# Supplementary Material

# Synthesis of 4′-alkyl-[1,1′-biphenyl]-2,3′-dicarbonitriles via dimerisation of phthalonitrile radical anion in liquid ammonia

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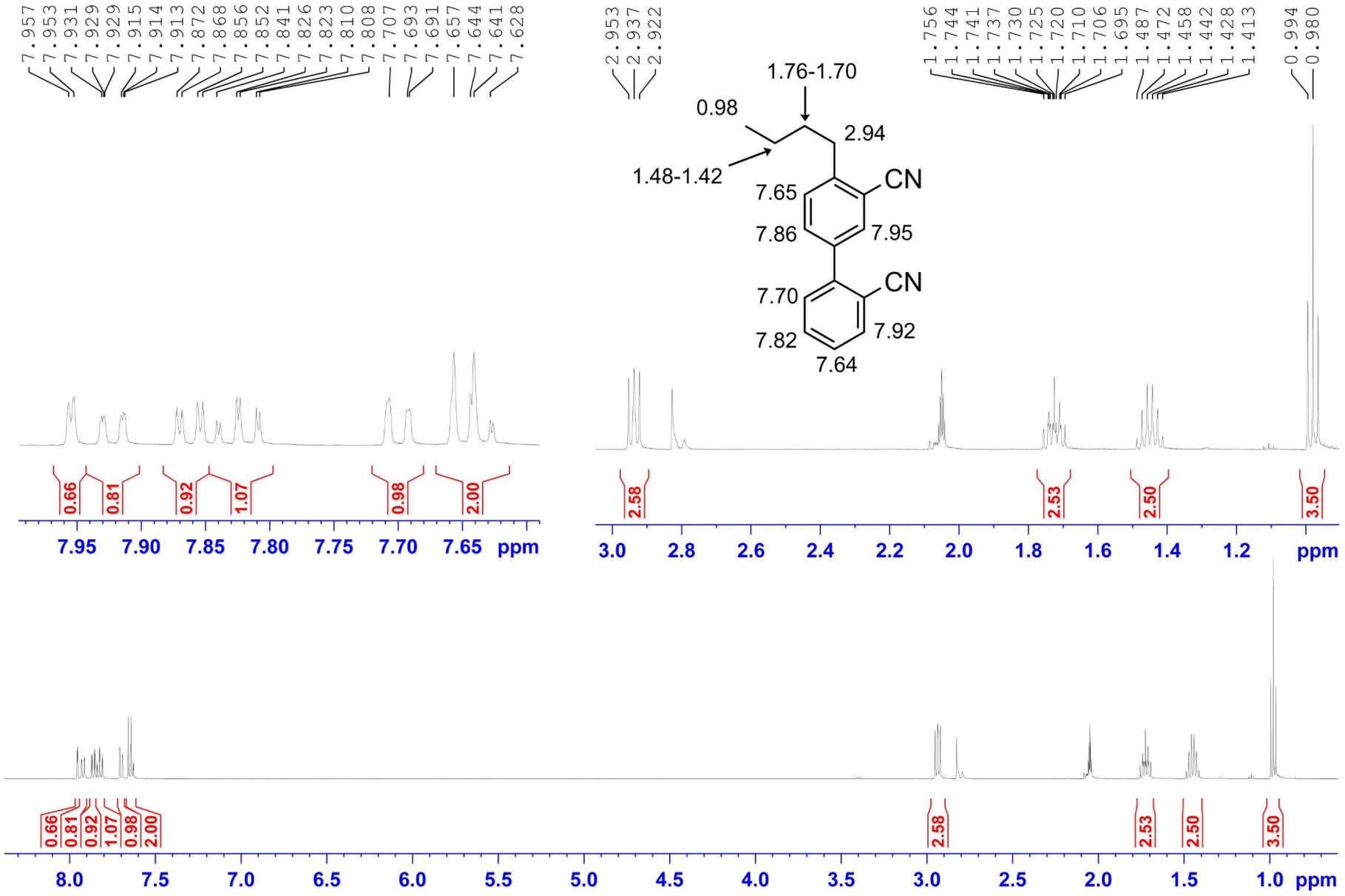
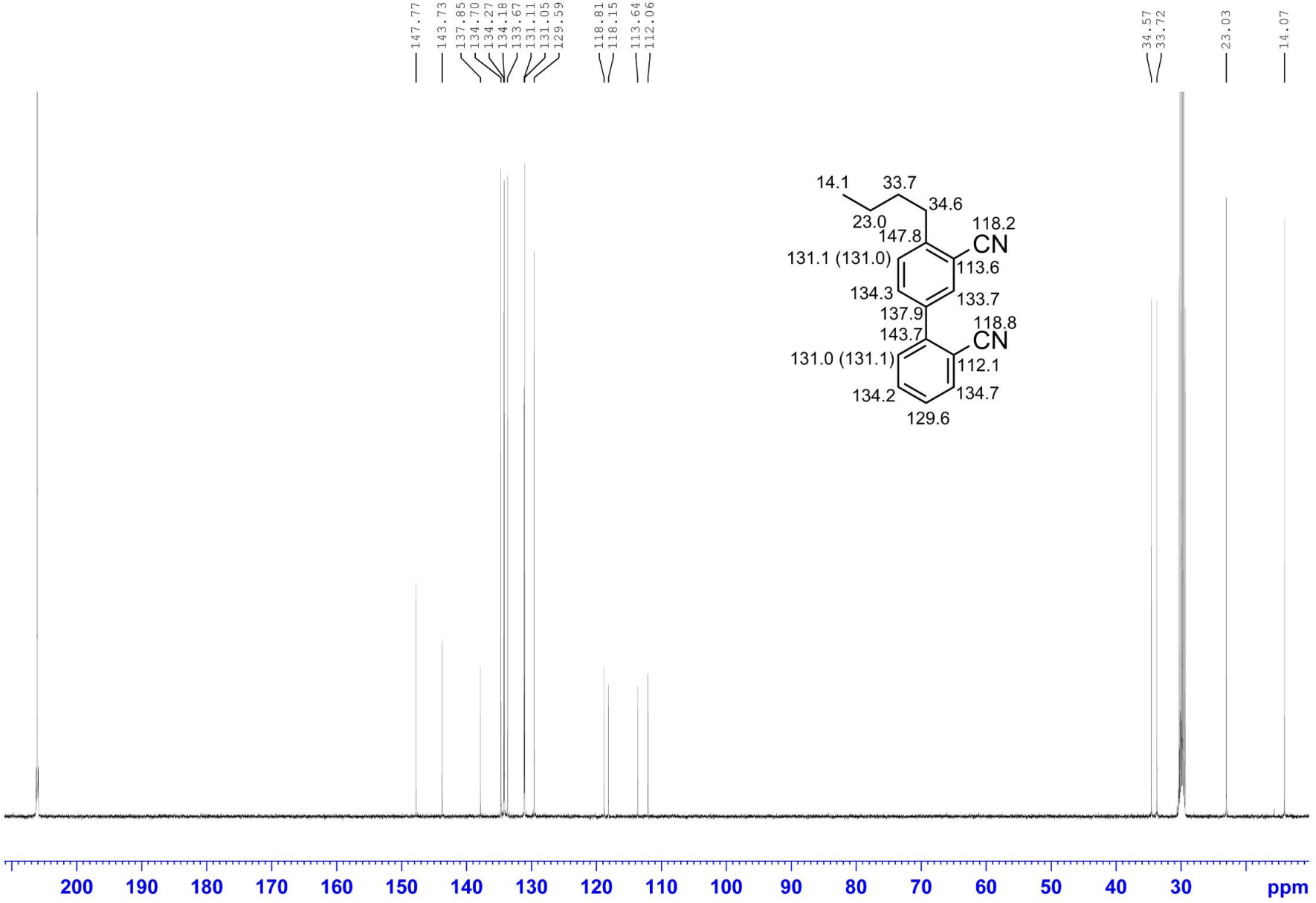
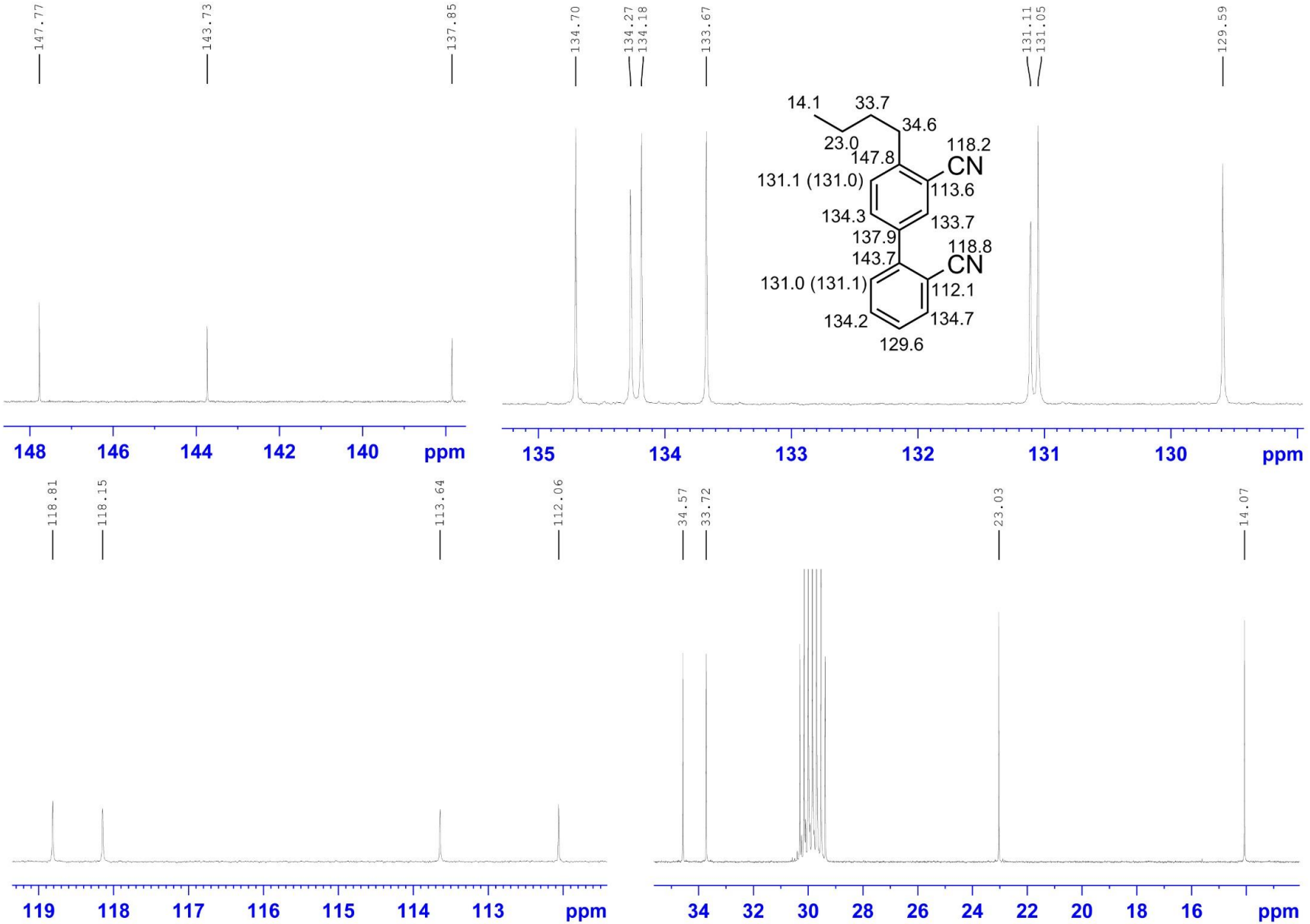
## $^1$H NMR for 4'-butyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7a)



