	5, 8, 3	0.235	8, 0, 4, 4	0.103	0.00	19061.83	-
26	27	32	22	4, 4, 5	0.293	9, 0, 2, 2	0.144	0.00	19155.42	-
27	27	28	26	6, 12, 1	0.204	2, 0, 11, 11	0.152	0.00	19228.60	-
28	27	34	20	1, 4, 7	0.463	6, 2, 2, 2	0.203	0.00	19252.40	-
29	27	30	24	3, 12, 3	0.248	6, 0, 6, 6	0.155	0.00	19334.06	-
30	27	32	22	2, 8, 5	0.286	6, 1, 4, 4	0.121	0.00	19372.14	-
31	27	34	20	2, 2, 7	0.396	4, 3, 3, 3	0.191	0.00	19418.95	-
32	27	34	20	3, 0, 7	0.604	9, 1, 0, 0	0.226	0.00	19540.33	-
33	27	28	26	4, 16, 1	0.252	4, 1, 8, 8	0.142	0.00	19560.93	-
34	27	34	20	2, 2, 7	0.383	6, 2, 2, 2	0.163	0.00	19662.93	-
35	27	36	18	0, 0, 9	1.000	5, 4, 0, 0	0.492	20247.02	20247.06	-0.05
1	33	34	32	6, 18, 1	0.209	6, 2, 8, 8	0.090	0.00	20094.14	-
2	33	34	32	9, 12, 1	0.174	4, 1, 11, 11	0.082	0.00	20366.83	-
3	33	34	32	11, 8, 1	0.180	3, 0, 13, 13	0.070	0.00	20624.17	-
4	33	36	30	5, 14, 3	0.238	7, 0, 8, 8	0.122	0.00	20770.67	-
5	33	34	32	12, 6, 1	0.173	3, 0, 13, 13	0.084	0.00	20863.71	-
6	33	36	30	7, 10, 3	0.195	6, 0, 9, 9	0.098	0.00	21031.79	-
7	33	34	32	14, 2, 1	0.203	2, 0, 14, 14	0.083	0.00	21081.16	-
8	33	34	32	15, 0, 1	0.253	11, 5, 0, 0	0.076	0.00	21264.58	-
9	33	36	30	9, 6, 3	0.153	5, 0, 10, 10	0.070	0.00	21277.50	-
10	33	34	32	15, 0, 1	0.410	11, 5, 0, 0	0.123	0.00	21426.16	-
11	33	36	30	10, 4, 3	0.208	4, 0, 11, 11	0.064	0.00	21497.68	-
12	33	38	28	3, 12, 5	0.282	8, 0, 6, 6	0.123	0.00	21563.77	-
13	33	34	32	14, 2, 1	0.225	2, 0, 14, 14	0.085	0.00	21609.57	-
14	33	36	30	11, 2, 3	0.232	12, 2, 1, 1	0.071	0.00	21691.51	-
15	33	38	28	5, 8, 5	0.214	10, 0, 4, 4	0.105	0.00	21808.51	-
16	33	34	32	14, 2, 1	0.161	1, 0, 15, 15	0.103	0.00	21827.40	-
17	33	36	30	12, 0, 3	0.409	13, 2, 0, 0	0.118	0.00	21852.30	-
18	33	36	30	12, 0, 3	0.215	2, 1, 12, 12	0.091	0.00	22010.66	-
19	33	38	28	7, 4, 5	0.240	12, 0, 2, 2	0.093	0.00	22031.50	-
20	33	34	32	13, 4, 1	0.181	1, 0, 15, 15	0.154	0.00	22078.04	-
21	33	36	30	11, 2, 3	0.213	2, 1, 12, 12	0.119	0.00	22212.20	-
22	33	38	28	8, 2, 5	0.285	13, 0, 1, 1	0.089	0.00	22227.08	-
23	33	34	32	0, 30, 1	0.170	1, 0, 15, 15	0.170	0.00	22346.86	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
24	33	38	28	9, 0, 5	0.436	13, 1, 0, 0	0.122	0.00	22385.49	-
25	33	36	30	10, 4, 3	0.184	2, 1, 12, 12	0.126	0.00	22445.80	-
26	33	40	26	2, 8, 7	0.346	8, 1, 4, 4	0.135	0.00	22461.30	-
27	33	38	28	9, 0, 5	0.299	3, 2, 9, 9	0.094	0.00	22530.57	-
28	33	34	32	0, 30, 1	0.144	1, 0, 15, 15	0.144	0.00	22634.95	-
29	33	40	26	4, 4, 7	0.283	4, 3, 6, 6	0.115	0.00	22679.34	-
30	33	36	30	9, 6, 3	0.154	2, 1, 12, 12	0.096	0.00	22706.36	-
31	33	38	28	8, 2, 5	0.233	3, 2, 9, 9	0.103	0.00	22711.61	-
32	33	40	26	5, 2, 7	0.318	4, 3, 6, 6	0.128	0.00	22868.55	-
33	33	38	28	7, 4, 5	0.204	12, 0, 2, 2	0.079	0.00	22925.90	-
34	33	34	32	10, 10, 1	0.101	2, 0, 14, 14	0.092	0.00	22939.39	-
35	33	36	30	1, 22, 3	0.114	4, 0, 11, 11	0.057	0.00	22993.31	-
36	33	40	26	6, 0, 7	0.475	13, 0, 0, 0	0.199	0.00	23019.12	-
37	33	40	26	6, 0, 7	0.295	13, 0, 0, 0	0.124	0.00	23147.42	-
38	33	38	28	5, 8, 5	0.210	10, 0, 4, 4	0.103	0.00	23169.03	-
39	33	36	30	6, 12, 3	0.129	5, 0, 10, 10	0.066	0.00	23256.11	-
40	33	34	32	9, 12, 1	0.107	2, 0, 14, 14	0.096	0.00	23306.72	-
41	33	40	26	4, 4, 7	0.262	6, 2, 5, 5	0.097	0.00	23314.12	-
42	33	38	28	3, 12, 5	0.265	8, 0, 6, 6	0.116	0.00	23428.41	-
43	33	42	24	1, 4, 9	0.453	5, 4, 3, 3	0.191	0.00	23446.03	-
44	33	40	26	2, 8, 7	0.302	8, 1, 4, 4	0.118	0.00	23517.36	-
45	33	36	30	4, 16, 3	0.209	6, 0, 9, 9	0.120	0.00	23589.77	-
46	33	42	24	2, 2, 9	0.433	5, 4, 3, 3	0.178	0.00	23618.06	-
47	33	34	32	7, 16, 1	0.154	3, 0, 13, 13	0.111	0.00	23644.33	-
48	33	42	24	3, 0, 9	0.616	11, 1, 0, 0	0.198	0.00	23744.62	-
49	33	42	24	2, 2, 9	0.410	9, 2, 1, 1	0.145	0.00	23858.05	-
50	33	34	32	4, 22, 1	0.234	4, 1, 11, 11	0.132	0.00	23998.95	-
51	33	44	22	0, 0, 11	0.999	6, 5, 0, 0	0.451	24474.85	24474.88	-0.03
Symmetry Π_g										
1	4	5	3	0, 1, 1	1.000	1, 0, 1, 0	1.000	3004.01	3004.05	-0.04
1	6	7	5	0, 3, 1	0.522	1, 0, 2, 1	0.522	4247.71	4247.65	0.05
2	6	7	5	1, 1, 1	0.522	2, 0, 1, 0	0.522	4390.63	4390.65	-0.02
1	8	9	7	1, 3, 1	0.498	2, 0, 2, 1	0.498	5475.07	5474.96	0.11
2	8	9	7	2, 1, 1	0.598	3, 0, 1, 0	0.449	5632.77	5632.73	0.04
3	8	9	7	1, 3, 1	0.502	2, 0, 2, 1	0.502	5790.58	5790.58	-0.01
1	10	11	9	1, 5, 1	0.427	2, 0, 3, 2	0.427	6688.17	6688.17	0.00
2	10	11	9	3, 1, 1	0.441	1, 0, 4, 3	0.308	6863.56	6863.47	0.09
3	10	11	9	3, 1, 1	0.421	1, 0, 4, 3	0.316	7023.67	7023.66	0.01
4	10	11	9	1, 5, 1	0.435	2, 0, 3, 2	0.435	7203.83	7203.91	-0.09
5	10	13	7	0, 1, 3	1.000	2, 1, 1, 0	0.750	7602.51	7602.56	-0.05
1	12	13	11	2, 5, 1	0.364	2, 0, 4, 3	0.332	0.00	7889.53	-
2	12	13	11	3, 3, 1	0.332	1, 0, 5, 4	0.230	8081.84	8081.85	-0.02
3	12	13	11	4, 1, 1	0.500	4, 1, 1, 0	0.281	8250.63	8250.55	0.08
4	12	13	11	3, 3, 1	0.358	1, 0, 5, 4	0.259	8425.01	8425.09	-0.09
5	12	13	11	1, 7, 1	0.361	2, 0, 4, 3	0.361	0.00	8629.07	-
6	12	15	9	0, 3, 3	0.564	2, 1, 2, 1	0.423	8803.27	8803.33	-0.06
7	12	15	9	1, 1, 3	0.564	2, 1, 2, 1	0.327	8944.14	8944.10	0.04
1	14	15	13	2, 7, 1	0.355	3, 0, 4, 3	0.266	0.00	9080.91	-
2	14	15	13	4, 3, 1	0.326	2, 0, 5, 4	0.217	0.00	9288.38	-
3	14	15	13	5, 1, 1	0.437	1, 0, 6, 5	0.222	0.00	9469.25	-
4	14	15	13	5, 1, 1	0.348	1, 0, 6, 5	0.249	0.00	9642.57	-
5	14	15	13	4, 3, 1	0.288	1, 0, 6, 5	0.212	0.00	9838.17	-
6	14	17	11	1, 3, 3	0.490	2, 1, 3, 2	0.260	9987.37	9987.41	-0.04

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
7	14	15	13	2, 7, 1	0.360	2, 0, 5, 4	0.291	0.00	10064.30	-
8	14	17	11	2, 1, 3	0.593	5, 0, 1, 0	0.370	10145.49	10145.47	0.02
9	14	17	11	1, 3, 3	0.502	4, 0, 2, 1	0.251	10297.08	10297.03	0.05
1	16	17	15	2, 9, 1	0.311	3, 0, 5, 4	0.233	0.00	10263.78	-
2	16	17	15	4, 5, 1	0.259	2, 0, 6, 5	0.225	0.00	10484.31	-
3	16	17	15	6, 1, 1	0.310	1, 0, 7, 6	0.176	0.00	10678.36	-
4	16	17	15	6, 1, 1	0.436	1, 0, 7, 6	0.213	0.00	10855.34	-
5	16	17	15	5, 3, 1	0.310	1, 0, 7, 6	0.230	0.00	11044.24	-
6	16	19	13	1, 5, 3	0.442	4, 0, 3, 2	0.221	0.00	11157.48	-
7	16	17	15	4, 5, 1	0.293	2, 0, 6, 5	0.223	0.00	11261.88	-
8	16	19	13	3, 1, 3	0.399	6, 0, 1, 0	0.250	0.00	11334.20	-
9	16	19	13	3, 1, 3	0.457	6, 0, 1, 0	0.286	0.00	11490.98	-
10	16	17	15	2, 9, 1	0.341	3, 0, 5, 4	0.256	0.00	11508.19	-
11	16	19	13	1, 5, 3	0.417	5, 0, 2, 1	0.210	0.00	11662.30	-
12	16	21	11	0, 1, 5	1.000	3, 2, 1, 0	0.625	12101.57	12101.61	-0.04
1	22	23	21	4, 11, 1	0.267	4, 1, 6, 5	0.150	0.00	13772.17	-
2	22	23	21	6, 7, 1	0.234	3, 0, 8, 7	0.139	0.00	14021.19	-
3	22	23	21	8, 3, 1	0.214	2, 0, 9, 8	0.161	0.00	14248.60	-
4	22	23	21	9, 1, 1	0.262	2, 0, 9, 8	0.117	0.00	14452.33	-
5	22	25	19	2, 9, 3	0.325	5, 0, 5, 4	0.203	0.00	14605.30	-
6	22	23	21	9, 1, 1	0.408	7, 3, 1, 0	0.153	0.00	14640.04	-
7	22	25	19	4, 5, 3	0.277	7, 0, 3, 2	0.152	0.00	14826.66	-
8	22	23	21	8, 3, 1	0.232	1, 0, 10, 9	0.183	0.00	14836.81	-
9	22	25	19	6, 1, 3	0.261	2, 1, 7, 6	0.146	0.00	15021.90	-
10	22	23	21	8, 3, 1	0.217	1, 0, 10, 9	0.198	0.00	15059.51	-
11	22	25	19	6, 1, 3	0.447	2, 1, 7, 6	0.160	0.00	15196.65	-
12	22	23	21	6, 7, 1	0.200	1, 0, 10, 9	0.159	0.00	15309.03	-
13	22	25	19	5, 3, 3	0.290	2, 1, 7, 6	0.159	0.00	15377.29	-
14	22	27	17	1, 5, 5	0.453	5, 1, 3, 2	0.226	0.00	15527.33	-
15	22	25	19	4, 5, 3	0.139	2, 0, 9, 8	0.125	0.00	15579.18	-
16	22	25	19	4, 5, 3	0.150	2, 0, 9, 8	0.086	0.00	15588.42	-
17	22	27	17	3, 1, 5	0.350	3, 2, 4, 3	0.217	0.00	15706.36	-
18	22	25	19	2, 9, 3	0.328	5, 0, 5, 4	0.205	0.00	15818.28	-
19	22	27	17	3, 1, 5	0.495	8, 0, 1, 0	0.217	0.00	15861.37	-
20	22	23	21	3, 13, 1	0.285	3, 0, 8, 7	0.174	0.00	15881.39	-
21	22	27	17	1, 5, 5	0.391	5, 1, 3, 2	0.195	0.00	16023.92	-
22	22	29	15	0, 1, 7	1.000	4, 3, 1, 0	0.547	16501.57	16501.59	-0.02
1	28	29	27	5, 15, 1	0.236	5, 1, 8, 7	0.118	0.00	17235.72	-
2	28	29	27	8, 9, 1	0.196	3, 0, 11, 10	0.086	0.00	17501.49	-
3	28	29	27	9, 7, 1	0.190	3, 0, 11, 10	0.105	0.00	17749.80	-
4	28	29	27	11, 3, 1	0.209	2, 0, 12, 11	0.116	0.00	17978.04	-
5	28	31	25	4, 11, 3	0.255	6, 0, 7, 6	0.158	0.00	17988.28	-
6	28	29	27	12, 1, 1	0.256	2, 0, 12, 11	0.113	0.00	18184.98	-
7	28	31	25	6, 7, 3	0.229	5, 0, 8, 7	0.114	0.00	18236.79	-
8	28	29	27	12, 1, 1	0.377	9, 4, 1, 0	0.127	0.00	18378.82	-
9	28	31	25	7, 5, 3	0.225	9, 1, 3, 2	0.084	0.00	18464.51	-
10	28	29	27	12, 1, 1	0.210	1, 0, 13, 12	0.130	0.00	18582.73	-
11	28	31	25	8, 3, 3	0.237	2, 1, 10, 9	0.092	0.00	18669.01	-
12	28	29	27	11, 3, 1	0.219	1, 0, 13, 12	0.168	0.00	18811.00	-
13	28	33	23	2, 9, 5	0.332	6, 1, 5, 4	0.140	0.00	18848.16	-
14	28	31	25	9, 1, 3	0.397	11, 1, 1, 0	0.128	0.00	18854.73	-
15	28	31	25	9, 1, 3	0.238	2, 1, 10, 9	0.136	0.00	19043.11	-
16	28	29	27	10, 5, 1	0.204	1, 0, 13, 12	0.183	0.00	19064.91	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
17	28	33	23	4, 5, 5	0.286	9, 0, 3, 2	0.141	0.00	19071.29	-
18	28	31	25	8, 3, 3	0.217	2, 1, 10, 9	0.136	0.00	19255.64	-
19	28	33	23	5, 3, 5	0.270	3, 2, 7, 6	0.134	0.00	19269.00	-
20	28	29	27	9, 7, 1	0.193	1, 0, 13, 12	0.154	0.00	19341.00	-
21	28	33	23	6, 1, 5	0.439	11, 0, 1, 0	0.198	0.00	19442.67	-
22	28	31	25	7, 5, 3	0.210	2, 1, 10, 9	0.103	0.00	19495.15	-
23	28	33	23	5, 3, 5	0.253	10, 0, 2, 1	0.124	0.00	19615.91	-
24	28	29	27	8, 9, 1	0.180	2, 0, 12, 11	0.173	0.00	19638.62	-
25	28	31	25	5, 9, 3	0.216	4, 0, 9, 8	0.095	0.00	19757.37	-
26	28	35	21	1, 5, 7	0.458	6, 2, 3, 2	0.200	0.00	19797.89	-
27	28	33	23	4, 5, 5	0.262	9, 0, 3, 2	0.129	0.00	19813.42	-
28	28	29	27	6, 13, 1	0.195	2, 0, 12, 11	0.140	0.00	19956.67	-
29	28	35	21	0, 7, 7	0.364	4, 3, 4, 3	0.199	0.00	19980.06	-
30	28	33	23	2, 9, 5	0.205	6, 1, 5, 4	0.087	0.00	20024.79	-
31	28	31	25	3, 13, 3	0.173	6, 0, 7, 6	0.108	0.00	20055.24	-
32	28	35	21	3, 1, 7	0.524	9, 1, 1, 0	0.197	0.00	20134.74	-
33	28	35	21	2, 3, 7	0.390	6, 2, 3, 2	0.156	0.00	20289.42	-
34	28	29	27	4, 17, 1	0.253	4, 1, 9, 8	0.142	0.00	20296.32	-
35	28	37	19	0, 1, 9	0.999	5, 4, 1, 0	0.492	20803.02	20802.97	0.05
Symmetry Π_u										
1	1	1	1	0, 1, 0	1.000	0, 0, 1, 0	1.000	667.38	667.39	-0.01
1	3	3	3	0, 3, 0	0.503	0, 0, 2, 1	0.503	1932.47	1932.38	0.09
2	3	3	3	1, 1, 0	0.503	0, 0, 2, 1	0.497	2076.86	2076.89	-0.03
1	5	5	5	1, 3, 0	0.500	0, 0, 3, 2	0.289	3181.46	3181.33	0.13
2	5	5	5	2, 1, 0	0.598	0, 0, 3, 2	0.402	3339.36	3339.37	-0.02
3	5	5	5	1, 3, 0	0.500	0, 0, 3, 2	0.309	3500.67	3500.64	0.03
1	7	7	7	1, 5, 0	0.418	1, 0, 3, 2	0.418	4416.15	4416.19	-0.04
2	7	7	7	3, 1, 0	0.459	0, 0, 4, 3	0.298	4591.12	4591.15	-0.03
3	7	7	7	3, 1, 0	0.401	0, 0, 4, 3	0.326	4753.45	4753.46	0.00
4	7	7	7	1, 5, 0	0.442	1, 0, 3, 2	0.442	4938.35	4938.28	0.07
5	7	9	5	0, 1, 2	1.000	1, 1, 1, 0	0.500	5315.71	5315.76	-0.05
1	9	9	9	2, 5, 0	0.369	1, 1, 3, 2	0.185	0.00	5639.09	-
2	9	9	9	3, 3, 0	0.319	0, 0, 5, 4	0.218	5830.80	5830.96	-0.16
3	9	9	9	4, 1, 0	0.495	0, 0, 5, 4	0.272	6000.53	6000.57	-0.04
4	9	9	9	3, 3, 0	0.363	0, 0, 5, 4	0.271	6179.04	6178.98	0.06
5	9	9	9	1, 7, 0	0.371	1, 0, 4, 3	0.371	6388.08	6388.01	0.07
6	9	11	7	0, 3, 2	0.543	1, 1, 2, 1	0.271	6537.96	6537.96	0.00
7	9	11	7	1, 1, 2	0.543	1, 1, 2, 1	0.229	6679.71	6679.70	0.01
1	11	11	11	2, 7, 0	0.353	1, 1, 4, 3	0.176	0.00	6851.90	-
2	11	11	11	4, 3, 0	0.330	0, 0, 6, 5	0.154	0.00	7059.07	-
3	11	11	11	5, 1, 0	0.449	0, 0, 6, 5	0.215	7240.00	7240.08	-0.07
4	11	11	11	5, 1, 0	0.328	0, 0, 6, 5	0.254	0.00	7416.21	-
5	11	11	11	4, 3, 0	0.277	0, 0, 6, 5	0.223	7616.63	7616.62	0.02
6	11	13	9	1, 3, 2	0.495	3, 0, 2, 1	0.371	7743.70	7743.65	0.05
7	11	11	11	2, 7, 0	0.358	1, 1, 4, 3	0.179	7847.82	7848.01	-0.19
8	11	13	9	2, 1, 2	0.597	4, 0, 1, 0	0.447	7901.47	7901.42	0.05
9	11	13	9	1, 3, 2	0.503	3, 0, 2, 1	0.377	8056.03	8056.03	0.00
1	13	13	13	2, 9, 0	0.304	1, 1, 5, 4	0.152	0.00	8056.10	-
2	13	13	13	5, 3, 0	0.253	1, 0, 6, 5	0.222	0.00	8276.56	-
3	13	13	13	6, 1, 0	0.331	0, 0, 7, 6	0.167	0.00	8470.47	-
4	13	13	13	6, 1, 0	0.425	0, 0, 7, 6	0.212	0.00	8649.15	-
5	13	13	13	5, 3, 0	0.314	0, 0, 7, 6	0.237	0.00	8842.35	-
6	13	15	11	1, 5, 2	0.435	3, 0, 3, 2	0.326	0.00	8935.27	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
7	13	13	13	4, 5, 0	0.292	0, 0, 7, 6	0.180	0.00	9065.14	-
8	13	15	11	3, 1, 2	0.421	1, 1, 4, 3	0.159	0.00	9111.16	-
9	13	15	11	3, 1, 2	0.440	1, 1, 4, 3	0.153	0.00	9269.51	-
10	13	13	13	2, 9, 0	0.345	1, 1, 5, 4	0.172	0.00	9316.77	-
11	13	15	11	1, 5, 2	0.427	3, 0, 3, 2	0.320	0.00	9445.24	-
12	13	17	9	0, 1, 4	1.000	2, 2, 1, 0	0.375	9864.85	9864.50	0.36
1	19	19	19	4, 11, 0	0.269	2, 2, 6, 5	0.101	0.00	11627.91	-
2	19	19	19	6, 7, 0	0.233	1, 1, 8, 7	0.092	0.00	11877.70	-
3	19	19	19	8, 3, 0	0.226	1, 0, 9, 8	0.157	0.00	12105.50	-
4	19	19	19	9, 1, 0	0.282	0, 0, 10, 9	0.100	0.00	12309.50	-
5	19	21	17	2, 9, 2	0.318	4, 0, 5, 4	0.239	0.00	12446.86	-
6	19	19	19	9, 1, 0	0.404	0, 0, 10, 9	0.138	0.00	12498.95	-
7	19	21	17	4, 5, 2	0.269	3, 0, 6, 5	0.169	0.00	12667.70	-
8	19	19	19	8, 3, 0	0.245	0, 0, 10, 9	0.184	0.00	12699.85	-
9	19	21	17	6, 1, 2	0.287	1, 1, 7, 6	0.093	0.00	12862.21	-
10	19	19	19	8, 3, 0	0.207	0, 0, 10, 9	0.204	0.00	12927.59	-
11	19	21	17	6, 1, 2	0.443	1, 1, 7, 6	0.107	0.00	13037.87	-
12	19	19	19	6, 7, 0	0.209	0, 0, 10, 9	0.167	0.00	13182.36	-
13	19	21	17	5, 3, 2	0.302	1, 1, 7, 6	0.111	0.00	13222.58	-
14	19	23	15	1, 5, 4	0.448	4, 1, 3, 2	0.252	0.00	13354.83	-
15	19	21	17	4, 5, 2	0.290	3, 0, 6, 5	0.167	0.00	13434.68	-
16	19	19	19	5, 9, 0	0.234	1, 0, 9, 8	0.212	0.00	13462.15	-
17	19	23	15	3, 1, 4	0.376	2, 2, 4, 3	0.127	0.00	13532.60	-
18	19	21	17	2, 9, 2	0.333	4, 0, 5, 4	0.250	0.00	13675.24	-
19	19	23	15	3, 1, 4	0.473	7, 0, 1, 0	0.258	0.00	13688.47	-
20	19	19	19	3, 13, 0	0.290	1, 1, 8, 7	0.122	0.00	13764.45	-
21	19	23	15	1, 5, 4	0.405	4, 1, 3, 2	0.228	0.00	13855.17	-
22	19	25	13	0, 1, 6	1.000	3, 3, 1, 0	0.312	14313.92	14313.96	-0.04
1	25	25	25	5, 15, 0	0.235	3, 2, 8, 7	0.147	0.00	15154.29	-
2	25	25	25	8, 9, 0	0.199	2, 1, 10, 9	0.121	0.00	15421.69	-
3	25	25	25	9, 7, 0	0.185	1, 1, 11, 10	0.069	0.00	15671.33	-
4	25	27	23	4, 11, 2	0.264	5, 0, 7, 6	0.156	0.00	15892.24	-
5	25	25	25	11, 3, 0	0.220	1, 0, 12, 11	0.113	0.00	15900.72	-
6	25	25	25	12, 1, 0	0.275	6, 6, 1, 0	0.062	0.00	16108.40	-
7	25	27	23	6, 7, 2	0.232	4, 0, 8, 7	0.138	0.00	16140.97	-
8	25	25	25	12, 1, 0	0.377	0, 0, 13, 12	0.086	0.00	16304.48	-
9	25	27	23	7, 5, 2	0.219	3, 0, 9, 8	0.123	0.00	16368.37	-
10	25	25	25	11, 3, 0	0.205	0, 0, 13, 12	0.127	0.00	16512.57	-
11	25	27	23	9, 1, 2	0.239	1, 1, 10, 9	0.057	0.00	16572.31	-
12	25	29	21	2, 9, 4	0.330	6, 0, 5, 4	0.155	0.00	16739.08	-
13	25	25	25	11, 3, 0	0.211	0, 0, 13, 12	0.164	0.00	16745.64	-
14	25	27	23	9, 1, 2	0.401	9, 2, 1, 0	0.141	0.00	16758.96	-
15	25	27	23	9, 1, 2	0.226	1, 1, 10, 9	0.091	0.00	16951.31	-
16	25	29	21	4, 5, 4	0.281	8, 0, 3, 2	0.153	0.00	16961.28	-
17	25	25	25	10, 5, 0	0.206	0, 0, 13, 12	0.187	0.00	17004.59	-
18	25	29	21	5, 3, 4	0.276	2, 2, 7, 6	0.075	0.00	17157.25	-
19	25	27	23	8, 3, 2	0.226	1, 1, 10, 9	0.094	0.00	17169.27	-
20	25	25	25	9, 7, 0	0.193	0, 0, 13, 12	0.161	0.00	17286.20	-
21	25	29	21	6, 1, 4	0.446	10, 0, 1, 0	0.183	0.00	17331.62	-
22	25	27	23	7, 5, 2	0.205	1, 1, 10, 9	0.075	0.00	17413.49	-
23	25	29	21	5, 3, 4	0.274	2, 2, 7, 6	0.076	0.00	17508.41	-
24	25	25	25	8, 9, 0	0.179	0, 0, 13, 12	0.101	0.00	17589.14	-
25	25	31	19	1, 5, 6	0.456	5, 2, 3, 2	0.192	0.00	17675.01	-

