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ARTICLE TYPE

π-Complexes from acyl cyanides and lithium dimethylcuprate(I)

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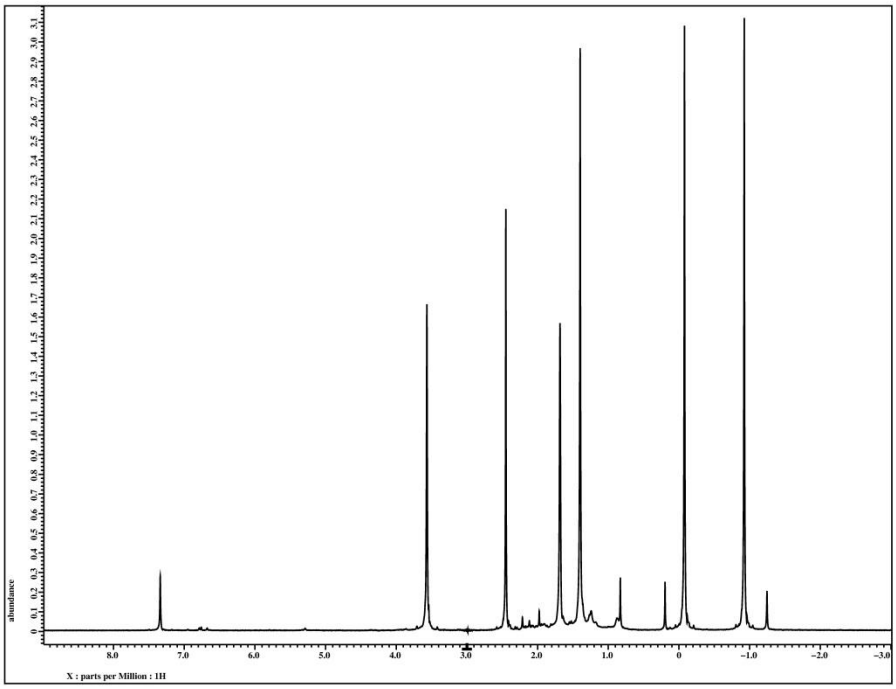
Electronic Supplementary Information

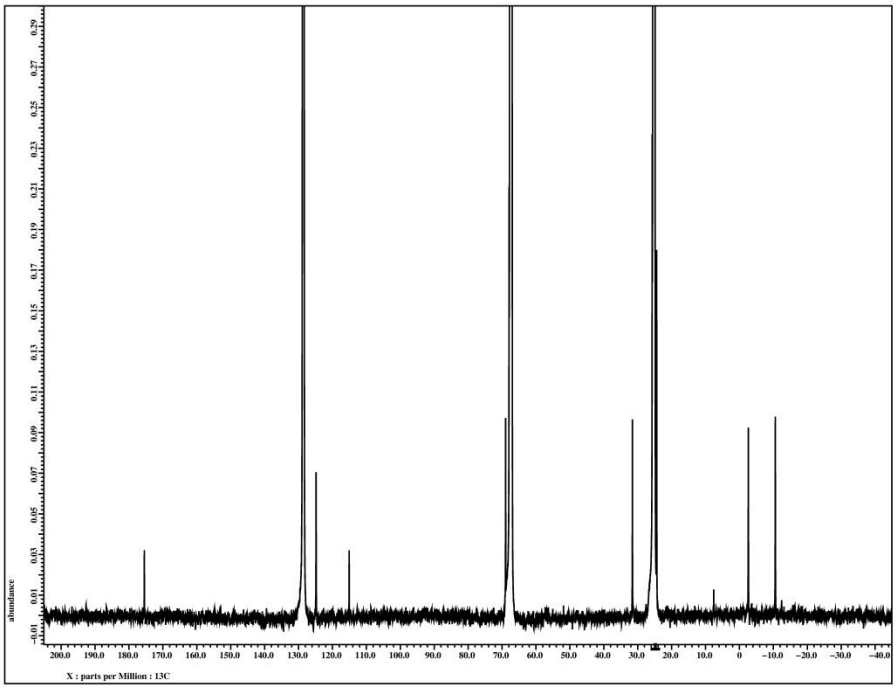
Pyruvonitrile / $Me_2CuLi{\cdot}LiI$ π-Complex

^{1}H NMR (–100 °C)



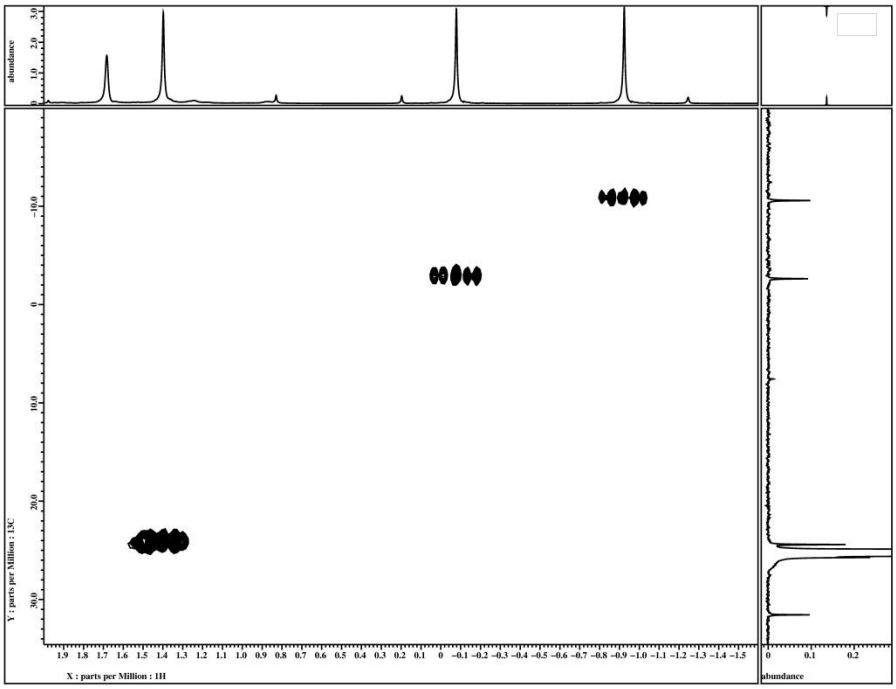
Pyruvonitrile / $Me_2CuLi{\cdot}LiI$ π-Complex

