

Energies (in cm^{-1}) of $^{12}\text{CO}_2$ up to polyad 14 provided by the fit using the Hamiltonian (61) involving experimental energies up to polyad 11. The rms deviation obtained is $0,75 \text{ cm}^{-1}$. The number of bosons were taken to be $N_s = 160$ and $N = 150$

State	Polyad	State (normal)	Contribution (normal)	State (local)	Contribution (local)	Exp.	Energies Theor.	ΔE
Symmetry	Σ_g^+							
1	2	1 0 0	0.510	0 0 1 1	0.490	1285.41	1286.36	-0.95
2	2	0 2 0	0.510	0 0 1 1	0.510	1388.19	1387.67	0.52
1	4	1 2 0	0.514	0 0 2 2	0.291	2548.37	2549.73	-1.37
2	4	2 0 0	0.660	0 0 2 2	0.335	2671.14	2671.23	-0.09
3	4	1 2 0	0.482	0 0 2 2	0.374	2797.14	2796.01	1.12
4	4	0 0 2	1.000	1 1 0 0	0.503	4673.33	4673.1	0.22
1	6	1 4 0	0.434	1 0 2 2	0.434	3792.7	3793.69	-0.99
2	6	3 0 0	0.514	0 0 3 3	0.248	3942.49	3942.41	0.08
3	6	3 0 0	0.387	0 0 3 3	0.310	4064.28	4063.98	0.29
4	6	1 4 0	0.459	0 0 3 3	0.277	4225.1	4223.62	1.48
5	6	0 2 2	0.548	1 1 1 1	0.276	5915.21	5915.43	-0.22
6	6	1 0 2	0.548	1 1 1 1	0.227	6016.69	6016.56	0.14
1	8	2 4 0	0.389	1 1 2 2	0.194	-	5022.01	-
2	8	3 2 0	0.336	0 0 4 4	0.186	5197.25	5196.33	0.92
3	8	4 0 0	0.555	0 0 4 4	0.217	-	5328.84	-
4	8	3 2 0	0.373	0 0 4 4	0.302	5475.56	5475.5	0.07
5	8	1 6 0	0.414	1 0 3 3	0.414	-	5666.4	-
6	8	1 2 2	0.507	3 0 1 1	0.378	7133.82	7133.75	0.06
7	8	2 0 2	0.660	4 0 0 0	0.495	7259.74	7259.78	-0.04
8	8	1 2 2	0.492	3 0 1 1	0.367	7377.68	7377.94	-0.26
9	8	0 0 4	1.000	2 2 0 0	0.379	-	9246.85	-
1	10	2 6 0	0.366	1 1 3 3	0.182	-	6237.21	-
2	10	4 2 0	0.352	2 2 1 1	0.130	-	6433.05	-
3	10	5 0 0	0.531	3 2 0 0	0.328	-	6586.12	-
4	10	5 0 0	0.295	0 0 5 5	0.233	-	6725.03	-
5	10	3 4 0	0.315	0 0 5 5	0.278	-	6904.93	-
6	10	1 8 0	0.364	1 0 4 4	0.364	-	7121.6	-
7	10	1 4 2	0.454	3 0 2 2	0.338	-	8332.98	-
8	10	3 0 2	0.454	5 0 0 0	0.287	-	8487.74	-
9	10	3 0 2	0.452	1 1 3 3	0.144	-	8607.61	-
10	10	1 4 2	0.451	3 0 2 2	0.336	-	8758.01	-
11	10	0 2 4	0.606	2 2 1 1	0.230	-	10444.8	-
12	10	1 0 4	0.606	4 1 0 0	0.345	-	10547.1	-
1	12	3 6 0	0.326	1 1 4 4	0.149	-	7440.98	-
2	12	5 2 0	0.266	1 0 5 5	0.219	-	7654.96	-
3	12	6 0 0	0.377	0 0 6 6	0.123	-	7830.7	-
4	12	6 0 0	0.460	0 0 6 6	0.162	-	7972.46	-
5	12	5 2 0	0.317	0 0 6 6	0.248	-	8140.03	-
6	12	4 4 0	0.264	0 0 6 6	0.247	-	8348.62	-
7	12	2 8 0	0.335	1 1 4 4	0.166	-	8587.37	-
8	12	2 4 2	0.376	4 0 2 2	0.282	-	9517.	-
9	12	3 2 2	0.368	5 0 1 1	0.233	-	9696.85	-
10	12	4 0 2	0.576	6 0 0 0	0.278	-	9832.95	-
11	12	3 2 2	0.376	1 1 4 4	0.138	-	9971.32	-
12	12	1 6 2	0.397	3 0 3 3	0.296	-	10153.2	-
13	12	1 2 4	0.493	2 2 2 2	0.146	-	11618.	-
14	12	2 0 4	0.644	6 0 0 0	0.293	-	11749.5	-
15	12	1 2 4	0.493	4 1 1 1	0.281	-	11862.2	-
16	12	0 0 6	1.000	3 3 0 0	0.318	-	13722.1	-
1	14	3 8 0	0.319	2 1 4 4	0.238	-	8634.55	-
2	14	5 4 0	0.288	3 2 2 2	0.178	-	8864.23	-
3	14	6 2 0	0.301	3 3 1 1	0.092	-	9060.48	-
4	14	7 0 0	0.522	4 3 0 0	0.280	-	9215.51	-
5	14	6 2 0	0.300	0 0 7 7	0.185	-	9372.51	-
6	14	5 4 0	0.274	0 0 7 7	0.249	-	9571.71	-
7	14	4 6 0	0.272	0 0 7 7	0.216	-	9804.09	-
8	14	2 10 0	0.331	1 1 5 5	0.164	-	10062.3	-
9	14	2 6 2	0.373	4 0 3 3	0.279	-	10688.3	-
10	14	4 2 2	0.335	3 0 4 4	0.168	-	10888.8	-
11	14	5 0 2	0.485	6 1 0 0	0.197	-	11048.	-
12	14	5 0 2	0.363	1 1 5 5	0.113	-	11182.7	-
