

Phase Transformations of Azithromycin Crystals Investigated by Thermal and Spectroscopic Analyses Combined with *ab Initio* Calculations

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SUPPORTING INFORMATION

Contents:

Calculated vibrational wavenumbers unscaled and scaled by the scale factors 0.9630 (20 to 2000 cm^{-1}) and 0.940 (2500 to 4000 cm^{-1}), experimental Raman and absorbance band positions and assignment of vibrational modes of orthorhombic AZM-DH crystal – Table S1.

Table S1.

ω_{calc}	ω_{scal}	ω_{Raman}	ω_{IR}	Assignment with PED* [%]
3762	3536	3557vw	3560	$\nu(\text{O49H124})$ [100]
3739	3515	3496vw	3490	$\nu(\text{O13H122})$ [100]
3643	3424		3420	$\nu(\text{O27H83})$ [96]
3615	3398			$\nu(\text{O24H123})$ [95]
3308	3110	3111vw	3100	$\nu(\text{O13H63})$ [99]
3182	2991	3010w	2993	$\nu_{\text{as}}(\text{C20H}_2)$ [98]
3166	2976	2979m	2979	$\nu(\text{C9H60})$ [86]
3162	2972	2971m	2971	$\nu(\text{C14H65})$ [81]
3158	2969			$\nu_{\text{as}}(\text{C22H}_2)$ [94]
3156	2967			$\nu_{\text{as}}(\text{C45H}_2)$ [92]
3154	2965			$\nu_{\text{as}}(\text{C5H}_2)$ [96]
3151	2962			$\nu_{\text{as}}(\text{C26H}_2)$ [89]
3144	2955			$\nu(\text{C47H114})$ [89]
3143	2954	2955m	2958	$\nu_{\text{as}}(\text{C26H}_2)$ [94]

3138	2950			$\nu(C_{51}H_{119})$ [74]
3134	2946			$\nu_{as}(C_{22}H_3)$ [98]
3132	2944			$\nu_{as}(C_5H_2)$ [74]
3132	2944			$\nu(C_{40}H_{105})$ [26] + $\nu(C_{50}H_{118})$ [26] + $\nu(C_{51}H_{120})$ [20]
3129	2941			$\nu_{as}(C_{40}H_2)$ [60] + $\nu(C_{50}H_{118})$ [19] + $\nu(C_{51}H_{120})$ [11]
3127	2939			$\nu_{as}(C_{29}H_2)$ [43] + $\nu_{as}(C_{30}H_2)$ [43]
3125	2938			$\nu_{as}(C_{40}H_2)$ [89]
3124	2937			$\nu_{as}(C_{14}H_2)$ [81]
3123	2936			$\nu_{as}(C_{45}H_2)$ [90]
3120	2933	2933vs	2934	$\nu_{as}(C_{30}H_3)$ [78] + $\nu(C_{28}H_{87})$ [17]
3119	2932			$\nu(C_{17}H_{72})$ [39] + $\nu(C_{20}H_{77})$ [21]
3119	2932			$\nu_{as}(C_{36}H_2)$ [86]
3118	2931			$\nu(C_{17}H_{72})$ [23] + $\nu(C_{20}H_{77})$ [53]
3116	2929			$\nu(C_6H_{57})$ [53] + $\nu(C_{10}H_{62})$ [18]
3115	2928			$\nu_{as}(C_9H_2)$ [62] + $\nu(C_9H_{61})$ [36] + $\nu(C_{10}H_{62})$ [14]
3114	2927			$\nu(C_{43}H_2)$ [76]
3112	2925			$\nu(C_6H_{57})$ [14] + $\nu(C_{43}H_{109})$ [17] + $\nu(C_{50}H_{118})$ [24] + $\nu_{as}(C_{51}H_2)$ [25]
3112	2925			$\nu(C_{28}H_{87})$ [62] + $\nu_{as}(C_{30}H_2)$ [28]
3110	2923			$\nu_{as}(C_{37}H_2)$ [96]
3109	2922			$\nu(C_6H_{57})$ [18] + $\nu(C_{10}H_{62})$ [54]
3107	2921			$\nu(C_{15}H_{67})$ [83]
3103	2917			$\nu(C_{29}H_{88})$ [39] + $\nu_{as}(C_{30}H_2)$ [35]
3103	2917			$\nu_{as}(C_{17}H_2)$ [53] + $\nu(C_{23}H_{82})$ [12]
3101	2915			$\nu_{as}(C_{17}H_2)$ [27] + $\nu(C_{23}H_{82})$ [54]
3101	2915			$\nu_{as}(C_{38}H_3)$ [91]
3100	2914	2911m	2912	$\nu(C_4H_{53})$ [56] + $\nu(C_{42}H_{108})$ [31]
3095	2909			$\nu(C_4H_{53})$ [22] + $\nu(C_{42}H_{108})$ [54]
3091	2906			$\nu(C_{21}H_{78})$ [68] + $\nu(C_{23}H_{82})$ [14]
3085	2900			$\nu_{as}(C_{47}H_2)$ [93]
3075	2891			$\nu(C_{16}H_{69})$ [44] + $\nu(C_{18}H_{74})$ [14]
3073	2889	2889m	2892	$\nu_s(C_{26}H_3)$ [84]
3069	2885			$\nu(C_{36}H_{97})$ [93]
3069	2885			$\nu_s(C_{43}H_2)$ [66] + $\nu_s(C_{45}H_2)$ [20]
3065	2881			$\nu_{as}(C_{37}H_3)$ [96]
3065	2881			$\nu(C_8H_{58})$ [27] + $\nu_s(C_9H_2)$ [32]
3064	2880			$\nu_s(C_{22}H_3)$ [77]
3063	2879			$\nu_s(C_5H_3)$ [92]
3063	2879			$\nu_s(C_{14}H_2)$ [44] + $\nu(C_{18}H_{74})$ [19]
3063	2879			$\nu_s(C_{29}H_2)$ [92]
3060	2876			$\nu_s(C_{45}H_3)$ [68] + $\nu(C_{43}H_{110})$ [20]
3060	2876			$\nu(C_8H_{58})$ [62] + $\nu_s(C_9H_2)$ [29]
3056	2873	2875		$\nu_s(C_{40}H_3)$ [54] + $\nu(C_{34}H_{95})$ [17] + $\nu(C_{38}H_{102})$ [16]
3056	2873			$\nu(C_{16}H_{69})$ [33] + $\nu(C_{18}H_{74})$ [43]
3053	2870			$\nu_s(C_{40}H_3)$ [43] + $\nu(C_{34}H_{95})$ [34]
3053	2870			$\nu_s(C_{51}H_3)$ [98]
3049	2866			$\nu_s(C_{30}H_3)$ [99]

