

## Supplementary Material (ESI)

### The cyclic ground state structure of HF trimer revealed by far infrared jet-cooled Fourier transform spectroscopy

Assigned infrared lines and fitted molecular parameters of the ground state, and of the  $\nu_6 = 1$  and  $\nu_4 = 1$  vibrational states of  $(\text{HF})_3$ .

J'	K'	l'	J''	K''	l''	EXP.FREQ.	CALC. FREQ.	DIFF.
18	17	1	19	18	0	488.70710	488.70903	-0.00193
17	15	1	18	16	0	488.74120	488.73870	0.00250
18	18	1	19	19	0	489.03590	489.03593	-0.00003
17	16	1	18	17	0	489.05880	489.05695	0.00185
16	14	1	17	15	0	489.08780	489.08596	0.00184
17	17	1	18	18	0	489.37680	489.37923	-0.00243
16	15	1	17	16	0	489.39980	489.39948	0.00032
15	13	1	16	14	0	489.42840	489.42787	0.00053
14	11	1	15	12	0	489.46700	489.46486	0.00214
16	16	1	17	17	0	489.71800	489.71713	0.00087
15	14	1	16	15	0	489.73610	489.73663	-0.00053
14	12	1	15	13	0	489.76390	489.76442	-0.00052
13	10	1	14	11	0	489.80290	489.80089	0.00201
12	8	1	13	9	0	489.84970	489.84638	0.00332
15	15	1	16	16	0	490.04960	490.04964	-0.00004
13	11	1	14	12	0	490.09620	490.09562	0.00058
12	9	1	13	10	0	490.13170	490.13159	0.00011
11	7	1	12	8	0	490.18050	490.17660	0.00390
14	14	1	15	15	0	490.37640	490.37678	-0.00038
13	12	1	14	13	0	490.39380	490.39487	-0.00107
12	10	1	13	11	0	490.42140	490.42148	-0.00008
11	8	1	12	9	0	490.45760	490.45694	0.00066
13	13	1	14	14	0	490.69730	490.69855	-0.00125
12	11	1	13	12	0	490.71510	490.71597	-0.00087
11	9	1	12	10	0	490.74160	490.74201	-0.00041
10	7	1	11	8	0	490.77760	490.77696	0.00064
9	5	1	10	6	0	490.82300	490.82101	0.00199
8	3	1	9	4	0	490.87820	490.87423	0.00397
12	12	1	13	13	0	491.01370	491.01496	-0.00126
11	10	1	12	11	0	491.03030	491.03174	-0.00144
10	8	1	11	9	0	491.05710	491.05722	-0.00012
9	6	1	10	7	0	491.09240	491.09166	0.00074
7	2	1	8	3	0	491.19140	491.18790	0.00350
11	11	1	12	12	0	491.32480	491.32603	-0.00123
10	9	1	11	10	0	491.34140	491.34218	-0.00078
9	7	1	10	8	0	491.36570	491.36711	-0.00141
8	5	1	9	6	0	491.40200	491.40103	0.00097
10	10	1	11	11	0	491.63020	491.63176	-0.00156
9	8	1	10	9	0	491.64580	491.64729	-0.00149
8	6	1	9	7	0	491.67060	491.67167	-0.00107
7	4	1	8	5	0	491.70510	491.70508	0.00002

