Pontificia Universidad JAVERIANA Bogotá

Univ.Sci. 26(2): 69–79, 2021
doi:10.11144/Javeriana.SC26-2.saco

SUPPLEMENTARY MATERIAL 1

Synthesis and characterization of four N-acylhydrazones as potential O,N,O donors for Cu^{2+}: An experimental and theoretical study

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Table 1. Vibrational assignments of experimental and calculated (unscaled and scaled) fundamental frequencies of compound 4a.

Calculated		Experimental	Assignment
Wavenumber	**Scaled wavenumber**	**Wavenumber**	
cm^{-1}			(PED %)
3532.4	3395.7	3180.6	ν NH (100)
3415.2	3283.1	3163.3	ν OH (99)
3222.9	3098.2		ν CH (12) + ν CH (85)
3219.1	3094.5		ν CH (93)
3217.8	3093.2		ν CH (13) + ν CH (13) + ν CH (73)
3209.7	3085.5		ν CH (80) + ν CH (13)
3208.6	3084.4		ν CH (87) + ν CH (12)
3188.7	3065.3		ν CH (82) + ν CH (13)
3177.8	3054.8		ν CH (96)
3171.8	3049		ν CH (92)
3101.4	2981.4	2922.2	ν CH (99)
3054.5	2936.3	2889.4	ν CH (99)
3049	2931		ν CH (99)
1799.7	1730	1656.9	ν OC (85)
1691.6	1626.1	1622.1	ν NC (69)
1676.1	1611.2	1610.6	ν CC (62) + δ HCC (13)
1651.6	1587.7	1597.1	ν CC (58) + δ HCC (20)
1627.3	1564.3	1554.6	ν CH (62)
1622.9	1560.1		ν CH (45)
1560.9	1500.5		ν CC (10) + δ HNN (53)
1533	1473.7		δ HCC (58)
1531.1	1471.9		ν CC (10) + δ HCC (34) + δ CCC (10)
1507.4	1449		ν CC (29) + δ HCC (28)
1489	1431.3		δ HCH (86)
1450.4	1394.3		ν CC (18) + δ HCC (45)
1434.2	1378.7		δ HOC (50) + δ HCC (10) + δ HCC (10)
1393.1	1339.2		δ HCC (61)
1370	1317		ν OC (55)

1362.2	1309.4		ν CC (25) + δ HCC (15) + δ HCC (20)
1330.6	1279.1		ν CC (21) + δ HCC (51)
1329.2	1277.8	1274.9	ν CC (58)
1315.1	1264.2		ν CC (12) + τ HCCC (34)
1272	1222.7	1230.6	ν CC (14) + δ HCC (12) + τ HCCC (22)
1266.6	1217.6		δ HCC (37)
1236.7	1188.9	1197.8	ν CC (35) + δ HCC (16)
1217.5	1170.4		ν CC (48) + δ HCC (10) + δ CCC (14)
1210.1	1163.3		ν CC (20) + δ HCC (76)
1185.1	1139.2		δ HCC (65)
1174.1	1128.6		ν NN (35) + δ HCC (15) + δ HCC (11)
1146	1101.6		δ HCC (15) + δ HCC (15)
1137.8	1093.8		ν CC (17) + δ HCC (27)
1111.2	1068.2		ν CC (12) + ν CC (21) + ν ClC (11) + δ HCC (10)
1106.2	1063.4		ν CC (14) + ν NN (10) + ν CC (17) + δ HCC (18)
1060	1019		ν CC (55) + δ HCC (21)
1030.7	990.8		δ CCC (62) + δ CCC (21)
1003.7	964.8		ν CC (38)
985.1	947		τ HCCC (80)
982.6	944.6		τ HCCC (69) + τ CCCC (12)
971.8	934.2		τ HCCC (11) + τ HCNN (81)
958.5	921.4		τ HCCC (76)
940.2	903.8		δ HCC (10) + τ HCCC (11) + τ HCCC (32)
937.8	901.5		τ HCCC (80)
897.3	862.6		δ CCC (53)
869	835.3		τ HCCC (84)
866.3	832.8		τ HCCC (30) + ω OCNC (10)
844.9	812.2		τ HCCC (85)
821.5	789.7		ν CC (15) + τ HCCC (36)
796.1	765.3		ν OC (10) + ν CC (12) + δ CCC (29)
777.6	747.5		δ CCC (11) + ω OCNC (13)
774	744		τ HOCC (33) + τ HCCC (41)
757.5	728.1		τ HOCC (54) + τ HCCC (31)
736.7	708.2		τ CCCC (61)
708.1	680.7		ω OCNC (11) + τ CCCC (64)
692.7	665.9		ν ClC (13) + δ CCC (10) + δ CCC (13)
653.5	628.2		δ CCC (41)
644.7	619.8		δ CCC (62)
603	579.7		ν ClC (14) + ω OCNC (22)
571.3	549.2		δ CCC (37)
560.7	539		τ HCCC (14) + τ CCCN (11) + τ CCCN (56)
507.8	488.1		τ HCCC (10) + ω CCCC (66)
482.3	463.6		τ HCCC (13) + τ CCCC (58)
479.1	460.6		δ CCO (70)
467.3	449.2		δ CCC (48)
453.4	435.9		τ HNNC (74)

421.9	405.6		τ CCCC (84)
413.3	397.3		δ CCC (45) + δ CCC (21)
388.3	373.3		ν ClC (20) + δ CCC (22)
356.9	343		δ CCCl (61)
348.4	334.9		τ CCNN (60)
327.6	314.9		ω CCCC (40)
270.9	260.4		τ CCCN (12) + τ CCCN (44)
253.9	244.1		δ CCC (10) + δ CCC (19)
245	235.5		δ CCC (61)
218.2	209.7		δ CCN (54)
217.4	209		τ CCCN (64) + τ CCCC (10)
147.2	141.5		δ CCC (22) + τ CCCN (14) + τ CCCC (28)
122.6	117.8		δ CCC (15) + τ CCCC (47) + τ CCCC (14)
85	81.7		δ CNN (12) + τ CCCC (36)
67.6	65		δ CNN (48)
54.2	52.1		τ CCCN (13) + τ CCCN (67)
31.9	30.6		δ CNN (22) + τ CCCC (51)
21.8	20.9		δ CCC (12) + τ CCCN (45) + τ CCCC (16)
9.3	9		τ CCCN (79)