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Table 4 – *Continued from previous page*

Number	Polyad ^a			Normal	Normal	Local	Local	Experimental	Theoretical	Δ
State ^a	P_{213}	P_{214}	P_{212}	state ^b	coefficient ^b	state ^c	coefficient ^c	energy ^d	energy	
26	25	27	23	5, 9, 2	0.218	3, 0, 9, 8	0.147	0.00	17681.08	-
27	25	29	21	4, 5, 4	0.263	8, 0, 3, 2	0.144	0.00	17711.47	-
28	25	31	19	0, 7, 6	0.355	3, 3, 4, 3	0.111	0.00	17855.51	-
29	25	25	25	6, 13, 0	0.198	1, 1, 11, 10	0.090	0.00	17912.17	-
30	25	29	21	2, 9, 4	0.300	6, 0, 5, 4	0.141	0.00	17936.07	-
31	25	27	23	3, 13, 2	0.258	5, 0, 7, 6	0.161	0.00	17977.48	-
32	25	31	19	3, 1, 6	0.511	9, 0, 1, 0	0.168	0.00	18010.15	-
33	25	31	19	2, 3, 6	0.378	7, 1, 2, 1	0.165	0.00	18168.64	-
34	25	25	25	4, 17, 0	0.252	2, 2, 9, 8	0.095	0.00	18255.68	-
35	25	33	17	0, 1, 8	1.000	4, 4, 1, 0	0.273	18664.57	18664.57	0.00
Symmetry Δ_g										
1	2	2	2	0, 2, 0	1.000	0, 0, 2, 0	1.000	1335.13	1335.14	-0.01
1	4	4	4	1, 2, 0	0.503	0, 0, 3, 1	0.497	2585.02	2584.88	0.14
2	4	4	4	0, 4, 0	0.503	0, 0, 3, 1	0.503	2760.73	2760.68	0.05
1	6	6	6	1, 4, 0	0.499	0, 0, 4, 2	0.272	3822.01	3821.89	0.12
2	6	6	6	2, 2, 0	0.569	0, 0, 4, 2	0.430	4007.91	4007.80	0.12
3	6	6	6	1, 4, 0	0.500	0, 0, 4, 2	0.298	4197.36	4197.23	0.13
1	8	8	8	1, 6, 0	0.402	1, 0, 4, 2	0.402	0.00	5047.47	-
2	8	8	8	3, 2, 0	0.443	0, 0, 5, 3	0.314	5245.28	5245.43	-0.15
3	8	8	8	3, 2, 0	0.390	0, 0, 5, 3	0.342	5436.50	5437.07	-0.57
4	8	8	8	1, 6, 0	0.431	1, 0, 4, 2	0.431	5644.90	5644.69	0.21
5	8	10	6	0, 2, 2	1.000	1, 1, 2, 0	0.500	5958.51	5958.59	-0.08
1	10	10	10	2, 6, 0	0.373	1, 1, 4, 2	0.186	0.00	6263.01	-
2	10	10	10	3, 4, 0	0.295	0, 0, 6, 4	0.218	0.00	6473.30	-
3	10	10	10	4, 2, 0	0.461	0, 0, 6, 4	0.296	0.00	6670.51	-
4	10	10	10	3, 4, 0	0.347	0, 0, 6, 4	0.273	0.00	6874.98	-
5	10	10	10	1, 8, 0	0.354	1, 0, 5, 3	0.354	0.00	7102.12	-
6	10	12	8	0, 4, 2	0.530	1, 1, 3, 1	0.265	7166.02	7166.00	0.02
7	10	12	8	1, 2, 2	0.530	1, 1, 3, 1	0.235	7338.16	7338.12	0.04
1	14	14	14	3, 8, 0	0.307	1, 1, 6, 4	0.143	0.00	8668.97	-
2	14	14	14	5, 4, 0	0.266	1, 0, 7, 5	0.224	0.00	8901.48	-
3	14	14	14	6, 2, 0	0.322	0, 0, 8, 6	0.173	0.00	9115.29	-
4	14	14	14	6, 2, 0	0.394	0, 0, 8, 6	0.231	0.00	9321.50	-
5	14	14	14	5, 4, 0	0.295	0, 0, 8, 6	0.242	0.00	9538.61	-
6	14	16	12	1, 6, 2	0.418	3, 0, 4, 2	0.313	0.00	9543.28	-
7	14	16	12	3, 2, 2	0.415	1, 1, 5, 3	0.165	0.00	9740.23	-
8	14	14	14	4, 6, 0	0.286	0, 0, 8, 6	0.171	0.00	9778.11	-
9	14	16	12	3, 2, 2	0.420	1, 1, 5, 3	0.163	0.00	9927.24	-
10	14	14	14	2, 10, 0	0.337	1, 1, 6, 4	0.169	0.00	10042.25	-
11	14	16	12	1, 6, 2	0.416	3, 0, 4, 2	0.312	0.00	10126.45	-
12	14	18	10	0, 2, 4	1.000	2, 2, 2, 0	0.375	10482.43	10482.49	-0.06
1	20	20	20	4, 12, 0	0.267	2, 2, 7, 5	0.100	0.00	12229.62	-
2	20	20	20	6, 8, 0	0.220	1, 1, 9, 7	0.092	0.00	12486.52	-
3	20	20	20	8, 4, 0	0.236	1, 0, 10, 8	0.157	0.00	12725.26	-
4	20	20	20	9, 2, 0	0.275	0, 0, 11, 9	0.102	0.00	12947.69	-
5	20	22	18	2, 10, 2	0.301	4, 0, 6, 4	0.226	0.00	13037.47	-
6	20	20	20	9, 2, 0	0.367	0, 0, 11, 9	0.151	0.00	13163.33	-
7	20	22	18	5, 4, 2	0.244	3, 0, 7, 5	0.172	0.00	13269.27	-
8	20	20	20	8, 4, 0	0.216	0, 0, 11, 9	0.194	0.00	13388.13	-
9	20	22	18	6, 2, 2	0.288	1, 1, 8, 6	0.095	0.00	13481.68	-
10	20	20	20	8, 4, 0	0.218	0, 0, 11, 9	0.205	0.00	13632.83	-
11	20	22	18	6, 2, 2	0.407	1, 1, 8, 6	0.117	0.00	13683.63	-
12	20	22	18	5, 4, 2	0.277	1, 1, 8, 6	0.109	0.00	13892.63	-

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Table 4 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
13	20	20	20	7, 6, 0	0.199	0, 0, 11, 9	0.155	0.00	13900.47	-
14	20	24	16	1, 6, 4	0.434	4, 1, 4, 2	0.244	0.00	13939.77	-
15	20	22	18	4, 6, 2	0.277	3, 0, 7, 5	0.173	0.00	14122.28	-
16	20	24	16	3, 2, 4	0.379	2, 2, 5, 3	0.130	0.00	14136.84	-
17	20	20	20	5, 10, 0	0.228	1, 0, 10, 8	0.208	0.00	14190.07	-
18	20	24	16	3, 2, 4	0.449	7, 0, 2, 0	0.245	0.00	14320.01	-
19	20	22	18	2, 10, 2	0.329	4, 0, 6, 4	0.247	0.00	14375.78	-
20	20	20	20	3, 14, 0	0.287	1, 1, 9, 7	0.116	0.00	14501.21	-
21	20	24	16	1, 6, 4	0.395	4, 1, 4, 2	0.222	0.00	14511.27	-
22	20	26	14	0, 2, 6	1.000	3, 3, 2, 0	0.312	14907.22	14907.19	0.04
Symmetry Δ_u										
1	5	6	4	0, 2, 1	1.000	1, 0, 2, 0	1.000	3659.27	3659.33	-0.06
1	7	8	6	0, 4, 1	0.513	1, 0, 3, 1	0.513	4887.97	4887.90	0.06
2	7	8	6	1, 2, 1	0.513	2, 0, 2, 0	0.513	5061.78	5061.75	0.03
1	9	10	8	1, 4, 1	0.499	2, 0, 3, 1	0.499	6103.68	6103.58	0.11
2	9	10	8	2, 2, 1	0.570	1, 0, 4, 2	0.430	6288.49	6288.37	0.12
3	9	10	8	1, 4, 1	0.501	2, 0, 3, 1	0.501	6474.53	6474.50	0.04
1	11	12	10	1, 6, 1	0.411	2, 0, 4, 2	0.411	7307.67	7307.78	-0.11
2	11	12	10	3, 2, 1	0.430	1, 0, 5, 3	0.322	7505.25	7505.13	0.12
3	11	12	10	3, 2, 1	0.405	1, 0, 5, 3	0.334	7694.40	7694.34	0.07
4	11	12	10	1, 6, 1	0.424	2, 0, 4, 2	0.424	7897.55	7897.70	-0.15
5	11	14	8	0, 2, 3	1.000	2, 1, 2, 0	0.750	8232.88	8232.96	-0.08
1	13	14	12	2, 6, 1	0.370	2, 0, 5, 3	0.309	0.00	8501.99	-
2	13	14	12	3, 4, 1	0.307	1, 0, 6, 4	0.229	0.00	8711.88	-
3	13	14	12	4, 2, 1	0.464	1, 0, 6, 4	0.297	0.00	8907.42	-
4	13	14	12	3, 4, 1	0.341	1, 0, 6, 4	0.262	0.00	9108.23	-
5	13	14	12	2, 6, 1	0.359	2, 0, 5, 3	0.344	0.00	9330.56	-
6	13	16	10	0, 4, 3	0.548	2, 1, 3, 1	0.411	9419.12	9419.21	-0.09
7	13	16	10	1, 2, 3	0.548	2, 1, 3, 1	0.339	9589.82	9589.83	-0.01
1	15	16	14	2, 8, 1	0.347	3, 0, 5, 3	0.260	0.00	9687.51	-
2	15	16	14	4, 4, 1	0.322	2, 0, 6, 4	0.231	0.00	9909.08	-
3	15	16	14	5, 2, 1	0.411	1, 0, 7, 5	0.238	0.00	10112.94	-
4	15	16	14	5, 2, 1	0.336	1, 0, 7, 5	0.265	0.00	10314.01	-
5	15	16	14	4, 4, 1	0.294	2, 0, 6, 4	0.207	0.00	10530.92	-
6	15	18	12	1, 4, 3	0.494	4, 0, 3, 1	0.247	0.00	10592.30	-
7	15	16	14	2, 8, 1	0.344	2, 0, 6, 4	0.262	0.00	10771.87	-
8	15	18	12	2, 2, 3	0.547	5, 0, 2, 0	0.342	10776.11	10775.75	0.36
9	15	18	12	1, 4, 3	0.501	4, 0, 3, 1	0.251	0.00	10955.61	-
1	17	18	16	3, 8, 1	0.303	3, 0, 6, 4	0.220	0.00	10865.49	-
2	17	18	16	5, 4, 1	0.256	2, 0, 7, 5	0.227	0.00	11097.51	-
3	17	18	16	6, 2, 1	0.306	1, 0, 8, 6	0.181	0.00	11310.46	-
4	17	18	16	6, 2, 1	0.402	1, 0, 8, 6	0.232	0.00	11514.40	-
5	17	18	16	5, 4, 1	0.290	1, 0, 8, 6	0.236	0.00	11727.52	-
6	17	20	14	1, 6, 3	0.427	4, 0, 4, 2	0.213	0.00	11753.93	-
7	17	20	14	3, 2, 3	0.394	2, 1, 5, 3	0.253	0.00	11950.69	-
8	17	18	16	4, 6, 1	0.283	2, 0, 7, 5	0.229	0.00	11962.20	-
9	17	20	14	3, 2, 3	0.435	6, 0, 2, 0	0.272	0.00	12135.79	-
10	17	18	16	2, 10, 1	0.334	3, 0, 6, 4	0.251	0.00	12220.96	-
11	17	20	14	1, 6, 3	0.406	5, 0, 3, 1	0.215	0.00	12330.95	-
12	17	22	12	0, 2, 5	1.000	3, 2, 2, 0	0.625	12707.19	12707.21	-0.02
1	23	24	22	4, 12, 1	0.267	4, 1, 7, 5	0.150	0.00	14362.99	-
2	23	24	22	6, 8, 1	0.224	3, 0, 9, 7	0.139	0.00	14618.79	-
3	23	24	22	8, 4, 1	0.227	2, 0, 10, 8	0.161	0.00	14856.54	-

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Table 4 – Continued from previous page

