

Supplementary Information

C₂₀ and Nitrogen-Substituted Fullerenes: Anharmonic IR and UV–Vis Spectra for Astrophysical Environments

Venkata Lakshmi Karri¹, Ajay Chaudhari², Takashi Onaka³, Mahadevappa Naganathappa^{1*}

Table S1. Average bond length (in Å) of CC for C₂₀ fullerene, CC & CN for C₁₂N₈, and CC, CN, & NN for N₁₀C₁₀ fullerene

States	Type	C ₂₀	C ₁₂ N ₈		N ₁₀ C ₁₀		
		CC	CC	CN	CC	CN	NN
Neutral In Gas Phase	Harmonic	1.451	1.329	1.481	1.374	1.486	1.49
	Anharmonic	1.451	1.329	1.481	1.374	1.486	1.49
Neutral In Solvent	Harmonic	1.451	1.329	1.481	1.373	1.485	1.486
	Anharmonic	1.451	1.329	1.481	1.373	1.485	1.486
Cation In Gas Phase	Harmonic	1.447	1.34	1.46	1.379	1.477	1.48
	Anharmonic	1.456	1.34	1.46	1.379	1.477	1.48
Anion In Gas Phase	Harmonic	1.456	1.355	1.459	1.387	1.477	1.48
	Anharmonic	1.456	1.355	1.459	1.387	1.477	1.48

Table S2. Cartesian coordinates (in Å) for C₂₀ fullerene and its nitrogen-substituted heterofullerenes N₁₀C₁₀ and C₁₂N₈ molecules optimized at B3LYP/6-311++G (d, p) level of theory in the neutral and ionic charge states in the gas phase, and water solvent states.

C ₂₀ Carti Coord	Neutral			Solvent		
	X	Y	Z	X	Y	Z
C ₁	1.186582	-0.412221	1.658415	1.186289	-0.411394	1.657246
C ₂	0.057343	-1.24307	1.658614	0.056214	-1.242764	1.657941
C ₃	-1.179827	1.671499	0.377787	-1.179468	1.670361	0.377799
C ₄	-1.094351	-0.363424	1.606323	-1.095777	-0.364261	1.606604
C ₅	1.101064	1.596313	0.386988	1.102578	1.597187	0.386577
C ₆	-0.696073	1.025371	1.662972	-0.696064	1.024835	1.662294
C ₇	1.838308	-0.629282	0.382983	1.839007	-0.628266	0.382463
C ₈	0.70722	1.0276	1.656612	0.707635	1.027775	1.656211
C ₉	0.053075	-2.039267	0.370972	0.051961	-2.038936	0.370904
C ₁₀	-1.808087	-0.597073	0.375348	-1.809549	-0.597957	0.375747
C ₁₁	-0.053075	2.039267	-0.370972	-0.051961	2.038936	-0.370904
C ₁₂	1.808087	0.597073	-0.375348	1.809549	0.597957	-0.375747
C ₁₃	1.179827	-1.671499	-0.377787	1.179468	-1.670361	-0.377799
C ₁₄	-1.101064	-1.596313	-0.386988	-1.102578	-1.597187	-0.386577
C ₁₅	-1.838308	0.629282	-0.382983	-1.839007	0.628266	-0.382463
C ₁₆	-0.057343	1.24307	-1.658614	-0.056214	1.242764	-1.657941
C ₁₇	1.094351	0.363424	-1.606323	1.095777	0.364261	-1.606604
C ₁₈	0.696073	-1.025371	-1.662972	0.696064	-1.024835	-1.662294
C ₁₉	-0.70722	-1.0276	-1.656612	-0.707635	-1.027775	-1.656211
C ₂₀	-1.186582	0.412221	-1.658415	-1.186289	0.411394	-1.657246
Cation			Anion			
C ₁	1.179409	-0.382763	1.591035	-0.305303	1.634339	1.124237
C ₂	0.026327	-1.229438	1.598804	-1.612169	1.087118	0.699604
C ₃	-1.238527	1.690717	0.407609	0.406592	0.590872	-1.814588
C ₄	-1.158612	-0.373951	1.607563	-1.613623	1.085608	-0.698747
C ₅	1.149162	1.614286	0.374763	1.67966	1.145464	-0.002766
C ₆	-0.723617	1.000494	1.59137	-0.307728	1.631713	-1.127028
C ₇	1.882647	-0.620882	0.355081	0.410481	0.594911	1.812659

C ₈	0.718086	1.00415	1.594941	0.470216	2.06735	-0.002556	
C ₉	0.031984	-1.979813	0.367426	-1.699555	-0.329342	1.177694	
C ₁₀	-1.88044	-0.610427	0.39512	-1.702152	-0.332052	-1.173761	
C ₁₁	-0.031984	1.979813	-0.367426	1.699555	0.329342	-1.177694	
C ₁₂	1.88044	0.610427	-0.39512	1.702152	0.332052	1.173761	
C ₁₃	1.238527	-1.690717	-0.407609	-0.406592	-0.590872	1.814588	
C ₁₄	-1.149162	-1.614286	-0.374763	-1.67966	-1.145464	0.002766	
C ₁₅	-1.882647	0.620882	-0.355081	-0.410481	-0.594911	-1.812659	
C ₁₆	-0.026327	1.229438	-1.598804	1.612169	-1.087118	-0.699604	
C ₁₇	1.158612	0.373951	-1.607563	1.613623	-1.085608	0.698747	
C ₁₈	0.723617	-1.000494	-1.59137	0.307728	-1.631713	1.127028	
C ₁₉	-0.718086	-1.00415	-1.594941	-0.470216	-2.06735	0.002556	
C ₂₀	-1.179409	0.382763	-1.591035	0.305303	-1.634339	-1.124237	
N ₁₀ C ₁₀		Neutral			Solvent		
Carti	Coord	X	Y	Z	X	Y	Z
N ₁	-0.78383569	-1.85100019	-1.16365056	1.747647	1.31924	0.073135	
N ₂	-1.6248049	-1.5467499	0.12649071	1.747966	0.477287	-1.231577	
N ₃	-0.72015668	-1.67515908	1.38237274	1.748082	-1.024404	-0.83372	
N ₄	0.73242378	-2.00160389	0.87705542	1.748137	-1.109888	0.716214	
N ₅	0.69188952	-2.0202955	-0.6943519	1.747505	0.338867	1.276827	
N ₆	1.60924985	1.5393441	-0.30323253	-1.747755	-0.477283	1.231764	
N ₇	0.54205951	1.74461171	-1.42486843	-1.748267	1.024173	0.834145	
N ₈	-0.83222106	1.96081911	-0.72339878	-1.748132	1.109635	-0.716813	
N ₉	-0.5764095	2.07417186	0.8296916	-1.747371	-0.33847	-1.277007	
N ₁₀	0.95123462	1.77699777	1.08171448	-1.747817	-1.319076	-0.07298	
C ₁₁	-0.43719481	-0.2019584	1.52023727	0.369424	-1.453062	-1.182895	
C ₁₂	0.7109519	0.32314768	1.38840311	-0.368989	-1.871845	-0.1033	
C ₁₃	1.19347108	-0.57042461	0.86239102	0.369164	-1.574479	1.016099	
C ₁₄	1.51238476	0.07558352	-0.19662502	-0.369056	-0.676372	1.747278	
C ₁₅	-1.5147515	-0.08047776	0.10429626	0.369346	0.676248	-1.747016	
C ₁₆	-1.01585104	0.64771518	1.02388805	-0.368734	-0.480042	-1.810927	
C ₁₇	-1.20954294	0.5426666	-0.75352914	-0.369154	1.574603	-1.016336	
C ₁₈	1.05629735	-0.61498441	-0.93930719	0.368903	0.480065	1.810664	
C ₁₉	0.34499698	0.23818552	-1.56318697	-0.369605	1.453157	1.183136	
C ₂₀	-0.63019124	-0.36058931	-1.43432015	0.368705	1.871633	0.103312	
Cation				Anion			
N ₁	1.763183	1.211887	-0.299584	1.670877	-0.678444	-1.224583	
N ₂	1.871985	-0.078704	-1.143755	1.596689	-1.457014	0.121801	
N ₃	1.74377	-1.255633	-0.155979	1.710227	-0.436779	1.292556	
N ₄	1.584798	-0.685479	1.225976	1.855414	1.008757	0.673342	
N ₅	1.594513	0.805102	1.140517	1.829942	0.8529	-0.902962	
N ₆	-1.88592	0.0794	1.154582	-1.597166	1.456916	-0.119095	
N ₇	-1.755362	1.258312	0.151553	-1.71046	0.433947	-1.292991	
N ₈	-1.563434	0.664864	-1.198078	-1.854879	-1.007957	-0.675683	
N ₉	-1.575712	-0.782867	-1.117752	-1.830693	-0.851902	0.902746	
N ₁₀	-1.776174	-1.216793	0.29677	-1.669973	0.679678	1.224817	
C ₁₁	0.414067	-1.801169	-0.428523	0.339071	-0.430468	1.840974	
C ₁₂	-0.440109	-1.785476	0.647708	-0.282596	0.773217	1.718404	
C ₁₃	0.202327	-0.994084	1.580677	0.546084	1.631933	0.974787	
C ₁₄	-0.566261	0.1127	1.866623	-0.182197	1.86221	-0.179241	
C ₁₅	0.563338	-0.110795	-1.837877	0.181432	-1.862337	0.179663	
C ₁₆	-0.213582	-1.203281	-1.508893	-0.510315	-1.4063	1.278239	
C ₁₇	-0.198929	1.023414	-1.637631	-0.545183	-1.632288	-0.975403	
C ₁₈	0.216358	1.168177	1.455126	0.508977	1.406985	-1.278452	
C ₁₉	-0.416531	1.853044	0.434968	-0.339206	0.429953	-1.840937	
C ₂₀	0.437401	1.737367	-0.635469	0.28396	-0.773021	-1.717975	

