Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information:

Differentiating the role of organic additives to assemble open framework aluminosilicates using INS spectroscopy

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The Gaussian calculated Infrared spectra and vibrational modes for 18-crown-6 ether (18C6) in the C_i and D_{3d} conformations is present herein. Also included are the simulated INS spectra using the AbINS algorithm, the experimental INS spectra from the 0-700 cm^{-1} wavenumber range, and the xyz coordinates of the molecular clusters used for Gaussian calculation.

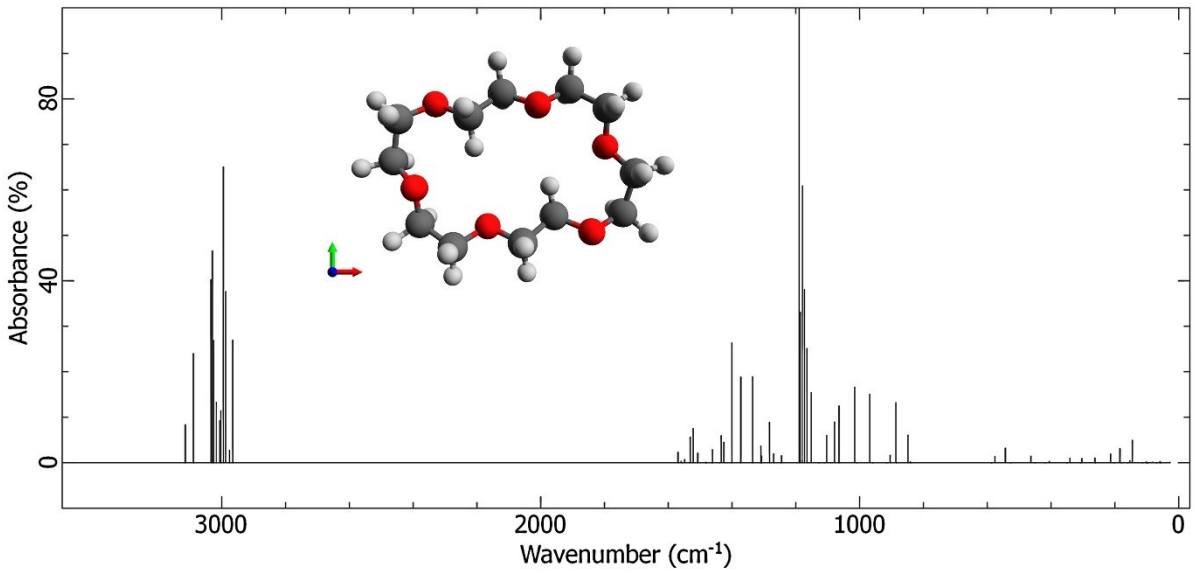

Figure S1. Gasussian calculated Infrared spectrum for the isolated 18C6 molecule in the C_i conformation. Included is the molecular structure used.

