

Supplementary data

Figure 9 – Highest Occupied Molecular Orbital (HOMO) of isoprene

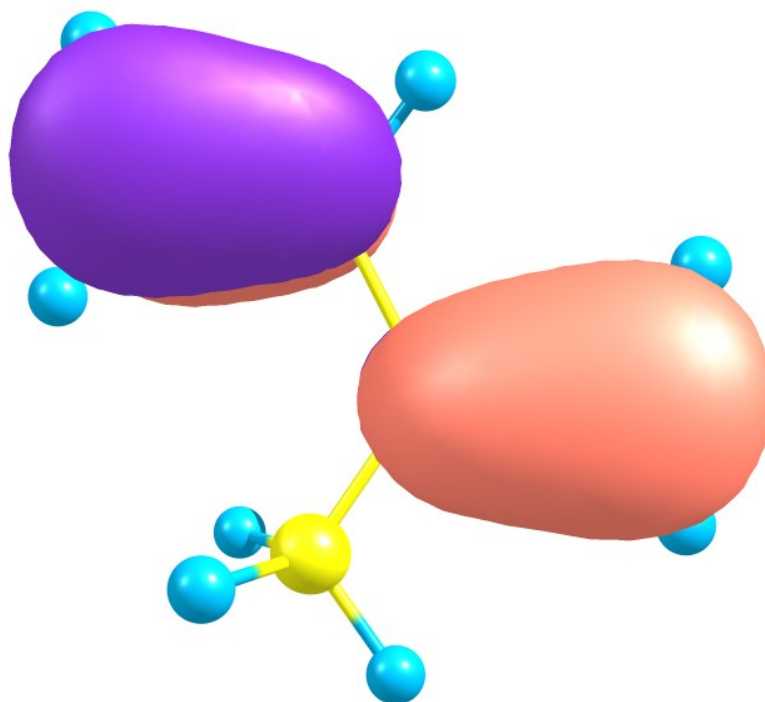


