Application of the Variable Oxygen Probe to determine the π-electron donor ability of the alkyne group.

Benjamin L. Harris\textsuperscript{1} and Jonathan M. White\textsuperscript{1*}

1) School of Chemistry and the BIO-21 Institute, The University of Melbourne, Parkville VIC 3010.

Supporting Information

Cambridge Database structures and REFCODES Page 2
NMR Data for new Compounds 1a, 1c, 1d, 1d, 1f, 1g Pages 3-13
Structures harvested from The Cambridge Crystallographic Database from the search fragment shown on the right. The structures shown below represent the ROH moiety of those obtained.
$^1$H nmr Compound 1a

![Chemical Structure](image)

ppm (δ)
$^{13}$C nmr Compound 1a

\[ \text{NC} \quad \text{O} \]

- 157.493 ppm
- 130.360 ppm
- 125.335 ppm
- 120.148 ppm
- 118.511 ppm
- 118.018 ppm
- 113.261 ppm
- 77.397 ppm
- 76.495 ppm
- 56.038 ppm
$^1H$ nmr Compound 1c

\begin{center}
\includegraphics[width=\textwidth]{nmr_spectrum.png}
\end{center}
$^{13}$C nmr Compound 1c
$^{13}$C nmr Compound 1d
\[ ^1\text{H} \text{nmr Compound 1e} \]

![NMR Spectrum Diagram](image-url)
$^{13}$C nmr Compound 1e
$^1$H nmr Compound 1f

![NMR spectrum of compound 1f](image)

- Peak at 9.258 ppm
- Peak at 9.254 ppm
- Peak at 9.251 ppm
- Peak at 9.200 ppm
- Peak at 9.196 ppm
- Peak at 7.260 ppm
- Peak at 5.055 ppm
- Peak at 5.051 ppm
- Peak at 2.620 ppm
- Peak at 2.616 ppm
- Peak at 2.612 ppm

Compound 1f structure:
$^{13}$C nmr Compound 1f

![Chemical structure diagram with ppm values](image)
$^1$H nmr Compound 1g

![Chemical structure diagram](image-url)

- Chemical shifts: 7.958, 7.754, 7.701, 7.660, 4.936, 2.557
$^{13}$C nmr Compound 1g

![Chemical Structure](image)