

Supplementary Information

Table A1: Optimized parameters of 3-FMC.

Bond length	Parameters	Bond Angles	Parameters
C1-C2	1.389	C2-C1-C6	118.7
C1-C6	1.407	C2-C1-H14	118.8
C1-H14	1.082	C6-C1-H14	122.4
C2-C3	1.391	C1-C2-C3	122.8
C2-F7	1.392	C1-C2-F7	118.3
C3-C4	1.401	C3-C2-F7	118.7
C3-H15	1.083	C2-C3-C4	118.1
C4-C5	1.396	C2-C3-H15	119.8
C4-H16	1.085	C4-C3-H15	121.9
C5-C6	1.409	C3-C4-C5	120.3
C5-H17	1.083	C3-C4-H16	119.5
C6-C8	1.493	C5-C4-H16	120.0
C8-O9	1.249	C4-C5-C6	120.5
C8-C10	1.529	C4-C5-H17	121.2
C10-C11	1.562	C6-C5-H17	118.1
C10-N12	1.452	C1-C6-C5	119.2
C10-H18	1.099	C1-C6-C8	122.6
C11-H20	1.096	C5-C6-C8	118.0
C11-H21	1.095	C6-C8-O9	120.0
N12-C13	1.096	C6-C8-C10	120.6
N12-H22	1.453	O9-C8-C10	119.1
C13-H23	1.095	C8-C10-C11	108.1
C13-H24	1.106	C8-C10-N12	108.2
C13-H25	1.098	C8-C10-H18	109.6
		C11-C10-N12	114.7
		C11-C10-H18	107.9
		N12-C10-H18	108.0
		C10-C11-H19	109.8
		C10-C11-H20	109.9
		C10-C11-H21	111.9
		H19-C11-H20	108.4
		H19-C11-H21	108.5
		H20-H11-H21	108.0
		C10-N12-H22	119.3
		C13-N12-H22	113.2
		N12-C13-H23	117.2
		N12-C13-H24	109.0
		N12-C13-H25	115.3
		H23-C13-H24	109.9
		H23-C13-H25	107.3
		H24-C13-H25	107.3

Table A2: Optimized parameters of 4-FMC.

Bond length	Parameters	Bond Angles	Parameters
C1-C2	1.396	C2-C1-C6	120.5
C1-C6	1.409	C2-C1-H14	119.8
C1-H14	1.082	C6-C1-H14	119.5
C2-C3	1.392	C1-C2-C3	118.5
C2-H15	1.083	C1-C2-H15	121.6
C3-C4	1.393	C3-C2-H15	119.8
C3-F7	1.39	C2-C3-C4	122.7
C4-C5	1.394	C2-C3-F7	118.6
C4-H16	1.083	C4-C3-F7	118.6
C5-C6	1.410	C3-C4-C5	118.2
C5-H17	1.084	C3-C4-H16	119.9
C6-C8	1.489	C5-C4-H16	121.8
C8-O9	1.249	C4-C5-C6	120.8
C8-C10	1.541	C4-C5-H17	120.7
C10-C11	1.538	C6-C5-H17	118.3
C10-N12	1.476	C1-C6-C5	119.1
C10-H18	1.100	C1-C6-C8	123.0
C11-H19	1.094	C5-C6-C8	117.7
C11-H20	1.095	C6-C8-O9	120.2
C11-H21	1.095	C6-C8-C10	120.0
N12-C13	1.466	O9-C8-C10	119.6
N12-H22	1.017	C8-C10-C11	111.2
C13-H23	1.094	C8-C10-N12	108.0
C13-H24	1.104	C8-C10-H18	107.3
C13-H25	1.097	C11-C10-N12	114.8
		C11-C10-H18	108.9
		N12-C10-H18	106.0
		C10-C11-H19	110.5
		C10-C11-H20	110.3
		C10-C11-H21	111.1
		H19-C11-H20	109.1
		H19-C11-H21	107.3
		H20-H11-H21	108.2
		H10-H12-H13	117.1
		C10-N12-H22	112.2
		C13-N12-H22	113.1
		N12-C13-H23	109.0
		N12-C13-H24	114.8
		N12-C13-H25	109.3
		H23-C13-H24	108.0
		H23-C13-H25	107.6
		H24-C13-H25	107.6

Table A3: Optimized parameters of 4-MMC.

Bond length	Parameters	Bond Angles	parameters
C1-C2	1.349	C2-C1-C6	120.1
C1-C6	1.351	C2-C1-H14	117.8
C1-H14	1.086	C6-C1-H14	122.1
C2-C3	1.353	C1-C2-C3	121.0
C2-H15	1.089	C1-C2-H15	118.9
C3-C4	1.354	C3-C2-H15	120.1
C3-C7	1.506	C2-C3-C4	118.6
C4-C5	1.349	C2-C3-C7	120.2
C4-H16	1.088	C4-C3-C7	121.1
C5-C6	1.353	C3-C4-C5	120.7
C5-H17	1.088	C3-C4-H16	120.4
C6-C8	1.515	C5-C4-H16	118.9
C7-H18	1.096	C4-C5-C6	120.4
C7-H19	1.095	C4-C5-H17	118.9
C7-H20	1.095	C6-C5-H17	120.7
C8-C9	1.553	C1-C6-C5	119.3
C8-O13	1.238	C1-C6-C8	123.4
C9-C10	1.524	C5-C6-C8	117.0
C9-N11	1.485	C3-C7-H18	111.0
C9-H21	1.097	C3-C7-H19	111.5
C10-H22	1.095	C3-C7-H20	110.8
C10-H23	1.097	H18-C7-H19	106.4
C10-H24	1.093	H18-C7-H20	108.4
N11-C12	1.456	H19-C7-H20	108.5
N11-H25	1.027	C6-C8-C9	119.7
C12-H26	1.096	C6-C8-O13	119.7
C12-H27	1.094	C9-C8-O13	120.6
C12-H28	1.094	C8-C9-C10	111.8
		C8-C9-N11	109.2
		C8-C9-H21	107.3
		C10-C9-N11	107.0
		C10-C9-H21	111.2
		N11-C9-H21	110.3
		C9-C10-H22	110.8
		C9-C10-H23	111.2
		C9-C10-H24	112.3
		H22-C10-H23	108.1
		H22-C10-H24	107.5
		H23-C10-H24	106.9
		C9-N11-C12	112.1
		C9-N11-H25	107.9
		C12-N11-H25	109.7
		N11-C12-H26	109.6
		N11-C12-H27	111.1
		N11-C12-H28	111.3
		H26-C12-H27	108.0
		H26-C12-H28	107.5
		H27-C12-H28	109.2

Table A4: Optimized parameters of buphedrone.

Bond length	Parameters	Bond Angles	Parameters
C1-C2	1.349	C2-C1-C6	120.8
C1-C6	1.355	C2-C1-H14	118.2
C1-H14	1.087	C6-C1-H14	120.8
C2-C3	1.346	C1-C2-C3	119.7
C2-H15	1.087	C1-C2-H15	120.2
C3-C4	1.346	C3-C2-H15	119.9
C3-H16	1.087	C2-C3-C4	119.9
C4-C5	1.351	C2-C3-H16	119.9
C4-H17	1.087	C4-C3-H16	120.1
C5-C6	1.354	C3-C4-C5	120.3
C5-H18	1.083	C3-C4-H17	119.5
C6-C7	1.518	C5-C4-H17	120.0
C7-O8	1.237	C4-C5-H18	120.2
C7-C9	1.549	C4-C5-H18	117.1
C7-C10	1.538	C6-C5-H18	122.6
C9-N12	1.491	C1-C6-C5	118.8
C9-H19	1.092	C1-C6-C7	116.9
C10-C11	1.52	C5-C6-C7	124.2
C10-H20	1.098	C3-C7-O8	119.7
C10-H21	1.099	C3-C7-C9	120.4
C11-H22	1.094	O8-C7-C9	119.7
C11-H23	1.093	C7-C9-C10	110.5
C11-H24	1.094	C7-C9-N12	109.9
N12-C13	1.459	C7-C9-H19	112.1
N12-H25	1.026	C10-C9-N12	106.1
C13-H26	1.096	C10-C9-H19	110.0
C13-H27	1.094	N12-C9-H19	107.9
C13-H28	1.095	C9-C10-C11	114.4
		C9-C10-H20	110.3
		C9-C10-H21	109.0
		C11-C10-H20	108.0
		C11-C10-H21	107.6
		H20-C10-H21	106.7
		C10-C11-H22	109.5
		C10-C11-H23	111.3
		C10-C11-H24	111.6
		H22-C11-H23	107.3
		H22-C11-H24	107.8
		H23-C11-H24	108.8
		C9-N12-C13	113.0
		C9-N12-H25	107.2
		C13-N12-H25	108.3
		N12-C13-H26	108.9
		N12-C13-H27	111.8
		N12-C13-H28	111.6
		H26-C13-H27	107.6
		H26-C13-H28	107.4
		H27-C13-H28	109.1

Table A5: Optimized parameters of butylone.

Bond length	Parameters	Bond Angles	Parameters
C ₁ -C ₂	1.378	C ₂ -C ₁ -C ₆	117.2
C ₁ -C ₆	1.419	C ₂ -C ₁ -H ₁₇	120.2
C ₁ -H ₁₇	1.081	C ₁ -C ₂ -C ₃	122.3
C ₂ -C ₃	1.396	C ₁ -C ₂ -O ₁₂	127.6
C ₂ -O ₁₂	1.407	C ₆ -C ₁ -H ₁₇	122.6
C ₃ -C ₄	1.386	C ₁ -C ₆ -C ₅	119.9
C ₃ -O ₁₀	1.398	C ₁ -C ₆ -C ₇	122.5
C ₄ -C ₅	1.401	C ₃ -C ₂ -O ₁₂	110.1
C ₄ -H ₁₈	1.082	C ₂ -C ₃ -C ₄	121.8
C ₅ -C ₆	1.411	C ₂ -C ₃ -C ₁₀	110.4
C ₅ -H ₁₉	1.083	C ₂ -O ₁₂ -C ₁₁	106.3
C ₆ -C ₇	1.487	C ₄ -C ₃ -O ₁₀	127.8
C ₇ -O ₈	1.253	C ₃ -C ₄ -C ₅	116.7
C ₇ -C ₉	1.545	C ₃ -C ₄ -H ₁₈	121.2
C ₉ -C ₁₃	1.551	C ₃ -O ₁₀ -C ₁₁	106.4
C ₉ -N ₁₅	1.469	C ₅ -C ₄ -H ₁₈	122.0
C ₉ -H ₂₀	1.095	C ₄ -C ₅ -C ₆	122.0
O ₁₀ -C ₁₁	1.477	C ₄ -C ₅ -H ₁₉	120.4
C ₁₁ -O ₁₂	1.471	C ₆ -C ₅ -H ₁₉	117.5
C ₁₁ -H ₂₁	1.091	C ₅ -C ₆ -C ₇	117.6
C ₁₁ -H ₂₂	1.091	C ₆ -C ₇ -O ₈	120.2
C ₁₃ -C ₁₄	1.536	C ₆ -C ₇ -C ₉	122.5
C ₁₃ -H ₂₃	1.096	O ₈ -C ₇ -C ₉	117.3
C ₁₃ -H ₂₄	1.099	C ₇ -C ₉ -C ₁₃	109.9
C ₁₄ -H ₂₅	1.096	C ₇ -C ₉ -N ₁₅	111.1
C ₁₄ -H ₂₆	1.097	C ₇ -C ₉ -H ₂₀	111.0
C ₁₄ -H ₂₇	1.096	C ₁₃ -C ₉ -N ₁₅	108.6
N ₁₅ -H ₁₆	1.469	C ₁₃ -C ₉ -H ₂₀	109.0
N ₁₅ -H ₂₈	1.019	C ₉ -C ₁₃ -C ₁₄	115.3
C ₁₆ -H ₂₉	1.094	C ₉ -C ₁₃ -H ₂₃	106.3
C ₁₆ -H ₃₀	1.105	C ₉ -C ₁₃ -H ₂₄	107.6
C ₁₆ -H ₃₁	1.096	N ₁₅ -C ₉ -H ₂₀	107.1
		C ₉ -N ₁₅ -C ₁₆	116.2
		C ₉ -N ₁₅ -H ₂₈	109.9
		O ₁₀ -C ₁₁ -O ₁₂	106.8
		O ₁₀ -C ₁₁ -H ₂₁	109.1
		O ₁₀ -C ₁₁ -H ₂₂	109.1
		O ₁₂ -C ₁₁ -H ₂₁	109.5
		O ₁₂ -C ₁₁ -H ₂₂	109.5
		H ₂₁ -C ₁₁ -H ₂₂	112.6
		C ₁₄ -C ₁₃ -H ₂₃	110.5
		C ₁₄ -C ₁₃ -H ₂₄	109.8
		C ₁₃ -C ₁₄ -H ₂₅	110.3
		C ₁₃ -C ₁₄ -H ₂₆	111.4

Continued **Table A5:** Optimized parameters of butylone.

Bond length	Parameters	Bond Angles	Parameters
		C ₁₃ -C ₁₄ -H ₂₇	112.1
		H ₂₃ -C ₁₃ -H ₂₄	107.1
		H ₂₅ -C ₁₄ -H ₂₆	107.5
		H ₂₅ -C ₁₄ -H ₂₇	107.5
		H ₂₆ -C ₁₄ -H ₂₇	107.8
		C ₁₆ -N ₁₅ -H ₂₈	111.7
		N ₁₅ -C ₁₆ -H ₂₉	108.9
		N ₁₅ -C ₁₆ -H ₃₀	114.7
		N ₁₅ -C ₁₆ -H ₃₁	109.4
		H ₂₉ -C ₁₆ -H ₃₀	107.9
		H ₂₉ -C ₁₆ -H ₃₁	107.6
		H ₃₀ -C ₁₆ -H ₃₁	108.0

Table A6: Optimized parameters of ethylone.

Bond length	Parameters	Bond Angles	Parameters
C1-C2	1.346	C2-C1-C6	119.1
C1-C6	1.357	C2-C1-H17	117.1
C1-H17	1.082	C6-C1-H17	123.7
C2-C3	1.327	C1-C2-C3	121.2
C2-O12	1.378	C1-C2-O12	125.5
C3-C4	1.343	C3-C2-O12	113.2
C3-O10	1.376	C2-C3-C4	120.9
C4-C5	1.353	C2-C3-O10	113.1
C4-H18	1.087	C4-C3-O10	125.8
C5-C6	1.361	C3-C4-C5	118.6
C5-H19	1.089	C3-C4-H18	120.1
C6-C7	1.518	C5-C4-H18	121.2
C7-O8	1.239	C4-C5-C6	120.8
C7-C9	1.548	C4-C5-H19	118.2
C9-C13	1.529	C6-C5-H19	120.8
C9-N14	1.478	C1-C6-C5	119.1
C9-H20	1.089	C1-C6-C7	124.0
O10-C11	1.446	C5-C6-C7	116.8
C11-O12	1.446	C6-C7-O8	119.8
C11-H21	1.096	C6-C7-C9	120.5
C11-H22	1.096	O8-C7-C9	119.6
C13-H23	1.094	C7-C9-C13	107.6
C13-H24	1.096	C7-C9-N14	107.6
C13-H25	1.096	C7-C9-H20	111.2
N14-C15	1.458	C13-C9-N14	113.1
N14-H26	1.024	C13-C9-H20	108.5
C15-C16	1.522	N14-C9-H20	108.5

Continued **Table A6:** Optimized parameters of ethylone.

Bond length	Parameters	Bond Angles	Parameters
C15-H27	1.095	C3-O10-C11	100.4
C15-H28	1.097	O10-C11-O12	112.9
C16-H29	1.095	O10-C11-H21	108.7
C16-H30	1.095	O10-C11-H22	108.7
C16-H31	1.095	O12-C11-H21	108.7
		O12-C11-H22	108.6
		H21-C11-H22	108.9
		C2-O12-C11	100.5
		C9-C13-H23	111.5
		C9-C13-H24	111.4
		C9-C13-H25	110.7
		H23-C13-H24	108.1
		H23-C13-H25	107.5
		H24-C13-H25	107.2
		C9-N14-C15	113.6
		C9-N14-H26	108.5
		C15-N14-H26	110.8
		N14-C15-C16	110.2
		N14-C15-H27	111.5
		N14-C15-H28	110.0
		C16-C15-H27	108.3
		C16-C15-H28	108.4
		H27-C15-H28	108.0
		C15-C16-H29	109.7
		C15-C16-H30	111.5
		H29-C16-H30	111.3
		C15-C16-H31	107.8
		H29-C16-H31	107.8
		H30-C16-H31	108.4

Table A7: Optimized parameters of MDPV.

Bond length	Parameters	Bond Angles	Parameters
C ₁ -C ₂	1.379	C ₂ -C ₁ -C ₆	117.3
C ₁ -C ₆	1.419	C ₂ -C ₁ -H ₂₁	120.1
C ₁ -H ₂₁	1.081	C ₁ -C ₂ -C ₃	122.4
C ₂ -C ₃	1.395	C ₁ -C ₂ -O ₁₄	127.5
C ₂ -O ₁₄	1.407	C ₆ -C ₁ -H ₂₁	122.6
C ₃ -C ₄	1.386	C ₁ -C ₆ -C ₅	119.7
C ₃ -O ₁₂	1.398	C ₁ -C ₆ -C ₇	123.2
C ₄ -C ₅	1.401	C ₃ -O ₁₄	110.1
C ₄ -H ₂₂	1.082	C ₂ -C ₃ -C ₄	121.7
C ₅ -C ₆	1.412	C ₂ -C ₃ -O ₁₂	110.4
C ₅ -H ₂₃	1.083	C ₂ -O ₁₄ -C ₁₃	106.3
C ₆ -C ₇	1.492	C ₄ -C ₃ -O ₁₂	127.9
C ₇ -C ₈	1.249	C ₃ -C ₄ -C ₅	116.8
C ₇ -C ₉	1.543	C ₃ -C ₄ -H ₂₂	121.3
C ₉ -C ₁₀	1.546	C ₃ -O ₁₂ -C ₁₃	106.4
C ₉ -N ₁₁	1.473	C ₅ -C ₄ -H ₂₂	122.0
C ₉ -H ₂₄	1.108	C ₄ -C ₅ -C ₆	122.2
C ₁₀ -C ₁₉	1.540	C ₄ -C ₅ -H ₂₃	120.4
C ₁₀ -H ₂₅	1.096	C ₆ -C ₅ -H ₂₃	117.5
C ₁₀ -H ₂₆	1.097	C ₅ -C ₆ -C ₇	117.0
N ₁₁ -C ₁₅	1.485	C ₆ -C ₇ -C ₈	119.8
N ₁₁ -C ₁₆	1.478	C ₆ -C ₇ -C ₉	121.5
O ₁₂ -C ₁₃	1.477	C ₈ -C ₇ -C ₉	118.6
C ₁₃ -O ₁₄	1.471	C ₇ -C ₉ -C ₁₀	108.7
C ₁₃ -H ₂₇	1.091	C ₇ -C ₉ -N ₁₁	109.1
C ₁₃ -H ₂₈	1.091	C ₇ -C ₉ -H ₂₄	110.0
C ₁₅ -C ₁₈	1.555	C ₁₀ -C ₉ -N ₁₁	111.0
C ₁₅ -H ₂₉	1.094	C ₁₀ -C ₉ -H ₂₄	107.7
C ₁₅ -H ₃₀	1.108	C ₉ -C ₁₀ -H ₁₉	113.7
C ₁₆ -C ₁₇	1.534	C ₉ -C ₁₀ -H ₂₅	107.3
C ₁₆ -H ₃₁	1.094	C ₉ -C ₁₀ -H ₂₆	108.9
C ₁₆ -H ₃₂	1.110	C ₁₁ -C ₉ -H ₂₄	110.2
C ₁₇ -C ₁₈	1.552	C ₉ -C ₁₁ -C ₁₅	116.1
C ₁₇ -H ₃₃	1.095	C ₉ -C ₁₁ -C ₁₆	117.7
C ₁₇ -H ₃₄	1.094	C ₁₉ -C ₁₀ -H ₂₅	110.4
C ₁₈ -H ₃₅	1.094	C ₁₉ -C ₁₀ -H ₂₆	108.7
C ₁₈ -H ₃₆	1.096	C ₁₀ -C ₁₉ -C ₂₀	112.3
C ₁₉ -C ₂₀	1.537	C ₁₀ -C ₁₉ -H ₃₇	109.6
C ₁₉ -H ₃₇	1.100	C ₁₀ -C ₁₉ -H ₃₈	109.7
C ₁₉ -H ₃₈	1.099	H ₂₅ -C ₁₀ -H ₂₆	107.7
C ₂₀ -H ₃₉	1.097	C ₁₅ -N ₁₁ -C ₁₆	107.8
C ₂₀ -H ₄₀	1.098	N ₁₁ -C ₁₅ -C ₁₈	105.0
C ₂₀ -H ₄₁	1.096	N ₁₁ -C ₁₅ -H ₂₉	110.4

Continued **Table A7:** Optimized parameters of MDPV.

Bond length	Parameters	Bond Angles	Parameters
		N ₁₁ -C ₁₅ -H ₃₀	111.5
		N ₁₁ -C ₁₆ -C ₁₇	102.3
		N ₁₁ -C ₁₆ -H ₃₁	110.6
		N ₁₁ -C ₁₆ -H ₃₂	112.7
		O ₁₂ -C ₁₃ -C ₁₄	106.8
		O ₁₂ -C ₁₃ -H ₂₇	109.1
		O ₁₂ -C ₁₃ -H ₂₈	109.1
		O ₁₄ -C ₁₃ -H ₂₇	109.5
		O ₁₄ -C ₁₃ -H ₂₈	109.5
		H ₂₇ -C ₁₃ -H ₂₈	112.6
		C ₁₈ -C ₁₅ -H ₂₉	112.2
		C ₁₈ -C ₁₅ -H ₃₀	110.4
		C ₁₅ -C ₁₈ -C ₁₇	105.1
		C ₁₅ -C ₁₈ -H ₃₅	111.9
		C ₁₅ -C ₁₈ -H ₃₆	110.2
		H ₂₉ -C ₁₅ -H ₃₀	107.4
		C ₁₇ -C ₁₆ -H ₃₁	113.0
		C ₁₇ -C ₁₆ -H ₃₂	110.4
		C ₁₆ -C ₁₇ -C ₁₈	103.3
		C ₁₆ -C ₁₇ -H ₃₃	109.4
		C ₁₆ -C ₁₇ -H ₃₄	112.7
		H ₃₁ -C ₁₆ -H ₃₂	108.0
		C ₁₈ -C ₁₇ -H ₃₃	110.5
		C ₁₈ -C ₁₇ -H ₃₄	112.7
		C ₁₇ -C ₁₈ -H ₃₅	111.8
		C ₁₇ -C ₁₈ -H ₃₆	110.5
		H ₃₃ -C ₁₇ -H ₃₄	108.3
		H ₃₅ -C ₁₈ -H ₃₆	107.3
		C ₂₀ -C ₁₉ -H ₃₇	109.4
		C ₂₀ -C ₁₉ -H ₃₈	109.1
		C ₁₉ -C ₂₀ -H ₃₉	110.9
		C ₁₉ -C ₂₀ -H ₄₀	111.1
		C ₁₉ -C ₂₀ -H ₄₁	111.3
		H ₃₇ -C ₁₉ -H ₃₈	106.5
		H ₃₉ -C ₂₀ -H ₄₀	107.7
		H ₃₉ -C ₂₀ -H ₄₁	107.8
		H ₄₀ -C ₂₀ -H ₄₁	107.8

Table A8: Optimized parameters of Methcathinone.