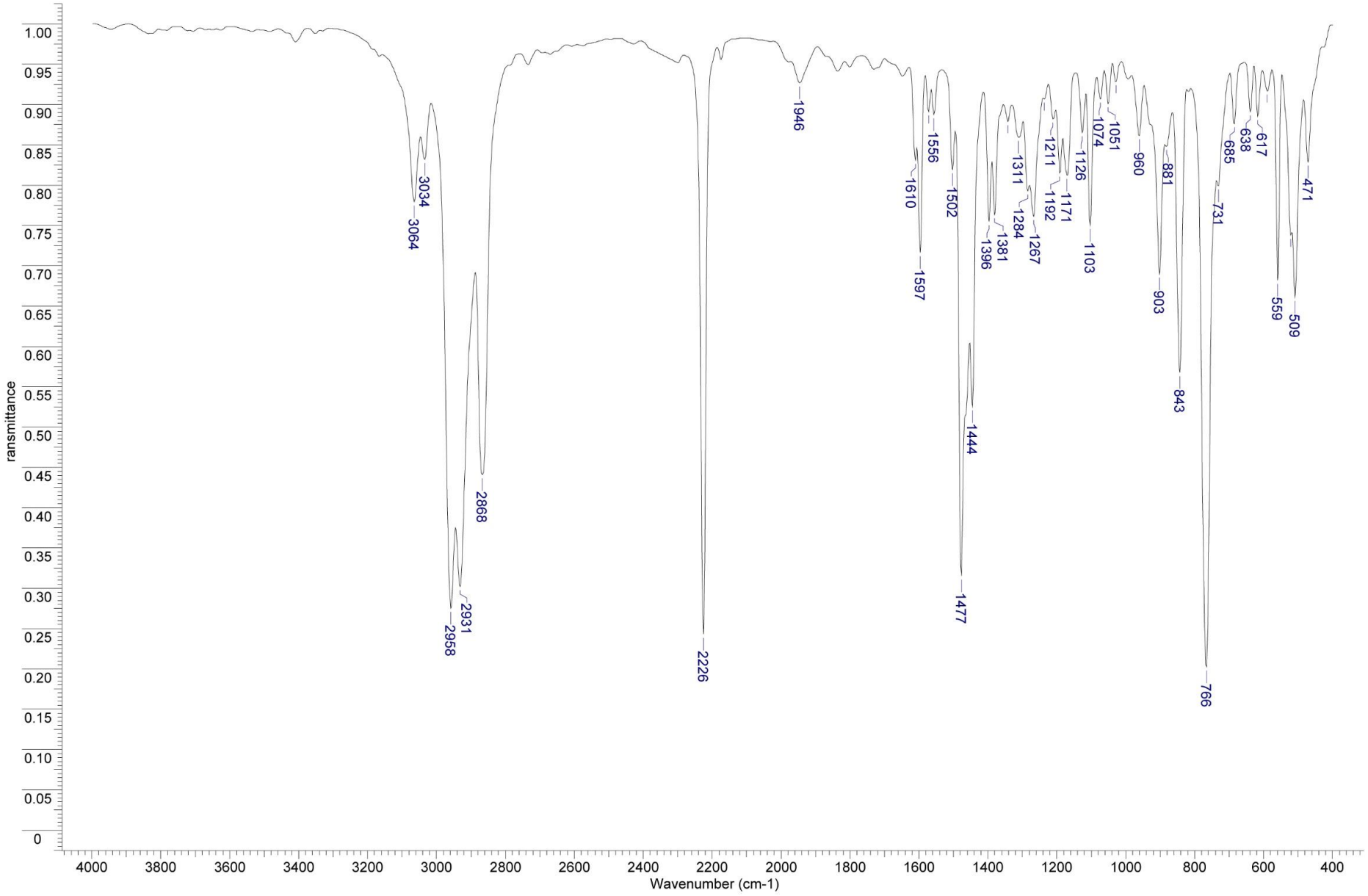
## $^{13}$C NMR (overview) for 4'-butyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7a)