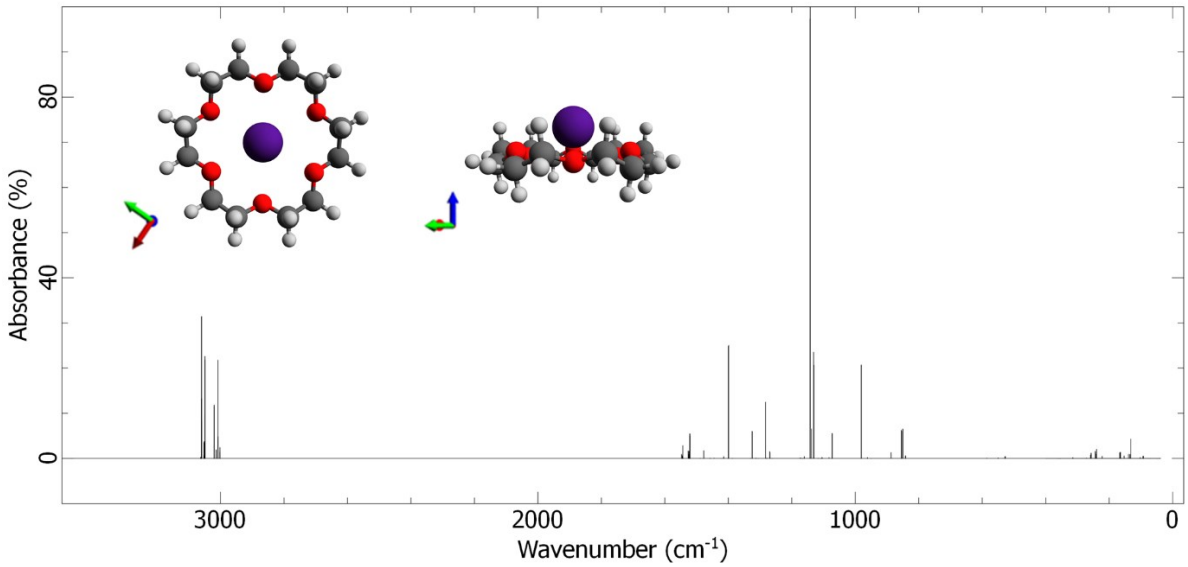

Figure S2. Gaussian calculated Infrared spectrum for the Cs^+-18C6 complex. Here the 18C6 oxyethylene chain is in the D_{3d} conformation. Included is the molecular structure used, viewing perpendicular and along the plane of the 18C6 molecule.

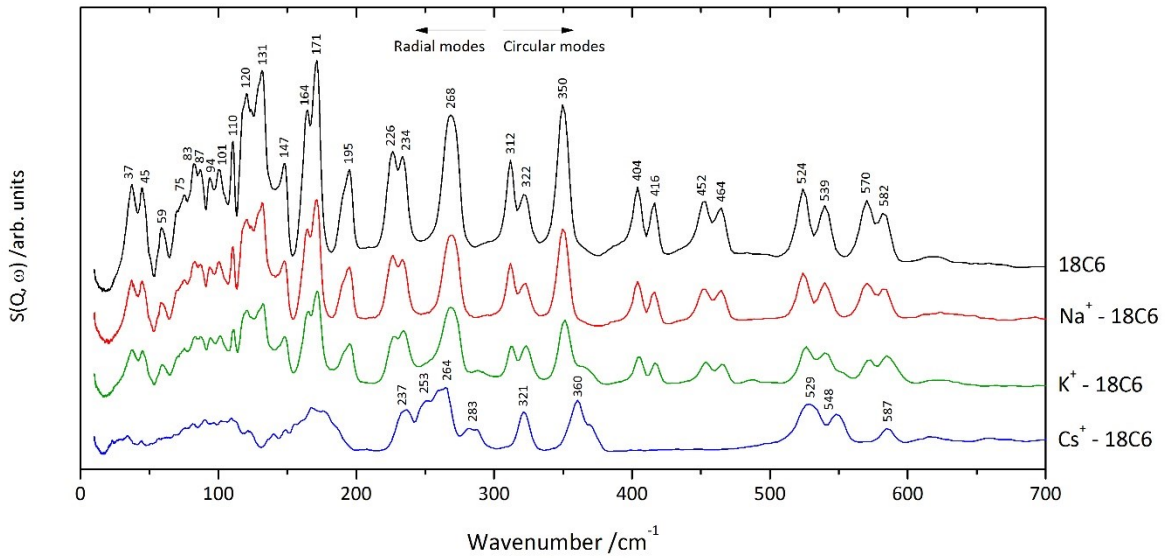

Figure S3. INS spectra of 18C6 and the metal cation-crown complexes in the 0-700 cm^{-1} region of skeletal vibrations. The spectrum in black corresponds to the isolated 18C6, red to the Na^+ complex, green to the K^+ complex and blue to the Cs^+ complex. The spectra have been normalised to the mass of samples loaded onto the spectrometer.