^{13}C NMR (–100 °C)



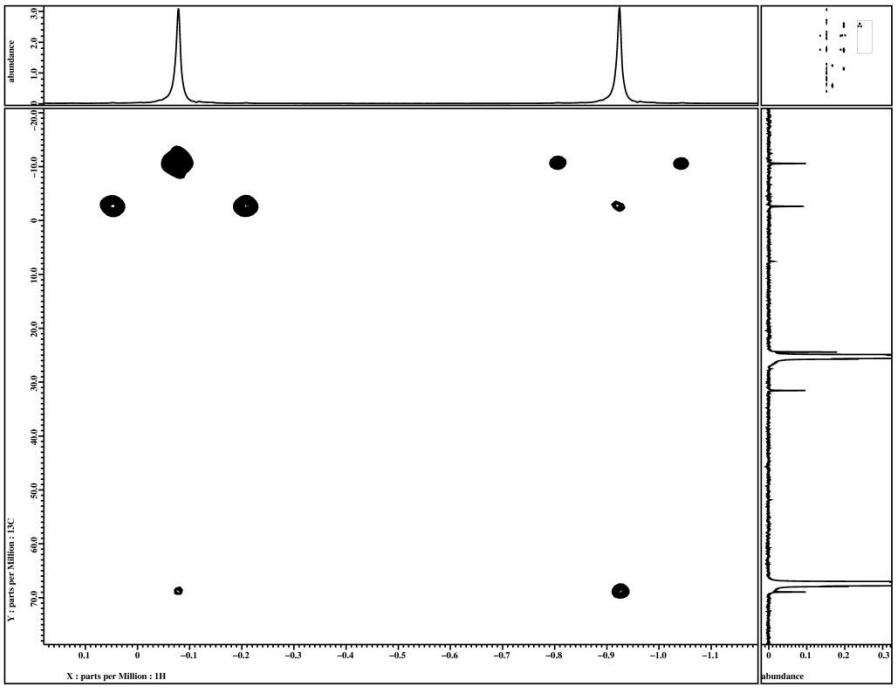
Pyruvonitrile / $Me_2CuLi{\cdot}LiI$ π-Complex

HMQC (–100 °C)



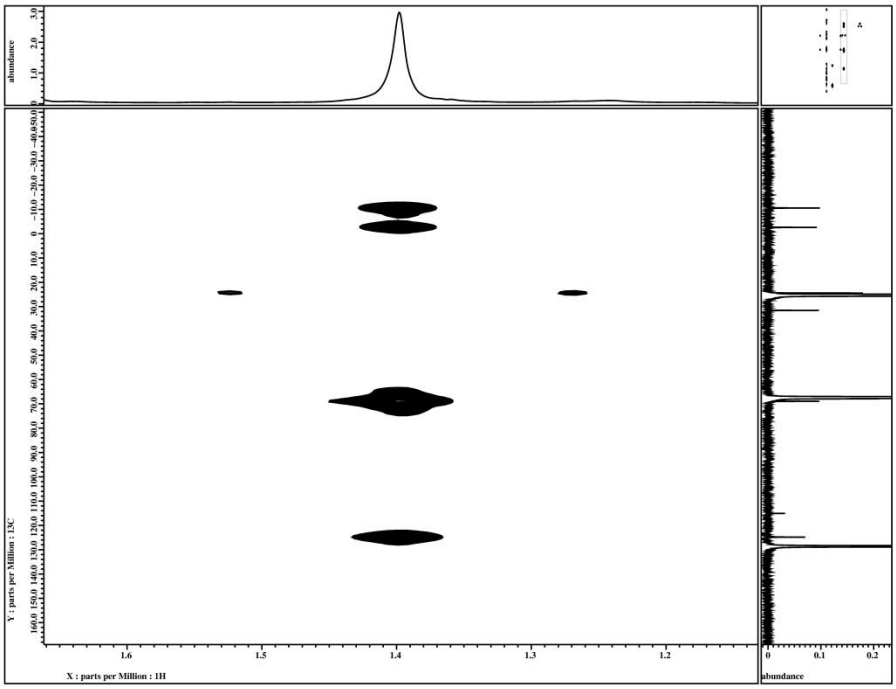
Pyruvonitrile / $Me_2CuLi{\cdot}LiI$ π-Complex

HMBC (–100 °C)



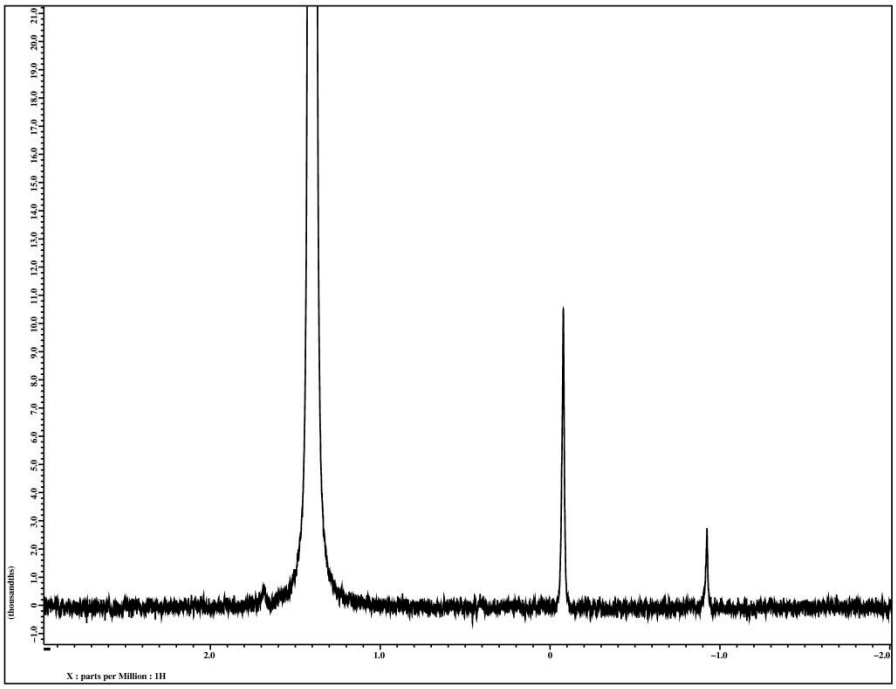
Pyruvonitrile / $Me_2CuLi{\cdot}LiI$ π-Complex

