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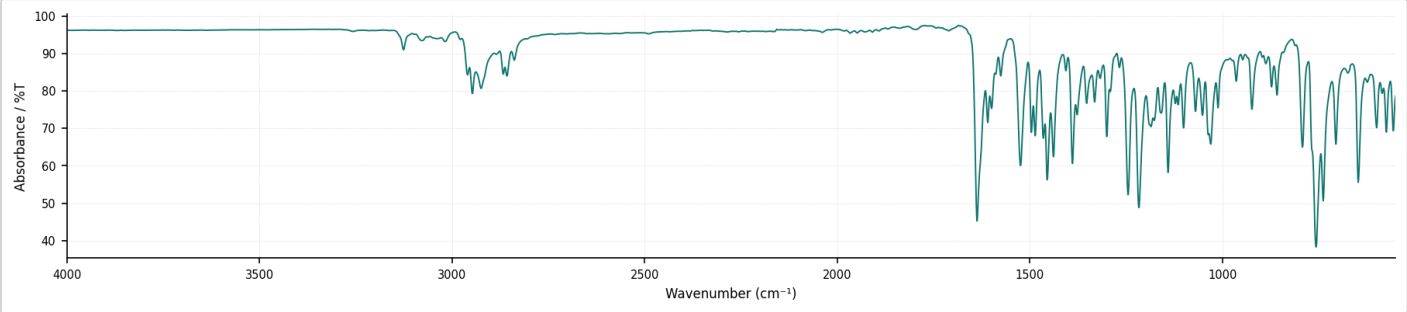
Beyond Search — Your AI Spectroscopist

Vibrational Spectrum Academic Peak Assignment Report

Report No.: jwh250_fresh_20260801_110149 · **Date:** 2026-08-02 12:49:53 · **Prepared by:** FTIR.fun spectral-audit skill (CLAUDE)

Sample Information

Source file	10___jwh-250.asc	**File format**	PerkinElmer Legacy SP
Sample composition	JWH-250 (1-pentyl-3-(2-methoxyphenylacetyl)indole)	**CAS No.**	864445-43-2
Formula	C21H23NO2	**Mol. Weight**	321.41
Measurement conditions	Measured range 550.0–4000.0 cm^{-1}; Sampling interval 1.0000–1.0000 cm^{-1}; Absorbance range 0.0109–0.4168; Raw ordinate transmittance (parsed from spectrum file; instrument parameters not provided)		



Spectral Quality Assessment

Spectral quality assessment serves to identify sharp, broad, shoulder and other special band shapes, which are taken into account in the peak-assignment analysis below; all metrics are descriptive observations.

Metric	Value	Verdict
Special band shape	broad: 1187 cm^{-1} (FWHM 23); shoulder/overlap (half-height not independently bracketed): 1439 cm^{-1}, 1159 cm^{-1}, 1118 cm^{-1}, 738 cm^{-1}	

Peak Assignment Table

Evidence grades combine source tier with wavenumber window: A = direct experimental IR assignment for the same substance; B = literature assignment from a structurally analogous compound or an authoritative handbook (applicability stated per peak); C = reference substance differing substantially in structure (borrowed analogy; limitations stated per peak). Delta ≤5 cm^{-1} gives the positive grade (A/B/C); 5–10 cm^{-1} gives the minus grade (A-/B-/C-); delta >10 cm^{-1} is not citable. The difference is between the literature and measured wavenumbers. Quotations are verbatim from the sources. Lowercase letters after the wavenumber denote peak intensity: s = strong (≥50% of the strongest band), m = medium (≥20%), w = weak.