3044	2861			$\nu(C_{31}H_{93}) [14] + \nu(C_{34}H_{95}) [21] + \nu(C_{38}H_{102}) [48]$
3038	2856			$\nu_s(C_{17}H_3) [97]$
3038	2856			$\nu(C_{31}H_{93}) [71] + \nu(C_{34}H_{95}) [22]$
3025	2844	2849w		$\nu_s(C_{47}H_2) [89]$
3024	2843			$\nu(C_{15}H_{68}) [91]$
3019	2838	2837w	2850	$\nu(C_{39}H_{104}) [93]$
3008	2828	2828w	2829	$\nu(C_{32}H_{94}) [80]$
3003	2823			$\nu_s(C_{37}H_3) [89]$
3001	2821			$\nu(C_{20}H_{76}) [92]$
2990	2811			$\nu(C_{48}H_{117}) [94]$
2960	2782	2782w	2783	$\nu(C_{18}H_{73}) [95]$
2959	2781			$\nu(C_{36}H_{98}) [93]$
1776	1705	1719w	1720	$\nu(O_3=C_2) [87]$
1554	1492			$\delta(H_{81}C_{22}H_{80}) [29] + \delta(H_{76}C_{20}H_{75}) [19] + \delta(H_{79}C_{22}H_{81}) [11]$
1553	1491			$\delta(H_{96}C_{36}H_{98}) [30] + \delta(H_{101}C_{37}H_{100}) [13] + \delta(H_{98}C_{36}H_{97}) [16] + \delta(H_{100}C_{37}H_{99}) [19]$
1549	1487			$\delta(H_{60}C_9H_{59}) [42] + \delta(H_{61}C_9H_{60}) [19]$
1547	1485			$\delta(H_{84}C_{26}H_{86}) [10] + \delta(H_{85}C_{26}H_{84}) [59]$
1543	1481			$\delta(H_{75}C_{20}H_{77}) [24] + \delta(H_{77}C_{20}H_{76}) [14] + \delta(H_{79}C_{22}H_{81}) [11]$
1543	1481			$\delta(H_{114}C_{47}H_{116}) [36] + \delta(H_{115}C_{47}H_{114}) [26]$
1542	1480			$\delta(H_{54}C_5H_{56}) [26] + \delta(H_{56}C_5H_{55}) [37]$
1539	1477			$\delta(H_{96}C_{36}H_{98}) [19] + \delta(H_{101}C_{37}H_{100}) [26] + \delta(H_{98}C_{36}H_{97}) [10] + \delta(H_{100}C_{37}H_{99}) [24]$
1539	1477			$\delta(H_{114}C_{47}H_{116}) [11] + \delta(H_{113}C_{45}H_{112}) [12] + \delta(H_{115}C_{47}H_{114}) [16] + \delta(H_{116}C_{47}H_{115}) [20]$
1537	1476			$\delta(H_{90}C_{30}H_{92}) [33] + \delta(H_{92}C_{30}H_{91}) [26]$
1536	1475			$\delta(H_{77}C_{20}H_{76}) [31] + \delta(H_{81}C_{22}H_{80}) [15]$
1535	1474			$\delta(H_{59}C_9H_{61}) [11] + \delta(H_{64}C_{14}H_{66}) [11] + \delta(H_{71}C_{17}H_{70}) [10]$
1534	1473			$\delta(H_{59}C_9H_{61}) [27] + \delta(H_{61}C_9H_{60}) [26]$
1532	1471			$\delta(H_{112}C_{45}H_{111}) [20] + \delta(H_{116}C_{47}H_{115}) [21]$
1531	1470			$\delta(H_{71}C_{17}H_{70}) [14] + \delta(H_{119}C_{51}H_{121}) [25] + \delta(H_{120}C_{51}H_{119}) [11] + \delta(H_{106}C_{40}H_{105}) [11]$
1531	1470			$\delta(H_{120}C_{51}H_{119}) [12] + \delta(H_{106}C_{40}H_{105}) [41] + \delta(H_{107}C_{40}H_{106}) [10]$
1530	1469			$\delta(H_{55}C_5H_{54}) [14] + \delta(H_{91}C_{30}H_{90}) [26] + \delta(H_{92}C_{30}H_{91}) [11]$
1530	1469	1470		$\delta(H_{70}C_{17}H_{72}) [39] + \delta(H_{71}C_{17}H_{70}) [13]$
1528	1467			$\delta(H_{64}C_{14}H_{66}) [17] + \delta(H_{70}C_{17}H_{72}) [11] + \delta(H_{72}C_{17}H_{71}) [19]$
1528	1467			$\delta(H_{54}C_5H_{56}) [11] + \delta(H_{55}C_5H_{54}) [26] + \delta(H_{91}C_{30}H_{90}) [19]$
1526	1465			$\delta(H_{97}C_{36}H_{96}) [19] + \delta(H_{101}C_{37}H_{100}) [10] + \delta(H_{98}C_{36}H_{97}) [24] + \delta(H_{100}C_{37}H_{99}) [10]$
1524	1463	1460vs		$\delta(H_{111}C_{45}H_{113}) [35] + \delta(H_{112}C_{45}H_{111}) [14] + \delta(H_{116}C_{47}H_{115}) [15]$
1524	1463			$\delta(H_{63}O_{13}C_{12}) [14] + \delta(H_{64}C_{14}H_{66}) [14] + \delta(H_{65}C_{14}H_{64}) [33]$
1521	1460			$\delta(H_{68}C_{15}H_{67}) [12] + \delta(H_{74}C_{18}H_{73}) [50]$
1519	1458			$\delta(H_{84}C_{26}H_{86}) [26] + \delta(H_{86}C_{26}H_{85}) [25]$
1518	1457			$\delta(H_{105}C_{40}H_{107}) [14] + \delta(H_{120}C_{51}H_{119}) [11] + \delta(H_{121}C_{51}H_{120}) [34]$
1517	1456			$\delta(H_{80}C_{22}H_{79}) [31] + \delta(H_{79}C_{22}H_{81}) [26]$
1516	1455			$\delta(H_{105}C_{40}H_{107}) [24] + \delta(H_{107}C_{40}H_{106}) [30] + \delta(H_{121}C_{51}H_{120}) [10]$ sci.