$C_{12}N_8$		Neutral			Solvent		
Carti	Coord	X	Y	Z	X	Y	Z
C ₁	0		0.664768	-1.799819	0	0.664768	-1.799819
C ₂	0.664768		1.799819	0	0.664768	1.799819	0
C ₃	-1.799819		0	-0.664768	-1.799819	0	-0.664768
C ₄	-0.664768		1.799819	0	-0.664768	1.799819	0
C ₅	0		-0.664768	-1.799819	0	-0.664768	-1.799819
C ₆	1.799819		0	-0.664768	1.799819	0	-0.664768
C ₇	-1.799819		0	0.664768	-1.799819	0	0.664768
C ₈	1.799819		0	0.664768	1.799819	0	0.664768
C ₉	0		0.664768	1.799819	0	0.664768	1.799819
C ₁₀	-0.664768		-1.799819	0	-0.664768	-1.799819	0
C ₁₁	0.664768		-1.799819	0	0.664768	-1.799819	0
C ₁₂	0		-0.664768	1.799819	0	-0.664768	1.799819
N ₁	-1.245593		-1.245593	1.245593	-1.245593	-1.245593	1.245593
N ₂	1.245593		-1.245593	1.245593	1.245593	-1.245593	1.245593
N ₃	-1.245593		1.245593	1.245593	-1.245593	1.245593	1.245593
N ₄	1.245593		1.245593	1.245593	1.245593	1.245593	1.245593
N ₅	-1.245593		1.245593	-1.245593	-1.245593	1.245593	-1.245593
N ₆	1.245593		1.245593	-1.245593	1.245593	1.245593	-1.245593
N ₇	-1.245593		-1.245593	-1.245593	-1.245593	-1.245593	-1.245593
N ₈	1.245593		-1.245593	-1.245593	1.245593	-1.245593	-1.245593
		Cation			Anion		
C ₁	0		0.670387	-1.812607	0	-1.720992	-0.625054
C ₂	0.670387		1.812607	0	0.717625	0	-2.011409
C ₃	-1.812607		0	-0.670387	-1.784887	-0.664785	-0.00599
C ₄	-0.670387		1.812607	0	-0.717625	0	-2.011409
C ₅	0		-0.670387	-1.812607	0	-1.891152	0.713536
C ₆	1.812607		0	-0.670387	1.784887	-0.664785	-0.00599
C ₇	-1.812607		0	0.670387	-1.784887	0.664785	-0.00599
C ₈	1.812607		0	0.670387	1.784887	0.664785	-0.00599
C ₉	0		0.670387	1.812607	0	1.720992	-0.625054
C ₁₀	-0.670387		-1.812607	0	-0.670066	0	1.803686
C ₁₁	0.670387		-1.812607	0	0.670066	0	1.803686
C ₁₂	0		-0.670387	1.812607	0	1.891152	0.713536
N ₁	-1.216912		-1.216912	1.216912	-1.261662	1.236603	1.266032
N ₂	1.216912		-1.216912	1.216912	1.261662	1.236603	1.266032
N ₃	-1.216912		1.216912	1.216912	-1.196438	1.23821	-1.209795
N ₄	1.216912		1.216912	1.216912	1.196438	1.23821	-1.209795
N ₅	-1.216912		1.216912	-1.216912	-1.196438	-1.23821	-1.209795
N ₆	1.216912		1.216912	-1.216912	1.196438	-1.23821	-1.209795
N ₇	-1.216912		-1.216912	-1.216912	-1.261662	-1.236603	1.266032
N ₈	1.216912		-1.216912	-1.216912	1.261662	-1.236603	1.266032

Each vibrational mode is labeled as fundamental (F) or combination band (CB). All 54 modes for each molecule (fundamentals and combination bands) are listed here; missing labels in earlier versions have been corrected.

Table S3. The harmonic and anharmonic infrared vibrational frequencies (in cm^{-1}) with relative intensity I (in KM mol^{-1}), including fundamental and combination modes for neutral C_{20} fullerene in the gas and water solvent states.

C_{20}	Neutral in the gas phase			Neutral in water solvent		
Vibrational Modes	Harmonic Freq (Int)	Anharmonic Freq (Int)	Mode	Harmonic Freq (Int)	Anharmonic Freq (Int)	Mode
C-C stretch	1376(0)	1378(0)	V_{54} (F)	1375(0)	1445(0)	V_{48} (F)
			V_6+V_{54} (CB)			V_9+V_{48} (CB)
	1374(0)	1372(0)	V_{53} (F)	1373(0)	1400(0)	V_{54} (F)
			V_6+V_{53} (CB)			$\text{V}_{18}+\text{V}_{54}$ (CB)
	1350(0)	1343(0)	V_{52} (F)	1349(0)	1319(68)	V_{51} (F)
			V_6+V_{52} (CB)			V_1+V_{51} (CB)
	1298(118)	1310(48)	V_{49} (F)	1292(346)	1288(0)	V_{46} (F)
			V_1+V_{49} (CB)			$\text{V}_{19}+\text{V}_{46}$ (CB)
			V_2+V_{49} (CB)			$\text{V}_{20}+\text{V}_{46}$ (CB)
	1296(122)	1298(27)	V_{50} (F)	1289(343)	1277(0)	V_{53} (F)
			V_2+V_{50} (CB)			$\text{V}_{18}+\text{V}_{53}$ (CB)
	1289(4)	1289(29)	V_{51} (F)	1284(5)	1270(1811)	V_{44} (F)
			V_1+V_{51} (CB)			V_1+V_{44} (CB)
	1255(0)	1283(0)	V_{48} (F)	1250(0)	1244(0)	V_{41} (F)
			$\text{V}_{48}+\text{V}_{50}$ (CB)			$\text{V}_{20}+\text{V}_{41}$ (CB)
	1249(0)	1276(0)	V_{45} (F)	1246(0)	1237(173)	V_{49} (F)
			$\text{V}_{21}+\text{V}_{45}$ (CB)			V_1+V_{49} (CB)
	1236(0)	1244(18)	V_{44} (F)	1234(0)	1231(288)	V_{38} (F)
			V_1+V_{44} (CB)			V_1+V_{38} (CB)
	1229(0)	1240(30)	V_{43} (F)	1227(0)	1214(0)	V_{52} (F)
			V_1+V_{43} (CB)			V_6+V_{52} (CB)
	1228(3)	1223(0)	V_{41} (F)	1226(11)	1208(434)	V_{43} (F)
			$\text{V}_{20}+\text{V}_{41}$ (CB)			$\text{V}_{19}+\text{V}_{47}$ (CB)
			---			V_2+V_{43} (CB)
	1226(6)	1195(16)	V_{42} (F)	1225(20)	1189.6(0)	V_{47} (F)
			V_2+V_{42} (CB)			V_2+V_{50} (CB)
	1199(2)	1192(2)	V_{39} (F)	1199(5)	1189(301)	V_{50} (F)
			V_1+V_{39} (CB)			V_2+V_{50} (CB)
			V_2+V_{39} (CB)			---

CCC bend	1173(0)	1191(0)	V ₄₆ (F) V ₁₉ +V ₄₆ (CB) V ₂₀ +V ₄₆ (CB)	1173(0)	1179(6)	V ₃₆ (F) V ₁ +V ₃₆ (CB) V ₂ +V ₃₆ (CB)
	1171(0)	1185(0)	V ₁₈ (F) V ₁₈ +V ₄₀ (CB) ---	1171(0)	1166(50)	V ₃₅ (F) V ₁ +V ₃₅ (CB) V ₂ +V ₃₅ (CB)
	1151(10)	1181(0)	V ₄₇ (F) V ₁₀ +V ₄₇ (CB)	1150(29)	1162(0)	V ₃₇ (F) V ₆ +V ₃₇ (CB)
	1150(9)	1171(6)	V ₃₈ (F) V ₁ +V ₃₈ (CB) V ₂₁ +V ₄₇ (CB)	1149(26)	1151(60)	V ₄₂ (F) V ₂ +V ₄₂ (CB) ---
	1126(0)	1159(3)	V ₃₆ (F) V ₁ +V ₃₆ (CB) V ₂ +V ₃₆ (CB)	1126(0)	1117(95)	V ₃₉ (F) V ₁ +V ₃₉ (CB) V ₂ +V ₃₉ (CB)
	1118(0.2)	1150(0)	V ₃₇ (F) V ₆ +V ₃₇ (CB) ---	1118(0.2)	1097.2(48)	V ₃₄ (F) V ₁ +V ₃₄ (CB) V ₃ +V ₃₄ (CB)
	1113(2)	1124(0.6)	V ₃₅ (F) V ₂ +V ₃₅ (CB)	1113(5)	1097(0)	V ₃₀ (F) V ₆ +V ₃₀ (CB)
	1112(2)	1102(0.4)	V ₃₄ (F) V ₂ +V ₃₄ (CB)	1112(6)	1080(0)	V ₄₀ (F) V ₁₈ +V ₄₀ (CB)
	1079(0)	1078(1.5)	V ₃₁ (F) V ₁ +V ₃₁ (CB)	1079(0)	1044(166)	V ₃₁ (F) V ₁ +V ₃₁ (CB)
	1078(0)	1076(0)	V ₃₂ (F) V ₃₁ +V ₃₂ (CB)	1078(0)	1004(0)	V ₃₂ (F) V ₁₉ +V ₃₂ (CB)
	1040(7)	1073(0)	V ₃₃ (F) V ₃₁ +V ₃₃ (CB)	1040(20)	986(0)	V ₃₃ (F) V ₃₁ +V ₃₃ (CB)
	963(0)	1001(0)	V ₃₀ (F) V ₆ +V ₃₀ (CB)	958(0)	924(23)	V ₂₈ (F) V ₂ +V ₂₈ (CB)
	959(0)	993(0)	V ₂₉ (F) V ₆ +V ₂₉ (CB)	955(0)	902(0)	V ₂₉ (F) V ₆ +V ₂₉ (CB)
	887(8)	905(15)	V ₂₈ (F) V ₂₈ +V ₅₂ (CB)	886(24)	899(87)	V ₂₆ (F) V ₁ +V ₂₆ (CB)
	885(9)	901(22)	V ₂₇ (F) V ₁ +V ₂₇ (CB)	885(27)	858(218)	V ₂₇ (F) V ₁ +V ₂₇ (CB)

854(25)	884(14)	V ₂₆ (F) V ₂ +V ₂₆ (CB)	853(70)	823(87)	V ₂₅ (F) V ₁₇ +V ₂₅ (CB)
796(0)	820(0)	V ₂₅ (F) V ₁₆ +V ₂₅ (CB)	796(0)	784(0)	V ₂₄ (F) V ₉ +V ₂₄ (CB)
755(0)	774(0)	V ₂₄ (F) V ₉ +V ₂₄ (CB)	755(0)	761(0)	V ₂₃ (F) V ₉ +V ₂₃ (CB)
754(0)	770(0)	V ₂₃ (F) V ₉ +V ₂₃ (CB)	754(0)	752(0)	V ₄₅ (F) V ₃₁ +V ₄₅ (CB)
743(0)	734(0)	V ₁₉ (F) V ₁₁ +V ₁₉ (CB)	745(0)	740(150)	V ₁₉ (F) V ₁ +V ₁₉ (CB)
706(45)	732(13)	V ₂₁ (F) V ₂ +V ₂₁ (CB)	704(0)	736(0)	V ₂₁ (F) V ₁₂ +V ₂₁ (CB)
705(42)	726(12)	V ₂₀ (F) V ₂ +V ₂₀ (CB)	703(134)	727(210)	V ₂₀ (F) V ₁ +V ₂₀ (CB)
703(0)	720(14)	V ₂₂ (F) V ₁₀ +V ₂₂ (CB)	702(129)	710(0)	V ₆ +V ₁₅ (CB) V ₁₆ +V ₁₅ (CB)
629(1.3)	665(0)	V ₁₇ (F) V ₆ +V ₁₇ (CB) V ₁₇ +V ₄₃ (CB)	629(3)	704(150)	V ₄₆ (F) V ₁₉ +V ₄₆ (CB) ---
616(0)	636(0.4)	V ₁₈ (F) V ₂ +V ₁₈ (CB) V ₁₈ +V ₄₀ (CB)	615(16)	682(21)	V ₁₃ (F) V ₁ +V ₁₃ (CB) ---
615(5)	627(0)	V ₁₆ (F) V ₁ +V ₁₆ (CB)	612(17)	668(15)	V ₂₂ (F) V ₁₀ +V ₂₂ (CB)
614(0)	619(2)	V ₁₅ (F) V ₆ +V ₁₅ (CB) V ₁₄ +V ₁₅ (CB)	611(0)	657(81)	V ₁₈ (F) V ₂ +V ₁₈ (CB) ---
613(5)	607(3)	V ₁₄ (F) V ₁ +V ₁₄ (CB) ---	609(0)	646(26)	V ₁₇ (F) V ₁ +V ₁₇ (CB) V ₂ +V ₁₇ (CB)
612(0)	591(2)	V ₁₂ (F) V ₁ +V ₁₂ (CB) ---	591(6)	584(152)	V ₈ (F) V ₁ +V ₈ (CB) V ₂ +V ₈ (CB)
592(1.6)	582(7)	V ₁₃ (F) V ₂ +V ₁₃ (CB)	588(7)	573(41)	V ₁₀ +V ₂₂ (CB) V ₁ +V ₁₀ (CB)