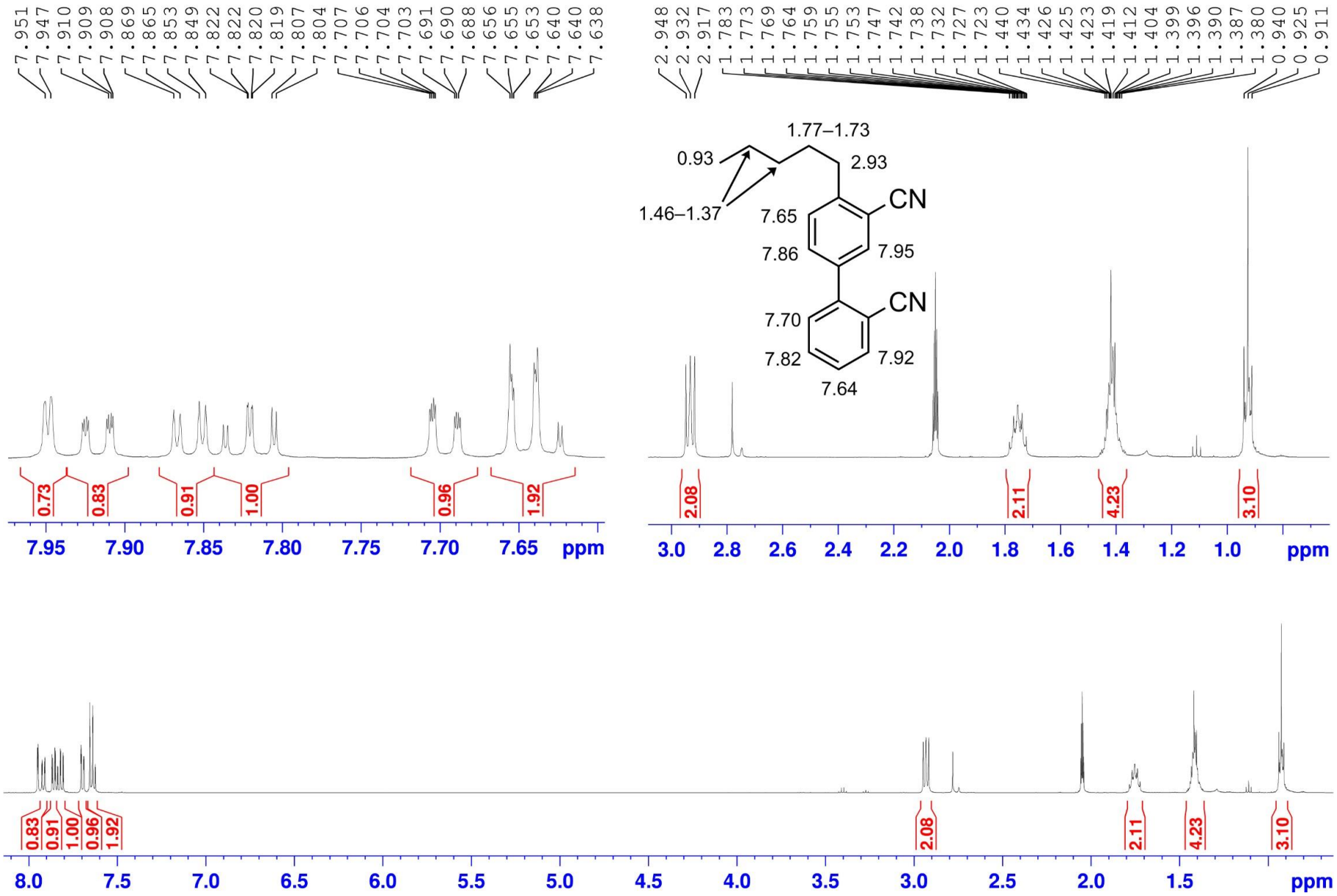
## $^{13}$C NMR (detailed) for 4'-butyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7a)



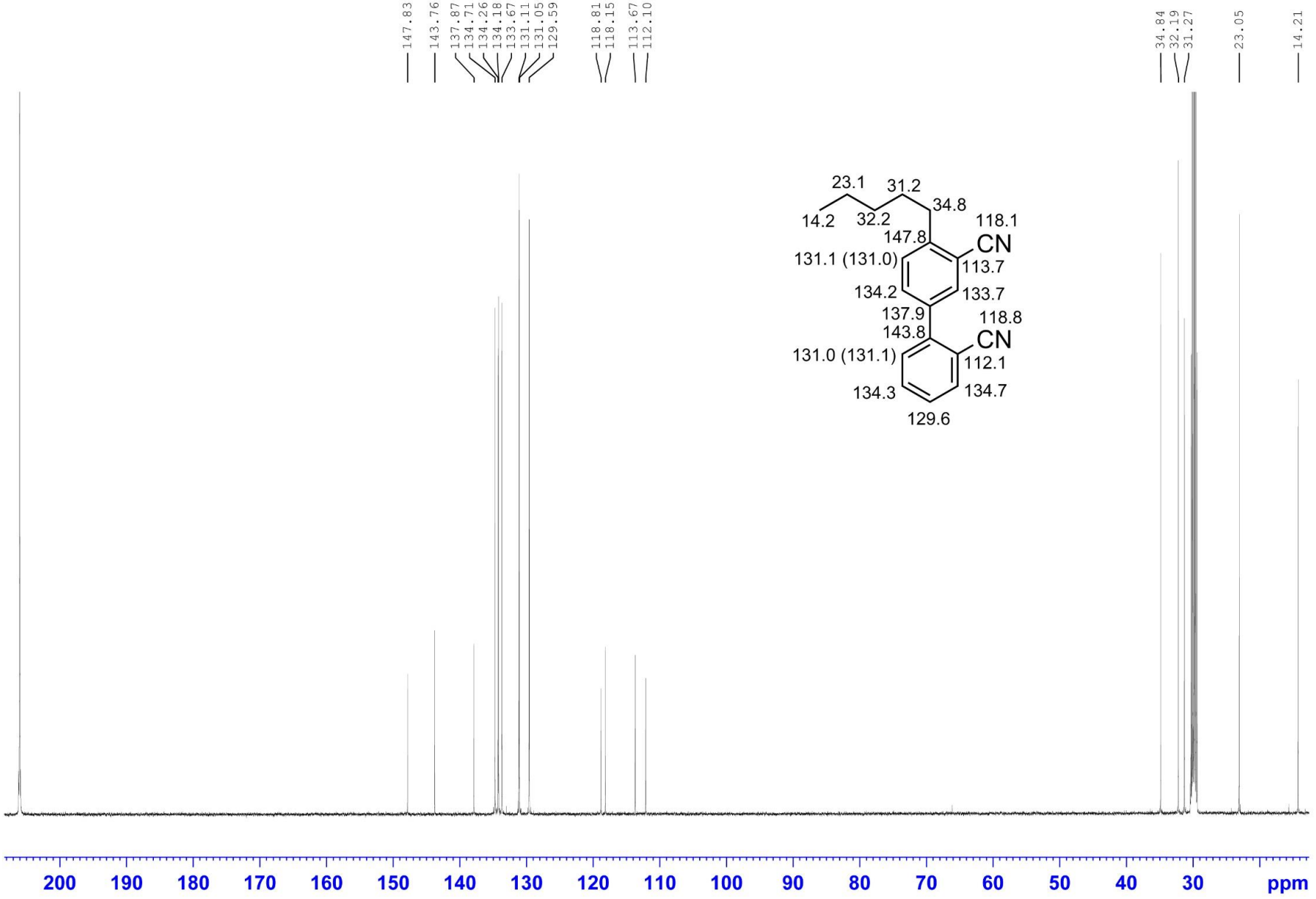
## IR for 4’-butyl-[1,1’-biphenyl]-2,3’-dicarbonitrile (7a)