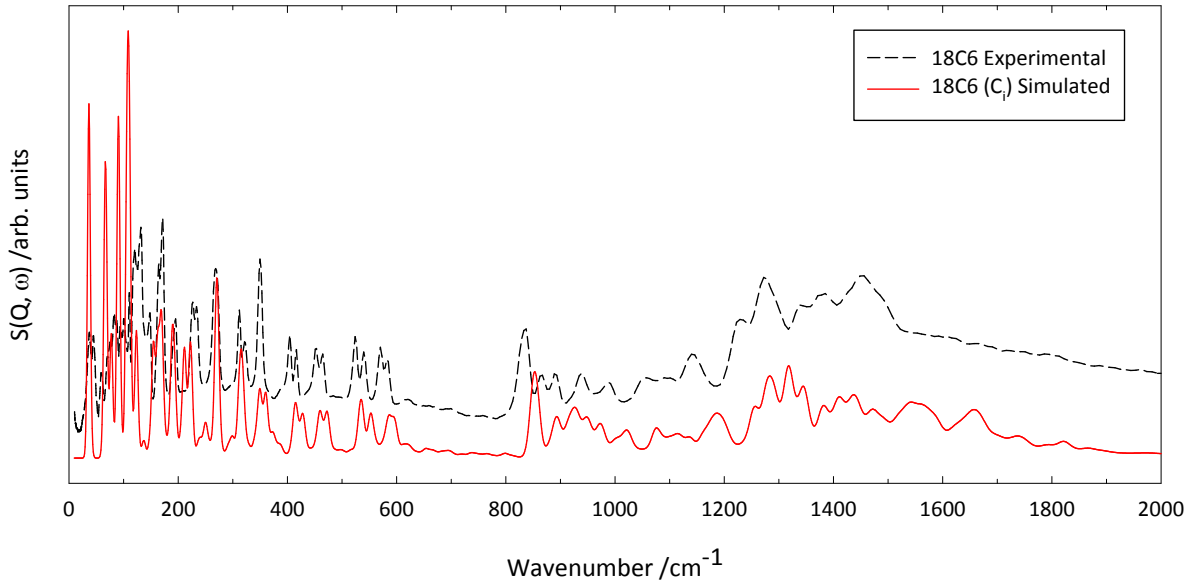

Figure S4. The experimental INS spectra of 18C6 (black, dashed) alongside the simulated INS spectra of 18C6 in the C_i conformation (red, solid), covering the 0-2000 cm^{-1} region. The simulated spectrum was calculated using the AbINS algorithm on the Gaussian output data.