HMBC (–100 °C)



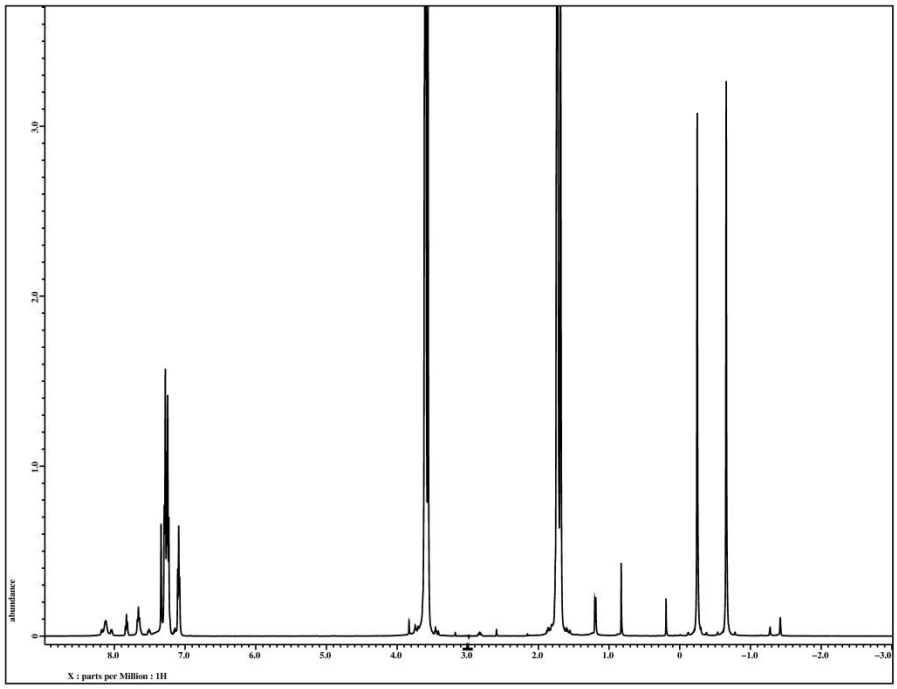
Pyruvonitrile / $Me_2CuLi{\cdot}LiI$ π-Complex

1-D NOE (irradiation offset = 1.40 ppm) (–100 °C)



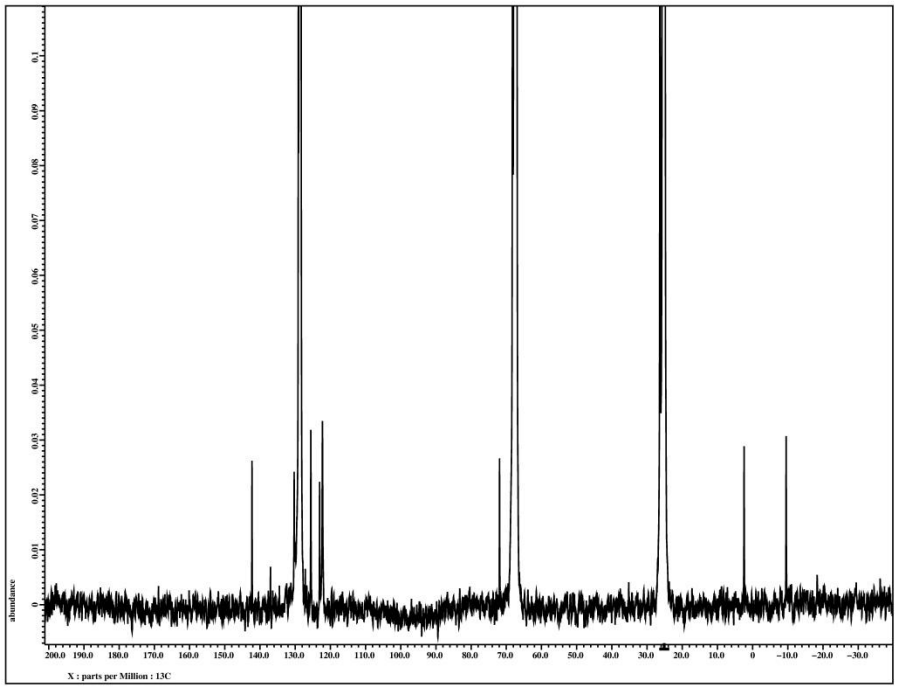
Benzoyl cyanide / $Me_2CuLi{\cdot}LiI$ π-Complex

^{1}H NMR (–100 °C)



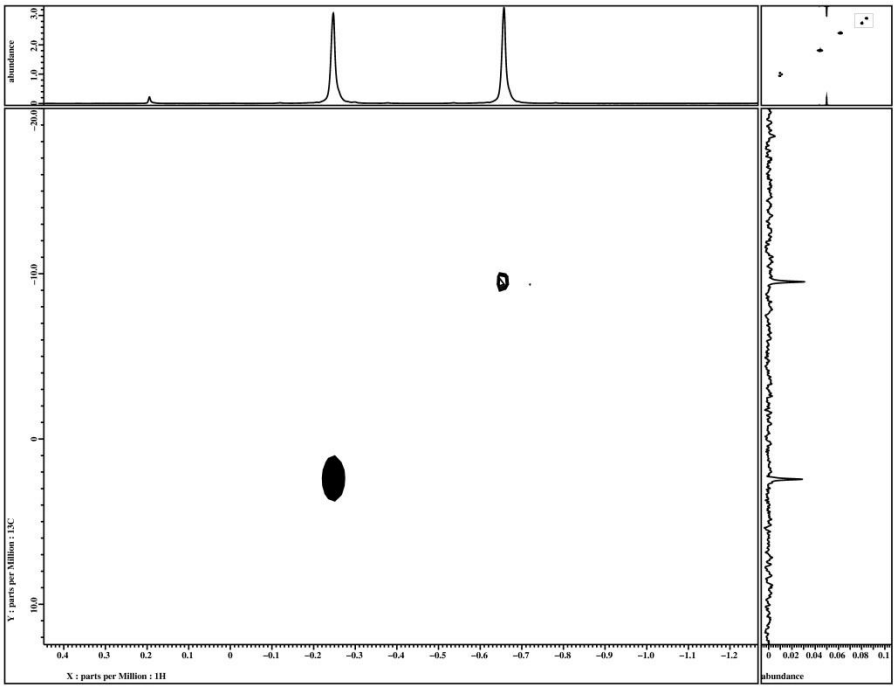
Benzoyl cyanide / $Me_2CuLi{\cdot}LiI$ π-Complex