1511	1451			$\delta(H97C36H96)$ [17] + $\delta(H101C37H100)$ [15] + $\delta(H99C37H101)$ [13] $\delta(H103C38H102)$ [11]
1511	1451	1451vs	1452	$\delta(H86C26H85)$ [14] + $\delta(H89C29H88)$ [55]
1510	1450			$\delta(H68C15H67)$ [48]
1510	1450			$\delta(H112C45H111)$ [10] + $\delta(H113C45H112)$ [18] + $\delta(H115C47H114)$ [23]
1506	1446			$\delta(H103C38H102)$ [60]
1502	1442			$\delta(H97C36H96)$ [16] + $\delta(H98C36H97)$ [12] + $\delta(H99C37H101)$ [43]
1499	1439			$\delta(H63O13C12)$ [48] + $\delta(H65C14H64)$ [15] + $\delta(H66C14H65)$ [17]
1496	1436			$\delta(H114C47H116)$ [17] + $\delta(H110C43H109)$ [64]
1480	1421		1430	$\delta(H75C20H77)$ [28] + $\delta(H77C20H76)$ [11] + $\delta(H76C20H75)$ [34]
1469				$\delta(H97C36H96)$ [16] + $\delta(H96C36H98)$ [15] + $\delta(H98C36H97)$ [13]
	1410			$\delta(H99C37H101)$ [12] + $\delta(H100C37H99)$ [13]
1466	1407			$\delta(H78C21N19)$ [17] $\delta(H82C23O24)$ [11]
1462	1404			$\delta(H57C6O7)$ [26] + $\delta(H108C42O52)$ [27] + $\tau(H108C42O52C50)$ [16]
1458	1400		1408	$\delta(H83O27C25)$ [19] + $\delta(H84C26H86)$ [10] + $\tau(H87C28O1C2)$ [12]
1457	1399	1403m		$\tau(H93C31O41C39)$ [16]
1453	1395			$\tau(H93C31O41C39)$ [14]
1452	1394			$\delta(H117C48O49)$ [10] + $\gamma(C48C50C44H117)$ [10]
1450	1392			$\delta(H78C21N19)$ [14] + $\delta(H82C23O24)$ [14] + $\gamma(C23C25C21H82)$ [11]
1445	1387	1391m	1393	$\delta(H93C31O41)$ [12]
1442	1384			$\delta(N35C34H95)$ [20]
1441	1383			$\delta(H90C30H92)$ [30] + $\delta(H91C30H90)$ [30] + $\delta(H92C30H91)$ [28]
1439				$\delta(H70C17H72)$ [20] + $\delta(H71C17H70)$ [19] + $\delta(H72C17H71)$ [21] + $\delta(H78C21N19)$ [12]
1437	1380			$\tau(H104C39O41C31)$ [16]
1436				$\delta(H123O24C23)$ [13] + $\delta(H80C22H79)$ [23] + $\delta(H81C22H80)$ [16] + $\delta(H79C22H81)$ [23]
1436	1379			$\delta(H64C14H66)$ [11] + $\delta(H65C14H64)$ [20] + $\delta(H66C14H65)$ [25]
1432	1375			$\delta(H57C6O7)$ [10] + $\delta(H120C51H119)$ [12] + $\delta(H121C51H120)$ [13]
1431	1374			$\delta(H84C26H86)$ [10] + $\delta(H86C26H85)$ [14] + $\tau(H87C28O1C2)$ [11]
1430	1373			$\delta(H57C6O7)$ [10] + $\delta(H108C42O52)$ [11] + $\delta(H121C51H120)$ [11]
1428	1371			$\delta(H111C45H113)$ [24] + $\delta(H112C45H111)$ [22] + $\delta(H113C45H112)$ [18]
1426	1369	1371m	1377	$\delta(H56C5H55)$ [10] wag.
1421	1364			$\tau(H104C39O41C31)$ [21]
1419	1362			$\delta(H62C10O11)$ [10]
1415	1358	1364m		$\delta(H78C21N19)$ [17] wag.
1413				$\delta(H62C10O11)$ [10] + $\delta(H117C48O49)$ [10] + $\tau(H118C50O52C42)$ [10] + $\gamma(C48C50C44H117)$ [10]
1410	1354			$\delta(C43C42H108)$ [10] + $\delta(C8C6H57)$ [15] + $\delta(C25O27H83)$ [10]
1410	1354			$\delta(H95C34C38)$ [22]
1409	1353			$\delta(C25C23H82)$ [20] + $\delta(C21C23H82)$ [12] + $\delta(C43C42H108)$ [22]
1405	1349	1354m		$\tau(H69C16C18N19)$ [26]
1399	1343		1343	$\delta(H123O24C23)$ [11] + $\tau(H78C21N19C18)$ [25] + $\gamma(O24C21C25C23)$ [13]
1394	1338			$\delta(H93C31O41)$ [12] + $\delta(H104C39C40)$ [10] + $\tau(H62C10O11C31)$ [10]
1392	1336			$\delta(H57C6O7)$ [20] + $\tau(H108C42O52C50)$ [20] + $\tau(H110C43C44C45)$ [15]
1383	1328	1334m		$\delta(H87C28O1)$ [32]