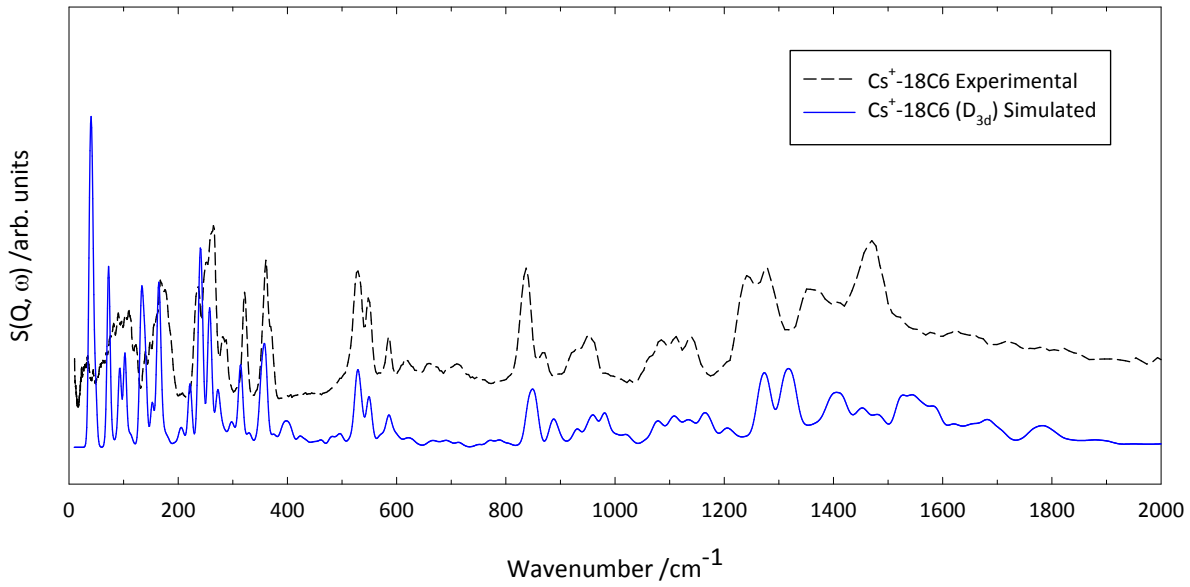

Figure S5. The experimental INS spectra of the Cs^+-18C6 complex (black, dashed) alongside the simulated INS spectra of the complex where 18C6 is in the D_{3d} conformation (blue, solid), covering the 0-2000 cm^{-1} region. The simulated spectrum was calculated using the AbINS algorithm on the Gaussian output data.

