Electronic Supplementary Information

Size of the Hydrogen Bond Network in Liquid Methanol: A Quantum Cluster Equilibrium Model with Extensive Structure Search

Soon Teh[†‡], Po-Jen Hsu*[†], Jer-Lai Kuo*[†]

[†]*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.*

[‡]Current address: *Experimental Quantum Information Physics Unit, Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan*

* Corresponding authors: pjhsu@gate.sinica.edu.tw (P.-J.H), jlkuo@pub.iams.sinica.edu.tw (J.-L.K.).

Contents

Table S1 The local minima of the cluster size n=1-13 sorted by the counterpoise corrected energies (E_0+E_{cp}) in Hartree at B3LYP/6-31+G(d,p). The cluster probabilities and the natural logarithms of the four cluster partition functions were computed at 300 K. Those with a probability lower than 0.0001 were not shown (e.g., n>13). The cluster indices (*n-i*) cannot be cross-referenced in the other tables.

n-i	E_0	E_0+E_{zpe}	E_0+E_{cp}	E_0+E_{cp}+E_{zpe}	E_{bind}	*P(300K)*	$lnq_{i,elec}$	$lnq_{i,vib}$	$lnq_{i,rot}$	$lnq_{i,trans}$
1-1	-115.73487	-115.68363	-115.73487	-115.68363	0.00000	0.00170	5.03007	-53.67002	8.07300	60.64010
2-1	-231.47914	-231.37447	-231.47793	-231.37326	-0.00300	0.00036	18.67823	-102.26136	11.46844	61.67982
3-1	-347.23226	-347.07284	-347.22977	-347.07035	-0.00649	0.00030	41.56787	-156.18379	13.01924	62.28802
3-2	-347.23079	-347.07170	-347.22841	-347.06933	-0.00615	0.00010	40.14160	-154.76780	11.93652	62.28802
4-1	-462.98894	-462.77547	-462.98386	-462.77039	-0.00897	0.00803	66.83095	-207.24998	13.11982	62.71954
4-2	-462.98715	-462.77392	-462.98224	-462.76901	-0.00862	0.00877	65.12730	-206.15910	13.82124	62.71954
5-1	-578.73957	-578.47284	-578.73271	-578.46598	-0.00957	0.17832	86.57102	-254.11932	14.51821	63.05426
5-2	-578.73348	-578.46675	-578.72717	-578.46044	-0.00846	0.00013	80.73849	-255.50226	14.48984	63.05426
5-3	-578.73263	-578.46593	-578.72633	-578.45962	-0.00830	0.00030	79.85134	-253.78061	14.51974	63.05426
5-7	-578.73138	-578.46482	-578.72523	-578.45868	-0.00811	0.00014	78.69794	-253.39808	14.53085	63.05426
5-9	-578.73102	-578.46470	-578.72504	-578.45872	-0.00811	0.00044	78.49526	-252.12790	14.59044	63.05426
6-1	-694.49008	-694.16994	-694.48169	-694.16155	-0.00996	0.03805	106.44861	-303.75982	14.00709	63.32774
6-2	-694.48805	-694.16823	-694.47986	-694.16004	-0.00971	0.16943	104.52955	-301.42657	15.08651	63.32774
6-3	-694.48781	-694.16784	-694.47955	-694.15958	-0.00963	0.03372	104.19889	-302.72643	15.10282	63.32774
6-4	-694.48433	-694.16421	-694.47620	-694.15608	-0.00905	0.00056	100.67737	-303.24915	15.04205	63.32774
6-5	-694.48418	-694.16389	-694.47605	-694.15576	-0.00900	0.00015	100.51795	-304.38639	15.04101	63.32774
6-6	-694.48390	-694.16381	-694.47586	-694.15577	-0.00900	0.00026	100.31791	-303.68042	15.06213	63.32774
6-7	-694.48376	-694.16367	-694.47570	-694.15561	-0.00897	0.00077	100.14534	-302.43003	15.07929	63.32774
6-8	-694.48383	-694.16368	-694.47570	-694.15555	-0.00896	0.00018	100.14429	-303.90997	15.07780	63.32774
6-9	-694.48375	-694.16366	-694.47566	-694.15557	-0.00897	0.00028	100.10575	-303.40592	15.07347	63.32774
6-11	-694.48336	-694.16340	-694.47530	-694.15534	-0.00893	0.00085	99.72462	-301.91407	15.08005	63.32774
6-15	-694.48063	-694.16038	-694.47314	-694.15289	-0.00852	0.00016	97.45205	-301.31830	15.11466	63.32774
6-59	-694.46809	-694.14966	-694.46180	-694.14337	-0.00693	0.01996	85.51692	-286.55874	17.09256	63.32774
7-1	-810.23754	-809.86437	-810.22785	-809.85468	-0.00990	0.21237	123.36625	-349.22350	15.61380	63.55897
7-2	-810.23748	-809.86424	-810.22781	-809.85457	-0.00988	0.08727	123.31732	-350.06571	15.61561	63.55897
7-3	-810.23732	-809.86372	-810.22741	-809.85381	-0.00977	0.00834	122.89788	-351.90394	15.52498	63.55897
7-4	-810.23719	-809.86363	-810.22730	-809.85375	-0.00976	0.00975	122.78669	-351.64109	15.52999	63.55897
7-5	-810.23669	-809.86302	-810.22679	-809.85313	-0.00968	0.00246	122.25175	-352.45285	15.50087	63.55897
7-6	-810.23665	-809.86292	-810.22670	-809.85297	-0.00965	0.00174	122.15216	-352.67325	15.47273	63.55897
7-7	-810.23653	-809.86299	-810.22667	-809.85313	-0.00968	0.00669	122.11802	-351.30942	15.49026	63.55897
7-8	-810.23419	-809.86072	-810.22456	-809.85110	-0.00939	0.00070	119.90246	-351.44451	15.58911	63.55897
7-9	-810.23409	-809.86049	-810.22447	-809.85087	-0.00935	0.00024	119.80812	-352.42651	15.58057	63.55897
7-10	-810.23402	-809.86042	-810.22438	-809.85078	-0.00934	0.00020	119.70985	-352.49141	15.57476	63.55897
7-16	-810.23294	-809.85940	-810.22324	-809.84970	-0.00919	0.00011	118.51604	-351.82616	15.53214	63.55897
7-17	-810.23283	-809.85936	-810.22319	-809.84971	-0.00919	0.00018	118.45681	-351.28550	15.51316	63.55897