Ring distort	588(1.7)	571(0.08)	V ₁₀ (F)	583(13)	559(102)	V ₉ (F)
			V ₁₀ +V ₂₂ (CB)			V ₁ +V ₉ (CB)
	555(0.03)	569(5)	V ₁₁ (F)	552(0.3)	552(14)	V ₆ (F)
			V ₁ +V ₁₁ (CB)			V ₁ +V ₆ (CB)
	553(0.02)	568(0.5)	V ₉ (F)	551(0.1)	532(0)	V ₇ (F)
			V ₉ +V ₂₂ (CB)			V ₇ +V ₂₇ (CB)
	528(0.02)	557(0.1)	V ₈ (F)	526(0.08)	531(24)	V ₁₆ (F)
			V ₁ +V ₈ (CB)			V ₂ +V ₁₆ (CB)
			---			V ₁₅ +V ₁₆ (CB)
	510(0)	543(8)	V ₆ (F)	508(0)	499(20)	V ₁₄ (F)
			V ₆ +V ₁₇ (CB)			V ₁₄ +V ₁₇ (CB)
	505(18)	523(0)	V ₄ (F)	497(58)	482(551)	V ₁₁ (F)
			V ₄ +V ₁₁ (CB)			V ₁ +V ₁₁ (CB)
			---			V ₁₁ +V ₂₁ (CB)
	464(0)	505(0)	V ₇ (F)	463(0)	464(31)	V ₁₂ (F)
			V ₇ +V ₁₃ (CB)			V ₁ +V ₁₂ (CB)
			---			V ₁₂ +V ₂₁ (CB)
	461(0)	481(0)	V ₅ (F)	460(0)	461(0)	V ₅ (F)
			V ₅ +V ₂₁ (CB)			---
	342(0)	337(0)	V ₃ (F)	318(0)	380(0)	V ₄ (F)
			V ₃ +V ₄₄ (CB)			V ₄ +V ₁₉ (CB)
	118(0)	84(0)	V ₂ (F)	77(0)	168(0)	V ₃ (F)
			V ₂ +V ₄₉ (CB)			V ₃ +V ₄₄ (CB)
	85(0)	57(0)	V ₁ (F)	25(0)	82.5(0)	V ₂ (F)
			V ₁ +V ₄₄ (CB)			V ₂ +V ₄₂ (CB)
			V ₁ +V ₄₉ (CB)			V ₂ +V ₄₉ (CB)

Table S4. The harmonic and anharmonic infrared vibrational frequencies (in cm⁻¹) with relative intensity I (in KM mol⁻¹), including fundamental and combination modes for C₂₀ fullerene in the cationic and anionic forms in the gas phase.

C ₂₀	Cation in the gas phase			Anion in the gas phase		
Vibrational Modes	Harmonic Freq (Int)	Anharmonic Freq (Int)	Mode	Harmonic Freq (Int)	Anharmonic Freq (Int)	Mode
C-C stretch	1369(0)	1396(0)	V ₅₄ (F)	1369(0)	1361(0)	V ₅₄ (F)
			V ₁₉ +V ₅₄ (CB)			V ₁₇ +V ₅₄ (CB)
	1365(0)	1395(0)	V ₅₃ (F)	1303(0)	1250(0)	V ₅₃ (F)

		$V_{42}+V_{53}$ (CB)			$V_{11}+V_{53}$ (CB)
1364(0)	1342(0)	V_{52} (F)	1295(102)	1299(47)	V_{52} (F)
		$V_{48}+V_{52}$ (CB)			V_1+V_{52} (CB)
1229(0.9)	1307(0)	V_{51} (F)	1262(0)	1301(0)	V_{51} (F)
		$V_{20}+V_{51}$ (CB)			$V_{33}+V_{51}$ (CB)
1217(1.2)	1301(0)	V_{50} (F)	1246(92)	1254(30)	V_{50} (F)
		$V_{19}+V_{50}$ (CB)			V_2+V_{50} (CB)
1216.9(0)	1294(0.08)	V_{49} (F)	1244(10)	1243(262)	V_{49} (F)
		V_1+V_{49} (CB)			V_1+V_{49} (CB)
1216.8(1.2)	1266(0.6)	V_{48} (F)	1207(0)	1232(0)	V_{48} (F)
		V_2+V_{48} (CB)			$V_{39}+V_{48}$ (CB)
1216.5(0)	1265(0.5)	V_{47} (F)	1199(0)	1218(0.09)	V_{47} (F)
		V_1+V_{47} (CB)			V_1+V_{47} (CB)
1214(0)	1254(0)	V_{46} (F)	1195(10)	1191(62)	V_{46} (F)
		$V_{20}+V_{46}$ (CB)			V_2+V_{46} (CB)
1208(0)	1250(0)	V_{45} (F)	1193(0)	1190(0.8)	V_{44} (F)
		$V_{10}+V_{45}$ (CB)			V_1+V_{44} (CB)
1197.2(0)	1220(0.4)	V_{44} (F)	1173(19)	1185(0)	V_{45} (F)
		$V_{22}+V_{44}$ (CB)			$V_{11}+V_{45}$ (CB)
1197(0)	1205(0)	V_{43} (F)	1172(0)	1178(8)	V_{40} (F)
		$V_{19}+V_{43}$ (CB)			$V_{40}+V_{44}$ (CB)
		$V_{20}+V_{43}$ (CB)			---
1183(6.4)	1203(9)	V_{42} (F)	1169(0)	1164.5(0)	V_{42} (F)
		$V_{42}+V_{43}$ (CB)			V_1+V_{42} (CB)
1182(6.3)	1198(10)	V_{41} (F)	1167(89)	1164.5(0.3)	V_{39} (F)
		$V_{41}+V_{43}$ (CB)			$V_{39}+V_{48}$ (CB)
1174(0.01)	1182(0)	V_{40} (F)	1152(0)	1159(25)	V_{41} (F)
		$V_{18}+V_{40}$ (CB)			V_1+V_{41} (CB)
1165(6.4)	1159(0.6)	V_{38} (F)	1144(8)	1145(0)	V_{43} (F)
		$V_{22}+V_{38}$ (CB)			$V_{36}+V_{43}$ (CB)
1164(6.5)	1156(0.6)	V_{39} (F)	1119(33)	1129(14)	V_{38} (F)
		$V_{22}+V_{39}$ (CB)			V_2+V_{38} (CB)
1134(5)	1136(0)	V_{36} (F)	1112(0)	1117(1)	V_{35} (F)
		$V_{17}+V_{36}$ (CB)			V_5+V_{35} (CB)
		$V_{34}+V_{36}$ (CB)			---

CCC bend	1121(0)	1127(0)	V ₃₇ (F)	1109(0.4)	1114(0)	V ₃₇ (F)
			V ₇ +V ₃₇ (CB)			V ₁₇ +V ₃₇ (CB)
	1093.6(4)	1107(0.07)	V ₃₂ (F)	---	---	---
			V ₁ +V ₃₂ (CB)	---	---	---
	1093.5(0)	1106(0)	V ₃₄ (F)	1087(1.5)	1109(0.05)	V ₃₆ (F)
			V ₈ +V ₃₄ (CB)			V ₁ +V ₃₆ (CB)
						V ₃ +V ₃₆ (CB)
	1093(0)	1105(0.2)	V ₃₃ (F)	1083(0)	1086(0)	V ₃₄ (F)
			V ₂ +V ₃₃ (CB)			V ₂₁ +V ₃₄ (CB)
	1092(4)	1104(0)	V ₃₅ (F)	1022(3)	1045(0.8)	V ₃₃ (F)
			V ₈ +V ₃₅ (CB)			V ₂ +V ₃₃ (CB)
	1053(0)	1037(1.4)	V ₃₁ (F)	1001(0)	983(0)	V ₃₂ (F)
			V ₃₁ +V ₅₀ (CB)			V ₃₂ +V ₄₁ (CB)
	1019(0)	981(0)	V ₃₀ (F)	936(0)	944(0)	V ₂₉ (F)
			V ₂₀ +V ₃₀ (CB)			V ₂₀ +V ₂₉ (CB)
	1018(0)	977(0)	V ₂₉ (F)	932(0)	936(0)	V ₃₁ (F)
			V ₁₉ +V ₂₉ (CB)			V ₈ +V ₃₁ (CB)
			---			V ₃₁ +V ₃₃ (CB)
	896(3)	895(4)	V ₂₈ (F)	885(0)	909(0)	V ₃₀ (F)
			V ₂₈ +V ₅₂ (CB)			V ₂₀ +V ₃₀ (CB)
	895(2)	894(3)	V ₂₇ (F)	873(29)	893(33)	V ₂₈ (F)
			V ₄ +V ₂₇ (CB)			V ₃ +V ₂₈ (CB)
	880(5)	866(8)	V ₂₆ (F)	854(31)	877(27)	V ₂₇ (F)
			V ₁ +V ₂₆ (CB)			V ₄ +V ₂₇ (CB)
	808(0)	808(0)	V ₂₅ (F)	848(39)	866(43)	V ₂₆ (F)
			V ₂₅ +V ₄₈ (CB)			V ₅ +V ₂₆ (CB)
	750.7(0)	770(0)	V ₂₄ (F)	787(0)	807(0)	V ₂₅ (F)
			V ₈ +V ₂₄ (CB)			V ₁₁ +V ₂₅ (CB)
	750(0)	769(0)	V ₂₃ (F)	751(0)	768(0)	V ₂₄ (F)
			V ₂₃ +V ₃₈ (CB)			V ₁₂ +V ₂₄ (CB)
	738(0)	758(0)	V ₂₂ (F)	746(0)	761(0)	V ₂₃ (F)
			V ₂₂ +V ₃₉ (CB)			V ₁₁ +V ₂₃ (CB)
	737(0)	746(0)	V ₂₁ (F)	706(0)	722(0)	V ₂₂ (F)
			V ₁₄ +V ₂₁ (CB)			V ₉ +V ₂₂ (CB)
	712(0)	679(0.2)	V ₁₉ (F)	705(92)	699(58)	V ₂₁ (F)