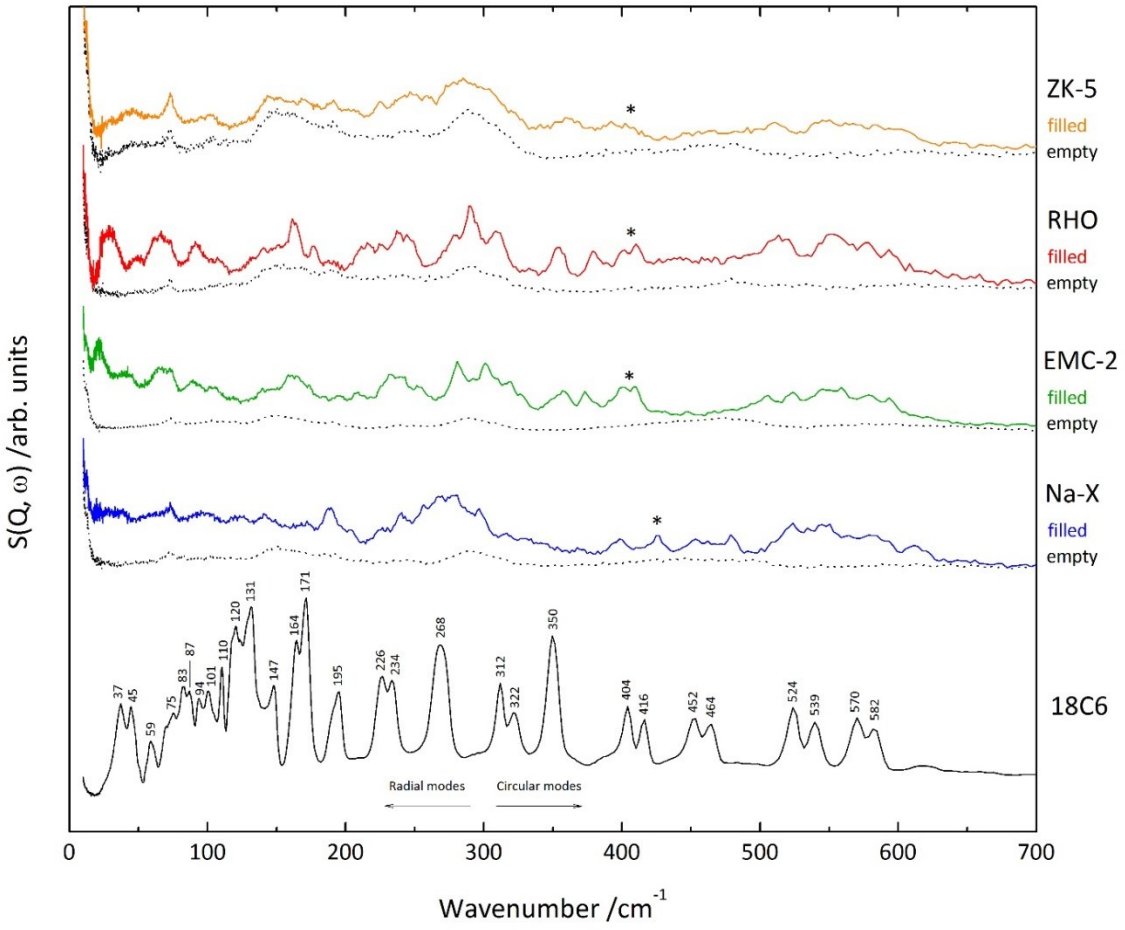

Figure S6. INS spectra of 18C6 and the filled zeolite samples in the 0-700 cm^{-1} region. The spectrum in black corresponds to the isolated 18C6, orange to zeolite ZK-5, red to RHO, green to EMC-2 and blue to Na-X. The block dotted spectra correspond to the empty zeolites as labelled. The spectra have been normalised to the mass of samples loaded onto the spectrometer, and the mass% content of 18C6.

Table S1. Gaussian calculated vibrational modes (ν_{calc}) for the isolated 18C6 molecule in the C_i conformation. Included is the estimated Infrared active intensity of each vibrational mode.

ν_{calc} /cm^{-1}	Intensity /km mol^{-1}	ν_{calc} /cm^{-1}	Intensity /km mol^{-1}	ν_{calc} /cm^{-1}	Intensity /km mol^{-1}
27.7726	0.0881464	1010.21	0	1461.47	2.87187
56.2379	0	1015.64	16.5789	1463.34	0
58.4867	0.289907	1064.85	12.473	1481.76	0
68.312	0	1066.81	0	1483.06	0.127265
81.5726	0.141634	1078.71	8.96519	1507.44	0
97.8484	0	1090.58	0	1507.5	2.13746
101.213	0	1103.37	5.98558	1522.03	0
101.958	0.212265	1111.16	0	1522.11	7.49695
114.24	0	1129	0	1531.3	5.66904
145.041	4.93471	1151.96	15.4399	1531.58	0
153.031	0.492609	1161.13	0	1548.34	0
160.257	0	1165.12	25.1638	1548.6	0.752242
179.894	0	1171.81	0	1557.43	0
184.239	3.12444	1172.95	38.101	1559.69	0.413059
202.91	0	1179.34	60.8852	1569.32	0
213.21	1.90325	1179.77	0	1569.53	2.295
261.867	0	1185.65	33.1532	2965.4	26.9405
262.635	1.04497	1188.78	0	2965.52	0
303.578	0.953136	1189.65	100	2975.34	0
308.12	0	1196.52	0	2975.35	2.81345
340.741	1.0177	1244.88	1.54734	2987.79	0
351.313	0	1246.1	0	2987.83	37.6516
405.6	0.302046	1268.75	0	2994.79	65.0156
419.486	0	1269.72	1.99276	2995.77	0
450.336	0	1282.66	8.88482	3002.59	11.4984
463.279	1.44015	1282.93	0	3002.63	0
526.535	0	1307.52	1.5251	3006.59	9.29243
543.194	3.20397	1308.6	0	3006.83	0
576.118	1.35532	1309.75	3.65463	3017.1	13.3609
587.663	0	1310.09	0	3017.13	0
840.033	0	1335.64	18.8976	3025.02	0
841.35	0.239467	1336.23	0	3025.11	26.9516
848.518	6.07323	1372.68	18.8389	3028.38	0
848.799	0	1373.78	0	3029.26	46.5745
883.633	0	1400.72	26.3343	3033.67	0
886.498	13.1839	1401.25	0	3033.86	40.2643
904.442	1.6535	1420.21	0	3088.72	23.9999
915.563	0	1425.73	4.54494	3088.82	0
960.889	0	1434.32	5.94621	3114.19	8.35738
968.599	15.0503	1438.7	0	3115.21	0

Table S2. Gaussian calculated vibrational modes (ν_{calc}) for the Cs^+-18C6 complex, with the 18C6 oxyethylene chain in the D_{3d} conformation. Included is the estimated Infrared active intensity of each vibrational mode.