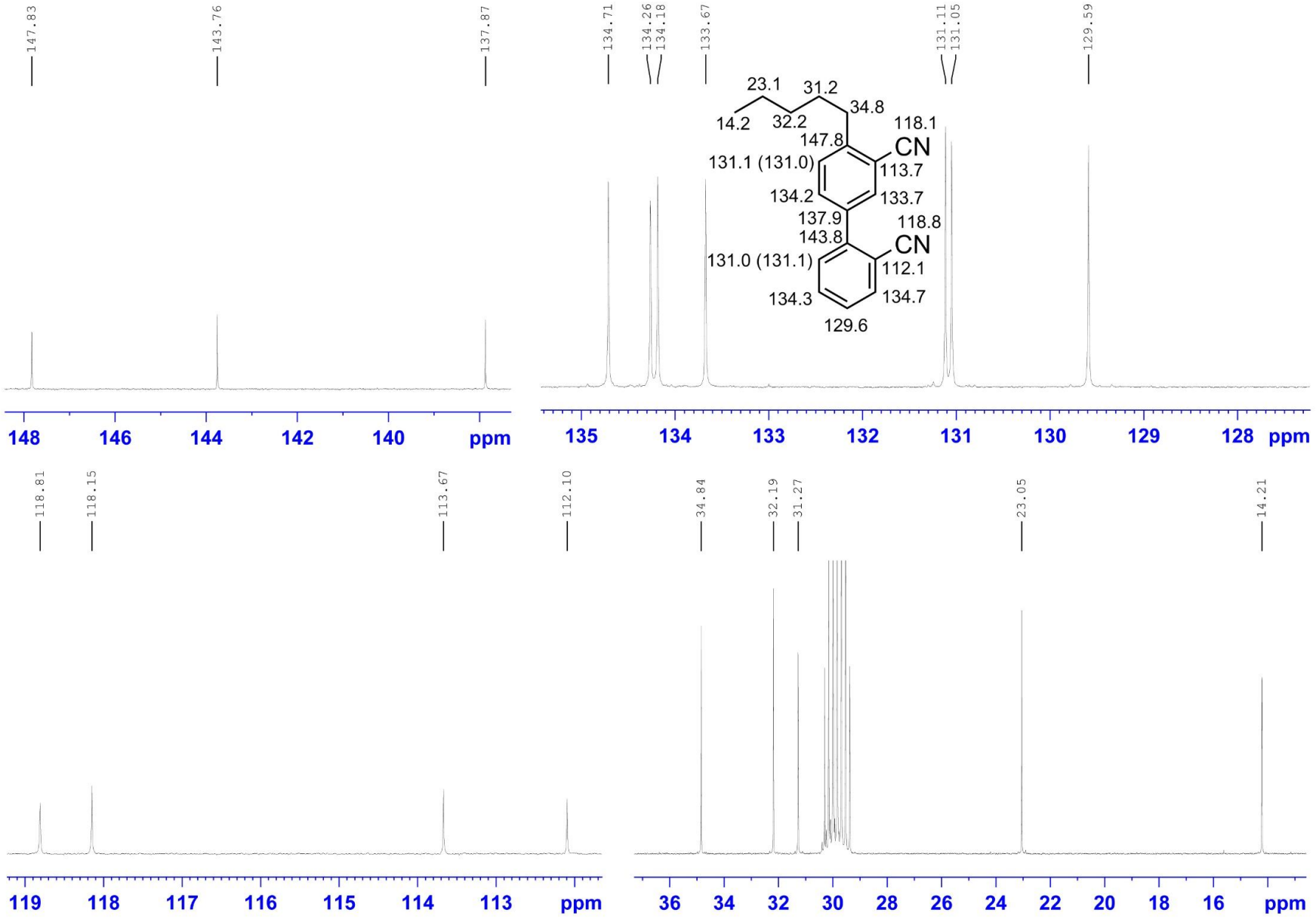
## $^1$H NMR for 4'-pentyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7b)