1381	1326			$\delta(H118C50C51)$ [30] + $\tau(H118C50O52C42)$ [10]
1377	1322	1327m		$\tau(H108C42O52C50)$ [10]
1376	1321			$\delta(H118C50C51)$ [27] + $\delta(H93C31O41)$ [12]
1365	1310			$\tau(H95C34N35C36)$ [29]
1364	1309			$\delta(H67C15C16)$ [12] + $\delta(H69C16C17)$ [12]
1362	1308		1317	$\delta(H53C4C2)$ [14] + $\delta(H87C28O1)$ [14] + $\tau(H53C4C2O1)$ [23]
1360	1306			$\delta(H73C18N19)$ [25]
1354	1300			$\delta(H82C23O24)$ [12] + $\gamma(C23C25C21H82)$ [11]
1349	1295	1295w		$\delta(H53C4C2)$ [11] + $\delta(H58C8C9)$ [16] + $\tau(H58C8C10C12)$ [11]
1337	1284			$\delta(H94C32O33)$ [16] + $\gamma(C32C34C31H94)$ [13]
1333	1280			$\delta(H109C43C44)$ [16] + $\tau(H62C10O11C31)$ [10]
1330	1277			$\delta(H67C15C16)$ [10] + $\delta(H69C16C17)$ [17] + $\delta(H109C43C44)$ [13]
1329	1276		1283	$\delta(H83O27C25)$ [14] + $\delta(H88C29C30)$ [19] + $\tau(H87C28O1C2)$ [35]
1326	1273			$\tau(H58C8C10C12)$ [16] + $\tau(H62C10O11C31)$ [16]
1323	1270			$\tau(H98C36N35C34)$ [14]
1319	1266	1272m	1269	$\delta(H117C48O49)$ [18] + $\tau(H118C50O52C42)$ [15] + $\gamma(C48C50C44H117)$ [11] + $\gamma(O49C44C50C48)$ [11]
1319	1266			$\delta(H88C29C30)$ [23] + $\tau(H88C29C28C25)$ [12] + $\tau(H89C29C28C25)$ [26] +
1313	1260			$\delta(H58C8C9)$ [13] + $\tau(H57C6O7C42)$ [10]
1311	1259			$\delta(H123O24C23)$ [20] + $\delta(H122O33C32)$ [15] + $\tau(H78C21N19C18)$ [13]
1310	1258			$\delta(H122O33C32)$ [12] + $\delta(H58C8C9)$ [12] + $\tau(H57C6O7C42)$ [10]
1301	1249	1251w	1250	$\delta(H67C15C16)$ [12] + $\tau(H68C15C16C17)$ [12] + $\tau(H69C16C18N19)$ [12]
1297	1245	1232m		$\tau(H103C38C39C40)$ [22]
1271	1220	1225m		$\delta(H124O49C48)$ [34]
1250	1200			$\tau(H74C18N19C20)$ [11] + $\tau(H76C20N19C18)$ [19]
1239	1189			$\tau(H115C47O46C44)$ [16] + $\tau(H116C47O46C44)$ [16]
1235	1186	1187m	1188	$\delta(H95C34C38)$ [10] + $\delta(H102C38C39)$ [19]
1232	1183			$\tau(H85C26C25C23)$ [10]
1224	1175			$v(N19C20)$ [20] + $\delta(C18N19C21)$ [16]
1218	1169			$\delta(C34C32H94)$
1216	1167			$\tau(H110C43C44C45)$ [10]
1210	1162		1166	$v(O1C2)$ [36] + $\delta(H53C4C2)$ [14]
1201	1153			$\tau(H97C36N35C34)$ [18] + $\tau(H101C37N35C34)$ [21]
1198	1150	1154m	1156	$\tau(H66C14C12C10)$ [13]
1194	1146			$v(C25O27) + v(C25C28) + \delta(C30C29C28)$
1193	1145			$v(C12C10) + \delta(C14C12C10)$
1191	1143			$\delta(H114C47H116)$ [13] + $\delta(H115C47H114)$ [13] + $\tau(H114C47O46C44)$ [28] + $\tau(H115C47O46C44)$ [19] + $\tau(H116C47O46C44)$ [20]
1189	1141		1145	$\delta(C25O27H83) + \delta(N19C20H76) + v(C25C28)$
1189	1141			$v(C45C44)$ [10]
1186	1139			$\tau(H106C40C39C38)$ [11]
1182	1135			$\delta(C48O49H124) + v(C42O7) + v(O46C47)$
1172	1125			$\tau(H75C20N19C18)$ [10] + $\tau(H77C20N19C18)$ [21]
1170	1123			$\delta(C34C38C39) + v(C32C31)$
1169	1122		1123	$v(C50C51) + v(C50C48)$
1169	1122			$v(C39O41) + v(C48C50)$