Figure 10 – The Second Highest Occupied Molecular Orbital (SHOMO) of isoprene

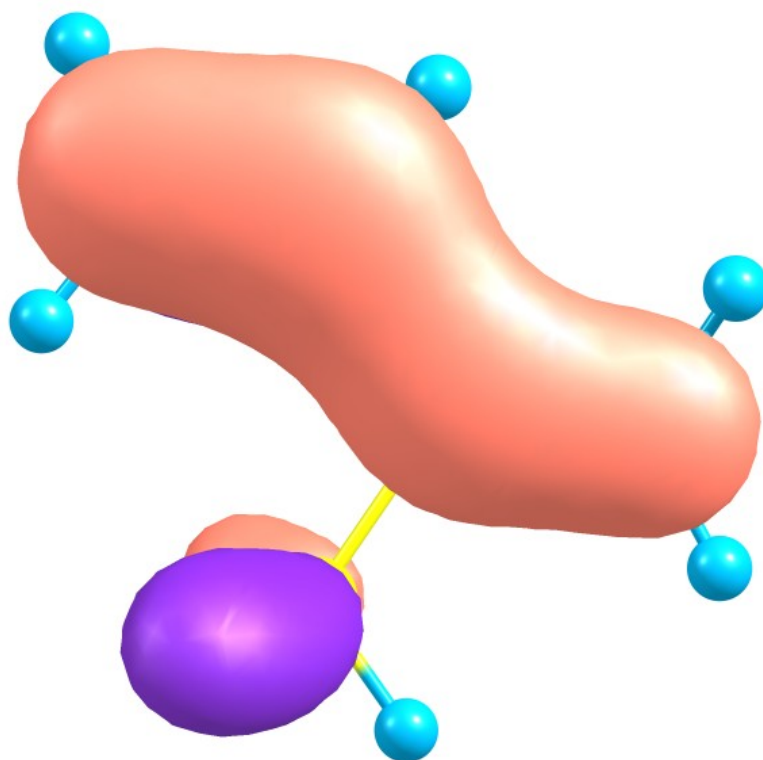


Figure 11 – The Lowest Unoccupied Molecular