7-18	-810.23270	-809.85933	-810.22310	-809.84973	-0.00919	0.00053	118.36333	-350.13096	15.53404	63.55897
7-21	-810.23238	-809.85913	-810.22289	-809.84964	-0.00918	0.00039	118.14665	-350.24603	15.56489	63.55897
7-22	-810.23225	-809.85897	-810.22279	-809.84951	-0.00916	0.00082	118.03987	-349.38043	15.54388	63.55897
7-24	-810.23223	-809.85856	-810.22271	-809.84904	-0.00909	0.00016	117.95045	-350.98065	15.56826	63.55897
8-1	-925.98651	-925.55989	-925.97540	-925.54878	-0.00997	0.01075	141.73668	-398.29866	14.72750	63.75926
8-2	-925.98581	-925.55895	-925.97450	-925.54764	-0.00983	0.00474	140.78925	-399.41612	15.97391	63.75926
8-3	-925.98561	-925.55892	-925.97447	-925.54777	-0.00984	0.01125	140.76056	-398.54338	15.99380	63.75926
8-4	-925.98563	-925.55901	-925.97442	-925.54780	-0.00985	0.01334	140.71232	-398.30989	15.97919	63.75926
8-6	-925.98556	-925.55873	-925.97422	-925.54739	-0.00980	0.00311	140.49993	-399.54220	15.96746	63.75926
8-7	-925.98563	-925.55855	-925.97422	-925.54713	-0.00976	0.00110	140.49223	-400.52117	15.91119	63.75926
8-8	-925.98532	-925.55798	-925.97369	-925.54634	-0.00966	0.00016	139.93470	-401.79982	15.85028	63.75926
8-10	-925.98475	-925.55784	-925.97342	-925.54651	-0.00969	0.00059	139.65263	-400.36335	15.96494	63.75926
8-14	-925.98217	-925.55540	-925.97110	-925.54433	-0.00941	0.00024	137.21355	-398.86625	16.00362	63.75926
8-15	-925.98202	-925.55528	-925.97106	-925.54432	-0.00941	0.00027	137.17188	-398.71134	16.00875	63.75926
8-17	-925.98191	-925.55522	-925.97098	-925.54428	-0.00941	0.00032	137.08646	-398.42533	15.99932	63.75926
8-19	-925.98190	-925.55518	-925.97092	-925.54420	-0.00940	0.00031	137.02005	-398.43976	16.02186	63.75926
8-20	-925.98186	-925.55524	-925.97090	-925.54428	-0.00941	0.00030	137.00011	-398.42372	16.01514	63.75926
8-26	-925.98160	-925.55493	-925.97074	-925.54407	-0.00938	0.00059	136.83280	-397.57753	16.01266	63.75926
8-27	-925.98166	-925.55497	-925.97070	-925.54402	-0.00937	0.00026	136.79492	-398.37883	16.02130	63.75926
8-36	-925.98147	-925.55481	-925.97053	-925.54387	-0.00935	0.00020	136.60816	-398.41216	15.99860	63.75926
9-3	-1041.73429	-1041.25414	-1041.72159	-1041.24144	-0.00986	0.00274	158.68301	-446.82334	16.37198	63.93594
9-4	-1041.73424	-1041.25391	-1041.72146	-1041.24113	-0.00983	0.00118	158.55075	-447.49776	16.33811	63.93594
9-5	-1041.73413	-1041.25397	-1041.72146	-1041.24130	-0.00985	0.00249	158.54190	-446.75001	16.34450	63.93594
9-7	-1041.73387	-1041.25399	-1041.72127	-1041.24139	-0.00986	0.01078	158.34137	-445.14950	16.40864	63.93594
9-10	-1041.73362	-1041.25312	-1041.72080	-1041.24030	-0.00974	0.00014	157.85657	-448.89417	16.30894	63.93594
9-11	-1041.73361	-1041.25307	-1041.72061	-1041.24007	-0.00971	0.00013	157.65184	-448.72885	16.26347	63.93594
9-13	-1041.73312	-1041.25287	-1041.72039	-1041.24014	-0.00972	0.00052	157.42224	-447.20595	16.35539	63.93594
9-14	-1041.73268	-1041.25310	-1041.72030	-1041.24073	-0.00979	0.02420	157.32597	-443.31938	16.40287	63.93594
9-15	-1041.73271	-1041.25312	-1041.72030	-1041.24071	-0.00978	0.04904	157.32438	-442.60252	16.39367	63.93594
9-16	-1041.73306	-1041.25276	-1041.72022	-1041.23992	-0.00970	0.00030	157.23588	-447.54584	16.31435	63.93594
9-17	-1041.73279	-1041.25285	-1041.72020	-1041.24025	-0.00973	0.00333	157.21892	-445.13508	16.34113	63.93594
9-19	-1041.73277	-1041.25261	-1041.72008	-1041.23992	-0.00970	0.00079	157.09775	-446.42522	16.31379	63.93594
9-20	-1041.73275	-1041.25250	-1041.71998	-1041.23973	-0.00968	0.00018	156.99101	-447.81058	16.30554	63.93594
9-21	-1041.73265	-1041.25251	-1041.71996	-1041.23982	-0.00968	0.00048	156.96401	-446.81355	16.33189	63.93594
9-23	-1041.73266	-1041.25264	-1041.71989	-1041.23988	-0.00969	0.00215	156.89636	-445.19851	16.29118	63.93594
9-24	-1041.73272	-1041.25244	-1041.71987	-1041.23960	-0.00966	0.00012	156.87380	-448.01625	16.25345	63.93594
9-25	-1041.73249	-1041.25228	-1041.71980	-1041.23959	-0.00966	0.00034	156.80143	-446.96738	16.30224	63.93594
9-32	-1041.73068	-1041.25092	-1041.71842	-1041.23866	-0.00956	0.00122	155.34212	-444.37060	16.45122	63.93594
9-33	-1041.73068	-1041.25086	-1041.71842	-1041.23860	-0.00955	0.00050	155.34193	-445.26593	16.44658	63.93594
9-63	-1041.73010	-1041.25020	-1041.71772	-1041.23781	-0.00946	0.00024	154.60504	-445.18319	16.37284	63.93594
9-70	-1041.73008	-1041.24993	-1041.71761	-1041.23746	-0.00942	0.00014	154.49761	-445.62009	16.34407	63.93594

10-2	-1157.48258	-1156.94921	-1157.46847	-1156.93509	-0.00988	0.00266	176.34861	-493.41813	16.73495	64.09398
10-5	-1157.48254	-1156.94895	-1157.46840	-1156.93481	-0.00985	0.00039	176.27607	-495.21349	16.66798	64.09398
10-7	-1157.48250	-1156.94904	-1157.46837	-1156.93492	-0.00986	0.00181	176.25206	-493.70079	16.73047	64.09398
10-11	-1157.48226	-1156.94889	-1157.46816	-1156.93479	-0.00985	0.00072	176.03114	-494.36006	16.69056	64.09398
10-12	-1157.48229	-1156.94868	-1157.46814	-1156.93453	-0.00982	0.00014	176.00707	-495.95180	16.67755	64.09398
10-16	-1157.48230	-1156.94865	-1157.46802	-1156.93437	-0.00981	0.00011	175.87466	-496.10745	16.66771	64.09398
10-18	-1157.48202	-1156.94877	-1157.46794	-1156.93469	-0.00984	0.00489	175.79318	-492.21181	16.69117	64.09398
10-19	-1157.48215	-1156.94858	-1157.46793	-1156.93437	-0.00981	0.00034	175.78856	-494.89477	16.69772	64.09398
10-22	-1157.48198	-1156.94845	-1157.46787	-1156.93433	-0.00980	0.00027	175.72248	-495.08281	16.72759	64.09398
10-24	-1157.48214	-1156.94840	-1157.46783	-1156.93409	-0.00978	0.00010	175.68324	-495.94074	16.67302	64.09398
10-26	-1157.48189	-1156.94840	-1157.46777	-1156.93428	-0.00980	0.00025	175.61859	-495.04048	16.70009	64.09398
10-27	-1157.48197	-1156.94831	-1157.46776	-1156.93410	-0.00978	0.00016	175.60132	-495.41115	16.64317	64.09398
10-28	-1157.48184	-1156.94823	-1157.46775	-1156.93414	-0.00979	0.00022	175.59325	-495.13072	16.69872	64.09398
10-29	-1157.48190	-1156.94830	-1157.46772	-1156.93411	-0.00978	0.00016	175.56341	-495.41265	16.69080	64.09398
10-33	-1157.48177	-1156.94820	-1157.46759	-1156.93403	-0.00977	0.00023	175.42979	-494.89231	16.66537	64.09398
10-37	-1157.48162	-1156.94818	-1157.46754	-1156.93410	-0.00978	0.00027	175.37736	-494.71017	16.70788	64.09398
10-38	-1157.48177	-1156.94815	-1157.46749	-1156.93387	-0.00976	0.00011	175.32332	-495.51765	16.63547	64.09398
10-39	-1157.48163	-1156.94800	-1157.46746	-1156.93383	-0.00976	0.00011	175.29047	-495.46974	16.65777	64.09398
10-55	-1157.48081	-1156.94772	-1157.46696	-1156.93386	-0.00976	0.00362	174.76443	-491.48321	16.69160	64.09398
10-66	-1157.48090	-1156.94726	-1157.46661	-1156.93297	-0.00967	0.00010	174.39857	-494.63724	16.62061	64.09398
10-96	-1157.47907	-1156.94507	-1157.46556	-1156.93156	-0.00953	0.01067	173.28753	-489.90481	17.67096	64.09398
11-6	-1273.23088	-1272.64436	-1273.21543	-1272.62891	-0.00991	0.01611	194.10965	-538.22823	17.07236	64.23694
11-9	-1273.23090	-1272.64425	-1273.21534	-1272.62869	-0.00989	0.00057	194.01087	-541.38278	16.97849	64.23694
11-13	-1273.23101	-1272.64398	-1273.21525	-1272.62822	-0.00985	0.00014	193.91423	-542.71087	16.99762	64.23694
11-21	-1273.23073	-1272.64372	-1273.21499	-1272.62797	-0.00982	0.00011	193.64389	-542.60917	16.96178	64.23694
11-26	-1273.23049	-1272.64369	-1273.21495	-1272.62815	-0.00984	0.00164	193.60143	-539.90625	16.97138	64.23694
11-27	-1273.23049	-1272.64372	-1273.21495	-1272.62818	-0.00984	0.00145	193.60074	-540.01840	16.96551	64.23694
11-37	-1273.23029	-1272.64350	-1273.21478	-1272.62800	-0.00983	0.00027	193.42611	-541.59901	17.01811	64.23694
11-41	-1273.23016	-1272.64354	-1273.21467	-1272.62804	-0.00983	0.00071	193.30699	-540.48325	17.01207	64.23694
11-46	-1273.23048	-1272.64355	-1273.21462	-1272.62769	-0.00980	0.00024	193.25970	-541.39308	16.86237	64.23694
11-54	-1273.22990	-1272.64310	-1273.21447	-1272.62766	-0.00980	0.00034	193.09489	-541.03180	17.03488	64.23694
11-59	-1273.23021	-1272.64319	-1273.21439	-1272.62737	-0.00977	0.00021	193.01112	-541.30991	16.91763	64.23694
11-61	-1273.22987	-1272.64310	-1273.21436	-1272.62758	-0.00979	0.00030	192.97606	-541.03874	17.01949	64.23694
11-62	-1273.22973	-1272.64310	-1273.21435	-1272.62771	-0.00980	0.00153	192.96934	-539.40051	17.03288	64.23694
12-7	-1388.97961	-1388.33944	-1388.96250	-1388.32234	-0.00990	0.00017	211.97970	-589.37719	17.28210	64.36746
12-32	-1388.97903	-1388.33888	-1388.96190	-1388.32175	-0.00985	0.00018	211.35074	-588.59067	17.23026	64.36746
13-12	-1504.72783	-1504.03387	-1504.70916	-1504.01521	-0.00985	0.00013	229.41586	-635.79926	17.52218	64.48752