12	10	1	12	9	0	491.89370	491.89372	-0.00002
9	9	1	10	10	0	491.93070	491.93215	-0.00145
8	7	1	9	8	0	491.94640	491.94708	-0.00068
7	5	1	8	6	0	491.97060	491.97093	-0.00033
6	3	1	7	4	0	492.00400	492.00381	0.00019
5	1	1	6	2	0	492.04840	492.04577	0.00263
8	8	1	9	9	0	492.22620	492.22722	-0.00102
7	6	1	8	7	0	492.24030	492.24156	-0.00126
6	4	1	7	5	0	492.26520	492.26486	0.00034
5	2	1	6	3	0	492.29740	492.29722	0.00018
7	7	1	8	8	0	492.51590	492.51696	-0.00106
6	5	1	7	6	0	492.52900	492.53073	-0.00173
5	3	1	6	4	0	492.55310	492.55349	-0.00039
6	6	1	7	7	0	492.80100	492.80137	-0.00037
5	4	1	6	5	0	492.81380	492.81458	-0.00078
4	2	1	5	3	0	492.83700	492.83680	0.00020
14	4	1	14	3	0	492.86900	492.86761	0.00139
5	5	1	6	6	0	493.07990	493.08047	-0.00057
4	3	1	5	4	0	493.09260	493.09312	-0.00052
4	4	1	5	5	0	493.35430	493.35425	0.00005
3	2	1	4	3	0	493.36610	493.36634	-0.00024
3	3	1	4	4	0	493.62170	493.62271	-0.00101
2	2	1	3	3	0	493.88510	493.88585	-0.00075
5	3	2	5	2	0	494.02070	494.02162	-0.00092
4	3	2	4	2	0	494.07320	494.07235	0.00085
9	1	2	9	0	0	494.18620	494.18344	0.00276
8	1	2	8	0	0	494.27840	494.27602	0.00238
5	1	2	5	0	0	494.49330	494.49087	0.00243
7	2	2	7	3	0	495.10150	495.09769	0.00381
6	2	2	6	3	0	495.17100	495.16947	0.00153
5	2	2	5	3	0	495.23120	495.23086	0.00034
2	2	2	1	1	0	495.35490	495.35405	0.00085
3	3	2	2	2	0	495.58090	495.58036	0.00054
4	4	2	3	3	0	495.80160	495.80130	0.00030
7	5	2	7	6	0	495.88040	495.88160	-0.00120
5	5	2	4	4	0	496.01770	496.01686	0.00084
4	3	2	3	2	0	496.03020	496.02879	0.00141
6	6	2	5	5	0	496.22850	496.22704	0.00146
5	4	2	4	3	0	496.24060	496.23947	0.00113
7	7	2	6	6	0	496.43310	496.43182	0.00128
6	5	2	5	4	0	496.44540	496.44475	0.00065
5	3	2	4	2	0	496.46600	496.46681	-0.00081
8	8	2	7	7	0	496.63270	496.63118	0.00152
7	6	2	6	5	0	496.64550	496.64462	0.00088
6	4	2	5	3	0	496.66670	496.66715	-0.00045
5	2	2	4	1	0	496.69570	496.69895	-0.00325
9	9	2	8	8	0	496.82640	496.82513	0.00127
8	7	2	7	6	0	496.83960	496.83907	0.00053
7	5	2	6	4	0	496.86190	496.86206	-0.00016
6	3	2	5	2	0	496.89310	496.89432	-0.00122
10	10	2	9	9	0	497.01460	497.01363	0.00097
9	8	2	8	7	0	497.02960	497.02808	0.00152
8	6	2	7	5	0	497.05170	497.05153	0.00017
7	4	2	6	3	0	497.08170	497.08423	-0.00253
11	11	2	10	10	0	497.19840	497.19668	0.00172

10	9	2	9	8	0	497.21230	497.21165	0.00065
9	7	2	8	6	0	497.23530	497.23554	-0.00024
8	5	2	7	4	0	497.26670	497.26867	-0.00197
7	3	2	6	2	0	497.30740	497.31120	-0.00380
12	12	2	11	11	0	497.37610	497.37426	0.00184
11	10	2	10	9	0	497.39020	497.38975	0.00045
10	8	2	9	7	0	497.41380	497.41409	-0.00029
9	6	2	8	5	0	497.44620	497.44763	-0.00143
8	4	2	7	3	0	497.48650	497.49058	-0.00408
13	13	2	12	12	0	497.54740	497.54635	0.00105
12	11	2	11	10	0	497.56340	497.56237	0.00103
11	9	2	10	8	0	497.58740	497.58716	0.00024
10	7	2	9	6	0	497.62000	497.62110	-0.00110
9	5	2	8	4	0	497.66130	497.66444	-0.00314
14	14	2	13	13	0	497.71380	497.71294	0.00086
13	12	2	12	11	0	497.73070	497.72950	0.00120
12	10	2	11	9	0	497.75470	497.75473	-0.00003
10	6	2	9	5	0	497.83020	497.83277	-0.00257
15	15	2	14	14	0	497.87480	497.87399	0.00081
14	13	2	13	12	0	497.89160	497.89111	0.00049
13	11	2	12	10	0	497.91770	497.91679	0.00091
12	9	2	11	8	0	497.95200	497.95150	0.00050
11	7	2	10	6	0	497.99280	497.99557	-0.00277
16	16	2	15	15	0	498.02910	498.02950	-0.00040
15	14	2	14	13	0	498.04770	498.04719	0.00051
14	12	2	13	11	0	498.07400	498.07333	0.00067
13	10	2	12	9	0	498.10760	498.10841	-0.00081
12	8	2	11	7	0	498.15010	498.15281	-0.00271
15	13	2	14	12	0	498.22490	498.22431	0.00059
13	9	2	12	8	0	498.30260	498.30448	-0.00188
17	16	2	16	15	0	498.34210	498.34266	-0.00056
12	7	2	11	6	0	498.35480	498.35878	-0.00398
15	12	2	14	11	0	498.40530	498.40554	-0.00024
11	5	2	10	4	0	498.42160	498.42285	-0.00125
14	10	2	13	9	0	498.44920	498.45057	-0.00137
16	13	2	15	12	0	498.54610	498.54574	0.00036
18	16	2	17	15	0	498.64290	498.64378	-0.00088
17	14	2	16	13	0	498.67980	498.68033	-0.00053
15	10	2	14	9	0	498.77890	498.78102	-0.00212
13	1	3	14	1	0	594.85550	594.85675	-0.00125
13	3	3	14	3	0	594.87260	594.87497	-0.00237
13	9	3	14	9	0	595.03750	595.04050	-0.00300
12	3	3	13	3	0	595.46520	595.46614	-0.00094
12	9	3	13	9	0	595.63080	595.63308	-0.00228
12	11	3	13	11	0	595.72680	595.72702	-0.00022
11	1	3	12	1	0	596.03010	596.03145	-0.00135
11	4	3	12	4	0	596.06620	596.06621	-0.00001
11	9	3	12	9	0	596.21740	596.21825	-0.00085
10	1	3	11	1	0	596.60730	596.60772	-0.00042
10	2	3	11	2	0	596.61530	596.61471	0.00059
10	3	3	11	3	0	596.62590	596.62638	-0.00048
10	6	3	11	6	0	596.68880	596.68963	-0.00083
10	7	3	11	7	0	596.72030	596.72023	0.00007
10	8	3	11	8	0	596.75540	596.75564	-0.00024