Orbitals (LUMO) of isoprene

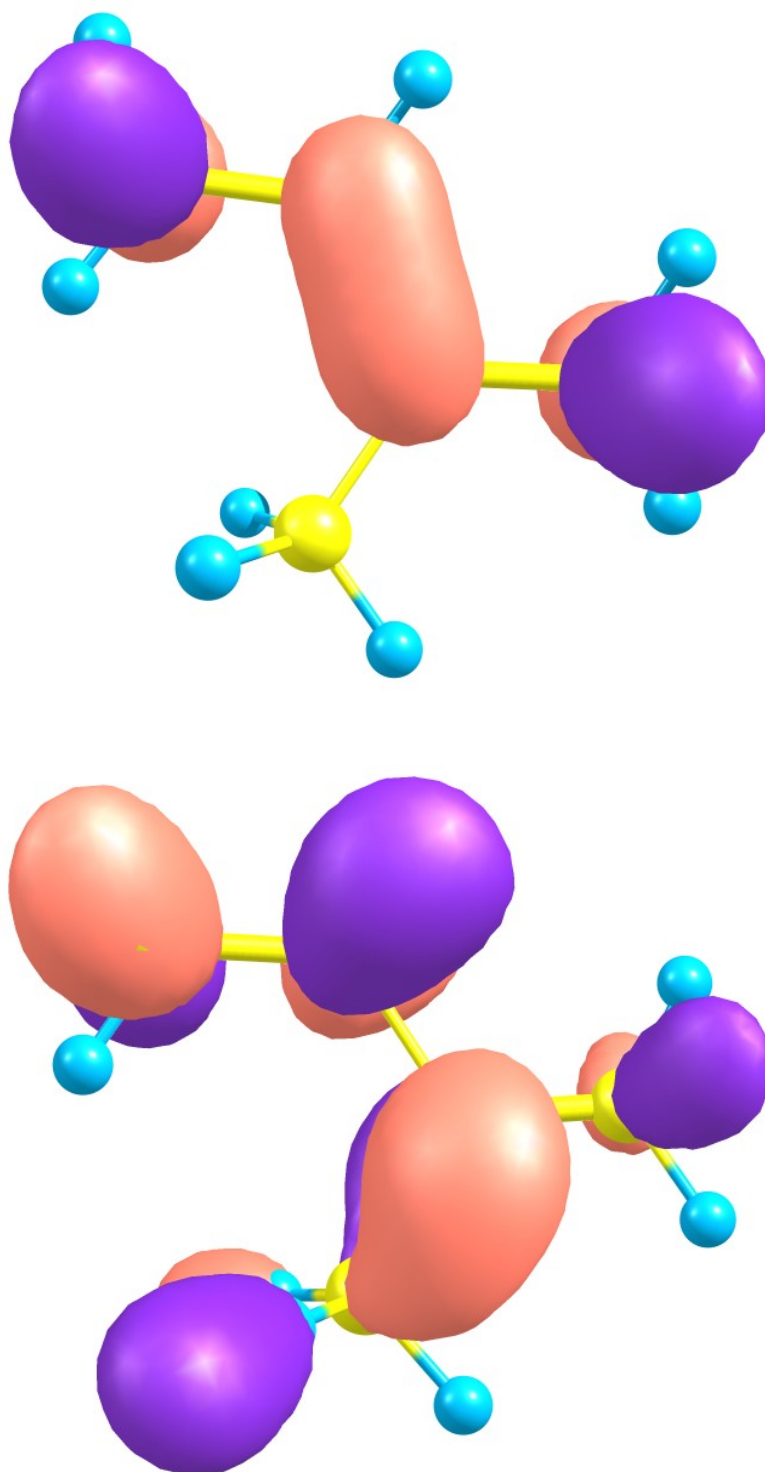
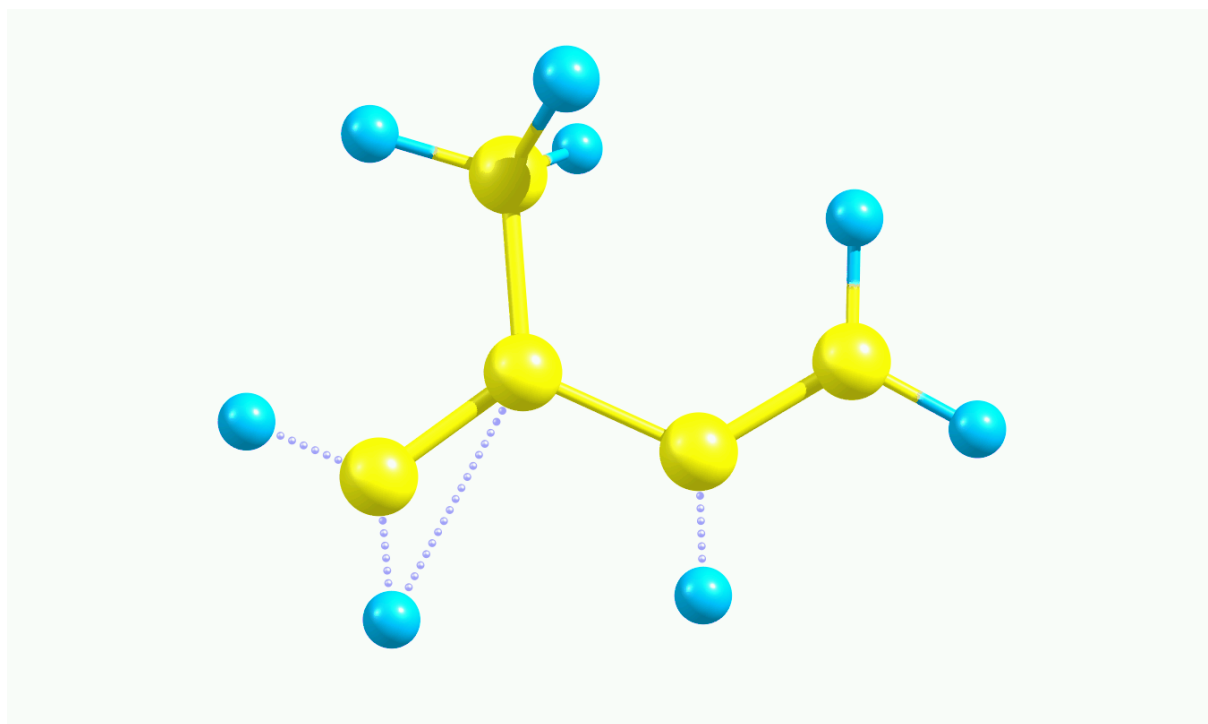
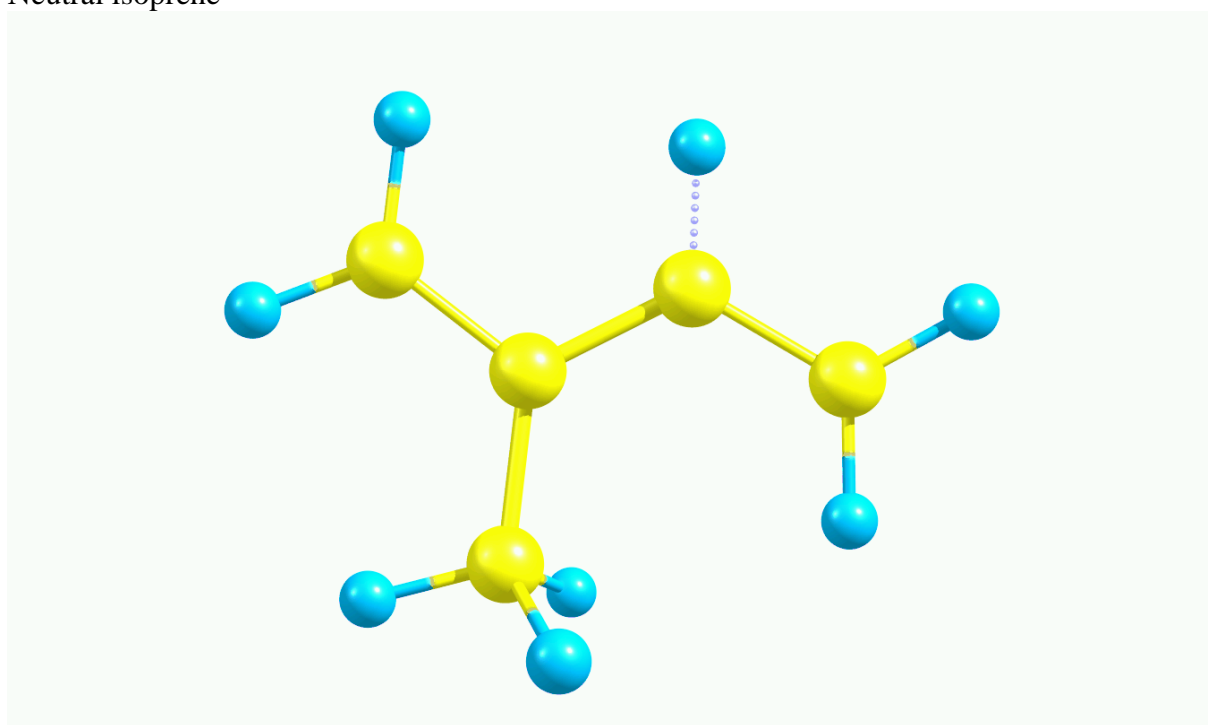