1167	1120	1121m		$v(C9C8) [12] + v(C6C8)$
1158	1112			$v(C15C16) + v(C16C18)$
1153	1107		1106	$v(O52C42) [31] + v(C43C42) [19]$
1143	1097			$v(C31O11) + v(C16C15)$
1140	1094			$v(C32O33) + \delta(C31C32C34)$
1139	1093	1096m		$v(C4C6) + v(C4C5) + v(C9C8)$
1136	1091		1096	$\delta(N35C36H98) + \tau(C34N35C36H97)$
1135	1090			$\tau(H91C30C29C28) [10]$
1130	1085			$\tau(H97C36N35C34) [16] + \tau(H101C37N35C34) [11]$
1126	1081			$v(C4C6) [13] + \tau(H56C5C4C6) [15]$
1122	1077			$v(O46C47) [40]$
1116	1071		1083	$v(O11C31) [14]$
1109	1065			$v(O49C48) [21]$
1107	1063			$v(C22C21) + v(C21N19)$
1104	1060	1062m		$v(O46C47) [10] + v(O49C48) [16]$
1094	1050			$v(C29C28) [18]$
1092	1048			$v(N35C36) [11] + v(O33C32) [21] + v(N35C34) [10]$
1088	1044		1049	$v(O49C48) [10] + v(O52C50) [12] + \tau(H121C51C50C48) [10]$
1087	1044			$v(C21N19) v(C21C23) \delta(C18C16C15)$
1083	1040			$v(N35C36) [10] + v(N35C37) [14] + \tau(H98C36N35C34) [10]$
1081	1038	1042m		$v(C16C17) + v(C16C15) + v(C4C5)$
1077	1034			$v(C5C4) [10]$
1075	1032		1032	$v(O41C31) [20]$
1071	1028			$v(C4C6) + v(C4C5) + v(C9C8)$
1070	1027			$v(N19C18) [13]$
1065	1022			$v(C32C31) + v(C34C32)$
1059	1017		1018	$v(C30C29) [27]$
1055	1013			$v(C34C38) + v(C34C32) + v(C8C10)$
1045	1003	1000w	1004	$v(N35C34) [12] + v(C40C39) [15]$
1031	990	988w	992	$v(O7C42) [18] + v(O11C10) [10]$
1022	981		978	$v(O11C10) [14]$
1019	978	980w	977	$v(O24C23) [10]$
1013	972		966	$v(O7C6) [13] + v(C43C42) [15]$
1001	961	963m	956	$v(O7C6) [12]$
998	958			$v(C12C15) [14] + \tau(H64C14C12C10) [15]$
989	949			$v(O24C23) [20] + \tau(H78C21N19C18) [10]$
985	946			$\delta(H102C38C39) [13]$
977	938		943	$v(C30C29) [27]$
975	936			$v(O13C12) [15]$
966	927	930m	931	$v(C23C25) [11] + \tau(H85C26C25C23) [14]$
964	925			$v(C50C51) + v(C50C48) + v(C43C44)$
963	924			$v(C18C16) + v(N19C21)$
957	919			$v(C18C16) + v(C16C17)$
951	913		910	$v(C39C38) [10] + v(O41C39) [12] + \tau(H106C40C39C38) [23]$
943	905	908m	903	$v(C21N19) + \tau(C21N19C18H74) + v(C25O27)$
936	899			$v(C6C8) [12]$