Table S2 The local minima of the cluster size n=1-14 sorted by counterpoise corrected energies (E_0+E_{cp}) in Hartree at B3LYP+D3/6-31+G(d,p). The cluster probabilities and the natural logarithms of the four cluster partition functions were computed at 300 K. Those with a probability lower than 0.0001 were not shown. The cluster indices (*n-i*) cannot be cross-referenced in the other tables.

n-i	E_0	E_0+E_{zpe}	E_0+E_{cp}	E_0+E_{cp}+E_{zpe}	E_{bind}	*P(300K)*	$lnq_{i,elec}$	$lnq_{i,vib}$	$lnq_{i,rot}$	$lnq_{i,trans}$
1-1	-115.73600	-115.68480	-115.73600	-115.68480	0.00000	0.00024	2.36275	-53.63142	8.07490	61.39809
4-1	-463.00334	-462.78976	-462.99805	-462.78446	-0.01132	0.00371	66.35561	-207.82474	13.07373	63.47753
4-2	-463.00187	-462.78864	-462.99668	-462.78345	-0.01107	0.00910	64.91207	-206.15564	13.74666	63.47753
5-1	-578.75860	-578.49182	-578.75139	-578.48461	-0.01213	0.13008	86.97231	-254.98301	14.45269	63.81225
5-2	-578.75856	-578.49166	-578.75131	-578.48441	-0.01209	0.04772	86.88937	-255.83254	14.38227	63.81225
5-3	-578.75806	-578.49078	-578.75090	-578.48363	-0.01193	0.00221	86.46576	-258.38099	14.28015	63.81225
5-4	-578.75721	-578.49016	-578.75009	-578.48304	-0.01181	0.04010	85.60480	-254.69340	14.35378	63.81225
6-1	-694.51387	-694.19285	-694.50474	-694.18372	-0.01249	0.00355	107.60790	-308.21608	14.83107	64.08573
6-2	-694.51393	-694.19281	-694.50466	-694.18355	-0.01246	0.00258	107.52700	-308.41446	14.78857	64.08573
6-3	-694.51354	-694.19254	-694.50447	-694.18347	-0.01245	0.00201	107.31973	-308.49449	14.82992	64.08573
6-4	-694.51338	-694.19258	-694.50444	-694.18364	-0.01248	0.00541	107.28882	-307.45485	14.81006	64.08573
6-5	-694.51326	-694.19252	-694.50428	-694.18355	-0.01246	0.00474	107.12668	-307.44216	14.82708	64.08573
6-6	-694.51330	-694.19221	-694.50419	-694.18311	-0.01239	0.00209	107.03172	-308.14239	14.80183	64.08573
6-7	-694.51272	-694.19272	-694.50403	-694.18403	-0.01254	0.29378	106.85928	-302.19750	13.97624	64.08573
6-8	-694.51277	-694.19217	-694.50384	-694.18323	-0.01241	0.00747	106.65706	-306.49303	14.80187	64.08573
6-10	-694.51156	-694.19041	-694.50271	-694.18156	-0.01213	0.00011	105.47273	-309.48812	14.79820	64.08573
6-11	-694.51159	-694.19031	-694.50262	-694.18134	-0.01210	0.00010	105.37786	-309.45024	14.73125	64.08573
6-13	-694.51103	-694.19007	-694.50211	-694.18115	-0.01206	0.00017	104.83899	-308.44732	14.81519	64.08573
6-14	-694.51104	-694.19009	-694.50209	-694.18115	-0.01206	0.00013	104.81855	-308.72855	14.80245	64.08573
6-15	-694.51066	-694.18975	-694.50193	-694.18103	-0.01204	0.00017	104.65381	-308.25698	14.79804	64.08573
6-18	-694.51053	-694.18959	-694.50185	-694.18091	-0.01202	0.00012	104.56293	-308.49345	14.77907	64.08573
6-21	-694.50985	-694.18883	-694.50110	-694.18008	-0.01188	0.00012	103.77733	-307.83880	14.89019	64.08573
6-22	-694.50978	-694.18910	-694.50102	-694.18034	-0.01193	0.00018	103.69561	-307.19419	14.76089	64.08573
6-24	-694.50835	-694.18818	-694.49988	-694.17971	-0.01182	0.00549	102.49229	-302.88371	15.04965	64.08573
6-70	-694.48543	-694.16713	-694.47896	-694.16065	-0.00865	0.00069	80.47289	-284.96515	17.06972	64.08573
7-1	-810.26883	-809.89424	-810.25792	-809.88332	-0.01282	0.01194	128.05149	-356.40248	15.23747	64.31695
7-2	-810.26886	-809.89436	-810.25789	-809.88340	-0.01283	0.00849	128.02647	-356.73045	15.25034	64.31695
7-3	-810.26866	-809.89361	-810.25774	-809.88269	-0.01273	0.00027	127.87073	-359.97441	15.18324	64.31695
7-4	-810.26827	-809.89369	-810.25738	-809.88280	-0.01275	0.00185	127.48303	-357.74874	15.28957	64.31695
7-5	-810.26815	-809.89386	-810.25734	-809.88305	-0.01278	0.02440	127.44078	-355.10092	15.26175	64.31695
7-6	-810.26803	-809.89347	-810.25725	-809.88269	-0.01273	0.00132	127.35379	-357.93077	15.25757	64.31695
7-8	-810.26797	-809.89368	-810.25709	-809.88280	-0.01275	0.00498	127.18779	-356.44738	15.27169	64.31695
7-9	-810.26783	-809.89332	-810.25704	-809.88253	-0.01271	0.00361	127.12853	-356.79742	15.36031	64.31695
7-10	-810.26770	-809.89324	-810.25691	-809.88244	-0.01270	0.00205	126.98870	-357.14823	15.28181	64.31695
7-11	-810.26758	-809.89324	-810.25690	-809.88256	-0.01271	0.00327	126.97917	-356.69222	15.30409	64.31695