Bond length	Parameters	Bond Angles	Parameters
C ₁ -C ₂	1.395	C ₂ -C ₁ -C ₆	120.5
C ₁ -C ₆	1.409	C ₂ -C ₁ -H ₁₃	121.2
C ₁ -H ₁₃	1.084	C ₁ -C ₂ -C ₃	120.0
C ₂ -C ₃	1.402	C ₁ -C ₂ -H ₁₄	120.0
C ₂ -H ₁₄	1.085	C ₆ -C ₁ -H ₁₃	118.3
C ₃ -C ₄	1.4	C ₁ -C ₆ -C ₅	119.1
C ₃ -H ₁₅	1.086	C ₁ -C ₆ -C ₇	117.9
C ₄ -C ₅	1.397	C ₃ -C ₂ -H ₁₄	120.1
C ₄ -H ₁₆	1.085	C ₂ -C ₃ -C ₄	119.9
C ₅ -C ₆	1.408	C ₂ -C ₃ -H ₁₅	120.1
C ₅ -H ₁₇	1.083	C ₄ -C ₃ -H ₁₅	120.0
C ₆ -C ₇	1.49	C ₃ -C ₄ -C ₅	120.2
C ₇ -O ₈	1.249	C ₃ -C ₄ -H ₁₆	120.0
C ₇ -C ₉	1.541	C ₅ -C ₄ -H ₁₆	119.8
C ₉ -C ₁₀	1.537	C ₄ -C ₅ -C ₆	120.2
C ₉ -N ₁₁	1.476	C ₄ -C ₅ -H ₁₇	120.1
C ₉ -H ₁₈	1.099	C ₆ -C ₅ -H ₁₇	119.7
C ₁₀ -H ₁₉	1.094	C ₅ -C ₆ -C ₇	122.9
C ₁₀ -H ₂₀	1.095	C ₆ -C ₇ -O ₈	120.5
C ₁₀ -H ₂₁	1.095	C ₆ -C ₇ -C ₉	120.0
N ₁₁ -C ₁₂	1.465	O ₈ -C ₇ -C ₉	119.5
N ₁₁ -H ₂₂	1.016	C ₇ -C ₉ -C ₁₀	111.4
C ₁₂ -H ₂₃	1.094	C ₇ -C ₉ -N ₁₁	107.4
C ₁₂ -H ₂₄	1.104	C ₇ -C ₉ -H ₁₈	107.7
C ₁₂ -H ₂₅	1.097	C ₁₀ -C ₉ -N ₁₁	114.8
		C ₁₀ -C ₉ -C ₁₈	109.0
		C ₉ -C ₁₀ -H ₁₉	110.4
		C ₉ -C ₁₀ -H ₂₀	110.4
		C ₉ -C ₁₀ -H ₂₁	111.1
		N ₁₁ -C ₉ -H ₁₈	106.2
		C ₉ -C ₁₁ -C ₁₂	117.4
		C ₉ -C ₁₁ -H ₂₂	112.3
		H ₁₉ -C ₁₀ -H ₂₀	109.2
		H ₁₉ -C ₁₀ -H ₂₁	107.4
		H ₂₀ -C ₁₀ -H ₂₁	108.2
		C ₁₂ -N ₁₁ -H ₂₂	113.4
		N ₁₁ -C ₁₂ -H ₂₃	109.0
		N ₁₁ -C ₁₂ -H ₂₄	114.9
		N ₁₁ -C ₁₂ -H ₂₅	109.4
		H ₂₃ -C ₁₂ -H ₂₄	108.0
		H ₂₃ -C ₁₂ -H ₂₅	107.6
		C ₂₄ -C ₁₂ -H ₂₅	107.6

Table A9: Optimized parameters of Methylone.

Bond length	Parameters	Bond Angles	Parameters
C ₁ -C ₂	1.378	C ₂ -C ₁ -C ₆	117.2
C ₁ -C ₆	1.419	C ₂ -C ₁ -H ₁₆	120.2
C ₁ -H ₁₆	1.081	C ₆ -C ₁ -H ₁₆	122.5
C ₂ -C ₃	1.395	C ₁ -C ₂ -C ₃	122.2
C ₂ -O ₁₅	1.406	C ₁ -C ₂ -O ₁₅	127.5
C ₃ -C ₄	1.385	C ₃ -C ₂ -O ₁₅	110.1
C ₃ -O ₁₃	1.390	C ₂ -C ₃ -C ₄	121.8
C ₄ -C ₅	1.401	C ₂ -C ₃ -O ₁₃	110.3
C ₄ -H ₁₇	1.082	C ₄ -C ₃ -O ₁₃	127.8
C ₅ -C ₆	1.409	C ₃ -C ₄ -C ₅	116.7
C ₅ -H ₁₈	1.083	C ₃ -C ₄ -H ₁₇	121.2
C ₆ -C ₇	1.486	C ₅ -C ₄ -H ₁₇	121.9
C ₇ -O ₈	1.251	C ₄ -C ₅ -C ₆	121.9
C ₇ -C ₉	1.531	C ₄ -C ₅ -H ₁₈	120.3
C ₉ -C ₁₀	1.561	C ₆ -C ₅ -H ₁₈	117.6
C ₉ -N ₁₁	1.452	C ₁ -C ₆ -C ₅	119.9
C ₉ -H ₁₉	1.099	C ₁ -C ₆ -C ₇	122.3
C ₁₀ -H ₂₀	1.095	C ₅ -C ₆ -C ₇	117.6
C ₁₀ -H ₂₁	1.094	C ₆ -C ₇ -O ₈	120.5
C ₁₀ -H ₂₂	1.095	C ₆ -C ₇ -C ₉	120.6
N ₁₁ -C ₁₂	1.452	O ₈ -C ₇ -C ₉	118.7
N ₁₁ -H ₂₃	1.012	C ₇ -C ₉ -C ₁₀	108.1
C ₁₂ -H ₂₄	1.094	C ₇ -C ₉ -N ₁₁	108.1
C ₁₂ -H ₂₅	1.106	C ₇ -C ₉ -H ₁₉	109.6
C ₁₂ -H ₂₆	1.098	H ₁₀ -C ₉ -N ₁₁	114.7
O ₁₃ -C ₁₄	1.476	C ₁₀ -C ₉ -H ₁₉	108.0
C ₁₄ -O ₁₅	1.471	N ₁₁ -C ₉ -H ₁₉	108.1
C ₁₄ -H ₂₇	1.090	C ₉ -C ₁₀ -H ₂₀	109.7
C ₁₄ -H ₂₈	1.090	C ₉ -C ₁₀ -H ₂₁	110.0
		C ₉ -C ₁₀ -H ₂₂	111.9
		H ₂₀ -C ₁₀ -H ₂₁	108.4
		H ₂₀ -C ₁₀ -H ₂₂	108.4
		H ₂₁ -C ₁₀ -H ₂₂	108.0
		C ₉ -N ₁₁ -C ₁₂	119.3
		C ₉ -N ₁₁ -H ₂₃	113.0
		C ₁₂ -N ₁₁ -H ₂₃	117.2
		N ₁₁ -C ₁₂ -H ₂₄	109.0
		N ₁₁ -C ₁₂ -H ₂₅	115.3
		N ₁₁ -C ₁₂ -H ₂₆	109.9
		H ₂₄ -C ₁₂ -H ₂₅	107.5
		H ₂₄ -C ₁₂ -H ₂₆	107.3
		H ₂₅ -C ₁₂ -H ₂₆	107.3
		C ₃ -O ₁₃ -C ₁₄	106.4
		O ₁₃ -C ₁₄ -O ₁₅	106.7
		O ₁₃ -C ₁₄ -H ₂₇	109.1
		O ₁₃ -C ₁₄ -H ₂₈	109.1
		O ₁₅ -C ₁₄ -H ₂₇	109.5
		O ₁₅ -C ₁₄ -H ₂₈	109.5
		H ₂₇ -C ₁₄ -H ₂₈	112.6
		C ₂ -O ₁₅ -C ₁₄	106.2

Table A10: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of 3-FMC.

s.no	Unscaled	Scaled	IR intensity	Raman intensity	Assignment
1	3597	3456	16.16	66.70	γ N ₁₂ -H ₂₂ (99),
2	3255	3128	1.091	75.63	γ [C ₁ -H ₁₄ (98)],
3	3248	3121	6.960	166.7	γ [C ₃ -H ₁₅ (49)], γ [C ₄ -H ₁₆ (14)], γ [C ₅ -H ₁₇ (34)],
4	3243	3116	0.611	57.20	γ [C ₃ -H ₁₅ (42)], γ [C ₅ -H ₁₇ (57)],
5	3217	3091	8.942	83.27	γ [C ₄ -H ₁₆ (85)],
6	3137	3014	20.33	73.60	γ [C ₁₁ -H ₁₉ (39)],
7	3131	3008	34.05	57.03	γ [C ₁₁ -H ₁₉ (24)], γ [C ₁₁ -H ₂₀ (12)], γ [C ₁₁ -H ₂₁ (63)],
8	3117	2995	36.61	117.6	γ [C ₁₁ -H ₂₀ (60)], γ [C ₁₃ -H ₂₅ (14)],
9	3051	2932	41.94	50.93	γ [C ₁₁ -H ₂₁ (30)], γ [C ₁₃ -H ₂₅ (15)],
10	3049	2930	36.17	143.8	[C ₁₃ -H ₂₃ (11)],
11	3027	2908	32.30	60.29	γ [C ₁₀ -H ₁₈ (98)],
12	2946	2831	122.4	127.7	γ [C ₁₃ -H ₂₄ (95)],
13	1682	1616	60.31	21.85	γ [O ₉ -C ₈ (56)], γ [C ₃ -C ₂ (10)],
14	1661	1596	1.327	180.8	γ [O ₉ -C ₈ (11)], γ [C ₂ -C ₁ (14)], γ [C ₅ -C ₄ (23)], γ [C ₆ -C ₁ (16)],
15	1637	1573	111.2	47.68	γ [C ₃ -C ₂ (29)],
16	1566	1504	20.12	16.07	β [H ₂₄ -C ₁₃ -H ₂₃ (23)], β [H ₂₅ -C ₁₃ -H ₂₄ (58)], τ [H ₂₄ -C ₁₃ -N ₁₂ -C ₁₀ (10)],
17	1545	1484	18.96	1.693	β [H ₁₉ -C ₁₁ -H ₂₁ (19)], β [H ₂₀ -C ₁₁ -H ₁₉ (11)], β [H ₂₁ -C ₁₁ -H ₂₀ (33)], β [H ₂₄ -C ₁₃ -H ₂₃ (17)],
18	1545	1487	10.00	14.95	β [H ₂₂ -N ₁₂ -C ₁₃ (15)],
19	1537	1477	5.795	16.45	β [H ₁₉ -C ₁₁ -H ₂₁ (18)],
20	1530	1470	8.009	26.83	β [H ₁₉ -C ₁₁ -H ₂₁ (24)], β [H ₂₀ -C ₁₁ -H ₁₉ (24)], β [H ₂₁ -C ₁₁ -H ₂₀ (10)], β [H ₂₄ -C ₁₃ -H ₂₃ (20)],
21	1516	1456	43.38	14.60	β [H ₂₂ -N ₁₂ -C ₁₃ (41)], β [H ₂₃ -C ₁₃ -H ₂₅ (11)],
22	1497	1438	7.171	24.70	β [H ₂₃ -C ₁₃ -H ₂₅ (62)], β [H ₂₄ -C ₁₃ -H ₂₃ (11)],
23	1485	1427	16.07	2.102	γ [C ₂ -C ₁ (18)], γ [C ₆ -C ₁ (22)], β [H ₁₅ -C ₃ -C ₄ (13)], β [H ₁₇ -C ₅ -C ₄ (11)],
24	1438	1381	12.50	14.66	β [H ₁₉ -C ₁₁ -H ₂₁ (33)], β [H ₁₉ -C ₁₁ -H ₂₁ (19)], β [H ₂₀ -C ₁₁ -H ₁₉ (33)], β [H ₂₁ -C ₁₁ -H ₂₀ (30)],
25	1401	1346	20.82	13.20	β [H ₁₈ -C ₁₀ -N ₁₂ (44)],
26	1382	1328	2.814	1.170	γ [C ₅ -C ₄ (23)], γ [C ₄ -C ₃ (19)],
27	1352	1299	52.14	9.235	τ [H ₁₈ -C ₁₀ -C ₈ -C ₆ (38)],
28	1337	1284	15.83	3.851	β [H ₁₄ -C ₁ -C ₂ (24)], β [H ₁₄ -C ₁ -C ₂ (11)], τ [H ₁₈ -C ₁₀ -C ₈ -C ₆ (11)],
29	1294	1243	106.2	60.04	γ [C ₈ -C ₆ (16)], γ [F ₇ -C ₂ (11)]
30	1263	1213	49.27	4.093	γ [N ₁₂ -C ₁₀ (31)], γ [F ₇ -C ₂ (10)]
31	1222	1174	15.60	3.532	β [H ₁₄ -C ₁ -C ₂ (11)], β [H ₁₆ -C ₄ -C ₅ (36)], β [H ₁₇ -C ₅ -C ₄ (19)],
32	1199	1152	87.60	6.438	γ [N ₁₂ -C ₁₃ (11)], γ [F ₇ -C ₂ (12)], β [H ₁₄ -C ₁ -C ₂ (22)], β [H ₁₄ -C ₁ -C ₂ (13)],
33	1188	1141	21.19	7.353	γ [N ₁₂ -C ₁₃ (36)], τ [H ₂₄ -C ₁₃ -N ₁₂ -C ₁₀ (20)],
34	1173	1127	1.402	5.493	β [H ₂₃ -C ₁₃ -H ₂₅ (13)], τ [H ₂₃ -C ₁₃ -N ₁₂ -C ₁₀ (18)], τ [H ₂₅ -C ₁₃ -N ₁₂ -C ₁₀ (50)],

Continued **Table A10:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of 3-FMC.

s.no	Unscaled	Scaled	IR intensity	Raman intensity	Assignment
35	1125	1081	10.11	2.523	γ [C_4-C_3 (16)], β [$H_{14}-C_1-C_2$ (20)],
36	1112	1068	7.038	21.29	τ [$H_{19}-C_{11}-C_{10}-N_{12}$ (14)], τ [$H_{20}-C_{11}-C_{10}-N_{12}$ (10)],
37	1073	1031	3.359	7.482	τ [$H_{18}-C_{10}-C_8-C_6$ (19)], τ [$H_{20}-C_{11}-C_{10}-N_{12}$ (16)], τ [$H_{21}-C_{11}-C_{10}-N_{12}$ (14)],
38	1037	996	10.63	34.39	β [$C_3-C_2-C_1$ (11)], β [$C_5-C_4-C_3$ (30)], β [$C_4-C_3-C_2$ (10)],
39	1032	991	1.417	0.260	τ [$H_{16}-C_4-C_3-C_2$ (43)], τ [$H_{17}-C_5-C_4-C_3$ (34)], τ [$C_5-C_4-C_3-C_2$ (14)],
40	1026	985	15.81	6.265	γ [$C_{11}-C_{10}$ (13)], τ [$H_{19}-C_{11}-C_{10}-N_{12}$ (10)],
41	1009	969	45.77	6.224	γ [$C_{10}-C_8$ (12)], γ [$C_{11}-C_{10}$ (17)]
42	963	925	0.406	2.265	τ [$H_{15}-N_3-C_4-C_5$ (49)], τ [$H_{17}-C_5-C_4-C_3$ (34)],
43	915	879	28.65	6.588	γ [F_7-C_2 (14)], τ [$H_{14}-N_1-C_2-C_3$ (13)],
44	906	870	28.11	1.262	τ [$H_{14}-N_1-C_2-C_3$ (56)],
45	858	824	12.92	7.319	γ [$N_{12}-C_{10}$ (12)], γ [$C_{11}-C_{10}$ (33)]
46	836	803	29.22	2.226	τ [$H_{15}-N_3-C_4-C_5$ (24)], τ [$H_{16}-C_4-C_3-C_2$ (34)],
47	776	745	16.79	2.300	τ [$H_{21}-C_{11}-C_{10}-N_{12}$ (13)], ρ_o [$O_9-C_{10}-C_6-C_8$ (16)], ρ_o [$C_{11}-N_{12}-C_8-C_{10}$ (10)]
48	752	722	29.35	6.471	γ [$C_{11}-C_{10}$ (10)], ρ_o [$O_9-C_{10}-C_6-C_8$ (18)],
49	691	664	4.736	2.098	τ [$C_5-C_4-C_3-C_2$ (18)], τ [$C_4-C_3-C_2-C_1$ (14)], τ [$C_6-C_1-C_2-C_3$ (22)],
50	685	658	3.707	5.254	β [$O_9-C_8-C_6$ (12)], β [$C_4-C_3-C_2$ (11)], τ [$C_5-C_4-C_3-C_2$ (11)], τ [$C_6-C_1-C_2-C_3$ (13)],
51	565	542	74.11	1.039	β [$C_{10}-C_8-C_6$ (12)], τ [$H_{22}-N_{12}-C_{10}-C_{11}$ (44)],
52	541	519	0.758	0.331	τ [$C_4-C_3-C_2-C_1$ (15)], τ [$C_6-C_1-C_2-C_3$ (11)], ρ_o [$F_7-C_1-C_3-C_2$ (34)],
53	532	511	19.32	4.773	γ [F_7-C_2 (14)], β [$C_3-C_2-C_1$ (25)], [$H_{22}-N_{12}-C_{10}-C_{11}$ (14)],
54	492	472	50.53	3.868	β [$C_8-C_6-C_1$ (10)], β [$F_7-C_2-C_3$ (11)], [$H_{22}-N_{12}-C_{10}-C_{11}$ (14)],
55	461	443	10.10	1.337	β [$C_{11}-C_{10}-N_{12}$ (12)], τ [$C_5-C_4-C_3-C_2$ (15)],
56	448	430	3.049	0.562	β [$C_{11}-C_{10}-N_{12}$ (19)]
57	386	370	8.817	3.528	β [$O_9-C_8-C_6$ (35)], β [$F_7-C_2-C_3$ (18)]
58	371	356	3.541	2.147	β [$C_{10}-C_8-C_6$ (12)], β [$F_7-C_2-C_3$ (27)]
59	305	293	2.310	4.558	γ [C_8-C_6 (15)], β [$C_6-C_1-C_2$ (17)], β [$C_{13}-N_{12}-C_{10}$ (10)]
60	260	249	1.342	0.272	β [$C_{11}-C_{10}-N_{12}$ (27)], ρ_o [$C_{11}-N_{12}-C_8-C_{10}$ (14)]
61	248	238	1.258	2.954	τ [$C_4-C_3-C_2-C_1$ (35)], τ [$C_6-C_1-C_2-C_3$ (11)], ρ_o [$F_7-C_1-C_3-C_2$ (27)]
62	230	221	1.984	1.168	β [$N_{12}-C_{10}-C_8$ (11)], τ [$H_{19}-C_{11}-C_{10}-N_{12}$ (19)], τ [$H_{20}-C_{11}-C_{10}-N_{12}$ (14)], τ [$H_{21}-C_{11}-C_{10}-N_{12}$ (12)], ρ_o [$C_{11}-N_{12}-C_8-C_{10}$ (11)]
63	224	215	9.514	0.588	β [$C_8-C_6-C_1$ (19)], β [$N_{12}-C_{10}-C_8$ (18)], β [$C_{13}-N_{12}-C_{10}$ (13)]

Table A10: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of 3-FMC.

s.no	Unscaled	Scaled	IR intensity	Raman intensity	Assignment
64	196	188	1.982	0.591	τ [H ₂₃ -C ₁₃ -N ₁₂ -C ₁₀ (41)], τ [H ₂₄ -C ₁₃ -N ₁₂ -C ₁₀ (18)],
65	149	143	0.636	3.870	τ [C ₆ -C ₁ -C ₂ -C ₃ (12)], ρ_e [O ₉ -C ₁₀ -C ₆ -C ₈ (15)], ρ_o [C ₈ -C ₅ -C ₁ -C ₆ (37)]
66	129	123	1.637	0.152	β [C ₈ -C ₆ -C ₁ (13)], β [C ₁₀ -C ₈ -C ₆ (13)], τ [N ₁₃ -C ₁₂ -C ₁₀ -C ₁₁ (32)],
67	94	90	0.779	1.003	β [C ₈ -C ₆ -C ₁ (13)], β [C ₁₀ -C ₈ -C ₆ (24)], τ [N ₁₃ -C ₁₂ -C ₁₀ -C ₁₁ (30)],
68	53	50	0.440	1.370	τ [N ₁₂ -C ₁₀ -C ₈ -C ₆ (50)], τ [C ₉ -C ₁₀ -C ₆ -C ₅ (19)],
69	35	33	2.638	3.423	τ [N ₁₂ -C ₁₀ -C ₈ -C ₆ (12)],

Table A11: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of 4-FMC.

s.no	Unscaled	Scaled	IR intensity	Raman intensity	Assignment
1	3533	3395	0.5854	67.24	γ N ₁ -H ₂₂ (99),
2	3258	3121	3.097	113.29	γ [C ₁ -H ₁₄ (81)], γ [C ₁ -H ₁₄ (17)]
3	3248	3112	5.217	119.33	γ [C ₃ -H ₁₅ (62)], γ [C ₄ -H ₁₆ (36)], γ [C ₅ -H ₁₇ (34)],
4	3239	3106	2.189	90.25	γ [C ₃ -H ₁₅ (42)], γ [C ₅ -H ₁₇ (57)],
5	3233	3022	0.216	35.31	γ [C ₄ -H ₁₆ (62)],
6	3145	3008	19.99	44.22	γ [C ₁₁ -H ₁₉ (72)],
7	3131	3005	24.36	83.41	γ [C ₁₁ -H ₁₉ (24)], γ [C ₁₁ -H ₂₀ (12)], γ [C ₁₁ -H ₂₁ (63)],
8	3127	2952	33.72	75.23	γ [C ₁₁ -H ₂₀ (60)], γ [C ₁₃ -H ₂₅ (14)],
9	3072	2938	39.99	63.08	γ [C ₁₁ -H ₂₁ (30)], γ [C ₁₃ -H ₂₅ (15)],
10	3058	2908	21.66	137.08	[C ₁₃ -H ₂₃ (11)],
11	3027	2859	22.56	49.05	γ [C ₁₀ -H ₁₈ (98)],
12	2976	1614	104.2	133.4	γ [C ₁₃ -H ₂₄ (95)],
13	1680	1591	71.51	22.68	γ [O ₉ -C ₈ (56)], γ [C ₃ -C ₂ (10)],
14	1656	1570	136.8	131.3	γ [O ₉ -C ₈ (11)], γ [C ₂ -C ₁ (14)], γ [C ₅ -C ₄ (23)], γ [C ₆ -C ₁ (16)],
15	1634	1503	51.45	40.22	γ [C ₃ -C ₂ (29)],
16	1564	1498	1.504	10.71	β [H ₂₄ -C ₁₃ -H ₂₃ (23)], β [H ₂₅ -C ₁₃ -H ₂₄ (58)], τ [H ₂₄ -C ₁₃ -N ₁₂ -C ₁₀ (10)],
17	1559	1482	28.26	12.41	β [H ₁₉ -C ₁₁ -H ₂₁ (19)], β [H ₂₀ -C ₁₁ -H ₁₉ (11)], β [H ₂₁ -C ₁₁ -H ₂₀ (33)], β [H ₂₄ -C ₁₃ -H ₂₃ (17)],
18	1543	1474	6.240	19.34	β [H ₂₂ -N ₁₂ -C ₁₃ (15)],
19	1534	1466	5.545	8.747	β [H ₁₉ -C ₁₁ -H ₂₁ (18)],
20	1526	1456	7.512	23.83	β [H ₁₉ -C ₁₁ -H ₂₁ (24)], β [H ₂₀ -C ₁₁ -H ₁₉ (24)], β [H ₂₁ -C ₁₁ -H ₂₀ (10)], β [H ₂₄ -C ₁₃ -H ₂₃ (20)],
21	1516	1437	10.26	5.191	β [H ₂₂ -N ₁₂ -C ₁₃ (41)], β [H ₂₃ -C ₁₃ -H ₂₅ (11)],
22	1496	1400	2.774	14.42	β [H ₂₃ -C ₁₃ -H ₂₅ (62)], β [H ₂₄ -C ₁₃ -H ₂₃ (11)],
23	1457	1395	17.34	6.001	γ [C ₂ -C ₁ (18)], γ [C ₆ -C ₁ (22)], β [H ₁₅ -C ₃ -C ₄ (13)], β [H ₁₇ -C ₅ -C ₄ (11)],