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
4	23	24	22	9, 2, 1	0.260	2, 0, 10, 8	0.131	0.00	15077.71	-
5	23	26	20	2, 10, 3	0.309	5, 0, 6, 4	0.193	0.00	15184.88	-
6	23	24	22	9, 2, 1	0.369	1, 0, 11, 9	0.155	0.00	15290.92	-
7	23	26	20	4, 6, 3	0.254	7, 0, 4, 2	0.139	0.00	15416.70	-
8	23	24	22	9, 2, 1	0.215	1, 0, 11, 9	0.194	0.00	15511.82	-
9	23	26	20	6, 2, 3	0.268	2, 1, 8, 6	0.149	0.00	15628.85	-
10	23	24	22	8, 4, 1	0.225	1, 0, 11, 9	0.200	0.00	15751.78	-
11	23	26	20	6, 2, 3	0.409	2, 1, 8, 6	0.176	0.00	15829.09	-
12	23	24	22	7, 6, 1	0.205	2, 0, 10, 8	0.155	0.00	16013.84	-
13	23	26	20	5, 4, 3	0.262	2, 1, 8, 6	0.164	0.00	16034.83	-
14	23	28	18	1, 6, 5	0.440	5, 1, 4, 2	0.220	0.00	16100.81	-
15	23	26	20	4, 6, 3	0.272	7, 0, 4, 2	0.149	0.00	16258.60	-
16	23	28	18	3, 2, 5	0.341	3, 2, 5, 3	0.211	0.00	16298.12	-
17	23	24	22	5, 10, 1	0.209	2, 0, 10, 8	0.188	0.00	16299.26	-
18	23	28	18	3, 2, 5	0.459	8, 0, 2, 0	0.201	0.00	16479.87	-
19	23	26	20	2, 10, 3	0.320	5, 0, 6, 4	0.200	0.00	16506.60	-
20	23	24	22	3, 14, 1	0.284	3, 0, 9, 7	0.166	0.00	16605.23	-
21	23	28	18	1, 6, 5	0.382	5, 1, 4, 2	0.191	0.00	16667.46	-
22	23	30	16	0, 2, 7	1.000	4, 3, 2, 0	0.547	17082.59	17082.48	0.12
Symmetry Φ_g										
1	6	7	5	0, 3, 1	1.000	1, 0, 3, 0	1.000	4314.91	4314.98	-0.07
1	8	9	7	0, 5, 1	0.508	1, 0, 4, 1	0.508	5531.30	5531.20	0.11
2	8	9	7	1, 3, 1	0.508	2, 0, 3, 0	0.508	5730.61	5730.53	0.08
1	10	11	9	1, 5, 1	0.499	2, 0, 4, 1	0.499	6736.76	6736.71	0.05
2	10	11	9	2, 3, 1	0.554	1, 0, 5, 2	0.446	6944.73	6944.54	0.19
3	10	11	9	1, 5, 1	0.501	2, 0, 4, 1	0.501	7154.63	7154.46	0.17
1	12	13	11	1, 7, 1	0.400	2, 0, 5, 2	0.400	0.00	7932.58	-
2	12	13	11	3, 3, 1	0.423	1, 0, 6, 3	0.330	0.00	8149.90	-
3	12	13	11	3, 3, 1	0.395	1, 0, 6, 3	0.346	0.00	8362.78	-
4	12	13	11	1, 7, 1	0.418	2, 0, 5, 2	0.418	0.00	8586.86	-
5	12	15	9	0, 3, 3	1.000	2, 1, 3, 0	0.750	8863.68	8863.73	-0.05
1	18	19	17	3, 9, 1	0.308	3, 0, 7, 4	0.209	0.00	11472.67	-
2	18	19	17	5, 5, 1	0.264	2, 0, 8, 5	0.228	0.00	11716.89	-
3	18	19	17	6, 3, 1	0.303	1, 0, 9, 6	0.185	0.00	11947.38	-
4	18	19	17	6, 3, 1	0.381	1, 0, 9, 6	0.245	0.00	12173.06	-
5	18	21	15	1, 7, 3	0.416	4, 0, 5, 2	0.208	0.00	12355.14	-
6	18	19	17	5, 5, 1	0.277	1, 0, 9, 6	0.241	0.00	12406.67	-
7	18	21	15	3, 3, 3	0.397	2, 1, 6, 3	0.260	0.00	12570.60	-
8	18	19	17	4, 7, 1	0.276	2, 0, 8, 5	0.236	0.00	12657.53	-
9	18	21	15	3, 3, 3	0.419	6, 0, 3, 0	0.262	0.00	12778.68	-
10	18	19	17	2, 11, 1	0.327	3, 0, 7, 4	0.245	0.00	12929.09	-
11	18	21	15	1, 7, 3	0.399	5, 0, 4, 1	0.217	0.00	12994.97	-
12	18	23	13	0, 3, 5	1.000	3, 2, 3, 0	0.625	13313.28	13313.17	0.11
Symmetry Φ_u										
1	3	3	3	0, 3, 0	1.000	0, 0, 3, 0	1.000	2003.25	2003.26	-0.02
1	5	5	5	1, 3, 0	0.506	0, 0, 4, 1	0.494	3240.62	3240.47	0.15
2	5	5	5	0, 5, 0	0.506	0, 0, 4, 1	0.506	3442.22	3442.10	0.11
1	7	7	7	1, 5, 0	0.499	0, 0, 5, 2	0.261	4467.12	4467.10	0.01
2	7	7	7	2, 3, 0	0.553	0, 0, 5, 2	0.446	4676.79	4676.61	0.18
3	7	7	7	1, 5, 0	0.500	0, 0, 5, 2	0.293	4890.10	4889.88	0.22
1	9	9	9	1, 7, 0	0.392	1, 0, 5, 2	0.392	0.00	5684.13	-
2	9	9	9	3, 3, 0	0.434	0, 0, 6, 3	0.322	0.00	5902.72	-
3	9	9	9	3, 3, 0	0.382	0, 0, 6, 3	0.353	0.00	6118.32	-

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Table 4 – Continued from previous page

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
4	9	9	9	1, 7, 0	0.424	1, 0, 5, 2	0.424	6346.71	6346.54	0.17
5	9	11	7	0, 3, 2	1.000	1, 1, 3, 0	0.500	6601.71	6601.79	-0.08
1	15	15	15	3, 9, 0	0.310	1, 1, 7, 4	0.136	0.00	9287.52	-
2	15	15	15	5, 5, 0	0.272	1, 0, 8, 5	0.224	0.00	9532.77	-
3	15	15	15	6, 3, 0	0.315	0, 0, 9, 6	0.177	0.00	9764.79	-
4	15	15	15	6, 3, 0	0.376	0, 0, 9, 6	0.243	0.00	9993.14	-
5	15	17	13	1, 7, 2	0.408	3, 0, 5, 2	0.306	0.00	10156.26	-
6	15	15	15	5, 5, 0	0.283	0, 0, 9, 6	0.247	0.00	10230.68	-
7	15	17	13	3, 3, 2	0.411	1, 1, 6, 3	0.169	0.00	10372.52	-
8	15	15	15	4, 7, 0	0.279	0, 0, 9, 6	0.165	0.00	10486.29	-
9	15	17	13	3, 3, 2	0.407	1, 1, 6, 3	0.169	0.00	10582.90	-
10	15	15	15	2, 11, 0	0.330	1, 1, 7, 4	0.165	0.00	10763.11	-
11	15	17	13	1, 7, 2	0.408	3, 0, 5, 2	0.306	0.00	10803.06	-
12	15	19	11	0, 3, 4	1.000	2, 2, 3, 0	0.375	11100.85	11100.84	0.01
Symmetry Γ_g										
1	4	4	4	0, 4, 0	1.000	0, 0, 4, 0	1.000	2671.14	2671.75	-0.61
1	6	6	6	1, 4, 0	0.510	0, 0, 5, 1	0.490	3898.33	3898.20	0.12
2	6	6	6	0, 6, 0	0.510	0, 0, 5, 1	0.510	4122.27	4122.12	0.15
1	8	8	8	1, 6, 0	0.499	0, 0, 6, 2	0.254	5115.30	5115.64	-0.34
2	8	8	8	2, 4, 0	0.542	0, 0, 6, 2	0.456	5345.60	5345.80	-0.20
3	8	8	8	1, 6, 0	0.500	0, 0, 6, 2	0.290	0.00	5579.91	-
Symmetry Γ_u										
1	7	8	6	0, 4, 1	1.000	1, 0, 4, 0	1.000	4970.93	4971.00	-0.07
1	9	10	8	0, 6, 1	0.503	1, 0, 5, 1	0.503	6176.65	6176.61	0.04
2	9	10	8	1, 4, 1	0.503	2, 0, 4, 0	0.503	6398.07	6397.92	0.15
Symmetry H_g										
1	8	9	7	0, 5, 1	1.000	1, 0, 5, 0	1.000	5627.25	5627.38	-0.12
1	10	11	9	1, 5, 1	0.501	2, 0, 5, 0	0.501	0.00	6823.65	-
2	10	11	9	0, 7, 1	0.501	1, 0, 6, 1	0.501	7064.52	7064.42	0.10
Symmetry H_u										
1	5	5	5	0, 5, 0	1.000	0, 0, 5, 0	1.000	3340.72	3340.60	0.12
1	7	7	7	1, 5, 0	0.512	0, 0, 6, 1	0.488	4557.59	4557.58	0.01
2	7	7	7	0, 7, 0	0.512	0, 0, 6, 1	0.512	4801.36	4801.21	0.15
Symmetry I_g										
1	6	6	6	0, 6, 0	1.000	0, 0, 6, 0	1.000	4009.67	4009.81	-0.14
1	8	8	8	1, 6, 0	0.515	0, 0, 7, 1	0.485	5218.70	5218.32	0.38
2	8	8	8	0, 8, 0	0.515	0, 0, 7, 1	0.515	0.00	5479.68	-
Symmetry I_u										
1	9	10	8	0, 6, 1	1.000	1, 0, 6, 0	1.000	6283.98	6284.12	-0.15
Symmetry J_u										
1	7	7	7	0, 7, 0	1.000	0, 0, 7, 0	1.000	4679.15	4679.40	-0.25

[a] The column labeled state indicates the state position from lower to higher energy inside the polyad for a given symmetry. The second column, labeled Polyad, indicates the polyad to which the state belongs. [b] The third and fourth columns, with headings normal state and coefficient, assign normal-mode labels ($\nu_1\nu_2\nu_3$) the state according to the square value of the largest contribution in this basis. [c] The fifth and sixth columns, with headings local state and coefficient, assign local-mode labels ($\nu_1\nu_2n_+n_-$) the state and its squared maximum component in the local basis is shown. [d] Experimental vibrational energies are taken from Ref.[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

Table 5: Fit of energies (in cm^{-1}) of $^{12}\text{CO}_2$ provided by the Hamiltonian (19) associated with Polyad P_{214} .

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
	P_{214}	P_{212}	P_{213}							
Symmetry Σ_g										
1	2	2	2	0, 2, 0	0.507	0, 0, 1, 1	0.507	1285.41	1285.52	-0.11
2	2	2	2	1, 0, 0	0.507	0, 0, 1, 1	0.493	1388.18	1388.30	-0.11
1	4	4	4	1, 2, 0	0.503	0, 0, 2, 2	0.319	2548.37	2548.41	-0.04
2	4	4	4	2, 0, 0	0.664	0, 0, 2, 2	0.335	2671.14	2671.43	-0.29
3	4	4	4	1, 2, 0	0.496	0, 0, 2, 2	0.346	2797.14	2797.18	-0.05
1	6	6	6	1, 4, 0	0.443	1, 0, 2, 2	0.443	3792.68	3792.55	0.13
2	6	6	6	3, 0, 0	0.495	0, 0, 3, 3	0.262	3942.54	3942.74	-0.20
3	6	6	6	3, 0, 0	0.411	0, 0, 3, 3	0.299	4064.28	4064.55	-0.28
4	6	6	6	1, 4, 0	0.461	0, 0, 3, 3	0.244	4225.10	4225.00	0.10
1	8	4	6	0, 0, 2	1.000	1, 1, 0, 0	0.500	4673.33	4673.15	0.18
2	8	8	8	2, 4, 0	0.367	1, 1, 2, 2	0.184	-	5022.01	-
3	8	8	8	3, 2, 0	0.354	0, 0, 4, 4	0.211	5197.15	5197.19	-0.04
4	8	8	8	4, 0, 0	0.568	0, 0, 4, 4	0.222	5330.60	5329.81	0.79
5	8	8	8	3, 2, 0	0.383	0, 0, 4, 4	0.280	5475.57	5475.74	-0.17
6	8	8	8	1, 6, 0	0.403	1, 0, 3, 3	0.403	-	5667.41	-
1	10	6	8	0, 2, 2	0.563	1, 1, 1, 1	0.281	5915.21	5915.28	-0.07
2	10	6	8	1, 0, 2	0.562	1, 1, 1, 1	0.219	6016.69	6016.62	0.07
3	10	10	10	2, 6, 0	0.366	1, 1, 3, 3	0.183	-	6239.54	-
4	10	10	10	4, 2, 0	0.337	0, 0, 5, 5	0.158	-	6435.13	-
5	10	10	10	5, 0, 0	0.519	0, 0, 5, 5	0.177	-	6588.00	-
6	10	10	10	5, 0, 0	0.322	0, 0, 5, 5	0.231	-	6725.30	-
7	10	10	10	3, 4, 0	0.300	0, 0, 5, 5	0.246	-	6904.11	-
8	10	10	10	2, 6, 0	0.349	1, 1, 3, 3	0.174	-	7121.49	-
1	12	8	10	1, 2, 2	0.494	3, 0, 1, 1	0.370	7133.82	7133.88	-0.06
2	12	8	10	2, 0, 2	0.661	4, 0, 0, 0	0.496	7259.75	7259.86	-0.11
3	12	8	10	1, 2, 2	0.502	3, 0, 1, 1	0.377	7377.62	7377.66	-0.04
4	12	12	12	2, 8, 0	0.322	1, 1, 4, 4	0.161	-	7446.97	-
5	12	12	12	4, 4, 0	0.281	1, 0, 5, 5	0.223	-	7659.24	-
6	12	12	12	6, 0, 0	0.348	0, 0, 6, 6	0.148	-	7833.84	-
7	12	12	12	6, 0, 0	0.484	0, 0, 6, 6	0.173	-	7973.64	-
8	12	12	12	5, 2, 0	0.332	0, 0, 6, 6	0.237	-	8138.54	-
9	12	12	12	4, 4, 0	0.288	0, 0, 6, 6	0.208	-	8345.85	-
10	12	12	12	2, 8, 0	0.350	1, 1, 4, 4	0.175	-	8585.20	-
1	16	8	12	0, 0, 4	1.000	2, 2, 0, 0	0.375	9246.93	9246.75	0.19
2	16	12	14	1, 6, 2	0.374	3, 0, 3, 3	0.280	-	9520.08	-
3	16	12	14	3, 2, 2	0.377	1, 1, 4, 4	0.121	-	9698.62	-
4	16	12	14	4, 0, 2	0.582	6, 0, 0, 0	0.273	-	9833.38	-
5	16	16	16	3, 10, 0	0.290	2, 1, 5, 5	0.218	-	9836.70	-
6	16	12	14	3, 2, 2	0.380	1, 1, 4, 4	0.126	-	9969.55	-
7	16	16	16	5, 6, 0	0.233	1, 1, 6, 6	0.088	-	10074.79	-
8	16	12	14	1, 6, 2	0.383	3, 0, 3, 3	0.287	-	10150.05	-
9	16	16	16	7, 2, 0	0.284	0, 0, 8, 8	0.089	-	10284.08	-
10	16	16	16	8, 0, 0	0.436	4, 4, 0, 0	0.119	-	10454.31	-
11	16	16	16	8, 0, 0	0.380	0, 0, 8, 8	0.145	-	10602.75	-
12	16	16	16	7, 2, 0	0.290	0, 0, 8, 8	0.207	-	10786.46	-
13	16	16	16	6, 4, 0	0.254	0, 0, 8, 8	0.212	-	11008.48	-
14	16	16	16	4, 8, 0	0.230	0, 0, 8, 8	0.140	-	11259.70	-
15	16	16	16	2, 12, 0	0.307	1, 1, 6, 6	0.153	-	11535.86	-
1	18	10	14	0, 2, 4	0.622	2, 2, 1, 1	0.233	10444.89	10445.14	-0.25
2	18	10	14	1, 0, 4	0.622	4, 1, 0, 0	0.350	10546.61	10546.55	0.06