7-12	-810.26750	-809.89292	-810.25684	-809.88227	-0.01267	0.00176	126.92371	-357.14561	15.19175	64.31695
7-14	-810.26751	-809.89267	-810.25671	-809.88188	-0.01262	0.00010	126.78029	-359.82817	15.17522	64.31695
7-15	-810.26735	-809.89304	-810.25661	-809.88230	-0.01268	0.00153	126.67565	-357.09820	15.25130	64.31695
7-17	-810.26669	-809.89276	-810.25612	-809.88219	-0.01266	0.02733	126.16670	-353.86739	15.41555	64.31695
7-18	-810.26670	-809.89204	-810.25596	-809.88129	-0.01253	0.00019	125.98970	-358.44561	15.20787	64.31695
7-29	-810.26456	-809.88992	-810.25439	-809.87975	-0.01231	0.00064	124.34342	-355.81814	15.44041	64.31695
7-36	-810.26425	-809.88983	-810.25378	-809.87937	-0.01226	0.00024	123.70194	-356.05539	15.31464	64.31695
7-38	-810.26386	-809.88963	-810.25366	-809.87943	-0.01227	0.00044	123.57133	-355.39230	15.39662	64.31695
7-42	-810.26344	-809.88950	-810.25330	-809.87936	-0.01226	0.00066	123.19684	-354.69162	15.48961	64.31695
7-46	-810.26323	-809.88946	-810.25306	-809.87929	-0.01225	0.00168	122.94076	-353.49199	15.47813	64.31695
8-1	-926.02598	-925.59723	-926.01307	-925.58432	-0.01324	0.00080	150.57586	-409.80666	14.92076	64.51725
8-2	-926.02595	-925.59745	-926.01304	-925.58454	-0.01327	0.00583	150.54391	-407.78995	14.91942	64.51725
8-5	-926.02294	-925.59484	-926.01031	-925.58221	-0.01298	0.00199	147.67337	-406.74660	15.67019	64.51725
8-7	-926.02268	-925.59440	-926.01023	-925.58195	-0.01295	0.00175	147.58745	-406.74444	15.62451	64.51725
8-8	-926.02281	-925.59479	-926.01020	-925.58218	-0.01298	0.00227	147.55927	-406.49970	15.67029	64.51725
8-9	-926.02267	-925.59415	-926.01010	-925.58158	-0.01290	0.00021	147.45629	-408.71979	15.59321	64.51725
8-10	-926.02266	-925.59448	-926.01010	-925.58191	-0.01294	0.00243	147.45250	-406.27762	15.62509	64.51725
8-13	-926.02275	-925.59433	-926.01006	-925.58164	-0.01291	0.00012	147.41297	-409.21870	15.55546	64.51725
8-14	-926.02257	-925.59423	-926.01001	-925.58168	-0.01291	0.00052	147.36459	-407.77780	15.66778	64.51725
8-15	-926.02251	-925.59435	-926.00999	-925.58183	-0.01293	0.00202	147.33948	-406.35340	15.62876	64.51725
8-18	-926.02209	-925.59417	-926.00975	-925.58183	-0.01293	0.00262	147.08178	-405.97252	15.76385	64.51725
8-21	-926.02206	-925.59385	-926.00941	-925.58119	-0.01285	0.00033	146.72761	-407.55323	15.63684	64.51725
8-22	-926.02194	-925.59358	-926.00940	-925.58104	-0.01284	0.00020	146.72066	-408.06340	15.62209	64.51725
8-23	-926.02182	-925.59345	-926.00935	-925.58098	-0.01283	0.00041	146.66185	-407.24705	15.60539	64.51725
8-26	-926.02177	-925.59331	-926.00925	-925.58080	-0.01280	0.00019	146.55830	-407.89612	15.60167	64.51725
8-29	-926.02162	-925.59322	-926.00902	-925.58062	-0.01278	0.00012	146.32202	-408.15770	15.63064	64.51725
8-37	-926.02100	-925.59323	-926.00875	-925.58098	-0.01283	0.00103	146.03512	-405.72030	15.62545	64.51725
8-41	-926.02092	-925.59273	-926.00863	-925.58044	-0.01276	0.00033	145.91039	-406.77075	15.64578	64.51725
8-43	-926.02088	-925.59269	-926.00857	-925.58038	-0.01275	0.00045	145.84504	-406.45407	15.72714	64.51725
8-64	-926.01998	-925.59172	-926.00779	-925.57952	-0.01265	0.00031	145.01909	-406.04424	15.75299	64.51725
8-106	-926.01888	-925.59074	-926.00673	-925.57859	-0.01253	0.00035	143.90643	-404.87862	15.83121	64.51725
8-119	-926.01852	-925.59049	-926.00649	-925.57846	-0.01251	0.00021	143.65006	-405.13128	15.81712	64.51725
8-121	-926.01840	-925.59049	-926.00641	-925.57849	-0.01252	0.00025	143.56540	-404.80054	15.74874	64.51725
8-125	-926.01842	-925.59051	-926.00634	-925.57844	-0.01251	0.00011	143.49724	-405.52573	15.75333	64.51725
8-127	-926.01842	-925.59067	-926.00631	-925.57855	-0.01252	0.00027	143.46046	-404.68896	15.81163	64.51725
8-135	-926.01798	-925.58937	-926.00605	-925.57745	-0.01239	0.00012	143.19561	-405.20068	15.82407	64.51725
8-153	-926.01705	-925.58942	-926.00544	-925.57781	-0.01243	0.00099	142.54900	-402.54729	15.90027	64.51725
8-162	-926.01665	-925.59017	-926.00521	-925.57873	-0.01255	0.08200	142.30241	-396.69243	14.70718	64.51725
8-163	-926.01661	-925.59015	-926.00519	-925.57873	-0.01255	0.16697	142.28944	-396.66351	15.40228	64.51725
8-229	-926.01333	-925.58633	-926.00169	-925.57469	-0.01204	0.00021	138.60319	-400.16313	15.89989	64.51725
9-2	-1041.77989	-1041.29774	-1041.76533	-1041.28318	-0.01334	0.00136	170.06441	-458.25819	15.95557	64.69393

9-6	-1041.77947	-1041.29708	-1041.76493	-1041.28254	-0.01326	0.00038	169.64387	-459.06625	15.91762	64.69393
9-7	-1041.77931	-1041.29715	-1041.76481	-1041.28265	-0.01328	0.00068	169.51420	-458.39882	15.95730	64.69393
9-9	-1041.77888	-1041.29652	-1041.76441	-1041.28205	-0.01321	0.00025	169.09305	-458.98263	15.96082	64.69393
9-11	-1041.77880	-1041.29644	-1041.76429	-1041.28193	-0.01320	0.00019	168.96336	-459.11188	15.95427	64.69393
9-12	-1041.77817	-1041.29623	-1041.76382	-1041.28188	-0.01319	0.00121	168.47682	-456.82137	15.98732	64.69393
9-14	-1041.77819	-1041.29602	-1041.76382	-1041.28165	-0.01317	0.00019	168.47366	-458.66127	15.95572	64.69393
9-17	-1041.77783	-1041.29565	-1041.76369	-1041.28151	-0.01315	0.00045	168.33714	-457.63131	15.94091	64.69393
9-21	-1041.77764	-1041.29584	-1041.76329	-1041.28149	-0.01315	0.00232	167.90990	-455.59295	15.97839	64.69393
9-24	-1041.77765	-1041.29547	-1041.76326	-1041.28108	-0.01310	0.00014	167.88127	-458.34350	15.92190	64.69393
9-31	-1041.77728	-1041.29524	-1041.76310	-1041.28105	-0.01310	0.00030	167.71245	-457.46026	15.98170	64.69393
9-33	-1041.77732	-1041.29526	-1041.76298	-1041.28093	-0.01309	0.00040	167.59195	-457.07595	16.01761	64.69393
9-36	-1041.77707	-1041.29518	-1041.76285	-1041.28096	-0.01309	0.00056	167.45036	-456.55423	15.97883	64.69393
9-50	-1041.77674	-1041.29423	-1041.76254	-1041.28003	-0.01299	0.00019	167.12871	-457.33983	16.02274	64.69393
9-55	-1041.77671	-1041.29466	-1041.76245	-1041.28041	-0.01303	0.00019	167.03524	-457.27749	16.02987	64.69393
9-56	-1041.77680	-1041.29483	-1041.76245	-1041.28047	-0.01304	0.00208	167.02917	-454.93443	16.08947	64.69393
9-61	-1041.77669	-1041.29463	-1041.76237	-1041.28031	-0.01302	0.00025	166.94955	-456.90948	16.03566	64.69393
9-64	-1041.77668	-1041.29488	-1041.76231	-1041.28051	-0.01304	0.00062	166.88122	-455.95570	16.04575	64.69393
9-65	-1041.77626	-1041.29455	-1041.76225	-1041.28054	-0.01304	0.00114	166.81819	-455.33419	16.10309	64.69393
9-67	-1041.77631	-1041.29466	-1041.76224	-1041.28058	-0.01305	0.00149	166.80430	-455.01557	16.06577	64.69393
9-77	-1041.77619	-1041.29446	-1041.76208	-1041.28035	-0.01302	0.00220	166.64319	-454.50980	16.10927	64.69393
9-81	-1041.77632	-1041.29429	-1041.76205	-1041.28002	-0.01298	0.00018	166.61082	-456.93726	16.05880	64.69393
9-95	-1041.77574	-1041.29438	-1041.76184	-1041.28048	-0.01304	0.00509	166.39098	-453.49040	16.17880	64.69393
9-119	-1041.77534	-1041.29400	-1041.76146	-1041.28011	-0.01300	0.00172	165.98430	-454.06657	16.07743	64.69393
9-146	-1041.77508	-1041.29329	-1041.76103	-1041.27924	-0.01290	0.00070	165.53366	-454.57665	16.13727	64.69393
9-157	-1041.77495	-1041.29332	-1041.76089	-1041.27926	-0.01290	0.00017	165.38639	-455.69803	15.97341	64.69393
9-163	-1041.77487	-1041.29286	-1041.76081	-1041.27879	-0.01285	0.00015	165.30485	-455.80548	16.07393	64.69393
9-165	-1041.77486	-1041.29331	-1041.76080	-1041.27925	-0.01290	0.00072	165.29117	-454.14512	15.97144	64.69393
9-297	-1041.77297	-1041.29132	-1041.75926	-1041.27760	-0.01272	0.00029	163.66891	-453.55186	16.10492	64.69393
10-1	-1157.53590	-1156.99965	-1157.51929	-1156.98303	-0.01351	0.00027	191.32911	-509.86038	16.23042	64.85197
10-6	-1157.53462	-1156.99857	-1157.51816	-1156.98212	-0.01342	0.00012	190.14510	-509.44671	16.24364	64.85197
10-8	-1157.53454	-1156.99808	-1157.51807	-1156.98161	-0.01337	0.00016	190.04839	-509.08993	16.24699	64.85197
10-10	-1157.53442	-1156.99853	-1157.51797	-1156.98209	-0.01341	0.00051	189.94892	-507.84940	16.25304	64.85197
10-13	-1157.53433	-1156.99837	-1157.51788	-1156.98193	-0.01340	0.00015	189.85400	-508.97613	16.22179	64.85197
10-15	-1157.53419	-1156.99845	-1157.51785	-1156.98210	-0.01342	0.00045	189.81317	-507.84345	16.25490	64.85197
10-16	-1157.53386	-1156.99798	-1157.51776	-1156.98188	-0.01339	0.00040	189.72010	-507.90739	16.29848	64.85197
10-21	-1157.53371	-1156.99796	-1157.51749	-1156.98174	-0.01338	0.00056	189.43470	-507.20391	16.21062	64.85197
10-25	-1157.53372	-1156.99807	-1157.51743	-1156.98178	-0.01338	0.00058	189.37746	-507.15911	16.25824	64.85197
10-27	-1157.53365	-1156.99790	-1157.51741	-1156.98165	-0.01337	0.00030	189.35508	-507.80831	16.27102	64.85197
10-33	-1157.53342	-1156.99777	-1157.51725	-1156.98160	-0.01337	0.00092	189.18736	-506.59323	16.34553	64.85197
10-40	-1157.53318	-1156.99794	-1157.51703	-1156.98179	-0.01338	0.00110	188.95151	-505.41368	15.58748	64.85197
10-50	-1157.53291	-1156.99714	-1157.51675	-1156.98098	-0.01330	0.00038	188.66408	-506.83806	16.24383	64.85197