928	891			$\nu(C28O1)$
919	882			$\nu(C48C50)$
915	878	881m	898	$\nu(O46C44)$ [14]
909	873	874m	880	$\delta(C28O1C2)$
903	867	868m	866	$\tau(H103C38C39C40)$ [10] + $\tau(C38C39C40H105)$
893	857			$\nu(C5C4) + \nu(C4C6)$
882	847			$\nu(C15C16)$ [10] + $\tau(H67C15C16C17)$ [13]
879	844		848	$\tau(H102C38C39C40)$ [17]
876	841			$\nu(C5C4) + \nu(C4C6)$
872	837			$\nu(C9C8)$ [22]
861	827	834m	834	$\delta(C43C42O52)$
854	820			$\nu(O52C50)$ [14]
847	813			$\nu(N35C36)$ [25] + $\nu(N35C37)$ [16] + $\nu(N35C34)$ [17]
845	811	811m	813	$\nu(C44C48)$ [12]
830	797		805	$\nu(O27C25)$ [11] + $\nu(C22C21)$ [16] + $\tau(H63O13C12C10)$ [23]
812	780		796	$\tau(C15C12O13H63)$
808	776			$\tau(H63O13C12C10)$ [27]
803	771	774m	776	$\nu(N19C21)$ [18] + $\tau(H63O13C12C10)$ [30]
785	754		756	$\delta(H88C29C30)$ [13] + $\tau(H88C29C28C25)$ [23] + $\tau(H90C30C29C28)$ [15]
775	744		745	$\nu(C14C12)$ [17] + $\nu(C12C15)$ [17] + $\delta(C12C15C16)$ [11]
764	733	731m	731	$\gamma(O3C4O1C2)$ [55]
741	711		722	$\nu(O46C44)$ [30] + $\nu(C45C44)$ [10]
727	698	696vw	697	$\tau(C25C23O24H123) + \delta(C26C25C28)$
705	677	667vw	674	$\delta(O3C2O1)$ [19]
679	652		663	$\nu(C21C22) + \delta(C21N19C20)$
668	641		639	$\tau(H83O27C25C23) + \tau(H123O24C23C21)$
656	630		629	$\tau(H123O24C23C21)$ [49] + $\tau(H83O27C25C23)$ [29]
640	614	612m	611	$\delta(C38C39O41) + \tau(C25C23O24H123) + \delta(C32C31O11)$
631	606			$\delta(C033C32C31) + \tau(C32C34C38H102)$
620	595		601	$\delta(O52C42O7)$ [20] + $\delta(C50O52C42)$ [10]
613	588		591	$\delta(C10C8C6)$
608	584	584vw	581	$\nu(C45C44)$ [12]
582	559	565vw	571	$\tau(C25C23O24H123) + \gamma(N19C18C21C20)$
575	552	561vw	561	$\delta(C22C21N19) + \tau(C25C23O24H123)$
570	547	551vw		$\delta(O52C42O7)$ [11]
549	527	537w	540	$\tau(H123O24C23C21)$ [34] + $\tau(H83O27C25C23)$ [49]
546	524	523w	524	$\delta(C40C39O41)$ [12]
541	519		517	$\delta(C39O41C31) + \tau(C32C34C38H102)$
530	509			$\nu(C26C25)$ [11]
523	502		506	$\delta(C44C48C50) + \delta(C48C44C43)$ breathing
506	486	497m	494	$\delta(O13C12C14)$ [10]
502	482		487	$\delta(C44C48C50) + \delta(C48C50C51)$
493	473			$\delta(C50O52C42)$ [10]
489	469	468m	460	$\gamma(C39C39O41C40) + \delta(C45C44C48)$ breathing
477	458			$\delta(C37N35C36)$ [18]
468	449			$\delta(C48C50O52) + \delta(C50C48C44)$