ν_{calc} /cm^{-1}	Intensity /km mol^{-1}	ν_{calc} /cm^{-1}	Intensity /km mol^{-1}	ν_{calc} /cm^{-1}	Intensity /km mol^{-1}
38.5255	0.0172226	961.453	0.158282	1456.68	0.0298256
42.7182	0.0176058	961.59	0.161518	1456.87	0.0302514
48.4983	0.00404487	980.785	20.6042	1477.56	1.69476
72.2435	0.00444936	981.091	20.7023	1477.73	1.65812
92.0192	0.497051	1072.75	5.505	1488.01	0.0294211
93.0888	0.459625	1073.14	5.44684	1520.46	0.00877098
102.746	0.192323	1082.54	0.196645	1521.21	5.44991
102.874	0.218827	1104.59	0.154642	1521.46	4.98564
131.585	4.27928	1104.72	0.217295	1523.74	1.57141
134.469	0.889701	1108.67	0.00155408	1524.17	0.854979
139.091	0.935323	1116.56	0.0253762	1526.56	1.63106
152.783	0.561172	1130.16	20.6735	1542.5	0.0024695
162.321	0.00308687	1131.19	23.5181	1542.64	0.0799607
164.422	1.36069	1138.22	6.52669	1543.31	2.82291
166.453	1.22536	1141.83	100	1544.78	0.48581
221.675	0.466118	1142.72	97.316	1545.11	0.553253
239.435	2.00689	1160.37	0.397547	1546.87	0.881845
240.255	0.969725	1160.75	0.0897109	3001.45	1.14568
243.315	1.53784	1164.96	0.0161156	3001.84	1.42405
256.683	1.15145	1166.07	0.00217146	3001.94	2.40261
258.316	0.73293	1171.24	0.0984606	3008.06	4.79432
272.025	0.0772357	1174.93	0.0714665	3008.22	4.09943
314.054	0.154727	1262.02	0.00232048	3008.64	21.7413
314.499	0.138271	1268.46	1.25123	3014.03	1.65999
352.847	0.00180955	1269.15	1.51761	3014.16	1.90603
359.091	0.00087284	1278.86	0.0233964	3014.27	1.90324
359.847	0.00185212	1279.04	0.0400016	3020.2	11.8026
527.171	0.393161	1282.84	12.4767	3020.29	11.5068
527.945	0.379834	1305.09	0.00344878	3020.71	3.25169
534.307	0.000723819	1312.62	0.0420028	3048.64	21.7681
549.115	0.0978007	1312.73	0.0678048	3049.04	22.5857
549.419	0.105401	1324.29	5.92122	3049.53	9.61936
585.365	0.0500074	1325.1	6.00037	3051.6	3.71483
841.588	0.583334	1330	0.0248227	3051.87	3.45132
841.782	0.546121	1387.43	0.0292934	3052.46	0.635534
850.044	6.52242	1398.87	25.0199	3059.79	31.3951
854.015	6.03684	1399.47	24.8315	3059.8	8.33905
854.772	6.2123	1414.13	0.375981	3059.96	13.1647
886.863	1.28606	1414.87	0.189002	3062.86	0.247716
931.009	0.00100057	1421.88	0.00421518	3062.96	0.17493
950.304	0.00251208	1444.76	0.0609924	3063.16	0.0459199

Table S3. The xyz coordinates of the 18C6 cluster from the .PDB file used as input for Gaussian and the AbINS algorithm to calculate the vibrational modes and INS spectra respectively.