10-53	-1157.53282	-1156.99715	-1157.51670	-1156.98104	-0.01331	0.00065	188.60982	-506.33257	16.32317	64.85197
10-74	-1157.53234	-1156.99622	-1157.51621	-1156.98009	-0.01321	0.00019	188.09553	-507.01753	16.29820	64.85197
10-85	-1157.53205	-1156.99673	-1157.51600	-1156.98069	-0.01327	0.00014	187.87353	-507.08674	16.24839	64.85197
10-94	-1157.53174	-1156.99616	-1157.51578	-1156.98020	-0.01322	0.00039	187.64318	-506.02905	16.46379	64.85197
10-135	-1157.53156	-1156.99611	-1157.51539	-1156.97994	-0.01320	0.00117	187.23231	-504.45080	16.40017	64.85197
10-141	-1157.53099	-1156.99547	-1157.51532	-1156.97979	-0.01318	0.00012	187.14981	-506.53923	16.27521	64.85197
10-148	-1157.53118	-1156.99609	-1157.51526	-1156.98017	-0.01322	0.00024	187.09115	-505.05928	15.58345	64.85197
10-155	-1157.53118	-1156.99558	-1157.51521	-1156.97962	-0.01317	0.00013	187.03969	-506.40771	16.37958	64.85197
10-157	-1157.53123	-1156.99554	-1157.51519	-1156.97949	-0.01315	0.00020	187.01861	-506.05243	16.45638	64.85197
10-172	-1157.53098	-1156.99564	-1157.51505	-1156.97972	-0.01318	0.00043	186.87527	-505.07055	16.38297	64.85197
10-190	-1157.53086	-1156.99546	-1157.51491	-1156.97951	-0.01316	0.00050	186.72496	-504.84853	16.46609	64.85197
10-211	-1157.53061	-1156.99592	-1157.51472	-1156.98002	-0.01321	0.00234	186.52169	-502.23313	15.58629	64.85197
10-226	-1157.53052	-1156.99497	-1157.51454	-1156.97899	-0.01310	0.00050	186.33010	-504.39739	16.39889	64.85197
10-236	-1157.53024	-1156.99457	-1157.51447	-1156.97880	-0.01309	0.00019	186.25983	-505.26002	16.37396	64.85197
10-381	-1157.52905	-1156.99359	-1157.51319	-1156.97773	-0.01298	0.00016	184.91457	-504.25643	16.54080	64.85197
10-469	-1157.52781	-1156.99238	-1157.51249	-1156.97705	-0.01291	0.00046	184.17226	-502.56713	16.65017	64.85197
10-494	-1157.52770	-1156.99229	-1157.51224	-1156.97683	-0.01289	0.00013	183.90807	-503.49676	16.53672	64.85197
10-582	-1157.52655	-1156.99104	-1157.51133	-1156.97583	-0.01279	0.00011	182.95743	-502.81522	16.71341	64.85197
11-11	-1273.28980	-1272.70000	-1273.27167	-1272.68187	-0.01356	0.00017	210.94454	-558.57715	16.47085	64.99493
11-21	-1273.28937	-1272.69972	-1273.27117	-1272.68152	-0.01353	0.00012	210.41392	-558.43065	16.48692	64.99493
11-40	-1273.28849	-1272.69870	-1273.27068	-1272.68090	-0.01347	0.00017	209.90425	-557.60719	16.56930	64.99493
11-45	-1273.28863	-1272.69946	-1273.27065	-1272.68147	-0.01352	0.00056	209.86281	-556.36759	16.54800	64.99493
11-52	-1273.28841	-1272.69888	-1273.27048	-1272.68094	-0.01347	0.00013	209.68924	-557.58341	16.51281	64.99493
11-79	-1273.28770	-1272.69812	-1273.26995	-1272.68038	-0.01342	0.00018	209.13553	-556.79659	16.55120	64.99493
11-86	-1273.28792	-1272.69858	-1273.26990	-1272.68056	-0.01344	0.00095	209.08174	-555.12496	16.61211	64.99493
11-141	-1273.28732	-1272.69787	-1273.26939	-1272.67994	-0.01338	0.00017	208.54652	-556.28183	16.60991	64.99493
11-148	-1273.28675	-1272.69768	-1273.26923	-1272.68016	-0.01340	0.00210	208.36970	-553.72792	16.72402	64.99493
11-174	-1273.28680	-1272.69744	-1273.26900	-1272.67965	-0.01335	0.00016	208.13004	-555.91056	16.58765	64.99493
11-223	-1273.28610	-1272.69720	-1273.26857	-1272.67967	-0.01336	0.00347	207.68160	-552.54631	16.73564	64.99493
11-233	-1273.28650	-1272.69731	-1273.26847	-1272.67929	-0.01332	0.00018	207.57749	-555.22843	16.56669	64.99493
11-309	-1273.28554	-1272.69644	-1273.26806	-1272.67896	-0.01329	0.00061	207.14588	-553.82790	16.81719	64.99493
11-345	-1273.28531	-1272.69615	-1273.26775	-1272.67859	-0.01326	0.00042	206.81113	-553.86148	16.79620	64.99493
12-20	-1389.04575	-1388.40222	-1389.02562	-1388.38209	-0.01371	0.00016	232.20628	-608.52411	16.69744	65.12545
12-23	-1389.04538	-1388.40226	-1389.02540	-1388.38228	-0.01373	0.00056	231.97058	-607.05688	16.75690	65.12545
12-108	-1389.04373	-1388.40081	-1389.02390	-1388.38098	-0.01362	0.00036	230.38700	-605.98032	16.82316	65.12545
12-111	-1389.04366	-1388.40055	-1389.02385	-1388.38075	-0.01360	0.00014	230.34355	-606.86223	16.80811	65.12545
12-171	-1389.04286	-1388.39965	-1389.02329	-1388.38008	-0.01355	0.00013	229.75140	-606.38803	16.83997	65.12545
13-7	-1504.80361	-1504.10610	-1504.78111	-1504.08361	-0.01394	0.00011	255.08718	-660.28890	16.84566	65.24551
13-109	-1504.79993	-1504.10277	-1504.77772	-1504.08056	-0.01371	0.00014	251.51786	-656.45469	16.86459	65.24551
14-26	-1620.55818	-1619.80690	-1620.53432	-1619.78304	-0.01399	0.00026	275.56283	-708.43098	17.05970	65.35668
14-34	-1620.55810	-1619.80757	-1620.53389	-1619.78336	-0.01402	0.00054	275.11512	-707.28715	17.09302	65.35668

