

Supplementary Materials: A Study of the Conformers of the (Nonafluorobutanesulfonyl)Imide Ion by Means of Infrared Spectroscopy and Density Functional Theory (DFT) Calculations

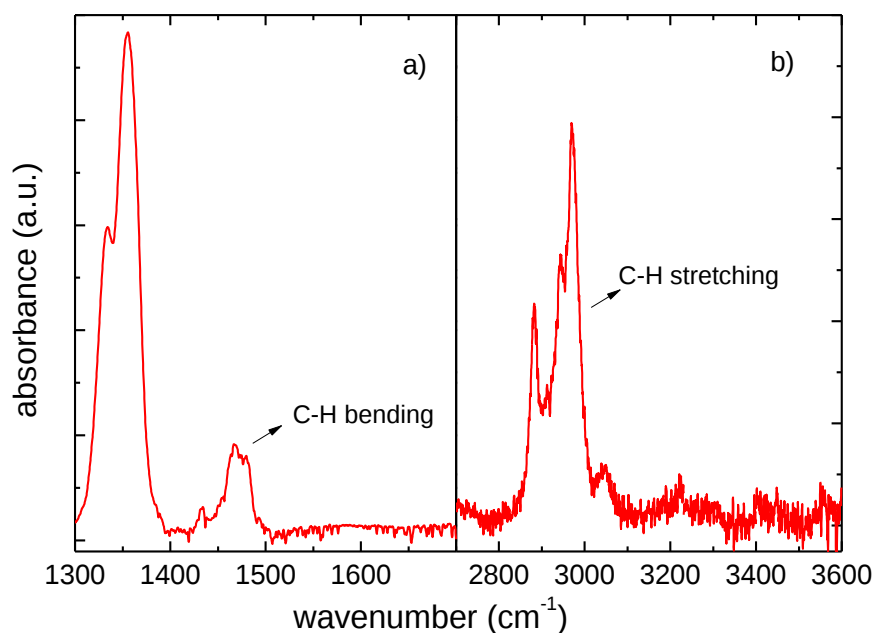


Figure S1. Absorbance of the PYR₁₄-IM₁₄ measured at 300 K in the frequency range between 1300 and 1700 cm⁻¹ (panel **a**) and between 2700 and 3600 cm⁻¹ (panel **b**). Lines due to C-H bending and stretching modes are indicated, while the absence of absorptions lines in the range between 1600 and 1700 cm⁻¹ (O-H bending modes) and between 3200 and 3600 cm⁻¹ (O-H stretching modes) rules out the presence of water.

Table S1. Atomic positions of conformer *tg* IM₁₄ of the trifluoromethanesulfonyl) (nonafluorobutanesulfonyl)imides ion (the three coordinates are reported in Å).

N	1.8768222173	-0.1750322657	0.9692600042
S	2.6824556092	0.9614108226	0.1638395013
S	0.8450830772	-1.1944068142	0.2922717176
O	3.1019852200	1.9841084010	1.1152288601
O	2.1285149638	1.3716958114	-1.1226395582
O	0.9921833491	-1.4296316948	-1.1415234816
O	0.6725796672	-2.3345090347	1.1843800742
C	4.2564917021	0.0879716049	-0.2708873438
C	-0.7675476822	-0.2559095684	0.4474953633
F	4.9193583151	-0.2782106014	0.8257710943
F	5.0411588844	0.9105285442	-0.9754707471
F	4.0212634304	-0.9969983634	-1.0041655893
F	-0.5774807471	1.0289292343	0.0961595390
F	-1.1724149502	-0.2967690299	1.7313135663

Table S1. *Cont.*

C	−1.9002206667	−0.8086754485	0.4386102368
C	−3.3358260884	−0.3303786044	−0.0885131105
C	−3.5911585674	1.1879649267	−0.0248124374
F	−3.0209917110	1.7254444790	1.0485686380
F	−4.9118333139	1.3936930002	0.0579422950
F	−3.1399960594	1.7967550555	−1.1173741062
F	−4.1486355558	−0.8172380948	−1.0528253337
F	−3.7156254081	−0.8544479899	1.0900579358
F	−1.6772959106	−0.4643573080	−1.7162913857
F	−1.9426877749	−2.1513320616	−0.3380732587

Table S2. Atomic positions of conformer *tt* IM₁₄ of the trifluoromethanesulfonyl) (nonafluorobutanesulfonyl)imides ion (the three coordinates are reported in Å).