Continued **Table A11:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of 4-FMC.

s.no	Unscaled	Scaled	IR intensity	Raman intensity	Assignment
24	1452	1399	15.32	2.839	β [H ₁₉ -C ₁₁ -H ₂₁ (33)], β [H ₁₉ -C ₁₁ -H ₂₁ (19)], β [H ₂₀ -C ₁₁ -H ₁₉ (33)], β [H ₂₁ -C ₁₁ -H ₂₀ (30)],
25	1385	1330	10.18	7.488	β [H ₁₈ -C ₁₀ -N ₁₂ (44)],
26	1378	1324			γ [C ₅ -C ₄ (23)], γ [C ₄ -C ₃ (19)],
27	1368	1314	11.19	3.351	τ [H ₁₈ -C ₁₀ -C ₈ -C ₆ (38)],
28	1355	1302	0.868	0.727	β [H ₁₄ -C ₁ -C ₂ (24)], β [H ₁₄ -C ₁ -C ₂ (11)], τ [H ₁₈ -C ₁₀ -C ₈ -C ₆ (11)],
29	1271	1221	177.9	51.45	γ [C ₈ -C ₆ (16)], γ [F ₇ -C ₂ (11)]
30	1266	1216	15.613	1.513	γ [N ₁₂ -C ₁₀ (31)], γ [F ₇ -C ₂ (10)]
31	1219	1171	12.59	1.764	β [H ₁₄ -C ₁ -C ₂ (11)], β [H ₁₆ -C ₄ -C ₅ (36)], β [H ₁₇ -C ₅ -C ₄ (19)],
32	1208	1160	79.58	10.40	γ [N ₁₂ -C ₁₃ (11)], γ [F ₇ -C ₂ (12)], β [H ₁₄ - C ₁ -C ₂ (22)], β [H ₁₄ -C ₁ -C ₂ (13)],
33	1171	1125	27.46	3.797	γ [N ₁₂ -C ₁₃ (36)], τ [H ₂₄ -C ₁₃ -N ₁₂ -C ₁₀ (20)],
34	1158	1112	30.40	6.805	β [H ₂₃ -C ₁₃ -H ₂₅ (13)], τ [H ₂₃ -C ₁₃ -N ₁₂ - C ₁₀ (18)], τ [H ₂₅ -C ₁₃ -N ₁₂ -C ₁₀ (50)],
35	1147	1102	4.449	2.100	γ [C ₄ -C ₃ (16)], β [H ₁₄ -C ₁ -C ₂ (20)],
36	1125	1081	12.20	12.78	τ [H ₁₉ -C ₁₁ -C ₁₀ -N ₁₂ (14)], τ [H ₂₀ -C ₁₁ -C ₁₀ - N ₁₂ (10)],
37	1092	1049	2.769	9.369	τ [H ₁₈ -C ₁₀ -C ₈ -C ₆ (19)], τ [H ₂₀ -C ₁₁ -C ₁₀ - N ₁₂ (16)], τ [H ₂₁ -C ₁₁ -C ₁₀ -N ₁₂ (14)],
38	1053	1011	3.835	1.007	β [C ₃ -C ₂ -C ₁ (11)], β [C ₅ -C ₄ -C ₃ (30)], β [C ₄ -C ₃ -C ₂ (10)],
39	1051	1010	11.65	1.115	τ [H ₁₆ -C ₄ -C ₃ -C ₂ (43)], τ [H ₁₇ -C ₅ -C ₄ - C ₃ (34)], τ [C ₅ -C ₄ -C ₃ -C ₂ (14)],
40	1021	981	0.403	0.915	γ [C ₁₁ -C ₁₀ (13)], τ [H ₁₉ -C ₁₁ -C ₁₀ -N ₁₂ (10)],
41	992	953	1.489	1.993	γ [C ₁₀ -C ₈ (12)], γ [C ₁₁ -C ₁₀ (17)]
42	986	947	63.89	7.761	τ [H ₁₅ -N ₃ -C ₄ -C ₅ (49)], τ [H ₁₇ -C ₅ -C ₄ - C ₃ (34)],
43	892	857	22.75	3.431	γ [F ₇ -C ₂ (14)], τ [H ₁₄ -N ₁ -C ₂ -C ₃ (13)],
44	875	840	48.77	2.810	τ [H ₁₄ -N ₁ -C ₂ -C ₃ (56)],
45	855	821	3.264	5.593	γ [N ₁₂ -C ₁₀ (12)], γ [C ₁₁ -C ₁₀ (33)]
46	837	804	14.09	32.89	τ [H ₁₅ -N ₃ -C ₄ -C ₅ (24)], τ [H ₁₆ -C ₄ -C ₃ - C ₂ (34)],
47	788	757	17.58	2.426	τ [H ₂₁ -C ₁₁ -C ₁₀ -N ₁₂ (13)], ρ_o [O ₉ -C ₁₀ -C ₆ - C ₈ (16)], ρ_o [C ₁₁ -N ₁₂ -C ₈ -C ₁₀ (10)]
48	744	714	12.68	1.145	γ [C ₁₁ -C ₁₀ (10)], ρ_o [O ₉ -C ₁₀ -C ₆ -C ₈ (18)],
49	694	666	29.84	0.745	τ [C ₅ -C ₄ -C ₃ -C ₂ (18)], τ [C ₄ -C ₃ -C ₂ -C ₁ (14)], τ [C ₆ -C ₁ -C ₂ -C ₃ (22)],
50	661	635	4.039	8.884	β [O ₉ -C ₈ -C ₆ (12)], β [C ₄ -C ₃ -C ₂ (11)], τ [C ₅ -C ₄ -C ₃ -C ₂ (11)], τ [C ₆ -C ₁ -C ₂ -C ₃ (13)],
51	640	615	56.65	4.157	β [C ₁₀ -C ₈ -C ₆ (12)], τ [H ₂₂ -N ₁₂ -C ₁₀ -C ₁₁ (44)],
52	600	576	109.4	0.531	τ [C ₄ -C ₃ -C ₂ -C ₁ (15)], τ [C ₆ -C ₁ -C ₂ -C ₃ (11)], ρ_o [F ₇ -C ₁ -C ₃ -C ₂ (34)],
53	532	511	0.754	1.334	γ [F ₇ -C ₂ (14)], β [C ₃ -C ₂ -C ₁ (25)], [H ₂₂ -N ₁₂ - C ₁₀ -C ₁₁ (14)],

Table A11: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of 4-FMC.

s.no	Unscaled	Scaled	IR intensity	Raman intensity	Assignment
54	505	485	8.874	0.330	β [C ₈ -C ₆ -C ₁ (10)], β [F ₇ -C ₂ -C ₃ (11)], [H ₂₂ -N ₁₂ -C ₁₀ -C ₁₁ (14)],
55	434	417	0.607	0.042	β [C ₁₁ -C ₁₀ -N ₁₂ (12)], τ [C ₅ -C ₄ -C ₃ -C ₂ (15)],
56	422	405	3.997	1.869	β [C ₁₁ -C ₁₀ -N ₁₂ (19)]
57	400	384	3.563	1.919	β [O ₉ -C ₈ -C ₆ (35)], β [F ₇ -C ₂ -C ₃ (18)]
58	369	354	4.459	1.755	β [C ₁₀ -C ₈ -C ₆ (12)], β [F ₇ -C ₂ -C ₃ (27)]
59	317	304	0.078	3.735	γ [C ₈ -C ₆ (15)], β [C ₆ -C ₁ -C ₂ (17)], β [C ₁₃ -N ₁₂ -C ₁₀ (10)]
60	293	281	8.836	0.159	β [C ₁₁ -C ₁₀ -N ₁₂ (27)], ρ_o [C ₁₁ -N ₁₂ -C ₈ -C ₁₀ (14)]
61	279	268	0.992	1.817	τ [C ₄ -C ₃ -C ₂ -C ₁ (35)], τ [C ₆ -C ₁ -C ₂ -C ₃ (11)], ρ_o [F ₇ -C ₁ -C ₃ -C ₂ (27)]
62	220	211	0.825	0.665	β [N ₁₂ -C ₁₀ -C ₈ (11)], τ [H ₁₉ -C ₁₁ -C ₁₀ -N ₁₂ (19)], τ [H ₂₀ -C ₁₁ -C ₁₀ -N ₁₂ (14)], τ [H ₂₁ -C ₁₁ -C ₁₀ -N ₁₂ (12)], ρ_o [C ₁₁ -N ₁₂ -C ₈ -C ₁₀ (11)]
63	215	206	0.842	0.162	β [C ₈ -C ₆ -C ₁ (19)], β [N ₁₂ -C ₁₀ -C ₈ (18)], β [C ₁₃ -N ₁₂ -C ₁₀ (13)]
64	193	185	0.827	0.273	τ [H ₂₃ -C ₁₃ -N ₁₂ -C ₁₀ (41)], τ [H ₂₄ -C ₁₃ -N ₁₂ -C ₁₀ (18)],
65	139	133	0.794	0.180	τ [C ₆ -C ₁ -C ₂ -C ₃ (12)], ρ_o [O ₉ -C ₁₀ -C ₆ -C ₈ (15)], ρ_o [C ₈ -C ₅ -C ₁ -C ₆ (37)]
66	103	98	3.755	0.178	β [C ₈ -C ₆ -C ₁ (13)], β [C ₁₀ -C ₈ -C ₆ (13)], τ [N ₁₃ -C ₁₂ -C ₁₀ -C ₁₁ (32)],
67	78	74	0.852	0.485	β [C ₈ -C ₆ -C ₁ (13)], β [C ₁₀ -C ₈ -C ₆ (24)], τ [N ₁₃ -C ₁₂ -C ₁₀ -C ₁₁ (30)],
68	46	44	0.445	5.361	τ [N ₁₂ -C ₁₀ -C ₈ -C ₆ (50)], τ [C ₉ -C ₁₀ -C ₆ -C ₅ (19)],
69	36	34	1.847	1.437	τ [N ₁₂ -C ₁₀ -C ₈ -C ₆ (12)],

Table A12: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Butylone.

Calculated Wavenumber (cm ⁻¹)		IR intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
3513	3379	1.44	62.67	ν (N ₁₅ -H ₂₈)(99)
3265	3141	1.43	60.22	ν (C ₁ -H ₁₇)(99)
3252	3128	5.43	137.1	ν (C ₄ -H ₁₈)(65), ν (C ₅ -H ₁₉)(34)
3237	3114	0.38	39.22	ν (C ₅ -H ₁₉)(65), ν (C ₄ -H ₁₈)(35)
3170	3049	31.12	161.3	ν (C ₁₁ -H ₂₁)(51), ν (C ₁₁ -H ₂₂)(49)
3128	3009	36.12	111.6	ν (C ₁₆ -H ₂₉)(70), ν (C ₁₆ -H ₃₁)(27)
3127	3008	53.35	39.10	ν (C ₁₄ -H ₂₇)(51), ν (C ₁₃ -H ₂₃)(18), ν (C ₁₄ -H ₂₅)(18)
3116	2998	46.45	72.35	ν (C ₁₄ -H ₂₅)(53), ν (C ₁₄ -H ₂₆)(32)
3099	2981	2.47	127.1	ν (C ₁₃ -H ₂₃)(40), ν (C ₁₄ -H ₂₇)(20), ν (C ₉ -H ₂₀)(16), ν (C ₁₄ -H ₂₆)(14)
3097	2980	89.63	261.1	ν (C ₉ -H ₂₀)(77), ν (C ₁₁ -H ₂₂)(51), ν (C ₁₁ -H ₂₁)(49)
3085	2968	20.44	48.28	ν (C ₁₃ -H ₂₃)(19)
3077	2960	44.61	83.97	ν (C ₁₆ -H ₃₁)(68), ν (C ₁₆ -H ₂₉)(25)
3045	2929	24.90	45.70	ν (C ₁₃ -H ₂₄)(71), ν (C ₁₃ -H ₂₃)(15)

Continued **Table A12:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Butylone.

Calculated Wavenumber (cm ⁻¹)		IR intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
3043	2927	16.19	153.3	$\nu(\text{C}_{14}\text{-H}_{26})(45)$, $\nu(\text{C}_{14}\text{-H}_{27})(24)$, $\nu(\text{C}_{14}\text{-H}_{25})(21)$
2965	2853	83.80	88.70	$\nu(\text{C}_{16}\text{-H}_{30})(63)$
1682	1618	17.19	9.33	$\nu(\text{O}_{8}\text{-C}_7)(27)$, $\nu(\text{C}_2\text{-C}_1)(24)$, $\nu(\text{C}_6\text{-C}_5)(13)$, $\nu(\text{C}_3\text{-C}_2)(11)$
1654	1591	15.46	113.1	$\nu(\text{C}_4\text{-C}_3)(37)$, $\nu(\text{C}_2\text{-C}_1)(14)$, $\beta(\text{C}_3\text{-C}_2\text{-C}_1)(12)$
1636	1574	157.8	219.1	$\nu(\text{O}_{8}\text{-C}_7)(54)$
1572	1512	0.05	36.05	$\beta(\text{H}_{22}\text{-C}_{11}\text{-H}_{21})(93)$
1562	1503	16.31	19.90	$\beta(\text{H}_{28}\text{-N}_{15}\text{-C}_{16})(11)$, $\beta(\text{H}_{30}\text{-C}_{16}\text{-H}_{29})(35)$, $\tau(\text{H}_{30}\text{-C}_{16}\text{-N}_{15}\text{-C}_9)(17)$
1550	1491	12.73	20.03	$\beta(\text{H}_{25}\text{-C}_{14}\text{-H}_{27})(46)$, $\beta(\text{H}_{26}\text{-C}_{14}\text{-H}_{25})(26)$, $\tau(\text{H}_{25}\text{-C}_{14}\text{-C}_{13}\text{-C}_9)(13)$
1547	1488	9.57	6.17	$\beta(\text{H}_{27}\text{-C}_{14}\text{-H}_{26})(39)$, $\beta(\text{H}_{26}\text{-C}_{14}\text{-H}_{25})(20)$, $\beta(\text{H}_{24}\text{-C}_{13}\text{-H}_{23})(18)$, $\tau(\text{H}_{26}\text{-C}_{14}\text{-C}_{13}\text{-C}_9)(10)$
1541	1482	60.98	8.44	$\beta(\text{H}_{28}\text{-N}_{15}\text{-C}_{16})(27)$, $\beta(\text{H}_{30}\text{-C}_{16}\text{-H}_{29})(13)$
1536	1477	3.63	16.99	$\beta(\text{H}_{24}\text{-C}_{13}\text{-H}_{23})(30)$, $\beta(\text{H}_{30}\text{-C}_{16}\text{-H}_{29})(12)$, $\beta(\text{H}_{29}\text{-C}_{16}\text{-H}_{31})(11)$
1535	1476	37.57	24.73	$\beta(\text{H}_{24}\text{-C}_{13}\text{-H}_{23})(28)$, $\beta(\text{H}_{30}\text{-C}_{16}\text{-H}_{29})(13)$, $\beta(\text{H}_{29}\text{-C}_{16}\text{-H}_{31})(11)$
1532	1474	32.45	5.76	$\beta(\text{H}_{28}\text{-N}_{15}\text{-C}_{16})(34)$
1498	1441	2.07	12.25	$\beta(\text{H}_{29}\text{-C}_{16}\text{-H}_{31})(58)$, $\beta(\text{H}_{30}\text{-C}_{16}\text{-H}_{29})(15)$
1482	1426	60.69	21.24	$\nu(\text{C}_2\text{-C}_1)(20)$, $\nu(\text{C}_5\text{-C}_4)(18)$, $\beta(\text{H}_{19}\text{-C}_5\text{-C}_6)(20)$
1464	1408	1.86	4.40	$\beta(\text{H}_{26}\text{-C}_{14}\text{-H}_{25})(34)$, $\beta(\text{H}_{25}\text{-C}_{14}\text{-H}_{27})(33)$, $\beta(\text{H}_{27}\text{-C}_{14}\text{-H}_{26})(32)$
1417	1363	8.98	11.53	$\tau(\text{H}_{22}\text{-C}_{11}\text{-O}_{12}\text{-C}_2)(34)$, $\tau(\text{H}_{21}\text{-C}_{11}\text{-O}_{12}\text{-C}_2)(20)$
1412	1359	34.29	26.08	$\beta(\text{H}_{20}\text{-C}_9\text{-N}_{15})(30)$, $\tau(\text{H}_{24}\text{-C}_{13}\text{-C}_9\text{-N}_{15})(10)$
1396	1343	19.92	33.57	$\nu(\text{C}_6\text{-C}_5)(34)$, $\nu(\text{C}_3\text{-C}_2)(11)$
1374	1322	4.36	5.15	$\beta(\text{H}_{20}\text{-C}_9\text{-N}_{15})(20)$, $\tau(\text{H}_{24}\text{-C}_{13}\text{-C}_9\text{-N}_{15})(14)$, $\tau(\text{H}_{23}\text{-C}_{13}\text{-C}_9\text{-N}_{15})(11)$
1346	1295	4.09	12.53	$\beta(\text{H}_{23}\text{-C}_{13}\text{-C}_{14})(30)$, $\tau(\text{H}_{20}\text{-C}_9\text{-C}_7\text{-C}_6)(34)$
1321	1270	12.24	4.54	$\beta(\text{H}_{17}\text{-C}_1\text{-C}_6)(27)$, $\beta(\text{H}_{18}\text{-C}_4\text{-C}_5)(18)$, $\beta(\text{H}_{19}\text{-C}_5\text{-C}_6)(17)$
1297	1248	252.6	24.11	$\nu(\text{C}_5\text{-C}_4)(12)$, $\beta(\text{H}_{23}\text{-C}_{13}\text{-C}_{14})(17)$
1285	1236	245.5	38.74	$\nu(\text{C}_5\text{-C}_4)(12)$, $\tau(\text{H}_{20}\text{-C}_9\text{-C}_7\text{-C}_6)(12)$
1252	1204	30.50	0.83	$\nu(\text{C}_7\text{-C}_6)(11)$, $\nu(\text{O}_{10}\text{-C}_3)(11)$, $\beta(\text{H}_{17}\text{-C}_1\text{-C}_6)(18)$
1230	1183	2.99	12.37	$\nu(\text{N}_{15}\text{-C}_9)(10)$, $\tau(\text{H}_{30}\text{-C}_{16}\text{-N}_{15}\text{-C}_9)(17)$
1180	1136	3.69	3.46	$\nu(\text{C}_5\text{-C}_4)(13)$, $\beta(\text{H}_{19}\text{-C}_5\text{-C}_6)(26)$, $\beta(\text{H}_{18}\text{-C}_4\text{-C}_5)(25)$
1174	1130	21.43	2.79	$\nu(\text{N}_{15}\text{-C}_{16})(10)$, $\beta(\text{H}_{29}\text{-C}_{16}\text{-H}_{31})(11)$, $\tau(\text{H}_{31}\text{-C}_{16}\text{-N}_{15}\text{-C}_9)(33)$, $\tau(\text{H}_{29}\text{-C}_{16}\text{-N}_{15}\text{-C}_9)(17)$
1168	1123	0.01	10.84	$\beta(\text{H}_{21}\text{-C}_{11}\text{-O}_{12})(58)$, $\tau(\text{H}_{22}\text{-C}_{11}\text{-O}_{12}\text{-C}_2)(31)$
1155	1111	18.13	5.89	$\nu(\text{N}_{15}\text{-C}_9)(24)$, $\nu(\text{N}_{15}\text{-C}_{16})(10)$
1134	1091	1.75	1.43	$\tau(\text{H}_{21}\text{-C}_{11}\text{-O}_{12}\text{-C}_2)(36)$, $\tau(\text{H}_{26}\text{-C}_{14}\text{-C}_{13}\text{-C}_9)(29)$
1117	1075	9.83	1.61	$\beta(\text{H}_{21}\text{-C}_{11}\text{-O}_{12})(40)$, $\tau(\text{C}_{11}\text{-O}_{12}\text{-C}_2\text{-C}_1)(17)$
1115	1072	36.94	4.59	$\beta(\text{C}_3\text{-C}_2\text{-C}_1)(12)$
1105	1063	45.03	12.01	$\beta(\text{C}_3\text{-C}_2\text{-C}_1)(15)$
1065	1025	2.43	7.13	$\nu(\text{C}_{14}\text{-C}_{13})(46)$, $\nu(\text{C}_{13}\text{-C}_9)(18)$
1021	982	128.5	3.89	$\nu(\text{O}_{12}\text{-C}_{11})(28)$, $\beta(\text{C}_{11}\text{-O}_{12}\text{-C}_2)(16)$, $\beta(\text{O}_{10}\text{-C}_3\text{-C}_4)(12)$, $\beta(\text{O}_{12}\text{-C}_2\text{-C}_3)(12)$
1010	972	33.37	3.05	$\tau(\text{H}_{19}\text{-C}_5\text{-C}_6\text{-C}_7)(25)$
1007	969	24.22	3.15	$\tau(\text{H}_{19}\text{-C}_5\text{-C}_6\text{-C}_7)(37)$, $\tau(\text{H}_{18}\text{-C}_4\text{-C}_5\text{-C}_6)(11)$, $\tau(\text{C}_6\text{-C}_5\text{-C}_4\text{-C}_3)(12)$
990	953	22.22	1.70	$\nu(\text{C}_{14}\text{-C}_{13})(15)$, $\nu(\text{N}_{15}\text{-C}_{16})(10)$, $\nu(\text{C}_9\text{-C}_7)(10)$
930	895	9.11	6.67	$\nu(\text{C}_{13}\text{-C}_9)(11)$, $\tau(\text{H}_{27}\text{-C}_{14}\text{-C}_{13}\text{-C}_9)(11)$
907	873	9.91	2.35	$\nu(\text{O}_{12}\text{-C}_2)(11)$, $\tau(\text{H}_{17}\text{-C}_1\text{-C}_6\text{-C}_7)(34)$

Continued **Table A12:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Butylone.