			V ₁₇ +V ₁₉ (CB)			V ₁₀ +V ₂₁ (CB)
	711(0)	677(0.2)	V ₂₀ (F)	679(4)	685(0.5)	V ₂₀ (F)
			V ₂₀ +V ₄₆ (CB)			V ₁ +V ₂₀ (CB)
	682(2)	667(0.8)	V ₁₈ (F)	664(0)	625(0)	V ₁₉ (F)
			V ₁₈ +V ₄₀ (CB)			V ₁₂ +V ₁₉ (CB)
			---			V ₁₉ +V ₃₉ (CB)
			---			V ₁₇ +V ₃₇ (CB)
	646(0.8)	656(0)	V ₁₇ (F)	639(0)	623(0.05)	V ₁₆ (F)
			V ₉ +V ₁₇ (CB)			V ₁₀ +V ₁₆ (CB)
			V ₁₇ +V ₁₉ (CB)			---
	645(0.8)	645(0)	V ₁₆ (F)	635(16)	621(3)	V ₁₅ (F)
			V ₈ +V ₁₆ (CB)			V ₁₀ +V ₁₅ (CB)
	620(0.06)	611(0.7)	V ₁₅ (F)	619(0.6)	599(12)	V ₁₄ (F)
			V ₁₅ +V ₄₃ (CB)			V ₃ +V ₁₄ (CB)
	619(0.08)	610(1)	V ₁₄ (F)	616(5)	572.5(0.4)	V ₁₁ +V ₅₃ (CB)
			V ₁₄ +V ₅₂ (CB)			V ₁₁ +V ₁₉ (CB)
			V ₁₄ +V ₄₅ (CB)			---
	590(4)	608(0.1)	V ₁₃ (F)	583(2)	572(0.3)	V ₁₁ (F)
			V ₃ +V ₁₃ (CB)			V ₂ +V ₁₁ (CB)
			V ₁₃ +V ₄₆ (CB)			V ₁₁ +V ₁₉ (CB)
	589(1.6)	586(0.2)	V ₁₂ (F)	582(9)	571(12)	V ₁₃ (F)
			V ₂ +V ₁₂ (CB)			V ₁₃ +V ₁₉ (CB)
			V ₁₁ +V ₄₃ (CB)			---
	554(0)	585(0.2)	V ₁₁ (F)	558(4)	562(0)	V ₁₈ (F)
			V ₂ +V ₁₁ (CB)			V ₉ +V ₁₈ (CB)
			V ₁₁ +V ₄₃ (CB)			V ₁₅ +V ₁₈ (CB)
	542(0.3)	568(0.002)	V ₁₀ (F)	555.5(4.5)	557(18)	V ₁₂ (F)
			V ₁₀ +V ₄₅ (CB)			V ₁ +V ₁₂ (CB)
Ring distort	541(0.3)	567(0.01)	V ₉ (F)	555(0)	542(6)	V ₉ (F)
			V ₉ +V ₁₇ (CB)			V ₉ +V ₁₈ (CB)
	527(0)	564(0.002)	V ₈ (F)	533(0.7)	527(4)	V ₈ (F)
			V ₈ +V ₁₆ (CB)			V ₁ +V ₈ (CB)
			V ₈ +V ₃₅ (CB)			V ₈ +V ₁₈ (CB)
	523(2)	549(3)	V ₇ (F)	509(9)	510(9)	V ₇ (F)
			V ₂ +V ₇ (CB)			V ₁ +V ₂ (CB)

522(0)	533(0)	V ₆ (F)	483(17)	479(0)	V ₁₀ (F)
		V ₆ +V ₄₉ (CB)			V ₁₀ +V ₁₅ (CB)
		---			V ₁₀ +V ₁₆ (CB)
521(0)	495(0)	V ₅ (F)	475.8(0)	463(0)	V ₆ (F)
		V ₅ +V ₂₀ (CB)			V ₆ +V ₂₀ (CB)
469(0)	492(0)	V ₄ (F)	395(0)	299(0)	V ₅ (F)
		V ₄ +V ₁₉ (CB)			V ₅ +V ₃₉ (CB)
		---			V ₅ +V ₄₉ (CB)
411(0)	453(0)	V ₃ (F)	389(0)	266(0)	V ₄ (F)
		V ₃ +V ₄₉ (CB)			V ₄ +V ₂₇ (CB)
308(0)	379(0)	V ₂ (F)	262(0)	252(0)	V ₃ (F)
		V ₂ +V ₇ (CB)			V ₃ +V ₄₉ (CB)
306(0)	377(0)	V ₁ (F)	196(0)	138(0)	V ₂ (F)
		V ₁ +V ₂₆ (CB)			V ₂ +V ₃₃ (CB)
---	---	---	169(0)	140(0)	V ₁ (F)
		---			V ₁ +V ₄₉ (CB)

Table S5. The harmonic and anharmonic infrared vibrational frequencies (in cm⁻¹) with relative intensity I (in KM mol⁻¹), including fundamental and combination modes for neutral N₁₀C₁₀ heterofullerene in the gas and water solvent states.

N ₁₀ C ₁₀	Neutral in the gas phase			Neutral in water solvent		
Vibrational Modes	Harmonic Freq (Int)	Anharmonic Freq (Int)	Mode	Harmonic Freq (Int)	Anharmonic Freq (Int)	Mode
C-C stretch	1499.7(0)	1517(0.002)	V ₅₄ (F)	1506(0.002)	1525(0)	V ₅₄ (F)
			V ₁ +V ₅₄ (CB)	1506(0.002)		V ₁ +V ₅₄ (CB)
	1499(0)	1516(0.001)	V ₅₃ (F)	1480(0.001)	1524(0)	V ₅₃ (F)
			V ₁ +V ₅₃ (CB)	1480(0.001)		V ₁ +V ₅₃ (CB)
	1475.6(0)	1493(0)	V ₅₁ (F)	---	1497(0.3)	V ₅₂ (F)
			V ₂₀ +V ₅₁ (CB)			V ₂₁ +V ₅₂ (CB)
	1475(0)	1492(0)	V ₅₂ (F)	---	1496(0.4)	V ₅₁ (F)
			V ₂₀ +V ₅₂ (CB)			V ₂₁ +V ₅₁ (CB)
	1403(0)	1405(0)	V ₅₀ (F)	1403(0)	1411(0)	V ₅₀ (F)
			V ₁ +V ₅₀ (CB)			V ₁ +V ₅₀ (CB)
	1369(0)	1382(0.001)	V ₄₈ (F)	---	1391(0)	V ₄₉ (F)
			V ₁₁ +V ₄₈ (CB)			V ₁₄ +V ₄₉ (CB)
			---		1391(0)	V ₄₈ (F)

			---			$V_{13}+V_{48}$ (CB)
	1368(0)	1381(0)	V_{49} (F)	1373(0)	1347(4)	V_{47} (F)
			$V_{12}+V_{49}$ (CB)			$V_{22}+V_{47}$ (CB)
			---	1373(0)	1347(4)	V_{46} (F)
			---			$V_{21}+V_{46}$ (CB)
	1325(6.5)	1346(2)	V_{47} (F)	1330(17)	1257(0.009)	V_{45} (F)
	1325(6.5)		$V_{38}+V_{47}$ (CB)	1330(17)		$V_{21}+V_{45}$ (CB)
	1201(0)	1345(3)	V_{46} (F)	1210(0.03)	1002(0)	V_{44} (F)
			$V_{20}+V_{46}$ (CB)			V_3+V_{44} (CB)
			---		1002(0)	V_{43} (F)
			---			$V_{43}+V_{52}$ (CB)
C-N stretch	988(0)	1251(0)	V_{45} (F)	992(0)	936(0.003)	V_{42} (F)
			$V_{20}+V_{45}$ (CB)	992(0)		V_5+V_{42} (CB)
	987(0)	985(0)	V_{43} (F)	927(0.003)	935(0.002)	V_{41} (F)
			V_2+V_{43} (CB)	927(0.003)		V_4+V_{41} (CB)
	919.4(0)	984(0)	V_{44} (F)	916(0.6)	929.6(1.1)	V_{40} (F)
			V_2+V_{44} (CB)	916(0.6)		$V_{21}+V_{40}$ (CB)
	919(0)	926.8(0)	V_{42} (F)	888(0)	929(1)	V_{39} (F)
		926.8(0)	V_5+V_{42} (CB)	888(0)		$V_{22}+V_{39}$ (CB)
			V_{41} (F)			---
			V_4+V_{41} (CB)		---	
	912(0.2)	925.8(0.1)	V_{40} (F)	875(0.4)	898(0)	V_{37} (F)
	912(0.2)		$V_{20}+V_{40}$ (CB)			$V_{37}+V_{45}$ (CB)
	879(0.001)	925(0.07)	V_{39} (F)	811(0)	895(2)	V_{38} (F)
			$V_{21}+V_{39}$ (CB)	811(0)	895(2)	V_8+V_{38} (CB)
			---			V_{36} (F)
			---			$V_{36}+V_{54}$ (CB)
	878(0)	891(0.08)	V_{38} (F)	---	800(0)	V_{31}
			$V_{38}+V_{45}$ (CB)			$V_{31}+V_{35}$ (CB)
	863(2)	886(0.06)	V_{37} (F)	---	836(0.006)	V_{35} (F)
			$V_{37}+V_{45}$ (CB)			$V_{11}+V_{35}$ (CB)
CNN/CCN bend	807(0)	859(5)	V_{36} (F)	790(0)	842(0.004)	V_{34} (F)
			$V_{15}+V_{36}$ (CB)	790(0)		$V_{11}+V_{34}$ (CB)