## $^{13}$C NMR (overview) for 4'-pentyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7b)

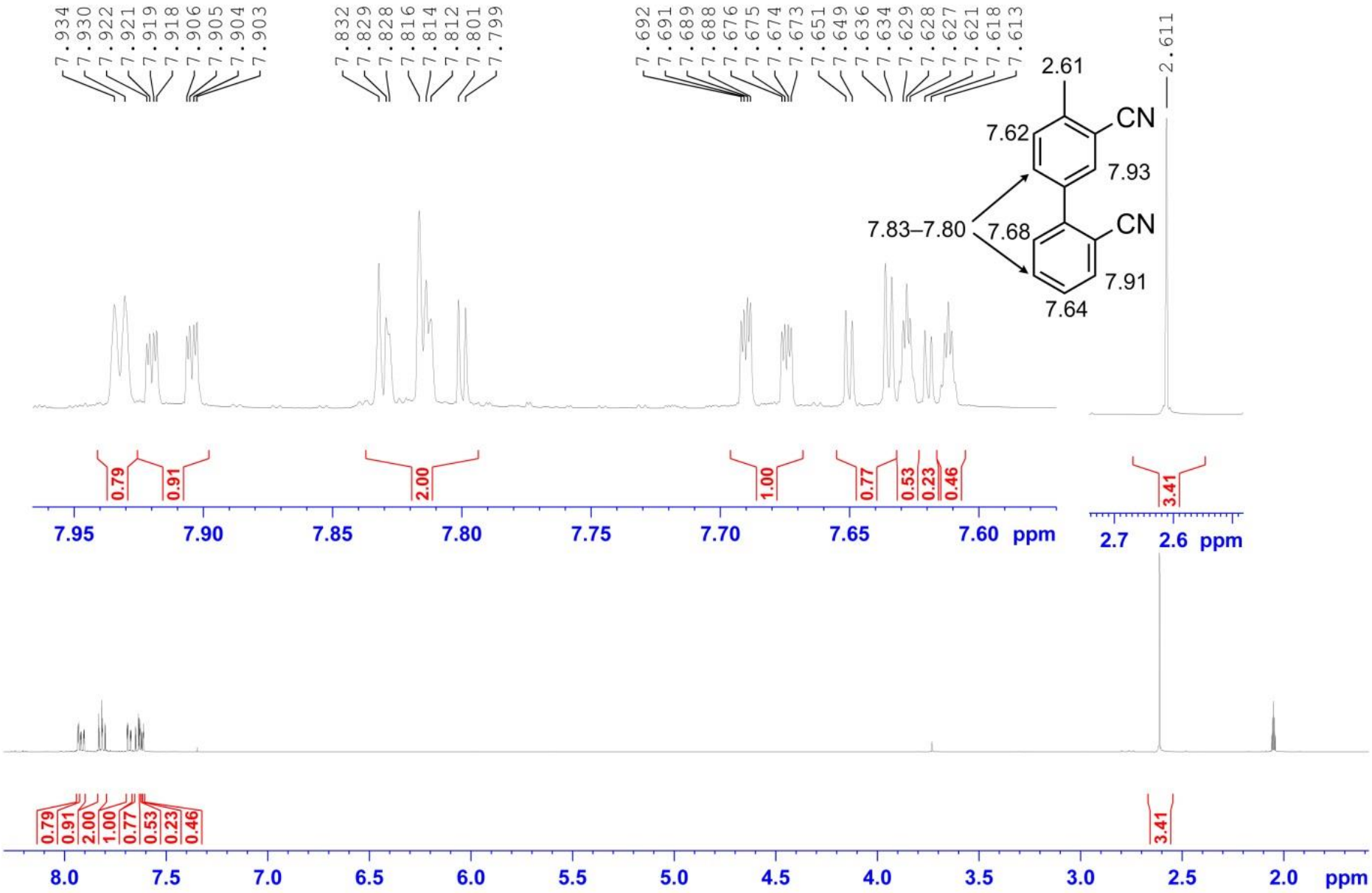


## $^{13}$C NMR (detailed) for 4'-pentyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7b)