Calculated Wavenumber (cm ⁻¹)		IR intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
896	862	9.42	3.08	$\Gamma(\text{H}_{17}-\text{C}_1-\text{C}_6-\text{C}_7)$ (41)
877	844	47.25	2.83	$\nu(\text{C}_{13}-\text{C}_9)$ (36), $\beta(\text{C}_{11}-\text{O}_{12}-\text{C}_2)$ (21), $\beta(\text{O}_{10}-\text{C}_3-\text{C}_4)$ (12)
869	836	26.01	1.48	$\Gamma(\text{H}_{18}-\text{C}_4-\text{C}_5-\text{C}_6)$ (56), $\Gamma(\text{H}_{19}-\text{C}_5-\text{C}_6-\text{C}_7)$ (27)
849	817	17.00	2.85	$\Gamma(\text{H}_{25}-\text{C}_{14}-\text{C}_{13}-\text{C}_9)$ (16)
816	785	14.56	23.51	$\nu(\text{C}_3-\text{C}_2)$ (29), $\nu(\text{O}_{10}-\text{C}_3)$ (15), $\nu(\text{C}_2-\text{C}_1)$ (11)
773	744	14.38	7.34	$\gamma(\text{O}_8-\text{C}_9-\text{C}_6-\text{C}_7)$ (17), $\gamma(\text{C}_7-\text{C}_1-\text{C}_5-\text{C}_6)$ (16)
752	724	19.02	3.07	$\Gamma(\text{H}_{23}-\text{C}_{13}-\text{C}_9-\text{N}_{15})$ (11)
720	693	44.56	3.35	$\beta(\text{O}_{12}-\text{C}_2-\text{C}_3)$ (26), $\beta(\text{C}_{11}-\text{O}_{12}-\text{C}_2)$ (20), $\beta(\text{O}_{10}-\text{C}_3-\text{C}_4)$ (15)
711	684	7.11	2.47	$\Gamma(\text{C}_6-\text{C}_5-\text{C}_4-\text{C}_3)$ (18), $\Gamma(\text{C}_4-\text{C}_3-\text{C}_2-\text{C}_1)$ (14), $\Gamma(\text{C}_5-\text{C}_4-\text{C}_3-\text{C}_2)$ (11), $\gamma(\text{O}_{10}-\text{C}_2-\text{C}_4-\text{C}_3)$ (14), $\gamma(\text{O}_{12}-\text{C}_1-\text{C}_3-\text{C}_2)$ (15)
707	680	143.5	21.37	$\Gamma(\text{H}_{28}-\text{N}_{15}-\text{C}_9-\text{C}_{13})$ (30)
677	651	8.05	1.80	$\beta(\text{O}_8-\text{C}_7-\text{C}_6)$ (13), $\beta(\text{C}_4-\text{C}_3-\text{C}_2)$ (11), $\Gamma(\text{H}_{28}-\text{N}_{15}-\text{C}_9-\text{C}_{13})$ (10)
593	571	9.20	6.06	$\nu(\text{C}_4-\text{C}_3)$ (17), $\nu(\text{O}_{12}-\text{C}_2)$ (11), $\beta(\text{C}_5-\text{C}_4-\text{C}_3)$ (12), $\beta(\text{C}_3-\text{C}_2-\text{C}_1)$ (11)
585	563	1.72	0.48	$\Gamma(\text{C}_6-\text{C}_5-\text{C}_4-\text{C}_3)$ (22), $\Gamma(\text{C}_4-\text{C}_3-\text{C}_2-\text{C}_1)$ (12), $\gamma(\text{C}_7-\text{C}_1-\text{C}_5-\text{C}_6)$ (14), $\gamma(\text{O}_{12}-\text{C}_1-\text{C}_3-\text{C}_2)$ (21), $\gamma(\text{O}_{10}-\text{C}_2-\text{C}_4-\text{C}_3)$ (14)
483	465	3.01	1.87	$\nu(\text{C}_9-\text{C}_7)$ (14), $\beta(\text{C}_6-\text{C}_5-\text{C}_4)$ (12), $\beta(\text{O}_8-\text{C}_7-\text{C}_6)$ (10), $\beta(\text{C}_9-\text{C}_7-\text{C}_6)$ (10)
441	424	4.33	0.72	$\beta(\text{C}_{16}-\text{N}_{15}-\text{C}_9)$ (14), $\Gamma(\text{H}_{18}-\text{C}_4-\text{C}_5-\text{C}_6)$ (13), $\Gamma(\text{C}_5-\text{C}_4-\text{C}_3-\text{C}_2)$ (23), $\gamma(\text{O}_{12}-\text{C}_1-\text{C}_3-\text{C}_2)$ (13)
431	414	3.47	2.31	$\beta(\text{C}_{16}-\text{N}_{15}-\text{C}_9)$ (12)
423	407	7.74	3.16	$\nu(\text{C}_{13}-\text{C}_9)$ (11), $\beta(\text{C}_{14}-\text{C}_{13}-\text{C}_9)$ (17), $\beta(\text{C}_{13}-\text{C}_9-\text{N}_{15})$ (19)
385	370	11.23	6.78	$\beta(\text{O}_8-\text{C}_7-\text{C}_6)$ (27), $\beta(\text{C}_5-\text{C}_4-\text{C}_3)$ (14)
324	312	1.21	2.77	$\gamma(\text{O}_{10}-\text{C}_2-\text{C}_4-\text{C}_3)$ (29), $\gamma(\text{O}_{12}-\text{C}_1-\text{C}_3-\text{C}_2)$ (10)
319	307	16.87	1.74	$\beta(\text{N}_{15}-\text{C}_9-\text{C}_7)$ (18), $\beta(\text{C}_9-\text{C}_7-\text{C}_6)$ (18)
303	292	0.28	1.90	$\nu(\text{C}_7-\text{C}_6)$ (16), $\beta(\text{C}_{14}-\text{C}_{13}-\text{C}_9)$ (15), $\beta(\text{C}_9-\text{C}_7-\text{C}_6)$ (12)
268	258	2.65	0.30	$\Gamma(\text{H}_{25}-\text{C}_{14}-\text{C}_{13}-\text{C}_9)$ (24), $\Gamma(\text{H}_{26}-\text{C}_{14}-\text{C}_{13}-\text{C}_9)$ (13)
236	227	0.07	2.27	$\Gamma(\text{C}_4-\text{C}_3-\text{C}_2-\text{C}_1)$ (41), $\Gamma(\text{H}_{29}-\text{C}_{16}-\text{C}_{15}-\text{C}_9)$ (13), $\gamma(\text{O}_{12}-\text{C}_1-\text{C}_3-\text{C}_2)$ (21)
220	212	0.80	0.52	$\beta(\text{C}_6-\text{C}_5-\text{C}_4)$ (15), $\Gamma(\text{H}_{26}-\text{C}_{14}-\text{N}_{15}-\text{C}_9)$ (11), $\Gamma(\text{H}_{31}-\text{C}_{16}-\text{N}_{15}-\text{C}_9)$ (10), $\gamma(\text{C}_{13}-\text{N}_{15}-\text{C}_7-\text{C}_9)$ (13)
182	175	0.66	0.93	$\beta(\text{C}_{13}-\text{C}_9-\text{N}_{15})$ (15), $\beta(\text{N}_{15}-\text{C}_9-\text{C}_7)$ (13), $\beta(\text{C}_{14}-\text{C}_{13}-\text{C}_9)$ (11), $\gamma(\text{C}_{13}-\text{N}_{15}-\text{C}_7-\text{C}_9)$ (14), $\gamma(\text{O}_8-\text{C}_9-\text{C}_6-\text{C}_7)$ (10)
177	170	4.46	0.37	$\beta(\text{C}_{13}-\text{C}_9-\text{N}_{15})$ (19), $\beta(\text{C}_{16}-\text{N}_{15}-\text{C}_9)$ (14), $\beta(\text{N}_{15}-\text{C}_9-\text{C}_7)$ (11), $\Gamma(\text{H}_{29}-\text{C}_{16}-\text{N}_{15}-\text{C}_9)$ (11), $\Gamma(\text{H}_{30}-\text{C}_{16}-\text{N}_{15}-\text{C}_9)$ (16)
125	120	11.17	0.22	$\Gamma(\text{C}_5-\text{C}_4-\text{C}_3-\text{C}_2)$ (21), $\gamma(\text{C}_7-\text{C}_1-\text{C}_5-\text{C}_6)$ (21), $\gamma(\text{O}_{10}-\text{C}_2-\text{C}_4-\text{C}_3)$ (10)
113	108	0.18	0.73	$\beta(\text{C}_9-\text{C}_7-\text{C}_6)$ (30), $\beta(\text{C}_7-\text{C}_6-\text{C}_5)$ (26), $\beta(\text{C}_{13}-\text{C}_9-\text{N}_{15})$ (10)
97	94	7.41	0.40	$\Gamma(\text{C}_{16}-\text{N}_{15}-\text{C}_9-\text{C}_{13})$ (49), $\Gamma(\text{C}_{14}-\text{C}_{13}-\text{C}_9-\text{N}_{15})$ (14)
89	85	3.74	0.85	$\Gamma(\text{C}_{11}-\text{O}_{12}-\text{C}_2-\text{C}_1)$ (53), $\Gamma(\text{H}_{21}-\text{C}_{11}-\text{O}_{12}-\text{C}_2)$ (12)
79	76	1.06	0.35	$\Gamma(\text{C}_{14}-\text{C}_{13}-\text{C}_9-\text{N}_{15})$ (44), $\Gamma(\text{C}_{16}-\text{N}_{15}-\text{C}_9-\text{C}_{13})$ (24)
34	32	0.62	3.11	$\Gamma(\text{N}_{15}-\text{C}_9-\text{C}_7-\text{C}_6)$ (51), $\Gamma(\text{C}_9-\text{C}_7-\text{C}_6-\text{C}_1)$ (24)
27	26	0.02	4.26	$\Gamma(\text{C}_9-\text{C}_7-\text{C}_6-\text{C}_1)$ (59), $\Gamma(\text{N}_{15}-\text{C}_9-\text{C}_7-\text{C}_6)$ (20)

Table A13: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Ethylone.

Calculated wave number (cm ⁻¹)		IR intensity	Raman intensity	Assignment based on PED (%)
Unscaled	Scaled			
3566	3426	13.535	70.105	n(N14-H26)(100)
3258	3130	1.0101	83.660	n(C1-H17)(97)
3252	3125	5.4504	119.42	n(C4-H18)(62), n(C5-H19)(35)
3238	3111	0.3707	41.122	n(C4-H18)(36), n(C5-H19)(64)
3170	3046	31.57	163.66	n(C11-H21)(50), n(C11-H22)(50)
3137	3014	37.311	81.409	n(C13-H23)(59), n(C13-H24)(38)
3136	3013	20.338	65.159	n(C16-H29)(25), n(C16-H30)(69)
3129	3006	40.358	55.840	n(C13-H24)(25), n(C13-H25)(63)
3113	2991	46.266	78.941	n(C16-H29)(45), n(C16-H31)(47)
3097	2976	90.443	270.67	n(C11-H21)(50), n(C11-H22)(50)
3049	2930	21.488	123.63	n(C13-H23)(28), n(C13-H24)(36), n(C13-H25)(36)
3043	2924	34.697	115.73	n(C16-H29)(30), n(C16-H30)(22), n(C16-H31)(47)
3035	2916	43.976	73.784	n(C9-H20)(96)
3028	2909	23.384	61.354	n(C15-H28)(94)
2918	2804	105.82	107.07	n(C15-H27)(98)
1687	1621	29.971	10.635	n(O8-C7)(35), n(C6-C5)(12)
1656	1591	22.971	167.24	n(C2-C1)(21), n(C4-C3)(33), b(C3-C2-C1)(11)
1643	1578	135.18	221.45	n(O8-C7)(45), n(C2-C1)(18), n(C4-C3)(12), n(C3-C2)(10)
1573	1511	4.516	7.377	b(H28-C15-C17)(76)
1571	1509	0.017	36.656	b(H22-C11-H21)(93)
1549	1488	15.403	16.356	b(H29-C16-H31)(20), b(H30-C16-H29)(31), t(H31-C16-C15-N14)(10)
1543	1482	38.785	26.956	b(H23-C13-H23)(18), b(H25-C13-H24)(16), b(H31-C16-H30)(19)
1539	1478	2.002	8.646	b(H23-C13-H23)(25), b(H24-C13-H23)(42), t(H23-C13-C9-N14)(11)
1537	1477	78.535	10.688	b(H17-C1-C6)(14), b(H18-C4-C5)(11), b(H24-C13-H23)(10), b(H25-C13-H24)(17)
1536	1476	20.166	26.770	b(H29-C16-H31)(29), b(H30-C16-H29)(31), t(H29-C13-C9-N14)(11)
1514	1454	48.171	24.719	b(H26-N14-C15)(52)
1483	1425	60.866	23.742	n(C2-C1)(20), n(C5-C4)(17), b(H19-C5-C6)(20)
1454	1397	8.739	2.916	b(H29-C16-H31)(29), b(H30-C16-H29)(29), b(H31-C16-H30)(27)
1442	1385	9.127	5.555	b(H23-C13-H23)(23), b(H24-C13-H23)(27), b(H25-C13-H24)(31)
1436	1379	62.475	27.492	b(H20-C9-N14)(17), t(H27-C15-N14-C9)(19), t(H28-C15-N14-C9)(24)
1417	1361	2.0125	16.982	t(H21-C11-O12-C2)(24), t(H22-C11-O12-C2)(38)
1402	1347	59.706	60.245	n(C3-C2)(11), n(C6-C5)(40)
1384	1330	3.615	1.5507	b(H20-C9-N14)(22), b(H27-C15-C16)(25), t(H20-C9-C7-C6)(13)
1349	1296	82.794	6.876	t(H20-C9-C7-C6)(39)

Table A13: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Ethylone.

Calculated wave number (cm ⁻¹)		IR intensity	Raman intensity	Assignment based on PED (%)
Unscaled	Scaled			
1322	1270	7.848	13.441	b(H17-C1-C6)(21), b(H18-C4-C5)(13), b(H19-C5-C6)(12), b(H27-C15-C16)(16)
1318	1266	31.888	22.812	b(H27-C15-C16)(31), t(H28-C15-N14-C9)(15)
1288	1237	374.24	64.180	n(C3-C2)(10), n(C5-C4)(21), n(C7-C6)(12), n(O10-C3)(10)
1265	1215	49.66	0.753	n(O10-C3)(11), n(N14-C9)(12), b(H17-C1-C6)(12)
1227	1179	63.023	10.121	n(N14-C9)(23), b(H17-C1-C6)(11)
1205	1158	49.261	4.972	n(N14-C15)(38), t(H30-C16-C15-N14)(15), t(H27-C15-N14-C9)(11)
1181	1134	5.714	2.399	n(C5-C4)(15), b(H18-C4-C5)(29), b(H19-C5-C6)(29)
1168	1122	0.0002	11.065	b(H21-C11-O12)(59)
1162	1116	11.832	13.495	t(H31-C16-C15-N14)(26)
1121	1077	24.239	10.101	n(C16-C15)(10), b(C3-C2-C1)(11)
1116	1072	9.612	1.597	b(H21-C11-O12)(40), t(H21-C11-O12-C2)(36), t(H22-C11-O12-C2)(30), t(C11-O12-C2-C1)(18)
1103	1059	55.050	29.346	b(C4-C3-C2)(10), b(C3-C2-C1)(15), b(C5-C4-C3)(10)
1074	1032	4.137	4.4060	t(H20-C9-C7-C6)(17), t(H23-C13-C9-N14)(16), t(H25-C13-C9-N14)(13)
1046	1005	8.358	5.8294	n(N14-C9)(15), n(C16-C15)(33), n(C13-C9)(16)
1022	982	97.205	3.6764	n(O12-C11)(24), b(O10-C3-C4)(12), b(O12-C2-C3)(11), b(C11-O12-C2)(14)
1007	967	18.179	2.6913	t(H18-C4-C5-C6)(15), t(H19-C5-C6-C7)(53)
1004	964	142.65	3.3917	n(C9-C7)(11), n(O12-C11)(11)
963	925	11.431	6.967	n(C16-C15)(26), n(C13-C9)(23), t(H30-C16-C15-N14)(10)
909	873	7.779	7.457	n(O12-C2)(17), t(H17-C1-C6-C16)(23)
905	869	20.496	1.1673	t(H17-C1-C6-C16)(56)
879	844	23.802	3.597	b(O10-C3-C4)(11), b(C11-O12-C2)(18)
871	837	18.692	3.761	t(H18-C4-C5-C6)(41), t(H19-C5-C6-C7)(19)
866	832	11.111	7.273	t(H18-C4-C5-C6)(18), t(H19-C5-C6-C7)(10)
844	811	3.765	1.574	n(O12-C11)(30), t(H29-C13-C9-N14)(27), t(H27-C15-N14-C9)(17), t(H28-C15-N14-C9)(16)
817	785	15.231	24.954	n(C2-C1)(12), n(C3-C2)(28), n(O10-C3)(17)
776	745	11.515	2.0847	t(H25-C13-C9-N14)(11), r ₀ (O8-C9-C6-C7)(20)
756	726	15.404	6.117	r ₀ (O8-C9-C6-C7)(16), r ₀ (C7-C1-C5-C6)(12)
718	689	1.330	6.117	b(O10-C3-C4)(20), b(O12-C2-C3)(24), b(C11-O12-C2)(22)
708	680	1.553	1.584	t(C4-C3-C2-C1)(13), t(C6-C5-C4-C3)(17), r ₀ (C10-C2-C4-C3)(16), r ₀ (O12-C1-C3-C2)(16)
680	653	11.692	4.693	b(O8-C7-C6)(16), b(C4-C3-C2)(15)
594	570	22.307	6.547	n(C4-C3)(13), b(C5-C4-C3)(11), t(H26-N14-C15-C16)(14)
591	567	67.010	2.682	t(H26-N14-C15-C16)(43)

Continued **Table A13:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Ethylone.

Calculated wave number (cm ⁻¹)		IR intensity	Raman intensity	Assignment based on PED (%)
Unscaled	Scaled			
579	556	9.824	1.498	t(C4-C3-C2-C1)(10), t(C6-C5-C4-C3)(23), r ₀ (C7-C1-C5-C6)(11), r ₀ (C10-C2-C4-C3)(13), r ₀ (O12-C1-C3-C2)(19)
544	522	48.713	5.562	b(C13-C9-N14)(13), t(H26-N14-C15-C16)(14)
452	434	8.925	0.849	b(C6-C5-C4)(18)
438	420	2.343	0.288	t(H18-C4-C5-C6)(14), t(C6-C5-C4-C3)(15), r ₀ (O12-C1-C3-C2)(12)
390	374	9.792	7.868	b(O8-C7-C6)(28), b(C5-C4-C3)(13)
371	356	8.925	1.892	b(O8-C7-C6)(10), r ₀ (C13-N14-C7-C9)(14)
360	345	1.716	2.034	b(N14-C9-C7)(13), b(C9-C7-C6)(10)
322	309	0.873	2.136	b(C13-C9-N14)(12), r ₀ (C10-C2-C4-C3)(35), r ₀ (O12-C1-C3-C2)(12)
267	256	0.558	2.170	b(C15-N14-C9)(15)
261	250	1.916	0.369	t(H29-C13-C9-N14)(22), t(H30-C16-C15-N14)(15), t(H31-C16-C15-N14)(12)
254	244	0.328	0.651	b(C13-C9-N14)(11), r ₀ (O12-C1-C3-C2)(10)
239	229	0.088	1.032	t(H24-C13-C9-N14)(21), t(H25-C13-C9-N14)(22), t(C4-C3-C2-C1)(13)
220	211	0.670	2.289	b(C13-C9-N14)(10), t(C4-C3-C2-C1)(28), r ₀ (O8-C9-C6-C7)(11), r ₀ (C13-N14-C7-C9)(16)
170	163	4.159	0.485	b(C7-C6-C5)(21), b(C15-N14-C9)(11)
124	119	7.104	0.275	r ₀ (O8-C9-C6-C7)(10), r ₀ (C7-C1-C5-C6)(20)
113	108	1.529	0.380	b(C15-N14-C9)(19), t(C15-N14-C9-C13)(35)
87	83	5.602	0.486	b(C9-C7-C6)(13), t(C16-C15-C14-C9)(16), t(C11-O12-C2-C1)(21)
81	77	2.128	0.965	t(C15-N14-C9-C13)(26), t(C16-C15-C14-C9)(29)
76	73	3.439	1.293	t(C11-O12-C2-C1)(35)
44	42	0.225	2.234	t(C9-C7-C6-C1)(70)
30	28	0.791	2.194	t(N14-C9-C7-C6)(49), t(C15-N14-C9-C13)(13), t(C9-C7-C6-C1)(13)

Table A14: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of MDPV.