13	14	3 4 2	0.292	1 1 5 5	0.127	-	11352.7	-
14	14	1 8 2	0.342	3 0 4 4	0.255	-	11560.7	-
15	14	1 4 4	0.467	4 1 2 2	0.266	-	12772.7	-
16	14	3 0 4	0.388	2 2 3 3	0.117	-	12933.6	-
17	14	3 0 4	0.513	7 0 0 0	0.275	-	13053.8	-
18	14	1 4 4	0.436	4 1 2 2	0.248	-	13195.2	-
19	14	0 2 6	0.660	3 3 1 1	0.210	-	14875.2	-
20	14	1 0 6	0.660	5 2 0 0	0.287	-	14980.1	-

State	Polyad	State (normal)	Contribution (normal)	State (local)	Contribution (local)	Exp.	Energies Theor.	ΔE
Symmetry	Σ_u^+							
1	2	0 0 1	1.000	1 0 0 0	1.000	2349.14	2349.02	0.12
1	4	0 2 1	0.519	1 0 1 1	0.519	3612.84	3613.42	-0.58
2	4	1 0 1	0.519	2 0 0 0	0.519	3714.78	3714.46	0.33
1	6	1 2 1	0.512	2 0 1 1	0.512	4853.62	4854.27	-0.65
2	6	2 0 1	0.662	3 0 0 0	0.500	4977.84	4977.9	-0.07
3	6	1 2 1	0.488	2 0 1 1	0.488	5099.66	5099.24	0.42
4	6	0 0 3	1.000	2 1 0 0	0.754	6972.58	6972.34	0.24
1	8	1 4 1	0.445	2 0 2 2	0.445	6075.98	6075.84	0.14
2	8	3 0 1	0.485	1 0 3 3	0.263	6227.92	6227.56	0.36
3	8	3 0 1	0.420	1 0 3 3	0.298	6347.85	6348.02	-0.17
4	8	1 4 1	0.456	2 0 2 2	0.456	6503.08	6503.03	0.05
5	8	0 2 3	0.578	2 1 1 1	0.436	8192.55	8192.51	0.04
6	8	1 0 3	0.578	2 1 1 1	0.319	8293.95	8294.07	-0.12
1	10	2 4 1	0.383	2 0 3 3	0.335	7283.98	7281.98	2.00
2	10	3 2 1	0.354	1 0 4 4	0.202	7460.52	7459.09	1.43
3	10	4 0 1	0.568	4 1 0 0	0.316	7593.69	7593.19	0.50
4	10	3 2 1	0.376	1 0 4 4	0.289	7734.45	7735.57	-1.12
5	10	1 6 1	0.407	2 0 3 3	0.407	7920.84	7921.97	-1.13
6	10	1 2 3	0.501	2 1 2 2	0.272	9388.99	9388.31	0.68
7	10	2 0 3	0.654	5 0 0 0	0.404	9516.97	9516.93	0.04
8	10	1 2 3	0.494	3 1 1 1	0.252	9631.35	9632.23	-0.88
9	10	0 0 5	1.000	3 2 0 0	0.632	-	11496.7	-
1	12	2 6 1	0.370	3 0 3 3	0.279	-	8475.2	-
2	12	4 2 1	0.345	2 0 4 4	0.228	-	8673.38	-
3	12	5 0 1	0.511	5 1 0 0	0.255	-	8829.48	-
4	12	5 0 1	0.328	1 0 5 5	0.229	-	8965.97	-
5	12	3 4 1	0.305	1 0 5 5	0.265	-	9140.94	-
6	12	1 8 1	0.353	2 0 4 4	0.353	-	9353.29	-
7	12	1 4 3	0.461	3 1 2 2	0.235	-	10565.2	-
8	12	3 0 3	0.421	6 0 0 0	0.263	-	10723.	-
9	12	3 0 3	0.483	6 0 0 0	0.302	-	10842.8	-
10	12	1 4 3	0.444	3 1 2 2	0.226	-	10988.7	-
11	12	0 2 5	0.634	3 2 1 1	0.401	-	12672.3	-
12	12	1 0 5	0.633	5 1 0 0	0.317	-	12775.8	-
1	14	3 6 1	0.320	3 0 4 4	0.233	-	9657.14	-
2	14	4 4 1	0.270	2 0 5 5	0.225	-	9873.08	-
3	14	6 0 1	0.342	5 2 0 0	0.140	-	10052.	-
4	14	6 0 1	0.486	5 2 0 0	0.198	-	10194.	-
5	14	5 2 1	0.324	1 0 6 6	0.243	-	10356.6	-
6	14	4 4 1	0.274	1 0 6 6	0.235	-	10560.6	-
7	14	2 8 1	0.338	2 0 5 5	0.303	-	10795.1	-
8	14	2 4 3	0.367	5 0 2 2	0.227	-	11727.2	-
9	14	3 2 3	0.378	6 0 1 1	0.236	-	11909.7	-
10	14	4 0 3	0.577	7 0 0 0	0.322	-	12048.2	-
11	14	3 2 3	0.373	6 0 1 1	0.233	-	12182.9	-
12	14	1 6 3	0.387	5 0 2 2	0.202	-	12360.2	-
13	14	1 2 5	0.483	3 2 2 2	0.258	-	13823.1	-
14	14	2 0 5	0.631	6 1 0 0	0.275	-	13957.4	-
15	14	1 2 5	0.490	5 1 1 1	0.245	-	14068.1	-
16	14	0 0 7	1.000	4 3 0 0	0.557	-	15923.1	-
Symmetry	Π_g							
1	3	0 1 1	1.000	1 0 1 0	1.00	3004.01	3004.07	-0.05
1	5	1 1 1	0.507	2 0 1 0	0.507	4247.71	4248.42	-0.71
2	5	0 3 1	0.507	1 0 2 1	0.507	4390.63	4390.26	0.37
1	7	1 3 1	0.509	2 0 2 1	0.509	5475.08	5475.54	-0.47
2	7	2 1 1	0.594	3 0 1 0	0.448	5632.77	5632.94	-0.17
3	7	1 3 1	0.488	2 0 2 1	0.488	5790.58	5790.22	0.36
4	7	0 1 3	1.00	2 1 1 0	0.754	7602.52	7602.42	0.09
