

Table 1 Simulated Raman scattering data (cm^{-1}) of four candidate structures of ice XIX. The listed peaks with intensities (\AA^4) are those for calculated phonons that are Raman mostly detectable. The experimentally obtained Raman peaks are listed in the first column.

Exp. [3]	Struct. 1	intensities	Struct. 2	intensities	Struct. 3	intensities	Struct. 4	intensities
	91	0.1711119	91	0.1342524	89	0.1809947	94	0.1474833
115	119	0.1019048	118	0.2227925	120	0.1049694	118	0.2973343
	127	0.2331842	133	0.3218784	129	0.1397504	130	0.2139002
	130	0.2539532	134	0.2928524	130	0.2284373	136	0.2748820
					131	0.3698570		
	135	0.3701034	145	0.2545186	135	0.6255397	138	0.2961073
131	148	1.5021780	148	1.4752949	148	1.2161666	148	1.2782497
			162	0.1756806	166	0.5556212		
160	166	1.0640794	166	1.1514516	168	0.5169759	166	0.6553584
			169	0.3667606	169	0.9146208	170	0.5677969
	180	1.5732085	177	1.1067290	181	0.3001562	173	0.9505691
			180	0.2760239	182	1.2880306	174	0.4671250
			183	0.5514221	185	0.2487282	181	0.6846465
			189	0.5431890	187	0.1832105	187	0.1375926
182	194	163837.07	193	3.6520939	192	4.3667210	193	4.3765791
			209	0.2587864	207	0.2279065	208	0.3616320
			229	0.2698043	229	0.3157040	231	0.2440198
			237	0.1203552	239	0.1029373	237	0.2313913
303	269	159.11713	275	1.3274303	275	1.5948712	280	1.1819855
	274	1.8454369	294	0.3906757	292	0.3261544	291	0.5765032
510			497	0.2351641	495	0.3375007	496	0.5428712
	525	3.2298426	528	1.9280807	532	1.2190256	537	1.2725561
	555	1.4328419	550	8.1352495	564	3.6469592	557	1.5075703
	560	9.0826532	558	2.1535129	565	4.0847907	565	4.9705862
	579	1.5755779	580	2.9985734	583	4.2349492	581	0.6503527
	588	2.5359765			586	5.2198678	585	10.407531
	604	12.415012	597	10.894359	601	13.090268	588	8.9270257
	610	5.2720770	600	5.8215921	603	4.3048322	591	6.0173801
	638	1.1694649			647	0.9899631	652	0.2341606
			651	0.4129857	649	0.4967194	657	1.3014885
	660	0.1804954	653	1.5374447	673	7.1102278	673	0.5993068
	676	2.8230338	668	2.8239645	679	0.3571049	686	3.0735708
	684	1.6042955	681	1.5339236	688	1.7643165	686	5.6466433
	696	3.3732870	696	1.1215886	695	0.2639007	691	0.5020224
			702	0.4092358	699	0.9697884	700	0.8266923
	707	0.7879297	707	0.8653995			719	0.5789473
	720	3.2074905	711	4.5322275	717	0.5234664	722	1.7246955

	726	2.3294236	721	1.4859902	727	1.8692400	730	2.1132175
			736	3.1512567	737	3.6098377	743	1.3036955
	747	1.3466998	742	0.8694161			755	0.9539743
	773	2.0907569	757	1.7560344	770	3.6495030	766	0.8143160
	775	5.0106141			776	3.0305038		
	787	6.3136314	785	4.6698773	778	0.9738215		
			788	4.6838343				
	804	3.3133260					803	9.4193811
			832	4.6306849	836	3.0702942	813	1.5699847
	879	0.7365376	851	1.2213161	878	3.3508879	851	2.4352838
					909	0.5599628	919	0.1659854
	932	2.2623592	915	1.4779113	922	0.3513371	953	1.6722976
	951	1.2038752	966	3.9250434	962	3.0323323	959	3.6241219
	978	1.4285933	971	0.8196471	974	2.6153460	967	1.0671273
	996	2.1958127	984	4.9321544	984	1.6769591	982	5.1212487
	1027	0.9851965	1018	0.7256582	1024	0.4703492	1017	0.1092593
	1617	10.399359	1623	7.9198791	1609	1.0321190	1606	1.2199889
	1641	6.5130427	1639	11.871310	1631	3.3639327	1625	4.3549306
	1647	8003.1270	1650	0.3158595	1637	4.8833906	1640	6.5870310
	1654	2.1042735	1659	0.1609391	1644	1.7811537	1655	0.2539494
	1655	3.2877297						
			1664	1.2609117	1665	9.3403868	1661	10.420090
	1680	4.2716177	1672	4.9458998	1667	0.5981186	1670	0.6131287
			1687	0.3044754	1686	0.6407600		
	1695	1.5623793	1695	3.2377123	1690	1.7482389	1699	0.1138995
					1693	0.3209194		
			1701	0.3585601	1702	0.2881202	1701	3.3757403
	3214	7.1988115	3209	5.1681058	3208	2.9072146	3206	17.929830
3206	3215	7352.6161	3210	6994.3137	3209	6921.2374	3208	7116.8694
			3248	30.545747	3249	11.273783	3242	26.152243
	3251	1218.0575	3249	1493.0470	3250	1515.5357	3244	1233.2802
	3252	51.409099	3258	0.2240370			3250	0.1259293
	3286	484.81981	3283	434.60602	3289	450.23201	3285	10.970670
	3287	36.062549			3290	20.479532	3286	437.85790
					3292	0.3958752		
	3301	587.72114	3303	491.07643	3293	345.01200	3296	476.82249
	3302	54.594409	3304	202.30881	3295	421.49237	3297	280.25722
			3330	254.49952	3327	470.99021	3330	241.23671
	3327	471.56429	3331	225.37684	3329	84.549156	3331	245.74137
	3328	78.860350						
	3361	29.802408	3361	151.34309	3362	649.08121	3361	550.44081
	3364	669.95134	3364	492.51669	3364	58.567203	3365	108.47659
	3387	173.74774	3389	305.44793	3387	441.10763	3389	705.68180

	3397	382.90535	3401	272.49450	3402	14.463054	3401	121.94425
	3407	80.961916	3403	554.49768	3408	164.58592	3409	166.24546
	3410	156.44227	3411	29.457424	3410	577.22156		
	3422	479.18166					3418	110.78688
	3436	122.82502	3428	149.85105	3429	293.35959	3421	600.09284
	3437	1.9796247	3434	285.71590	3430	36.680399	3437	3.8247831
	3462	150.40342	3466	227.54016	3459	165.19095	3462	251.47520
	3470	436.36889	3474	345.43436	3469	415.40090	3473	338.11313