	806.7(0)	837(0)	V ₃₅ (F)	780(0)	799(0)	V ₃₀ (F)
			V ₁₄ +V ₃₅ (CB)	780(0)		V ₃₀ +V ₃₄ (CB)
	789(0)	836(0)	V ₃₄ (F)	749(0)	793(0.003)	V ₃₃ (F)
			V ₁₄ +V ₃₄ (CB)	749(0)		V ₁ +V ₃₃ (CB)
			---		793(0.003)	V ₃₂ (F)
			---			V ₁ +V ₃₂ (CB)
	788(0)	797(0.001)	V ₃₁ (F)	746(0)	751(0.001)	V ₂₇ (F)
		797(0.001)	V ₃ +V ₃₁ (CB)			V ₁ +V ₂₇ (CB)
			V ₃₀ (F)			---
			V ₁₁ +V ₃₀ (CB)			---
	773(0)	793(0.008)	V ₃₃ (F)	720(101)	726(71)	V ₂₆ (F)
		793(0.008)	V ₁ +V ₃₃ (CB)			V ₁₇ +V ₂₆ (CB)
			V ₃₂ (F)	720(101)	726(71)	V ₂₅ (F)
			V ₁ +V ₃₂ (CB)			V ₁₇ +V ₂₅ (CB)
	772(0)	745(0)	V ₂₇ (F)	---	722(0.002)	V ₂₉ (F)
			V ₁ +V ₂₇ (CB)			V ₁ +V ₂₉ (CB)
	748.4(0)	734(25)	V ₂₅ (F)	---	720.5(0.009)	V ₂₈ (F)
			V ₂₅ +V ₅₀ (CB)			V ₁₁ +V ₂₈ (CB)
	748(0)	733(26)	V ₂₆ (F)	---	701(0.003)	V ₂₄ (F)
			V ₂₆ +V ₅₀ (CB)			V ₁₄ +V ₂₄ (CB)
			---		701(0.003)	V ₂₃ (F)
			---			V ₁₃ +V ₂₃ (CB)
	742(0)	722(0.002)	V ₂₈ (F)	---	673(0.002)	V ₂₂ (F)
			V ₁₃ +V ₂₈ (CB)			V ₂₂ +V ₄₅ (CB)
		722(0.002)	V ₂₉ (F)			
			V ₁₄ +V ₂₉ (CB)			
CCC bend	723(41)	701(0.01)	V ₂₃ (F)	695(0)	668(0.001)	V ₂₁ (F)
	723(41)		V ₁₁ +V ₂₃ (CB)	695(0)		V ₂₁ +V ₄₅ (CB)
	693(0.01)	700(0.01)	V ₂₄ (F)			
	693(0.01)	700(0.01)	V ₁₂ +V ₂₄ (CB)			
			V ₂₃ (F)			---
			V ₁₁ +V ₂₃ (CB)			
	657(0)	671(0)	V ₂₂ (F)			---

Ring distort			V ₂₂ +V ₄₀ (CB)			
	652(0.08)	656(0.02)	V ₂₁ (F)	666(0)	676(0)	V ₂₀ (F)
			V ₂₁ +V ₄₅ (CB)			V ₂₀ +V ₄₀ (CB)
	652(0.08)	657(0.02)	V ₂₀ (F)	665(0)	633(0.05)	V ₁₉ (F)
			V ₂₀ +V ₄₅ (CB)			V ₁₉ +V ₃₇ (CB)
	621(0.5)	625(0.01)	V ₁₇ (F)	661(0)	632(0.04)	V ₁₈ (F)
			V ₁ +V ₁₇ (CB)			V ₁₈ +V ₃₈ (CB)
	620(0.5)	624(0.006)	V ₁₉ (F)	628(2)	621(0)	V ₁₇ (F)
	620(0.5)		V ₁₉ +V ₃₈ (CB)	628(2)		V ₁ +V ₁₇ (CB)
	603(14)	623(0.004)	V ₁₈ (F)	618(0)	595(23)	V ₁₆ (F)
			V ₁₈ +V ₂₀ (CB)			V ₁₆ +V ₅₃ (CB)
	563(0)	592(9)	V ₁₆ (F)	605(37)	532(0.006)	V ₁₃ (F)
			V ₁₆ +V ₅₃ (CB)			V ₁₃ +V ₄₈ (CB)
	515(0.05)	590(0.006)	V ₁₅ (F)	564(0)	530(0.08)	V ₁₄
	515(0.05)		V ₉ +V ₁₅ (CB)			V ₅ +V ₁₄ (CB)
			V ₁₀ +V ₁₅ (CB)			---
	512(0)	525(0.007)	V ₁₁ (F)	523(0.005)	507(0)	V ₁₅ (F)
			V ₁₁ +V ₄₈ (CB)	523(0.005)		V ₁₅ +V ₃₆ (CB)
	511(0)	524(0.004)	V ₁₂ (F)	522(0.004)	487(0.004)	V ₁₂ (F)
			V ₁₂ +V ₁₄ (CB)			V ₁₂ +V ₃₄ (CB)
			---	522(0.004)	487(0.004)	V ₁₁ (F)
			---			V ₁₁ +V ₃₄ (CB)
	493(0)	495(0.05)	V ₁₀ (F)	502(0.03)	504(0.2)	V ₁₀ (F)
			V ₁₀ +V ₂₁ (CB)			V ₁₀ +V ₃₈ (CB)
	492(0)	496(0.06)	V ₉ (F)	502(0.03)	504(0.2)	V ₉ (F)
			V ₉ +V ₂₀ (CB)			V ₉ +V ₂₁ (CB)
	463(0)	486(0.3)	V ₁₄ (F)	467(0.003)	483(0.002)	V ₈ (F)
			V ₁₄ +V ₃ (CB)			V ₈ +V ₂₁ (CB)
	447(0)	484(2)	V ₁₃ (F)	450(0)	454(0)	V ₇ (F)
			V ₁₃ +V ₃₄ (CB)			V ₇ +V ₄₅ (CB)
	446(0)	479(0)	V ₈ (F)	450(0)	453(0)	V ₆ (F)
			V ₈ +V ₂₀ (CB)			V ₆ +V ₄₅ (CB)
	344(0.02)	452(0.001)	V ₆ (F)	351(0.004)	353.4(0.003)	V ₄ (F)

			V ₁ +V ₆ (CB)			V ₄ +V ₄₁ (CB)
	452(0.001)		V ₇ (F)			---
			V ₁ +V ₇ (CB)			---
342(0)	349(0.004)		V ₄ (F)	351(0.004)	353(0.03)	V ₅ (F)
			V ₄ +V ₁₁ (CB)			V ₄ +V ₄₁ (CB)
336(0)	347(0.1)		V ₅ (F)	339(0.2)	327(301)	V ₁ (F)
			V ₅ +V ₅₂ (CB)			V ₁ +V ₅₄ (CB)
335(0)	329(161)		V ₁ (F)	339(0.2)	309(0.6)	V ₃ (F)
			V ₁ +V ₅₄ (CB)			V ₃ +V ₄₄ (CB)
264(211)	306(0.002)		V ₂ (F)	289(468)	307(0.02)	V ₂ (F)
			V ₂ +V ₄₃ (CB)			V ₂ +V ₄₄ (CB)

Table S6. The harmonic and anharmonic infrared vibrational frequencies (in cm⁻¹) with relative intensity I (in KM mol⁻¹), including fundamental and combination modes for N₁₀C₁₀ heterofullerene in the cationic and anionic forms in the gas phase.

N ₁₀ C ₁₀	Cation in the gas phase			Anion in the gas phase		
Vibrational Modes	Harmonic Freq (Int)	Anharmonic Freq (Int)	Mode	Harmonic Freq (Int)	Anharmonic Freq (Int)	Mode
C-C stretch	1464(32)	1775(14)	V ₅₄ (F)	1494(0)	1533(50)	V ₅₂ (F)
			V ₅ +V ₅₄ (CB)			V ₅ +V ₅₂ (CB)
			---			V ₄₈ +V ₅₂ (CB)
	1454(20)	1774(2)	V ₅₃ (F)	1470(2)	1474(199)	V ₅₁ (F)
			V ₅ +V ₅₃ (CB)			V ₁ +V ₅₁ (CB)
	1432(1)	1757(15)	V ₅₂ (F)	1377(0.2)	1357(50)	V ₄₇ (F)
			V ₅ +V ₅₂ (CB)			V ₁ +V ₄₇ (CB)
	1411(12)	1737(47)	V ₅₁ (F)	1376(5)	1371(0.006)	V ₄₅ (F)
			V ₃₃ +V ₅₁ (CB)			V ₁ +V ₄₅ (CB)
			V ₄₁ +V ₅₁ (CB)			V ₄₆ +V ₅₂ (CB)
	1347(1.5)	1684(4)	V ₅₀ (F)	1359(0)	1294(134)	V ₄₆ (F)
			V ₅ +V ₅₀ (CB)			V ₁ +V ₄₆ (CB)
	1334(17)	1656(4)	V ₄₉ (F)	1328(0)	1270(322)	V ₅₃ (F)
			V ₆ +V ₄₉ (CB)			V ₁ +V ₅₃ (CB)
	1313(0.02)	1642(165)	V ₄₈ (F)	1325(73)	1261(128)	V ₅₀ (F)
			V ₁ +V ₄₈ (CB)			V ₅ +V ₅₀ (CB)
	1290(0.4)	1573(0.2)	V ₄₇ (F)	1275(17)	1153(0.4)	V ₄₉ (F)

			V ₂ +V ₄₇ (CB)			V ₅ +V ₄₉ (CB)
		1573(0.2)	V ₄₆ (F)			---
			V ₂ +V ₄₆ (CB)			---
		1573(0.2)	V ₄₅ (F)			---
			V ₂ +V ₄₅ (CB)			---
	1289(1.3)	1486(62)	V ₄₄ (F)	1254(0.07)	1150(127)	V ₄₈ (F)
			V ₁ +V ₄₄ (CB)			V ₁ +V ₄₈ (CB)
			V ₃₃ +V ₄₄ (CB)			V ₄₈ +V ₅₂ (CB)
	1264(16)	1406(5)	V ₄₃ (F)	1232(0)	1087(2)	V ₅₄ (F)
			V ₃₀ +V ₄₃ (CB)			V ₅ +V ₅₄ (CB)
	1045(0.02)	1368(14)	V ₄₂ (F)	---	1054(0.4)	V ₄₉ (F)
			V ₃ +V ₄₂ (CB)			V ₅ +V ₄₉ (CB)
	1028(0.6)	1346(30)	V ₄₁ (F)	---	1002(0.01)	V ₄₄ (F)
			V ₃₀ +V ₄₁ (CB)			V ₅ +V ₄₄ (CB)
			V ₄₁ +V ₄₄ (CB)			---
			V ₄₁ +V ₄₈ (CB)			---
C-N stretch	985(0.5)	1300(3)	V ₃₉ (F)	991(10)	999(0.001)	V ₄₃ (F)
			V ₁ +V ₃₉ (CB)	991(10)		V ₄ +V ₄₃ (CB)
	971(5)	1297(14)	V ₄₀ (F)	944(0.4)	963(0.3)	V ₃₆ (F)
			V ₃₀ +V ₄₀ (CB)			V ₇ +V ₃₆ (CB)
	953(2)	1288(5)	V ₃₈ (F)	931(0.1)	948(8)	V ₄₂ (F)
			V ₃₀ +V ₃₈ (CB)			V ₆ +V ₄₆ (CB)
	926(3)	1250(5)	V ₃₇ (F)	909(0.004)	943(2)	V ₄₁ (F)
			V ₁ +V ₃₇ (CB)			V ₃ +V ₄₁ (CB)
	903(3)	1247(21)	V ₃₆ (F)	907(3.5)	914(9)	V ₃₇ (F)
			V ₃₆ +V ₄₄ (CB)			V ₁₀ +V ₃₇ (CB)
	888(6)	1231(138)	V ₃₅ (F)	902(3)	911(19)	V ₃₈ (F)
			V ₂ +V ₃₅ (CB)			V ₁ +V ₃₈ (CB)
			---			V ₈ +V ₃₈ (CB)
	887(0.3)	1205(331)	V ₃₃ (F)	896(0.3)	900(19)	V ₃₉ (F)
			V ₃₃ +V ₄₈ (CB)			V ₁₀ +V ₃₉ (CB)
			V ₃₃ +V ₄₄ (CB)			---
	844(2)	1199(10)	V ₃₄ (F)	856(0)	832(16)	V ₃₄ (F)