Figure 12 – CC stretching of neutral isoprene and CCC deformation of ionic isoprene



Neutral isoprene



Ionic isoprene

Table 8 – Experimental photoabsorption cross section for the isoprene molecule, as determined by the electron impact method (9 – 28 eV)

Energy (eV)	Cross Section (Mb)
9.0	41.5
9.2	44.3
9.4	46.7
9.6	48.5
9.8	50.0
10.0	53.3
10.2	55.6
10.4	56.9
10.6	59.0
10.8	61.4
11.0	63.3
11.2	65.4
11.4	66.1
11.6	67.9
11.8	70.4
12.0	72.4
12.2	75.8
12.4	76.5
12.6	80.1
12.8	82.3
13.0	84.6
13.2	86.1
13.4	88.1
13.6	90.9
13.8	94.6
14.0	98.3
14.2	97.8
14.4	99.6
14.6	102.4
14.8	102.6
15.0	104.0
15.2	106.7
15.4	108.7
15.6	109.2
15.8	109.2
16.0	113.1
16.2	112.8
16.4	112.7
16.6	117.5
16.8	114.7
17.0	117.2
17.2	117.3
17.4	118.5
17.6	118.0
17.8	115.9
18.0	116.6
18.2	118.9
18.4	118.4

Energy (eV)	Cross Section (Mb)
18.6	118.2
18.8	116.5
19.0	117.4
19.2	116.1
19.4	118.3
19.6	118.7
19.8	116.3
20.0	119.8
20.2	116.4
20.4	117.3
20.6	117.0
20.8	118.3
21.0	115.8
21.2	117.4
21.4	116.1
21.6	114.8
21.8	116.8
22.0	113.6
22.2	115.2
22.4	114.0
22.6	112.3
22.8	110.2
23.0	112.0
23.2	109.5
23.4	110.4
23.6	107.9
23.8	106.8
24.0	105.5
24.2	105.4
24.4	106.6
24.6	103.9
24.8	102.5
25.0	103.4
25.2	100.0
25.4	100.8
25.6	99.8
25.8	97.9
26.0	98.2
26.2	97.2
26.4	97.7
26.6	98.1
26.8	96.3
27.0	95.1
27.2	94.1
27.4	94.4
27.6	92.6
27.8	93.3
28.0	89.6