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
3	18	14	16	2, 6, 2	0.366	4, 0, 3, 3	0.275	-	10694.44	-
4	18	14	16	4, 2, 2	0.315	1, 1, 5, 5	0.092	-	10892.41	-
5	18	18	18	4, 10, 0	0.274	2, 2, 5, 5	0.103	-	11020.88	-
6	18	14	16	5, 0, 2	0.468	6, 1, 0, 0	0.198	-	11049.70	-
7	18	14	16	5, 0, 2	0.389	1, 1, 5, 5	0.108	-	11181.48	-
8	18	18	18	6, 6, 0	0.244	1, 1, 7, 7	0.094	-	11269.19	-
9	18	14	16	4, 2, 2	0.276	1, 1, 5, 5	0.111	-	11348.46	-
10	18	18	18	7, 4, 0	0.234	1, 0, 8, 8	0.156	-	11491.53	-
11	18	14	16	2, 6, 2	0.358	4, 0, 3, 3	0.268	-	11554.71	-
12	18	18	18	9, 0, 0	0.295	0, 0, 9, 9	0.086	-	11679.28	-
13	18	18	18	9, 0, 0	0.481	5, 4, 0, 0	0.237	-	11831.93	-
14	18	18	18	8, 2, 0	0.296	0, 0, 9, 9	0.166	-	12003.20	-
15	18	18	18	7, 4, 0	0.248	0, 0, 9, 9	0.209	-	12215.69	-
16	18	18	18	6, 6, 0	0.239	0, 0, 9, 9	0.191	-	12459.33	-
17	18	18	18	5, 8, 0	0.237	0, 0, 9, 9	0.114	-	12728.63	-
18	18	18	18	3, 12, 0	0.286	1, 1, 7, 7	0.138	-	13020.59	-
1	24	12	18	0, 0, 6	1.000	3, 3, 0, 0	0.312	13721.14	13721.07	0.07
2	24	16	20	1, 6, 4	0.397	4, 1, 3, 3	0.223	-	13918.58	-
3	24	16	20	3, 2, 4	0.385	7, 0, 1, 1	0.210	-	14100.76	-
4	24	20	22	3, 10, 2	0.297	5, 0, 5, 5	0.186	-	14163.51	-
5	24	16	20	4, 0, 4	0.572	8, 0, 0, 0	0.313	-	14239.46	-
6	24	16	20	3, 2, 4	0.360	7, 0, 1, 1	0.197	-	14366.92	-
7	24	20	22	5, 6, 2	0.248	3, 0, 7, 7	0.136	-	14402.03	-
8	24	16	20	2, 4, 4	0.361	4, 1, 3, 3	0.201	-	14535.67	-
9	24	24	24	5, 14, 0	0.241	3, 2, 7, 7	0.151	-	14538.56	-
10	24	20	22	7, 2, 2	0.257	3, 0, 7, 7	0.119	-	14613.49	-
11	24	20	22	8, 0, 2	0.369	1, 1, 8, 8	0.062	-	14788.59	-
12	24	24	24	8, 8, 0	0.203	2, 1, 9, 9	0.123	-	14810.11	-
13	24	20	22	8, 0, 2	0.442	8, 2, 0, 0	0.146	-	14933.31	-
14	24	24	24	9, 6, 0	0.206	1, 1, 10, 10	0.070	-	15061.01	-
15	24	20	22	7, 2, 2	0.305	1, 1, 8, 8	0.099	-	15104.35	-
16	24	24	24	11, 2, 0	0.212	1, 0, 11, 11	0.109	-	15287.19	-
17	24	20	22	6, 4, 2	0.265	1, 1, 8, 8	0.098	-	15314.68	-
18	24	24	24	12, 0, 0	0.297	6, 6, 0, 0	0.067	-	15479.86	-
19	24	20	22	5, 6, 2	0.234	3, 0, 7, 7	0.171	-	15554.52	-
20	24	24	24	12, 0, 0	0.456	6, 6, 0, 0	0.103	-	15640.21	-
21	24	20	22	2, 12, 2	0.295	4, 0, 6, 6	0.221	-	15819.14	-
22	24	24	24	11, 2, 0	0.268	0, 0, 12, 12	0.105	-	15820.18	-
23	24	24	24	10, 4, 0	0.201	0, 0, 12, 12	0.157	-	16039.58	-
24	24	24	24	0, 24, 0	0.191	0, 0, 12, 12	0.191	-	16288.59	-
25	24	24	24	0, 24, 0	0.184	0, 0, 12, 12	0.184	-	16561.84	-
26	24	24	24	7, 10, 0	0.194	0, 0, 12, 12	0.130	-	16856.45	-
27	24	24	24	6, 12, 0	0.203	1, 0, 11, 11	0.180	-	17170.44	-
28	24	24	24	3, 18, 0	0.261	2, 1, 9, 9	0.196	-	17502.37	-
1	26	14	20	0, 2, 6	0.681	3, 3, 1, 1	0.213	14874.78	14875.25	-0.47
2	26	14	20	1, 0, 6	0.681	5, 2, 0, 0	0.287	14978.78	14978.49	0.29
3	26	18	22	2, 6, 4	0.361	4, 1, 4, 4	0.173	-	15049.99	-
4	26	18	22	4, 2, 4	0.284	2, 2, 5, 5	0.080	-	15250.61	-
5	26	22	24	4, 10, 2	0.269	5, 0, 6, 6	0.163	-	15305.35	-
6	26	18	22	5, 0, 4	0.398	9, 0, 0, 0	0.196	-	15413.07	-
7	26	18	22	5, 0, 4	0.459	9, 0, 0, 0	0.226	-	15541.87	-
8	26	22	24	6, 6, 2	0.240	4, 0, 7, 7	0.140	-	15553.63	-
9	26	18	22	4, 2, 4	0.308	8, 0, 1, 1	0.168	-	15696.54	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
10	26	26	26	6, 14, 0	0.230	3, 3, 7, 7	0.072	-	15701.03	-
11	26	22	24	7, 4, 2	0.250	3, 0, 8, 8	0.123	-	15777.37	-
12	26	18	22	2, 6, 4	0.364	6, 0, 3, 3	0.170	-	15891.25	-
13	26	22	24	8, 2, 2	0.273	1, 1, 9, 9	0.052	-	15969.36	-
14	26	26	26	8, 10, 0	0.190	2, 1, 10, 10	0.109	-	15978.40	-
15	26	22	24	9, 0, 2	0.501	9, 2, 0, 0	0.177	-	16123.30	-
16	26	26	26	10, 6, 0	0.205	1, 1, 11, 11	0.062	-	16236.33	-
17	26	22	24	8, 2, 2	0.272	1, 1, 9, 9	0.082	-	16282.94	-
18	26	26	26	11, 4, 0	0.222	1, 1, 11, 11	0.056	-	16471.46	-
19	26	22	24	7, 4, 2	0.229	1, 1, 9, 9	0.100	-	16483.17	-
20	26	26	26	12, 2, 0	0.258	6, 6, 1, 1	0.058	-	16676.70	-
21	26	22	24	6, 6, 2	0.229	1, 1, 9, 9	0.087	-	16715.33	-
22	26	26	26	13, 0, 0	0.470	7, 6, 0, 0	0.197	-	16845.12	-
23	26	22	24	5, 8, 2	0.241	3, 0, 8, 8	0.164	-	16973.15	-
24	26	26	26	13, 0, 0	0.247	0, 0, 13, 13	0.074	-	17016.14	-
25	26	26	26	12, 2, 0	0.237	0, 0, 13, 13	0.120	-	17226.54	-
26	26	22	24	3, 12, 2	0.290	4, 0, 7, 7	0.196	-	17253.42	-
27	26	26	26	11, 4, 0	0.220	0, 0, 13, 13	0.167	-	17468.77	-
28	26	26	26	10, 6, 0	0.203	0, 0, 13, 13	0.190	-	17736.05	-
29	26	26	26	9, 8, 0	0.192	0, 0, 13, 13	0.171	-	18025.02	-
30	26	26	26	8, 10, 0	0.180	0, 0, 13, 13	0.113	-	18333.53	-
31	26	26	26	6, 14, 0	0.200	1, 1, 11, 11	0.090	-	18660.03	-
32	26	26	26	4, 18, 0	0.246	2, 2, 9, 9	0.092	-	19003.29	-
1	32	16	24	0, 0, 8	1.000	4, 4, 0, 0	0.273	18096.36	18096.45	-0.09
2	32	20	26	1, 6, 6	0.417	5, 2, 3, 3	0.176	-	18217.59	-
3	32	24	28	3, 10, 4	0.300	7, 0, 5, 5	0.164	-	18391.72	-
4	32	20	26	3, 2, 6	0.376	3, 3, 4, 4	0.095	-	18403.63	-
5	32	20	26	4, 0, 6	0.532	10, 0, 0, 0	0.218	-	18547.79	-
6	32	24	28	5, 6, 4	0.257	9, 0, 3, 3	0.126	-	18630.94	-
7	32	20	26	4, 0, 6	0.325	10, 0, 0, 0	0.133	-	18668.56	-
8	32	28	30	5, 14, 2	0.244	6, 1, 7, 7	0.103	-	18696.81	-
9	32	20	26	2, 4, 6	0.377	7, 1, 2, 2	0.165	-	18824.97	-
10	32	24	28	6, 4, 4	0.234	10, 0, 2, 2	0.096	-	18844.65	-
11	32	28	30	8, 8, 2	0.193	5, 0, 9, 9	0.104	-	18967.24	-
12	32	24	28	8, 0, 4	0.290	2, 2, 8, 8	0.054	-	19024.98	-
13	32	32	32	7, 18, 0	0.207	4, 3, 9, 9	0.113	-	19162.50	-
14	32	24	28	8, 0, 4	0.490	11, 1, 0, 0	0.158	-	19169.26	-
15	32	28	30	9, 6, 2	0.212	4, 0, 10, 10	0.107	-	19218.02	-
16	32	24	28	7, 2, 4	0.306	2, 2, 8, 8	0.069	-	19327.61	-
17	32	28	30	10, 4, 2	0.219	3, 0, 11, 11	0.090	-	19445.67	-
18	32	32	32	10, 12, 0	0.174	3, 2, 11, 11	0.089	-	19453.11	-
19	32	24	28	6, 4, 4	0.268	2, 2, 8, 8	0.066	-	19525.67	-
20	32	28	30	11, 2, 2	0.249	3, 0, 11, 11	0.078	-	19642.89	-
21	32	32	32	12, 8, 0	0.180	2, 2, 12, 12	0.043	-	19726.99	-
22	32	24	28	5, 6, 4	0.248	4, 1, 7, 7	0.125	-	19753.86	-
23	32	28	30	12, 0, 2	0.475	11, 3, 0, 0	0.145	-	19804.16	-
24	32	28	30	11, 2, 2	0.236	1, 1, 12, 12	0.055	-	19971.90	-
25	32	32	32	13, 6, 0	0.183	1, 1, 14, 14	0.042	-	19981.93	-
26	32	24	28	3, 10, 4	0.293	7, 0, 5, 5	0.160	-	20006.77	-
27	32	28	30	11, 2, 2	0.216	1, 1, 12, 12	0.079	-	20178.63	-
28	32	32	32	15, 2, 0	0.189	1, 1, 14, 14	0.047	-	20214.08	-
29	32	32	32	16, 0, 0	0.256	8, 8, 0, 0	0.050	-	20415.17	-
30	32	28	30	10, 4, 2	0.205	1, 1, 12, 12	0.093	-	20416.01	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
31	32	32	32	16, 0, 0	0.448	8, 8, 0, 0	0.088	-	20583.92	-
32	32	28	30	9, 6, 2	0.191	1, 1, 12, 12	0.086	-	20677.75	-
33	32	32	32	15, 2, 0	0.221	1, 0, 15, 15	0.092	-	20766.99	-
34	32	28	30	7, 10, 2	0.183	3, 0, 11, 11	0.130	-	20960.74	-
35	32	32	32	15, 2, 0	0.215	0, 0, 16, 16	0.069	-	20988.14	-
36	32	32	32	14, 4, 0	0.206	0, 0, 16, 16	0.109	-	21238.19	-
37	32	28	30	6, 12, 2	0.206	4, 0, 10, 10	0.133	-	21262.92	-
38	32	32	32	13, 6, 0	0.189	0, 0, 16, 16	0.152	-	21511.38	-
39	32	28	30	3, 18, 2	0.254	5, 0, 9, 9	0.159	-	21582.80	-
40	32	32	32	0, 32, 0	0.179	0, 0, 16, 16	0.179	-	21804.71	-
41	32	32	32	0, 32, 0	0.173	0, 0, 16, 16	0.173	-	22116.23	-
42	32	32	32	10, 12, 0	0.167	0, 0, 16, 16	0.130	-	22444.50	-
43	32	32	32	1, 30, 0	0.168	1, 0, 15, 15	0.168	-	22788.38	-
44	32	32	32	7, 18, 0	0.180	1, 1, 14, 14	0.090	-	23146.97	-
45	32	32	32	4, 24, 0	0.234	2, 2, 12, 12	0.088	-	23519.50	-
1	40	20	30	0, 0, 10	1.000	5, 5, 0, 0	0.246	22373.15	22373.30	-0.15
2	40	24	32	1, 6, 8	0.433	7, 2, 3, 3	0.169	-	22417.22	-
3	40	28	34	3, 10, 6	0.299	7, 1, 6, 6	0.112	-	22521.27	-
4	40	24	32	3, 2, 8	0.352	4, 4, 4, 4	0.091	-	22607.41	-
5	40	32	36	5, 14, 4	0.240	9, 0, 7, 7	0.118	-	22757.71	-
6	40	24	32	4, 0, 8	0.462	11, 1, 0, 0	0.149	-	22758.03	-
7	40	28	34	5, 6, 6	0.254	11, 0, 3, 3	0.115	-	22761.48	-
8	40	24	32	4, 0, 8	0.413	11, 1, 0, 0	0.133	-	22875.15	-
9	40	28	34	6, 4, 6	0.257	12, 0, 2, 2	0.116	-	22977.50	-
10	40	24	32	2, 4, 8	0.385	8, 2, 2, 2	0.127	-	23018.80	-
11	40	32	36	7, 10, 4	0.195	7, 0, 9, 9	0.090	-	23027.18	-
12	40	36	38	7, 18, 2	0.210	8, 1, 9, 9	0.082	-	23154.01	-
13	40	28	34	7, 2, 6	0.283	13, 0, 1, 1	0.119	-	23163.02	-
14	40	32	36	9, 6, 4	0.208	12, 1, 3, 3	0.070	-	23277.90	-
15	40	28	34	8, 0, 6	0.506	14, 0, 0, 0	0.185	-	23310.27	-
16	40	36	38	10, 12, 2	0.176	6, 0, 12, 12	0.059	-	23442.49	-
17	40	28	34	7, 2, 6	0.283	13, 0, 1, 1	0.119	-	23456.95	-
18	40	32	36	10, 4, 4	0.227	4, 1, 11, 11	0.074	-	23506.94	-
19	40	28	34	6, 4, 6	0.259	12, 0, 2, 2	0.117	-	23642.08	-
20	40	32	36	11, 2, 4	0.268	14, 1, 1, 1	0.073	-	23708.40	-
21	40	36	38	12, 8, 2	0.173	5, 0, 13, 13	0.072	-	23715.00	-
22	40	40	40	10, 20, 0	0.189	5, 5, 10, 10	0.046	-	23723.04	-
23	40	28	34	5, 6, 6	0.256	11, 0, 3, 3	0.116	-	23858.40	-
24	40	32	36	12, 0, 4	0.454	14, 2, 0, 0	0.121	-	23873.51	-
25	40	36	38	13, 6, 2	0.188	4, 0, 14, 14	0.071	-	23969.56	-
26	40	40	40	13, 14, 0	0.158	4, 3, 13, 13	0.070	-	24024.06	-
27	40	32	36	12, 0, 4	0.285	2, 2, 12, 12	0.043	-	24030.79	-
28	40	28	34	3, 10, 6	0.299	7, 1, 6, 6	0.114	-	24099.49	-
29	40	36	38	14, 4, 2	0.204	4, 0, 14, 14	0.075	-	24202.98	-
30	40	32	36	11, 2, 4	0.243	2, 2, 12, 12	0.059	-	24224.09	-
31	40	40	40	15, 10, 0	0.157	3, 3, 14, 14	0.032	-	24310.63	-
32	40	36	38	15, 2, 2	0.244	13, 4, 1, 1	0.067	-	24408.52	-
33	40	32	36	10, 4, 4	0.221	2, 2, 12, 12	0.067	-	24449.48	-
34	40	36	38	16, 0, 2	0.445	14, 4, 0, 0	0.114	-	24579.26	-
35	40	40	40	16, 8, 0	0.158	2, 2, 16, 16	0.033	-	24581.19	-
36	40	32	36	9, 6, 4	0.203	2, 2, 12, 12	0.059	-	24699.58	-
37	40	36	38	16, 0, 2	0.257	3, 0, 15, 15	0.066	-	24750.44	-
38	40	40	40	18, 4, 0	0.169	2, 2, 16, 16	0.032	-	24833.42	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
39	40	36	38	15, 2, 2	0.238	1, 1, 16, 16	0.038	-	24958.34	-
40	40	32	36	8, 8, 4	0.185	4, 1, 11, 11	0.098	-	24970.87	-
41	40	40	40	19, 2, 0	0.204	10, 9, 1, 1	0.072	-	25063.03	-
42	40	36	38	14, 4, 2	0.210	1, 1, 16, 16	0.058	-	25196.53	-
43	40	40	40	20, 0, 0	0.297	10, 10, 0, 0	0.052	-	25261.12	-
44	40	32	36	6, 12, 4	0.206	4, 1, 11, 11	0.086	-	25261.18	-
45	40	40	40	20, 0, 0	0.415	10, 10, 0, 0	0.073	-	25432.66	-
46	40	36	38	13, 6, 2	0.184	1, 1, 16, 16	0.077	-	25458.20	-
47	40	32	36	4, 16, 4	0.251	8, 0, 8, 8	0.137	-	25568.96	-
48	40	40	40	19, 2, 0	0.219	10, 9, 1, 1	0.077	-	25625.52	-
49	40	36	38	0, 32, 2	0.175	1, 1, 16, 16	0.088	-	25740.03	-
50	40	40	40	19, 2, 0	0.204	1, 0, 19, 19	0.075	-	25854.06	-
51	40	36	38	11, 10, 2	0.164	1, 1, 16, 16	0.082	-	26039.93	-
52	40	40	40	18, 4, 0	0.196	1, 0, 19, 19	0.100	-	26109.05	-
53	40	36	38	10, 12, 2	0.166	1, 1, 16, 16	0.060	-	26356.42	-
54	40	40	40	17, 6, 0	0.169	0, 0, 20, 20	0.065	-	26385.39	-
55	40	40	40	16, 8, 0	0.141	0, 0, 20, 20	0.103	-	26680.33	-
56	40	36	38	9, 14, 2	0.165	3, 0, 15, 15	0.121	-	26688.34	-
57	40	40	40	16, 8, 0	0.143	0, 0, 20, 20	0.142	-	26992.04	-
58	40	36	38	7, 18, 2	0.179	4, 0, 14, 14	0.131	-	27034.77	-
59	40	40	40	0, 40, 0	0.169	0, 0, 20, 20	0.169	-	27319.16	-
60	40	36	38	4, 24, 2	0.230	5, 0, 13, 13	0.108	-	27394.93	-
61	40	40	40	0, 40, 0	0.169	0, 0, 20, 20	0.169	-	27660.61	-
62	40	40	40	0, 40, 0	0.137	0, 0, 20, 20	0.137	-	28015.51	-
63	40	40	40	1, 38, 0	0.152	0, 0, 20, 20	0.087	-	28383.15	-
64	40	40	40	10, 20, 0	0.147	1, 1, 18, 18	0.070	-	28762.91	-
65	40	40	40	8, 24, 0	0.161	1, 1, 18, 18	0.071	-	29154.27	-
66	40	40	40	5, 30, 0	0.215	2, 2, 16, 16	0.070	-	29556.81	-
1	48	28	38	1, 6, 10	0.438	8, 3, 3, 3	0.160	-	26517.54	-
2	48	24	36	0, 0, 12	0.979	6, 6, 0, 0	0.221	26552.21	26552.11	0.10
3	48	32	40	3, 10, 8	0.283	10, 1, 5, 5	0.104	-	26552.30	-
4	48	28	38	0, 8, 10	0.357	5, 5, 4, 4	0.088	-	26712.39	-
5	48	36	42	5, 14, 6	0.238	11, 0, 7, 7	0.107	-	26721.21	-
6	48	32	40	5, 6, 8	0.245	7, 2, 7, 7	0.087	-	26793.57	-
7	48	28	38	4, 0, 10	0.377	13, 1, 0, 0	0.119	-	26870.01	-
8	48	28	38	4, 0, 10	0.498	13, 1, 0, 0	0.157	-	26987.22	-
9	48	36	42	7, 10, 6	0.200	13, 0, 5, 5	0.084	-	26989.77	-
10	48	32	40	6, 4, 8	0.264	14, 0, 2, 2	0.097	-	27012.11	-
11	48	40	44	7, 18, 4	0.211	10, 0, 10, 10	0.076	-	27049.73	-
12	48	28	38	2, 4, 10	0.382	10, 2, 2, 2	0.126	-	27118.17	-
13	48	32	40	7, 2, 8	0.301	15, 0, 1, 1	0.118	-	27202.55	-
14	48	36	42	9, 6, 6	0.194	15, 0, 3, 3	0.059	-	27240.52	-
15	48	40	44	10, 12, 4	0.172	8, 0, 12, 12	0.074	-	27336.01	-
16	48	32	40	8, 0, 8	0.474	16, 0, 0, 0	0.186	-	27355.51	-
17	48	36	42	10, 4, 6	0.219	5, 2, 11, 11	0.058	-	27470.88	-
18	48	32	40	8, 0, 8	0.294	16, 0, 0, 0	0.115	-	27493.13	-
19	48	44	46	10, 20, 2	0.186	9, 2, 11, 11	0.064	-	27549.35	-
20	48	40	44	12, 8, 4	0.160	7, 0, 13, 13	0.067	-	27607.05	-
21	48	32	40	6, 4, 8	0.231	15, 0, 1, 1	0.087	-	27664.68	-
22	48	36	42	11, 2, 6	0.257	16, 1, 1, 1	0.071	-	27676.14	-
23	48	36	42	12, 0, 6	0.387	17, 1, 0, 0	0.110	-	27847.01	-
24	48	44	46	13, 14, 2	0.155	8, 1, 13, 13	0.050	-	27847.56	-
25	48	40	44	13, 6, 4	0.180	7, 0, 13, 13	0.051	-	27861.16	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
26	48	32	40	5, 6, 8	0.256	13, 0, 3, 3	0.080	-	27868.93	-
27	48	36	42	12, 0, 6	0.354	17, 1, 0, 0	0.100	-	27997.21	-
28	48	40	44	14, 4, 4	0.203	16, 2, 2, 2	0.052	-	28095.51	-
29	48	32	40	3, 10, 8	0.300	10, 1, 5, 5	0.110	-	28098.18	-
30	48	44	46	15, 10, 2	0.149	6, 1, 15, 15	0.045	-	28131.97	-
31	48	36	42	11, 2, 6	0.261	3, 3, 12, 12	0.048	-	28176.43	-
32	48	48	48	13, 22, 0	0.172	6, 6, 12, 12	0.038	-	28222.91	-
33	48	40	44	15, 2, 4	0.243	17, 2, 1, 1	0.055	-	28304.85	-
34	48	36	42	10, 4, 6	0.226	3, 3, 12, 12	0.052	-	28389.50	-
35	48	44	46	16, 8, 2	0.161	6, 0, 16, 16	0.045	-	28401.18	-
36	48	40	44	16, 0, 4	0.394	17, 3, 0, 0	0.095	-	28480.13	-
37	48	48	48	16, 16, 0	0.145	8, 8, 8, 8	0.028	-	28528.94	-
38	48	36	42	9, 6, 6	0.208	3, 3, 12, 12	0.044	-	28627.85	-
39	48	40	44	16, 0, 4	0.318	17, 3, 0, 0	0.076	-	28642.07	-
40	48	44	46	17, 6, 2	0.166	5, 0, 17, 17	0.050	-	28653.18	-
41	48	48	48	18, 12, 0	0.144	4, 4, 16, 16	0.027	-	28821.83	-
42	48	40	44	15, 2, 4	0.247	2, 2, 16, 16	0.031	-	28836.00	-
43	48	44	46	18, 4, 2	0.178	5, 0, 17, 17	0.050	-	28884.47	-
44	48	36	42	8, 8, 6	0.196	5, 2, 11, 11	0.073	-	28887.45	-
45	48	40	44	14, 4, 4	0.201	2, 2, 16, 16	0.046	-	29061.99	-
46	48	44	46	20, 0, 2	0.216	16, 6, 0, 0	0.051	-	29087.61	-
47	48	48	48	20, 8, 0	0.142	10, 10, 4, 4	0.025	-	29100.38	-
48	48	36	42	6, 12, 6	0.201	12, 0, 6, 6	0.091	-	29165.93	-
49	48	44	46	20, 0, 2	0.426	16, 6, 0, 0	0.100	-	29259.04	-
50	48	40	44	13, 6, 4	0.169	2, 2, 16, 16	0.059	-	29312.03	-
51	48	48	48	21, 6, 0	0.163	11, 10, 3, 3	0.055	-	29362.83	-
52	48	44	46	20, 0, 2	0.222	4, 0, 18, 18	0.053	-	29438.68	-
53	48	36	42	4, 16, 6	0.255	10, 0, 8, 8	0.104	-	29461.66	-
54	48	40	44	0, 32, 4	0.170	2, 2, 16, 16	0.064	-	29582.31	-
55	48	48	48	22, 4, 0	0.187	11, 11, 2, 2	0.031	-	29606.31	-
56	48	44	46	19, 2, 2	0.224	3, 0, 19, 19	0.060	-	29653.99	-
57	48	48	48	23, 2, 0	0.230	12, 11, 1, 1	0.074	-	29824.91	-
58	48	40	44	0, 32, 4	0.152	2, 2, 16, 16	0.057	-	29870.61	-
59	48	44	46	18, 4, 2	0.194	3, 0, 19, 19	0.075	-	29897.10	-
60	48	48	48	24, 0, 0	0.392	12, 12, 0, 0	0.063	-	30010.39	-
61	48	44	46	17, 6, 2	0.155	3, 0, 19, 19	0.075	-	30161.94	-
62	48	40	44	10, 12, 4	0.161	4, 1, 15, 15	0.082	-	30175.36	-
63	48	48	48	24, 0, 0	0.320	12, 12, 0, 0	0.052	-	30187.80	-
64	48	48	48	23, 2, 0	0.235	12, 11, 1, 1	0.076	-	30397.98	-
65	48	44	46	17, 6, 2	0.150	1, 1, 20, 20	0.055	-	30445.44	-
66	48	40	44	9, 14, 4	0.168	4, 1, 15, 15	0.086	-	30495.36	-
67	48	48	48	23, 2, 0	0.166	1, 1, 22, 22	0.033	-	30638.82	-
68	48	44	46	16, 8, 2	0.151	1, 1, 20, 20	0.073	-	30745.66	-
69	48	40	44	7, 18, 4	0.175	6, 0, 14, 14	0.078	-	30829.67	-
70	48	48	48	22, 4, 0	0.180	1, 1, 22, 22	0.043	-	30902.53	-
71	48	44	46	0, 40, 2	0.168	1, 1, 20, 20	0.084	-	31061.17	-
72	48	40	44	4, 24, 4	0.223	8, 0, 12, 12	0.122	-	31177.51	-
73	48	48	48	21, 6, 0	0.161	1, 1, 22, 22	0.043	-	31185.30	-
74	48	44	46	0, 40, 2	0.163	1, 1, 20, 20	0.081	-	31390.88	-
75	48	48	48	20, 8, 0	0.130	1, 0, 23, 23	0.097	-	31484.83	-
76	48	44	46	13, 14, 2	0.138	1, 1, 20, 20	0.064	-	31733.90	-
77	48	48	48	20, 8, 0	0.138	0, 0, 24, 24	0.055	-	31799.54	-
78	48	44	46	1, 38, 2	0.151	3, 0, 19, 19	0.113	-	32089.50	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
79	48	48	48	19, 10, 0	0.138	0, 0, 24, 24	0.090	-	32128.17	-
80	48	44	46	10, 20, 2	0.148	4, 0, 18, 18	0.108	-	32457.06	-
81	48	48	48	18, 12, 0	0.134	0, 0, 24, 24	0.129	-	32469.74	-
82	48	48	48	0, 48, 0	0.160	0, 0, 24, 24	0.160	-	32823.42	-
83	48	44	46	3, 34, 2	0.160	5, 0, 17, 17	0.100	-	32836.06	-
84	48	48	48	0, 48, 0	0.169	0, 0, 24, 24	0.169	-	33188.54	-
85	48	44	46	5, 30, 2	0.212	6, 1, 15, 15	0.090	-	33226.06	-
86	48	48	48	0, 48, 0	0.148	0, 0, 24, 24	0.148	-	33564.51	-
87	48	48	48	1, 46, 0	0.129	0, 0, 24, 24	0.105	-	33950.84	-
88	48	48	48	1, 46, 0	0.142	1, 0, 23, 23	0.142	-	34347.10	-
89	48	48	48	2, 44, 0	0.146	1, 1, 22, 22	0.073	-	34752.95	-
90	48	48	48	3, 42, 0	0.152	2, 1, 21, 21	0.114	-	35168.09	-
91	48	48	48	6, 36, 0	0.198	3, 3, 18, 18	0.062	-	35592.27	-
Symmetry Σ_u										
1	4	2	3	0, 0, 1	1.000	1, 0, 0, 0	1.000	2349.14	2349.03	0.11
1	6	4	5	0, 2, 1	0.534	1, 0, 1, 1	0.534	3612.84	3612.89	-0.05
2	6	4	5	1, 0, 1	0.534	2, 0, 0, 0	0.534	3714.79	3714.78	0.02
1	8	6	7	1, 2, 1	0.499	2, 0, 1, 1	0.499	4853.62	4853.64	-0.01
2	8	6	7	2, 0, 1	0.664	3, 0, 0, 0	0.498	4977.84	4977.98	-0.14
3	8	6	7	1, 2, 1	0.500	2, 0, 1, 1	0.500	5099.66	5099.67	-0.01
1	10	8	9	1, 4, 1	0.451	2, 0, 2, 2	0.451	6075.98	6075.79	0.19
2	10	8	9	3, 0, 1	0.467	1, 0, 3, 3	0.275	6227.92	6227.97	-0.06
3	10	8	9	3, 0, 1	0.441	1, 0, 3, 3	0.287	6347.85	6348.06	-0.21
4	10	8	9	1, 4, 1	0.456	2, 0, 2, 2	0.456	6503.08	6503.07	0.02
1	12	6	9	0, 0, 3	1.000	2, 1, 0, 0	0.750	6972.58	6972.38	0.20
2	12	10	11	1, 6, 1	0.361	2, 0, 3, 3	0.361	7283.98	7283.49	0.49
3	12	10	11	3, 2, 1	0.367	1, 0, 4, 4	0.226	7460.52	7460.31	0.21
4	12	10	11	4, 0, 1	0.578	4, 1, 0, 0	0.325	7593.69	7593.77	-0.08
5	12	10	11	3, 2, 1	0.383	1, 0, 4, 4	0.267	7734.45	7734.74	-0.29
6	12	10	11	1, 6, 1	0.394	2, 0, 3, 3	0.394	7920.83	7920.90	-0.07
1	14	8	11	0, 2, 3	0.592	2, 1, 1, 1	0.444	8192.55	8192.69	-0.14
2	14	8	11	1, 0, 3	0.592	2, 1, 1, 1	0.306	8293.95	8293.86	0.09
3	14	12	13	2, 6, 1	0.366	3, 0, 3, 3	0.275	-	8479.40	-
4	14	12	13	4, 2, 1	0.327	2, 0, 4, 4	0.205	8676.72	8676.15	0.56
5	14	12	13	5, 0, 1	0.496	5, 1, 0, 0	0.248	8831.48	8831.11	0.37
6	14	12	13	5, 0, 1	0.355	1, 0, 5, 5	0.224	8965.23	8965.39	-0.16
7	14	12	13	3, 4, 1	0.287	1, 0, 5, 5	0.234	9137.80	9138.36	-0.56
8	14	12	13	2, 6, 1	0.354	2, 0, 4, 4	0.328	-	9350.22	-
1	16	10	13	1, 2, 3	0.486	2, 1, 2, 2	0.291	9388.99	9389.15	-0.16
2	16	10	13	2, 0, 3	0.653	5, 0, 0, 0	0.408	9516.97	9517.08	-0.11
3	16	10	13	1, 2, 3	0.502	4, 0, 1, 1	0.251	9631.35	9631.24	0.12
4	16	14	15	2, 8, 1	0.328	3, 0, 4, 4	0.246	-	9665.35	-
5	16	14	15	4, 4, 1	0.290	2, 0, 5, 5	0.225	-	9878.38	-
6	16	14	15	6, 0, 1	0.314	1, 0, 6, 6	0.159	-	10055.05	-
7	16	14	15	6, 0, 1	0.505	5, 2, 0, 0	0.213	-	10194.53	-
8	16	14	15	5, 2, 1	0.336	1, 0, 6, 6	0.230	-	10353.65	-
9	16	14	15	4, 4, 1	0.294	2, 0, 5, 5	0.201	-	10555.26	-
10	16	14	15	2, 8, 1	0.350	2, 0, 5, 5	0.268	-	10789.04	-
1	18	12	15	1, 4, 3	0.463	4, 0, 2, 2	0.232	-	10567.47	-
2	18	12	15	3, 0, 3	0.401	6, 0, 0, 0	0.251	10724.03	10724.05	-0.02
3	18	12	15	3, 0, 3	0.504	6, 0, 0, 0	0.315	-	10842.18	-
4	18	16	17	3, 8, 1	0.310	3, 0, 5, 5	0.201	10842.06	10842.68	-0.62
5	18	12	15	1, 4, 3	0.441	4, 0, 2, 2	0.221	10986.27	10986.05	0.23