^{13}C NMR (–100 °C)



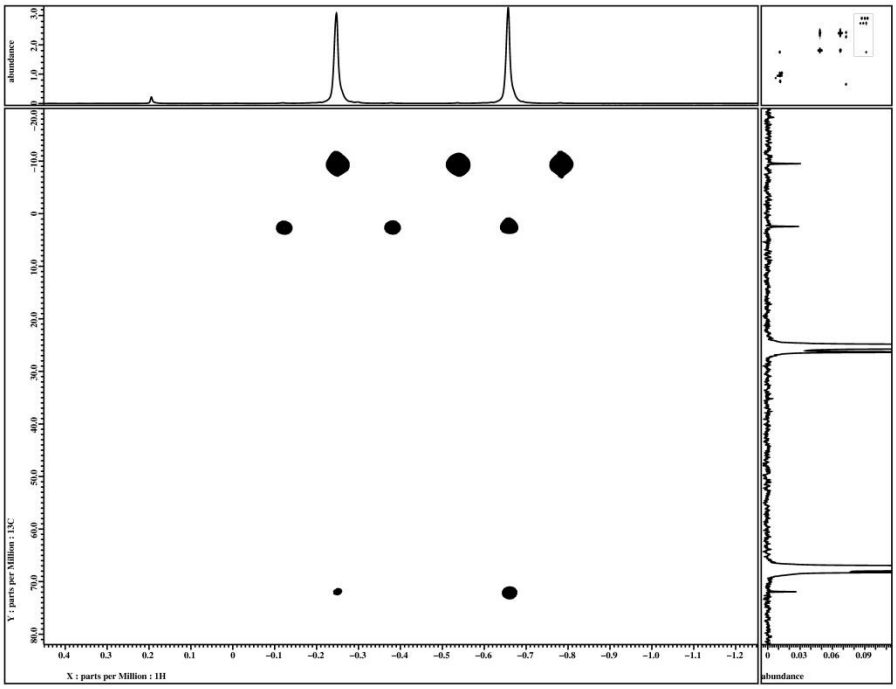
Benzoyl cyanide / $Me_2CuLi{\cdot}LiI$ π-Complex

HMQC (–100 °C)



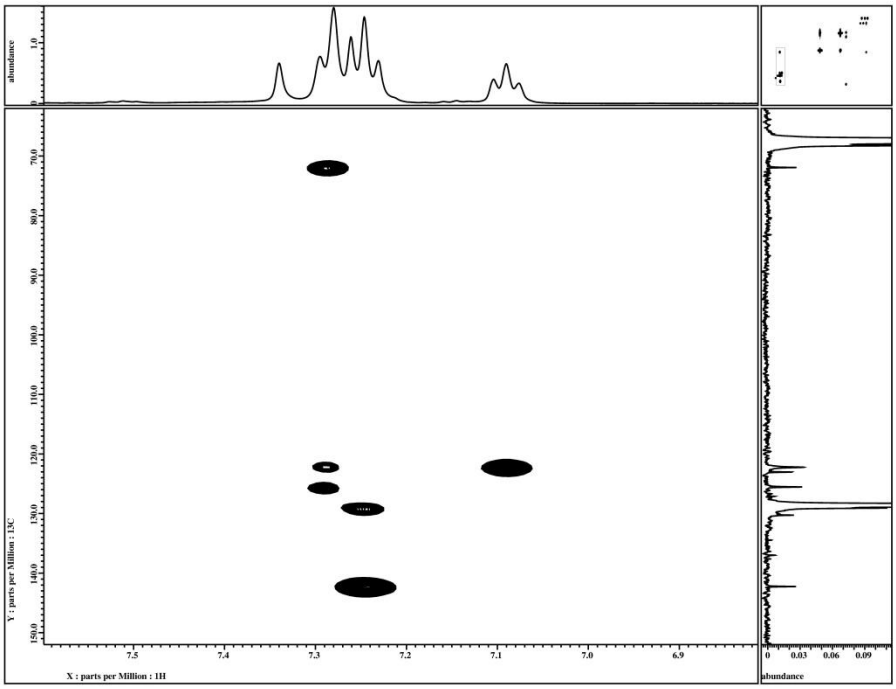
Benzoyl cyanide / $Me_2CuLi{\cdot}LiI$ π-Complex

HMBC (–100 °C)

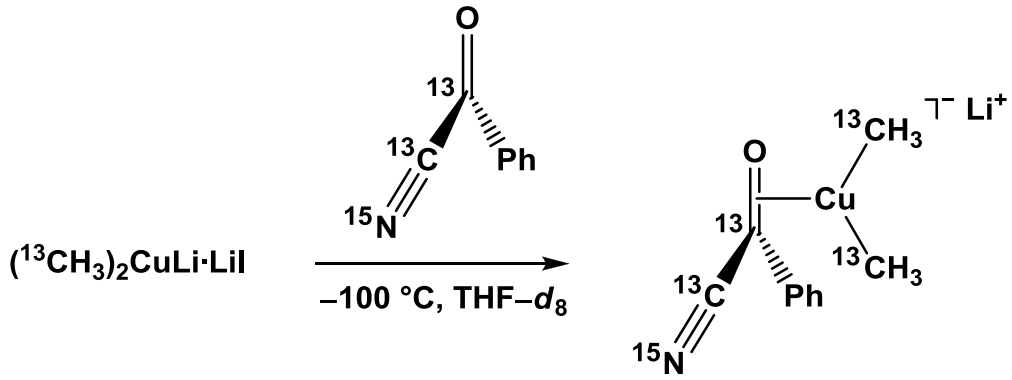


Benzoyl cyanide / $Me_2CuLi{\cdot}LiI$ π-Complex

HMBC (–100 °C)



Study of the benzoyl cyanide / $Me_2CuLi{\cdot}LiI$ π-complex using isotopic labelling.