Calculated Wavenumber (cm ⁻¹)		IR Intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
3264	3139	1.01	67.81	ν (C ₁ -H ₂₁) (99)
3252	3128	5.57	136.1	ν (C ₄ -H ₂₂) (63), ν (C ₅ -H ₂₃) (36)
3238	3114	0.50	40.14	ν (C ₅ -H ₂₃) (63), ν (C ₄ -H ₂₂) (36)
3168	3047	31.60	163.6	ν (C ₁₃ -H ₂₇) (51), ν (C ₁₃ -H ₂₈) (51)
3131	3012	53.56	90.53	ν (C ₁₇ -H ₃₃) (33), ν (C ₁₇ -H ₃₄) (30), ν (C ₁₈ -H ₃₅) (19), ν (C ₁₈ -H ₃₆) (13)
3120	3001	53.42	50.71	ν (C ₁₀ -H ₂₅) (44), ν (C ₁₀ -H ₂₆) (21), ν (C ₂₀ -H ₃₉) (19)
3115	2996	52.39	58.71	ν (C ₂₀ -H ₄₁) (59), ν (C ₁₈ -H ₃₅) (26), ν (C ₂₀ -H ₃₉) (23)
3114	2995	9.47	147.7	ν (C ₂₀ -H ₃₉) (19), ν (C ₁₇ -H ₃₄) (26)
3110	2991	26.55	74.86	ν (C ₁₆ -H ₃₁) (92)
3107	2988	19.05	17.23	ν (C ₂₀ -H ₄₀) (43), ν (C ₁₀ -H ₂₅) (17)
3096	2978	91.65	274.4	ν (C ₁₃ -H ₂₈) (51), ν (C ₁₃ -H ₂₇) (49)
3086	2968	38.40	60.56	ν (C ₁₅ -H ₂₉) (85)
3075	2958	38.82	120.5	ν (C ₁₇ -H ₃₃) (53), ν (C ₁₈ -H ₃₆) (16)
3067	2950	33.15	60.09	ν (C ₁₈ -H ₃₅) (57), ν (C ₁₇ -H ₃₄) (27), ν (C ₁₈ -H ₃₅) (27), ν (C ₁₇ -H ₃₄) (11)
3064	2947	31.13	42.63	ν (C ₁₉ -H ₃₈) (48), ν (C ₁₀ -H ₂₅) (19), ν (C ₁₀ -H ₂₆) (16)
3055	2938	9.25	117.4	ν (C ₁₀ -H ₂₆) (53), ν (C ₁₉ -H ₃₈) (22), ν (C ₁₀ -H ₂₅) (11), ν (C ₁₉ -H ₃₇) (10)
3037	2921	36.11	115.9	ν (C ₂₀ -H ₄₀) (41), ν (C ₂₀ -H ₃₉) (31), ν (C ₂₀ -H ₄₁) (26)
3022	2907	31.56	63.39	ν (C ₁₉ -H ₃₇) (76), ν (C ₁₉ -H ₃₈) (21)
2931	2819	133.2	116.3	ν (C ₁₅ -H ₃₀) (55), ν (C ₉ -H ₂₄) (36)
2923	2811	33.15	25.53	ν (C ₉ -H ₂₄) (59), ν (C ₉ -H ₂₄) (40)
2905	2794	64.20	39.15	ν (C ₁₆ -H ₃₂) (91)
1687	1622	24.85	9.65	ν (C ₇ -O ₈) (39), ν (C ₁ -C ₂) (18), ν (C ₆ -C ₅) (10)
1653	1590	20.54	153.4	ν (C ₄ -C ₃) (35), ν (C ₁ -C ₂) (20)
1643	1580	141.8	207.4	ν (O ₈ -C ₇) (43), ν (C ₃ -C ₂) (11), ν (C ₄ -C ₃) (10)
1573	1513	4.94	14.95	β (H ₃₀ -C ₁₅ -H ₂₉) (66), β (H ₃₆ -C ₁₈ -H ₃₅) (10), β (H ₃₂ -C ₁₆ -H ₃₁) (10)
1570	1510	0.12	35.63	β (H ₂₈ -C ₁₃ -H ₂₇) (93)
1554	1494	3.82	6.16	β (H ₃₂ -C ₁₆ -H ₃₁) (42), β (H ₃₀ -C ₁₅ -H ₂₉) (11), β (H ₃₈ -C ₁₉ -H ₃₇) (14),
1553	1493	3.87	1.37	β (H ₃₈ -C ₁₉ -H ₃₇) (28), β (H ₄₀ -C ₂₀ -H ₃₉) (20), β (H ₃₂ -C ₁₆ -H ₃₁) (18)
1547	1488	3.89	13.53	β (H ₃₆ -C ₁₈ -H ₃₅) (61), β (H ₃₂ -C ₁₆ -H ₃₁) (16), β (H ₃₄ -C ₁₇ -H ₃₃) (10)
1544	1485	7.03	22.62	β (H ₃₉ -C ₂₀ -C ₄₁) (39), β (H ₄₁ -C ₂₀ -C ₄₀) (38), τ (H ₄₁ -C ₂₀ -C ₁₉ -C ₁₀) (14)
1540	1481	2.35	24.10	β (H ₄₁ -C ₂₀ -C ₄₀) (11), β (H ₃₈ -C ₁₉ -H ₃₇) (30), β (H ₄₀ -C ₂₀ -H ₃₉) (27)
1536	1477	3.82	18.71	ν (C ₃ -C ₂) (11), β (H ₃₄ -C ₁₇ -H ₃₃) (81), β (H ₃₆ -C ₁₈ -H ₃₅) (17), β (H ₂₂ -C ₄ -C ₅) (15)
1535	1476	94.91	8.89	β (H ₂₁ -C ₁ -C ₂) (21), β (H ₂₃ -C ₅ -C ₆) (12)
1528	1469	15.73	13.29	β (H ₂₆ -C ₁₀ -H ₂₅) (72), β (H ₃₈ -C ₁₉ -H ₃₇) (19)
1482	1425	64.53	20.97	ν (C ₅ -C ₄) (16), ν (C ₁ -C ₂) (18)
1459	1403	1.34	5.13	β (H ₃₉ -C ₂₀ -C ₄₁) (33), β (H ₄₁ -C ₂₀ -C ₄₀) (31), β (H ₄₀ -C ₂₀ -H ₃₉) (29)
1430	1375	29.17	3.89	β (H ₂₄ -C ₉ -C ₇) (23), τ (H ₂₆ -C ₁₀ -C ₁₉ -C ₂₀) (12)
1420	1366	6.22	8.52	τ (H ₂₄ -C ₉ -C ₇ -C ₆) (10), τ (H ₃₂ -C ₁₆ -N ₁₁ -C ₉) (13)
1416	1362	0.39	19.34	τ (H ₂₇ -C ₁₃ -O ₁₄ -C ₂) (25), τ (H ₂₈ -C ₁₃ -O ₁₄ -C ₂) (41)
1407	1353	20.53	21.10	β (H ₂₄ -C ₉ -C ₇) (14), τ (H ₂₅ -C ₁₀ -C ₁₉ -C ₂₀) (10), τ (H ₃₈ -C ₁₉ -C ₁₀ -C ₉) (14), τ (H ₃₇ -C ₁₉ -C ₁₀ -C ₉) (13)

Continued **Table A14:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of MDPV.

Calculated Wavenumber (cm ⁻¹)		IR Intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
1394	1341	14.61	31.82	ν (C ₆ -C ₉) (32), ν (C ₃ -C ₂) (11)
1384	1331	0.60	9.53	τ (H ₃₃ -C ₁₇ -C ₁₈ -C ₁₅) (14), τ (H ₃₀ -C ₁₅ -N ₁₁ -C ₉) (11), τ (H ₃₂ -C ₁₆ -N ₁₁ -C ₉) (12)
1379	1326	14.29	1.91	τ (H ₂₄ -C ₉ -C ₇ -C ₆) (37), τ (H ₂₅ -C ₁₀ -C ₁₉ -C ₂₀) (12)
1370	1317	1.10	4.47	τ (H ₃₃ -C ₁₇ -C ₁₈ -C ₁₅) (17), τ (H ₃₄ -C ₁₇ -C ₁₈ -C ₁₅) (14), τ (H ₃₀ -C ₁₅ -N ₁₁ -C ₉) (12)
1356	1304	2.26	11.01	β (H ₂₅ -C ₁₀ -C ₁₉) (50), β (H ₃₇ -C ₁₉ -C ₂₀) (22), β (H ₃₃ -C ₁₇ -C ₁₈) (12), τ (H ₃₆ -C ₁₈ -C ₁₇ -C ₁₆) (19)
1353	1301	7.29	17.35	β (H ₂₅ -C ₁₀ -C ₁₉) (13), β (H ₃₇ -C ₁₉ -C ₂₀) (11), β (H ₃₃ -C ₁₇ -C ₁₈) (10), τ (H ₃₆ -C ₁₈ -C ₁₇ -C ₁₆) (12)
1333	1282	14.83	6.32	τ (H ₂₆ -C ₁₀ -C ₁₉ -C ₂₀) (19), τ (H ₂₄ -C ₉ -C ₇ -C ₆) (21)
1317	1266	11.94	4.23	β (H ₂₁ -C ₁ -C ₂) (24), β (H ₂₃ -C ₅ -C ₆) (24), β (H ₂₂ -C ₄ -C ₅) (17)
1297	1247	112.3	27.99	β (H ₃₁ -C ₁₆ -C ₁₇) (13), β (H ₃₅ -C ₁₈ -C ₁₇) (12)
1294	1244	104.8	21.98	β (H ₃₅ -C ₁₈ -C ₁₇) (11), β (H ₃₁ -C ₁₆ -C ₁₇) (10)
1283	1234	290.1	51.66	ν (C ₅ -C ₄) (15)
1258	1210	4.23	10.22	β (H ₂₉ -C ₁₅ -C ₁₈) (36), β (H ₃₁ -C ₁₆ -C ₁₇) (11), τ (H ₂₉ -C ₁₅ -N ₁₁ -C ₉) (11)
1246	1198	12.47	4.79	β (H ₂₁ -C ₁ -C ₂) (24)
1245	1197	35.04	9.59	ν (C ₇ -C ₆) (11), β (H ₂₃ -C ₅ -C ₆) (16), τ (H ₃₄ -C ₁₇ -C ₁₈ -C ₁₅) (12)
1230	1183	7.75	4.63	β (H ₃₃ -C ₁₇ -C ₁₈) (10), τ (H ₃₄ -C ₁₇ -C ₁₈ -C ₁₅) (18), τ (H ₃₆ -C ₁₈ -C ₁₇ -C ₁₆) (11)
1182	1137	8.69	3.89	ν (N ₁₁ -C ₁₅) (20), β (H ₂₂ -C ₄ -C ₅) (25)
1180	1135	11.37	0.98	ν (C ₅ -C ₄) (12), β (H ₂₃ -C ₅ -C ₆) (26)
1173	1128	47.56	11.86	ν (N ₁₁ -C ₉) (30), ν (N ₁₁ -C ₁₆) (15), β (C ₉ -N ₁₁ -C ₁₅) (11)
1168	1123	0.01	11.05	β (H ₂₇ -C ₁₃ -O ₁₄) (58), τ (H ₂₈ -C ₁₃ -O ₁₄ -C ₂) (31)
1158	1113	12.02	5.87	τ (C ₁₈ -C ₁₇ -C ₁₆ -N ₁₁) (11)
1156	1112	4.13	3.85	τ (H ₃₉ -C ₂₀ -C ₁₉ -C ₁₀) (11)
1129	1086	7.28	3.25	ν (N ₁₁ -C ₁₅) (13)
1116	1073	9.43	1.63	β (H ₂₇ -C ₁₃ -O ₁₄) (40), τ (H ₂₇ -C ₁₃ -O ₁₄ -C ₂) (37), τ (C ₁₃ -O ₁₄ -C ₂ -C ₁) (17)
1110	1067	79.87	14.84	β (C ₁ -C ₂ -C ₃) (25), β (C ₅ -C ₄ -C ₃) (15), β (C ₄ -C ₃ -C ₂) (14)
1080	1038	1.03	19.08	ν (C ₁₉ -C ₁₀) (26), ν (C ₂₀ -C ₁₉) (22), ν (C ₁₀ -C ₉) (18)
1068	1027	3.67	6.44	ν (C ₁₇ -C ₁₆) (28), ν (C ₁₈ -C ₁₇) (22)
1042	1002	3.41	3.33	ν (C ₂₀ -C ₁₉) (36), ν (C ₁₀ -C ₉) (12)
1019	980	157.1	2.86	ν (C ₁₃ -O ₁₄) (33), β (O ₁₂ -C ₃ -C ₄) (13), β (O ₁₄ -C ₂ -C ₃) (13), β (C ₁₃ -O ₁₄ -C ₂) (19)
1010	972	0.05	1.49	β (H ₃₃ -C ₁₇ -C ₁₈) (12), β (H ₃₅ -C ₁₈ -C ₁₇) (12), τ (H ₂₂ -C ₄ -C ₃ -C ₂) (20), τ (H ₂₃ -C ₅ -C ₆ -C ₇) (59)
1009	971	0.49	0.64	β (C ₉ -N ₁₁ -C ₁₅) (10), τ (C ₆ -C ₅ -C ₄ -C ₃) (10)
993	955	66.59	3.40	ν (C ₉ -C ₇) (12), ν (C ₁₀ -C ₉) (10)
974	936	0.30	4.72	ν (C ₁₇ -C ₁₆) (27), β (C ₁₈ -C ₁₇ -C ₁₆) (10)
946	910	4.73	2.71	β (H ₂₅ -C ₁₀ -C ₁₉) (10), τ (H ₄₁ -C ₂₀ -C ₁₉ -C ₁₀) (11)
930	894	4.31	16.43	ν (C ₁₉ -C ₁₀) (22), ν (C ₂₀ -C ₁₉) (12), τ (H ₃₉ -C ₂₀ -C ₁₉ -C ₁₀) (10), τ (H ₄₀ -C ₂₀ -C ₁₉ -C ₁₀) (13)
922	886	4.50	9.94	ν (C ₁₈ -C ₁₇) (26), ν (C ₁₇ -C ₁₆) (17)
912	877	11.74	4.77	ν (C ₁₈ -C ₁₇) (12), τ (H ₂₁ -C ₁ -C ₂ -C ₃) (31)

Continued **Table A14:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of MDPV.

Calculated Wavenumber (cm ⁻¹)		IR Intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
902	867	11.46	3.51	ν (C ₁₈ -C ₁₇) (13), ν (N ₁₁ -C ₁₅) (10), τ (H ₂₁ -C ₁ -C ₂ -C ₃) (29)
894	860	6.68	2.72	ν (C ₂ -O ₁₄) (20), ν (C ₃ -O ₁₂) (12), ν (C ₁₃ -O ₁₄) (10)
876	842	5.87	2.51	τ (H ₂₂ -C ₄ -C ₃ -C ₂) (40), τ (H ₂₃ -C ₅ -C ₆ -C ₇) (19)
874	840	30.14	4.02	ν (C ₁₃ -O ₁₄) (33), β (C ₁₃ -O ₁₄ -C ₂) (25), β (O ₁₂ -C ₃ -C ₄) (13)
849	816	35.18	3.87	(N ₁₁ -C ₁₆) (20), τ (H ₂₂ -C ₄ -C ₃ -C ₂) (10)
834	802	6.48	1.04	β (H ₃₅ -C ₁₈ -C ₁₇) (12), τ (H ₃₅ -C ₁₈ -C ₁₇ -C ₁₆) (29)
816	784	13.98	24.49	ν (C ₃ -C ₂) (26), ν (C ₃ -O ₁₂) (17), ν (C ₁ -C ₂) (10)
801	770	5.23	2.40	τ (H ₃₇ -C ₁₉ -C ₁₀ -C ₉) (12)
788	758	17.04	2.05	γ (O ₈ -C ₉ -C ₆ -C ₇) (22)
742	713	4.02	5.61	τ (H ₂₅ -C ₁₀ -C ₁₉ -C ₂₀) (13)
719	691	0.66	3.68	β (O ₁₄ -C ₂ -C ₃) (14), β (C ₁₃ -O ₁₄ -C ₂) (12), β (O ₁₂ -C ₃ -C ₄) (10), τ (C ₆ -C ₅ -C ₄ -C ₃) (12)
715	687	0.62	4.89	τ (C ₆ -C ₅ -C ₄ -C ₃) (15), γ (C ₁₂ -C ₄ -C ₂ -C ₃) (10)
683	657	8.83	3.46	β (C ₄ -C ₃ -C ₂) (16), β (O ₈ -C ₇ -C ₆) (14)
651	626	7.67	4.37	β (C ₁₈ -C ₁₇ -C ₁₆) (13)
620	596	1.90	1.10	β (C ₁₇ -C ₁₆ -N ₁₁) (21), β (C ₁₈ -C ₁₇ -C ₁₆) (20), τ (H ₃₃ -C ₁₇ -C ₁₈ -C ₁₅) (10)
594	571	11.61	6.00	ν (C ₄ -C ₃) (16), ν (C ₂ -O ₁₄) (10), β (C ₁ -C ₂ -C ₃) (12), β (O ₈ -C ₇ -C ₆) (10),
580	557	3.93	1.21	τ (C ₁ -C ₂ -C ₃ -C ₄) (10), τ (C ₆ -C ₅ -C ₄ -C ₃) (18), γ (O ₁₄ -C ₁ -C ₃ -C ₂) (16)
511	491	3.87	1.63	β (C ₂₀ -C ₁₉ -C ₁₀) (16)
450	432	11.31	0.42	β (C ₇ -C ₆ -C ₁) (19), β (C ₁ -C ₂ -C ₃) (10), γ (C ₁₀ -N ₁₁ -C ₇ -C ₉) (10)
437	420	1.46	0.36	β (O ₈ -C ₇ -C ₆) (23), τ (C ₅ -C ₄ -C ₃ -C ₂) (33), τ (H ₂₁ -C ₁ -C ₂ -C ₃) (14), τ (C ₆ -C ₅ -C ₄ -C ₃) (16), γ (O ₁₄ -C ₁ -C ₃ -C ₂) (11)
385	370	4.80	8.19	ν (C ₇ -C ₆) (12), β (C ₅ -C ₄ -C ₃) (19)
352	338	3.72	0.85	β (C ₉ -C ₇ -C ₆) (13), β (O ₈ -C ₇ -C ₆) (11), β (C ₉ -N ₁₁ -C ₁₅) (10)
324	311	0.10	3.88	γ (O ₁₂ -C ₄ -C ₂ -C ₃) (24)
318	305	0.46	2.82	ν (C ₁₀ -C ₉) (10), β (C ₁₉ -C ₁₀ -C ₉) (12), γ (O ₁₂ -C ₄ -C ₂ -C ₃) (10)
290	278	1.16	1.13	β (C ₂₀ -C ₁₉ -C ₁₀) (18), τ (C ₁₈ -C ₁₇ -C ₁₆ -N ₁₁) (11), γ (C ₁₀ -N ₁₁ -C ₇ -C ₉) (19)
284	273	3.96	0.40	β (C ₁₀ -C ₉ -C ₇) (23)
258	248	0.37	2.64	ν (C ₉ -C ₇) (15), ν (C ₇ -C ₆) (11)
242	232	0.03	0.25	τ (H ₄₁ -C ₂₀ -C ₁₉ -C ₁₀) (42), τ (H ₃₉ -C ₂₀ -C ₁₉ -C ₁₀) (15), τ (H ₄₀ -C ₂₀ -C ₁₉ -C ₁₀) (16)
236	227	0.06	2.60	τ (C ₁ -C ₂ -C ₃ -C ₄) (43), γ (O ₁₄ -C ₁ -C ₃ -C ₂) (21)
189	181	0.87	0.88	β (C ₁₉ -C ₁₀ -C ₉) (15), β (C ₁₀ -C ₉ -C ₇) (13), τ (C ₁₇ -N ₁₆ -C ₁₁ -C ₉) (14)
154	148	0.41	0.56	β (C ₇ -C ₆ -C ₁) (31), β (C ₉ -C ₇ -C ₆) (14)
139	133	0.62	0.78	β (N ₁₁ -C ₉ -C ₇) (28), β (C ₉ -N ₁₁ -C ₁₅) (10)
120	115	12.16	0.33	τ (C ₅ -C ₄ -C ₃ -C ₂) (19), (C ₁ -C ₂ -C ₃ -C ₄) (10), γ (O ₈ -C ₉ -C ₆ -C ₇) (10), γ (C ₇ -C ₅ -C ₁ -C ₆) (29)
88	84	0.02	0.16	τ (C ₁₉ -C ₁₀ -C ₉ -N ₁₁) (62)
78	75	0.36	0.38	β (C ₁₉ -C ₁₀ -C ₉) (12), τ (C ₂₀ -C ₁₉ -C ₁₀ -C ₉) (18)
74	71	6.47	0.92	τ (H ₂₇ -C ₁₃ -O ₁₄ -C ₂) (14), τ (C ₁₃ -O ₁₄ -C ₂ -C ₁) (55)
71	68	1.79	1.02	β (C ₉ -C ₇ -C ₆) (10), τ (C ₂₀ -C ₁₉ -C ₁₀ -C ₉) (28)
56	53	0.64	0.06	τ (C ₁₇ -N ₁₆ -C ₁₁ -C ₉) (15), τ (C ₉ -C ₇ -C ₆ -C ₅) (12), τ (C ₁₉ -N ₁₀ -C ₉ -C ₇) (32), τ (C ₁₉ -C ₁₀ -C ₉ -N ₁₁) (12)
41	39	0.15	0.50	τ (C ₁₉ -N ₁₀ -C ₉ -C ₇) (34), τ (C ₁₈ -C ₁₇ -C ₁₆ -N ₁₁) (14), γ (C ₁₀ -N ₁₁ -C ₇ -C ₉) (12)

Calculated Wavenumber (cm ⁻¹)		IR Intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
26	25	0.18	5.0	τ (C ₁₇ -C ₁₆ -C ₁₁ -C ₉) (14), τ (C ₂₀ -C ₁₉ -C ₁₀ -C ₉) (83)
13	12	0.51	3.49	τ (N ₁₁ -C ₉ -C ₇ -C ₆) (75)

Table A15: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Methcathinone.

Calculated Wavenumber (cm ⁻¹)		IR intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
3536	3401	0.67	67.01	ν (N ₁₁ -H ₂₂) (99)
3249	3125	5.08	105.3	ν (C ₅ -H ₁₇) (93)
3234	3111	11.95	104.1	ν (C ₁ -H ₁₃) (82), ν (C ₂ -H ₁₄) (16)
3219	3096	27.24	140.3	ν (C ₄ -H ₁₆) (22), ν (C ₃ -H ₁₅) (47), ν (C ₂ -H ₁₄) (16), ν (C ₁ -H ₁₃) (11)
3205	3083	18.56	113.4	ν (C ₂ -H ₁₄) (47), ν (C ₄ -H ₁₆) (46)
3193	3071	0.18	57.13	ν (C ₃ -H ₁₅) (49), ν (C ₄ -H ₁₆) (26), ν (C ₂ -H ₁₄) (23)
3146	3026	19.26	42.83	ν (C ₁₀ -H ₁₉) (73), ν (C ₁₀ -H ₂₀) (18)
3129	3010	27.24	81.04	ν (C ₁₀ -H ₂₀) (44)
3125	3006	34.61	78.61	ν (C ₁₂ -H ₂₃) (77), ν (C ₁₀ -H ₂₁) (54), ν (C ₁₂ -H ₂₅) (22)
3069	2952	41.25	63.84	ν (C ₁₂ -H ₂₅) (73), ν (C ₁₂ -H ₂₃) (19)
3057	2940	21.63	139.4	ν (C ₁₀ -H ₁₉) (26), ν (C ₁₀ -H ₂₀) (36), ν (C ₁₀ -H ₂₁) (36),
3037	2921	23.21	42.69	ν (C ₉ -H ₁₈) (97)
2969	2856	109.9	138.2	ν (C ₁₂ -H ₂₄) (92)
1679	1615	80.43	25.32	ν (C ₇ -O ₈) (66)
1656	1593	38.20	137.8	ν (C ₁ -C ₂) (27), ν (C ₆ -C ₅) (13), ν (C ₅ -C ₄) (12)
1629	1567	34.45	27.95	ν (C ₄ -C ₃) (27), ν (C ₆ -C ₅) (12), ν (C ₇ -O ₈) (11)
1563	1503	9.85	25.40	β (H ₂₅ -C ₁₂ -H ₂₄) (69), β (H ₂₄ -C ₁₂ -H ₂₃) (30), τ (H ₂₄ -C ₁₂ -N ₁₁ -C ₉) (12)
1549	1490	0.15	3.97	β (H ₁₃ -C ₁ -C ₂) (16), β (H ₁₄ -C ₂ -C ₃) (17), β (H ₁₆ -C ₄ -C ₅) (16), β (H ₁₇ -C ₅ -C ₄) (17)
1543	1484	5.76	17.46	β (H ₂₁ -C ₁₀ -H ₂₀) (33), β (H ₁₀ -C ₁₀ -H ₂₁) (27), τ (H ₂₁ -C ₁₀ -C ₉ -N ₁₁) (13)
1535	1476	6.93	11.39	β (H ₂₅ -C ₁₂ -H ₂₄) (15), β (H ₂₃ -C ₁₂ -H ₂₅) (12), β (H ₂₂ -N ₁₁ -C ₁₂) (10), β (H ₁₀ -C ₁₀ -H ₂₁) (10)
1526	1468	7.61	23.24	β (H ₂₀ -C ₁₀ -H ₁₉) (42), β (H ₂₁ -C ₁₀ -H ₂₀) (12), β (H ₁₀ -C ₁₀ -H ₂₁) (10)
1517	1459	7.89	4.98	β (H ₂₂ -N ₁₁ -C ₁₂) (51)
1505	1447	17.88	5.77	β (H ₁₅ -C ₃ -C ₄) (28), β (H ₁₄ -C ₂ -C ₃) (14), β (H ₁₆ -C ₄ -C ₅) (14)
1494	1437	2.49	14.19	β (H ₂₃ -C ₁₂ -H ₂₅) (60)
1451	1395	17.43	2.73	β (H ₂₀ -C ₁₀ -H ₁₉) (36), β (H ₂₁ -C ₁₀ -H ₂₀) (31), β (H ₁₀ -C ₁₀ -H ₂₁) (29)
1394	1341	12.62	10.07	β (H ₁₈ -C ₉ -N ₁₁) (14), β (H ₁₃ -C ₁ -C ₂) (11), τ (H ₁₈ -C ₉ -C ₇ -C ₆) (32)
1384	1331	0.59	3.06	β (H ₁₇ -C ₅ -C ₄) (18), β (H ₁₃ -C ₁ -C ₂) (15), τ (H ₁₈ -C ₉ -C ₇ -C ₆) (22)
1373	1320	13.59	2.69	ν (C ₆ -C ₅) (16), ν (C ₅ -C ₄) (15), ν (C ₃ -C ₂) (12), β (H ₁₈ -C ₉ -N ₁₁) (14)
1365	1313	6.30	5.76	ν (C ₆ -C ₅) (13), β (H ₁₈ -C ₉ -N ₁₁) (27)
1272	1223	119.2	37.38	ν (C ₇ -C ₆) (32)
1234	1187	26.50	5.66	β (H ₁₆ -C ₄ -C ₅) (27), β (H ₁₆ -C ₄ -C ₅) (27), β (H ₁₇ -C ₅ -C ₄) (23), β (H ₁₃ -C ₁ -C ₂) (16)

Table A15: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Methcathinone.