1	9	1 5 1	0.408	2 0 3 2	0.408	6688.18	6687.38	0.80
2	9	3 1 1	0.468	1 0 4 3	0.285	6863.56	6863.23	0.33
3	9	3 1 1	0.387	1 0 4 3	0.337	7023.68	7024.17	-0.49
4	9	1 5 1	0.442	2 0 3 2	0.442	7203.82	7204.18	-0.36
5	9	0 3 3	0.536	2 1 2 1	0.404	8803.27	8803.12	0.15
6	9	1 1 3	0.536	2 1 2 1	0.350	8944.15	8944.43	-0.28
1	11	2 5 1	0.388	3 0 3 2	0.293	-	7885.9	-
2	11	3 3 1	0.300	2 0 4 3	0.214	8080.89	8080.11	0.78
3	11	4 1 1	0.487	4 1 1 0	0.270	8250.63	8250.69	-0.06
4	11	3 3 1	0.360	1 0 5 4	0.294	8425.	8426.87	-1.87
5	11	1 7 1	0.387	2 0 4 3	0.387	-	8630.71	-
6	11	1 3 3	0.506	3 1 2 1	0.258	9987.48	9986.14	1.34
7	11	2 1 3	0.594	5 0 1 0	0.366	10145.5	10145.6	-0.07
8	11	1 3 3	0.493	3 1 2 1	0.251	10297.1	10298.4	-1.39
9	11	0 1 5	1.00	3 2 1 0	0.633	-	12102.	-

State	Polyad	State (normal)	Contribution (normal)	State (local)	Contribution (local)	Exp.	Energies	
							Theor.	ΔE
1	13	2 7 1	0.349	3 0 4 3	0.263	-	9072.71	-
2	13	4 3 1	0.337	2 0 5 4	0.240	-	9283.89	-
3	13	5 1 1	0.455	5 1 1 0	0.228	-	9467.95	-
4	13	5 1 1	0.309	1 0 6 5	0.258	-	9644.48	-
5	13	3 5 1	0.274	1 0 6 5	0.258	-	9842.22	-
6	13	2 7 1	0.337	2 0 5 4	0.333	-	10068.2	-
7	13	1 5 3	0.429	3 1 3 2	0.218	-	11153.9	-
8	13	3 1 3	0.429	6 0 1 0	0.268	-	11333.1	-
9	13	3 1 3	0.429	6 0 1 0	0.268	-	11492.4	-
10	13	1 5 3	0.429	3 1 3 2	0.219	-	11665.6	-
11	13	0 3 5	0.578	3 2 2 1	0.365	-	13258.9	-
12	13	1 1 5	0.578	5 1 1 0	0.289	-	13400.6	-
Symmetry		Π_u						
1	1	0 1 0	1.000	0 0 1 0	1.000	667.38	667.584	-0.20
1	3	1 1 0	0.528	0 0 2 1	0.472	1932.47	1933.69	-1.22
2	3	0 3 0	0.528	0 0 2 1	0.528	2076.86	2076.18	0.68
1	5	1 3 0	0.508	1 0 2 1	0.508	3181.46	3182.85	-1.38
2	5	2 1 0	0.592	0 0 3 2	0.401	3339.36	3339.53	-0.18
3	5	1 3 0	0.484	0 0 3 2	0.351	3500.67	3499.36	1.31
4	5	0 1 2	1.00	1 1 1 0	0.503	5315.71	5315.64	0.07
1	7	1 5 0	0.396	1 0 3 2	0.396	4416.15	4416.74	-0.59
2	7	3 1 0	0.485	0 0 4 3	0.273	4591.12	4591.13	-0.01
3	7	3 1 0	0.366	0 0 4 3	0.345	4753.45	4753.29	0.16
4	7	1 5 0	0.446	0 0 4 3	0.251	4938.39	4936.93	1.45
5	7	0 3 2	0.515	1 1 2 1	0.259	6537.96	6538.2	-0.24
6	7	1 1 2	0.515	1 1 2 1	0.244	6679.71	6679.64	0.07
1	9	2 5 0	0.390	1 1 3 2	0.194	-	5637.23	-
2	9	4 1 0	0.317	0 0 5 4	0.178	-	5829.73	-
3	9	4 1 0	0.478	0 0 5 4	0.263	-	6000.22	-
4	9	3 3 0	0.360	0 0 5 4	0.306	6179.01	6179.38	-0.37
5	9	1 7 0	0.396	1 0 4 3	0.396	6388.08	6387.24	0.85
6	9	1 3 2	0.508	3 0 2 1	0.379	7743.7	7743.27	0.43
7	9	2 1 2	0.595	4 0 1 0	0.446	7901.48	7901.59	-0.11
8	9	1 3 2	0.492	3 0 2 1	0.366	8056.02	8056.54	-0.52
9	9	0 1 4	1.000	2 2 1 0	0.379	-	9864.51	-
1	11	2 7 0	0.342	1 1 4 3	0.170	-	6845.89	-
2	11	4 3 0	0.336	2 2 2 1	0.124	-	7055.39	-
3	11	5 1 0	0.465	0 0 6 5	0.187	-	7238.43	-
4	11	5 1 0	0.287	0 0 6 5	0.260	-	7416.89	-
5	11	3 5 0	0.286	0 0 6 5	0.270	7616.62	7618.49	-1.87
6	11	1 9 0	0.344	1 0 5 4	0.344	-	7848.58	-
7	11	1 5 2	0.419	3 0 3 2	0.312	-	8933.07	-
8	11	3 1 2	0.449	1 1 4 3	0.149	-	9110.52	-
9	11	3 1 2	0.408	1 1 4 3	0.165	-	9270.52	-
10	11	1 5 2	0.436	3 0 3 2	0.325	-	9447.02	-
11	11	0 3 4	0.557	2 2 2 1	0.211	-	11043.3	-
12	11	1 1 4	0.557	2 2 2 1	0.168	-	11184.7	-
1	13	3 7 0	0.330	1 1 5 4	0.131	-	8043.97	-
2	13	5 3 0	0.292	1 0 6 5	0.208	-	8268.95	-
3	13	6 1 0	0.370	0 0 7 6	0.127	-	8466.45	-