			V_1+V_{34} (CB)			V_1+V_{34} (CB)
			V_2+V_{34} (CB)			$V_{10}+V_{34}$ (CB)
	824(3)	1139(1)	V_{32} (F)	---	---	---
			$V_{30}+V_{41}$ (CB)			---
			$V_{30}+V_{33}$ (CB)			---
			$V_{30}+V_{12}$ (CB)			---
	823(1)	1097(17)	V_{31} (F)	---	---	---
			V_6+V_{31} (CB)			---
			$V_{11}+V_{31}$ (CB)			---
	781(0.1)	1067(10)	V_{30} (F)	---	---	---
			$V_{30}+V_{41}$ (CB)		---	---
			$V_{30}+V_{33}$ (CB)			---
			$V_{12}+V_{30}$ (CB)			---
CNN/CCN bend	769(15)	1057(3)	V_{29} (F)	800(2)	823(71)	V_{35} (F)
			$V_{29}+V_{44}$ (CB)			V_1+V_{35} (CB)
	762(3)	1045(1)	V_{28} (F)	799(3)	805(0.04)	V_{33} (F)
			$V_{28}+V_{41}$ (CB)			$V_{12}+V_{33}$ (CB)
	759(16)	949(19)	V_{27} (F)	786(0)	790(0.08)	V_{32} (F)
			$V_{27}+V_{44}$ (CB)			V_9+V_{32} (CB)
			$V_{19}+V_{27}$ (CB)			---
	752(4)	931(8)	V_{26} (F)	780(0)	776(0.09)	V_{31} (F)
			$V_{26}+V_4$ (CB)			---
			$V_{17}+V_{26}$ (CB)			$V_{13}+V_{31}$ (CB)
CCC bend	742(20)	892(7)	V_{25} (F)	774(0)	769(0.04)	V_{22} (F)
			V_1+V_{25} (CB)			$V_{22}+V_{27}$ (CB)
	738(13)	865(10)	V_{24} (F)	764(0.009)	766(0.06)	V_{30} (F)
			$V_{24}+V_{48}$ (CB)			$V_{16}+V_{30}$ (CB)
	729(6)	860(3)	V_{23} (F)	737(0.005)	750(0.016)	V_{29} (F)
			V_7+V_{23} (CB)			V_5+V_{29} (CB)
	728(0.2)	847(2)	V_{22} (F)	720(16)	733(0.02)	V_{21} (F)
			V_9+V_{22} (CB)			$V_{21}+V_{27}$ (CB)
	719(0.2)	838(1.2)	V_{21} (F)	712(62)	721(0.06)	V_{40} (F)
			$V_{10}+V_{21}$ (CB)			V_7+V_{40} (CB)

			V ₉ +V ₂₁ (CB)			---
			V ₁₇ +V ₂₆ (CB)			---
	675(2.4)	822(0.1)	V ₁₉ (F)	708(46)	720(768)	V ₂₆ (F)
			V ₁₉ +V ₂₇ (CB)			V ₁ +V ₂₆ (CB)
			---			V ₁₈ +V ₂₆ (CB)
	669(3)	816(0.2)	V ₂₀ (F)	706(19)	702(216)	V ₂₇ (F)
			V ₁₇ +V ₂₀ (CB)			V ₁ +V ₂₇ (CB)
			---			V ₁₇ +V ₂₇ (CB)
	658(2.3)	802(0.2)	V ₁₈ (F)	681(0.004)	695(99)	V ₂₅ (F)
			V ₆ +V ₁₈ (CB)			V ₃₀ +V ₂₅ (CB)
			---			V ₁ +V ₂₅ (CB)
	656(0.4)	794(3)	V ₁₇ (F)	663(0.003)	688(245)	V ₂₈ (F)
			V ₁₇ +V ₂₀ (CB)			V ₁ +V ₂₈ (CB)
			V ₁₇ +V ₂₆ (CB)			---
	---	---	---	660(0.004)	677(0.02)	V ₂₄ (F)
			---	660(0.004)		V ₉ +V ₂₄ (CB)
	---	---	---	---	654(0.4)	V ₈ (F)
			---			V ₄ +V ₈ (CB)
			---			V ₂ +V ₈ (CB)
Ring distort	636(0.2)	784(0.9)	V ₁₆ (F)	622(6)	629(27)	V ₁₉ (F)
			V ₁₆ +V ₁₉ (CB)			V ₁ +V ₁₉ (CB)

	617(8)	764(0.5)	V ₁₅ (F)	621(0.8)	614(0.04)	V ₁₈ (F)
			V ₁₃ +V ₁₅ (CB)			V ₁₈ +V ₂₆ (CB)
	561(34)	723(6)	V ₁₄ (F)	608(0)	613(15)	V ₂₀ (F)
			V ₁₇ +V ₁₄ (CB)			V ₃ +V ₂₀ (CB)
	560(0.3)	704(2)	V ₁₃ (F)	560(0.02)	600(0.3)	V ₁₇ (F)
			V ₁₃ +V ₁₅ (CB)			V ₅ +V ₁₇ (CB)
	542(0.3)	660(12)	V ₁₂ (F)	555(15)	561(10)	V ₁₆ (F)
			V ₁₂ +V ₃₀ (CB)			V ₁₆ +V ₃₀ (CB)
	529(0.7)	656(1)	V ₁₁ (F)	513(0)	512(82)	V ₁₄ (F)
			V ₁ +V ₁₁ (CB)			V ₁ +V ₁₄ (CB)
			V ₁₁ +V ₃₁ (CB)			---

512(12)	627(0.2)	V_{10} (F)	506(1.3)	498(29)	V_{12} (F)
		$V_{10}+V_{21}$ (CB)			V_1+V_{12} (CB)
502(84)	618(0.9)	V_8 (F)	497(16)	479(60)	V_{13} (F)
		V_4+V_8 (CB)			$V_{13}+V_{31}$ (CB)
		V_8+V_{30} (CB)			---
497(10)	613(1)	V_9 (F)	491(2)	438(0.03)	V_{11} (F)
		V_9+V_{21} (CB)			V_2+V_{11} (CB)
		---			V_4+V_{11} (CB)
		---			V_5+V_{11} (CB)
464(5)	606(1.3)	V_7 (F)	472(0.3)	410(0.4)	V_{10} (F)
		V_7+V_{23} (CB)			V_2+V_{10} (CB)
		V_7+V_{30} (CB)			V_4+V_{10} (CB)
459(95)	---	---	461(0.2)		V_1+V_9 (CB)
452(23)	---	---	457(30)	375(133)	V_9 (F)
					V_1+V_9 (CB)
429(4)	564(0.9)	V_6 (F)	443(0.01)	373(6)	V_6 (F)
		V_6+V_{30} (CB)			V_2+V_6 (CB)
		V_6+V_{31} (CB)			V_5+V_6 (CB)
378(2)	537(2)	V_5 (F)	428(22)	361(223)	V_5 (F)
		V_5+V_{33} (CB)			V_5+V_6 (CB)
		---			V_5+V_{52}
363(17)	535(1.2)	V_4 (F)	357(0.6)	253(1)	V_4 (F)
		V_4+V_{26} (CB)			V_4+V_8 (CB)
347(6)	518(5)	V_3 (F)	330(264)	279(1.4)	V_3+V_7 (CB)
		V_3+V_{34} (CB)			V_3+V_7 (CB)
340(85)	412(1.5)	V_2 (F)	291(0.02)	253(1.3)	V_4 (F)
		V_2+V_{35} (CB)			V_4+V_8 (CB)
49(9)	409.4(0.6)	V_1 (F)	281(293)	240(2)	V_{15} (F)
		V_1+V_{11} (CB)			V_4+V_{15} (CB)
---	---	---	254(265)	163(0.8)	V_2 (F)
					V_2+V_6 (CB)
---	---	---	30(31)	79(0.33)	V_1 (F)
					V_1+V_7 (CB)

Table S7. The harmonic and anharmonic infrared vibrational frequencies (in cm^{-1}) with relative intensity I (in KM mol^{-1}), including fundamental and combination modes for neutral C_{12}N_8 heterofullerene in the cationic and anionic forms in the gas phase.

C_{12}N_8	Neutral in the gas phase			Neutral in water solvent		
	Vibrational Modes	Harmonic Freq (Int)	Anharmonic Freq (Int) Mode	Harmonic Freq (Int)	Anharmonic Freq (Int) Mode	
C-C stretch	1613(0)	1632(0)	V_{54} (F)	1614(0)	1631(0)	V_{54} (F)
			V_6+V_{54} (CB)			V_4+V_{54} (CB)
	1613(0)	1632(0)	V_{53} (F)	1614(0)	1631(0)	V_{53} (F)
			V_4+V_{53} (CB)			V_6+V_{53} (CB)
	1601(31)	1620(14)	V_{52} (F)	1600(61)	1619(23)	V_{52} (F)
			V_2+V_{52} (CB)			V_1+V_{52} (CB)
	1601(31)	1620(14)	V_{51} (F)	1600(61)	1619(23)	V_{51} (F)
			V_1+V_{51} (CB)			V_2+V_{51} (CB)
	1601(31)	1620(14)	V_{50} (F)	1600(61)	1619(23)	V_{50} (F)
			V_3+V_{50} (CB)			V_3+V_{50} (CB)
	1575(0)	1591(0)	V_{49} (F)	1576(0)	1590(0)	V_{49} (F)
			V_6+V_{49} (CB)			V_4+V_{49} (CB)
	1138(0)	1146(0)	V_{48} (F)	1137(0)	1145(0)	V_{48} (F)
			V_5+V_{48} (CB)			V_4+V_{48} (CB)
	1138(0)	1146(0)	V_{47} (F)	1137(0)	1145(0)	V_{47} (F)
			V_4+V_{47} (CB)			V_4+V_{47} (CB)
	1138(0)	1146(0)	V_{46} (F)	1137(0)	1145(0)	V_{46} (F)
			V_6+V_{46} (CB)			V_5+V_{46} (CB)
	1121(0)	1135(0)	V_{45} (F)	1118(0)	1117(0)	V_{45} (F)
			$\text{V}_{32}+\text{V}_{45}$ (CB)			$\text{V}_{31}+\text{V}_{45}$ (CB)
	1083(0)	1089(0)	V_{44} (F)	1084(0)	1090(0)	V_{44} (F)
			V_2+V_{44} (CB)			V_1+V_{44} (CB)
	1083(0)	1089(0)	V_{43} (F)	1084(0)	1090(0)	V_{43} (F)
			$\text{V}_{39}+\text{V}_{43}$ (CB)			V_2+V_{43} (CB)
C-N stretch	1059(92)	1071(35)	V_{42} (F)	1057(191)	1062(56)	V_{42} (F)
			$\text{V}_{39}+\text{V}_{42}$ (CB)			$\text{V}_{38}+\text{V}_{42}$ (CB)
	1059(92)		---	1057(191)	1062(56)	V_{41} (F)
			---			$\text{V}_{39}+\text{V}_{41}$ (CB)