466	447			$\tau(H122O33C32C31)$ [38]
461	443			$\tau(H122O33C32C31)$ [23]
460	442	440w	437	$\tau(H122O33C32C31)$ [10]
442	424	426w		$\delta(C39O41C31) + \tau(C8C10C12O13)$
436	419		418	$\delta(C15C16C18)$ [18]
422	405			$\delta(C36N35C34)$ [12]
421	404		408	$\gamma(C51C48O52C50)$ [10]
406	390	399m		$\delta(C18N19C21)$ [11] + $\delta(C14C12C15)$ [11]
400	384			$\delta(C34C32C31) + \delta(C38C39O41)$
392	376			$\delta(C43C42O52)$ [11]
389	373	374w		$\delta(C20N19C18) + \delta(C26C25C23) + \gamma(C36C37C34N35)$
382	367			$\delta(C47O46C44) + \delta(C34N35C37)$
375	360			$\delta(C47O46C44)$ [16]
366	351	351m		$\delta(C36N35C37) + \gamma(N19C18C16C17)$
359	345			$\delta(C47O46C44)$ [13] + $\gamma(C37C34C36N35)$ [13]
355	341			$\delta(C47O46C44) + \delta(C34N35C37)$
348	334			$\gamma(C37C34C36N35)$ [10] + $\gamma(C14C10C15C12)$ [10]
346	332			$\delta(C45C44O46)$ [16]
343	329			$\tau(C23C25C26H85)$
342	328	324m		$\delta(C20N19C21)$ [20] + $\gamma(C22C23N19C21)$ [10]
331	318			$\delta(C28C29C30) + \delta(C21N19C20)$
329	316			$\delta(C32C34C38) + \delta(C31O41C39)$
320	307			$\delta(N19C18C16) + \delta(C16C15C12) + \delta(C37N35C34)$
315	302			$\tau(C10C12C14H64) + \tau(C50C48O49H124)$
313	300			$\delta(O49C48C50)$ [10]
310	298	299m		$\gamma(O27C23C28C25)$ [14] + $\tau(C44C48C49H124)$
306	294			$\tau(H124O49C48C44)$ [29]
303	291			$\delta(C5C4C2)$ [10]
297	285			$\tau(H54C5C4C6)$ [13] + $\tau(H55C5C4C6)$ [15] + $\tau(H56C5C4C6)$ [20]
295	283			$\tau(H59C9C8C6)$ [16] + $\tau(H60C9C8C6)$ [12] + $\tau(H61C9C8C6)$ [12]
294	282			$\tau(C10C8C9H59) + \tau(C28C29C30H90)$
290	278	279m		$\tau(C6C4C5H56) + \tau(C21N19C20H75)$
287	276			$\delta(C36N35C34)$ [12]
281	270			$\tau(C50C48O49H124) + \tau(C48C44C45H111)$
276	265			$\tau(H97C36N35C34)$ [14] + $\tau(H96C36N35C34)$ [13]
274	263			$\tau(C18N19C20H75)$
270	259	260m		$\tau(C50C48O49H124) + \tau(C18N19C20H75) + \tau(C23C21C22H80)$
266	255			$\tau(H80C22C21C23)$ [12] + $\tau(H79C22C21C23)$ [16]
265	254			$\gamma(C45C43O46C44)$ [14]
263	252			$\delta(C40C39O41)$ [12]
255	245			$\delta(C51C50O52)$ [14] + $\tau(H124O49C48C44)$ [11]
252	242			$\delta(C22C21C23)$ [18]
250	240			$\tau(C10C12C14H64) + \tau(C50C48O49H124)$
246	236			$\tau(H105C40C39C38)$ [15] + $\tau(H106C40C39C38)$ [16] + $\tau(H107C40C39C38)$ [16]
243	233			$\tau(C38C39C40H106) + \tau(C28C29C30H90) + \tau(C15C12C14H64)$