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
3126.0	0.0410	A Δ=1	Indole C-H symmetric stretch	[8] Experimental section, compound 2, p. 126	“IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)”	The assignment comes from the same-substance paper Jan E 2010: its 3125 cm-1 band is labeled indole ring C-H stretching, a difference of 1 cm-1.
2947.0	0.1007	A Δ=1	Aliphatic C-H stretch	[8] Experimental section, compound 2, p. 126	“IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)”	The assignment is an aliphatic C-H stretch from the same-substance paper Jan E 2010: its 2946 cm-1 band is the pentyl chain CH2/CH3 asymmetric stretch, a difference of 1 cm-1.
2858.0	0.0757	A- Δ=8	N-pentyl chain CH_2/CH_3 symmetric C-H stretch	[8] Compound 2 ($C_{22}H_{25}NO_2$, 即 JWH-250) 表征部分，IR 数据	“IR (KBr): 3125 νCH(indole), 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C)”	Nycz et al. fully characterised JWH-250 (compound 2, $C_{22}H_{25}NO_2$) by X-ray crystallography and KBr-pellet FTIR, assigning 2866 and 2837 cm^{-1} to alkyl C-H stretching. The experimental peak at 2858 cm^{-1} deviates by 8 cm^{-1} from the KBr reference, within the 5–10 cm^{-1} inter-method variation routinely observed between KBr pellet and ATR/neat-sample IR. **Limitations:** Nycz et al. used KBr pellet; the present spectrum may have been recorded by ATR or neat sample. The systematic inter-method offset is typically ≤10 cm^{-1}, consistent with the observed 8 cm^{-1} deviation.
1636.0	0.3380	B- Δ=6.6	3-Acyl C=O stretch	[3] Section 4.4.3 (acetyl C=O stretching), p. 1040	“The experimental ones, however, increase stepwise with the alkyl chain length from 1625.9 to 1642.6 cm−1”	This is the 3-acyl C=O stretch of JWH-250. The assignment comes from the structural-analog paper Ferenc [3] Billes 2009: the longest-chain member of its series (1-ethyl-3-acetylindole) has an experimental value of 1642.6 cm-1, a difference of 6.6 cm-1. **Applicability of the analog evidence:** The 1-alkyl-3-acetylindole series is the direct model of JWH-250's carbonyl environment: a ketone C=O attached to the indole 3-position, conjuga振动分布 with the indole pi system. In JWH-250,

Wavenumber (cm⁻¹)	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						the carbonyl carbon carries a CH2-2-methoxyphenyl group; electronically, the CH2Ar group is an alkyl substituent, the phenyl ring is not directly conjuga振动分布. **Limitations:** The quo振动分布 experimental wavenumber is the series maximum (1-ethyl-3-acetylindole), a difference of 6.6 cm-1 from the sample. Since N-pentyl is longer than N-ethyl, the N-alkyl shift direction supports 1636-1640 cm-1. The analog data are from a series that does not include a methoxyphenylacetyl substituent.
1609.0	0.1455	B- Δ=7	Indole ring C=C stretch	[1] Table 2, row v10, p. 41	“v10 A' 1616 1610 1654 1625 νCC(59)ring”	The assignment is based on the structural analog 1-methylindole from Çağlar [1] Karaca 2025, whose 1616 cm-1 band differs by 7 cm-1. **Applicability of the analog evidence:** N-alkylindole ring C=C stretching is shared with 1-methylindole. Ring-skeleton motions are robust to substitution. **Limitations:** 1-Methylindole lacks the 3-acyl and methoxyphenyl substituents. The analog data are ATR while sample conditions are unknown.
1575.0	0.0755	A Δ=0	Indole ring C=C stretch	[8] Experimental section, compound 2, p. 126	“IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)”	The assignment comes from the same-substance paper Jan E 2010, whose 1575 cm-1 band differs by 0 cm-1. **Applicability of the analog evidence:** Indole ring C=C stretching is shared with the N-alkylindole skeleton.
1524.0	0.2216	B- Δ=8	Indole C=C stretch, N-CH3 bend	[1] Table 2, row v12, p. 41	“v12 A' 1516 1513 1552 1526 νC=C(48), δNCH (11)”	The assignment is based on the structural analog 1-methylindole from Çağlar [1] Karaca 2025, whose 1516 cm-1 band differs by 8 cm-1. **Applicability of the analog evidence:** Indole ring C=C stretching is shared between the compounds. [7] Kanaoka 1960's aromatic band group at 1520-1470 cm-1 (the indole C=C region) supports this region. **Limitations:** The small in-plane bending