	1059(92)		---	1057(191)	1062(56)	V ₄₀ (F)
			---			V ₃₇ +V ₄₀ (CB)
	1002(0)	1069(42)	V ₄₁ (F)	1003(0)	1008(1.5)	V ₃₇ (F)
			V ₃₇ +V ₄₁ (CB)			V ₃₇ +V ₄₃ (CB)
	1002(0)	1069(42)	V ₄₀ (F)	1003(0)	1008(1.5)	V ₃₈ (F)
			V ₁₄ +V ₄₀ (CB)			V ₁₀ +V ₃₈ (CB)
	1002(0)		---	1003(0)	1008(1.5)	V ₃₉ (F)
			---			V ₁₁ +V ₃₉ (CB)
	926(8)	1004(0)	V ₃₉ (F)	926(19)	938(5)	V ₃₆ (F)
			V ₉ +V ₃₉ (CB)			V ₁₈ +V ₃₆ (CB)
	926(8)	1004(0)	V ₃₈ (F)	926(19)	938(5)	V ₃₅ (F)
			V ₁₁ +V ₃₈ (CB)			V ₁₇ +V ₃₅ (CB)
	926(8)	1004(0)	V ₃₇ (F)	926(19)	938(5)	V ₃₄ (F)
			V ₁₀ +V ₃₇ (CB)			V ₁₆ +V ₃₄ (CB)
	885(0)	938(3)	V ₃₆ (F)	886(0)	899(0.1)	V ₃₃ (F)
			V ₁ +V ₃₆ (CB)			V ₂₅ +V ₃₃ (CB)
	885(0)	938(3)	V ₃₅ (F)	886(0)	899(0.1)	V ₃₂ (F)
			V ₂ +V ₃₅ (CB)			V ₂₃ +V ₃₂ (CB)
	885(0)	938(3)	V ₃₄ (F)	886(0)	899(0.1)	V ₃₁ (F)
			V ₃ +V ₃₄ (CB)			V ₂₄ +V ₃₁ (CB)
	827(0)	898(0)	V ₃₃ (F)	828(0)	837(0.1)	V ₂₉ (F)
			V ₂₅ +V ₃₃ (CB)			V ₂₉ +V ₃₅ (CB)
	827(0)	898(0)	V ₃₂ (F)	828(0)	837(0.1)	V ₃₀ (F)
			V ₂₄ +V ₃₂ (CB)			V ₃₀ +V ₃₆ (CB)
	827(0)	898(0)	V ₃₁ (F)	---		---
			V ₂₃ +V ₃₁ (CB)			---
CNN bend	748(8)	835(0)	V ₃₀ (F)	749(19)	761(11)	V ₂₈ (F)
			V ₂₈ +V ₃₀ (CB)			V ₃₀ +V ₃₆ (CB)
	748(8)	835(0)	V ₂₉ (F)	749(19)	761(11)	V ₂₇ (F)
			V ₂₉ +V ₃₄ (CB)			V ₂₇ +V ₃₁ (CB)
			---	749(19)	761(11)	V ₂₆ (F)
			---			V ₂₆ +V ₃₂ (CB)
	726(28)	759(5.6)	V ₂₈ (F)	723(64)	733(0)	V ₂₁ (F)

			V ₁ +V ₂₈ (CB)			V ₂₁ +V ₅₂ (CB)
	726(28)	759(5.6)	V ₂₇ (F)	723(64)	733(0)	V ₂₀ (F)
			V ₃ +V ₂₇ (CB)			V ₂₀ +V ₅₀ (CB)
	726(28)	759(5.6)	V ₂₆ (F)	723(64)	733(0)	V ₁₉ (F)
			V ₂ +V ₂₆ (CB)			V ₁₉ +V ₅₁ (CB)
	723(0)	731(0)	V ₂₁ (F)	722(0)	728(52)	V ₂₅ (F)
			V ₂₁ +V ₅₂ (CB)			V ₂₅ +V ₃₃ (CB)
	723(0)	731(0)	V ₂₀ (F)		728(52)	V ₂₄ (F)
			V ₂₀ +V ₅₁ (CB)			V ₂₄ +V ₃₁ (CB)
	723(0)	731(0)	V ₁₉ (F)		728(52)	V ₂₃ (F)
			V ₁₉ +V ₅₀ (CB)			V ₂₃ +V ₃₂ (CB)
	716(0)	730(29)	V ₂₅ (F)	716.4(0)	718(0)	V ₁₈ (F)
			V ₁ +V ₂₅ (CB)			V ₁₈ +V ₅₂ (CB)
	716(0)	730(29)	V ₂₄ (F)	716.4(0)	718(0)	V ₁₇ (F)
			V ₃ +V ₂₄ (CB)			V ₁₇ +V ₅₁ (CB)
	716(0)	730(29)	V ₂₃ (F)	716.4(0)	718(0)	V ₁₆ (F)
			V ₂₃ +V ₃₁ (CB)			V ₁₆ +V ₅₀ (CB)
	708(0)	720(0)	V ₁₈ (F)	707(0)	707(25)	V ₁₅ (F)
			V ₁₈ +V ₅₂ (CB)			V ₂ +V ₁₅ (CB)
	708(0)	720(0)	V ₁₇ (F)	707(0)	---	V ₃ +V ₁₅ (CB)
			V ₁₇ +V ₅₁ (CB)			V ₃₇ +V ₁₅ (CB)
	708(0)	720(0)	V ₁₆ (F)	707(0)	---	V ₃₈ +V ₁₅ (CB)
			V ₁₆ +V ₁₅ (CB)			V ₃₉ +V ₁₅ (CB)
	692(0)	703(0)	V ₁₅ (F)	695(0)	699(0)	V ₁₄ (F)
			V ₃ +V ₁₅ (CB)			V ₄ +V ₁₄ (CB)
	676(0)	686(0)	V ₁₄ (F)	680(0)	644(0)	V ₂₂ (F)
			V ₆ +V ₁₄ (CB)			V ₆ +V ₂₂ (CB)
	591(0)	603(0)	V ₂₂ (F)	592(0)	---	---
			V ₆ +V ₂₂ (CB) 592(0)			
Ring distort	574(21)	602(0)	V ₁₃ (F)	573(46)	603(16)	V ₁₃ (F)
			V ₁₃ +V ₃₉ (CB) 573(46)			V ₁₃ +V ₃₇ (CB)
	574(21)	602(0)	V ₁₂ (F)	573(46)	603(16)	V ₁₂ (F)
			V ₁₂ +V ₃₇ (CB)			V ₁₂ +V ₃₈ (CB)

478(0)	583(22)	V ₁₁ (F)	478.5(0)	582.8(36)	V ₁₁ (F)
		V ₇ +V ₁₁ (CB)			V ₇ +V ₁₁ (CB)
478(0)	583(22)	V ₁₀ (F)	478.5(0)	582.8(36)	V ₁₀ (F)
		V ₈ +V ₁₀ (CB)			V ₇ +V ₁₀ (CB)
478(0)	583(22)	V ₉ (F)	---	582.8(36)	V ₉ (F)
		V ₇ +V ₉ (CB)			V ₈ +V ₉ (CB)
432(101)	483(0)	V ₈ (F)	426(230)	484(0)	V ₈ (F)
		V ₈ +V ₁₀ (CB)			V ₈ +V ₁₀ (CB)
432(101)	483(0)	V ₇ (F)	426(230)	484(0)	V ₇ (F)
		V ₇ +V ₉ (CB)			V ₇ +V ₁₀ (CB)
		V ₇ +V ₁₁ (CB)	426(230)		---
361(0)	433(91)	V ₆ (F)	362(0)	427(160)	V ₆ (F)
		V ₆ +V ₅₄ (CB)			V ₆ +V ₅₃ (CB)
361(0)	433(91)	V ₅ (F)	362(0)	427(160)	V ₅ (F)
		V ₅ +V ₄₈ (CB)			V ₅ +V ₅₃ (CB)
361(0)	433(91)	V ₄ (F)	362(0)	427(160)	V ₄ (F)
		V ₄ +V ₅₃ (CB)			V ₄ +V ₅₄ (CB)
---	365(0)	V ₃ (F)	---	365(0)	V ₃ (F)
		V ₃ +V ₁₅ (CB)			V ₃ +V ₁₅ (CB)
		V ₃ +V ₂₄ (CB)			V ₃ +V ₅₀ (CB)
---	365(0)	V ₂ (F)	---	365(0)	V ₂ (F)
		V ₂ +V ₁₅ (CB)			V ₂ +V ₁₅ (CB)
		V ₂ +V ₂₃ (CB)			V ₂ +V ₅₁ (CB)
---	365(0)	V ₁ (F)	---	365(0)	V ₁ (F)
		V ₁ +V ₁₅ (CB)			V ₁ +V ₅₂ (CB)
		V ₁ +V ₂₅ (CB)			V ₁ +V ₁₅ (CB)

Table S8. The harmonic and anharmonic infrared vibrational frequencies (in cm⁻¹) with relative intensity I (in KM mol⁻¹), including fundamental and combination modes for C₁₂N₈ heterofullerene in the cationic and anionic forms in the gas phase.