Table S3 The local minima of the cluster size n=1-13 sorted by the electronic energies (E_0) in Hartree at MP2/6-31+G(d,p). The cluster probabilities and the natural logarithms of the four cluster partition functions were computed at 300 K. Those with a probability lower than 0.0001 were not shown. The cluster indices (*n-i*) cannot be cross-referenced in the other tables. The coordinate files are available on our PyQCE website.[1]

n-i	E_0	E_0+E_{zpe}	E_{bind}	*P(300K)*	$lnq_{i,elec}$	$lnq_{i,vib}$	$lnq_{i,rot}$	$lnq_{i,trans}$
4-1	-461.63091	-461.41156	-0.01203	0.00137	65.17557	-213.02662	13.10492	63.89809
4-2	-461.62918	-461.41004	-0.01165	0.00124	63.35804	-211.99951	13.79324	63.89809
5-1	-577.04327	-576.76914	-0.01297	0.04720	86.34948	-261.98371	14.47388	64.23280
6-1	-692.45497	-692.12559	-0.01341	0.00261	106.82661	-315.57385	14.83917	64.50629
6-2	-692.45483	-692.12604	-0.01348	0.14748	106.67546	-310.52675	13.97795	64.50629
6-3	-692.45471	-692.12540	-0.01338	0.00273	106.54852	-315.28674	14.87394	64.50629
6-4	-692.45432	-692.12534	-0.01337	0.01174	106.13623	-313.41394	14.87391	64.50629
7-1	-807.86676	-807.48246	-0.01378	0.00459	127.39375	-365.80873	15.28974	64.73751
7-2	-807.86598	-807.48174	-0.01368	0.00218	126.57848	-365.75374	15.30442	64.73751
7-3	-807.86591	-807.48184	-0.01369	0.01381	126.50622	-363.85515	15.32521	64.73751
7-4	-807.86591	-807.48184	-0.01369	0.01794	126.50620	-363.59378	15.32561	64.73751
7-5	-807.86548	-807.48162	-0.01366	0.01257	126.04643	-363.56219	15.39784	64.73751
7-6	-807.86530	-807.48163	-0.01366	0.07241	125.85660	-361.59122	15.36803	64.73751
7-7	-807.86364	-807.47988	-0.01341	0.00030	124.11747	-365.31028	15.32451	64.73751
7-8	-807.86172	-807.47828	-0.01318	0.00334	122.09447	-361.04888	15.51096	64.73751
8-1	-923.28056	-922.84101	-0.01427	0.00295	150.08401	-418.33620	14.95333	64.93781
8-2	-923.27857	-922.83879	-0.01399	0.00015	147.98668	-419.92009	15.65103	64.93781
8-3	-923.27663	-922.83729	-0.01380	0.00019	145.94669	-417.76366	15.79139	64.93781
8-4	-923.27653	-922.83781	-0.01387	0.01734	145.84384	-413.15866	15.78866	64.93781
8-5	-923.27642	-922.83777	-0.01386	0.00571	145.73041	-414.11028	15.74266	64.93781
8-6	-923.27336	-922.83489	-0.01350	0.00046	142.50022	-413.46182	15.80933	64.93781
8-7	-923.27330	-922.83547	-0.01358	0.50017	142.44366	-405.32286	14.71500	64.93781
9-2	-1038.69110	-1038.19681	-0.01434	0.00256	169.33729	-468.45315	15.98657	65.11448
9-3	-1038.68807	-1038.19419	-0.01405	0.00111	166.14735	-466.20419	16.09388	65.11448
9-4	-1038.68771	-1038.19413	-0.01405	0.08650	165.77017	-461.59576	16.21564	65.11448
9-5	-1038.68758	-1038.19392	-0.01402	0.00071	165.63222	-466.05920	16.00769	65.11448
10-2	-1154.10390	-1153.55456	-0.01460	0.00044	190.97013	-521.74161	16.22007	65.27252
10-3	-1154.10335	-1153.55379	-0.01452	0.00030	190.38891	-521.59293	16.26542	65.27252
10-4	-1154.10198	-1153.55335	-0.01448	0.00639	188.94794	-516.41738	15.59448	65.27252
10-5	-1154.10137	-1153.55206	-0.01435	0.00039	188.31046	-519.31516	16.33536	65.27252
10-6	-1154.10121	-1153.55205	-0.01435	0.00027	188.13532	-519.51884	16.32951	65.27252
10-7	-1154.09902	-1153.55052	-0.01420	0.02380	185.83523	-512.00391	15.60851	65.27252
10-8	-1154.09533	-1153.54604	-0.01375	0.00016	181.95415	-514.22145	16.71888	65.27252
11-2	-1269.51581	-1268.91091	-0.01468	0.00014	211.67415	-573.54813	16.52762	65.41549

11-3	-1269.51502	-1268.91057	-0.01465	0.00012	210.83783	-572.88997	16.55478	65.41549
12-1	-1384.92735	-1384.26833	-0.01484	0.00013	231.97810	-623.79990	16.76402	65.54601
12-2	-1384.92690	-1384.26803	-0.01481	0.00060	231.50079	-621.77149	16.78409	65.54601
12-3	-1384.92411	-1384.26507	-0.01457	0.00034	228.57043	-619.54753	16.92890	65.54601
12-4	-1384.92271	-1384.26436	-0.01451	0.00072	227.08921	-617.29113	16.88846	65.54601
13-1	-1500.34241	-1499.62809	-0.01515	0.00443	255.99107	-673.95140	16.87308	65.66607
13-4	-1500.33714	-1499.62275	-0.01474	0.00011	250.44532	-672.35261	17.11335	65.66607
13-5	-1500.33203	-1499.61814	-0.01438	0.00169	245.06570	-664.49976	17.38482	65.66607

Table S4 The local minima of the cluster size n=1-9 sorted by counterpoise corrected energies (E_0+E_{cp}) in Hartree using MP2/6-311++G(d,p) single-point calculations level of theory. The E_{zpe} was obtained from the frequency calculations of MP2/6-31+G(d, p). The optimized structures were taken from **Table S3**. The cluster probabilities and the natural logarithms of the four cluster partition functions were computed at 300 K. Those with a probability lower than 0.0001 were not shown (e.g., $n > 9$). The cluster indices (n-i) correspond to those in **Table 2** and cannot be cross-referenced in **Table S1 – S3** and **S5**. The coordinate files are available on our PyQCE website.[1]