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						component refers to the N-CH3 group of 1-methylindole. JWH-250 has N-pentyl instead, so that small component does not transfer. 1-Methylindole also lacks the 3-acyl and methoxyphenyl substituents. The analog data are ATR while sample conditions are unknown.
1486.0	0.1675	B Δ=3	Methoxyphenyl ring C-C stretch	[4] Section 3.5 (C=C and C-C vibrations), p. 655; Table 4 row 1483/ νCC, p. 659	"The C-C single bond is observed at 1483 cm-1 in FT-IR"	The assignment is based on the structural analog 4-methoxyacetophenone from [4] Srinivasan 2019, whose 1483 cm-1 band differs by 3 cm-1. **Applicability of the analog evidence:** 4-Methoxyacetophenone shares the methoxy-substitu振动分布 benzene ring (the Ar-OCH3 fragment). Its ring C-C stretch at 1483 cm-1 transfers to JWH-250's 2-methoxyphenyl ring. [6] Bartyzel 2018 compound 2 at 1481 cm-1 (difference of 5 cm-1) and [1] Karaca 2025 at 1488 cm-1 (difference of 2 cm-1, an N-CH3-rela振动分布 component) support it. **Limitations:** The analog has para-methoxy substitution while JWH-250 is ortho. The side chain differs (Ar-CO-CH3 vs indolyl-CO-CH2Ar). The analog data are KBr pellets while sample conditions are unknown. The source is a single-author journal.
1454.0	0.2467	B Δ=2	Methoxy methyl in-plane bend	[5] Table 2, row 1452, p. 9	"1452 m 1435 δ(Me)"	The assignment comes from the structural-analog paper Julia [5] Polak 2024: its 1452 cm-1 band differs from the sample by 2 cm-1. **Applicability of the analog evidence:** The OCH3 methyl deformation of the analog's 5-methoxy group is shared with JWH-250's 2-methoxyphenyl OCH3: both are aryl methyl ether CH3 deformations. **Limitations:** The measured 1454 cm-1 band is composite. It also carries pentyl-chain CH2 scissoring (about 1465 cm-1), pentyl CH3 asymmetric deformation, and indole ring contributions not covered by this assignment. The analog also has COOH and N-H, which perturb ring

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						modes. KBr data vs unknown sample conditions.
1439.0	0.2040	B Δ=5	Indole five/six ring stretch	[5] Table 2, row 1434, p. 9	"1434 s 1431 ν(R5/R6)"	The assignment comes from the structural-analog paper Julia [5] Polak 2024: its 1434 cm-1 band differs from the sample by 5 cm-1. **Applicability of the analog evidence:** Indole ring stretching is shared: both are indole derivatives. The five/six-membered ring stretch at 1434-1439 cm-1 is robust to substitution. **Limitations:** The analog's ring substitution (5-OCH3, 2-COOH) differs from JWH-250 (3-acyl, N-pentyl). The analog has N-H rather than N-alkyl. KBr data vs unknown sample conditions.
1389.0	0.2175	A Δ=0	Indole ring stretch + C-H bend	[8] Experimental section, compound 2, p. 126	"IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)"	The assignment comes from the same-substance paper Jan E 2010: its 1389 cm-1 band differs from the sample by 0 cm-1. The vibration is a mixed mode, composed of ring C-C 39%, C-N 15%, and C-H bending 16%. **Applicability of the analog evidence:** Indole ring-skeleton stretching is shared with 1-methylindole: the same five-membered-ring C-C/C-N mix. **Limitations:** 1-Methylindole lacks the 3-acyl and methoxyphenyl substituents. [6] Bartyzel 2018 compound 2 at 1386 cm-1 (difference of 3 cm-1) supports the assignment. ATR data vs unknown sample conditions.
1352.0	0.1153	B Δ=1	Methyl C-H and C-N-C ring bend	[6] Table 3 (compound 2), p. 940	"1351 (m) 1400 1347 δHCH (15), CHCNC (30)"	The assignment comes from the structural-analog paper Agata [6] Bartyzel 2018: its 1351 cm-1 band differs from the sample by 1 cm-1, which is close to the analog. The vibration is a mixed mode, composed of C-H bending 15% and ring C-N-C deformation 30%. **Applicability of the analog evidence:** JWH-250 carries methyl groups (OCH3 and the pentyl terminal CH3) whose C-H deformation is the shared coordinate. The indole ring C-N-C deformation is shared with the indole skeleton. **Limitations:** The band is a mixed mode;