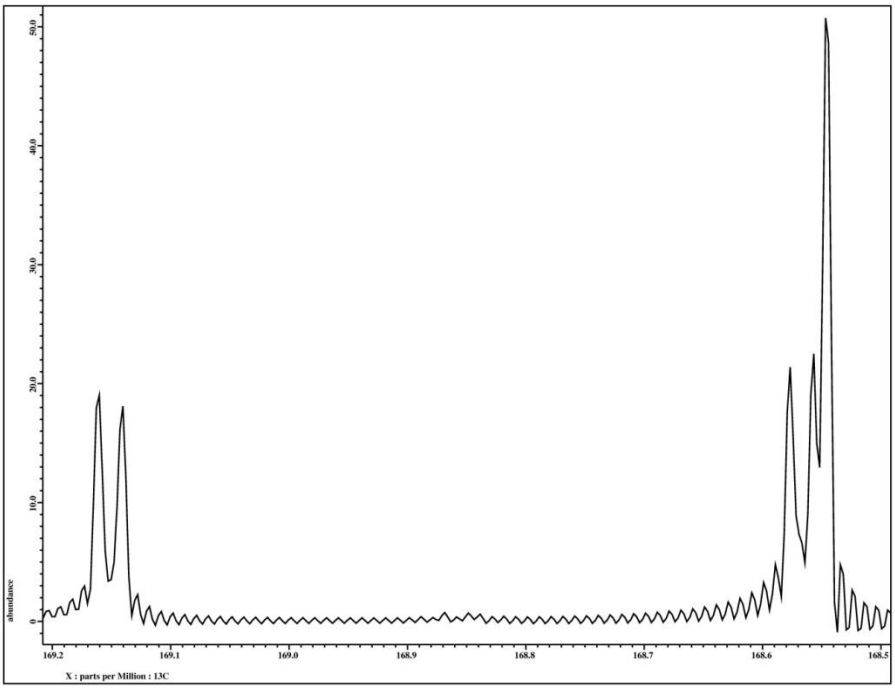
References

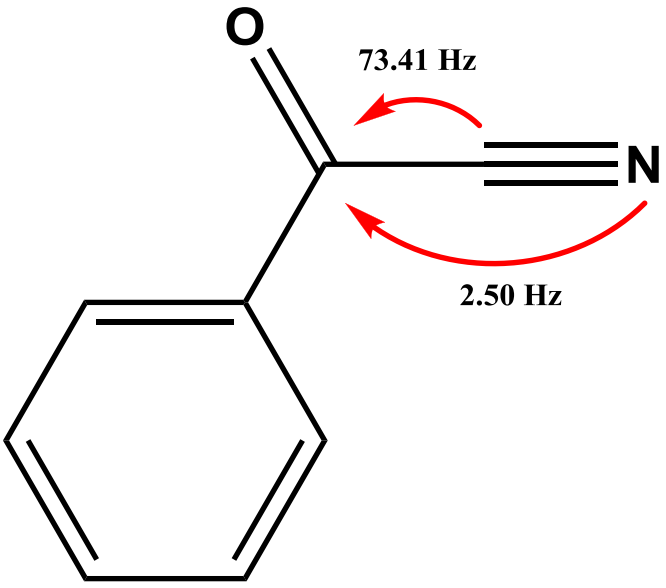
1. Preparation of CuCN: Reid, J.C.; Weaver, J.C. *Cancer Research* **1951**, *11*, 188-194.
2. Preparation of benzoyl cyanide: Oakwood, T.S.; Weisgerber, C.A. *Org. Synth.* **1944**, *24*, 14-16.

Note that in the titles below the number of stars (*) refers to the number of labeled atoms.

***Benzoyl cyanide (Substrate Only)

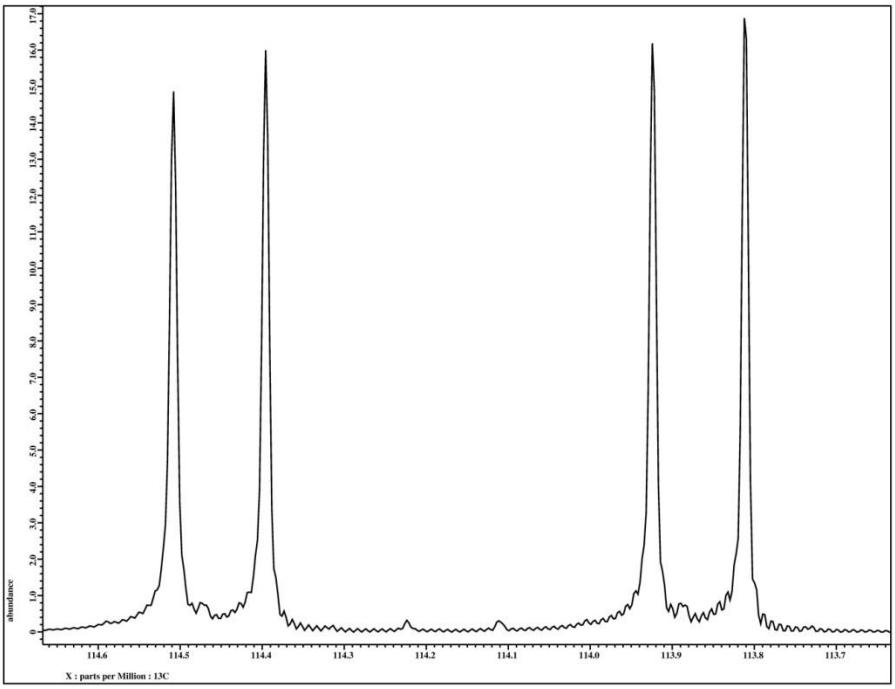
^{13}C (carbonyl carbon) (–100 °C)