Calculated Wavenumber (cm ⁻¹)		IR intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
1222	1175	0.96	8.54	β (H ₁₅ -C ₃ -C ₄) (10), β (H ₁₄ -C ₂ -C ₃) (25)
1218	1171	23.41	3.19	ν (N ₁₁ -C ₉) (19), τ (H ₂₄ -C ₁₂ -N ₁₁ -C ₉) (19)
1171	1126	29.76	3.89	ν (N ₁₁ -C ₁₂) (16), β (H ₂₃ -C ₁₂ -H ₂₅) (12), τ (H ₂₅ -C ₁₂ -N ₁₁ -C ₉) (35), τ (H ₂₃ -C ₁₂ -N ₁₁ -C ₉) (12),
1158	1113	27.83	7.22	ν (N ₁₁ -C ₁₂) (23), ν (N ₁₁ -C ₉) (12), τ (H ₂₅ -C ₁₂ -N ₁₁ -C ₉) (16)
1128	1085	5.89	4.63	ν (C ₅ -C ₄) (14), β (H ₁₃ -C ₁ -C ₂) (14)
1122	1079	8.91	4.35	ν (C ₁₀ -C ₉) (16)
1092	1050	1.66	8.83	ν (N ₁₁ -C ₁₂) (29), τ (H ₁₀ -C ₁₀ -C ₉ -N ₁₁) (18), τ (H ₂₁ -C ₁₀ -C ₉ -N ₁₁) (16)
1067	1026	0.83	8.63	ν (C ₃ -C ₂) (15), ν (C ₄ -C ₃) (13), β (C ₁ -C ₂ -C ₃) (16), β (C ₅ -C ₄ -C ₃) (14), β (H ₁₄ -C ₂ -C ₃) (11)
1051	1011	11.77	2.13	τ (H ₂₀ -C ₁₀ -C ₉ -N ₁₁) (11), τ (H ₂₄ -C ₁₂ -N ₁₁ -C ₉) (10)
1039	999	0.45	1.43	ν (C ₄ -C ₃) (13), β (C ₁ -C ₂ -C ₃) (31), β (C ₄ -C ₃ -C ₂) (16), τ (H ₁₃ -C ₁ -C ₂ -C ₃) (14), τ (H ₁₄ -C ₂ -C ₃ -C ₄) (25), τ (H ₁₅ -C ₃ -C ₄ -C ₅) (20)
1037	997	2.92	37.10	ν (C ₃ -C ₂) (15), β (C ₅ -C ₄ -C ₃) (11)
1013	974	0.41	0.69	τ (H ₁₆ -C ₄ -C ₃ -C ₂) (33), τ (H ₁₇ -C ₅ -C ₄ -C ₃) (10)
985	947	62.37	8.94	ν (C ₁₀ -C ₉) (16), ν (C ₉ -C ₇) (13), β (C ₄ -C ₃ -C ₂) (10)
972	935	2.20	3.56	τ (H ₁₅ -C ₃ -C ₄ -C ₅) (31), τ (H ₁₇ -C ₅ -C ₄ -C ₃) (30), τ (H ₁₃ -C ₁ -C ₂ -C ₃) (15)
886	852	13.06	3.27	ν (C ₁₀ -C ₉) (18), ν (N ₁₁ -C ₉) (17)
880	846	2.21	6.11	τ (H ₁₄ -C ₂ -C ₃ -C ₄) (28), τ (H ₁₇ -C ₅ -C ₄ -C ₃) (27), τ (H ₁₃ -C ₁ -C ₂ -C ₃) (13), τ (H ₁₆ -C ₄ -C ₃ -C ₂) (14),
826	794	10.67	1.06	τ (H ₁₆ -C ₄ -C ₃ -C ₂) (10), γ (O ₈ -C ₉ -C ₆ -C ₇) (18), γ (C ₇ -C ₅ -C ₁ -C ₆) (13)
781	751	24.70	9.60	ν (C ₉ -C ₇) (13), β (C ₄ -C ₃ -C ₂) (10), τ (H ₂₁ -C ₁₀ -C ₉ -N ₁₁) (10)
722	694	53.81	2.66	τ (H ₁₇ -C ₅ -C ₄ -C ₃) (14), τ (H ₁₃ -C ₁ -C ₂ -C ₃) (10), γ (O ₈ -C ₉ -C ₆ -C ₇) (13)
711	683	12.23	2.54	τ (C ₆ -C ₅ -C ₄ -C ₃) (26), τ (C ₁ -C ₂ -C ₃ -C ₄) (21), τ (H ₁₅ -C ₃ -C ₄ -C ₅) (17), γ (O ₈ -C ₉ -C ₆ -C ₇) (10)
685	658	7.04	2.30	β (C ₄ -C ₃ -C ₂) (15), β (O ₈ -C ₇ -C ₆) (12), τ (H ₂₂ -N ₁₁ -C ₉ -C ₁₀) (12)s
650	625	1.30	6.57	β (C ₅ -C ₄ -C ₃) (39), β (C ₁ -C ₂ -C ₃) (26), β (C ₆ -C ₅ -C ₄) (10)
619	595	158.1	2.61	ν (N ₁₁ -C ₉) (11), τ (H ₂₂ -N ₁₁ -C ₉ -C ₁₀) (42)
531	510	6.55	1.80	β (O ₈ -C ₇ -C ₆) (12), β (C ₇ -C ₆ -C ₁) (14), β (C ₉ -C ₇ -C ₆) (14)
465	447	4.92	0.70	β (C ₁₀ -C ₉ -N ₁₁) (84), τ (C ₅ -C ₄ -C ₃ -C ₂) (14), γ (C ₁₀ -N ₁₁ -C ₇ -C ₆) (18)
422	406	2.99	2.86	ν (C ₇ -C ₆) (11), β (O ₈ -C ₇ -C ₆) (13), β (C ₁₀ -C ₉ -N ₁₁) (13), τ (C ₁ -C ₂ -C ₃ -C ₄) (17), τ (C ₅ -C ₄ -C ₃ -C ₂) (24)
421	405	0.49	0.56	τ (C ₆ -C ₅ -C ₄ -C ₃) (17)
363	349	4.95	1.58	ν (C ₉ -C ₇) (11), β (C ₁₂ -N ₁₁ -C ₉) (20), β (O ₈ -C ₇ -C ₆) (17), γ (C ₁₀ -N ₁₁ -C ₇ -C ₆) (17)
311	299	1.01	3.04	ν (C ₇ -C ₆) (14), ν (C ₉ -C ₇) (12), $q\beta$ (C ₆ -C ₅ -C ₄) (10), β (C ₉ -C ₇ -C ₆) (10), β (C ₁₀ -C ₉ -N ₁₁) (13)
297	285	9.38	0.23	β (C ₁₀ -C ₉ -N ₁₁) (30), β (C ₁₂ -N ₁₁ -C ₉) (22), γ (C ₁₀ -N ₁₁ -C ₇ -C ₆) (14)
233	224	0.69	0.56	β (N ₁₁ -C ₉ -C ₇) (26), τ (H ₂₃ -C ₁₂ -N ₁₁ -C ₉) (13)
210	202	0.51	0.15	τ (H ₂₁ -C ₁₀ -C ₉ -N ₁₁) (32), τ (H ₂₀ -C ₁₀ -C ₉ -N ₁₁) (28), τ (H ₁₀ -C ₁₀ -C ₉ -N ₁₁) (24),
203	195	0.21	0.69	β (C ₇ -C ₆ -C ₁) (18), τ (H ₂₃ -C ₁₂ -N ₁₁ -C ₉) (25), τ (H ₂₄ -C ₁₂ -N ₁₁ -C ₉) (13)
153	147	0.50	0.36	β (C ₉ -C ₇ -C ₆) (32), β (C ₇ -C ₆ -C ₁) (21)
140	134	0.43	4.32	τ (C ₁ -C ₂ -C ₃ -C ₄) (12), τ (C ₆ -C ₅ -C ₄ -C ₃) (12), γ (O ₈ -C ₉ -C ₆ -C ₇) (17), γ (C ₁₀ -N ₁₁ -C ₇ -C ₆) (34)

Table A15: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Methcathinone.

Calculated Wavenumber (cm ⁻¹)		IR intensity	Raman Acti- vity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
75	72	1.74	0.48	τ (C ₁₂ -N ₁₁ -C ₉ -C ₁₀) (67)
43	41	0.32	5.94	τ (N ₁₁ -C ₉ -C ₇ -C ₆) (16), τ (C ₉ -C ₇ -C ₆ -C ₅) (66)
38	36	3.34	2.42	τ (N ₁₁ -C ₉ -C ₇ -C ₆) (51), τ (C ₉ -C ₇ -C ₆ -C ₅) (25)

Table A16: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of MMC.

Unscaled	Scaled	IR intensity	Raman Intensity	Assignment
3586	3446	29.160	89.167	γ(N11-H25) (99)
3234	3107	3.2040	90.385	γ(C5-H17) (94)
3225	3099	13.566	77.891	γ(C1-H14) (87), γ(C2-H15) (12)
3195	3070	16.920	67.222	γ(C1-H14) (11), γ(C2-H15) (73), γ(C4-H16) (15)
3193	3068	16.906	99.936	γ(C2-H15) (15), γ(C4-H16) (80)
3147	3024	22.360	51.449	γ(C10-H23) (67), γ(C10-H24) (29)
3137	3014	40.540	74.388	γ(C10-H22) (60), γ(C10-H24) (36)
3132	3009	16.070	66.698	γ(C7-H18) (70), γ(C7-H19) (28),
3122	3000	36.132	121.50	γ(C12-H26) (89), γ(C12-H28) (10)
3101	2980	20.830	107.71	γ(C7-H18) (12), γ(C7-H18) (48), γ(C7-H20) (40)
3057	2937	31.732	150.15	γ(C10-H22) (35), γ(C10-H23) (28), γ(C10-H24) (34)
3048	2929	54.240	68.399	γ(C12-H28) (86)
3039	2920	27.324	270.87	γ(C7-H18) (18), γ(C7-H19) (24), γ(C7-H20) (58)
2932	2817	82.440	93.780	γ(C9-H21) (92)
2921	2807	109.93	95.638	γ(C12-H27) (90)
1676	1610	31.314	19.751	γ(O13-C8) (33), γ(C5-C4) (17), γ(C3-C2) (11)
1659	1594	127.74	325.15	γ(O13-C8) (39), γ(5-C4) (12), γ(C1-C6) (11)
1616	1552	31.107	27.775	γ(O13-C8) (11), γ(C1-C6) (18), γ(C3-C2) (24)
1567	1505	2.3908	14.662	β(H14-C1-C2) (16), β(H15-C2-C3) (12), β(H16-C4-C5) (17), β(H17-C5-C4) (17)
1566	1504	25.029	17.928	β(H28-C12-H27) (73)
1543	1482	8.3203	36.129	β(H25-N11-C12) (12), β(H23-C10-H22) (21), β(H24-C10-H23) (27), τ(H23-C10-C9-N11) (10)
1537	1477	11.575	12.265	β(H22-C10-H24) (38), β(H23-C10-H22) (26), τ(H22-C10-C9-N11) (12)
1535	1475	6.3317	35.643	β(H19-C7-H18) (34), β(H20-C7-H19) (30), τ(H19-C7-C3-C2) (10)
1531	1471	7.4355	23.526	β(H18-C7-H20) (46), β(H19-C7-H18) (27), τ(H18-C7-C3-C2) (10)
1526	1466	3.1784	18.452	β(H24-C10-H23) (11), β(H26-C12-H28) (19), β(H27-C12-H26) (28), τ(H26-C12-N11-C9) (10)
1517	1457	50.824	6.8584	β(H25-N11-C12) (40), β(H26-C12-H28) (25)
1502	1443	28.202	41.270	β(H25-N11-C12) (22), β(H26-C12-H28) (29), β(H27-C12-H26) (28)
1463	1405	21.102	32.529	γ(C5-C4) (15), γ(C2-C1) (13), β(H15-C2-C3) (15)
1462	1404	0.7965	29.321	β(H18-C7-H20) (25), β(H19-C7-H18) (15), β(H20-C7-H19) (38)
1446	1389	6.6789	10.421	β(H22-C10-H24) (30), β(H23-C10-H22) (27), β(H24-C10-H23) (35)
1401	1346	8.5119	16.787	β(H21-C9-N11) (50), τ(H21-C9-C8-C6) (11)

Table A16: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of MMC.

Unscaled	Scaled	IR intensity	Raman Intensity	Assignment
1378	1324	3.6261	3.2609	β (H14-C1-C2) (23), β (H15-C2-C3) (13), β (H16-C4-C5) (13), β (H17-C5-C4) (16)
1370	1316	3.7945	0.7305	γ (C5-C4) (14), γ (C2-C1) (12), γ (C1-C6) (30), γ (C4-C3) (17)
1339	1286	42.999	12.179	τ (H21-C9-C8-C6) (46)
1288	1237	101.26	48.760	γ (C8-C6) (27)
1254	1205	8.1333	27.346	γ (C5-C4) (10), γ (C2-C1) (15), γ (C7-C3) (40), β (H17-C5-C4) (10)
1245	1196	8.9474	15.962	β (H14-C1-C2) (10), β (H15-C2-C3) (20), β (H16-C4-C5) (14), β (H17-C5-C4) (10)
1227	1179	96.660	17.102	γ (N11-C9) (29)
1194	1147	40.597	7.4565	γ (N11-C12) (40), τ (H27-C12-N11-C9) (19)
1172	1126	2.1154	6.2712	β (H17-C5-C4) (11), τ (H26-C12-N11-C9) (13), τ (H28-C12-N11-C9) (20)
1169	1123	5.9793	8.1617	β (H17-C5-C4) (10), τ (H28-C12-N11-C9) (24)
1138	1093	6.6036	26.257	γ (N11-C12) (10), β (H23-C10-H22) (10), τ (H22-C10-C9-N11) (21), τ (H23-C10-C9-N11) (14)
1100	1057	12.413	0.1346	β (H19-C7-H18) (14), τ (H18-C7-C3-C2) (48)
1096	1053	3.1577	2.2632	τ (H22-C10-C9-N11) (13), τ (H24-C10-C9-N11) (14), τ (H21-C9-C8-C6) (15)
1057	1015	1.6142	0.2438	β (C5-C4-C3) (41), β (C3-C2-C1) (25), β (C4-C3-C2) (15)
1041	1000	11.413	10.453	γ (C10-C9) (26), β (H20-C7-H19) (10)
1039	998	12.974	2.1180	τ (H18-C7-C3-C2) (17), τ (H20-C7-C3-C2) (28)
1026	985	3.1041	1.5142	τ (H16-C4-C5-C6) (24), τ (H17-C5-C4-C3) (49), τ (C5-C4-C3-C2) (13)
1005	965	41.514	3.2773	γ (C9-C8) (12), τ (H14-C1-C2-C3) (17), τ (H15-C2-C3-C7) (14)
995	956	36.435	1.4675	τ (H14-C1-C2-C3) (22), τ (H15-C2-C3-C7) (23)
888	853	3.3658	3.1794	γ (N11-C9) (17), γ (C10-C9) (24)
884	849	6.0067	5.4529	τ (H16-C4-C5-C6) (51), τ (H17-C5-C4-C3) (25)
861	827	16.044	2.4595	τ (H14-C1-C2-C3) (22), τ (H15-C2-C3-C7) (36)
827	794	3.9174	27.615	γ (C3-C2) (15), γ (C4-C3) (17), γ (C7-C3) (18)
784	753	22.119	4.5649	ρ_0 (O13-C9-C6-C8) (13)
755	725	2.1335	2.0859	τ (C3-C2-C1-C6) (22)
696	668	10.987	2.8561	τ (C3-C2-C1-C6) (22), ρ_0 (O13-C9-C6-C8) (21)
670	643	0.8619	7.1532	β (C5-C4-C3) (22),
618	593	13.418	0.4086	γ (C8-C6) (10), γ (C7-C3) (16), β (O13-C8-C6) (24), β (C4-C3-C2) (15)
592	568	89.001	2.4044	τ (H25-N11-C9-C10) (54)
512	492	6.2704	0.9174	τ (C4-C3-C2-C1) (13)
486	467	21.865	2.0088	β (C9-C8-C6) (10), ρ_0 (C7-C2-C4-C3) (21)
438	420	3.2124	1.8749	β (C10-C9-N11) (44)
427	410	0.1556	0.1801	τ (H14-C1-C2-C3) (14), τ (H17-C5-C4-C3) (10), τ (H16-C4-C5-C6) (10), τ (C5-C4-C3-C2) (25), τ (C3-C2-C1-C6) (18), τ (C4-C3-C2-C1) (14)
399	383	22.865	2.1392	β (C12-N11-C9) (18)
361	346	3.1616	0.6017	β (C7-C3-C4) (28)
307	295	2.2056	3.5219	β (N11-C9-C8) (20), ρ_0 (C7-C2-C4-C3) (14), ρ_0 (C8-C1-C5-C6) (15)
286	274	2.8365	2.4838	γ (C8-C6) (14)

Continued **Table A16:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of MMC.

Unscaled	Scaled	IR intensity	Raman Intensity	Assignment
251	241	5.8771	1.6949	β (C8-C6-C5) (24), β (C7-C3-C4) (11), β (N11-C9-C8) (11), β (C12-N11-C9) (25)
223	214	0.4070	0.1705	β (C12-N11-C9) (16), τ (H22-C10-C9-N11) (14), τ (H24-C10-C9-N11) (31)
216	207	0.8622	0.4110	τ (H23-C10-C9-N11) (23), ρ_o (O13-C9-C6-C8) (13), ρ_o (C10-C11-C8-C9) (19)
172	165	1.4669	0.6270	τ (H26-C12-N11-C9) (43), τ (H28-C12-N11-C9) (14), τ (H27-C12-N11-C9) (14), ρ_o (C10-C11-C8-C9) (12)
133	127	0.6772	0.3871	β (C8-C6-C5) (19), β (C9-C8-C6) (21), τ (N11-C9-C8-C6) (11)
103	98	0.5776	0.3068	β (C9-C8-C6) (14), τ (C4-C3-C2-C1) (10), τ (C12-N11-C9-C10) (10), ρ_o (C8-C1-C5-C6) (12)
85	81	1.0456	1.3027	τ (C4-C3-C2-C1) (10), τ (C12-N11-C9-C10) (45), ρ_o (C8-C1-C5-C6) (14)
70	67	0.2190	5.0206	τ (N11-C9-C8-C6) (13), τ (C9-C8-C6-C1) (55)
38	36	0.8428	2.2668	τ (N11-C9-C8-C6) (33), τ (C12-N11-C9-C10) (23), τ (C9-C8-C6-C1) (25)
29	27	0.3935	0.7650	τ (H18-C7-C3-C2) (23), τ (H18-C7-C3-C2) (37), τ (H20-C7-C3-C2) (35)

Table A17: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Buphedrone.

Unscaled	Scaled	IR intensity	Raman intensity	Assignment
3512	3375	1.3717	59.435	γ (N12-H25) (99)
3237	3110	6.5393	208.96	γ (C1-H14) (60), γ (C2-H15) (11), γ (C5-H18) (17)
3234	3107	16.572	24.391	γ (C1-H14) (26), γ (C4-H17) (11), γ (C5-H18) (60)
3220	3094	28.379	111.598	γ (C2-H15) (18), γ (C3-H16) (48), γ (C4-H17) (11), γ (C5-H18) (14)
3207	3081	12.499	115.283	γ (C2-H15) (46), γ (C4-H17) (44)
3196	3071	0.1258	52.628	γ (C2-H15) (24), γ (C3-H16) (46), γ (C4-H17) (27)
3127	3005	35.653	106.46	γ (C10-H21) (18), γ (C11-H22) (18), γ (C13-H26) (71), γ (C13-H28) (27)
3126	3004	52.113	34.981	γ (C11-H22) (18), γ (C11-H23) (52)
3115	2993	46.331	69.602	γ (C11-H22) (52), γ (C11-H24) (32)
3098	2977	2.328	114.547	γ (C9-H19) (18), γ (C10-H21) (38), γ (C11-H23) (19), γ (C11-H24) (14)
3086	2965	18.184	49.206	γ (C9-H19) (74), γ (C10-H21) (21)
3076	2956	45.014	83.227	γ (C13-H26) (24), γ (C13-H28) (69)
3043	2924	25.959	35.041	γ (C10-H20) (67), γ (C10-H21) (14)
3042	2923	15.141	152.92	γ (C10-H20) (13), γ (C11-H22) (19), γ (C11-H23) (22), γ (C11-H24) (44)
2964	2848	84.877	90.029	γ (C13-H27) (93)
1670	1604	38.796	9.6589	γ (O8-C7) (49), γ (C4-C3) (11)
1654	1589	45.836	148.08	γ (O8-C7) (14), γ (C1-C2) (22), γ (C5-C4) (10), γ (C6-C5) (19)
1627	1563	46.720	42.777	γ (O8-C7) (19), γ (C4-C3) (25)
1562	1501	13.082	19.058	β (H27-C13-H26) (34), β (H28-C13-H27) (35), τ (H27-C13-N12-C9) (12)
1551	1490	1.4013	4.1288	β (H14-C1-C2) (14), β (H15-C2-C3) (14), β (H17-C4-C5) (15), β (H18-C5-C4) (16)

Table A17: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Buphedrone.