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						only 45% of the potential-energy distribution is lis振动分布. The analog is 1,2,3,5-tetrasubstitu振动分布 (no C2-H/C3-H), so its ring deformation pattern differs from JWH-250's 1,3-disubstitu振动分布 indole. ATR data vs unknown sample conditions.
1331.0	0.1131	B Δ=0	Indole ring C-C/C-N stretch	[1] Table 2, row v20, p. 41	“v20 A' 1331 1331 1357 1334 νCC(53)ring1, νCN(19)”	The literature value of 1331 cm-1 is assigned to the indole ring C-C and C-N skeleton stretching vibration. The measured peak is at 1331 cm-1, a difference of 0 cm-1. **Applicability of the analog evidence:** This vibration is shared with 1-methylindole, as both contain the same indole ring. **Limitations:** The analog lacks the 3-acyl and methoxyphenyl substituents. Data were collec振动分布 in ATR mode; sample conditions are unknown.
1300.0	0.1687	B Δ=0	Indole ring in-plane bend	[5] Table 2, row 1300, p. 9	“1300 w 1282 δ(R5/R6)”	No qualifying literature assignment was found. This peak is most likely the indole ring in-plane bending vibration. **Applicability of the analog evidence:** The reference compound shares the indole ring skeleton. Its band at 1300/1282 cm^{-1} is assigned to in-plane ring deformation, which is transferable to the indole moiety in the target compound. **Limitations:** The reference compound carries different alkyl/methoxy substitution patterns; conjugation and substituent effects may shift peak positions by a few cm^{-1}.
1245.0	0.2821	B Δ=2	Indole C-H bend, C-C stretch	[1] Table 2, row v22, p. 41	“v22 A' 1243 1239 1268 1247 νCC(18), δCCH(41), δNCH(10)”	The literature value of 1243 cm-1 is assigned to indole ring C-H bending, mixed with C-C stretching and a minor N-CH3 component. The measured peak is at 1245 cm-1, a difference of 2 cm-1. This band may also contain contribution from the 2-methoxyphenyl C-O-C stretch. **Applicability of the analog evidence:** This vibration is shared with 1-methylindole, as both compounds

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						contain the same indole ring structure. **Limitations:** The N-CH3 group of 1-methylindole differs from the N-pentyl chain of JWH-250, so that component is not transferable. The measured peak may also have a strong methoxyphenyl C-O-C contribution not covered by this assignment. Data were collec振动分布 in ATR mode; sample conditions are unknown.
1216.0	0.3092	B Δ=4	Aryl methyl ether C-O stretch	[5] Table 2, row 1220, p. 9	“1220 vs 1205 ν(C5O3), δ(O3C5), δ(R5/R6)”	The literature value of 1220 cm-1 is assigned to the aryl methyl ether C-O stretch, mixed with O-C in-plane bending and ring bending. The measured peak is at 1216 cm-1, a difference of 4 cm-1. **Applicability of the analog evidence:** This vibration arises from the methoxy group attached to an aromatic ring. JWH-250 contains the same methoxy group on its 2-methoxyphenyl moiety. **Limitations:** The methoxy group of the analog is attached to the indole ring, while in JWH-250 it is on a separate phenyl ring, representing a positional difference. The analog also contains a carboxylic acid and N-H group. The measured peak may also contain indole C-H bending character, not covered by this assignment. Data were collec振动分布 in KBr; sample conditions are unknown.
1187.0	0.1499	B Δ=5	Methoxy C-O stretch	[6] Table 3 (compound 2), p. 940	“1182 (m) 1213 1167 νOC (26)”	This peak is assigned to the methoxy C-O stretch. A structural analog in the literature shows this vibration at 1182 cm-1, a wavenumber difference of 5 cm-1. **Applicability of the analog evidence:** The analog carries two aryl OCH3 groups. Its methoxy C-O stretch at 1182 cm-1 transfers to JWH-250's 2-methoxyphenyl OCH3. **Limitations:** The potential-energy distribution is partial: 26% is C-O stretch, the rest is unlis振动分布, and the band is mixed. The analog is