n-i	E_0	E_0+E_{zpe}	E_0+E_{cp}	E_0+E_{cp}+E_{zpe}	E_{bind}	P(300K)	$lnq_{i,elec}$	$lnq_{i,vib}$	$lnq_{i,rot}$	$lnq_{i,trans}$
1-1 (1-I)	-115.44509	-115.39243	-115.44509	-115.39243	0.00000	0.00268	5.85370	-55.17512	8.07103	60.32768
2-1 (2-I)	-230.90102	-230.79338	-230.89791	-230.79026	-0.00271	0.00044	19.84389	-105.82238	11.45460	61.36740
3-1 (3-I)	-346.36540	-346.20172	-346.35834	-346.19466	-0.00579	0.00038	41.84628	-160.25264	13.00939	61.97560
3-2 (3-II)	-346.36406	-346.20075	-346.35716	-346.19385	-0.00552	0.00076	40.60175	-157.21033	11.90907	61.97560
4-1 (4-I)	-461.83465	-461.61530	-461.82058	-461.60122	-0.00788	0.00201	65.74551	-213.02662	13.10492	62.40712
4-2 (4-II)	-461.83304	-461.61390	-461.81935	-461.60021	-0.00763	0.00306	64.45119	-211.99951	13.79324	62.40712
5-1 (5-I)	-577.29851	-577.02438	-577.27887	-577.00474	-0.00852	0.02314	85.49504	-261.98371	14.47388	62.74184
6-1 (6-I)	-692.76159	-692.43280	-692.73729	-692.40850	-0.00899	0.06450	105.37906	-310.52675	13.97795	63.01532
6-2 (6-II)	-692.76094	-692.43196	-692.73558	-692.40660	-0.00867	0.00145	103.57834	-313.41394	14.87391	63.01532
6-3 (6-III)	-692.76119	-692.43188	-692.73549	-692.40618	-0.00860	0.00020	103.48522	-315.28674	14.87394	63.01532
6-4 (6-IV)	-692.76132	-692.43193	-692.73544	-692.40606	-0.00858	0.00014	103.43790	-315.57385	14.83917	63.01532
7-1 (7-I)	-808.22331	-807.83964	-808.19320	-807.80953	-0.00893	0.00633	122.62207	-361.59122	15.36803	63.24655
7-2 (7-II)	-808.22346	-807.83938	-808.19314	-807.80907	-0.00887	0.00077	122.56415	-363.59378	15.32561	63.24655
7-4 (7-IV)	-808.22345	-807.83937	-808.19313	-807.80906	-0.00887	0.00059	122.55751	-363.85515	15.32521	63.24655
7-5 (7-V)	-808.22363	-807.83977	-808.19267	-807.80881	-0.00883	0.00052	122.06858	-363.56219	15.39784	63.24655
7-8 (7-VIII)	-808.21949	-807.83604	-808.19089	-807.80745	-0.00864	0.00111	120.19583	-361.04888	15.51096	63.24655
8-1 (8-I)	-923.68926	-923.24971	-923.65185	-923.21230	-0.00911	0.00001	142.75280	-418.33620	14.95333	63.44685
8-2 (8-II)	-923.68285	-923.24502	-923.65103	-923.21320	-0.00922	0.88913	141.89406	-405.32286	14.71500	63.44685
8-4 (8-IV)	-923.68601	-923.24735	-923.64963	-923.21098	-0.00895	0.00009	140.42149	-414.11028	15.74266	63.44685
8-5 (8-V)	-923.68593	-923.24721	-923.64958	-923.21085	-0.00893	0.00022	140.35883	-413.15866	15.78866	63.44685
9-2 (9-II)	-1039.14822	-1038.65464	-1039.10781	-1038.614227	-0.00915	0.00121	160.04808	-461.59576	16.21564	63.62352

Table S5 The local minima of the cluster size n=1-9 sorted by the electronic energies at MP2/6-31+G(d,p). The cluster probabilities and the natural logarithms of the four cluster partition functions were computed at 340 K. High probability clusters were marked by *, which were mainly contributed by electronic and vibrational partition functions. Those with a probability lower than 0.0001 were not shown.

n-i	*P (340 K)*	$lnq_{i,elec}$	$lnq_{i,vib}$	$lnq_{i,rot}$	$lnq_{i,trans}$
1-1*	0.40083	1.18256	-48.58148	8.25878	62.00639
2-1	0.01034	12.83757	-91.78983	11.64234	63.04611
3-1	0.00323	33.28117	-138.74499	13.19716	63.65431
3-2	0.00321	33.28112	-138.75140	13.19670	63.65431
3-3	0.00321	33.28098	-138.75053	13.19714	63.65431
3-4	0.00518	31.83661	-135.72787	12.09681	63.65431
3-5	0.00033	28.89629	-136.64184	13.20800	63.65431
4-1	0.03913	57.50786	-184.07133	13.29267	64.08583
4-2	0.04306	55.90416	-183.06017	13.98098	64.08583
5-1*	0.24583	76.19072	-225.62260	14.66162	64.42055
5-3	0.00014	71.94166	-228.67316	14.50418	64.42055
5-5	0.00046	71.42903	-227.05888	14.56907	64.42055
5-6	0.00051	71.05300	-226.57265	14.56834	64.42055
5-8	0.00013	68.74383	-225.63216	14.55341	64.42055
6-1	0.00271	94.25877	-271.79798	15.02691	64.69403
6-2*	0.15502	94.12541	-266.75767	14.16569	64.69403
6-3	0.00292	94.01340	-271.51450	15.06169	64.69403
6-4	0.01307	93.64961	-269.65145	15.06166	64.69403
7-1	0.00094	112.40625	-314.61871	15.47749	64.92526
7-2	0.00049	111.68689	-314.56590	15.49216	64.92526
7-3	0.00312	111.62313	-312.67397	15.51296	64.92526
7-4	0.00405	111.62311	-312.41242	15.51335	64.92526
7-5	0.00296	111.21744	-312.39323	15.58559	64.92526
7-6	0.01746	111.04994	-310.42046	15.55578	64.92526
7-8	0.00124	107.73042	-309.88788	15.69871	64.92526
8-4	0.00088	128.68574	-354.57760	15.97640	65.12555
8-5	0.00029	128.58565	-355.53972	15.93041	65.12555
8-7	0.03759	125.68558	-346.74974	14.90274	65.12555
9-4	0.00094	146.26779	-395.59464	16.40338	65.30223