Unscaled	Scaled	IR intensity	Raman intensity	Assignment
1547	1486	12.956	10.407	β (H21-C10-H20) (18), β (H23-C11-H22) (36), β (H24-C11-H23) (23), τ (H23-C11-C10-C9) (11)
1545	1484	8.7521	12.154	β (H22-C11-H24) (41), β (H23-C11-H22) (11), β (H24-C11-H23) (13), τ (H22-C11-C10-C9) (10), τ (H24-C11-C10-C9) (10)
1537	1477	7.4812	24.188	β (H25-N12-C13) (18), β (H26-C13-H28) (16), β (H27-C13-H26) (11), β (H27-C13-H26) (27)
1536	1476	5.5062	22.321	β (H21-C10-H20) (55), β (H24-C11-H23) (18)
1532	1472	16.946	7.0793	β (H25-N12-C13) (41), β (H26-C13-H28) (12), β (H27-C13-H26) (18)
1504	1445	16.434	4.5377	β (H15-C2-C3) (15), β (H16-C3-C4) (28), β (H16-C3-C4) (28), β (H17-C4-C5) (15)
1497	1438	1.7911	12.044	β (H26-C13-H28) (57), β (H27-C13-H26) (20), β (H27-C13-H26) (14)
1464	1406	2.1991	4.0330	β (H22-C11-H24) (36), β (H23-C11-H22) (31), β (H24-C11-H23) (31)
1410	1355	4.9372	4.6829	β (H19-C9-N12) (33), τ (H20-C10-C8-C12) (11)
1389	1334	6.8672	2.5223	β (H14-C1-C2) (17), β (H18-C5-C4) (21), β (H20-C10-C11) (11)
1374	1320	1.6270	2.492	γ (C1-C2) (15), γ (C3-C2) (14), γ (C5-C4) (17), γ (C6-C5) (21)
1360	1306	1.8869	2.9609	γ (C6-C5) (10), β (H19-C9-N12) (22), β (H20-C10-C11) (14)
1345	1292	1.2763	13.447	β (H20-C10-C11) (10), τ (H19-C9-C7-C6) (36), τ (H21-C10-C9-C12) (15)
1295	1244	24.193	5.1676	β (H20-C10-C11) (19), τ (H19-C9-C7-C6) (11), τ (H20-C10-C8-C12) (12), τ (H21-C10-C9-C12) (18)
1268	1218	135.58	25.087	γ (C7-C6) (31)
1238	1189	17.578	3.0344	γ (C5-C4) (10), β (H14-C1-C2) (13), β (H17-C4-C5) (28), β (H18-C5-C54) (18)
1231	1182	8.0520	15.426	γ (N12-C9) (11), τ (H27-C13-N12-C9) (18)
1223	1175	5.5381	10.454	γ (C3-C2) (10), β (H14-C1-C2) (11), β (H15-C2-C3) (14), β (H15-C2-C3) (26), β (H16-C3-C4) (35), β (H16-C3-C4) (35)
1175	1129	20.816	3.260	γ (N12-C13) (12), β (H26-C13-H28) (13), τ (H26-C13-N12-C9) (20), τ (H28-C13-C12-C9) (39)
1155	1109	20.629	5.5329	γ (N12-C9) (25), γ (N12-C13) (22)
1136	1091	3.1071	2.8717	τ (H20-C10-C8-C12) (10), τ (H24-C11-C10-C9) (20)
1125	1081	1.4755	0.5952	γ (C1-C2) (10), γ (C5-C4) (15), β (H14-C1-C2) (12)
1111	1067	21.432	0.7750	γ (N12-C13) (18), γ (C10-C9) (14), τ (H23-C11-C10-C9) (12), τ (H27-C13-N12-C9) (11)
1066	1024	1.854	7.1700	γ (C3-C2) (18), γ (C4-C3) (14), β (C1-C2-C3) (13), β (C5-C4-C3) (12)
1064	1022	1.2308	9.0262	γ (C11-C10) (40), γ (C10-C9) (15)
1046	1005	0.3208	1.0330	τ (H14-C1-C2-C3) (20), τ (H15-C2-C3-C4) (29), τ (H16-C3-C4-C5) (20), τ (C1-C2-C3-C4) (11)
1037	996	6.1901	28.176	γ (C3-C2) (12), γ (C4-C3)(10), β (C1-C2-C3) (27), β (C4-C3-C2) (16), β (C5-C4-C3) (13)
1017	977	0.7470	0.2303	τ (H14-C1-C2-C3) (27), τ (H16-C3-C4-C5) (11), τ (H17-C4-C5-C6) (30), τ (C6-C5-C4-C3) (10)
1009	969	14.401	7.5614	γ (N12-C13) (16), γ (C11-C10) (11), γ (C9-C7) (10)
988	949	11.918	4.5339	γ (C11-C10) (13), γ (C9-C7) (15)
971	933	2.462	3.0654	τ (H14-C1-C2-C3) (12), τ (H16-C3-C4-C5) (25), τ (H18-C5-C4-C3) (27)
917	881	3.8932	5.5640	γ (C10-C9) (18), τ (H23-C11-C10-C9) (11)

Table A17: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Buphedrone.

Unscaled	Scaled	IR intensity	Raman intensity	Assignment
882	847	0.5018	4.2253	τ (H14-C1-C2-C3) (18), τ (H15-C2-C3-C4) (30), τ (H17-C4-C5-C6) (18), τ (H18-C5-C4-C3) (31)
866	832	29.295	3.6410	τ (H21-C10-C9-C12) (18), τ (H22-C11-C10-C9) (22)
824	791	18.765	1.6608	τ (H16-C3-C4-C5) (10), τ (H17-C4-C5-C6) (18), τ (O8-C9-C6-C7) (16), ρ_0 (C7-C1-C5-C6) (15)
762	732	8.8581	5.1344	γ (C9-C7) (14), τ (H20-C10-C8-C12) (12)
728	699	50.152	4.8409	τ (H16-C3-C4-C5) (13), τ (H17-C4-C5-C6) (12), τ (H18-C5-C4-C3) (11), τ (O8-C9-C6-C7) (24)
716	688	41.040	1.8823	τ (C1-C2-C3-C4) (20), τ (C5-C4-C3-C2) (17), τ (C6-C5-C4-C3) (26)
708	680	138.78	9.0948	τ (H25-N12-C9-C10) (29)
679	652	16.578	1.5720	β (O8-C7-C6) (14), β (C4-C3-C2) (16), τ (H25-N12-C9-C10) (17)
649	623	0.3892	5.8949	β (C1-C2-C3) (24), β (C5-C4-C3) (39), β (C6-C5-C4) (18)
482	463	2.7500	1.2232	β (O8-C7-C6) (12), β (C13-N12-C9) (10), τ (C5-C4-C3-C2) (11), ρ_0 (C7-C1-C5-C6) (15)
477	458	3.3019	2.1203	β (O8-C7-C6) (24), β (C7-C6-C5) (10)
428	411	1.3133	6.3123	γ (N12-C9) (10), γ (C10-C9) (15), β (C10-C9-N12) (25)
422	405	0.6101	0.2905	τ (H18-C5-C4-C3) (11), τ (C1-C2-C3-C4) (36)
415	398	4.1920	0.3335	β (C13-N12-C9) (26), β (C11-C10-C9) (12), τ (C5-C4-C3-C2) (18), τ (C6-C5-C4-C3) (14)
331	318	18.168	1.2948	β (O8-C7-C6) (12), β (C6-C5-C4) (11), β (C7-C6-C5) (18), β (C9-C7-C6) (31)
322	309	7.9447	1.9692	γ (C7-C6) (12), γ (C9-C7) (14), β (C11-C10-C9) (15), ρ_0 (C10-N12-C7-C9) (11)
263	252	2.2505	1.0332	τ (H22-C11-C10-C9) (15), τ (H26-C13-N12-C9) (16)
224	215	0.7141	0.2550	β (C7-C6-C5) (21), β (C11-C10-C9) (10), τ (H22-C11-C10-C9) (13), τ (H24-C11-C10-C9) (14)
191	183	0.5757	2.9410	β (C10-C9-N12) (11), τ (H23-C11-C10-C9) (10), ρ_0 (C10-N12-C7-C9) (19)
182	174	4.3344	0.3359	β (N12-C9-C7) (15), β (C13-N12-C9) (11), β (C10-C9-N12) (11), τ (H26-C13-N12-C9) (15), τ (H27-C13-N12-C9) (16)
153	147	1.3931	3.3447	τ (C5-C4-C3-C2) (10), τ (O8-C9-C6-C7) (14), ρ_0 (C7-C1-C5-C6) (33)
137	131	0.3157	0.3939	β (C7-C6-C5) (16), β (C10-C9-N12) (21)
96	92	4.4624	0.1464	τ (C13-N12-C9-C10) (67)
77	73	0.3303	0.4609	τ (C13-N12-C9-C10) (17), τ (C11-C10-C9-N12) (53)
33	31	1.0556	4.3410	τ (N12-C9-C7-C6) (60), τ (C9-C7-C6-C1) (20)
25	24	0.0499	9.3411	τ (N12-C9-C7-C6) (15), τ (C9-C7-C6-C1) (67)

Table A18: Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Methylone.

Calculated Wavenumber (cm ⁻¹)		IR Intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
3594	3458	17.33	71.68	$\nu(\text{N}_{11}-\text{H}_{23})$ (99)
3259	3135	1.05	76.66	$\nu(\text{C}_1-\text{H}_{16})$ (99)
3253	3129	5.25	125.32	$\nu(\text{C}_4-\text{H}_{17})$ (64), $\nu(\text{C}_5-\text{H}_{18})$ (34)
3238	3115	0.34	40.52	$\nu(\text{C}_5-\text{H}_{18})$ (65), $\nu(\text{C}_4-\text{H}_{17})$ (35)
3170	3049	31.62	162.43	$\nu(\text{C}_{14}-\text{H}_{27})$ (51), $\nu(\text{C}_{14}-\text{H}_{28})$ (49)
3135	3016	21.24	75.60	$\nu(\text{C}_{10}-\text{H}_{20})$ (45), $\nu(\text{C}_{10}-\text{H}_{21})$ (53)
3130	3011	37.43	59.30	$\nu(\text{C}_{10}-\text{H}_{22})$ (64), $\nu(\text{C}_{10}-\text{H}_{20})$ (18), $\nu(\text{C}_{10}-\text{H}_{21})$ (17)
3116	2998	38.81	128.11	$\nu(\text{C}_{12}-\text{H}_{24})$ (85), $\nu(\text{C}_{12}-\text{H}_{26})$ (14)
3097	2980	90.17	267.23	$\nu(\text{C}_{14}-\text{H}_{28})$ (51), $\nu(\text{C}_{14}-\text{H}_{27})$ (49)
3050	2934	31.72	86.56	$\nu(\text{C}_{10}-\text{H}_{20})$ (34), $\nu(\text{C}_{10}-\text{H}_{22})$ (64), $\nu(\text{C}_{10}-\text{H}_{21})$ (27)
3047	2931	49.16	123.14	$\nu(\text{C}_{12}-\text{H}_{26})$ (80), $\nu(\text{C}_{12}-\text{H}_{24})$ (12)
3030	2915	34.96	63.84	$\nu(\text{C}_9-\text{H}_{19})$ (99)
2941	2829	127.70	135.19	$\nu(\text{C}_{12}-\text{H}_{25})$ (95)
1687	1623	30.22	10.92	$\nu(\text{O}_8-\text{H}_7)$ (35), $\nu(\text{C}_1-\text{C}_2)$ (22), $\nu(\text{C}_6-\text{C}_5)$ (12)
1656	1593	22.96	161.81	$\nu(\text{C}_1-\text{C}_2)$ (20)
1643	1581	134.40	217.23	$\nu(\text{O}_8-\text{H}_7)$ (85), $\nu(\text{C}_4-\text{C}_3)$ (12), $\nu(\text{C}_3-\text{C}_2)$ (10)
1572	1512	0.02	36.27	$\beta(\text{H}_{28}-\text{C}_{14}-\text{H}_{27})$ (93)
1566	1506	20.99	14.64	$\beta(\text{H}_{25}-\text{C}_{12}-\text{H}_{24})$ (21), $\beta(\text{H}_{26}-\text{C}_{12}-\text{H}_{25})$ (60), $\tau(\text{H}_{25}-\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (10)
1546	1487	38.57	0.95	$\beta(\text{H}_{22}-\text{C}_{10}-\text{H}_{21})$ (93), $\beta(\text{H}_{21}-\text{C}_{10}-\text{H}_{20})$ (14)
1545	1486	15.62	18.46	$\beta(\text{H}_{20}-\text{C}_{10}-\text{H}_{22})$ (25), $\beta(\text{H}_{25}-\text{C}_{12}-\text{H}_{24})$ (17), $\beta(\text{H}_{23}-\text{N}_{11}-\text{C}_{12})$ (13)
1537	1479	91.25	15.98	$\beta(\text{H}_{16}-\text{C}_1-\text{C}_2)$ (17), $\beta(\text{H}_{17}-\text{C}_4-\text{C}_5)$ (12), $\beta(\text{H}_{20}-\text{C}_{10}-\text{H}_{22})$ (11)
1531	1473	3.26	27.20	$\beta(\text{H}_{21}-\text{C}_{10}-\text{H}_{20})$ (23), $\beta(\text{H}_{25}-\text{C}_{12}-\text{H}_{24})$ (21)
1517	1460	34.03	22.37	$\beta(\text{H}_{23}-\text{N}_{11}-\text{C}_{12})$ (42), $\beta(\text{H}_{24}-\text{C}_{12}-\text{H}_{26})$ (13)
1499	1442	7.85	29.35	$\beta(\text{H}_{24}-\text{C}_{12}-\text{H}_{26})$ (58)
1484	1427	59.83	22.74	$\nu(\text{C}_1-\text{C}_2)$ (20), $\nu(\text{C}_5-\text{C}_4)$ (18), $\beta(\text{H}_{18}-\text{C}_5-\text{C}_4)$ (15)
1440	1386	20.34	18.82	$\beta(\text{H}_{20}-\text{C}_{10}-\text{H}_{22})$ (34), $\beta(\text{H}_{21}-\text{C}_{10}-\text{H}_{20})$ (20)
1417	1363	4.95	14.18	$\tau(\text{H}_{28}-\text{C}_{14}-\text{O}_{15}-\text{C}_2)$ (37), $\tau(\text{H}_{27}-\text{C}_{14}-\text{O}_{15}-\text{C}_2)$ (34)
1406	1352	81.57	60.47	$\nu(\text{C}_6-\text{C}_5)$ (18), $\beta(\text{H}_{19}-\text{C}_9-\text{N}_{11})$ (24)
1398	1345	5.94	14.83	$\nu(\text{C}_6-\text{C}_5)$ (24), $\nu(\text{C}_3-\text{C}_2)$ (10), $\beta(\text{H}_{19}-\text{C}_9-\text{N}_{11})$ (16)
1350	1299	77.69	6.94	$\beta(\text{H}_{19}-\text{C}_9-\text{N}_{11})$ (10), $\tau(\text{H}_{19}-\text{C}_9-\text{C}_7-\text{C}_6)$ (43)
1323	1272	5.86	1.31	$\beta(\text{H}_{16}-\text{C}_1-\text{C}_2)$ (32), $\beta(\text{H}_{17}-\text{C}_4-\text{C}_5)$ (19), $\beta(\text{H}_{18}-\text{C}_5-\text{C}_4)$ (17)
1293	1244	326.35	71.19	$\nu(\text{C}_5-\text{C}_4)$ (20), $\nu(\text{C}_7-\text{C}_6)$ (15)
1272	1223	111.90	1.94	$\nu(\text{N}_{11}-\text{C}_9)$ (18), $\nu(\text{O}_{13}-\text{C}_3)$ (12)
1235	1188	59.28	9.97	$\nu(\text{N}_{11}-\text{C}_9)$ (18), $\nu(\text{C}_7-\text{C}_6)$ (12), $\beta(\text{H}_{16}-\text{C}_1-\text{C}_2)$ (17)
1191	1145	32.17	7.50	$\nu(\text{N}_{11}-\text{C}_{12})$ (41), $\tau(\text{H}_{25}-\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (17)
1181	1136	7.17	2.09	$\nu(\text{C}_5-\text{C}_4)$ (15), $\beta(\text{H}_{18}-\text{C}_5-\text{C}_4)$ (30), $\beta(\text{H}_{17}-\text{C}_4-\text{C}_5)$ (17)
1174	1130	2.71	5.85	$\beta(\text{H}_{24}-\text{C}_{12}-\text{H}_{26})$ (13), $\tau(\text{H}_{24}-\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (17), $\tau(\text{H}_{26}-\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (50)
1168	1123	0.02	11.03	$\beta(\text{H}_{27}-\text{C}_{14}-\text{O}_{15})$ (59), $\tau(\text{H}_{28}-\text{C}_{14}-\text{O}_{15}-\text{C}_2)$ (30)
1126	1083	11.85	6.44	$\beta(\text{C}_1-\text{C}_2-\text{C}_3)$ (11)
1117	1075	9.62	1.59	$\beta(\text{H}_{27}-\text{C}_{14}-\text{O}_{15})$ (40), $\tau(\text{H}_{27}-\text{C}_{14}-\text{O}_{15}-\text{C}_2)$ (36), $\tau(\text{C}_{14}-\text{O}_{15}-\text{C}_2-\text{C}_1)$ (18)
1102	1060	58.54	39.77	$\beta(\text{C}_1-\text{C}_2-\text{C}_3)$ (20), $\beta(\text{C}_4-\text{C}_3-\text{C}_2)$ (11), $\beta(\text{C}_5-\text{C}_4-\text{C}_3)$ (10)
1074	1033	4.62	4.09	$\tau(\text{H}_{19}-\text{C}_9-\text{C}_7-\text{C}_6)$ (17), $\tau(\text{H}_{21}-\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (17), $\tau(\text{H}_{22}-\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (15)
1025	986	63.01	6.00	$\nu(\text{C}_{10}-\text{C}_9)$ (10)

Continued **Table A18:** Calculated vibrational wavenumbers along with the IR and Raman intensity along with their assignments of Methylone.

Calculated Wavenumber (cm ⁻¹)		IR Intensity	Raman Activity	Assignments based on Potential Energy Distributions
Unscaled	Scaled			
1019	980	58.56	3.24	$\nu(\text{C}_{10}-\text{C}_9)$ (12), $\beta(\text{C}_{14}-\text{O}_{15}-\text{C}_2)$ (12)
1008	969	22.97	2.90	$\nu(\text{O}_{15}-\text{C}_{14})$ (19), $\tau(\text{H}_{17}-\text{C}_4-\text{C}_5-\text{C}_6)$ (21)
1000	962	138.61	7.14	$\nu(\text{C}_9-\text{C}_7)$ (13)
913	879	7.26	4.58	$\nu(\text{O}_{15}-\text{C}_2)$ (17), $\tau(\text{H}_{18}-\text{C}_5-\text{C}_4-\text{C}_3)$ (52), $\tau(\text{H}_{16}-\text{C}_1-\text{C}_2-\text{C}_3)$ (18)
906	872	21.01	1.13	$\tau(\text{H}_{16}-\text{C}_1-\text{C}_2-\text{C}_3)$ (52)
878	845	26.44	2.99	$\nu(\text{O}_{15}-\text{C}_{14})$ (37), $\beta(\text{C}_{13}-\text{C}_3-\text{C}_4)$ (13), $\beta(\text{O}_{15}-\text{C}_2-\text{C}_3)$ (10), $\beta(\text{C}_{14}-\text{O}_{15}-\text{C}_2)$ (12)
870	837	22.05	2.74	$\tau(\text{H}_{17}-\text{C}_4-\text{C}_5-\text{C}_6)$ (56), $\tau(\text{H}_{18}-\text{C}_5-\text{C}_4-\text{C}_3)$ (21)
857	825	7.95	9.85	$\nu(\text{C}_{10}-\text{C}_9)$ (33), $\nu(\text{N}_{11}-\text{C}_9)$ (11)
817	786	15.01	23.04	$\nu(\text{C}_3-\text{C}_2)$ (27), $\nu(\text{O}_{13}-\text{C}_3)$ (12), $\nu(\text{C}_1-\text{C}_2)$ (11)
781	751	7.99	3.60	$\tau(\text{H}_{22}-\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (14), $\gamma(\text{O}_8-\text{C}_9-\text{C}_6-\text{C}_7)$ (14)
758	729	20.72	5.81	$\gamma(\text{O}_8-\text{C}_9-\text{C}_6-\text{C}_7)$ (20)
718	691	1.52	6.03	$\beta(\text{O}_{15}-\text{C}_2-\text{C}_3)$ (25), $\beta(\text{C}_{14}-\text{O}_{15}-\text{C}_2)$ (23), $\beta(\text{C}_{13}-\text{C}_3-\text{C}_4)$ (19)
708	681	1.71	1.53	$\tau(\text{C}_6-\text{C}_5-\text{C}_4-\text{C}_3)$ (17), $\tau(\text{C}_5-\text{C}_4-\text{C}_3-\text{C}_2)$ (14), $\gamma(\text{O}_{15}-\text{C}_1-\text{C}_3-\text{C}_2)$ (16), $\gamma(\text{O}_{13}-\text{C}_2-\text{C}_4-\text{C}_3)$ (15)
683	657	11.57	4.54	$\beta(\text{C}_4-\text{C}_3-\text{C}_2)$ (16), $\beta(\text{O}_8-\text{C}_7-\text{C}_6)$ (15)
593	571	11.04	6.57	$\nu(\text{C}_4-\text{C}_3)$ (17), $\nu(\text{O}_{15}-\text{C}_2)$ (11), $\beta(\text{C}_1-\text{C}_2-\text{C}_3)$ (15), $\beta(\text{C}_5-\text{C}_4-\text{C}_3)$ (12)
582	560	7.59	0.52	$\tau(\text{C}_6-\text{C}_5-\text{C}_4-\text{C}_3)$ (22), $\tau(\text{C}_1-\text{C}_2-\text{C}_3-\text{C}_4)$ (12), $\gamma(\text{O}_{15}-\text{C}_1-\text{C}_3-\text{C}_2)$ (17), $\gamma(\text{O}_{13}-\text{C}_2-\text{C}_4-\text{C}_3)$ (12)
566	545	87.80	2.50	$\tau(\text{H}_{23}-\text{N}_{11}-\text{C}_9-\text{C}_{10})$ (48)
497	478	44.49	3.56	$\beta(\text{C}_9-\text{N}_7-\text{C}_6)$ (10), $\beta(\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (14), $\tau(\text{H}_{23}-\text{N}_{11}-\text{C}_9-\text{C}_{10})$ (15)
446	429	13.71	1.35	$\beta(\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (18)
437	420	2.65	0.61	$\tau(\text{C}_5-\text{C}_4-\text{C}_3-\text{C}_2)$ (24), $\tau(\text{C}_6-\text{C}_5-\text{C}_4-\text{C}_3)$ (15)
391	376	14.30	7.51	$\beta(\text{O}_8-\text{C}_7-\text{C}_6)$ (36), $\beta(\text{C}_5-\text{C}_4-\text{C}_3)$ (12)
380	366	4.71	2.22	$\beta(\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (13), $\beta(\text{C}_9-\text{N}_7-\text{C}_6)$ (13)
326	314	1.50	2.95	$\gamma(\text{C}_7-\text{C}_1-\text{C}_5-\text{C}_6)$ (17), $\gamma(\text{O}_{13}-\text{C}_2-\text{C}_4-\text{C}_3)$ (16), $\gamma(\text{O}_{15}-\text{C}_1-\text{C}_3-\text{C}_2)$ (11)
284	273	1.33	2.34	$\nu(\text{C}_7-\text{C}_6)$ (12), $\beta(\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (12)
257	247	0.60	0.76	$\beta(\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (20), $\gamma(\text{O}_{15}-\text{C}_1-\text{C}_3-\text{C}_2)$ (10)
239	230	1.46	1.25	$\tau(\text{H}_{22}-\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (17), $\tau(\text{H}_{21}-\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (12), $\tau(\text{C}_1-\text{C}_2-\text{C}_3-\text{C}_4)$ (17), $\gamma(\text{O}_{15}-\text{C}_1-\text{C}_3-\text{C}_2)$ (13)
229	220	5.61	0.33	$\beta(\text{N}_{11}-\text{C}_9-\text{C}_7)$ (14), $\beta(\text{C}_7-\text{C}_6-\text{C}_5)$ (11), $\beta(\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (11)
220	211	1.49	1.64	$\tau(\text{H}_{24}-\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (11), $\tau(\text{H}_{20}-\text{C}_{10}-\text{C}_9-\text{N}_{11})$ (10), $\tau(\text{C}_1-\text{C}_2-\text{C}_3-\text{C}_4)$ (22)
196	189	2.68	0.95	$\beta(\text{N}_{11}-\text{C}_9-\text{C}_7)$ (10), $\tau(\text{H}_{24}-\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (27), $\tau(\text{H}_{25}-\text{C}_{12}-\text{N}_{11}-\text{C}_9)$ (19), $\gamma(\text{C}_{10}-\text{N}_{11}-\text{C}_7-\text{C}_6)$ (11)
131	126	1.78	0.32	$\beta(\text{C}_7-\text{C}_6-\text{C}_5)$ (15), $\beta(\text{C}_9-\text{N}_7-\text{C}_6)$ (11), $\tau(\text{C}_{12}-\text{N}_{11}-\text{C}_9-\text{C}_{10})$ (40)
125	120	7.09	0.29	$\gamma(\text{C}_7-\text{C}_1-\text{C}_5-\text{C}_6)$ (17), $\tau(\text{C}_5-\text{C}_4-\text{C}_3-\text{C}_2)$ (19)
93	89	6.26	0.90	$\beta(\text{C}_9-\text{N}_7-\text{C}_6)$ (19), $\beta(\text{C}_7-\text{C}_6-\text{C}_5)$ (13), $\tau(\text{C}_{14}-\text{O}_{15}-\text{C}_2-\text{C}_1)$ (17), $\tau(\text{C}_{12}-\text{N}_{11}-\text{C}_9-\text{C}_{10})$ (16)
83	80	4.42	1.72	$\tau(\text{C}_{14}-\text{O}_{15}-\text{C}_2-\text{C}_1)$ (43), $\tau(\text{C}_{12}-\text{N}_{11}-\text{C}_9-\text{C}_{10})$ (10)
56	53	0.19	1.54	$\tau(\text{C}_9-\text{C}_7-\text{C}_6-\text{C}_1)$ (41), $\tau(\text{N}_{11}-\text{C}_9-\text{C}_7-\text{C}_6)$ (29)
37	35	1.15	1.97	$\tau(\text{C}_9-\text{C}_7-\text{C}_6-\text{C}_1)$ (48), $\tau(\text{N}_{11}-\text{C}_9-\text{C}_7-\text{C}_6)$ (25)

Table A19: Donor-acceptor interactions along with their charge transfer for 3-FMC molecule.