	x	y	z		x	y	z
C	-3.87196	1.60806	0.26932	H	5.21786	0.05111	0.05811
C	-4.16536	0.21212	-0.26904	H	4.03115	-0.21417	1.36251
C	3.23699	1.98523	0.27575	C	3.87196	-1.60806	-0.26932
C	2.01105	2.71903	-0.23477	C	-2.01105	-2.71903	0.23477
C	-0.3557	2.57385	-0.25321	H	-4.14329	-2.57122	-0.04472
C	-1.4768	1.71954	0.32097	H	-3.16846	-1.88495	-1.37033
H	-4.03115	0.21417	-1.36251	O	2.69298	-2.19276	0.25059
H	3.16846	1.88495	1.37033	O	-0.86053	-2.08415	-0.28328
H	2.05533	3.77465	0.08492	H	-2.00537	-2.70048	1.33651
H	-0.50744	3.63374	0.00917	H	-2.05533	-3.77465	-0.08492
H	-1.30182	0.66497	0.0862	C	1.4768	-1.71954	-0.32097
H	-5.21786	-0.05111	-0.05811	C	0.3557	-2.57385	0.25321
H	4.14329	2.57122	0.04472	H	1.30182	-0.66497	-0.0862
H	2.00537	2.70048	-1.33651	H	1.50133	-1.82211	-1.41769
H	-0.35832	2.49836	-1.35227	H	0.35832	-2.49836	1.35227
H	-1.50133	1.82211	1.41769	H	0.50744	-3.63374	-0.00917
O	-2.69298	2.19276	-0.25059	H	-3.84063	1.57188	1.37026
O	3.28531	0.71364	-0.34086	H	-4.69123	2.27355	-0.02763
O	0.86053	2.08415	0.28328	H	3.84063	-1.57188	-1.37026
O	-3.28531	-0.71364	0.34086	H	4.69123	-2.27355	0.02763
C	4.16536	-0.21212	0.26904				
C	-3.23699	-1.98523	-0.27575				

Table S4. The xyz coordinates of the Na^+-18C6 complex cluster from the .PDB file used as input for Gaussian and the AbINS algorithm to calculate the vibrational modes and INS spectra respectively.

	x	y	z		x	y	z
C	-1.76048	2.68757	-0.62925	H	-0.37315	3.78295	0.59343
C	-0.41835	3.35263	-0.41781	H	3.89182	2.11505	-0.07275
C	1.89225	2.86577	-0.21507	H	4.3523	-0.10449	1.00679
C	2.89931	1.74929	-0.37197	H	2.57048	-1.29156	2.24897
C	3.43438	-0.40768	0.4824	H	2.17482	-3.58264	-0.43877
C	2.78568	-1.57257	1.214	H	-0.29076	-3.58794	-0.19893
C	1.59878	-2.65704	-0.57939	H	-2.21778	-2.77108	-1.91338
C	0.1839	-2.9979	-0.9922	H	-2.2807	-3.04075	0.55878
C	-1.94501	-1.91901	-1.27435	H	-3.88438	1.82308	0.79144
C	-2.56789	-2.08317	0.11195	H	-0.28492	4.16481	-1.14693
C	-3.08844	-0.08689	1.40636	Na	0.06459	0.05835	0.27868
C	-3.17436	1.06819	0.42248	O	-1.86734	1.6238	0.31362
H	-1.8489	2.29485	-1.65352	O	0.60322	2.3699	-0.56967
H	2.95288	1.42031	-1.42071	O	2.49295	0.66195	0.45555
H	3.71301	-0.68487	-0.54512	O	1.52437	-1.92676	0.64525
H	3.46496	-2.43618	1.22466	O	-0.52412	-1.77302	-1.20819
H	2.08364	-2.06318	-1.36695	O	-2.12139	-1.05789	1.00488
H	0.19442	-3.59385	-1.91528	H	2.17506	3.70706	-0.86423
H	-2.30834	-1.00649	-1.75602	H	1.87971	3.22087	0.82613
H	-3.66185	-2.07849	0.02133	H	-4.0757	-0.54806	1.53798
H	-3.52598	0.72683	-0.56353	H	-2.75329	0.28552	2.37938
H	-2.55796	3.42734	-0.47255				

Table S5. The xyz coordinates of the K^+-18C6 complex cluster from the .PDB file used as input for Gaussian and the AbINS algorithm to calculate the vibrational modes and INS spectra respectively.