N	2.0774721861	−0.2751632180	0.9392077723
S	2.9462936454	0.8796942687	0.2315884467
S	0.8849764808	−1.0673738495	0.2226222448
O	3.5559593616	1.6966236756	1.2747046812
O	2.3471082442	1.5365276286	−0.9258750934
O	0.8926982661	−1.0943073301	−1.2379868170
O	0.6521300948	−2.3067644417	0.9545787957
C	4.3681911321	−0.0786099336	−0.4686208554
C	−0.5939664598	−0.0035122571	0.6533822044
F	5.0818964869	−0.6524960946	0.4997572162
F	5.1735375839	0.7493856692	−1.1428615890
F	3.9488321880	−1.0269758827	−1.3022479232
F	−0.2902955865	1.2887765107	0.4606685082
F	−0.9014874200	−0.1877562226	1.9527360367
C	−1.8494011320	−0.3227900267	−0.1879867407
C	−3.1583334024	0.2447533252	0.4178919077
C	−4.3455228175	0.2873951389	−0.5708608788
F	−4.1776817417	1.2397841075	−1.4837162000
F	−5.4663156817	0.5537254495	0.1087503294
F	−4.4987588815	−0.8837970639	−1.1874385085
F	−3.5382508801	−0.5222961065	1.4552229176
F	−2.9643228251	1.5058884574	0.8490051415
F	−1.7091944533	0.2059868573	−1.4166068795
F	−2.0138583884	−1.6537886617	−0.2921167169

Table S3. Unscaled calculated frequency and intensity of the vibrations of the two conformers of the trifluoromethanesulfonyl(nonafluorobutanesulfonyl)imides ion, with the two theories: PBE0 and B3LYP.

Conf <i>tg</i> IM ₁₄ PBE0		Conf <i>tg</i> IM ₁₄ B3LYP		Conf <i>tt</i> IM ₁₄ PBE0		Conf <i>tt</i> IM ₁₄ B3LYP	
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
22.77	0.53706	22.05	0.6	20.01	0.41917	21.299	0.41
28.37	0.56875	26.631	0.21	26.98	0.53748	28.902	0.77
30.69	1.14891	30.022	1.27	31.03	0.87848	35.093	0.73
42.42	0.07479	45.619	0.13	40.07	0.01817	41.695	0.02
52.01	0.87383	52.059	0.87	49.51	0.21128	49.817	0.35
63.75	0.54889	63.841	0.61	59.87	1.2423	60.848	1.24
79.80	0.61692	79.584	0.63	61.96	0.7365	69.85	0.22
95.24	0.08366	92.223	0.09	90.34	0.3017	88.509	0.45
123.91	1.17384	120.644	1.11	106.6	1.19497	103.974	1.05
138.72	0.3748	138.705	0.37	155.77	0.23959	153.568	0.25
162.89	0.19311	158.853	0.21	170.72	0.56199	168.939	0.42
185.98	2.40473	181.404	2.38	182.11	0.14409	180.277	0.2
194.89	1.82542	195.875	1.68	193.68	3.00391	193.072	3.61
209.39	1.23216	208.297	1.11	198.05	2.10683	197.685	1.32
217.77	2.4698	217.797	2.18	214.76	0.68538	214.833	0.72
233.03	1.04835	230.086	1.26	239.75	8.54776	237.618	5.8
240.76	10.48347	238.83	10.45	242.47	0.01648	238.695	3.26
257.95	3.39815	257.183	3.55	245.78	2.50361	245.119	1.75
279.30	0.35325	272.449	0.33	278.43	0.69509	272.134	0.58
292.96	0.95243	285.542	0.79	291.93	5.18089	287.034	0.3
308.01	0.48171	301.645	0.32	295.67	0.17198	291.616	4.98
309.24	0.11958	303.126	0.36	308.81	0.05155	300.901	0.43
317.21	2.09543	308.991	2.93	317.18	2.74531	307.966	3.42
324.99	2.27712	317.841	1.94	335.43	7.44111	329.829	7.25
335.40	4.5441	329.297	4.59	340.61	0.27973	333.847	0.29
347.30	2.79179	340.112	2.86	350.45	3.11969	344.309	3.07
370.57	1.7671	363.506	1.52	365.81	0.53833	359.497	0.59
372.42	0.38156	365.926	0.41	380.31	0.01479	374.125	0.02
391.33	5.08243	382.065	4.16	389.69	5.06426	380.234	4.14
408.45	2.89574	400.078	2.27	402.35	1.91077	394.287	1.51
456.01	5.91401	448.315	6.82	471.01	1.34371	462.844	1
506.96	103.02783	497.286	101.59	504.5	127.28305	496.217	126.52
526.40	20.13282	518.046	21.96	528.93	22.37909	521.24	24.5
536.19	1.72781	526.104	1.95	538.83	8.10704	529.271	8.18
547.97	17.333	536.348	18.06	552.98	7.92619	541.783	7.29
554.80	8.08338	543.437	5.96	554.79	8.17169	544.467	8.74
571.42	41.16229	559.242	43.59	570.5	33.25004	559.427	32.4
586.82	0.50157	575.741	0.75	583.25	19.17954	571.131	13.2
600.69	145.87989	586.583	172.06	599.97	147.31614	586.908	214.9
619.37	3.80971	604.926	0.38	617.28	189.33282	603.654	125.26
626.02	198.57864	609.971	169.28	623.16	1.62851	610.307	2.33
657.39	9.0544	644.589	6.54	653.79	28.94172	638.158	21.53
691.01	23.56857	675.153	19.94	703.46	39.28405	686.185	41.46
740.77	34.65459	712.017	32.79	733.64	21.91091	711.535	13.13
761.47	16.68354	745.062	19.52	756.33	11.76168	736.84	19.76
785.55	13.47089	760.454	9	784.3	8.99271	760.246	7.14