238	228			$\tau(\text{H65C14C12C10})$ [12]
235	226			$\tau(\text{H100C37N35C34})$ [10] + $\tau(\text{H121C51C50C48})$ [10]
234	225			$\tau(\text{H101C37N35C34})$ [10] + $\tau(\text{H99C37N35C34})$ [16] + $\tau(\text{H100C37N35C34})$ [19]
232	223			$\tau(\text{C48C50C51H121})$ + $\tau(\text{C28C25C26H84})$
227	218	219m		$\tau(\text{H71C17C16C15})$ [15]
226	217			$\tau(\text{H111C45C44C43})$ [13] + $\tau(\text{H112C45C44C43})$ [12]
218	209			$\tau(\text{C28C29C30H90})$ + $\tau(\text{C28C25C26H84})$ + $\tau(\text{C43C44C45H111})$
212	204			$\tau(\text{H86C26C25C23})$ [13]
205	197	196m		$\delta(\text{C23C21N19})$ + $\delta(\text{C2C4C5})$ + $\delta(\text{C28C25C23})$
199	191			$\delta(\text{C8C10C12})$ + $\delta(\text{C2C4C5})$ + $\delta(\text{C28C25C23})$
198	190			$\delta(\text{O46C44C48})$ [28]
189	181			$\tau(\text{O49C48C44C45})$
174	167			$\tau(\text{C4C6C8C9})$
167	160	159m		$\tau(\text{C44C43C42O52})$
159	153			$\tau(\text{C22C21N19C20})$
152	146			$\delta(\text{O1C2C4})$ [13]
143	137	138m		$\gamma(\text{C40C38O41C39})$ [10]
133	128			$\tau(\text{O7C6C4C5})$
130	125			$\delta(\text{C34N35C37})$
128	123			$\gamma(\text{N35C32C38C34})$ [15]
125	120	122m		$\tau(\text{C23C12N19C20})$
123	118			lattice
118	113	113		lattice
115	110			lattice
111	107	107		lattice
107	103	100		lattice
96	92	95		lattice
95	91	91		lattice
88	84	83		lattice
80	77			lattice
79	76	75		lattice
76	73	71		lattice
71	68			lattice
68	65	66		lattice
64	61	60		lattice
60	58			lattice
57	55	52		lattice
44	42	43		lattice
43	41	39		lattice
34	33	36		lattice

*Only PED values greater than 9 % are given.

Modes without PED were visually determined.

Nomenclature: τ = torsion; δ = bending; wag. = wagging; γ = out of plane bending; v = stretching; v_{as} = asymmetric stretching; v_s = symmetric stretching. vs = very strong ; s = strong; m = medium; w = weak; vw = very weak.