C ₁₂ N ₈	Cation in the gas phase			Anion in the gas phase		
	Vibrational Modes	Harmonic Freq (Int)	Anharmonic Freq (Int) Mode	Harmonic Freq (Int)	Anharmonic Freq (Int) Mode	
C-C stretch	1547(0)	1354(1)	V ₅₁ (F)	1610(0.4)	1619(13)	V ₅₄ (F)
			V ₃₀ +V ₅₁ (CB)			V ₆ +V ₅₄ (CB)

	1547(0)	1354(1)	V_{50} (F)		1619(13)	V_{53} (F)
			$V_{30}+V_{50}$ (CB)			V_3+V_{53} (CB)
	1547(0)	1354(1)	V_{49} (F)			---
			$V_{29}+V_{49}$ (CB)			---
	1496(72)	1353(21)	V_{54} (F)	1604(58)	1563(5)	V_{52} (F)
			V_1+V_{54} (CB)			V_5+V_{52} (CB)
	1496(72)	1353(21)	V_{53} (F)			---
	1496(72)		V_2+V_{53} (CB)			---
			V_3+V_{53} (CB)			---
	---	1281(3)	V_{52} (F)	1549(34)	1486(1)	V_{51} (F)
			V_3+V_{52} (CB)			V_2+V_{50} (CB)
			$V_{49}+V_{52}$ (CB)			---
C-N stretch	1176(0)	1183(0)	V_{48} (F)	1502(73)	1468(33)	V_{50} (F)
			V_1+V_{48} (CB)			V_1+V_{51} (CB)
	1176(0)	1183(0)	V_{47} (F)			---
			V_2+V_{47} (CB)			---
	1176(0)	1183(0)	V_{46} (F)			---
			$V_{43}+V_{46}$ (CB)			---
	1140(0)	1140(0)	V_{45} (F)	1489(93)	1233(15)	V_{49} (F)
			V_5+V_{45} (CB)			$V_{49}+V_1$ (CB)
	1120(0)	1130(0)	V_{44} (F)	1240(45)	1222(20)	V_{48} (F)
	1120(0)		$V_{44}+V_{48}$ (CB)			$V_{48}+V_2$ (CB)
						$V_{48}+V_{47}$ (CB)
	1103(64)	1128(0)	V_{43} (F)	1211(77)	1192(42)	V_{47} (F)
	1103(64)		$V_{43}+V_{46}$ (CB)			V_4+V_{47} (CB)
	1033(0)	1100(20)	V_{42} (F)	1182(0)	1157(0.5)	V_{46} (F)
			$V_{42}+V_{53}$ (CB)			V_2+V_{46} (CB)
	1033(0)	1100(20)	V_{41} (F)			---
			$V_{41}+V_{40}$ (CB)			---
	1033(0)	1100(20)	V_{40} (F)			---
			$V_{31}+V_{40}$ (CB)			---
	967(17)	1033(0)	V_{39} (F)	1143(2)	1133(0)	V_{45} (F)
			V_3+V_{39} (CB)			V_2+V_{45} (CB)

967(17)	1033(0)	V_{38} (F)			---
		V_2+V_{38} (CB)			---
967(17)	1033(0)	V_{37} (F)			---
		V_1+V_{37} (CB)			---
905(0)	956(9)	V_{36} (F)	1126(0)	1102(0)	V_{44} (F)
		$V_{36}+V_{54}$ (CB)			V_5+V_{45} (CB)
905(0)	956(9)	V_{35} (F)			---
		$V_{35}+V_{53}$ (CB)			---
905(0)	956(9)	V_{34} (F)			---
		$V_{10}+V_{34}$ (CB)			---
882(0)	876(10)	V_{32} (F)	1097(0)	1071(19)	V_{43} (F)
882(0)		V_3+V_{32} (CB)			V_9+V_{43} (CB)
	868(10)	V_{33} (F)	1068(62)	1041(11)	V_{42} (F)
		V_2+V_{33} (CB)			V_9+V_{43} (CB)
	867(10)	V_{31} (F)	---		---
		V_1+V_{31} (CB)			---
778(10)	857(12)	V_{29} (F)	1039(86)	1035(14)	V_{41} (F)
778(10)		V_3+V_{29} (CB)			V_8+V_{37} (CB)
778(10)	853(14)	V_{30} (F)	1030(62)	1009(4)	V_{40} (F)
		V_1+V_{30} (CB)			V_9+V_{40} (CB)
769(0)	760(0)	V_{24} (F)	1005(5)	1000(5)	V_{39} (F)
		$V_{24}+V_{27}$ (CB)			$V_{12}+V_{39}$ (CB)
	760(0)	V_{23} (F)			---
		$V_{23}+V_{26}$ (CB)			---
	760(0)	V_{22} (F)			---
		$V_{22}+V_{28}$ (CB)			---
	752(1.1)	V_{25} (F)	985(25)	983(8)	V_{37} (F)
		V_7+V_{25} (CB)			V_8+V_{37} (CB)
			982(0)	977(0)	V_{38} (F)
					V_1+V_{38} (CB)
	---	---	976(16)	927(0)	V_{36} (F)
		---			V_1+V_{36} (CB)
	---	---	934(0)	913(0.2)	V_{35} (F)

			---			V_2+V_{35} (CB)
						$V_{20}+V_{35}$ (CB)
		---	---	902(4)	909(0.9)	V_{34} (F)
						$V_{22}+V_{34}$ (CB)
		---	---	899(0.04)	871(0)	V_{33} (F)
						$V_{18}+V_{33}$ (CB)
---	---	---	---	859(0)	838(4)	V_{32} (F)
						$V_{23}+V_{32}$ (CB)
---	---	---	---	833(4)	835(3)	V_{30} (F)
			---			$V_{23}+V_{30}$ (CB)
			---			$V_{29}+V_{30}$ (CB)
---		---	---	829(23)	819(14)	V_{31} (F)
						V_6+V_{31} (CB)
CNN bend	770(0)	695(64)	V_{28} (F)	828.9(2)	796(0.5)	V_{29} (F)
			V_1+V_{28} (CB)			V_3+V_{29} (CB)
		695(64)	V_{27} (F)			---
			$V_{20}+V_{27}$ (CB)			---
			V_{26} (F)			---
			$V_{19}+V_{26}$ (CB)			---
	743(0)	684(1.7)	V_{21} (F)	791(0.2)	764(9)	V_{28} (F)
			V_3+V_{21} (CB)			V_1+V_{28} (CB)
	743(0)	684(1.7)	V_{20} (F)			---
			V_1+V_{20} (CB)			---
	743(0)	684(1.7)	V_{19} (F)			---
			V_2+V_{19} (CB)			---
	689(0)	627(0.2)	V_{17} (F)	764(28)	760(11)	V_{26} (F)
			$V_{17}+V_{29}$ (CB)			V_3+V_{26} (CB)
	689(0)	627(0.2)	V_{16} (F)			V_7+V_{26} (CB)
			$V_{10}+V_{16}$ (CB)			---
	689(0)	627(0.2)	V_{15} (F)			---
			$V_{11}+V_{15}$ (CB)			---
	650(0)	---	---	752(3.5)	759(4)	V_{27} (F)
						$V_{25}+V_{27}$ (CB)

625(3)	621(0)	V_{14} (F)	748(5)	736(13)	V_{24} (F)
625(3)		$V_{14}+V_{33}$ (CB)			V_3+V_{24} (CB)
625(3)	621(0)	V_{13} (F)			---
		$V_{13}+V_{31}$ (CB)			---
613(0)	584(0)	V_{12} (F)	728(1.4)	730(0.03)	V_{25} (F)
613(0)		$V_{12}+V_{19}$ (CB)			$V_{25}+V_{27}$ (CB)
592(0)	533(2.4)	V_{18} (F)	726(24)	725(14)	V_{23} (F)
		V_1+V_{18} (CB)			V_4+V_{23} (CB)
					$V_{23}+V_{28}$ (CB)
499(0)	444(189)	V_7 (F)	717(10)	713(0)	V_{22} (F)
		V_7+V_{25} (CB)			$V_{22}+V_{34}$ (CB)
499(0)	444(189)	V_8 (F)			
		V_8+V_{18} (CB)			
	444(189)	V_9 (F)			
		V_9+V_{18} (CB)			
---	---	---	704(0)	706(9)	V_{20} (F)
					V_4+V_{20} (CB)
					$V_{11}+V_{20}$ (CB)
---	---	---	698.6(4)	703(14)	V_{21} (F)
---	---	---	698.6(4)		$V_{21}+V_{32}$ (CB)
---	---	---	691(2)	701(0.2)	V_{19} (F)
					$V_{13}+V_{19}$ (CB)
			689(0)	701(0.2)	V_{18} (F)
					$V_{18}+V_{33}$ (CB)
			674(62)	672(44)	V_{17} (F)
					$V_{17}+V_{31}$ (CB)
---	---	---	631(12)	630(5)	V_{16} (F)
					V_6+V_{16} (CB)
---	---	---	600(0)	600(0)	V_{15} (F)
					V_6+V_{15} (CB)
---	---	---	598(10)	588(0)	V_{13} (F)
					$V_{13}+V_{14}$ (CB)
---	---	---	584(0)	585(6)	V_{14} (F)

						$V_{14}+V_{49}$ (CB)
Ring distort	490(260)	427(0)	V_{11} (F)	555(4)	572(0.3)	V_{11} (F)
	490(260)	---	V_2+V_{11} (CB)			$V_{11}+V_{20}$ (CB)
			$V_{11}+V_{17}$ (CB)			---
	338(0)	281(0)	V_{10} (F)	554(0.003)	556(18)	V_{12} (F)
	338(0)		$V_{10}+V_{16}$ (CB)			$V_{12}+V_{39}$ (CB)
	338(0)					
	281(4)	153(0)	V_6 (F)	537(0)	539(0)	V_{10} (F)
			V_2+V_6 (CB)			$V_{10}+V_2$ (CB)
	281(4)	153(0)	V_5 (F)			V_4+V_{10} (CB)
			V_3+V_5 (CB)			---
	281(4)	153(0)	V_4 (F)			---
			V_4+V_{26} (CB)			---
			V_1+V_4 (CB)			---
	---	11.35(7)	V_2 (F)	532(10)	537(12)	V_9 (F)
	---	---	V_2+V_{53} (CB)			V_9+V_2 (CB)
		11.35(7)	V_1 (F)			---
			V_1+V_{54} (CB)			---
	---	10.44(7)	V_3 (F)	502(13)	504(10)	V_8 (F)
		---	V_3+V_{29} (CB)			V_8+V_{37} (CB)
				461(0.04)	454(0.01)	V_7 (F)
	---	---	---			V_7+V_{26} (CB)
				416(170)	406(166)	V_6 (F)
						V_6+V_{16} (CB)
	---	---	---	405(203)	395(172)	V_5 (F)
	---	---	---			V_4+V_5 (CB)
			---	319(52)	306(70)	V_4 (F)
			---			V_4+V_5 (CB)
	---	---	---			V_4+V_{23} (CB)
	---	---	---	290(0)	285(0)	V_3 (F)
						V_3+V_6 (CB)
						V_3+V_{19} (CB)
						V_3+V_{26} (CB)

---	---	---	288(136)	263(125)	V ₂ (F)
					V ₁ +V ₂ (CB)
---	---	---	271(2)	261(2)	V ₁ (F)
					V ₁ +V ₂ (CB)
					V ₁ +V ₂₈ (CB)
					V ₁ +V ₄₉ (CB)