	x	y	z		x	y	z
C	2.684	-2.464	0.303	H	-3.469	-1.025	1.402
C	1.569	-3.289	-0.302	H	-4.608	0.699	-0.002
C	-0.792	-3.557	-0.303	H	4.608	-0.699	0.002
C	-2.064	-3.003	0.302	H	3.612	-0.221	1.401
C	-3.477	-1.093	0.303	H	-3.651	2.897	-0.004
C	-3.633	0.286	-0.302	H	-2.621	2.492	-1.402
C	3.633	-0.286	0.302	H	3.469	1.025	-1.402
C	-2.684	2.464	-0.303	H	4.334	1.713	-0.004
C	3.477	1.093	-0.303	H	2.909	3.641	-0.002
C	2.064	3.003	-0.302	H	1.997	3.017	-1.401
C	0.792	3.557	0.303	H	0.847	3.516	1.402
C	-1.569	3.289	0.302	H	0.683	4.609	0.004
H	3.651	-2.897	0.004	H	-1.614	3.239	1.401
H	1.614	-3.239	-1.401	H	-1.698	4.34	0.002
H	-0.847	-3.516	-1.402	K	0	0	0
H	-2.909	-3.641	0.002	O	2.577	-1.122	-0.163
H	-4.334	-1.713	0.004	O	0.317	-2.792	0.163
H	-3.612	0.221	-1.401	O	-2.261	-1.67	-0.163
H	2.621	-2.492	1.402	O	-2.577	1.122	0.163
H	1.698	-4.34	-0.002	O	2.261	1.67	0.163
H	-0.683	-4.609	-0.004	O	-0.317	2.792	-0.163
H	-1.997	-3.017	1.401				

Table S6. The xyz coordinates of the Cs^+-18C6 complex cluster from the .PDB file used as input for Gaussian and the AbINS algorithm to calculate the vibrational modes and INS spectra respectively.

	x	y	z		x	y	z
C	-1.67182	-3.26146	-0.04265	H	3.71965	0.11166	1.06711
C	-2.75526	-2.38456	-0.63929	H	-0.59423	4.65181	-0.47283
C	0.69161	-3.59859	-0.05085	H	-0.7007	3.40863	-1.74728
C	1.97433	-3.05629	-0.65092	H	3.73559	2.77595	-0.38751
C	-3.64338	-0.18078	-0.62486	H	2.75381	2.48847	1.07
C	-3.45925	1.19923	-0.02364	H	1.87404	4.30099	-0.44129
C	3.44505	-1.19045	-0.63671	H	1.64487	3.08708	-1.72788
C	3.66068	0.18305	-0.03096	O	-0.39622	-2.76196	-0.43263
C	-1.99159	3.08224	-0.05754	O	-2.69939	-1.0851	-0.05727
C	-0.68854	3.57133	-0.65943	O	2.28729	-1.79474	-0.0663
C	2.76696	2.39786	-0.02822	O	-2.19795	1.72266	-0.42807
C	1.66308	3.23906	-0.63861	O	2.59162	1.03989	-0.4202
Cs	0.00213	0.00057	0.82687	O	0.40702	2.87326	-0.07359
H	-2.61586	-2.31673	-1.72833	H	4.33301	-1.81	-0.43976
H	-1.80786	-4.28838	-0.4129	H	3.32392	-1.09697	-1.72601
H	0.53464	-4.62111	-0.42517	H	-2.81117	3.7092	-0.43922
H	-1.75941	-3.28155	1.05566	H	-1.96844	3.18596	1.03933
H	-3.73499	-2.84647	-0.44446	H	-4.27292	1.84842	-0.37954
H	0.77498	-3.64799	1.04684	H	-3.52101	1.148	1.07544
H	-3.5071	-0.12773	-1.71509	H	2.7868	-3.77424	-0.46223
H	-4.66876	-0.52458	-0.42103	H	1.85447	-2.94835	-1.73907
H	4.61921	0.58087	-0.39611				