4	13	6 1 0	0.396	0 0 7 6	0.193	-	8648.82	-
5	13	5 3 0	0.307	0 0 7 6	0.257	-	8845.33	-
6	13	4 5 0	0.271	0 0 7 6	0.236	-	9069.47	-
7	13	2 9 0	0.335	1 1 5 4	0.166	-	9319.58	-
8	13	2 5 2	0.385	4 0 3 2	0.289	-	10109.7	-
9	13	3 3 2	0.316	1 1 5 4	0.103	-	10305.7	-
10	13	4 1 2	0.493	1 1 5 4	0.136	-	10476.6	-
11	13	3 3 2	0.357	1 1 5 4	0.142	-	10650.	-
12	13	1 7 2	0.377	3 0 4 3	0.281	-	10849.9	-
13	13	1 3 4	0.502	4 1 2 1	0.286	-	12204.3	-
14	13	2 1 4	0.590	2 2 3 2	0.154	-	12365.	-
15	13	1 3 4	0.494	4 1 2 1	0.281	-	12516.	-
16	13	0 1 6	1.000	3 3 1 0	0.318	-	14315.	-

State	Polyad	State (normal)	Contribution (normal)	State (local)	Contribution (local)	Exp.	Energies Theor.	ΔE
Symmetry	Δ_g							
1	2	0 2 0	1.000	0 0 2 0	1.000	1335.13	1335.47	-0.34
1	4	1 2 0	0.539	0 0 3 1	0.461	2585.02	2586.35	-1.32
2	4	0 4 0	0.539	0 0 3 1	0.539	2760.73	2759.96	0.77
1	6	1 4 0	0.505	1 0 3 1	0.505	3821.98	3823.28	-1.30
2	6	2 2 0	0.561	0 0 4 2	0.427	4007.91	4008.14	-0.23
3	6	1 4 0	0.484	0 0 4 2	0.345	4197.36	4195.99	1.37
4	6	0 2 2	1.000	1 1 2 0	0.503	5958.51	5958.48	0.03
1	8	2 4 0	0.387	1 1 3 1	0.193	-	5047.37	-
2	8	3 2 0	0.471	0 0 5 3	0.282	5245.47	5245.53	-0.06
3	8	0 8 0	0.365	0 0 5 3	0.365	-	5437.23	-
4	8	1 6 0	0.440	0 0 5 3	0.239	-	5643.56	-
5	8	1 2 2	0.504	1 1 3 1	0.249	7166.05	7166.14	-0.09
6	8	0 4 2	0.504	1 1 3 1	0.254	7338.15	7338.14	0.01
1	10	2 6 0	0.387	1 1 4 2	0.192	-	6259.77	-
2	10	4 2 0	0.329	0 0 6 4	0.174	-	6471.83	-
3	10	4 2 0	0.442	0 0 6 4	0.284	-	6670.62	-
4	10	3 4 0	0.351	0 0 6 4	0.313	-	6875.93	-
5	10	1 8 0	0.385	1 0 5 3	0.385	-	7101.84	-
6	10	1 4 2	0.507	3 0 3 1	0.378	-	8359.54	-
7	10	2 2 2	0.566	1 1 4 2	0.217	-	8544.58	-
8	10	1 4 2	0.491	3 0 3 1	0.366	-	8728.1	-
9	10	0 2 4	1.000	2 2 2 0	0.380	-	10482.5	-
1	12	3 6 0	0.323	1 1 5 3	0.160	-	7461.55	-
2	12	4 4 0	0.317	1 0 6 4	0.246	-	7687.22	-
3	12	5 2 0	0.434	0 0 7 5	0.197	-	7895.45	-
4	12	0 12 0	0.277	0 0 7 5	0.277	-	8102.26	-
5	12	3 6 0	0.269	0 0 7 5	0.269	-	8324.91	-
6	12	2 8 0	0.334	1 1 5 3	0.166	-	8569.79	-
7	12	1 6 2	0.396	3 0 4 2	0.295	-	9540.05	-
8	12	3 2 2	0.446	1 1 5 3	0.153	-	9739.52	-
9	12	3 2 2	0.384	1 1 5 3	0.177	-	9928.69	-
10	12	1 6 2	0.430	3 0 4 2	0.320	-	10128.9	-
11	12	0 4 4	0.531	2 2 3 1	0.201	-	11646.8	-
12	12	1 2 4	0.531	2 2 3 1	0.178	-	11818.	-
1	14	3 8 0	0.328	2 1 5 3	0.244	-	8653.63	-
2	14	5 4 0	0.299	1 0 7 5	0.200	-	8892.23	-
3	14	6 2 0	0.362	0 0 8 6	0.127	-	9111.18	-
4	14	6 2 0	0.364	0 0 8 6	0.208	-	9322.07	-
5	14	5 4 0	0.298	0 0 8 6	0.267	-	9542.82	-
6	14	4 6 0	0.272	0 0 8 6	0.231	-	9783.78	-
7	14	2 10 0	0.333	1 1 6 4	0.165	-	10046.4	-
8	14	2 6 2	0.386	4 0 4 2	0.290	-	10709.	-
9	14	4 2 2	0.293	1 1 6 4	0.099	-	10922.9	-
10	14	4 2 2	0.455	1 1 6 4	0.147	-	11120.8	-
11	14	3 4 2	0.346	1 1 6 4	0.147	-	11321.2	-
12	14	1 8 2	0.366	3 0 5 3	0.273	-	11539.9	-
13	14	1 4 4	0.505	4 1 3 1	0.287	-	12796.6	-
14	14	2 2 4	0.565	2 2 4 2	0.165	-	12982.6	-
15	14	1 4 4	0.494	4 1 3 1	0.282	-	13162.6	-
16	14	0 2 6	1.000	3 3 2 0	0.318	-	14908.3	-
Symmetry	Δ_u							
1	4	0 2 1	1.000	1 0 2 0	1.000	3659.27	3659.41	-0.14
1	6	1 2 1	0.522	2 0 2 0	0.522	4887.99	4888.69	-0.71
2	6	0 4 1	0.522	1 0 3 1	0.522	5061.78	5061.39	0.39
1	8	1 4 1	0.506	2 0 3 1	0.506	6103.68	6103.86	-0.18
2	8	2 2 1	0.564	1 0 4 2	0.430	6288.49	6288.72	-0.23