Donor (i)	Acceptor (j)	E_{orb} (kcal/mol)	$E_{\text{orb}} - E_{\text{orb}}$ (au)	F(i,j) (au)
σ (C1-H14)	σ^* (C1-C6)	2.98	1.29	0.055
σ (C1-C6)	σ^* (C2-F7)	4.32	0.89	0.056
n (C1-C6)	n^* (C2-C3)	22.11	0.27	0.069
n (C1-C6)	n^* (C4-C5)	18.54	0.28	0.066
n (C1-C6)	n^* (C8-C9)	19.38	0.26	0.067
n (C2-C3)	n^* (C1-C6)	20.78	0.29	0.070
n (C2-C3)	n^* (C4-C5)	17.58	0.30	0.066
n (C4-C5)	n^* (C1-C6)	20.75	0.27	0.067
n (C4-C5)	n^* (C2-C3)	21.92	0.26	0.068
n^* (C2-C3)	n^* (C4-C5)	159.50	0.02	0.080
n^* (C8-O9)	n^* (C10-C11)	97.88	0.02	0.073
σ (C13-H23)	σ^* (C10-N12)	4.22	0.87	0.054
σ (C11-H21)	σ^* (C10-N12)	3.62	0.88	0.050
σ (C10-C11)	n^* (C8-O9)	4.64	0.57	0.047
σ (C8-H10)	σ^* (N12-C13)	3.09	1.01	0.050
σ (C5-H17)	σ^* (C1-C6)	4.37	1.07	0.061
LP3 (F7)	n^* (C2-C3)	17.40	0.40	0.080
LP2 (O9)	n^* (C6-C8)	17.09	0.70	0.099
LP2 (F7)	n^* (C1-C2)	5.53	0.95	0.065
LP2 (O9)	σ^* (C8-C10)	17.22	0.64	0.094
LP2 (F7)	σ^* (C2-C3)	5.57	0.95	0.065
LP1 (N12)	σ^* (C10-C11)	11.26	0.56	0.072
LP1 (N12)	σ^* (C13-C24)	9.90	0.65	0.073

Table A20: Donor-acceptor interactions along with their charge transfer for 4-FMC molecule.

Donor (i)	Acceptor (j)	E_{orb} (kcal/mol)	$E_{\text{orb}} - E_{\text{orb}}$ (au)	F(i,j) (au)
σ (C1-C2)	σ^* (C1-C6)	2.99	1.26	0.055
σ (C1-C2)	σ^* (C1-H14)	1.43	1.19	0.037
σ (C1-C2)	σ^* (C2-C3)	3.97	1.29	0.064
σ (C1-C2)	σ^* (C3-H15)	1.61	1.17	0.039
σ (C1-C2)	σ^* (C6-C8)	3.37	1.15	0.056
σ (C1-C6)	σ^* (C1-C2)	2.59	1.27	0.051
σ (C1-C6)	σ^* (C1-H14)	1.52	1.18	0.038
σ (C1-C6)	σ^* (C2-H15)	2.22	1.16	0.046
σ (C1-C6)	σ^* (C5-C6)	3.82	1.25	0.062
σ (C1-C6)	σ^* (C5-H17)	1.88	1.18	0.042
σ (C1-C6)	σ^* (C6-C8)	2.27	1.14	0.046
σ (C1-C6)	σ^* (C8-O9)	1.61	1.21	0.039
n (C1-C6)	n^* (C1-C6)	0.63	0.27	0.012
n (C1-C6)	n^* (C2-C3)	19.27	0.26	0.063
n (C1-C6)	n^* (C4-C5)	22.11	0.27	0.071
LP(F7)	n^* (C1-C2)	1.15	0.72	0.026
n^* (C2-C3)	n^* (C2-H15)	1.98	1.19	0.043
n^* (C8-O9)	n^* (C4-C5)	2.43	1.30	0.050
n^* (C3-C4)	n^* (C5-H17)	2.26	1.21	0.047

Table A21: Donor-acceptor interactions along with their charge transfer for 4-MMC molecule.

Donor(i)	Acceptor(j)	E (2) Kcal/mol	$E_{\oplus}-E_{\ominus}$ (au)	F (i, j) au
$\sigma(C_1-C_2)$	$\sigma^*(C_1-C_6)$	2.96	1.25	0.054
$\sigma(C_1-C_2)$	$\sigma^*(C_2-C_3)$	2.65	1.26	0.052
$\sigma(C_1-C_2)$	$\sigma^*(C_6-C_7)$	2.93	1.15	0.052
$\pi(C_1-C_2)$	$\pi^*(C_3-C_4)$	21.90	0.27	0.069
$\pi(C_1-C_2)$	$\pi^*(C_5-C_6)$	19.15	0.27	0.065
$\sigma(C_1-C_6)$	$\sigma^*(C_2-H_{15})$	2.24	1.16	0.046
$\sigma(C_1-C_6)$	$\sigma^*(C_5-C_6)$	3.89	1.24	0.062
$\pi(C_3-C_4)$	$\pi^*(C_1-C_2)$	17.57	0.28	0.070
$\pi(C_3-C_4)$	$\pi^*(C_5-C_6)$	22.12	0.27	0.068
$\pi(C_5-C_6)$	$\pi^*(C_1-C_2)$	19.62	0.28	0.065
$\pi(C_5-C_6)$	$\pi^*(C_3-C_4)$	18.65	0.27	0.069
$\sigma(C_1-H_{14})$	$\sigma^*(C_2-C_3)$	3.61	1.08	0.056
$\sigma(C_1-H_{14})$	$\sigma^*(C_5-C_6)$	4.22	1.07	0.060
$\sigma(C_2-H_{15})$	$\sigma^*(C_3-C_4)$	3.47	1.09	0.055
LP (2) O ₈	$\sigma^*(C_6-C_7)$	16.53	0.70	0.097
LP (2) O ₈	$\sigma^*(C_7-C_9)$	17.25	0.62	0.092
LP (1) N ₁₂	$\sigma^*(C_7-C_9)$	9.52	0.60	0.068
LP (1) N ₁₂	$\sigma^*(C_{13}-H_{27})$	8.59	0.68	0.069
$\pi^*(C_7-O_8)$	$\pi^*(C_5-C_6)$	73.73	0.02	0.072

Table A22: Donor-acceptor interactions along with their charge transfer for Buphedrone molecule.

Donor(i)	Acceptor(j)	E(2) Kcal/mol	$E_{\oplus}-E_{\ominus}$ (au)	F(i, j) au
$\sigma(C_1-C_2)$	$\sigma^*(C_2-C_3)$	3.17	1.26	0.056
$\sigma(C_1-C_2)$	$\sigma^*(C_6-C_8)$	3.45	1.15	0.057
$\sigma(C_1-C_6)$	$\sigma^*(C_5-C_6)$	3.94	1.25	0.063
$\pi(C_1-C_6)$	$\pi^*(C_2-C_3)$	17.90	0.28	0.064
$\pi(C_1-C_6)$	$\pi^*(C_4-C_5)$	20.09	0.28	0.069
$\pi(C_1-C_6)$	$\pi^*(C_8-O_{13})$	21.33	0.25	0.069
$\sigma(C_1-H_{14})$	$\sigma^*(C_2-C_3)$	3.72	1.09	0.057
$\sigma(C_1-H_{14})$	$\sigma^*(C_5-C_6)$	3.83	1.09	0.058
$\pi(C_2-C_3)$	$\pi^*(C_1-C_6)$	23.94	0.27	0.072
$\pi(C_2-C_3)$	$\pi^*(C_4-C_5)$	16.74	0.28	0.062
$\sigma(C_4-C_5)$	$\sigma^*(C_3-C_4)$	3.15	1.26	0.056
$\pi(C_4-C_5)$	$\pi^*(C_1-C_6)$	18.30	0.27	0.064
$\pi(C_4-C_5)$	$\pi^*(C_2-C_3)$	22.83	0.28	0.071
$\sigma(C_5-H_{17})$	$\sigma^*(C_1-C_6)$	4.15	1.07	0.060
$\sigma(C_7-H_{20})$	$\pi^*(C_2-C_3)$	4.23	0.53	0.046
$\pi(C_8-O_{13})$	$\pi^*(C_1-C_6)$	5.33	0.39	0.045
LP (2) O ₁₃	$\sigma^*(C_6-C_8)$	16.55	0.71	0.098
LP (2) O ₁₃	$\sigma^*(C_8-C_9)$	17.01	0.63	0.094
$\pi^*(C_8-O_{13})$	$\pi^*(C_1-C_6)$	65.53	0.03	0.072

Table A23: Donor-acceptor interactions along with their charge transfer for Butylone molecule.

Donor(i)	Acceptor(j)	E(2) Kcal/mol	$E_{\text{orb}} - E_{\text{orb}}$ (au)	F(i, j) au
π (C ₁ -C ₂)	π^* (C ₃ -C ₄)	21.04	0.29	0.071
π (C ₁ -C ₂)	π^* (C ₅ -C ₆)	16.30	0.30	0.064
π (C ₃ -C ₄)	π^* (C ₁ -C ₂)	19.94	0.29	0.068
π (C ₃ -C ₄)	π^* (C ₅ -C ₆)	21.41	0.30	0.071
π (C ₅ -C ₆)	π^* (C ₁ -C ₂)	21.38	0.26	0.067
π (C ₅ -C ₆)	π^* (C ₃ -C ₄)	18.67	0.26	0.062
π (C ₅ -C ₆)	π^* (C ₇ -O ₈)	22.06	0.25	0.070
σ (C ₁ -C ₂)	σ^* (C ₂ -C ₃)	4.97	1.27	0.071
σ (C ₁ -C ₆)	σ^* (C ₂ -O ₁₂)	6.78	0.96	0.072
σ (C ₁ -H ₁₇)	σ^* (C ₂ -C ₃)	4.32	1.07	0.061
σ (C ₂ -C ₃)	σ^* (C ₁ -C ₂)	5.13	1.33	0.074
σ (C ₂ -C ₃)	σ^* (C ₃ -C ₄)	4.80	1.31	0.071
σ (C ₃ -C ₄)	σ^* (C ₂ -C ₃)	4.70	1.27	0.069
σ (C ₄ -C ₅)	σ^* (C ₃ -O ₁₀)	6.85	0.97	0.073
σ (C ₅ -H ₁₉)	σ^* (C ₁ -C ₆)	4.60	1.05	0.062
σ (C ₇ -O ₈)	σ^* (C ₅ -C ₆)	4.32	0.38	0.040
σ (C ₁₁ -O ₁₂)	σ^* (O ₁₀ -C ₁₁)	4.48	1.38	0.070
LP (2) O ₈	σ^* (C ₆ -C ₇)	16.56	0.70	0.020
LP (2) O ₈	σ^* (C ₇ -C ₉)	17.18	0.61	0.092
LP (2) O ₁₀	π^* (C ₃ -C ₄)	26.68	0.33	0.090
LP (2) O ₁₂	π^* (C ₁ -C ₂)	24.92	0.33	0.087
LP (1) N ₁₅	σ^* (C ₇ -C ₉)	9.50	0.60	0.068
LP (1) N ₁₅	σ^* (C ₁₆ -H ₃₀)	8.58	0.69	0.019

Table A24: Donor-acceptor interactions along with their charge transfer for Ethylone molecule.

Donor (i)	Acceptor (j)	E (2)	E (j)-E (i)	F (i,j)
σ (C1-C2)	σ^* (C2-C3)	4.97	1.27	0.071
π (C1-C2)	π^* (C3-C4)	20.87	0.29	0.071
π (C1-C2)	π^* (C5-C6)	16.34	0.30	0.064
σ (C1-C6)	σ^* (C2-O12)	6.78	0.96	0.072
σ (C2-C3)	σ^* (C1-C2)	5.14	1.33	0.74
σ (C2-C3)	σ^* (C3-C4)	4.80	1.31	0.071
σ (C3-C4)	σ^* (C2-C3)	4.70	1.27	0.069
π (C3-C4)	π^* (C1-C2)	19.96	0.29	0.068
π (C3-C4)	π^* (C5-C6)	20.93	0.30	0.071
σ (C4-C5)	σ^* (C3-O10)	6.86	0.97	0.073
π (C5-C6)	π^* (C1-C2)	21.34	0.26	0.067
π (C5-C6)	π^* (C3-C4)	18.56	0.26	0.062
π (C5-C6)	π^* (C7-O8)	21.98	0.25	0.070
LP (2)(O8)	σ^* (C6-C7)	16.77	0.71	0.091
LP (1)(O10)	σ^* (C2-C3)	3.47	1.14	0.056
LP (2)(O12)	π^* (C1-C2)	25.00	0.33	0.087
LP (1)(N14)	σ^* (C9-C13)	11.00	0.56	0.071
LP (2)(O10)	σ^* (C3-C4)	26.65	0.33	0.090
π^* (C1-C2)	π^* (C5-C6)	228.68	0.01	0.078
π^* (C3-C4)	π^* (C5-C6)	229.07	0.01	0.082

Table A25: Donor-acceptor interactions along with their charge transfer for MDPV molecule.

Donor(i)	Acceptor(j)	E(2) Kcal/mol	$E_{(i)}-E_{(j)}$ (au)	F(i, j) au
π (C ₁ -C ₂)	π^* (C ₃ -C ₄)	21.12	0.29	0.071
π (C ₁ -C ₂)	π^* (C ₅ -C ₆)	16.32	0.30	0.064
π (C ₃ -C ₄)	π^* (C ₁ -C ₂)	19.97	0.29	0.068
π (C ₃ -C ₄)	π^* (C ₅ -C ₆)	21.02	0.30	0.071
π (C ₅ -C ₆)	π^* (C ₁ -C ₂)	21.44	0.26	0.062
π (C ₅ -C ₆)	π^* (C ₃ -C ₄)	18.77	0.26	0.062
π (C ₇ -O ₈)	π^* (C ₅ -C ₆)	4.31	0.38	0.040
π (O ₁₂ -C ₁₃)	π^* (C ₃ -C ₄)	4.61	1.36	0.071
σ (C ₁ -C ₂)	σ^* (C ₂ -C ₃)	4.99	1.27	0.071
σ (C ₁ -H ₂₁)	σ^* (C ₂ -C ₃)	4.34	1.07	0.061
σ (C ₂ -C ₃)	σ^* (C ₁ -C ₂)	5.13	1.33	0.074
σ (C ₂ -C ₃)	σ^* (C ₃ -C ₄)	4.82	1.31	0.071
σ (C ₄ -C ₅)	σ^* (C ₃ -O ₁₂)	6.87	0.97	0.073
σ (C ₃ -C ₄)	σ^* (C ₂ -C ₃)	4.73	1.29	0.069
σ (C ₄ -H ₂₂)	σ^* (C ₂ -C ₃)	4.14	1.07	0.060
σ (C ₅ -H ₂₃)	σ^* (C ₁ -C ₆)	4.56	1.05	0.062
σ (C ₁₃ -O ₁₄)	σ^* (C ₁ -C ₂)	4.46	1.38	0.070
LP (2) O ₈	π^* (C ₆ -C ₇)	16.96	0.69	0.098
LP (2) O ₈	π^* (C ₇ -C ₉)	18.47	0.61	0.096
LP (2) O ₁₂	π^* (C ₃ -C ₄)	26.57	0.34	0.090
LP (2) O ₁₄	π^* (C ₁ -C ₂)	24.74	0.33	0.086
LP (1) N ₁₁	σ^* (C ₉ -H ₂₄)	7.66	0.66	0.065
LP (1) N ₁₁	σ^* (C ₁₅ -H ₃₀)	6.27	0.67	0.059
LP (2) O ₁₂	σ^* (C ₁₃ -H ₂₇)	3.46	1.14	0.056
LP (2) O ₁₂	σ^* (C ₁₃ -H ₂₈)	3.51	0.79	0.044
LP (2) O ₁₄	σ^* (C ₁₃ -H ₂₇)	3.69	0.76	0.048
LP (2) O ₁₄	σ^* (C ₁₃ -H ₂₈)	3.73	0.76	0.049

Table A26: Donor-acceptor interactions along with their charge transfer for Methcathinone molecule.

Donor(i)	Acceptor(j)	E(2) Kcal/mol	$E_{(i)}-E_{(j)}$ (au)	F(i, j) au
π (C ₁ -C ₂)	π^* (C ₃ -C ₄)	22.07	0.27	0.070
π (C ₁ -C ₂)	π^* (C ₅ -C ₆)	18.81	0.28	0.065
π (C ₃ -C ₄)	π^* (C ₅ -C ₆)	22.30	0.28	0.071
π (C ₃ -C ₄)	π^* (C ₁ -C ₂)	17.86	0.28	0.064
π (C ₅ -C ₆)	π^* (C ₁ -C ₂)	20.55	0.28	0.069
π (C ₅ -C ₆)	π^* (C ₃ -C ₄)	18.84	0.27	0.065
π (C ₅ -C ₆)	π^* (C ₇ -O ₈)	21.15	0.24	0.068
π (C ₇ -O ₈)	π^* (C ₅ -C ₆)	5.38	0.39	0.045
σ (C ₁ -H ₁₃)	σ^* (C ₅ -C ₆)	4.19	1.08	0.060
σ (C ₁₀ -H ₂₁)	σ^* (C ₉ -N ₁₁)	4.57	0.82	0.055
LP (2) O ₈	π^* (C ₆ -C ₇)	16.38	0.71	0.097
LP (2) O ₈	π^* (C ₆ -C ₇)	18.82	0.62	0.097
LP (2) O ₈	π^* (C ₁₀ -H ₂₀)	0.59	0.71	0.019
LP (1) O ₈	σ^* (C ₆ -C ₇)	1.78	1.14	0.129

continued **Table A26:** Donor-acceptor interactions along with their charge transfer for Methcathinone molecule.

Donor(i)	Acceptor(j)	E(2) Kcal/mol	$E_{(i)} - E_{(j)}$ (au)	F(i, j) au
LP (1) O ₈	σ^* (C ₇ -C ₉)	1.46	1.05	0.035
LP (1) N ₁₁	σ^* (C ₅ -H ₁₇)	0.70	0.74	0.021
LP (1) N ₁₁	σ^* (C ₇ -O ₈)	1.22	0.25	0.016
LP (1) N ₁₁	σ^* (C ₇ -C ₉)	1.65	0.62	0.029
LP (1) N ₁₁	σ^* (C ₉ -C ₁₀)	8.48	0.62	0.066
LP (1) N ₁₁	σ^* (C ₉ -H ₁₈)	1.06	0.68	0.024
LP (1) N ₁₁	σ^* (C ₁₀ -H ₂₁)	0.70	0.71	0.020
LP (1) N ₁₁	σ^* (C ₁₂ -H ₂₄)	8.79	0.68	0.024

Table A27: Donor-acceptor interactions along with their charge transfer for Methylone molecule.

Donor(i)	Acceptor(j)	E (2) Kcal/mol	$E_{(i)} - E_{(j)}$ (au)	F (i, j) au
π (C ₁ -C ₂)	π^* (C ₃ -C ₄)	20.88	0.29	0.071
π (C ₁ -C ₂)	π^* (C ₅ -C ₆)	16.34	0.30	0.064
π (C ₃ -C ₄)	π^* (C ₁ -C ₂)	19.97	0.29	0.068
π (C ₃ -C ₄)	π^* (C ₅ -C ₆)	20.93	0.30	0.071
π (C ₅ -C ₆)	π^* (C ₁ -C ₂)	21.33	0.26	0.667
π (C ₅ -C ₆)	π^* (C ₃ -C ₄)	18.55	0.26	0.662
π (C ₅ -C ₆)	π^* (C ₇ -O ₈)	22.00	0.25	0.070
σ (C ₁ -C ₂)	σ^* (C ₂ -C ₃)	4.97	1.27	0.071
σ (C ₁ -C ₆)	σ^* (C ₂ -O ₁₅)	6.78	0.96	0.072
σ (C ₁ -H ₁₇)	σ^* (C ₂ -C ₃)	4.30	1.07	0.061
σ (C ₄ -C ₅)	σ^* (C ₃ -O ₁₃)	6.86	0.97	0.073
σ (C ₂ -C ₃)	σ^* (C ₃ -C ₄)	4.80	1.31	0.071
σ (C ₂ -C ₃)	σ^* (C ₁ -C ₂)	5.15	1.33	0.074
σ (C ₃ -C ₄)	σ^* (C ₂ -C ₃)	4.71	1.27	0.069
σ (C ₅ -H ₁₈)	σ^* (C ₁ -C ₆)	4.61	1.05	0.062
σ (C ₇ -O ₈)	σ^* (C ₅ -C ₆)	4.26	0.38	0.039
σ (C ₁₂ -H ₂₄)	σ^* (C ₉ -N ₁₁)	4.22	0.87	0.054
LP (2) O ₈	σ^* (C ₆ -C ₇)	16.76	0.71	0.098
LP (2) O ₈	σ^* (C ₇ -C ₉)	17.25	0.63	0.094
LP (1) N ₁₁	π^* (C ₉ -C ₁₀)	11.16	0.56	0.071
LP (2) O ₁₃	π^* (C ₃ -C ₄)	26.64	0.33	0.090
LP (1) O ₁₅	π^* (C ₁ -C ₂)	25.01	0.33	0.087
LP (1) N ₁₁	σ^* (C ₁₂ -H ₂₅)	9.98	0.65	0.073