

TABLE 1: A compararison of the calculated restricted Hartree-Fock interaction energies for $H_3(^4A')$, in μE_h , with the fitted values from Eq. 5.

Number	shape	R_1	R_2	R_3	calc.	fit	error(%)
1	1	2.00	2.00	2.00	255870.62	255599.03	0.11
2	1	3.00	3.00	3.00	71578.66	70979.18	0.84
3	1	4.00	4.00	4.00	19137.06	19072.88	0.34
4	1	5.00	5.00	5.00	4637.59	4633.15	0.10
5	1	6.00	6.00	6.00	1015.77	1015.65	0.01
6	1	7.00	7.00	7.00	204.30	204.59	-0.14
7	1	8.00	8.00	8.00	38.41	38.58	-0.44
8	2	2.25	1.88	1.88	261754.22	261774.44	-0.01
9	2	3.38	2.81	2.81	77195.34	76967.39	0.30
10	2	4.50	3.75	3.75	21813.02	21806.05	0.03
11	2	5.63	4.69	4.69	5644.01	5642.94	0.02
12	2	6.75	5.63	5.63	1339.28	1339.44	-0.01
13	2	7.88	6.56	6.56	299.74	300.07	-0.11
14	2	9.00	7.50	7.50	62.50	62.66	-0.26
15	3	2.75	1.75	1.75	276311.33	278620.32	-0.84
16	3	3.75	2.63	2.63	92704.85	93784.57	-1.16
17	3	5.00	3.50	3.50	29513.21	29775.11	-0.89
18	3	6.25	4.38	4.38	8536.71	8561.96	-0.30
19	3	7.50	5.25	5.25	2318.59	2322.51	-0.17
20	3	8.75	6.13	6.13	580.76	581.62	-0.15
21	3	10.00	7.00	7.00	140.22	140.43	-0.15
22	4	2.75	1.63	1.63	317956.56	320895.49	-0.92
23	4	4.13	2.44	2.44	121622.00	124537.20	-2.40
24	4	5.50	3.25	3.25	42780.39	43477.86	-1.63
25	4	6.88	4.06	4.06	13818.05	13876.89	-0.43
26	4	8.25	4.88	4.88	4111.88	4118.98	-0.17
27	4	9.63	5.69	5.69	1173.82	1175.16	-0.11
28	4	11.00	6.50	6.50	319.57	319.80	-0.07
29	5	3.00	1.50	1.50	373411.99	377351.54	-1.06
30	5	4.50	2.25	2.25	171488.10	170692.73	0.46

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Number	shape	R_1	R_2	R_3	calc.	fit	error(%)
31	5	6.00	3.00	3.00	63857.63	64314.55	-0.72
32	5	7.50	3.75	3.75	22201.06	22123.98	0.35
33	5	9.00	4.50	4.50	7378.79	7350.67	0.38
34	5	10.50	5.25	5.25	2349.86	2344.85	0.21
35	5	12.00	6.00	6.00	719.05	718.21	0.12
36	6	2.25	2.25	1.50	289072.57	289216.77	-0.05
37	6	3.38	3.38	2.25	97503.76	97286.03	0.22
38	6	4.50	4.50	3.00	34110.48	33952.50	0.46
39	6	5.63	5.63	3.75	11582.88	11533.81	0.42
40	6	6.75	6.75	4.50	3792.27	3783.65	0.23
41	6	7.88	7.88	5.25	1194.01	1193.06	0.08
42	6	9.00	9.00	6.00	362.75	362.76	0.00
43	7	2.50	2.13	1.38	313059.70	313891.27	-0.27
44	7	3.75	3.19	2.06	118010.29	118399.15	-0.33
45	7	5.00	4.25	2.75	45949.85	45843.65	0.23
46	7	6.25	5.31	3.44	17461.82	17403.30	0.34
47	7	7.50	6.38	4.13	6424.73	6414.21	0.16
48	7	8.75	7.44	4.81	2318.91	2317.68	0.05
49	7	10.00	8.50	5.50	796.95	796.92	0.00
50	8	2.75	2.00	1.25	357478.06	360188.95	-0.76
51	8	4.13	3.00	1.88	150897.00	152357.96	-0.97
52	8	5.50	4.00	2.50	64858.54	64912.41	-0.08
53	8	6.88	5.00	3.13	26899.93	26838.14	0.23
54	8	8.25	6.00	3.75	11096.17	11085.00	0.10
55	8	9.63	7.00	4.38	4407.78	4406.62	0.03
56	8	11.00	8.00	5.00	1726.97	1726.90	0.00
57	9	1.88	3.00	1.13	416557.36	423482.60	-1.66
58	9	2.81	4.50	1.69	208327.13	204504.06	1.84
59	9	3.75	6.00	2.25	93850.41	92919.27	0.99
60	9	4.69	7.50	2.81	42008.10	41719.98	0.69
61	9	5.63	9.00	3.78	10989.50	10970.89	0.17
62	9	3.94	10.50	6.56	8362.91	8355.70	0.09