3	8	1 4 1	0.488	2 0 3 1	0.488	6474.53	6474.31	0.22
4	8	0 2 3	1.000	2 1 2 0	0.754	8232.89	8232.8	0.08
1	10	1 6 1	0.385	2 0 4 2	0.385	7307.65	7306.15	1.50
2	10	3 2 1	0.459	1 0 5 3	0.293	7505.22	7504.9	0.32
3	10	3 2 1	0.367	1 0 5 3	0.359	7694.42	7695.22	-0.80
4	10	1 6 1	0.436	2 0 4 2	0.436	7897.57	7898.4	-0.83
5	10	0 4 3	0.513	2 1 3 1	0.387	9419.19	9418.8	0.39
6	10	1 2 3	0.513	2 1 3 1	0.367	9589.93	9590.32	-0.39
1	12	2 6 1	0.387	3 0 4 2	0.292	-	8496.8	-
2	12	4 2 1	0.311	2 0 5 3	0.239	-	8709.74	-
3	12	4 2 1	0.450	1 0 6 4	0.289	-	8907.99	-
4	12	3 4 1	0.349	1 0 6 4	0.303	-	9110.72	-
5	12	1 8 1	0.376	2 0 5 3	0.376	-	9333.	-
6	12	1 4 3	0.507	3 1 3 1	0.258	-	10590.4	-
7	12	2 2 3	0.566	5 0 2 0	0.349	-	10775.8	-
8	12	1 4 3	0.493	3 1 3 1	0.251	-	10957.5	-
9	12	0 2 5	1.000	3 2 2 0	0.633	-	12707.6	-

State	Polyad	State (normal)	Contribution (normal)	State (local)	Contribution (local)	Exp.	Energies Theor.	ΔE
1	14	2 8 1	0.330	3 0 5 3	0.249	-	9676.9	-
2	14	4 4 1	0.322	2 0 6 4	0.248	-	9903.57	-
3	14	5 2 1	0.428	5 1 2 0	0.214	-	10111.9	-
4	14	5 2 1	0.293	1 0 7 5	0.276	-	10316.8	-
5	14	0 12 1	0.257	1 0 7 5	0.257	-	10536.1	-
6	14	2 8 1	0.339	2 0 6 4	0.320	-	10777.1	-
7	14	1 6 3	0.406	5 0 3 1	0.218	-	11749.2	-
8	14	3 2 3	0.431	6 0 2 0	0.269	-	11949.5	-
9	14	3 2 3	0.400	2 1 5 3	0.260	-	12137.7	-
10	14	1 6 3	0.424	3 1 4 2	0.216	-	12335.	-
11	14	0 4 5	0.549	3 2 3 1	0.347	-	13850.2	-
12	14	1 2 5	0.548	3 2 3 1	0.286	-	14021.4	-
Symmetry		Φ_g						
1	5	0 3 1	1.000	1 0 3 0	1.000	4314.92	4315.05	-0.14
1	7	1 3 1	0.533	2 0 3 0	0.533	5531.3	5531.88	-0.58
2	7	0 5 1	0.533	1 0 4 1	0.533	5730.61	5730.2	0.41
1	9	1 5 1	0.504	2 0 4 1	0.504	6736.79	6736.56	0.22
2	9	2 3 1	0.547	1 0 5 2	0.444	6944.87	6944.95	-0.08
3	9	1 5 1	0.487	2 0 4 1	0.487	7154.75	7154.47	0.28
4	9	0 3 3	1.000	2 1 3 0	0.755	8863.68	8863.48	0.20
1	11	2 5 1	0.390	2 0 5 2	0.368	-	7929.98	-
2	11	3 3 1	0.454	1 0 6 3	0.295	-	8149.56	-
3	11	0 9 1	0.373	1 0 6 3	0.373	-	8364.	-
4	11	1 7 1	0.433	2 0 5 2	0.433	-	8588.04	-
5	11	1 3 3	0.503	2 1 4 1	0.375	-	10037.3	-
6	11	0 5 3	0.503	2 1 4 1	0.380	-	10234.	-
1	13	2 7 1	0.384	3 0 5 2	0.290	-	9113.02	-
2	13	4 3 1	0.321	2 0 6 3	0.256	-	9344.12	-
3	13	4 3 1	0.427	1 0 7 4	0.301	-	9565.43	-
4	13	3 5 1	0.342	1 0 7 4	0.310	-	9790.59	-
5	13	1 9 1	0.370	2 0 6 3	0.370	-	10030.6	-
6	13	1 5 3	0.506	3 1 4 1	0.257	-	11198.9	-
7	13	2 3 3	0.550	5 0 3 0	0.339	-	11406.8	-
8	13	1 5 3	0.493	3 1 4 1	0.251	-	11612.5	-
9	13	0 3 5	1.000	3 2 3 0	0.633	-	13313.5	-
Symmetry		Φ_u						
1	3	0 3 0	1.000	0 0 3 0	1.000	2003.25	2003.65	-0.41
1	5	1 3 0	0.549	0 0 4 1	0.451	3240.62	3241.95	-1.33
2	5	0 5 0	0.549	0 0 4 1	0.549	3442.22	3441.39	0.82
1	7	1 5 0	0.502	1 0 4 1	0.502	-	4468.21	-
2	7	2 3 0	0.544	0 0 5 2	0.442	-	4677.05	-
3	7	1 5 0	0.483	0 0 5 2	0.345	4890.1	4888.72	1.37
4	7	0 3 2	1.000	1 1 3 0	0.503	6601.72	6601.63	0.09
1	9	2 5 0	0.399	1 1 4 1	0.198	-	5683.23	-
2	9	3 3 0	0.464	0 0 6 3	0.285	-	5902.8	-
3	9	0 9 0	0.379	0 0 6 3	0.379	-	6118.76	-
4	9	1 7 0	0.437	0 0 6 3	0.235	-	6345.7	-
5	9	1 3 2	0.518	1 1 4 1	0.242	-	7796.97	-
6	9	0 5 2	0.518	1 1 4 1	0.261	-	7994.36	-
1	11	2 7 0	0.382	1 1 5 2	0.190	-	6887.83	-
2	11	4 3 0	0.336	0 0 7 4	0.169	-	7118.66	-