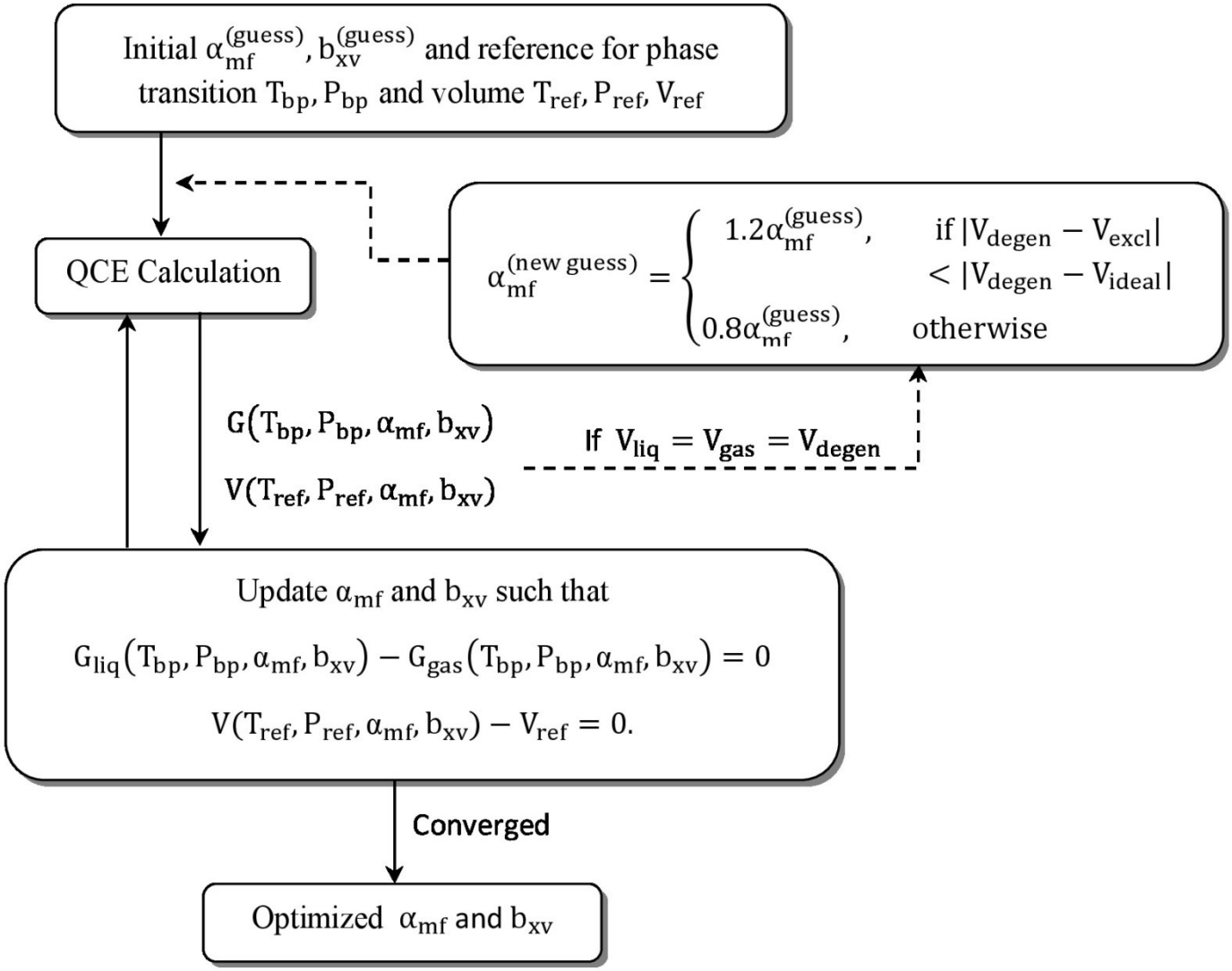

Figure S1 Parameter optimization implemented in PyQCE. For a pair of initial $\alpha_{mf}^{(guess)}$ and $b_{xv}^{(guess)}$, two QCE calculation (readers can refer to the multi-component systems section in Weinhold's original work for the setup[2]) was performed. One at the boiling point (T_{bp},P_{bp}) to determine the Gibbs free energy for the gas (G_{gas}) and the liquid phase (G_{liq}), another at a referenced condition (T_{ref},P_{ref}) to obtain the volume $V \in \{V_{gas},V_{liq}\}$ with respect to the referenced phase. The algorithm then checked whether the volume is degenerate and restarted the iteration with a new guess for the parameters if so (see the "**Parameter optimization in PyQCE"** section below). The optimizing cycle repeats until the parameters converge. The convergence criterion is 1E-5 for the population $\{N_i\}$, the Gibbs free energy G and the volume V. For parameter fitting, we set a strict constraint of 1E-10 for the convergence of α_{mf} and b_{xv}. Here, the convergence criterion for a property x is defined as $|x_k - x_{k+1}|/x_{k+1}$ in which the index k refers to the number of iteration.

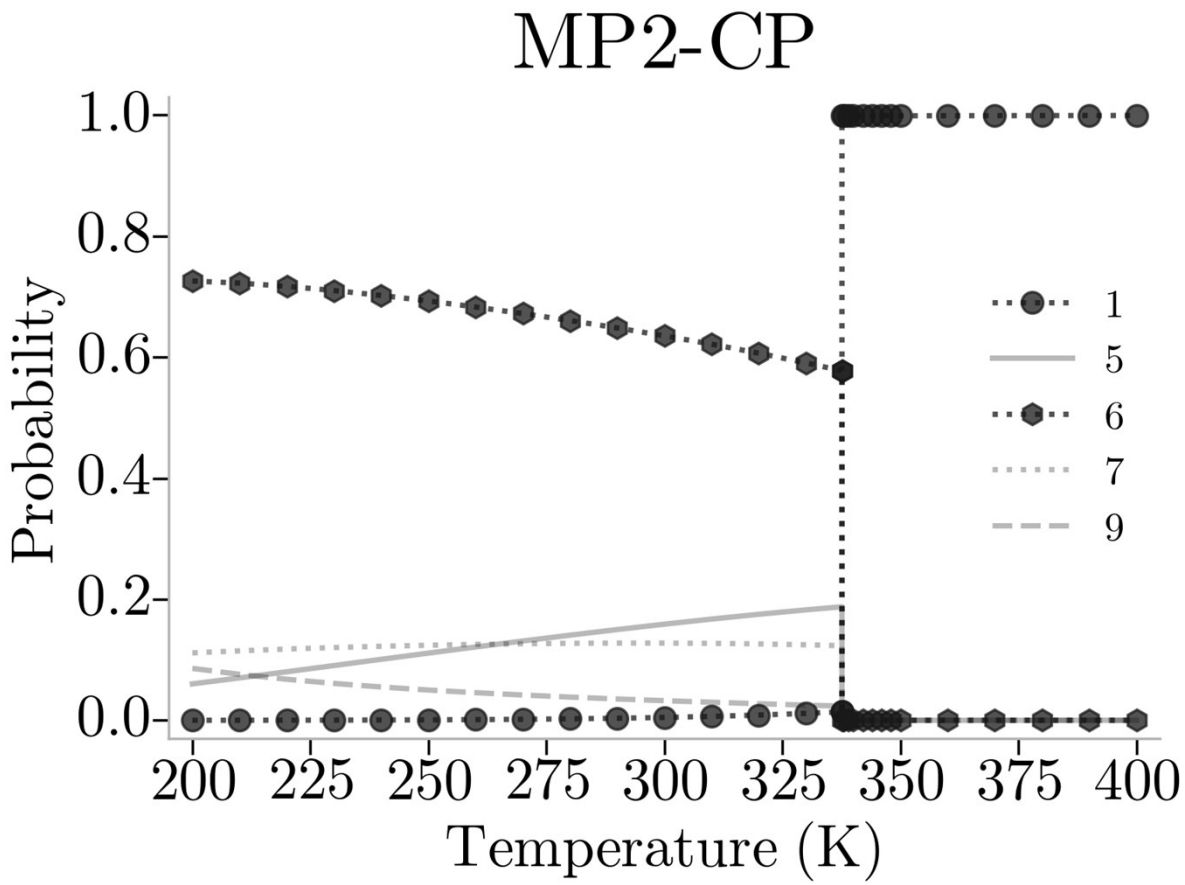

Figure S2 Temperature-dependent cluster probabilities at MP2-CP/6-311++G(d,p). Here, we manually removed the **8-II** structures in **Table 2** and plotted the cluster sizes with the maximal probability greater than 0.1. Without **8-II**, the cluster probability of the QCE model shows that cyclic hexamer (**6-I**) contributes more than 60% to the overall probability. The plot is nearly identical to the cluster probability done by Matisz, Kunsági-Máté, *et al.* [see **Fig.** 3 in *Ref.* 4 (constant $^{\alpha_{mf}}$ and $^{b_{xv}}$)].

Parameter optimization in PyQCE[1]

Eq. 15 implies a trivial minimum solution $V_{liquid} = V_{gas} = V_{deg}$ (deg stands for degenerate) that is unphysical. Such degeneracy is related to the parameters α_{mf} via the volume polynomial in Eq. 13. From Descartes' rule of sign, the polynomial can have either three positive real roots or one positive real root with two imaginary roots, and the degenerate case refers to the latter. At two limits of α_{mf}, only a single real positive degenerate root is obtained: (i) $\alpha_{mf} \ll 1$, $V_{deg} = k_B T \sum_i N_i / P + V_{excl} \approx V_{ideal}$ where V_{ideal} is the ideal gas volume at a given T and P; (ii) $1/(\alpha_{mf} N_A) \ll 1$, $V_{deg} = V_{excl}$. These limits of α_{mf} represent a bounded region in which the solutions are nondegenerate. The degeneracies are problematic for optimization as they solve Eq. 15 exactly but not Eq. 16, leading to further minimization iteration remained stuck in the vicinity of the local minima.

Therefore, during the optimization of parameters, once the degeneracy occurs (i.e., $V_{liquid} = V_{gas} = V_{deg}$), we restart the minimization with a new guess of α_{mf} determined by

$$\alpha_{mf}^{(new\ guess)} = \begin{cases} 1.2\alpha_{mf}^{(guess)} & , if\ |V_{deg} - V_{excl}| < |V_{deg} - V_{ideal}| \\ 0.8\alpha_{mf}^{(guess)} & , otherwise \end{cases} \quad (1)$$

The value of $b_{xv}^{(guess)}$ at each new iteration are chosen to be 1 due to its weak effect on condensed-phase cluster populations.[2] This modification attempts to lift the degeneracy by scaling the parameter α_{mf} in the opposite direction of the aforementioned limits. The minimization procedure uses the Powell's hybrid method.[3]

To compare with Fig. 3 in Ref. 4, we adopted *model 1* (constant α_{mf} and b_{xv}) proposed by Matisz, Kunsági-Máté, *et al.*, which assumed both parameters are independent with temperature and pressure. The different values of α_{mf} for the four datasets represent the amount of correction needed in the intermolecular interaction to fit the experimental data.

References

1. Teh Soon and Po-Jen Hsu. PyQCE, http://140.109.113.226:30000/gristlegrime/qce_si. 2020.
2. F. Weinhold. Quantum cluster equilibrium theory of liquids: General theory and computer implementation. *Journal of Chemical Physics*, 1998.
3. M. J. D. Powell "An efficient method for finding the minimum of a function of several variables without calculating derivatives". *Computer Journal*. 7 (2): 155–162, 1964.
4. G. Matisz, Walter M F Fabian, A. M. Kelterer, and S. Kunsági-Máté. Weinhold's QCE model - A modified parameter fit. Model study of liquid methanol based on MP2 cluster geometries. Journal of Molecular Structure: *THEOCHEM*, 956(1-3):103–109, 2010.