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
6	18	16	17	5, 4, 1	0.276	2, 0, 6, 6	0.208	-	11069.34	-
7	18	16	17	6, 2, 1	0.317	2, 0, 6, 6	0.135	-	11264.50	-
8	18	16	17	7, 0, 1	0.517	6, 2, 0, 0	0.226	-	11418.77	-
9	18	16	17	7, 0, 1	0.266	1, 0, 7, 7	0.190	-	11567.43	-
10	18	16	17	5, 4, 1	0.247	1, 0, 7, 7	0.221	-	11757.53	-
11	18	16	17	4, 6, 1	0.274	2, 0, 6, 6	0.223	-	11982.77	-
12	18	16	17	2, 10, 1	0.330	3, 0, 5, 5	0.248	-	12235.86	-
1	20	10	15	0, 0, 5	1.000	3, 2, 0, 0	0.625	11496.44	11496.30	0.14
2	20	14	17	1, 6, 3	0.386	5, 0, 2, 2	0.213	-	11731.77	-
3	20	14	17	3, 2, 3	0.383	6, 0, 1, 1	0.239	11912.44	11912.11	0.33
4	20	18	19	3, 10, 1	0.294	3, 0, 6, 6	0.153	-	12012.42	-
5	20	14	17	4, 0, 3	0.580	7, 0, 0, 0	0.317	12048.73	12048.62	0.11
6	20	14	17	3, 2, 3	0.372	6, 0, 1, 1	0.233	12179.97	12180.25	-0.28
7	20	18	19	5, 6, 1	0.242	2, 0, 7, 7	0.173	-	12250.69	-
8	20	14	17	1, 6, 3	0.371	5, 0, 2, 2	0.219	-	12354.95	-
9	20	18	19	7, 2, 1	0.272	2, 0, 7, 7	0.160	-	12461.06	-
10	20	18	19	8, 0, 1	0.405	7, 2, 0, 0	0.158	-	12633.65	-
11	20	18	19	8, 0, 1	0.412	7, 2, 0, 0	0.161	-	12779.85	-
12	20	18	19	7, 2, 1	0.298	1, 0, 8, 8	0.203	-	12957.27	-
13	20	18	19	6, 4, 1	0.260	1, 0, 8, 8	0.204	-	13173.51	-
14	20	18	19	1, 14, 1	0.228	2, 0, 7, 7	0.228	-	13419.08	-
15	20	18	19	2, 12, 1	0.301	3, 0, 6, 6	0.226	-	13689.50	-
1	22	12	17	0, 2, 5	0.652	3, 2, 1, 1	0.407	12672.28	12672.65	-0.37
2	22	12	17	1, 0, 5	0.652	5, 1, 0, 0	0.326	12774.73	12774.75	-0.01
3	22	16	19	2, 6, 3	0.364	5, 0, 3, 3	0.228	-	12884.64	-
4	22	16	19	4, 2, 3	0.300	7, 0, 1, 1	0.164	-	13083.90	-
5	22	20	21	4, 10, 1	0.272	4, 1, 5, 5	0.153	-	13175.39	-
6	22	16	19	5, 0, 3	0.435	8, 0, 0, 0	0.190	-	13243.70	-
7	22	16	19	5, 0, 3	0.424	8, 0, 0, 0	0.186	-	13373.62	-
8	22	20	21	6, 6, 1	0.243	3, 0, 7, 7	0.141	-	13423.66	-
9	22	16	19	4, 2, 3	0.292	7, 0, 1, 1	0.160	-	13534.49	-
10	22	20	21	7, 4, 1	0.243	2, 0, 8, 8	0.160	-	13646.68	-
11	22	16	19	2, 6, 3	0.361	5, 0, 3, 3	0.226	-	13735.02	-
12	22	20	21	9, 0, 1	0.260	2, 0, 8, 8	0.108	-	13836.56	-
13	22	20	21	9, 0, 1	0.494	7, 3, 0, 0	0.185	-	13989.50	-
14	22	20	21	8, 2, 1	0.287	1, 0, 9, 9	0.166	-	14154.85	-
15	22	20	21	7, 4, 1	0.240	1, 0, 9, 9	0.205	-	14361.30	-
16	22	20	21	6, 6, 1	0.235	1, 0, 9, 9	0.183	-	14599.24	-
17	22	20	21	5, 8, 1	0.239	2, 0, 8, 8	0.223	-	14862.82	-
18	22	20	21	3, 12, 1	0.288	3, 0, 7, 7	0.202	-	15148.96	-
1	24	14	19	1, 2, 5	0.465	3, 2, 2, 2	0.275	-	13824.81	-
2	24	14	19	2, 0, 5	0.623	6, 1, 0, 0	0.263	13957.22	13957.53	-0.31
3	24	18	21	2, 8, 3	0.340	5, 0, 4, 4	0.212	-	14027.80	-
4	24	14	19	1, 2, 5	0.493	5, 1, 1, 1	0.246	14065.69	14065.45	0.24
5	24	18	21	4, 4, 3	0.302	7, 0, 2, 2	0.165	-	14242.56	-
6	24	22	23	4, 12, 1	0.266	4, 1, 6, 6	0.149	-	14332.27	-
7	24	18	21	5, 2, 3	0.303	2, 1, 6, 6	0.137	-	14423.52	-
8	24	18	21	6, 0, 3	0.535	9, 0, 0, 0	0.175	-	14564.31	-
9	24	22	23	7, 6, 1	0.205	3, 0, 8, 8	0.133	-	14589.20	-
10	24	18	21	5, 2, 3	0.331	2, 1, 6, 6	0.158	-	14712.14	-
11	24	22	23	8, 4, 1	0.243	2, 0, 9, 9	0.142	-	14822.93	-
12	24	18	21	4, 4, 3	0.302	7, 0, 2, 2	0.165	-	14901.89	-
13	24	22	23	9, 2, 1	0.287	2, 0, 9, 9	0.126	-	15027.48	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
14	24	18	21	2, 8, 3	0.348	5, 0, 4, 4	0.217	-	15124.29	-
15	24	22	23	10, 0, 1	0.473	8, 3, 0, 0	0.173	-	15193.39	-
16	24	22	23	10, 0, 1	0.298	1, 0, 10, 10	0.126	-	15350.50	-
17	24	22	23	9, 2, 1	0.254	1, 0, 10, 10	0.180	-	15546.18	-
18	24	22	23	8, 4, 1	0.230	1, 0, 10, 10	0.200	-	15776.29	-
19	24	22	23	7, 6, 1	0.208	1, 0, 10, 10	0.162	-	16033.09	-
20	24	22	23	5, 10, 1	0.226	2, 0, 9, 9	0.210	-	16312.90	-
21	24	22	23	3, 14, 1	0.285	3, 0, 8, 8	0.177	-	16613.41	-
1	28	14	21	0, 0, 7	1.000	4, 3, 0, 0	0.547	15921.09	15921.10	-0.01
2	28	18	23	1, 6, 5	0.408	5, 1, 3, 3	0.204	-	16080.52	-
3	28	18	23	3, 2, 5	0.382	3, 2, 4, 4	0.180	-	16264.60	-
4	28	22	25	3, 10, 3	0.299	6, 0, 5, 5	0.187	-	16289.95	-
5	28	18	23	4, 0, 5	0.556	9, 0, 0, 0	0.274	-	16405.86	-
6	28	22	25	5, 6, 3	0.254	8, 0, 3, 3	0.111	-	16528.78	-
7	28	18	23	3, 2, 5	0.341	8, 0, 1, 1	0.149	-	16529.66	-
8	28	26	27	5, 14, 1	0.243	5, 1, 7, 7	0.122	-	16629.84	-
9	28	18	23	2, 4, 5	0.369	5, 1, 3, 3	0.171	-	16692.31	-
10	28	22	25	7, 2, 3	0.240	9, 1, 1, 1	0.090	-	16741.36	-
11	28	26	27	8, 8, 1	0.199	3, 0, 10, 10	0.086	-	16900.81	-
12	28	22	25	8, 0, 3	0.331	10, 1, 0, 0	0.121	-	16919.05	-
13	28	22	25	8, 0, 3	0.469	10, 1, 0, 0	0.172	-	17063.12	-
14	28	26	27	9, 6, 1	0.210	3, 0, 10, 10	0.106	-	17151.64	-
15	28	22	25	7, 2, 3	0.308	2, 1, 8, 8	0.144	-	17227.77	-
16	28	26	27	10, 4, 1	0.209	2, 0, 11, 11	0.115	-	17378.57	-
17	28	22	25	6, 4, 3	0.268	2, 1, 8, 8	0.139	-	17432.04	-
18	28	26	27	12, 0, 1	0.261	2, 0, 11, 11	0.103	-	17573.54	-
19	28	22	25	5, 6, 3	0.241	4, 0, 7, 7	0.113	-	17666.09	-
20	28	26	27	12, 0, 1	0.470	9, 4, 0, 0	0.158	-	17733.95	-
21	28	26	27	11, 2, 1	0.255	1, 0, 12, 12	0.108	-	17907.67	-
22	28	22	25	3, 10, 3	0.289	6, 0, 5, 5	0.181	-	17924.86	-
23	28	26	27	11, 2, 1	0.201	1, 0, 12, 12	0.158	-	18120.83	-
24	28	26	27	10, 4, 1	0.197	1, 0, 12, 12	0.189	-	18364.07	-
25	28	26	27	9, 6, 1	0.184	1, 0, 12, 12	0.178	-	18631.59	-
26	28	26	27	7, 10, 1	0.189	2, 0, 11, 11	0.171	-	18920.40	-
27	28	26	27	6, 12, 1	0.205	2, 0, 11, 11	0.174	-	19228.50	-
28	28	26	27	3, 18, 1	0.258	4, 1, 8, 8	0.136	-	19554.41	-
1	36	18	27	0, 0, 9	1.000	5, 4, 0, 0	0.492	20247.02	20247.16	-0.15
2	36	22	29	1, 6, 7	0.426	6, 2, 3, 3	0.186	-	20329.81	-
3	36	26	31	3, 10, 5	0.300	8, 0, 5, 5	0.131	-	20468.83	-
4	36	22	29	3, 2, 7	0.366	4, 3, 4, 4	0.174	-	20517.89	-
5	36	22	29	4, 0, 7	0.501	11, 0, 0, 0	0.162	-	20665.19	-
6	36	26	31	5, 6, 5	0.257	10, 0, 3, 3	0.127	-	20708.49	-
7	36	30	33	5, 14, 3	0.244	7, 0, 8, 8	0.115	-	20739.45	-
8	36	22	29	4, 0, 7	0.368	11, 0, 0, 0	0.119	-	20783.70	-
9	36	26	31	6, 4, 5	0.248	11, 0, 2, 2	0.112	-	20923.36	-
10	36	22	29	2, 4, 7	0.382	8, 1, 2, 2	0.149	-	20933.76	-
11	36	30	33	7, 10, 3	0.189	6, 0, 9, 9	0.104	-	21009.37	-
12	36	26	31	7, 2, 5	0.263	12, 0, 1, 1	0.102	-	21106.31	-
13	36	34	35	7, 18, 1	0.209	6, 2, 9, 9	0.091	-	21170.22	-
14	36	26	31	8, 0, 5	0.503	13, 0, 0, 0	0.158	-	21251.67	-
15	36	30	33	9, 6, 3	0.211	5, 0, 10, 10	0.089	-	21260.11	-
16	36	26	31	7, 2, 5	0.298	12, 0, 1, 1	0.115	-	21403.97	-
17	36	34	35	10, 12, 1	0.176	5, 1, 11, 11	0.071	-	21459.77	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
18	36	30	33	10, 4, 3	0.225	11, 2, 2, 2	0.065	-	21488.47	-
19	36	26	31	6, 4, 5	0.265	11, 0, 2, 2	0.120	-	21595.65	-
20	36	30	33	11, 2, 3	0.262	12, 2, 1, 1	0.080	-	21687.86	-
21	36	34	35	12, 8, 1	0.178	4, 1, 12, 12	0.063	-	21732.97	-
22	36	26	31	5, 6, 5	0.253	10, 0, 3, 3	0.124	-	21817.94	-
23	36	30	33	12, 0, 3	0.470	13, 2, 0, 0	0.135	-	21850.73	-
24	36	34	35	13, 6, 1	0.187	3, 0, 14, 14	0.067	-	21987.74	-
25	36	30	33	12, 0, 3	0.249	2, 1, 12, 12	0.084	-	22012.92	-
26	36	26	31	3, 10, 5	0.296	8, 0, 5, 5	0.130	-	22064.94	-
27	36	30	33	11, 2, 3	0.231	2, 1, 12, 12	0.119	-	22213.03	-
28	36	34	35	14, 4, 1	0.198	3, 0, 14, 14	0.073	-	22220.57	-
29	36	34	35	15, 2, 1	0.232	11, 5, 1, 1	0.070	-	22423.96	-
30	36	30	33	10, 4, 3	0.214	2, 1, 12, 12	0.136	-	22444.46	-
31	36	34	35	16, 0, 1	0.453	11, 6, 0, 0	0.126	-	22593.32	-
32	36	30	33	9, 6, 3	0.198	2, 1, 12, 12	0.123	-	22700.40	-
33	36	34	35	16, 0, 1	0.225	2, 0, 15, 15	0.091	-	22770.21	-
34	36	30	33	8, 8, 3	0.179	4, 0, 11, 11	0.087	-	22977.54	-
35	36	34	35	15, 2, 1	0.227	2, 0, 15, 15	0.097	-	22984.82	-
36	36	34	35	14, 4, 1	0.209	1, 0, 16, 16	0.113	-	23228.99	-
37	36	30	33	6, 12, 3	0.207	5, 0, 10, 10	0.113	-	23273.78	-
38	36	34	35	13, 6, 1	0.187	1, 0, 16, 16	0.153	-	23496.43	-
39	36	30	33	3, 18, 3	0.249	6, 0, 9, 9	0.156	-	23587.61	-
40	36	34	35	0, 32, 1	0.177	1, 0, 16, 16	0.177	-	23784.02	-
41	36	34	35	0, 32, 1	0.168	1, 0, 16, 16	0.168	-	24089.74	-
42	36	34	35	10, 12, 1	0.167	2, 0, 15, 15	0.135	-	24412.12	-
43	36	34	35	1, 30, 1	0.165	2, 0, 15, 15	0.165	-	24750.02	-
44	36	34	35	7, 18, 1	0.180	3, 0, 14, 14	0.133	-	25102.52	-
45	36	34	35	4, 24, 1	0.232	4, 1, 12, 12	0.131	-	25468.87	-
1	44	22	33	0, 0, 11	0.997	6, 5, 0, 0	0.450	24474.85	24474.92	-0.07
2	44	26	35	1, 6, 9	0.437	7, 3, 3, 3	0.164	-	24479.83	-
3	44	30	37	3, 10, 7	0.296	9, 1, 5, 5	0.111	-	24549.06	-
4	44	26	35	0, 8, 9	0.345	5, 4, 4, 4	0.170	-	24672.23	-
5	44	34	39	5, 14, 5	0.241	10, 0, 7, 7	0.119	-	24751.65	-
6	44	30	37	5, 6, 7	0.252	12, 0, 3, 3	0.097	-	24789.80	-
7	44	26	35	4, 0, 9	0.422	12, 1, 0, 0	0.142	-	24826.31	-
8	44	26	35	4, 0, 9	0.457	12, 1, 0, 0	0.153	-	24942.98	-
9	44	30	37	6, 4, 7	0.262	13, 0, 2, 2	0.110	-	25007.07	-
10	44	34	39	7, 10, 5	0.199	12, 0, 5, 5	0.077	-	25020.66	-
11	44	26	35	2, 4, 9	0.385	9, 2, 2, 2	0.136	-	25080.22	-
12	44	38	41	7, 18, 3	0.211	9, 1, 9, 9	0.079	-	25113.86	-
13	44	30	37	7, 2, 7	0.296	14, 0, 1, 1	0.124	-	25195.10	-
14	44	34	39	9, 6, 5	0.202	10, 0, 7, 7	0.059	-	25271.38	-
15	44	30	37	8, 0, 7	0.496	15, 0, 0, 0	0.195	-	25344.93	-
16	44	38	41	10, 12, 3	0.175	7, 0, 12, 12	0.072	-	25401.24	-
17	44	30	37	7, 2, 7	0.259	14, 0, 1, 1	0.108	-	25486.64	-
18	44	34	39	10, 4, 5	0.225	14, 1, 2, 2	0.069	-	25501.09	-
19	44	42	43	10, 20, 1	0.188	8, 3, 10, 10	0.069	-	25647.95	-
20	44	30	37	6, 4, 7	0.248	13, 0, 2, 2	0.104	-	25665.06	-
21	44	38	41	12, 8, 3	0.168	6, 0, 13, 13	0.074	-	25673.02	-
22	44	34	39	11, 2, 5	0.266	15, 1, 1, 1	0.080	-	25704.51	-
23	44	34	39	12, 0, 5	0.425	16, 1, 0, 0	0.116	-	25872.33	-
24	44	30	37	5, 6, 7	0.257	12, 0, 3, 3	0.099	-	25875.36	-
25	44	38	41	13, 6, 3	0.186	5, 0, 14, 14	0.062	-	25927.37	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
26	44	42	43	13, 14, 1	0.157	6, 2, 13, 13	0.056	-	25947.61	-
27	44	34	39	12, 0, 5	0.320	16, 1, 0, 0	0.087	-	26025.55	-
28	44	30	37	3, 10, 7	0.300	9, 1, 5, 5	0.112	-	26110.53	-
29	44	38	41	14, 4, 3	0.206	5, 0, 14, 14	0.063	-	26161.30	-
30	44	34	39	11, 2, 5	0.254	3, 2, 12, 12	0.098	-	26211.87	-
31	44	42	43	15, 10, 1	0.154	5, 1, 15, 15	0.052	-	26233.12	-
32	44	38	41	15, 2, 3	0.247	15, 3, 1, 1	0.064	-	26368.83	-
33	44	34	39	10, 4, 5	0.225	3, 2, 12, 12	0.108	-	26431.15	-
34	44	42	43	16, 8, 1	0.161	4, 1, 16, 16	0.052	-	26503.04	-
35	44	38	41	16, 0, 3	0.426	16, 3, 0, 0	0.099	-	26541.60	-
36	44	34	39	9, 6, 5	0.207	3, 2, 12, 12	0.093	-	26675.38	-
37	44	38	41	16, 0, 3	0.289	16, 3, 0, 0	0.067	-	26707.73	-
38	44	42	43	17, 6, 1	0.161	4, 1, 16, 16	0.047	-	26755.20	-
39	44	38	41	15, 2, 3	0.245	15, 3, 1, 1	0.063	-	26908.72	-
40	44	34	39	8, 8, 5	0.191	5, 1, 11, 11	0.087	-	26940.81	-
41	44	42	43	19, 2, 1	0.187	13, 7, 1, 1	0.050	-	26985.74	-
42	44	38	41	14, 4, 3	0.207	2, 1, 16, 16	0.089	-	27140.85	-
43	44	42	43	20, 0, 1	0.257	14, 7, 0, 0	0.067	-	27186.44	-
44	44	34	39	6, 12, 5	0.205	11, 0, 6, 6	0.092	-	27225.19	-
45	44	42	43	20, 0, 1	0.427	14, 7, 0, 0	0.111	-	27357.45	-
46	44	38	41	13, 6, 3	0.178	2, 1, 16, 16	0.117	-	27396.72	-
47	44	34	39	4, 16, 5	0.253	9, 0, 8, 8	0.125	-	27526.94	-
48	44	42	43	19, 2, 1	0.199	3, 0, 18, 18	0.055	-	27543.52	-
49	44	38	41	0, 32, 3	0.173	2, 1, 16, 16	0.130	-	27672.78	-
50	44	42	43	19, 2, 1	0.216	2, 0, 19, 19	0.078	-	27765.53	-
51	44	38	41	11, 10, 3	0.159	2, 1, 16, 16	0.118	-	27966.87	-
52	44	42	43	18, 4, 1	0.197	2, 0, 19, 19	0.100	-	28014.61	-
53	44	38	41	10, 12, 3	0.164	2, 1, 16, 16	0.085	-	28277.48	-
54	44	42	43	17, 6, 1	0.163	2, 0, 19, 19	0.104	-	28285.21	-
55	44	42	43	17, 6, 1	0.144	1, 0, 20, 20	0.106	-	28574.43	-
56	44	38	41	9, 14, 3	0.167	4, 0, 15, 15	0.079	-	28603.43	-
57	44	42	43	16, 8, 1	0.147	1, 0, 20, 20	0.144	-	28880.39	-
58	44	38	41	7, 18, 3	0.178	5, 0, 14, 14	0.107	-	28943.79	-
59	44	42	43	0, 40, 1	0.169	1, 0, 20, 20	0.169	-	29201.70	-
60	44	38	41	4, 24, 3	0.227	7, 0, 12, 12	0.124	-	29297.77	-
61	44	42	43	0, 40, 1	0.166	1, 0, 20, 20	0.166	-	29537.27	-
62	44	42	43	13, 14, 1	0.135	1, 0, 20, 20	0.133	-	29886.22	-
63	44	42	43	1, 38, 1	0.152	2, 0, 19, 19	0.152	-	30247.83	-
64	44	42	43	10, 20, 1	0.148	2, 0, 19, 19	0.127	-	30621.48	-
65	44	42	43	8, 24, 1	0.161	3, 0, 18, 18	0.103	-	31006.66	-
66	44	42	43	5, 30, 1	0.214	5, 1, 15, 15	0.107	-	31402.92	-
Symmetry Π_g										
1	5	3	4	0, 1, 1	1.000	1, 0, 1, 0	1.000	3004.01	3004.02	-0.01
1	7	5	6	0, 3, 1	0.515	1, 0, 2, 1	0.515	4247.71	4247.77	-0.07
2	7	5	6	1, 1, 1	0.515	2, 0, 1, 0	0.515	4390.63	4390.63	0.00
1	9	7	8	1, 3, 1	0.501	2, 0, 2, 1	0.501	5475.07	5475.02	0.05
2	9	7	8	2, 1, 1	0.598	3, 0, 1, 0	0.448	5632.77	5632.86	-0.09
3	9	7	8	1, 3, 1	0.499	2, 0, 2, 1	0.499	5790.58	5790.55	0.03
1	11	9	10	1, 5, 1	0.423	2, 0, 3, 2	0.423	6688.17	6687.87	0.30
2	11	9	10	3, 1, 1	0.448	1, 0, 4, 3	0.303	6863.56	6863.54	0.02
3	11	9	10	3, 1, 1	0.413	1, 0, 4, 3	0.322	7023.67	7023.85	-0.17
4	11	9	10	1, 5, 1	0.438	2, 0, 3, 2	0.438	7203.83	7203.82	0.01
1	13	7	10	0, 1, 3	1.000	2, 1, 1, 0	0.750	7602.51	7602.50	0.01