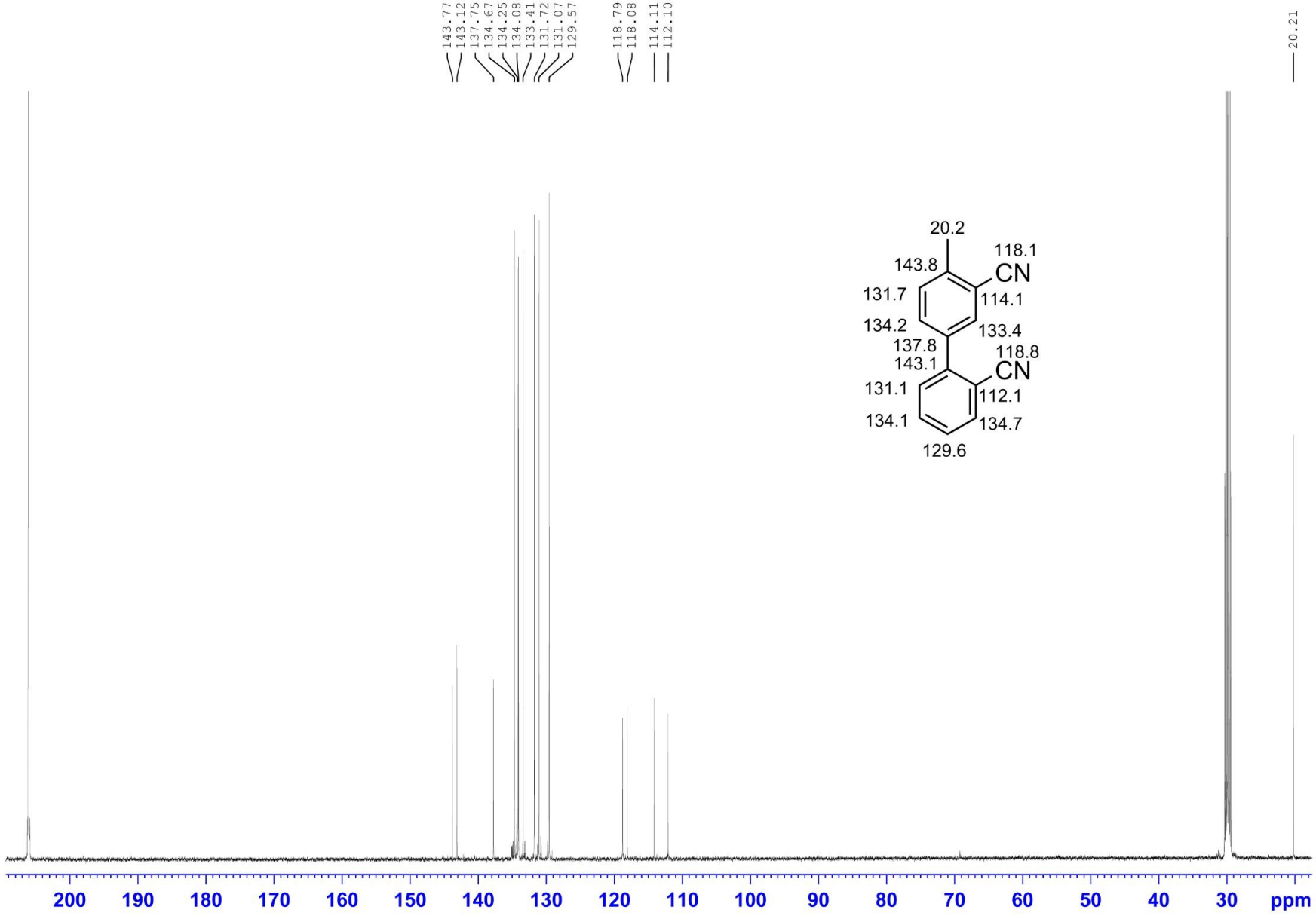


**IR for 4’-pentyl-[1,1’-biphenyl]-2,3’-dicarbonitrile (7b)**

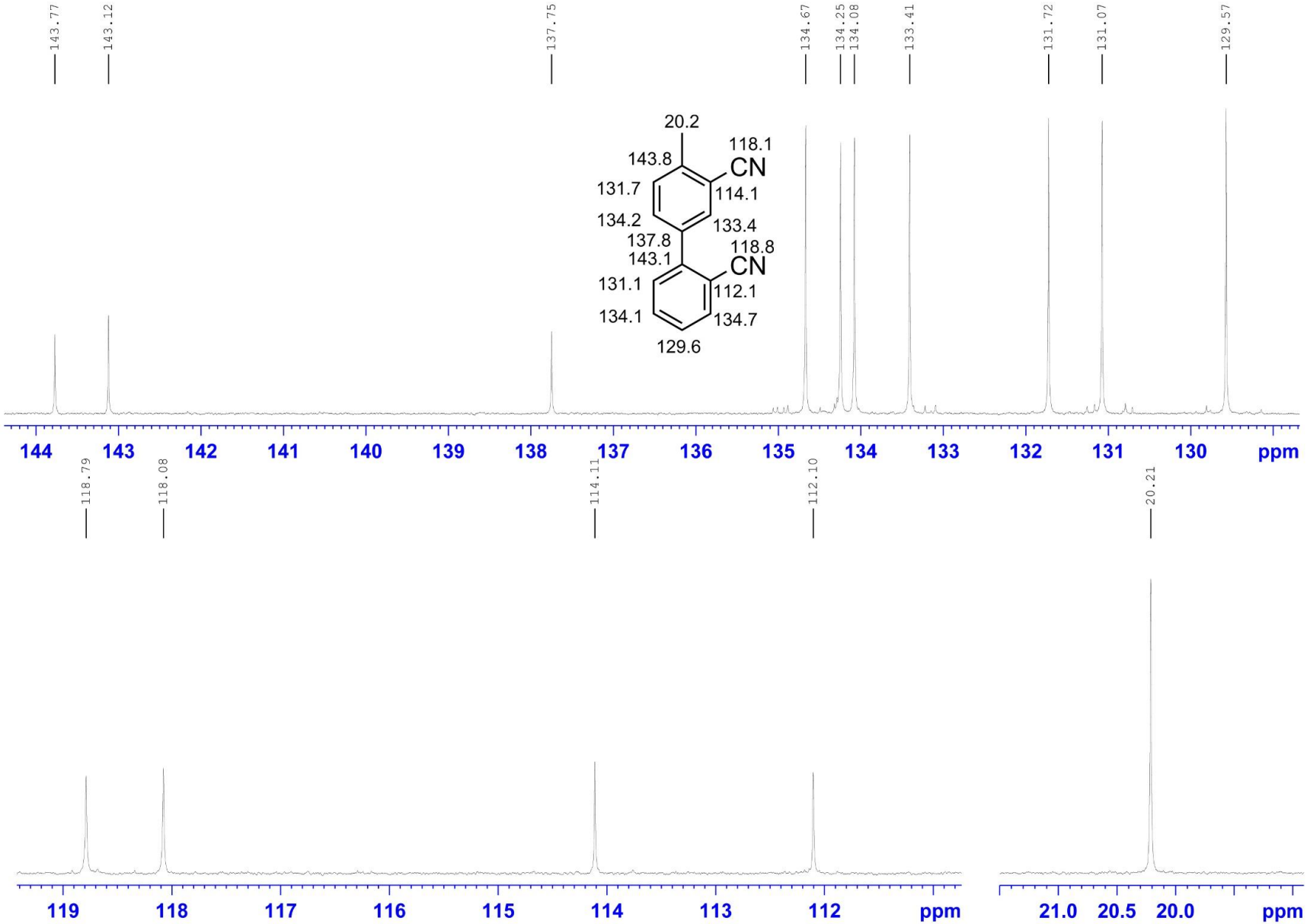
**$^1$H NMR for 4'-methyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7c).**