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						tetrasubstitu振动分布 while JWH-250 is 1,3-disubstitu振动分布. The sample band at 1187 cm-1 may also carry indole ring C-H in-plane bending. ATR data vs unknown sample conditions.
1159.0	0.1302	B Δ=5	Indole ring C-H in-plane bend	[1] Table 2, row v24, p. 41	“v24 A' 1154 1177 1157 νCC(18)ring1, δCCH(69)ring1”	This peak is assigned to the indole six-membered-ring C-H in-plane bend. A structural analog in the literature shows this vibration at 1154 cm-1, a wavenumber difference of 5 cm-1. **Applicability of the analog evidence:** Indole six-membered-ring C-H in-plane bending is the shared motion: the same ring of the N-alkylindole core. **Limitations:** 1-Methylindole lacks the 3-acyl and methoxyphenyl substituents. The sample band may carry OCH3 C-O-C character not in this assignment. ATR data vs unknown sample conditions.
1140.0	0.2293	B- Δ=6	Indole ring C-H in-plane bend	[1] Table 2, row v25, p. 41	“v25 A' 1134 1135 1157 1137 νCC(23)ring1, δCCH(42)ring1”	This peak is assigned to the indole six-membered-ring C-H in-plane bend. A structural analog in the literature shows this vibration at 1134 cm-1, a wavenumber difference of 6 cm-1. **Applicability of the analog evidence:** Indole six-membered-ring C-H in-plane bending with ring C-C stretch is shared with the N-alkylindole core. **Limitations:** 1-Methylindole has different substitution. The strong sample band at 1140 cm-1 may include methoxyphenyl-ring C-H in-plane character not covered by this assignment. ATR data vs unknown sample conditions.
1118.0	0.1053	B- Δ=10	Aromatic C-H in-plane bend	[6] Table 3 (compound 2), p. 940	“1108 (m) 1166 1122 δHCC (26)”	This peak is assigned to the aromatic C-H in-plane bend. A structural analog in the literature shows this vibration at 1108 cm-1, a wavenumber difference of 10 cm-1, which is relatively close for this type of analog. **Applicability of the analog evidence:** Aromatic C-H in-plane bending is the plausible motion for the 1118 cm-1 band: C-H in-plane bending of the indole ring and/or the methoxyphenyl ring. The

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						analog band is the same C-H bending motion. **Limitations:** The wavenumber difference is 10.0 cm-1. The potential-energy distribution is partial: 26% C-H bending, the rest unlis振动分布. The analog is tetrasubstitu振动分布, so its C-H pattern differs from JWH-250's 1,3-disubstitu振动分布 indole. ATR data vs unknown sample conditions.
1101.0	0.1541	B Δ=0	Indole benzene-ring C-H bend	[5] Table 2, row 1101, p. 9	"1101 w 1102 δ(C6H), δ(C7H)"	This peak is assigned to indole benzene-ring C-H in-plane bending, based on [5] Polak 2024 at 1101 cm-1 (difference of 0 cm-1). **Applicability of the analog evidence:** Indole benzene-ring C-H in-plane bending is present in the analog, and this vibration is relatively insensitive to ring substitution. **Limitations:** The analog has different ring substituents (2-COOH, 5-OCH3) compared to JWH-250 (3-acyl, N-pentyl). The analog was measured in KBr, while sample conditions are unknown.
1069.0	0.1268	B Δ=5	Methoxyphenyl C-H in-plane bend	[4] Section 3.5 (C-H vibrations), p. 655; Table 4 row 1064/ βCH, p. 659	"The FT-IR values are found at 1315, 1278, 1278, 1197 and 1064 cm-1"	This peak is most likely the methoxyphenyl ring C-H in-plane bending. No direct assignment at 1069 cm-1 was found in same-substance literature. **Applicability of the analog evidence:** This vibrational mode is applicable to JWH-250's 2-methoxyphenyl ring, as both share the same Ar-OCH3 fragment. **Limitations:** The analog has para-methoxy substitution, while JWH-250 has ortho-methoxy; this changes the ring C-H in-plane pattern. The band may also include indole ring C-H character. The analog was measured in KBr; sample conditions are unknown.
1052.0	0.1336	B Δ=1	Aryl methoxy (Ar-OCH_3) C-O-C stretch; possible indole ring C-O contribution	[9] Table 2 (solid-state column, C-O-C	"C-O-C 1280 cm–1 strong asym- metric. and 1053 cm–1 very weak asymmetric."	No direct assignment for 1052 cm−1 was found in same-substance literature. This assignment follows from Thaçi et al. 2023: B2MBCP (bis(2-methoxybenzylidene)cyclopentanone)