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
2	13	11	12	2, 5, 1	0.371	2, 0, 4, 3	0.323	-	7888.48	-
3	13	11	12	3, 3, 1	0.325	1, 0, 5, 4	0.221	8081.84	8081.60	0.24
4	13	11	12	4, 1, 1	0.498	4, 1, 1, 0	0.280	8250.63	8250.72	-0.09
5	13	11	12	3, 3, 1	0.360	1, 0, 5, 4	0.268	8425.01	8425.36	-0.36
6	13	11	12	1, 7, 1	0.368	2, 0, 4, 3	0.368	-	8628.84	-
1	15	9	12	0, 3, 3	0.557	2, 1, 2, 1	0.417	8803.27	8803.45	-0.18
2	15	9	12	1, 1, 3	0.557	2, 1, 2, 1	0.333	8944.14	8944.05	0.09
3	15	13	14	2, 7, 1	0.355	3, 0, 4, 3	0.266	-	9078.61	-
4	15	13	14	4, 3, 1	0.330	2, 0, 5, 4	0.224	-	9287.46	-
5	15	13	14	5, 1, 1	0.442	5, 1, 1, 0	0.221	-	9469.15	-
6	15	13	14	5, 1, 1	0.339	1, 0, 6, 5	0.252	-	9642.94	-
7	15	13	14	4, 3, 1	0.279	1, 0, 6, 5	0.223	-	9838.51	-
8	15	13	14	2, 7, 1	0.355	2, 0, 5, 4	0.302	-	10063.85	-
1	17	11	14	1, 3, 3	0.495	2, 1, 3, 2	0.251	9987.37	9987.44	-0.08
2	17	11	14	2, 1, 3	0.594	5, 0, 1, 0	0.371	10145.49	10145.55	-0.06
3	17	15	16	2, 9, 1	0.304	3, 0, 5, 4	0.228	-	10259.67	-
4	17	11	14	1, 3, 3	0.500	4, 0, 2, 1	0.250	10297.08	10296.89	0.20
5	17	15	16	5, 3, 1	0.251	2, 0, 6, 5	0.225	-	10482.28	-
6	17	15	16	6, 1, 1	0.320	1, 0, 7, 6	0.166	-	10677.69	-
7	17	15	16	6, 1, 1	0.432	1, 0, 7, 6	0.210	-	10855.55	-
8	17	15	16	5, 3, 1	0.312	1, 0, 7, 6	0.236	-	11044.86	-
9	17	15	16	4, 5, 1	0.291	2, 0, 6, 5	0.214	-	11262.26	-
10	17	15	16	2, 9, 1	0.343	3, 0, 5, 4	0.257	-	11507.36	-
1	21	11	16	0, 1, 5	1.000	3, 2, 1, 0	0.625	12101.57	12101.58	-0.01
2	21	15	18	2, 5, 3	0.359	5, 0, 3, 2	0.224	-	12314.64	-
3	21	15	18	3, 3, 3	0.349	6, 0, 2, 1	0.218	-	12509.36	-
4	21	19	20	3, 11, 1	0.278	4, 1, 5, 4	0.148	-	12598.75	-
5	21	15	18	4, 1, 3	0.502	7, 0, 1, 0	0.275	-	12677.70	-
6	21	19	20	6, 5, 1	0.234	2, 0, 8, 7	0.155	-	12843.70	-
7	21	15	18	3, 3, 3	0.344	6, 0, 2, 1	0.215	-	12844.98	-
8	21	15	18	2, 5, 3	0.359	5, 0, 3, 2	0.225	-	13038.02	-
9	21	19	20	7, 3, 1	0.278	2, 0, 8, 7	0.168	-	13064.33	-
10	21	19	20	8, 1, 1	0.368	7, 2, 1, 0	0.144	-	13260.26	-
11	21	19	20	8, 1, 1	0.364	1, 0, 9, 8	0.171	-	13446.30	-
12	21	19	20	7, 3, 1	0.285	1, 0, 9, 8	0.210	-	13649.41	-
13	21	19	20	6, 5, 1	0.255	1, 0, 9, 8	0.197	-	13879.81	-
14	21	19	20	5, 7, 1	0.236	2, 0, 8, 7	0.227	-	14135.91	-
15	21	19	20	2, 13, 1	0.287	3, 0, 7, 6	0.215	-	14415.10	-
1	29	15	22	0, 1, 7	1.000	4, 3, 1, 0	0.547	16501.57	16501.56	0.01
2	29	19	24	1, 7, 5	0.373	5, 1, 4, 3	0.187	-	16641.40	-
3	29	19	24	3, 3, 5	0.363	3, 2, 5, 4	0.171	-	16838.28	-
4	29	23	26	3, 11, 3	0.288	6, 0, 6, 5	0.180	-	16854.85	-
5	29	19	24	4, 1, 5	0.493	9, 0, 1, 0	0.243	-	17007.10	-
6	29	23	26	5, 7, 3	0.227	5, 0, 7, 6	0.109	-	17099.90	-
7	29	19	24	3, 3, 5	0.316	8, 0, 2, 1	0.138	-	17168.02	-
8	29	27	28	5, 15, 1	0.234	5, 1, 8, 7	0.117	-	17204.53	-
9	29	23	26	7, 3, 3	0.262	9, 1, 2, 1	0.098	-	17321.54	-
10	29	19	24	2, 5, 5	0.372	5, 1, 4, 3	0.158	-	17350.59	-
11	29	27	28	8, 9, 1	0.203	4, 0, 10, 9	0.080	-	17479.27	-
12	29	23	26	8, 1, 3	0.326	10, 1, 1, 0	0.119	-	17518.24	-
13	29	23	26	8, 1, 3	0.396	10, 1, 1, 0	0.145	-	17700.19	-
14	29	27	28	10, 5, 1	0.185	3, 0, 11, 10	0.104	-	17735.05	-
15	29	23	26	7, 3, 3	0.282	2, 1, 9, 8	0.151	-	17893.69	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
16	29	27	28	11, 3, 1	0.222	2, 0, 12, 11	0.109	-	17969.55	-
17	29	23	26	6, 5, 3	0.253	2, 1, 9, 8	0.134	-	18113.00	-
18	29	27	28	12, 1, 1	0.267	2, 0, 12, 11	0.115	-	18181.30	-
19	29	23	26	5, 7, 3	0.245	4, 0, 8, 7	0.111	-	18357.73	-
20	29	27	28	12, 1, 1	0.383	9, 4, 1, 0	0.129	-	18378.57	-
21	29	27	28	11, 3, 1	0.206	1, 0, 13, 12	0.119	-	18584.73	-
22	29	23	26	3, 11, 3	0.291	6, 0, 6, 5	0.182	-	18625.29	-
23	29	27	28	11, 3, 1	0.217	1, 0, 13, 12	0.164	-	18814.75	-
24	29	27	28	10, 5, 1	0.206	1, 0, 13, 12	0.189	-	19069.24	-
25	29	27	28	9, 7, 1	0.192	1, 0, 13, 12	0.173	-	19345.78	-
26	29	27	28	8, 9, 1	0.175	2, 0, 12, 11	0.174	-	19642.29	-
27	29	27	28	6, 13, 1	0.204	2, 0, 12, 11	0.165	-	19957.16	-
28	29	27	28	3, 19, 1	0.249	4, 1, 9, 8	0.138	-	20289.13	-
1	37	19	28	0, 1, 9	1.000	5, 4, 1, 0	0.492	20803.02	20802.84	0.18
2	37	23	30	1, 7, 7	0.396	6, 2, 4, 3	0.173	-	20868.82	-
3	37	27	32	3, 11, 5	0.294	8, 0, 6, 5	0.128	-	21012.46	-
4	37	23	30	3, 3, 7	0.364	4, 3, 5, 4	0.166	-	21068.41	-
5	37	23	30	4, 1, 7	0.467	11, 0, 1, 0	0.151	-	21238.97	-
6	37	27	32	5, 7, 5	0.241	10, 0, 4, 3	0.119	-	21257.89	-
7	37	31	34	5, 15, 3	0.239	8, 0, 8, 7	0.105	-	21293.07	-
8	37	23	30	4, 1, 7	0.335	11, 0, 1, 0	0.108	-	21395.00	-
9	37	27	32	7, 3, 5	0.236	12, 0, 2, 1	0.091	-	21480.83	-
10	37	31	34	8, 9, 3	0.197	6, 0, 10, 9	0.103	-	21566.50	-
11	37	23	30	2, 5, 7	0.379	8, 1, 3, 2	0.148	-	21567.28	-
12	37	27	32	8, 1, 5	0.274	3, 2, 9, 8	0.101	-	21679.09	-
13	37	35	36	8, 17, 1	0.203	6, 2, 10, 9	0.087	-	21736.22	-
14	37	31	34	9, 7, 3	0.197	5, 0, 11, 10	0.089	-	21821.78	-
15	37	27	32	8, 1, 5	0.416	13, 0, 1, 0	0.131	-	21858.57	-
16	37	35	36	10, 13, 1	0.164	5, 1, 12, 11	0.071	-	22027.99	-
17	37	27	32	7, 3, 5	0.262	3, 2, 9, 8	0.118	-	22043.14	-
18	37	31	34	11, 3, 3	0.194	4, 0, 12, 11	0.060	-	22056.75	-
19	37	27	32	6, 5, 5	0.241	11, 0, 3, 2	0.109	-	22251.28	-
20	37	31	34	12, 1, 3	0.218	12, 2, 2, 1	0.065	-	22269.37	-
21	37	35	36	12, 9, 1	0.173	4, 1, 13, 12	0.066	-	22304.04	-
22	37	31	34	12, 1, 3	0.383	13, 2, 1, 0	0.110	-	22464.25	-
23	37	27	32	5, 7, 5	0.250	10, 0, 4, 3	0.123	-	22484.50	-
24	37	35	36	14, 5, 1	0.171	3, 0, 15, 14	0.059	-	22562.73	-
25	37	31	34	12, 1, 3	0.248	2, 1, 13, 12	0.094	-	22661.94	-
26	37	27	32	3, 11, 5	0.295	8, 0, 6, 5	0.129	-	22740.32	-
27	37	35	36	15, 3, 1	0.201	3, 0, 15, 14	0.072	-	22801.88	-
28	37	31	34	11, 3, 3	0.236	2, 1, 13, 12	0.124	-	22880.94	-
29	37	35	36	16, 1, 1	0.235	2, 0, 16, 15	0.066	-	23020.10	-
30	37	31	34	10, 5, 3	0.214	2, 1, 13, 12	0.137	-	23124.08	-
31	37	35	36	16, 1, 1	0.363	11, 6, 1, 0	0.101	-	23224.38	-
32	37	31	34	9, 7, 3	0.200	2, 1, 13, 12	0.119	-	23389.14	-
33	37	35	36	16, 1, 1	0.230	2, 0, 16, 15	0.100	-	23435.50	-
34	37	35	36	15, 3, 1	0.226	2, 0, 16, 15	0.098	-	23668.29	-
35	37	31	34	8, 9, 3	0.186	4, 0, 12, 11	0.088	-	23674.00	-
36	37	35	36	14, 5, 1	0.196	1, 0, 17, 16	0.117	-	23924.06	-
37	37	31	34	6, 13, 3	0.202	5, 0, 11, 10	0.115	-	23977.00	-
38	37	35	36	13, 7, 1	0.170	1, 0, 17, 16	0.157	-	24200.59	-
39	37	31	34	4, 17, 3	0.250	6, 0, 10, 9	0.150	-	24296.86	-
40	37	35	36	0, 33, 1	0.178	1, 0, 17, 16	0.178	-	24495.84	-

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Table 5 – *Continued from previous page*