Table S3. Cont.

Conf <i>tg</i> IM₁₄PBE0	Conf <i>tg</i> IM₁₄ B3LYP	Conf <i>tt</i> IM₁₄PBE0	Conf <i>tt</i> IM₁₄ B3LYP	Conf <i>tg</i> IM₁₄PBE0	Conf <i>tg</i> IM₁₄ B3LYP	Conf <i>tt</i> IM₁₄PBE0	Conf <i>tt</i> IM₁₄ B3LYP
Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)	Frequency (cm ⁻¹)	Intensity (km/mol)
876.55	75.25954	851.235	83.13	833.15	42.36993	809.498	45.58
1041.55	70.15682	1001.754	443.88	1051.4	222.03988	1000.46	462.72
1058.80	599.43788	1019.463	239.7	1068.91	409.7273	1038.696	198.75
1154.77	143.39319	1110.237	258.15	1154.83	90.40415	1110.465	238.98
1160.77	305.58985	1118.631	165.34	1159.71	233.89537	1117.357	67.96
1184.07	37.47723	1149.823	32.43	1187.38	84.78931	1150.85	6.4
1196.08	91.74152	1157.656	86.89	1195.96	184.88126	1158.494	211.67
1221.79	43.77069	1175.025	41.87	1232.75	13.6247	1186.294	15.88
1246.95	37.59596	1203.791	38.36	1247.83	32.95383	1203.212	31.76
1251.74	128.20928	1208.85	107.23	1253.7	265.2752	1211.644	256.26
1255.48	301.30688	1214.289	341.09	1260.28	65.06594	1216.83	133.89
1264.17	131.87405	1222.2	128.1	1263.76	211.63797	1221.052	199.84
1274.04	120.74155	1231.521	114.63	1271.7	176.79534	1231.075	327.85
1283.29	479.27184	1241.38	443.26	1274.06	273.88973	1231.846	92.16
1310.05	296.96138	1268.807	266.78	1304.92	447.13565	1263.566	391.96
1319.91	49.55202	1281.778	44.71	1310.77	60.66888	1271.166	51.59
1341.69	8.2355	1299.174	64.85	1339.11	40.30282	1298.621	72.64
1349.77	90.05977	1301.363	26.04	1348.81	102.96149	1301.399	56.63
1373.71	487.30959	1323.917	465.37	1372.57	448.00399	1323.378	421.23
1403.67	51.49406	1364.048	51.36	1407.82	88.52253	1369.353	93.55



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