9	1	3	10	1	0	597.17570	597.17646	-0.00076
9	2	3	10	2	0	597.18400	597.18351	0.00049
9	4	3	10	4	0	597.21190	597.21173	0.00017
9	5	3	10	5	0	597.23480	597.23296	0.00184
9	6	3	10	6	0	597.25730	597.25895	-0.00165
9	9	3	10	9	0	597.36750	597.36597	0.00153
8	1	3	9	1	0	597.73790	597.73760	0.00030
8	3	3	9	3	0	597.75710	597.75652	0.00058
8	6	3	9	6	0	597.81970	597.82062	-0.00092
7	1	3	8	1	0	598.29040	598.29103	-0.00063
7	2	3	8	2	0	598.29800	598.29816	-0.00016
7	3	3	8	3	0	598.31050	598.31006	0.00044
7	4	3	8	4	0	598.32770	598.32675	0.00095
7	5	3	8	5	0	598.34980	598.34823	0.00157
7	6	3	8	6	0	598.37440	598.37456	-0.00016
6	1	3	7	1	0	598.83630	598.83668	-0.00038
6	2	3	7	2	0	598.84420	598.84386	0.00034
6	3	3	7	3	0	598.85640	598.85582	0.00058
6	4	3	7	4	0	598.87330	598.87260	0.00070
6	5	3	7	5	0	598.89640	598.89420	0.00220
5	1	3	6	1	0	599.37410	599.37448	-0.00038
5	2	3	6	2	0	599.38200	599.38168	0.00032
5	3	3	6	3	0	599.39360	599.39371	-0.00011
4	0	3	5	0	0	599.90010	599.90192	-0.00182
4	1	3	5	1	0	599.90490	599.90433	0.00057
4	2	3	5	2	0	599.91180	599.91157	0.00023
4	3	3	5	3	0	599.92340	599.92365	-0.00025
3	1	3	4	1	0	600.42590	600.42618	-0.00028
3	2	3	4	2	0	600.43320	600.43345	-0.00025
3	3	3	4	3	0	600.44440	600.44558	-0.00118
2	1	3	3	1	0	600.93960	600.93996	-0.00036
2	2	3	3	2	0	600.94740	600.94726	0.00014
18	15	3	18	15	0	601.55850	601.55676	0.00174
21	21	3	21	21	0	601.57560	601.57602	-0.00042
19	18	3	19	18	0	601.63600	601.63638	-0.00038
20	20	3	20	20	0	601.65310	601.65305	0.00005
18	18	3	18	18	0	601.79650	601.79558	0.00092
16	15	3	16	15	0	601.84700	601.84764	-0.00064
15	14	3	15	14	0	601.90970	601.91064	-0.00094
16	16	3	16	16	0	601.92270	601.92304	-0.00034
14	13	3	14	13	0	601.97010	601.96999	0.00011
15	15	3	15	15	0	601.98120	601.98121	-0.00001
13	12	3	13	12	0	602.02610	602.02572	0.00038
14	14	3	14	14	0	602.03670	602.03573	0.00097
10	6	3	10	6	0	602.06090	602.06249	-0.00159
12	11	3	12	11	0	602.07900	602.07787	0.00113
11	10	3	11	10	0	602.12660	602.12646	0.00014
12	12	3	12	12	0	602.13370	602.13393	-0.00023
10	9	3	10	9	0	602.17130	602.17152	-0.00022
11	11	3	11	11	0	602.17760	602.17767	-0.00007
9	8	3	9	8	0	602.21230	602.21307	-0.00077
10	10	3	10	10	0	602.21850	602.21788	0.00062
9	9	3	9	9	0	602.25360	602.25457	-0.00097
8	8	3	8	8	0	602.28660	602.28778	-0.00118
7	7	3	7	7	0	602.31790	602.31752	0.00038