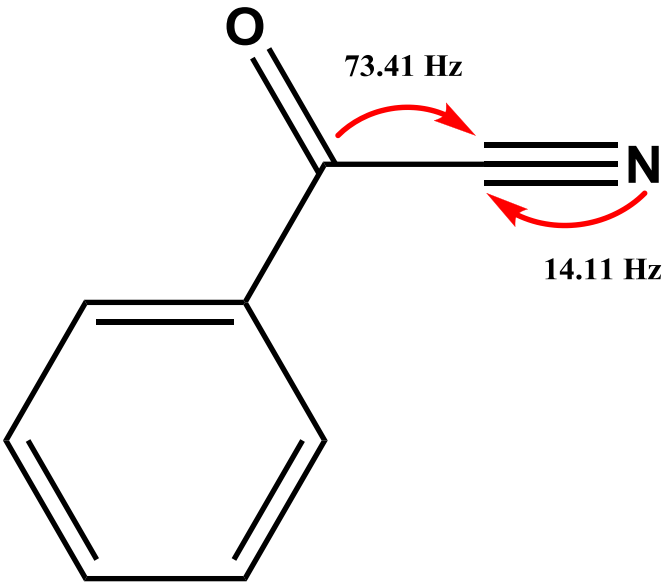




***Benzoyl cyanide (Substrate Only)

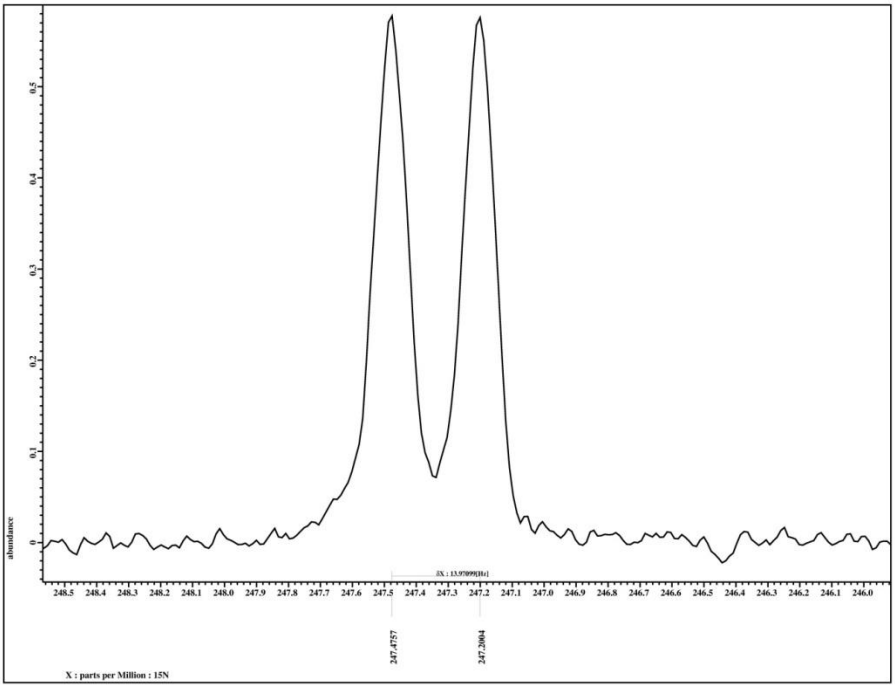
^{13}C (cyano carbon) (–100 °C)

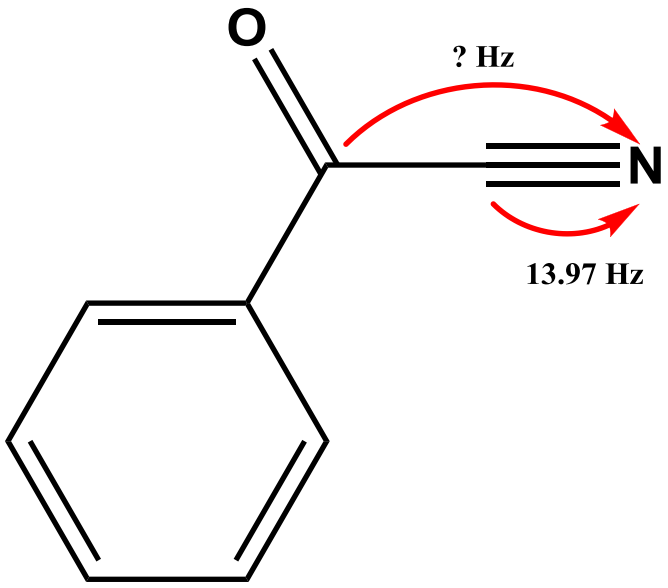




***Benzoyl cyanide (Substrate Only)

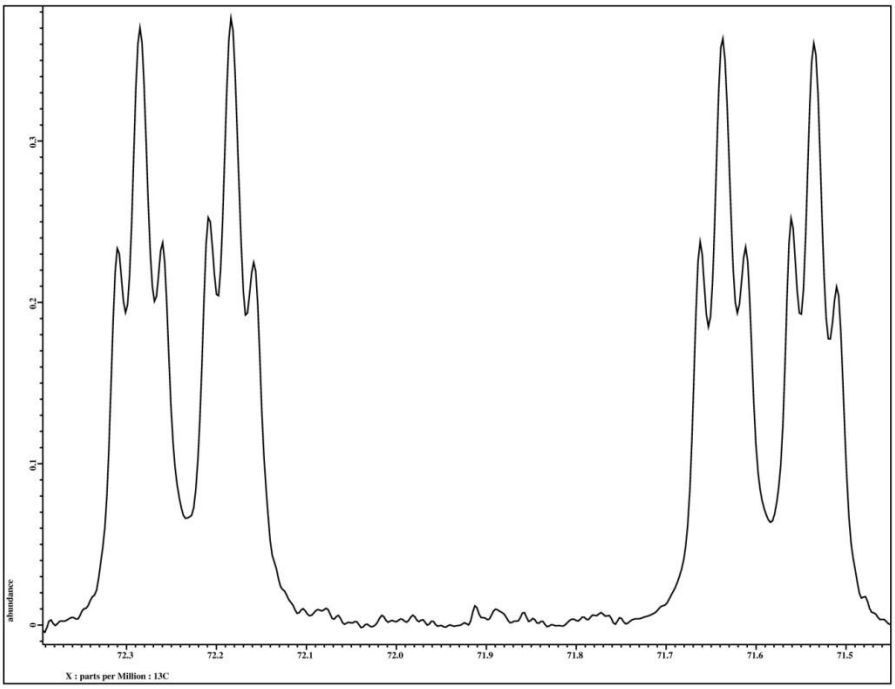
^{15}N (cyano nitrogen) (–100 °C)