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
				row), p. 182		contains the same ortho-methoxy-phenyl (Ar-OCH_3) fragment as JWH-250; the C-O-C asymmetric stretch appears at 1053 cm−1 (weak band) in solid-state KBr FTIR, delta 1 cm−1. **Applicability of the analog evidence:** The two 2-methoxybenzylidene units of B2MBCP provide the same Ar-OCH_3 fragment as the 2-methoxyphenyl group of JWH-250 (both ortho-methoxy); the local bonding environment of the methoxy C-O-C stretch (Ar-O-CH_3) matches one-to-one, so the vibrational coordinate transfers directly. **Limitations:** The 1053 cm−1 band is labelled very weak in the source table; the carbonyl of B2MBCP is a cyclopentanone (not an indole 3-acyl), but the C-O-C vibration involves only the methoxy–phenyl local environment; the source solid-state spectrum is KBr pellet and the sample measurement conditions are unknown.
1032.0	0.1750	A Δ=3	Aryl methyl ether C-O stretch mixed with ring stretch	[8] Experimental section, compound 2, p. 126	“IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)”	This peak is assigned to aryl methyl ether C-O stretch mixed with ring stretch, based on the same-substance paper Jan E 2010, whose 1029 cm-1 band differs by 3 cm-1. **Applicability of the analog evidence:** The aryl OCH3 C-O stretch (symmetric C-O-C of an aryl methyl ether) is shared between the analog and JWH-250's 2-methoxyphenyl group. **Limitations:** The analog's methoxy group is on the indole 5-position, while JWH-250's methoxy is on a separate phenyl ring. The analog also contains COOH and N-H groups. The analog was measured in KBr; sample conditions are unknown.
1011.0	0.1222	B Δ=3	Indole C-C stretch, C-H bend	[1] Table 2, row v29, p. 41	“v29 A' 1014 1010 1036 1018 νCC(61)ring1, δCCH(17)”	The assignment comes from the structural analog Çağlar [1] Karaca 2025. Its 1-methylindole 1014 cm^{-1} band differs from the sample by 3 cm^{-1}. **Applicability of the analog evidence:** Indole six-membered-ring C-C stretching

Wavenumber (cm⁻¹)	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						is shared with 1-methylindole (the same ring of the N-alkylindole core). **Limitations:** 1-Methylindole lacks the 3-acyl and methoxyphenyl substituents. ATR data vs unknown sample conditions.
964.0	w 0.0830	B Δ=5	Aromatic C-H out-of-plane bend	[1] Table 2, row v31, p. 41	"v31 A" 959 973 957 γCH(88)"	The assignment comes from the structural analog Çağlar [1] Karaca 2025. Its 1-methylindole 959 cm⁻¹ band differs from the sample by 5 cm⁻¹. **Applicability of the analog evidence:** Aromatic ring C-H out-of-plane bending is shared with the N-alkylindole core. [6] Bartyzel 2018 compound 2 at 963 cm⁻¹ (difference of 1 cm⁻¹) supports it. **Limitations:** 1-Methylindole has different substitution. The sample band may include methoxyphenyl-ring C-H out-of-plane character. ATR data vs unknown sample conditions.
923.0	m 0.1245	A Δ=1	Aromatic C-H out-of-plane bend	[8] Experimental section, compound 2, p. 126	"IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)"	The assignment comes from the same-substance paper Jan E 2010. Its 922 cm⁻¹ band differs from the sample by 1 cm⁻¹.
872.0	m 0.0911	B- Δ=9	Indole in-plane deformation	[1] Table 2, row v33, p. 41	"v33 A' 881 881 896 881 νCC(13), δCCC(40), δCCH(16)"	The assignment comes from the structural analog Çağlar [1] Karaca 2025. Its 1-methylindole 881 cm⁻¹ band differs from the sample by 9 cm⁻¹, which is relatively close for an analog. **Applicability of the analog evidence:** Indole ring in-plane deformation (domina振动分布 by ring-angle bending) is shared with the N-alkylindole skeleton. **Limitations:** The difference of 9 cm⁻¹ is near the limit. 1-Methylindole has different substitution. ATR data vs unknown sample conditions.
858.0	m 0.1029	B- Δ=10	Aromatic C-H out-of-plane bend	[6] Table 3 (compou	"848 (m) 887 853 CHCCC (71)"	The assignment comes from [6] Bartyzel 2018. Its experimental band at 848 cm⁻¹ differs by 10 cm⁻¹.