3	11	4 3 0	0.421	0 0 7 4	0.296	-	7340.9	-
4	11	3 5 0	0.344	0 0 7 4	0.320	-	7568.48	-
5	11	1 9 0	0.378	1 0 6 3	0.378	-	7811.83	-
6	11	1 5 2	0.505	3 0 4 1	0.377	-	8980.08	-
7	11	2 3 2	0.549	1 1 5 2	0.225	-	9188.17	-
8	11	1 5 2	0.490	3 0 4 1	0.365	-	9395.7	-
9	11	0 3 4	1.000	2 2 3 0	0.380	-	11100.7	-
1	13	3 7 0	0.333	1 1 6 3	0.152	-	8082.81	-
2	13	4 5 0	0.301	1 0 7 4	0.249	-	8324.87	-
3	13	5 3 0	0.416	0 0 8 5	0.201	-	8554.85	-
4	13	0 13 0	0.289	0 0 8 5	0.289	-	8784.81	-
5	13	0 13 0	0.270	0 0 8 5	0.270	-	9026.72	-
6	13	2 9 0	0.335	1 1 6 3	0.166	-	9286.44	-
7	13	2 5 2	0.381	4 0 4 1	0.285	-	10151.9	-
8	13	3 3 2	0.444	1 1 6 3	0.154	-	10371.6	-
9	13	0 9 2	0.367	1 1 6 3	0.185	-	10584.7	-
10	13	1 7 2	0.428	3 0 5 2	0.319	-	10806.	-
11	13	0 5 4	0.513	2 2 4 1	0.194	-	12253.1	-
12	13	1 3 4	0.513	2 2 4 1	0.185	-	12449.1	-

State	Polyad	State (normal)	Contribution (normal)	State (local)	Contribution (local)	Exp.	Energies Theor.	ΔE
Symmetry Γ_g								
1	4	0 4 0	1.000	0 0 4 0	1.000	2671.72	2672.14	-0.42
1	6	1 4 0	0.557	0 0 5 1	0.443	3898.33	3899.57	-1.24
2	6	0 6 0	0.557	0 0 5 1	0.557	4122.27	4121.41	0.86
1	8	1 6 0	0.499	1 0 5 1	0.499	-	5116.31	-
2	8	2 4 0	0.532	0 0 6 2	0.450	-	5346.27	-
3	8	1 6 0	0.483	0 0 6 2	0.347	-	5578.89	-
4	8	0 4 2	1.000	1 1 4 0	0.503	-	7245.07	-
1	10	2 6 0	0.408	1 1 5 1	0.203	-	6322.98	-
2	10	3 4 0	0.459	0 0 7 3	0.285	-	6561.96	-
3	10	0 10 0	0.388	0 0 7 3	0.388	-	6798.92	-
4	10	1 8 0	0.436	0 0 7 3	0.233	-	7044.61	-
5	10	1 4 2	0.529	1 1 5 1	0.237	-	8429.79	-
6	10	0 6 2	0.529	1 1 5 1	0.266	-	8649.19	-
1	12	2 8 0	0.378	1 1 6 2	0.188	-	7520.23	-
2	12	4 4 0	0.342	0 0 8 4	0.164	-	7768.65	-
3	12	4 4 0	0.406	0 0 8 4	0.303	-	8011.27	-
4	12	3 6 0	0.339	0 0 8 4	0.326	-	8258.47	-
5	12	1 10 0	0.375	1 0 7 3	0.375	-	8518.28	-
6	12	1 6 2	0.503	3 0 5 1	0.375	-	9603.68	-
7	12	2 4 2	0.537	1 1 6 2	0.229	-	9832.2	-
8	12	1 6 2	0.489	3 0 5 1	0.365	-	10060.7	-
9	12	0 4 4	1.000	2 2 4 0	0.380	-	11719.3	-
1	14	3 8 0	0.339	1 1 7 3	0.145	-	8708.65	-
2	14	4 6 0	0.286	1 0 8 4	0.250	-	8966.59	-
3	14	5 4 0	0.404	0 0 9 5	0.203	-	9215.86	-
4	14	0 14 0	0.297	0 0 9 5	0.297	-	9465.81	-
5	14	0 14 0	0.272	0 0 9 5	0.272	-	9725.31	-
6	14	2 10 0	0.336	1 1 7 3	0.167	-	9999.41	-
7	14	2 6 2	0.392	4 0 5 1	0.294	-	10767.5	-
8	14	3 4 2	0.443	1 1 7 3	0.153	-	11005.8	-
9	14	0 10 2	0.378	1 1 7 3	0.190	-	11239.6	-
10	14	1 8 2	0.427	3 0 6 2	0.318	-	11479.9	-
11	14	1 4 4	0.501	2 2 5 1	0.189	-	12861.3	-
12	14	0 6 4	0.501	2 2 5 1	0.191	-	13078.9	-
Symmetry Γ_u								
1	6	0 4 1	1.000	1 0 4 0	1.000	4970.93	4970.99	-0.06
1	8	1 4 1	0.543	2 0 4 0	0.543	6176.65	6177.08	-0.43
2	8	0 6 1	0.543	1 0 5 1	0.543	6398.07	6397.62	0.46
1	10	1 6 1	0.502	2 0 5 1	0.502	-	7372.39	-
2	10	2 4 1	0.535	1 0 6 2	0.453	-	7601.55	-
3	10	1 6 1	0.486	2 0 5 1	0.486	-	7832.03	-
4	10	0 4 3	1.000	2 1 4 0	0.755	-	9494.46	-
1	12	2 6 1	0.400	2 0 6 2	0.354	-	8557.62	-
2	12	3 4 1	0.451	1 0 7 3	0.295	-	8796.18	-
3	12	0 10 1	0.384	1 0 7 3	0.384	-	9031.49	-
4	12	1 8 1	0.432	2 0 6 2	0.432	-	9274.4	-
5	12	1 4 3	0.515	2 1 5 1	0.366	-	10657.8	-
6	12	0 6 3	0.515	2 1 5 1	0.389	-	10876.3	-
1	14	2 8 1	0.380	3 0 6 2	0.287	-	9733.46	-
2	14	4 4 1	0.328	2 0 7 3	0.268	-	9981.7	-
3	14	4 4 1	0.412	1 0 8 4	0.308	-	10223.1	-