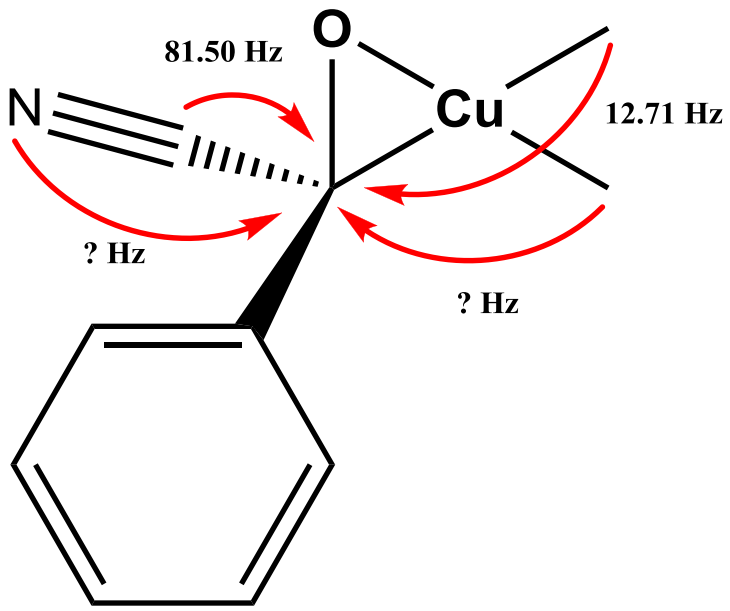




***Benzoyl cyanide / **$Me_2CuLi{\cdot}LiI$ π-Complex

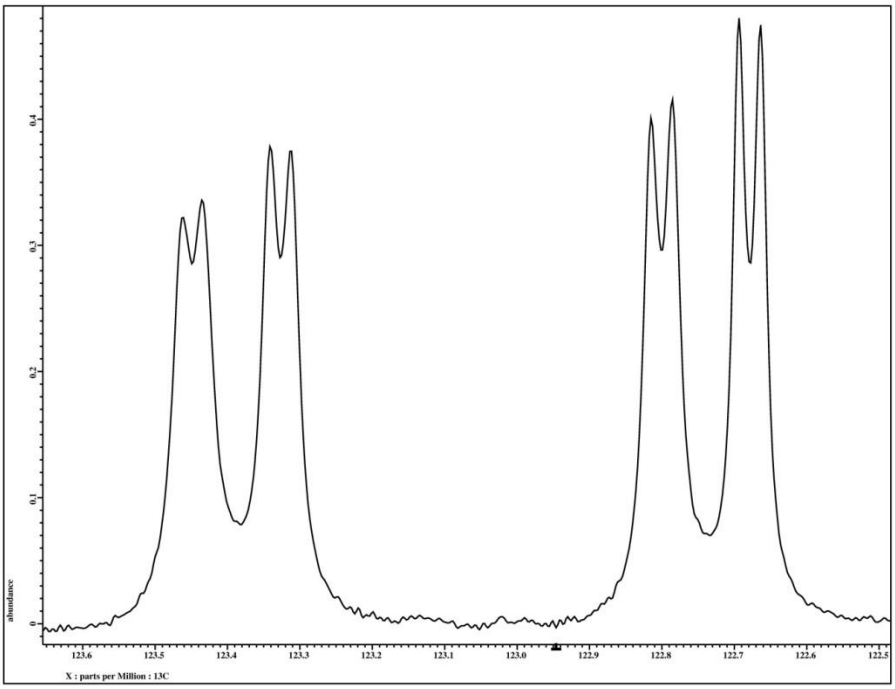
^{13}C (carbonyl carbon) (–100 °C)

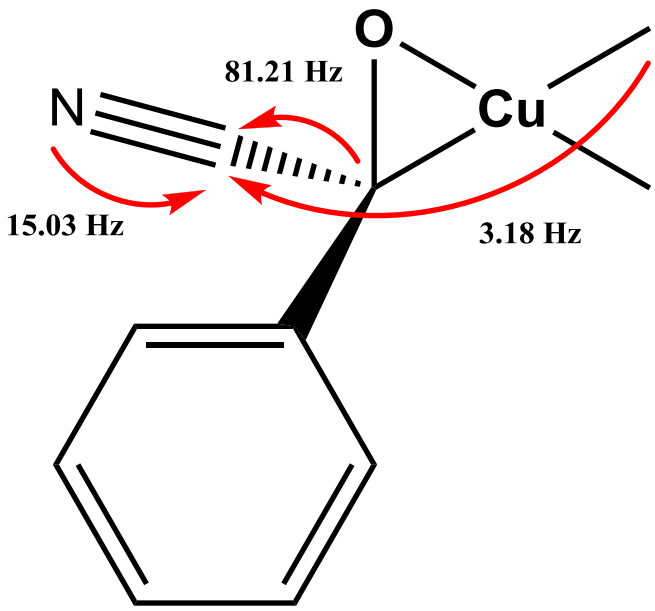




***Benzoyl cyanide / **$Me_2CuLi \cdot LiI$ π-Complex

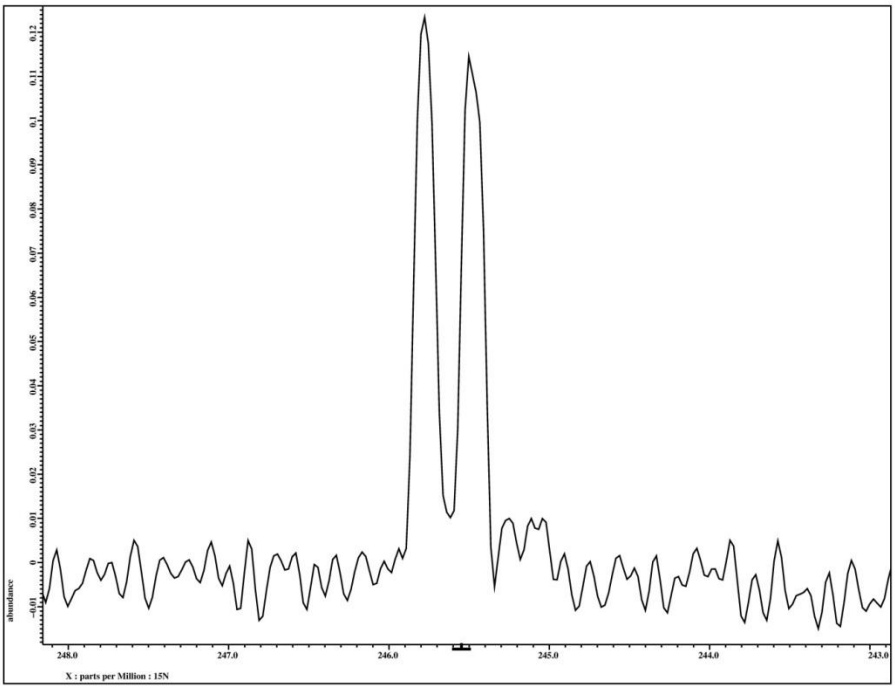
^{13}C (cyano carbon) (–100 °C)