Wavenumber (cm⁻¹)	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
				nd 2), p. 941		**Applicability of the analog evidence:** Aromatic C-H out-of-plane bending is the plausible motion for the 858 cm⁻¹ band: C-H out-of-plane bending of the indole ring and/or the methoxyphenyl ring. The analog band is the same motion. **Limitations:** The analog is tetrasubstitu振动分布, so its out-of-plane C-H pattern differs from JWH-250's 1,3-disubstitu振动分布 indole plus 1,2-disubstitu振动分布 benzene. ATR data vs unknown sample conditions.
792.0	m 0.1875	A Δ=0	Indole C3-H out-of-plane bend	[8] Experimental section, compound 2, p. 126	"IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)"	The assignment comes from the same-substance paper Jan E 2010, whose experimental band at 792 cm⁻¹ differs by 0 cm⁻¹. The C3-H out-of-plane detail comes from [7] Kanaoka 1960's characteristic 785-770 cm⁻¹ region for 3-substitu振动分布 indoles; measured to the upper bound, the difference is 7 cm⁻¹. **Applicability of the analog evidence:** JWH-250 is a 3-substitu振动分布 indole; the C3-H out-of-plane bending region 785-770 cm⁻¹ for 3-substitu振动分布 indoles matches the substitution pattern directly (Kanaoka compares indoles with and without C3-H). **Limitations:** This is a 1960 region-type tentative assignment, not a normal-mode analysis. The difference of 7 cm⁻¹ is measured to the upper bound of 785 cm⁻¹. The scan is OCR-transcribed, so individual characters may be imperfect. KBr data vs unknown sample conditions.
756.0	s 0.4167	A Δ=2	Indole ring deformation	[8] Experimental section, compound 2, p. 126	"IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)"	The assignment comes from the same-substance paper Jan E 2010, whose experimental band at 758 cm⁻¹ differs by 2 cm⁻¹. The vibration composition comes from a normal-mode analysis: ring C-C 47%, C-N 10%, ring-angle bending 13%. **Limitations:** 1-Methylindole lacks the 3-acyl and methoxyphenyl substituents. The sample's strongest band likely also carries methoxyphenyl-ring C-H out-of-plane character not covered by this

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
						assignment. ATR data vs unknown sample conditions.
738.0 s	0.2959	A Δ=1	Aromatic C-H out-of-plane bend	[8] Experimental section, compound 2, p. 126	“IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)”	The assignment comes from the same-substance paper Jan E 2010, whose experimental band at 737 cm^{-1} differs by 1 cm^{-1}. **Applicability of the analog evidence:** Aromatic ring C-H out-of-plane bending is shared with the N-alkylindole core, consistent with the ortho-disubstitu振动分布 benzene pattern. **Limitations:** 1-Methylindole has different substitution. [6] Bartyzel 2018 compound 2 at 738 cm^{-1} shows a ring-deformation motion at the same position, so the coordinate assignment at this position is ambiguous. ATR data vs unknown sample conditions.
705.0 m	0.1820	B- Δ=6	N-C(pentyl) stretch, ring bend	[1] Table 2, row v39, p. 41	“v39 A' 711 711 723 711 νC16-N(25), δCCC(23), δCCH(14)”	This peak is assigned to N-C(pentyl) stretching mixed with indole ring deformation, based on [1] Karaca 2025. Their experimental wavenumber is 711 cm-1, a difference of 6 cm-1 from the sample. The vibration is composed of 25% N-C, 23% ring angle bending, and 14% C-H bending. **Applicability of the analog evidence:** N-C(pentyl) stretching and indole ring deformation are shared with the N-alkylindole skeleton. 1-Methylindole has N-CH3 while JWH-250 has N-pentyl, but the N-C stretching motion persists. **Limitations:** The N-C component refers to the N-CH3 carbon of 1-methylindole; the chain length differs. 1-Methylindole lacks the 3-acyl and methoxyphenyl substituents. ATR data vs unknown sample conditions.