Number	Polyad ^a			Normal	Normal	Local	Local	Experimental	Theoretical	Δ
State ^a	P_{214}	P_{212}	P_{213}	state ^b	coefficient ^b	state ^c	coefficient ^c	energy ^d	energy	
41	37	35	36	0, 33, 1	0.165	1, 0, 17, 16	0.165	-	24808.25	-
42	37	35	36	10, 13, 1	0.161	2, 0, 16, 15	0.140	-	25136.58	-
43	37	35	36	9, 15, 1	0.164	2, 0, 16, 15	0.161	-	25479.84	-
44	37	35	36	7, 19, 1	0.176	3, 0, 15, 14	0.130	-	25837.20	-
45	37	35	36	4, 25, 1	0.227	4, 1, 13, 12	0.128	-	26207.96	-
Symmetry Π_u										
1	1	1	1	0, 1, 0	1.000	0, 0, 1, 0	1.000	667.38	667.43	-0.05
1	3	3	3	1, 1, 0	0.504	0, 0, 2, 1	0.496	1932.47	1932.54	-0.07
2	3	3	3	0, 3, 0	0.504	0, 0, 2, 1	0.504	2076.86	2076.90	-0.05
1	5	5	5	1, 3, 0	0.502	0, 0, 3, 2	0.280	3181.46	3181.43	0.04
2	5	5	5	2, 1, 0	0.597	0, 0, 3, 2	0.402	3339.36	3339.51	-0.15
3	5	5	5	1, 3, 0	0.497	0, 0, 3, 2	0.319	3500.67	3500.62	0.05
1	7	7	7	1, 5, 0	0.414	1, 0, 3, 2	0.414	4416.15	4415.93	0.21
2	7	7	7	3, 1, 0	0.465	0, 0, 4, 3	0.293	4591.12	4591.19	-0.07
3	7	7	7	3, 1, 0	0.393	0, 0, 4, 3	0.330	4753.45	4753.61	-0.16
4	7	7	7	1, 5, 0	0.444	1, 0, 3, 2	0.444	4938.35	4938.20	0.15
1	9	5	7	0, 1, 2	1.000	1, 1, 1, 0	0.500	5315.71	5315.71	0.01
2	9	9	9	2, 5, 0	0.375	1, 1, 3, 2	0.188	-	5638.12	-
3	9	9	9	3, 3, 0	0.311	0, 0, 5, 4	0.209	5830.80	5830.66	0.14
4	9	9	9	4, 1, 0	0.492	0, 0, 5, 4	0.270	6000.53	6000.62	-0.09
5	9	9	9	3, 3, 0	0.364	0, 0, 5, 4	0.279	6179.04	6179.19	-0.15
6	9	9	9	1, 7, 0	0.378	1, 0, 4, 3	0.378	6388.08	6387.81	0.27
1	11	7	9	0, 3, 2	0.535	1, 1, 2, 1	0.268	6537.96	6538.07	-0.11
2	11	7	9	1, 1, 2	0.535	1, 1, 2, 1	0.232	6679.71	6679.66	0.04
3	11	11	11	2, 7, 0	0.352	1, 1, 4, 3	0.176	-	6849.74	-
4	11	11	11	4, 3, 0	0.333	0, 0, 6, 5	0.144	-	7058.08	-
5	11	11	11	5, 1, 0	0.454	0, 0, 6, 5	0.209	-724.00	7239.75	0.25
6	11	11	11	5, 1, 0	0.318	0, 0, 6, 5	0.256	-	7416.38	-
7	11	11	11	4, 3, 0	0.268	0, 0, 6, 5	0.234	7616.63	7616.88	-0.25
8	11	11	11	2, 7, 0	0.352	1, 1, 4, 3	0.176	7847.82	7847.62	0.20
1	13	9	11	1, 3, 2	0.499	3, 0, 2, 1	0.374	7743.70	7743.69	0.00
2	13	9	11	2, 1, 2	0.597	4, 0, 1, 0	0.448	7901.47	7901.53	-0.06
3	13	13	13	3, 7, 0	0.309	1, 1, 5, 4	0.148	-	8052.19	-
4	13	9	11	1, 3, 2	0.500	3, 0, 2, 1	0.375	8056.03	8055.95	0.08
5	13	13	13	5, 3, 0	0.264	1, 0, 6, 5	0.221	-	8274.46	-
6	13	13	13	6, 1, 0	0.341	0, 0, 7, 6	0.157	-	8469.47	-
7	13	13	13	6, 1, 0	0.419	0, 0, 7, 6	0.208	-	8648.94	-
8	13	13	13	5, 3, 0	0.314	0, 0, 7, 6	0.243	-	8842.70	-
9	13	13	13	4, 5, 0	0.289	0, 0, 7, 6	0.194	-	9065.44	-
10	13	13	13	2, 9, 0	0.345	1, 1, 5, 4	0.172	-	9316.08	-
1	17	9	13	0, 1, 4	1.000	2, 2, 1, 0	0.375	9864.85	9864.45	0.40
2	17	13	15	2, 5, 2	0.366	4, 0, 3, 2	0.274	-	10113.99	-
3	17	13	15	3, 3, 2	0.338	1, 1, 5, 4	0.117	-	10307.84	-
4	17	17	17	3, 11, 0	0.273	2, 1, 6, 5	0.205	-	10433.80	-
5	17	13	15	4, 1, 2	0.501	1, 1, 5, 4	0.136	-	10476.41	-
6	17	13	15	3, 3, 2	0.354	1, 1, 5, 4	0.128	-	10647.28	-
7	17	17	17	6, 5, 0	0.241	1, 1, 7, 6	0.093	-	10678.81	-
8	17	13	15	1, 7, 2	0.357	3, 0, 4, 3	0.268	-	10845.55	-
9	17	17	17	7, 3, 0	0.283	1, 0, 8, 7	0.166	-	10899.06	-
10	17	17	17	8, 1, 0	0.385	0, 0, 9, 8	0.121	-	11094.93	-
11	17	17	17	8, 1, 0	0.346	0, 0, 9, 8	0.169	-	11283.54	-
12	17	17	17	7, 3, 0	0.283	0, 0, 9, 8	0.213	-	11491.58	-
13	17	17	17	6, 5, 0	0.254	0, 0, 9, 8	0.205	-	11727.45	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
14	17	17	17	5, 7, 0	0.230	0, 0, 9, 8	0.128	-	11989.17	-
15	17	17	17	2, 13, 0	0.293	1, 1, 7, 6	0.146	-	12274.12	-
1	25	13	19	0, 1, 6	1.000	3, 3, 1, 0	0.312	14313.92	14313.94	-0.01
2	25	17	21	1, 7, 4	0.361	4, 1, 4, 3	0.203	-	14490.44	-
3	25	17	21	3, 3, 4	0.357	7, 0, 2, 1	0.195	-	14686.18	-
4	25	21	23	3, 11, 2	0.283	5, 0, 6, 5	0.177	-	14739.11	-
5	25	17	21	4, 1, 4	0.499	8, 0, 1, 0	0.273	-	14854.59	-
6	25	21	23	6, 5, 2	0.225	4, 0, 7, 6	0.134	-	14984.07	-
7	25	17	21	3, 3, 4	0.332	7, 0, 2, 1	0.182	-	15018.54	-
8	25	25	25	5, 15, 0	0.231	3, 2, 8, 7	0.144	-	15123.86	-
9	25	21	23	7, 3, 2	0.272	3, 0, 8, 7	0.126	-	15205.16	-
10	25	17	21	2, 5, 4	0.366	4, 1, 4, 3	0.186	-	15206.34	-
11	25	25	25	8, 9, 0	0.203	2, 1, 10, 9	0.118	-	15399.29	-
12	25	21	23	8, 1, 2	0.348	1, 1, 9, 8	0.068	-	15401.38	-
13	25	21	23	8, 1, 2	0.381	1, 1, 9, 8	0.087	-	15585.18	-
14	25	25	25	10, 5, 0	0.194	1, 1, 11, 10	0.067	-	15655.35	-
15	25	21	23	7, 3, 2	0.285	1, 1, 9, 8	0.103	-	15783.43	-
16	25	25	25	11, 3, 0	0.232	1, 1, 11, 10	0.052	-	15889.67	-
17	25	21	23	6, 5, 2	0.255	1, 1, 9, 8	0.094	-	16008.31	-
18	25	25	25	12, 1, 0	0.290	6, 6, 1, 0	0.065	-	16101.18	-
19	25	21	23	5, 7, 2	0.241	3, 0, 8, 7	0.169	-	16258.74	-
20	25	25	25	12, 1, 0	0.376	6, 6, 1, 0	0.085	-	16300.22	-
21	25	25	25	11, 3, 0	0.221	0, 0, 13, 12	0.115	-	16510.93	-
22	25	21	23	3, 11, 2	0.289	4, 0, 7, 6	0.210	-	16532.13	-
23	25	25	25	11, 3, 0	0.206	0, 0, 13, 12	0.163	-	16746.45	-
24	25	25	25	10, 5, 0	0.200	0, 0, 13, 12	0.192	-	17006.56	-
25	25	25	25	9, 7, 0	0.188	0, 0, 13, 12	0.179	-	17288.80	-
26	25	25	25	7, 11, 0	0.178	0, 0, 13, 12	0.122	-	17591.10	-
27	25	25	25	6, 13, 0	0.203	1, 1, 11, 10	0.088	-	17911.88	-
28	25	25	25	3, 19, 0	0.253	2, 1, 10, 9	0.190	-	18249.89	-
1	33	17	25	0, 1, 8	1.000	4, 4, 1, 0	0.273	18664.57	18664.51	0.06
2	33	21	27	1, 7, 6	0.385	5, 2, 4, 3	0.162	-	18767.52	-
3	33	25	29	3, 11, 4	0.291	7, 0, 6, 5	0.159	-	18945.97	-
4	33	21	27	3, 3, 6	0.365	3, 3, 5, 4	0.090	-	18965.69	-
5	33	21	27	4, 1, 6	0.482	10, 0, 1, 0	0.198	-	19135.22	-
6	33	25	29	5, 7, 4	0.235	9, 0, 4, 3	0.116	-	19191.18	-
7	33	29	31	5, 15, 2	0.237	6, 1, 8, 7	0.100	-	19260.94	-
8	33	21	27	4, 1, 6	0.307	10, 0, 1, 0	0.126	-	19293.48	-
9	33	25	29	7, 3, 4	0.250	4, 1, 8, 7	0.093	-	19413.43	-
10	33	21	27	2, 5, 6	0.376	7, 1, 3, 2	0.165	-	19470.87	-
11	33	29	31	8, 9, 2	0.200	5, 0, 10, 9	0.102	-	19535.01	-
12	33	25	29	8, 1, 4	0.301	2, 2, 9, 8	0.057	-	19610.83	-
13	33	33	33	8, 17, 0	0.205	4, 4, 9, 8	0.056	-	19738.98	-
14	33	29	31	9, 7, 2	0.188	4, 0, 11, 10	0.104	-	19790.52	-
15	33	25	29	8, 1, 4	0.400	2, 2, 9, 8	0.065	-	19791.33	-
16	33	25	29	7, 3, 4	0.274	2, 2, 9, 8	0.073	-	19980.24	-
17	33	29	31	11, 3, 2	0.209	3, 0, 12, 11	0.086	-	20025.25	-
18	33	33	33	11, 11, 0	0.166	3, 2, 12, 11	0.088	-	20031.89	-
19	33	25	29	6, 5, 4	0.249	2, 2, 9, 8	0.063	-	20193.97	-
20	33	29	31	12, 1, 2	0.243	3, 0, 12, 11	0.087	-	20237.37	-
21	33	33	33	12, 9, 0	0.170	2, 2, 13, 12	0.045	-	20308.74	-
22	33	25	29	5, 7, 4	0.244	4, 1, 8, 7	0.121	-	20432.95	-
23	33	29	31	12, 1, 2	0.380	11, 3, 1, 0	0.116	-	20433.27	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
24	33	33	33	14, 5, 0	0.180	2, 1, 14, 13	0.081	-	20567.80	-
25	33	29	31	12, 1, 2	0.226	1, 1, 13, 12	0.061	-	20635.06	-
26	33	25	29	3, 11, 4	0.294	7, 0, 6, 5	0.161	-	20694.65	-
27	33	33	33	15, 3, 0	0.212	1, 1, 15, 14	0.046	-	20806.85	-
28	33	29	31	11, 3, 2	0.227	1, 1, 13, 12	0.082	-	20859.57	-
29	33	33	33	16, 1, 0	0.258	8, 8, 1, 0	0.051	-	21024.89	-
30	33	29	31	10, 5, 2	0.211	1, 1, 13, 12	0.093	-	21108.40	-
31	33	33	33	16, 1, 0	0.361	8, 8, 1, 0	0.071	-	21230.85	-
32	33	29	31	9, 7, 2	0.197	1, 1, 13, 12	0.083	-	21379.21	-
33	33	33	33	16, 1, 0	0.211	1, 0, 16, 15	0.100	-	21446.45	-
34	33	29	31	8, 9, 2	0.181	3, 0, 12, 11	0.131	-	21669.90	-
35	33	33	33	15, 3, 0	0.220	0, 0, 17, 16	0.073	-	21684.77	-
36	33	33	33	14, 5, 0	0.198	0, 0, 17, 16	0.114	-	21946.18	-
37	33	29	31	6, 13, 2	0.203	4, 0, 11, 10	0.136	-	21978.84	-
38	33	33	33	13, 7, 0	0.175	0, 0, 17, 16	0.155	-	22228.38	-
39	33	29	31	4, 17, 2	0.248	5, 0, 10, 9	0.153	-	22304.76	-
40	33	33	33	0, 33, 0	0.179	0, 0, 17, 16	0.179	-	22529.36	-
41	33	33	33	0, 33, 0	0.169	0, 0, 17, 16	0.169	-	22847.58	-
42	33	33	33	10, 13, 0	0.163	0, 0, 17, 16	0.125	-	23181.81	-
43	33	33	33	1, 31, 0	0.164	1, 0, 16, 15	0.164	-	23531.06	-
44	33	33	33	7, 19, 0	0.177	1, 1, 15, 14	0.088	-	23894.51	-
45	33	33	33	4, 25, 0	0.229	2, 2, 13, 12	0.086	-	24271.47	-
Symmetry Δ_g										
1	2	2	2	0, 2, 0	1.000	0, 0, 2, 0	1.000	1335.13	1335.19	-0.06
1	4	4	4	1, 2, 0	0.511	0, 0, 3, 1	0.489	2585.02	2585.05	-0.03
2	4	4	4	0, 4, 0	0.511	0, 0, 3, 1	0.511	2760.73	2760.70	0.02
1	6	6	6	1, 4, 0	0.501	0, 0, 4, 2	0.261	3822.01	3821.92	0.09
2	6	6	6	2, 2, 0	0.568	0, 0, 4, 2	0.430	4007.91	4007.99	-0.07
3	6	6	6	1, 4, 0	0.497	0, 0, 4, 2	0.309	4197.36	4197.22	0.14
1	8	8	8	1, 6, 0	0.396	1, 0, 4, 2	0.396	-	5047.02	-
2	8	8	8	3, 2, 0	0.451	0, 0, 5, 3	0.307	5245.28	5245.49	-0.21
3	8	8	8	3, 2, 0	0.381	0, 0, 5, 3	0.348	5436.50	5437.30	-0.80
4	8	8	8	1, 6, 0	0.434	1, 0, 4, 2	0.434	5644.90	5644.59	0.31
1	10	6	8	0, 2, 2	1.000	1, 1, 2, 0	0.500	5958.51	5958.61	-0.10
2	10	10	10	2, 6, 0	0.377	1, 1, 4, 2	0.189	-	6261.64	-
3	10	10	10	4, 2, 0	0.295	0, 0, 6, 4	0.208	-	6472.91	-
4	10	10	10	4, 2, 0	0.458	0, 0, 6, 4	0.294	-	6670.66	-
5	10	10	10	3, 4, 0	0.350	0, 0, 6, 4	0.282	-	6875.26	-
6	10	10	10	1, 8, 0	0.362	1, 0, 5, 3	0.362	-	7101.87	-
1	12	8	10	0, 4, 2	0.521	1, 1, 3, 1	0.261	7166.02	7166.14	-0.12
2	12	8	10	1, 2, 2	0.521	1, 1, 3, 1	0.239	7338.16	7338.11	0.04
3	12	12	12	2, 8, 0	0.340	1, 1, 5, 3	0.170	-	7467.00	-
4	12	12	12	4, 4, 0	0.324	0, 0, 7, 5	0.136	-	7690.51	-
5	12	12	12	5, 2, 0	0.425	0, 0, 7, 5	0.224	-	7896.48	-
6	12	12	12	5, 2, 0	0.310	0, 0, 7, 5	0.272	-	8101.07	-
7	12	12	12	4, 4, 0	0.276	0, 0, 7, 5	0.229	-	8322.46	-
8	12	12	12	2, 8, 0	0.353	1, 1, 5, 3	0.176	-	8567.86	-
1	18	10	14	0, 2, 4	1.000	2, 2, 2, 0	0.375	10482.43	10482.50	-0.07
2	18	14	16	2, 6, 2	0.372	4, 0, 4, 2	0.279	-	10714.59	-
3	18	14	16	3, 4, 2	0.311	1, 1, 6, 4	0.115	-	10925.46	-
4	18	18	18	4, 10, 0	0.275	2, 2, 6, 4	0.103	-	11037.13	-
5	18	14	16	4, 2, 2	0.465	1, 1, 6, 4	0.148	-	11120.19	-
6	18	18	18	6, 6, 0	0.247	1, 1, 8, 6	0.096	-	11291.04	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
7	18	14	16	3, 4, 2	0.339	1, 1, 6, 4	0.131	-	11317.54	-
8	18	18	18	7, 4, 0	0.272	1, 0, 9, 7	0.172	-	11525.05	-
9	18	14	16	2, 6, 2	0.357	4, 0, 4, 2	0.268	-	11534.37	-
10	18	18	18	8, 2, 0	0.359	0, 0, 10, 8	0.128	-	11743.32	-
11	18	18	18	8, 2, 0	0.325	0, 0, 10, 8	0.183	-	11959.20	-
12	18	18	18	7, 4, 0	0.272	0, 0, 10, 8	0.221	-	12188.81	-
13	18	18	18	6, 6, 0	0.248	0, 0, 10, 8	0.201	-	12439.80	-
14	18	18	18	5, 8, 0	0.235	0, 0, 10, 8	0.120	-	12713.04	-
15	18	18	18	3, 12, 0	0.285	1, 1, 8, 6	0.141	-	13007.46	-
1	26	14	20	0, 2, 6	1.000	3, 3, 2, 0	0.312	14907.22	14907.15	0.08
2	26	18	22	2, 6, 4	0.362	4, 1, 5, 3	0.188	-	15068.28	-
3	26	18	22	3, 4, 4	0.334	2, 2, 6, 4	0.095	-	15279.40	-
4	26	22	24	3, 12, 2	0.269	5, 0, 7, 5	0.168	-	15320.42	-
5	26	18	22	4, 2, 4	0.466	8, 0, 2, 0	0.255	-	15472.07	-
6	26	22	24	6, 6, 2	0.237	4, 0, 8, 6	0.142	-	15573.55	-
7	26	18	22	3, 4, 4	0.318	2, 2, 6, 4	0.089	-	15662.82	-
8	26	26	26	6, 14, 0	0.231	3, 3, 8, 6	0.072	-	15714.68	-
9	26	22	24	7, 4, 2	0.270	3, 0, 9, 7	0.131	-	15806.93	-
10	26	18	22	2, 6, 4	0.368	4, 1, 5, 3	0.179	-	15869.94	-
11	26	26	26	8, 10, 0	0.196	2, 1, 11, 9	0.113	-	15995.29	-
12	26	22	24	8, 2, 2	0.334	1, 1, 10, 8	0.071	-	16023.27	-
13	26	22	24	8, 2, 2	0.350	1, 1, 10, 8	0.095	-	16233.67	-
14	26	26	26	10, 6, 0	0.203	1, 1, 12, 10	0.065	-	16258.60	-
15	26	22	24	7, 4, 2	0.269	1, 1, 10, 8	0.107	-	16454.43	-
16	26	26	26	11, 4, 0	0.234	1, 1, 12, 10	0.058	-	16504.19	-
17	26	22	24	6, 6, 2	0.244	1, 1, 10, 8	0.093	-	16695.00	-
18	26	26	26	12, 2, 0	0.279	6, 6, 2, 0	0.063	-	16734.66	-
19	26	22	24	5, 8, 2	0.242	3, 0, 9, 7	0.168	-	16957.16	-
20	26	26	26	12, 2, 0	0.339	0, 0, 14, 12	0.079	-	16959.72	-
21	26	26	26	11, 4, 0	0.194	0, 0, 14, 12	0.123	-	17193.76	-
22	26	22	24	3, 12, 2	0.290	4, 0, 8, 6	0.201	-	17240.07	-
23	26	26	26	11, 4, 0	0.212	0, 0, 14, 12	0.169	-	17445.88	-
24	26	26	26	10, 6, 0	0.202	0, 0, 14, 12	0.194	-	17718.27	-
25	26	26	26	9, 8, 0	0.191	0, 0, 14, 12	0.175	-	18010.33	-
26	26	26	26	8, 10, 0	0.177	0, 0, 14, 12	0.116	-	18320.90	-
27	26	26	26	6, 14, 0	0.201	1, 1, 12, 10	0.090	-	18648.86	-
28	26	26	26	3, 20, 0	0.246	2, 1, 11, 9	0.184	-	18993.22	-
Symmetry Δ_u										
1	6	4	5	0, 2, 1	1.000	1, 0, 2, 0	1.000	3659.27	3659.36	-0.08
1	8	6	7	0, 4, 1	0.505	1, 0, 3, 1	0.505	4887.97	4888.05	-0.09
2	8	6	7	1, 2, 1	0.505	2, 0, 2, 0	0.505	5061.78	5061.76	0.02
1	10	8	9	1, 4, 1	0.501	2, 0, 3, 1	0.501	6103.68	6103.58	0.11
2	10	8	9	2, 2, 1	0.569	1, 0, 4, 2	0.431	6288.49	6288.56	-0.06
3	10	8	9	1, 4, 1	0.499	2, 0, 3, 1	0.499	6474.53	6474.47	0.06
1	12	10	11	1, 6, 1	0.405	2, 0, 4, 2	0.405	7307.67	7307.27	0.40
2	12	10	11	3, 2, 1	0.438	1, 0, 5, 3	0.315	7505.25	7505.20	0.04
3	12	10	11	3, 2, 1	0.396	1, 0, 5, 3	0.341	7694.40	7694.58	-0.18
4	12	10	11	1, 6, 1	0.428	2, 0, 4, 2	0.428	7897.55	7897.58	-0.03
1	14	8	11	0, 2, 3	1.000	2, 1, 2, 0	0.750	8232.88	8232.98	-0.09
2	14	12	13	2, 6, 1	0.375	2, 0, 5, 3	0.298	-	8500.52	-
3	14	12	13	3, 4, 1	0.298	1, 0, 6, 4	0.218	-	8711.51	-
4	14	12	13	4, 2, 1	0.462	1, 0, 6, 4	0.295	-	8907.64	-
5	14	12	13	3, 4, 1	0.345	1, 0, 6, 4	0.272	-	9108.55	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
6	14	12	13	1, 8, 1	0.353	2, 0, 5, 3	0.353	-	9330.27	-
1	16	10	13	0, 4, 3	0.539	2, 1, 3, 1	0.404	9419.12	9419.35	-0.23
2	16	10	13	1, 2, 3	0.539	2, 1, 3, 1	0.346	9589.82	9589.80	0.02
3	16	14	15	2, 8, 1	0.344	3, 0, 5, 3	0.258	-	9684.55	-
4	16	14	15	4, 4, 1	0.324	2, 0, 6, 4	0.237	-	9907.85	-
5	16	14	15	5, 2, 1	0.417	1, 0, 7, 5	0.231	-	10112.82	-
6	16	14	15	5, 2, 1	0.326	1, 0, 7, 5	0.269	-	10314.46	-
7	16	14	15	4, 4, 1	0.285	1, 0, 7, 5	0.219	-	10531.30	-
8	16	14	15	2, 8, 1	0.354	2, 0, 6, 4	0.286	-	10771.46	-
1	18	12	15	1, 4, 3	0.498	4, 0, 3, 1	0.249	-	10592.23	-
2	18	12	15	2, 2, 3	0.568	5, 0, 2, 0	0.355	10776.11	10775.69	0.43
3	18	16	17	3, 8, 1	0.311	3, 0, 6, 4	0.213	-	10860.42	-
4	18	12	15	1, 4, 3	0.500	4, 0, 3, 1	0.250	-	10955.41	-
5	18	16	17	5, 4, 1	0.266	2, 0, 7, 5	0.225	-	11094.94	-
6	18	16	17	6, 2, 1	0.317	1, 0, 8, 6	0.171	-	11309.62	-
7	18	16	17	6, 2, 1	0.397	1, 0, 8, 6	0.229	-	11514.65	-
8	18	16	17	5, 4, 1	0.295	1, 0, 8, 6	0.244	-	11728.25	-
9	18	16	17	4, 6, 1	0.285	2, 0, 7, 5	0.222	-	11962.52	-
10	18	16	17	2, 10, 1	0.337	3, 0, 6, 4	0.253	-	12220.07	-
1	22	12	17	0, 2, 5	1.000	3, 2, 2, 0	0.625	12707.19	12707.21	-0.02
2	22	16	19	2, 6, 3	0.368	5, 0, 4, 2	0.230	-	12903.84	-
3	22	16	19	3, 4, 3	0.323	6, 0, 3, 1	0.202	-	13114.75	-
4	22	20	21	4, 10, 1	0.272	4, 1, 6, 4	0.153	-	13191.05	-
5	22	16	19	4, 2, 3	0.467	7, 0, 2, 0	0.255	-	13308.33	-
6	22	20	21	6, 6, 1	0.242	3, 0, 8, 6	0.143	-	13444.53	-
7	22	16	19	3, 4, 3	0.330	6, 0, 3, 1	0.206	-	13502.28	-
8	22	20	21	7, 4, 1	0.272	2, 0, 9, 7	0.174	-	13678.17	-
9	22	16	19	2, 6, 3	0.363	5, 0, 4, 2	0.227	-	13714.23	-
10	22	20	21	8, 2, 1	0.347	7, 2, 2, 0	0.136	-	13895.38	-
11	22	20	21	8, 2, 1	0.338	1, 0, 10, 8	0.186	-	14108.41	-
12	22	20	21	7, 4, 1	0.271	1, 0, 10, 8	0.218	-	14333.55	-
13	22	20	21	6, 6, 1	0.247	1, 0, 10, 8	0.194	-	14579.33	-
14	22	20	21	5, 8, 1	0.239	2, 0, 9, 7	0.226	-	14847.05	-
15	22	20	21	3, 12, 1	0.288	3, 0, 8, 6	0.207	-	15135.73	-
1	30	16	23	0, 2, 7	1.000	4, 3, 2, 0	0.547	17082.59	17082.37	0.23
2	30	20	25	2, 6, 5	0.356	5, 1, 5, 3	0.174	-	17207.91	-
3	30	20	25	3, 4, 5	0.342	3, 2, 6, 4	0.167	-	17419.41	-
4	30	24	27	3, 12, 3	0.275	6, 0, 7, 5	0.172	-	17425.21	-
5	30	20	25	4, 2, 5	0.463	9, 0, 2, 0	0.228	-	17611.43	-
6	30	24	27	6, 6, 3	0.230	5, 0, 8, 6	0.116	-	17678.08	-
7	30	28	29	6, 14, 1	0.228	5, 1, 9, 7	0.112	-	17784.55	-
8	30	20	25	3, 4, 5	0.304	3, 2, 6, 4	0.140	-	17799.22	-
9	30	24	27	7, 4, 3	0.265	9, 1, 3, 1	0.099	-	17911.31	-
10	30	20	25	2, 6, 5	0.372	6, 1, 4, 2	0.157	-	18001.58	-
11	30	28	29	8, 10, 1	0.198	7, 2, 6, 4	0.077	-	18064.26	-
12	30	24	27	8, 2, 3	0.318	10, 1, 2, 0	0.116	-	18126.97	-
13	30	28	29	10, 6, 1	0.198	3, 0, 12, 10	0.101	-	18326.93	-
14	30	24	27	8, 2, 3	0.361	2, 1, 10, 8	0.144	-	18334.99	-
15	30	24	27	7, 4, 3	0.263	2, 1, 10, 8	0.157	-	18551.48	-
16	30	28	29	11, 4, 1	0.228	2, 0, 13, 11	0.105	-	18572.02	-
17	30	24	27	6, 6, 3	0.240	2, 1, 10, 8	0.132	-	18786.85	-
18	30	28	29	12, 2, 1	0.263	2, 0, 13, 11	0.123	-	18801.52	-
19	30	28	29	12, 2, 1	0.344	9, 4, 2, 0	0.115	-	19024.14	-