6	6	3	6	6	0	602.34410	602.34381	0.00029
5	5	3	5	5	0	602.36760	602.36667	0.00093
4	4	3	4	4	0	602.38610	602.38610	-0.00000
3	3	3	3	3	0	602.40190	602.40213	-0.00023
2	2	3	2	2	0	602.41420	602.41475	-0.00055
3	1	3	2	1	0	603.84940	603.85000	-0.00060
4	0	3	3	0	0	604.30340	604.30334	0.00006
5	1	3	4	1	0	604.75180	604.75316	-0.00136
5	2	3	4	2	0	604.75980	604.76055	-0.00075
5	3	3	4	3	0	604.77350	604.77289	0.00061
6	0	3	5	0	0	605.18980	605.18960	0.00020
6	2	3	5	2	0	605.19960	605.19945	0.00015
6	3	3	5	3	0	605.21180	605.21177	0.00003
6	4	3	5	4	0	605.22930	605.22905	0.00025
7	1	3	6	1	0	605.62140	605.62247	-0.00107
7	2	3	6	2	0	605.63090	605.62985	0.00105
7	3	3	6	3	0	605.64180	605.64217	-0.00037
7	4	3	6	4	0	605.65870	605.65943	-0.00073
8	0	3	7	0	0	606.04270	606.04191	0.00079
8	2	3	7	2	0	606.05180	606.05174	0.00006
8	3	3	7	3	0	606.06440	606.06404	0.00036
8	4	3	7	4	0	606.08110	606.08128	-0.00018
8	5	3	7	5	0	606.10520	606.10349	0.00171
9	0	3	8	0	0	606.45550	606.45530	0.00020
9	2	3	8	2	0	606.46580	606.46511	0.00069
9	3	3	8	3	0	606.47800	606.47739	0.00061
9	4	3	8	4	0	606.49510	606.49460	0.00050
10	1	3	9	1	0	606.86230	606.86260	-0.00030
10	2	3	9	2	0	606.86990	606.86995	-0.00005
10	6	3	9	6	0	606.94910	606.94859	0.00051
10	9	3	9	9	0	607.06110	607.06012	0.00098
11	1	3	10	1	0	607.25870	607.25892	-0.00022
11	2	3	10	2	0	607.26670	607.26625	0.00045
11	4	3	10	4	0	607.29710	607.29560	0.00150
11	5	3	10	5	0	607.31950	607.31766	0.00184
11	7	3	10	7	0	607.37740	607.37671	0.00069
11	9	3	10	9	0	607.45510	607.45593	-0.00083
13	0	3	12	0	0	608.02590	608.02354	0.00236
13	5	3	12	5	0	608.08630	608.08432	0.00198
13	9	3	12	9	0	608.22140	608.22169	-0.00029

MARQUARDT PARAMETER = 0, TRUST EXPANSION = 1.00

NEW PARAMETER (EST. ERROR) -- CHANGE THIS ITERATION

1	0	GS	0.000(100)E-36	0.000E-36
2	10000	A0	0.2446077( 67)	0.0000000
3	30000	B0/2	0.1224081(115)	-0.0000000
4	200	-Dj0	-2.0111(299)E-06	-0.0000E-06
5	211	-Dj0	-2.480( 38)E-06	-0.000E-06
6	233	-Dj0	-1.829( 37)E-06	-0.000E-06
7	1100	-Djk0	2.772( 37)E-06	0.000E-06
8	1111	-Djk0	3.690( 61)E-06	0.000E-06
9	1133	-Djk0	2.230( 58)E-06	0.000E-06
10	2000	-Dk0	-0.9800( 0)E-06	0.000E-06
11	2011	-Dk0	-1.4749(287)E-06	-0.00E-06

12	2033	-Dk0	-0.7132(268)E-06	-0.0000E-06
13	11	V11	494.763171(127)	0.000000
14	10011	A	0.2395364( 76)	0.0000000
15	30011	C	0.1197380(114)	-0.0000000
16	600011	-2CZeta11	0.0529(220)E-03	0.0000E-03
17	33	V33	602.429822(133)	0.000000
18	10033	A	0.2404624( 72)	0.0000000
19	30033	C	0.1207141(116)	-0.0000000

END OF ITERATION 2 OLD, NEW RMS ERROR= 2.61770 2.61770