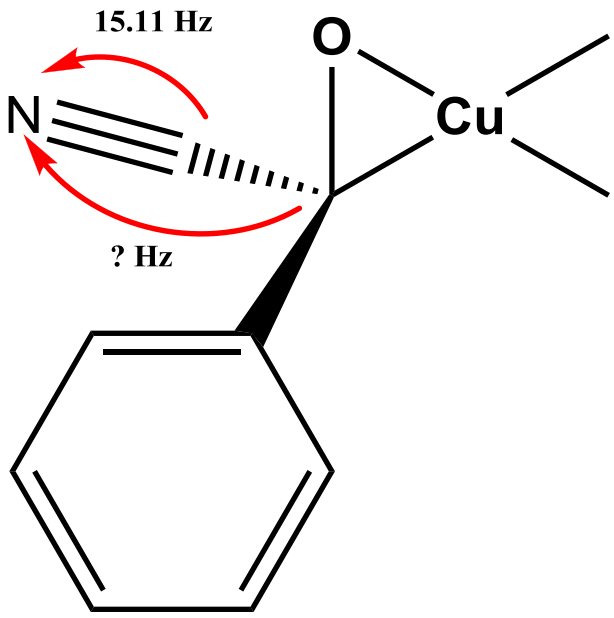




***Benzoyl cyanide / **$Me_2CuLi{\cdot}LiI$ π-Complex

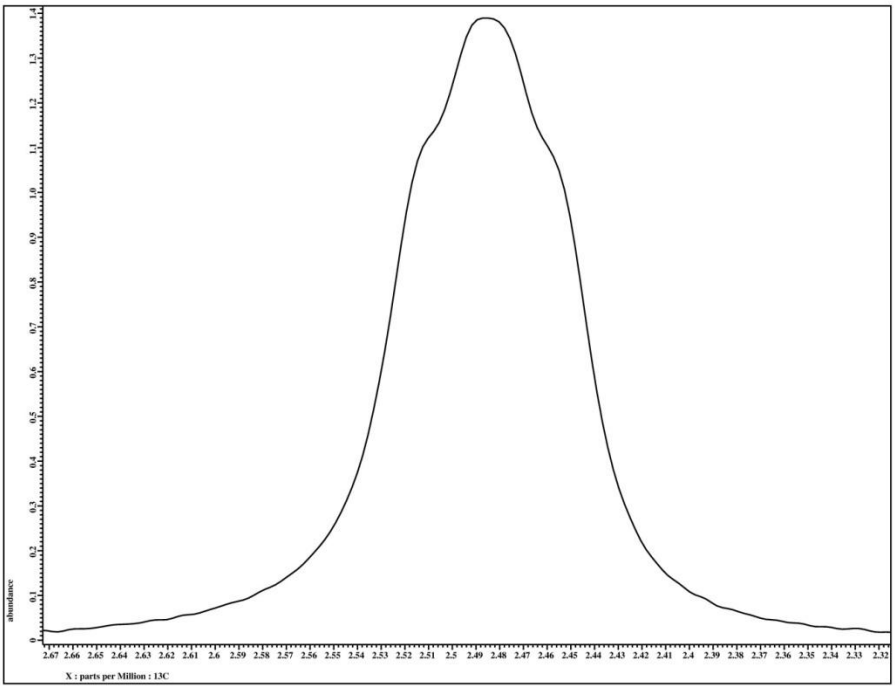
^{15}N (cyano nitrogen) (–100 °C)

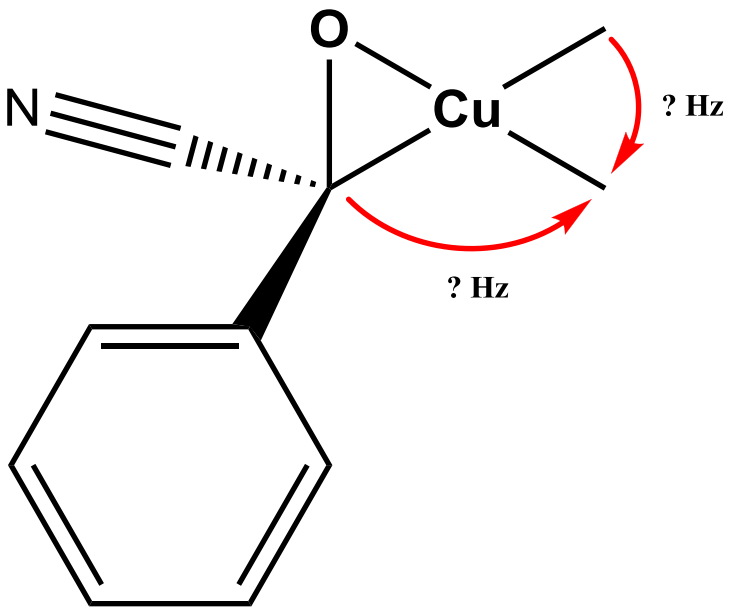




***Benzoyl cyanide / **$Me_2CuLi{\cdot}LiI$ π-Complex

^{13}C (CuMe *cis* to carbonyl C) (–100 °C)





***Benzoyl cyanide / **$Me_2CuLi{\cdot}LiI$ π-Complex

^{13}C (CuMe *trans* to carbonyl C) (–100 °C)