4	14	3 6 1	0.338	1 0 8 4	0.317	-	10467.9	-
5	14	1 10 1	0.367	2 0 7 3	0.367	-	10724.5	-
6	14	1 6 3	0.505	3 1 5 1	0.257	-	11810.3	-
7	14	2 4 3	0.539	2 1 6 2	0.345	-	12038.3	-
8	14	1 6 3	0.492	3 1 5 1	0.251	-	12265.	-
9	14	0 4 5	1.000	3 2 4 0	0.633	-	13919.6	-
Symmetry H_g								
1	7	0 5 1	1.000	1 0 5 0	1.000	5627.25	5627.24	0.02
1	9	1 5 1	0.551	2 0 5 0	0.551	-	6823.79	-
2	9	0 7 1	0.551	1 0 6 1	0.551	7064.52	7064.1	0.42
1	11	1 7 1	0.499	2 0 6 1	0.499	-	8010.63	-
2	11	2 5 1	0.526	1 0 7 2	0.458	-	8258.49	-
3	11	1 7 1	0.485	2 0 6 1	0.485	-	8507.75	-
4	11	0 5 3	1.000	2 1 5 0	0.755	-	10125.7	-
1	13	2 7 1	0.407	2 0 7 2	0.343	-	9188.3	-
2	13	3 5 1	0.450	1 0 8 3	0.293	-	9444.26	-
3	13	0 11 1	0.392	1 0 8 3	0.392	-	9698.15	-
4	13	1 9 1	0.432	2 0 7 2	0.432	-	9958.3	-
5	13	1 5 3	0.526	2 1 6 1	0.358	-	11279.8	-
6	13	0 7 3	0.526	2 1 6 1	0.397	-	11517.6	-

State	Polyad	State (normal)	Contribution (normal)	State (local)	Contribution (local)	Exp.	Energies Theor.	ΔE
Symmetry		Hu						
1	5	0 5 0	1.000	0 0 5 0	1.000	3340.72	3340.92	-0.20
1	7	1 5 0	0.564	0 0 6 1	0.436	-	4558.73	-
2	7	0 7 0	0.564	0 0 6 1	0.564	-	4800.49	-
1	9	1 7 0	0.496	1 0 6 1	0.496	-	5766.85	-
2	9	2 5 0	0.523	0 0 7 2	0.455	-	6015.78	-
3	9	1 7 0	0.481	0 0 7 2	0.351	-	6267.2	-
4	9	0 5 2	1.000	1 1 5 0	0.503	-	7888.81	-
1	11	2 7 0	0.414	1 1 6 1	0.206	-	6965.82	-
2	11	3 5 0	0.457	0 0 8 3	0.284	-	7222.55	-
3	11	0 11 0	0.396	0 0 8 3	0.396	-	7478.21	-
4	11	1 9 0	0.436	0 0 8 3	0.233	-	7741.08	-
5	11	1 5 2	0.539	1 1 6 1	0.232	-	9064.11	-
6	11	0 7 2	0.539	1 1 6 1	0.271	-	9303.12	-
1	13	2 9 0	0.373	1 1 7 2	0.186	-	8156.15	-
2	13	4 5 0	0.346	0 0 9 4	0.159	-	8421.01	-
3	13	4 5 0	0.394	0 0 9 4	0.308	-	8681.85	-
4	13	3 7 0	0.336	0 0 9 4	0.331	-	8946.69	-
5	13	1 11 0	0.373	1 0 8 3	0.373	-	9221.92	-
6	13	1 7 2	0.501	3 0 6 1	0.374	-	10229.7	-
7	13	2 5 2	0.529	1 1 7 2	0.232	-	10476.6	-
8	13	1 7 2	0.488	3 0 6 1	0.364	-	10723.9	-
9	13	0 5 4	1.000	2 2 5 0	0.380	-	12338.1	-
Symmetry		Ig						
1	6	0 6 0	1.000	0 0 6 0	1.000	4010.07	4010.	0.06
1	8	1 6 0	0.570	0 0 7 1	0.430	-	5219.13	-
2	8	0 8 0	0.570	0 0 7 1	0.570	-	5478.93	-
1	10	1 8 0	0.494	1 0 7 1	0.494	-	6419.38	-
2	10	2 6 0	0.516	0 0 8 2	0.458	-	6685.59	-
3	10	1 8 0	0.480	0 0 8 2	0.355	-	6954.13	-
4	10	0 6 2	1.000	1 1 6 0	0.503	-	8532.85	-
1	12	2 8 0	0.419	1 1 7 1	0.208	-	7611.21	-
2	12	3 6 0	0.455	0 0 9 3	0.282	-	7884.3	-
3	12	0 12 0	0.402	0 0 9 3	0.402	-	8156.92	-
4	12	1 10 0	0.436	0 0 9 3	0.235	-	8435.63	-
5	12	1 6 2	0.547	1 1 7 1	0.228	-	9699.67	-
6	12	0 8 2	0.547	1 1 7 1	0.275	-	9956.41	-
1	14	2 10 0	0.369	1 1 8 2	0.183	-	8795.03	-
2	14	4 6 0	0.351	0 0 10 4	0.155	-	9075.27	-
3	14	4 6 0	0.385	0 0 10 4	0.311	-	9352.65	-
4	14	0 14 0	0.337	0 0 10 4	0.337	-	9633.6	-
5	14	1 12 0	0.373	1 0 9 3	0.373	-	9923.27	-
6	14	1 8 2	0.499	3 0 7 1	0.372	-	10857.6	-
7	14	2 6 2	0.522	1 1 8 2	0.234	-	11121.3	-
8	14	1 8 2	0.487	3 0 7 1	0.363	-	11385.6	-
9	14	0 6 4	1.000	2 2 6 0	0.380	-	12957.3	-
Symmetry		Iu						
1	8	0 6 1	1.000	1 0 6 0	1.000	6283.98	6283.78	0.19
1	10	1 6 1	0.559	2 0 6 0	0.559	-	7471.75	-
2	10	0 8 1	0.559	1 0 7 1	0.559	-	7729.95	-
1	12	1 8 1	0.497	2 0 7 1	0.497	-	8650.83	-
2	12	2 6 1	0.519	1 0 8 2	0.462	-	8915.75	-
3	12	1 8 1	0.484	2 0 7 1	0.484	-	9182.08	-