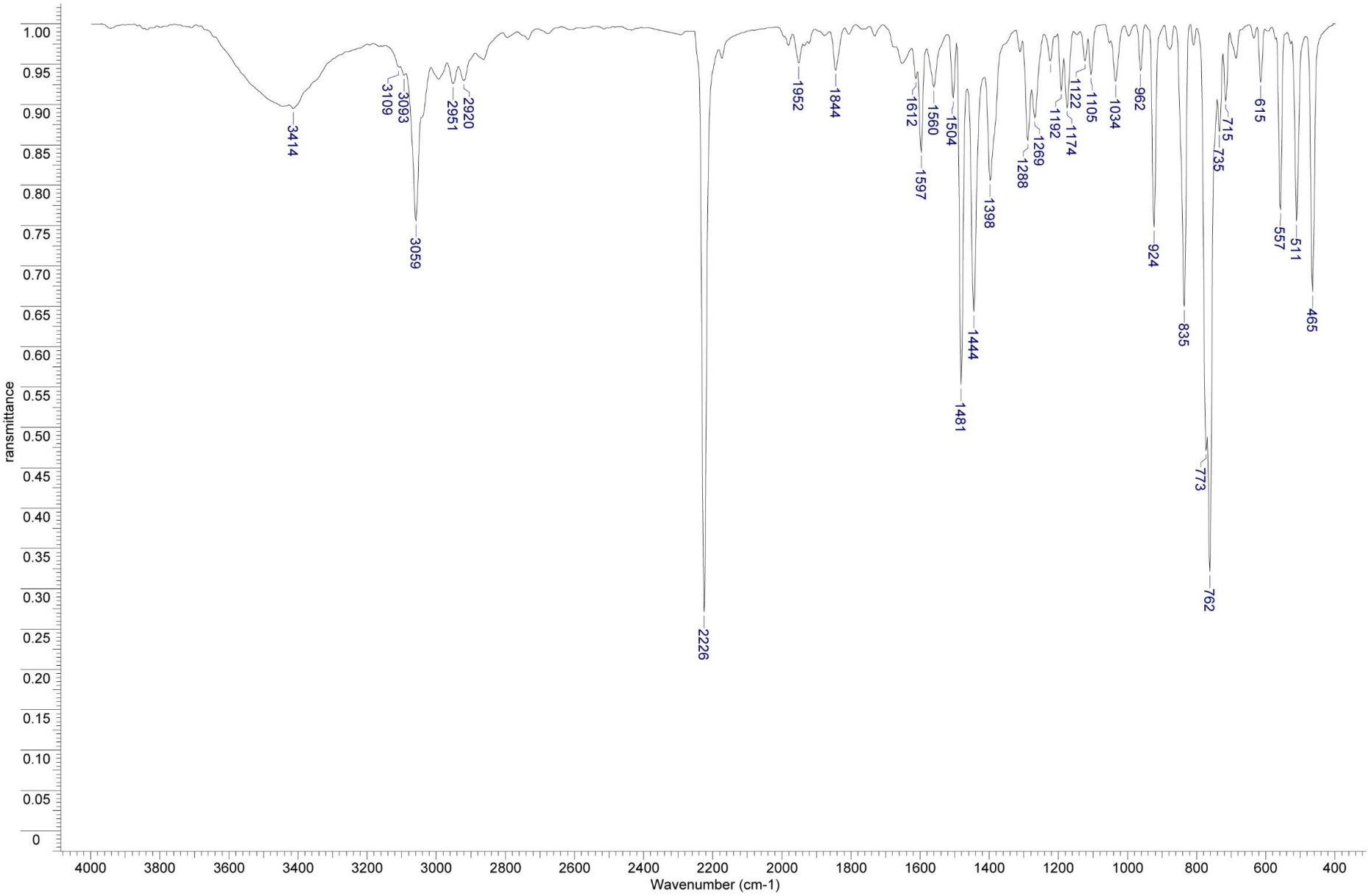
## $^{13}$C NMR (overview) for 4'-methyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7c)



## $^{13}$C NMR (detailed) for 4'-methyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7c)

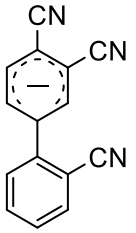


**IR for 4'-methyl-[1,1'-biphenyl]-2,3'-dicarbonitrile (7c).**



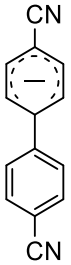
## Optimized geometries for anionic intermediates $2^{-}$ and $6^{-}$

1,2-dicyano-4-(2-cyanophenyl)-cyclohexa-2,5-dienyl anion (**6**$^{-}$)




C -0.060747 1.367417 1.210447
C 0.044285 1.298735 -0.196724
C 0.003691 2.509316 -0.907334
C -0.132434 3.733648 -0.257225
C -0.232762 3.787857 1.140786
C -0.197767 2.607280 1.873202
C 0.175127 -0.032451 -0.961359
C -1.100346 -0.340286 -1.735608
C -1.193338 -0.167520 -3.083084
C -0.074249 0.164171 -3.922132
C 1.212211 0.138994 -3.271616
C 1.357429 -0.022333 -1.913537
C -0.242265 0.361722 -5.304322
N -0.429359 0.532659 -6.452950
H -0.336001 4.742622 1.651023
H -0.159900 4.652155 -0.839924
H -0.272444 2.623762 2.957667
H 0.079937 2.471988 -1.990367
C -0.033108 0.183911 2.027951
H -1.969266 -0.659586 -1.162547
H 2.354275 -0.111856 -1.489333
H -2.153673 -0.332574 -3.570675
C 2.418200 0.224507 -4.053842
H 0.337912 -0.806387 -0.194798
N -0.021133 -0.729071 2.753084
N 3.414171 0.299553 -4.655296

1-cyano-4-(4-cyanophenyl)-cyclohexa-2,5-dienyl anion (**2**$^{-}$)




C 8.475502 -1.859692 1.138675
C 7.207296 -1.258652 1.130365
C 6.541280 -1.101271 2.359934
C 7.119021 -1.522998 3.551796
C 8.395601 -2.124295 3.544686
C 9.072024 -2.291336 2.322799
C 6.569774 -0.744665 -0.174177
C 5.129137 -1.205532 -0.344320
C 4.063142 -0.363778 -0.216953
C 4.199766 1.051614 -0.011399
C 5.536607 1.570963 -0.083241
C 6.638566 0.778075 -0.221781
C 3.082486 1.894467 0.111854
N 2.145167 2.600947 0.223742
C 8.998619 -2.566136 4.766921
N 9.493519 -2.928744 5.759150
H 3.056831 -0.774073 -0.308615
H 4.964485 -2.264534 -0.543313
H 7.198875 -1.170179 -0.981274
H 7.626940 1.228401 -0.310608
H 5.669456 2.653237 -0.066975
H 5.557614 -0.639697 2.362072
H 6.593886 -1.395019 4.495052
H 10.052963 -2.760540 2.311740
H 9.002616 -1.992185 0.194489