Wavenumber (cm⁻¹)	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
646.0	s 0.2472	A Δ=1	C-C out-of-plane deformation	[8] Experimental section, compound 2, p. 126	“IR (KBr) 3125 νCH(indole); 2946, 2924 νPhH, 2866, 2837 νCH(alkyl), 1707 νC=O, 1638, 1608 νC=N, 1575 νC=C, 1389 νC–O–C, 1029 δ(C–O–C), 922, 758, 737 δ(C–H out of the plane), 792, 647 δ(C–C out of the plane)”	This peak is assigned to C-C out-of-plane deformation, based on the same-substance paper Jan E 2010. Their experimental wavenumber is 647 cm-1, a difference of 1 cm-1 from the sample.
600.0	m 0.1528	B- Δ=6	Ring out-of-plane deformation	[6] Table 3 (compound 2), p. 941	“606 (m) 632 608 CHCCC (14), CCCCC (34), COCCC (20)”	This peak is assigned to aromatic ring out-of-plane deformation, based on [6] Bartyzel 2018. Their experimental wavenumber is 606 cm-1, a difference of 6 cm-1 from the sample. **Applicability of the analog evidence:** Indole ring out-of-plane deformation (ring-puckering type, 34% ring out-of-plane) is the shared motion. The C-O-C out-of-plane component relates to the aryl OCH3, a shared fragment. **Limitations:** The mode is mixed: 34% ring out-of-plane plus C-H out-of-plane and C-O-C out-of-plane. The analog is tetrasubstitu振动分布 vs JWH-250's 1,3-disubstitu振动分布 indole. ATR data vs unknown sample conditions.
574.0	m 0.1612	B Δ=1	Indole out-of-plane deformation	[1] Table 2, row v42, p. 41	“v42 A" 573 573 583 573 φPhenyl(44), τCCCN(25)”	This peak is assigned to indole ring out-of-plane deformation/torsion, based on [1] Karaca 2025. Their experimental wavenumber is 573 cm-1, a difference of 1 cm-1 from the sample. The vibration is composed of 44% phenyl torsion and 25% ring torsion. **Applicability of the analog evidence:** Indole ring out-of-plane deformation/torsion is shared with the N-alkylindole skeleton. **Limitations:** 1-Methylindole lacks the 3-acyl and methoxyphenyl substituents. The sample band may also carry C=O in-plane bending, so the coordinate at 574-578 cm-1 is ambiguous. ATR data vs unknown sample conditions.
555.0	m 0.1537	B- Δ=9	OCH3 C-O-C out-of-plane bend	[6] Table 3 (compou	“564 (w) 575 553 COCCC (10)”	This peak is assigned based on the work of Agata [6] Bartyzel 2018. In the structural analog, the methoxy C-O-C

Wavenumber (cm^{-1})	Absorbance	Evidence grade	Vibrational Assignment	Reference	Literature Excerpt (verbatim)	Note
				nd 2), p. 941		out-of-plane deformation appears at 564 cm^{-1}, which is a difference of 9 cm^{-1} from the JWH-250 peak. **Applicability of the analog evidence:** The aryl methyl ether C-O-C out-of-plane deformation exists in both the analog's OCH3 groups and JWH-250's 2-methoxyphenyl OCH3. **Limitations:** The assignment is weak: only 10% of the potential-energy distribution (C-O-C out-of-plane) is lis振动分布. The band is weak in the source. The analog is tetrasubstitu振动分布 vs JWH-250's 1,3-disubstitu振动分布 indole. The difference of 9 cm-1 is near the limit. ATR data vs unknown sample conditions.

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