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Number	shape	R_1	R_2	R_3	calc.	fit	error(%)
63	9	7.50	12.00	4.50	3666.21	3665.10	0.03
64	10	2.50	2.50	1.00	436834.96	436834.51	0.00
65	10	3.75	3.75	1.50	202200.39	201782.38	0.21
66	10	5.00	5.00	2.00	108070.49	107433.33	0.59
67	10	6.25	6.25	2.50	57590.17	57391.44	0.35
68	10	7.50	7.50	3.00	29985.97	29950.67	0.12
69	10	8.75	8.75	3.50	15221.43	15217.15	0.03
70	10	10.00	10.00	4.00	7530.20	7529.93	0.00
71	11	2.75	2.37	0.88	518915.37	519856.29	-0.18
72	11	4.13	3.56	1.31	257062.28	256521.42	0.21
73	11	5.50	4.75	1.75	147174.74	146172.65	0.68
74	11	6.88	5.94	2.19	85199.76	84924.38	0.32
75	11	8.25	7.13	2.63	48681.14	48637.98	0.09
76	11	9.63	8.31	3.06	27669.87	27664.63	0.02
77	11	11.00	9.50	3.50	15219.15	15219.03	0.00
78	12	3.00	2.25	0.75	650706.19	661990.48	-1.73
79	12	4.50	3.38	1.13	340943.81	336983.07	1.16
80	12	6.00	4.50	1.50	206284.79	201298.63	2.42
81	12	7.50	5.63	1.88	125813.33	124821.09	0.79
82	12	9.00	6.75	2.25	78981.76	78850.04	0.17
83	12	10.50	7.88	2.63	48658.16	48644.48	0.03
84	12	12.00	9.00	3.00	29967.03	29965.49	0.01
85	13	2.75	2.75	0.50	1155992.89	1136132.64	1.72
86	13	4.13	4.13	0.75	605043.70	605043.70	0.00
87	13	5.50	5.50	1.00	384475.86	384475.44	0.00
88	13	6.88	6.88	1.25	268961.35	268909.01	0.02
89	13	8.25	8.25	1.50	196329.37	196328.11	0.00
90	13	9.63	9.63	1.75	145123.83	145127.81	0.00
91	13	11.00	11.00	2.00	107182.97	107185.69	0.00
92	14	3.00	2.63	0.38	1696644.79	1672989.78	1.39
93	14	4.50	3.94	0.56	944406.50	947766.94	-0.36

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Number	shape	R_1	R_2	R_3	calc.	fit	error(%)
94	14	6.00	5.25	0.75	606453.24	607884.37	-0.24
95	14	7.50	6.56	0.94	427627.45	425021.53	0.61
96	14	9.00	7.87	1.13	317535.50	317076.63	0.14
97	14	10.50	9.19	1.31	248878.67	248874.07	0.00
98	14	12.00	10.50	1.50	196330.86	196351.41	-0.01
	1	9.00	9.00	9.00	6.83	6.90	-1.02
	1	11.00	11.00	11.00	0.16	0.16	0.00
	1	12.00	12.00	12.00	0.01	0.01	0.00
		8.54	8.54	10.00	10.51	10.64	-1.24