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Table 5 – *Continued from previous page*

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
20	30	24	27	5, 8, 3	0.244	4, 0, 9, 7	0.110	-	19043.44	-
21	30	28	29	12, 2, 1	0.207	1, 0, 14, 12	0.127	-	19254.03	-
22	30	24	27	3, 12, 3	0.292	6, 0, 7, 5	0.182	-	19320.56	-
23	30	28	29	11, 4, 1	0.219	1, 0, 14, 12	0.170	-	19501.09	-
24	30	28	29	10, 6, 1	0.206	1, 0, 14, 12	0.191	-	19768.04	-
25	30	28	29	9, 8, 1	0.194	1, 0, 14, 12	0.169	-	20054.47	-
26	30	28	29	8, 10, 1	0.181	2, 0, 13, 11	0.176	-	20359.27	-
27	30	28	29	6, 14, 1	0.200	2, 0, 13, 11	0.158	-	20681.32	-
28	30	28	29	4, 18, 1	0.247	4, 1, 10, 8	0.139	-	21019.64	-
Symmetry Φ_g										
1	7	5	6	0, 3, 1	1.000	1, 0, 3, 0	1.000	4314.91	4315.03	-0.12
1	9	7	8	1, 3, 1	0.502	2, 0, 3, 0	0.502	5531.30	5531.35	-0.05
2	9	7	8	0, 5, 1	0.502	1, 0, 4, 1	0.502	5730.61	5730.57	0.04
1	11	9	10	1, 5, 1	0.501	2, 0, 4, 1	0.501	6736.76	6736.62	0.14
2	11	9	10	2, 3, 1	0.553	1, 0, 5, 2	0.446	6944.73	6944.75	-0.02
3	11	9	10	1, 5, 1	0.498	2, 0, 4, 1	0.498	7154.63	7154.44	0.19
1	15	9	12	0, 3, 3	1.000	2, 1, 3, 0	0.750	8863.68	8863.79	-0.11
2	15	13	14	2, 7, 1	0.377	3, 0, 5, 2	0.282	-	9117.97	-
3	15	13	14	4, 3, 1	0.285	2, 0, 6, 3	0.219	-	9346.24	-
4	15	13	14	4, 3, 1	0.442	1, 0, 7, 4	0.310	-	9564.79	-
5	15	13	14	3, 5, 1	0.336	1, 0, 7, 4	0.277	-	9787.76	-
6	15	13	14	2, 7, 1	0.355	2, 0, 6, 3	0.343	-	10026.93	-
1	23	13	18	0, 3, 5	1.000	3, 2, 3, 0	0.625	13313.28	13313.17	0.11
2	23	17	20	2, 7, 3	0.372	5, 0, 5, 2	0.233	-	13498.01	-
3	23	17	20	3, 5, 3	0.304	6, 0, 4, 1	0.190	-	13724.87	-
4	23	21	22	4, 11, 1	0.275	4, 1, 7, 4	0.155	-	13788.64	-
5	23	17	20	4, 3, 3	0.447	7, 0, 3, 0	0.244	-	13939.74	-
6	23	21	22	6, 7, 1	0.244	3, 0, 9, 6	0.146	-	14051.64	-
7	23	17	20	3, 5, 3	0.321	6, 0, 4, 1	0.200	-	14155.74	-
8	23	21	22	7, 5, 1	0.263	2, 0, 10, 7	0.178	-	14298.79	-
9	23	17	20	2, 7, 3	0.365	5, 0, 5, 2	0.228	-	14385.51	-
10	23	21	22	8, 3, 1	0.334	1, 0, 11, 8	0.138	-	14534.71	-
11	23	21	22	8, 3, 1	0.321	1, 0, 11, 8	0.196	-	14769.16	-
12	23	21	22	7, 5, 1	0.260	1, 0, 11, 8	0.224	-	15013.30	-
13	23	21	22	6, 7, 1	0.238	1, 0, 11, 8	0.192	-	15274.02	-
14	23	21	22	5, 9, 1	0.239	2, 0, 10, 7	0.225	-	15553.59	-
15	23	21	22	3, 13, 1	0.289	3, 0, 9, 6	0.199	-	15852.04	-
Symmetry Φ_u										
1	3	3	3	0, 3, 0	1.000	0, 0, 3, 0	1.000	2003.25	2003.30	-0.06
1	5	5	5	1, 3, 0	0.516	0, 0, 4, 1	0.484	3240.62	3240.63	0.00
2	5	5	5	0, 5, 0	0.516	0, 0, 4, 1	0.516	3442.22	3442.13	0.08
1	7	7	7	1, 5, 0	0.501	1, 0, 4, 1	0.501	4467.12	4467.04	0.08
2	7	7	7	2, 3, 0	0.552	0, 0, 5, 2	0.446	4676.79	4676.82	-0.03
3	7	7	7	1, 5, 0	0.497	0, 0, 5, 2	0.304	4890.10	4889.86	0.24
1	9	9	9	1, 7, 0	0.385	1, 0, 5, 2	0.385	-	5683.45	-
2	9	9	9	3, 3, 0	0.442	0, 0, 6, 3	0.314	-	5902.77	-
3	9	9	9	3, 3, 0	0.372	0, 0, 6, 3	0.360	-	6118.60	-
4	9	9	9	1, 7, 0	0.429	1, 0, 5, 2	0.429	6346.71	6346.42	0.29
1	11	7	9	0, 3, 2	1.000	1, 1, 3, 0	0.500	6601.71	6601.85	-0.14
2	11	11	11	2, 7, 0	0.378	1, 1, 5, 2	0.189	-	6890.79	-
3	11	11	11	4, 3, 0	0.299	0, 0, 7, 4	0.206	-	7120.01	-
4	11	11	11	4, 3, 0	0.438	0, 0, 7, 4	0.308	-	7340.67	-
5	11	11	11	3, 5, 0	0.340	0, 0, 7, 4	0.286	-	7567.31	-

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Table 5 – Continued from previous page

Number State ^a	Polyad ^a			Normal state ^b	Normal coefficient ^b	Local state ^c	Local coefficient ^c	Experimental energy ^d	Theoretical energy	Δ
6	11	11	11	1, 9, 0	0.352	1, 0, 6, 3	0.352	-	7811.22	-
1	19	11	15	0, 3, 4	1.000	2, 2, 3, 0	0.375	11100.85	11100.89	-0.03
2	19	15	17	2, 7, 2	0.375	4, 0, 5, 2	0.281	-	11320.38	-
3	19	15	17	3, 5, 2	0.292	1, 1, 7, 4	0.113	-	11547.86	-
4	19	19	19	4, 11, 0	0.277	2, 2, 7, 4	0.104	-	11645.96	-
5	19	15	17	4, 3, 2	0.445	1, 1, 7, 4	0.156	-	11764.48	-
6	19	19	19	6, 7, 0	0.246	1, 1, 9, 6	0.098	-	11909.79	-
7	19	15	17	3, 5, 2	0.329	1, 1, 7, 4	0.133	-	11983.89	-
8	19	19	19	7, 5, 0	0.261	1, 0, 10, 7	0.176	-	12157.94	-
9	19	15	17	2, 7, 2	0.360	4, 0, 5, 2	0.270	-	12218.34	-
10	19	19	19	8, 3, 0	0.343	0, 0, 11, 8	0.132	-	12395.62	-
11	19	19	19	8, 3, 0	0.310	0, 0, 11, 8	0.193	-	12633.14	-
12	19	19	19	7, 5, 0	0.262	0, 0, 11, 8	0.227	-	12881.59	-
13	19	19	19	6, 7, 0	0.241	0, 0, 11, 8	0.199	-	13147.36	-
14	19	19	19	5, 9, 0	0.236	0, 0, 11, 8	0.114	-	13432.37	-
15	19	19	19	3, 13, 0	0.287	1, 1, 9, 6	0.136	-	13736.53	-
Symmetry Γ_g										
1	4	4	4	0, 4, 0	1.000	0, 0, 4, 0	1.000	2671.14	2671.76	-0.62
1	6	6	6	1, 4, 0	0.520	0, 0, 5, 1	0.480	3898.33	3898.31	0.02
2	6	6	6	0, 6, 0	0.520	0, 0, 5, 1	0.520	4122.27	4122.13	0.14
1	8	8	8	1, 6, 0	0.500	1, 0, 5, 1	0.500	5115.30	5115.46	-0.16
2	8	8	8	2, 4, 0	0.541	0, 0, 6, 2	0.455	5345.60	5346.01	-0.41
3	8	8	8	1, 6, 0	0.497	0, 0, 6, 2	0.303	-	5579.88	-
Symmetry Γ_u										
1	8	6	7	0, 4, 1	1.000	1, 0, 4, 0	1.000	4970.93	4971.06	-0.12
1	10	8	9	1, 4, 1	0.508	2, 0, 4, 0	0.508	6176.65	6176.73	-0.08
2	10	8	9	0, 6, 1	0.508	1, 0, 5, 1	0.508	6398.07	6397.97	0.10
Symmetry H_g										
1	9	7	8	0, 5, 1	1.000	1, 0, 5, 0	1.000	5627.25	5627.42	-0.17
1	11	9	10	1, 5, 1	0.513	2, 0, 5, 0	0.513	-	6823.72	-
2	11	9	10	0, 7, 1	0.513	1, 0, 6, 1	0.513	7064.52	7064.46	0.06
Symmetry H_u										
1	5	5	5	0, 5, 0	1.000	0, 0, 5, 0	1.000	3340.72	3340.56	0.16
1	7	7	7	1, 5, 0	0.524	0, 0, 6, 1	0.476	4557.59	4557.62	-0.03
2	7	7	7	0, 7, 0	0.524	0, 0, 6, 1	0.524	4801.36	4801.19	0.17
Symmetry I_g										
1	6	6	6	0, 6, 0	1.000	0, 0, 6, 0	1.000	4009.67	4009.70	-0.03
1	8	8	8	1, 6, 0	0.527	0, 0, 7, 1	0.473	5218.70	5218.25	0.45
2	8	8	8	0, 8, 0	0.527	0, 0, 7, 1	0.527	-	5479.61	-
Symmetry I_u										
1	10	8	9	0, 6, 1	1.000	1, 0, 6, 0	1.000	6283.98	6284.13	-0.15
Symmetry J_u										
1	7	7	7	0, 7, 0	1.000	0, 0, 7, 0	1.000	4679.15	4679.18	-0.03

[a] The column labeled state indicates the state position from lower to higher energy inside the polyad for a given symmetry. The second column, labeled Polyad, indicates the polyad to which the state belongs. [b] The third and fourth columns, with headings normal state and coefficient, assign normal-mode labels ($\nu_1\nu_2\nu_3$) the state according to the square value of the largest contribution in this basis. [c] The fifth and sixth columns, with headings local state and coefficient, assign local-mode labels ($\nu_1\nu_2n_+n_-$) the state and its squared maximum component in the local basis is shown. [d] Experimental vibrational energies are taken from Ref.[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

References

- [1] L. Rothman, R. Hawkins, R. Wattson, R. Gamache, *J. Quant. Spectr. Rad. Trans.* **1992**; *48*, 537–566.
- [2] A. Campargue, D. Bailly, J. Teffo, S. Tashkun, V. Perevalov, *J. Mol. Spectr.* **1999**; *193*, 204–212.
- [3] G. Weireauch, G. Wumaier, A. Campargue, S. Tashkun, V. Perevalov, J. Teffo, *J. Mol. Spectr.* **1999**; *198*, 187–188.
- [4] G. Weireauch, A. Campargue, *J. Mol. Spectr.* **2001**; *207*, 263–268.
- [5] C. Miller, L. Brown, *J. Mol. Spectrosc.* **2004**; *228*, 329–354.
- [6] B. Perevalov, S. Kassi, V. Perevalov, S. Tashkun, A. Campargue, *J. Mol. Spectr.* **2008**; *252*, 143–159.
- [7] S. Kassi, K. Song, A. Campargue, *J. Quant. Spectr. Rad. Trans.* **2009**; *110*, 1801–1814.
- [8] K. Song, S. Kassi, S. Tashkun, V. Perevalov, A. Campargue, *J. Quant. Spectr. Rad. Trans.* **2010**; *111*, 332–344.
- [9] R. Lemus, M. Sánchez-Castellanos, F. Pérez-Bernal, J. M. Fernández, M. Carvajal, *J. Chem. Phys.* **2014**; *141*, 054306.
- [10] E. Karlovets, S. Kassi, S. Tashkun, V. Perevalov, A. Campargue, *J. Quant. Spectr. Rad. Trans.* **2014**; *144*, 137–153.
- [11] Y. Tan, X.-Q. Zhao, A.-W. Liu, S.-M. Hu, O. Lyulin, S. Tashkun, V. Perevalov, *J. Quant. Spectr. Rad. Trans.* **2015**; *165*, 22–27.
- [12] D. Jaquemart, Y. Borkov, O. Lyulin, S. Tashkun, V. Perevalov, *J. Quant. Spectr. Rad. Trans.* **2015**; *160*, 1–9.
- [13] T. Petrova, A. Solodov, A. Solodov, O. Lyulin, Y. Borkov, S. Tashkun, V. Perevalov, *J. Quant. Spectr. Rad. Trans.* **2015**; *164*, 109–116.