4	12	0 6 3	1.000	2 1 6 0	0.755	-	10757.3	-
1	14	2 8 1	0.413	2 0 8 2	0.334	-	9821.48	-
2	14	3 6 1	0.449	1 0 9 3	0.291	-	10093.5	-
3	14	0 12 1	0.398	1 0 9 3	0.398	-	10364.2	-
4	14	1 10 1	0.432	2 0 8 2	0.432	-	10640.3	-
5	14	1 6 3	0.535	2 1 7 1	0.351	-	11903.	-
6	14	0 8 3	0.535	2 1 7 1	0.404	-	12158.4	-
Symmetry		Jg						
1	9	0 7 1	1.000	1 0 7 0	1.000	-	6940.62	-
1	11	1 7 1	0.566	2 0 7 0	0.566	-	8120.76	-
2	11	0 9 1	0.566	1 0 8 1	0.566	-	8395.34	-
1	13	1 9 1	0.495	2 0 8 1	0.495	-	9292.69	-
2	13	2 7 1	0.513	1 0 9 2	0.464	-	9573.32	-
3	13	1 9 1	0.482	2 0 8 1	0.482	-	9855.34	-
4	13	0 7 3	1.000	2 1 7 0	0.755	-	11389.2	-

State	Polyad	State (normal)	Contribution (normal)	State (local)	Contribution (local)	Exp.	Energies Theor.	ΔE
Symmetry Ju								
1	7	0 7 0	1.000	0 0 7 0	1.000	-	4679.39	-
1	9	1 7 0	0.577	0 0 8 1	0.423	-	5880.59	-
2	9	0 9 0	0.577	0 0 8 1	0.577	-	6156.91	-
1	11	1 9 0	0.492	1 0 8 1	0.492	-	7073.59	-
2	11	2 7 0	0.510	0 0 9 2	0.460	-	7355.71	-
3	11	1 9 0	0.479	0 0 9 2	0.359	-	7639.99	-
4	11	0 7 2	1.000	1 1 7 0	0.503	-	9177.19	-
1	13	2 9 0	0.423	1 1 8 1	0.210	-	8258.75	-
2	13	3 7 0	0.454	0 0 10 3	0.279	-	8547.04	-
3	13	0 13 0	0.407	0 0 10 3	0.407	-	8835.22	-
4	13	1 11 0	0.436	0 0 10 3	0.237	-	9128.64	-
5	13	1 7 2	0.554	1 1 8 1	0.224	-	10336.3	-
6	13	0 9 2	0.555	1 1 8 1	0.279	-	10609.3	-
Symmetry Kg								
1	8	0 8 0	1.000	0 0 8 0	1.000	-	5349.07	-
1	10	1 8 0	0.582	0 0 9 1	0.418	-	6542.98	-
2	10	0 10 0	0.582	0 0 9 1	0.582	-	6834.56	-
1	12	1 10 0	0.489	1 0 9 1	0.489	-	7729.24	-
2	12	2 8 0	0.505	0 0 10 2	0.462	-	8026.12	-
3	12	1 10 0	0.477	0 0 10 2	0.364	-	8324.99	-
4	12	0 8 2	1.000	1 1 8 0	0.503	-	9821.84	-
1	14	2 10 0	0.427	1 1 9 1	0.212	-	8908.18	-
2	14	3 8 0	0.453	0 0 11 3	0.276	-	9210.64	-
3	14	0 14 0	0.412	0 0 11 3	0.412	-	9513.24	-
4	14	1 12 0	0.436	0 0 11 3	0.240	-	9820.38	-
5	14	1 8 2	0.561	1 1 9 1	0.220	-	10973.8	-
6	14	0 10 2	0.561	1 1 9 1	0.283	-	11261.8	-
Symmetry Ku								
1	10	0 8 1	1.000	1 0 8 0	1.000	-	7597.77	-
1	12	1 8 1	0.572	2 0 8 0	0.572	-	8770.7	-
2	12	0 10 1	0.572	1 0 9 1	0.572	-	9060.41	-
1	14	1 10 1	0.493	2 0 9 1	0.493	-	9935.98	-
2	14	2 8 1	0.509	1 0 10 2	0.465	-	10231.2	-
3	14	1 10 1	0.481	2 0 9 1	0.481	-	10527.8	-
4	14	0 8 3	1.000	2 1 8 0	0.755	-	12021.4	-
Symmetry Lg								
1	11	0 9 1	1.000	1 0 9 0	1.000	-	8255.21	-
1	13	1 9 1	0.578	2 0 9 0	0.578	-	9421.47	-
2	13	0 11 1	0.578	1 0 10 1	0.578	-	9725.25	-
Symmetry Lu								
1	9	0 9 0	1.000	0 0 9 0	1.000	-	6019.06	-
1	11	1 9 0	0.588	0 0 10 1	0.412	-	7206.2	-
2	11	0 11 0	0.588	0 0 10 1	0.588	-	7511.98	-
1	13	1 11 0	0.487	1 0 10 1	0.487	-	8386.17	-
2	13	2 9 0	0.501	0 0 11 2	0.462	-	8696.84	-
3	13	1 11 0	0.475	0 0 11 2	0.369	-	9009.32	-
4	13	0 9 2	1.000	1 1 9 0	0.503	-	10466.8	-
Symmetry Mg								
1	10	0 10 0	1.000	0 0 10 0	1.000	-	6689.34	-
1	12	1 10 0	0.593	0 0 11 1	0.407	-	7870.18	-
2	12	0 12 0	0.593	0 0 11 1	0.593	-	8189.24	-
1	14	1 12 0	0.485	1 0 11 1	0.485	-	9044.26	-
2	14	2 10 0	0.497	0 0 12 2	0.462	-	9367.85	-
3	14	1 12 0	0.474	0 0 12 2	0.373	-	9693.09	-
4	14	0 10 2	1.000	1 1 10 0	0.503	-	11112.	-
Symmetry Mu								
1	12	0 10 1	1.000	1 0 10 0	1.000	-	8912.96	-
1	14	1 10 1	0.584	2 0 10 0	0.584	-	10073.	-
2	14	0 12 1	0.584	1 0 11 1	0.584	-	10389.9	-