Chemoselective Lactam Formation in the Addition of Benzenesulfonyl Bromide to *N*-Allyl Acrylamides and *N*-Allyl 3,3-Dimethylacrylamides

Chen Wang* and Glen A. Russell†

Department of Chemistry, Iowa State University, Ames, IA 50011-3111

Supporting Information

^{1}H NMR and ^{1}H - ^{1}H NOESY spectra were recorded in $CDCl_3$ or C_6D_6 at 400 MHz with δ measured relative to $CHCl_3$ (7.27 ppm) or C_6H_6 (7.16 ppm) respectively. ^{13}C NMR spectra were recorded at 100 MHz with δ relative to the central ^{13}C peak of $CDCl_3$ (77.23 ppm).

Figure 1. ^{1}H NMR spectrum of ***trans*-9a** in C_6D_6 (3 - 1).

Figure 2. ^{1}H NMR spectrum of ***trans*-9a** in C_6D_6 (3 - 2).

Figure 3. ^{1}H NMR spectrum of ***trans*-9a** in C_6D_6 (3 - 3).

Figure 4. ^{1}H - ^{1}H NOESY spectrum of ***trans*-9a** in C_6D_6.

Figure 5. ^{13}C NMR spectrum of ***trans*-9a** in $CDCl_3$.

Figure 6. ^{1}H NMR spectrum of ***cis*-9a** in C_6D_6 (3 - 1).

Figure 7. ^{1}H NMR spectrum of ***cis*-9a** in C_6D_6 (3 - 2).

Figure 8. ^{1}H NMR spectrum of ***cis*-9a** in C_6D_6 (3 - 3).

Figure 9. ^{1}H - ^{1}H NOESY spectrum of ***cis*-9a** in C_6D_6.

Figure 10. ^{13}C NMR spectrum of ***cis*-9a** in $CDCl_3$.

Figure 11. ^{1}H NMR spectrum of **9b** (c/t = 1 : 5) in C_6D_6.

Figure 12. ^{1}H - ^{1}H NOESY spectrum of **9b** (c/t = 1 : 5) in C_6D_6.

Figure 13. ^{13}C NMR spectrum of **9b** (c/t = 1 : 5) in $CDCl_3$.

Figure 14. ^{1}H NMR spectrum of ***trans*-9c** in $CDCl_3$.

Figure 15. ^{1}H - ^{1}H NOESY spectrum of ***trans*-9c** in $CDCl_3$.

Figure 16. ^{13}C NMR spectrum of ***trans*-9c** in $CDCl_3$.

Figure 17. ^{1}H NMR spectrum of ***cis*-9c** in C_6D_6.

Figure 18. ^{1}H - ^{1}H NOESY spectrum of ***cis*-9c** in C_6D_6.

Figure 19. ^{13}C NMR spectrum of ***cis*-9c** in $CDCl_3$.

Figure 20. ^{1}H NMR spectrum of ***trans*-9d** in C_6D_6.

Figure 21. ^{1}H - ^{1}H NOESY spectrum of ***trans*-9d** in C_6D_6.

Figure 22. ^{13}C NMR spectrum of ***trans*-9d** in $CDCl_3$.

Figure 23. ^{1}H NMR spectrum of ***cis*-9d** in C_6D_6.

Figure 24. ^{1}H - ^{1}H NOESY spectrum of ***cis*-9d** in C_6D_6.

Figure 25. ^{13}C NMR spectrum of ***cis*-9d** in $CDCl_3$.

Figure 26. ^{1}H NMR spectrum of ***trans*-9e** in $CDCl_3$.

Figure 27. ^{1}H - ^{1}H NOESY spectrum of ***trans*-9e** in $CDCl_3$.

Figure 28. ^{13}C NMR spectrum of ***trans*-9e** in $CDCl_3$.

Figure 29. ^{1}H NMR spectrum of **10c** (2 rotamers) in $CDCl_3$.

Figure 30. ^{13}C NMR spectrum of **10c** (2 rotamers) in $CDCl_3$.

Figure 31. ^{1}H NMR spectrum of **10d** (2 rotamers) in $CDCl_3$.

Figure 32. ^{13}C NMR spectrum of **10d** (2 rotamers) in $CDCl_3$.

Figure 33. ^{1}H NMR spectrum of **10e** in $CDCl_3$.

Figure 34. ^{13}C NMR spectrum of **10e** in $CDCl_3$.

Figure 35. ^{1}H NMR spectrum of **10f** in $CDCl_3$.

Figure 36. ^{13}C NMR spectrum of **10f** in $CDCl_3$.

Figure 37. ^{1}H NMR spectrum of **12a** and **13a** (2 : 1) in $CDCl_3$.

Figure 38. ^{1}H - ^{1}H NOESY spectrum of **12a** and **13a** (2 : 1) in $CDCl_3$.

Figure 39. ^{13}C NMR spectrum of **12a** and **13a** (2 : 1) in $CDCl_3$.

Figure 40. ^{1}H NMR spectrum of **12b** in $CDCl_3$.

Figure 41. ^{13}C NMR spectrum of **12b** in $CDCl_3$.

Figure 42. ^{1}H NMR spectrum of **12c** in C_6D_6.

Figure 43. ^{13}C NMR spectrum of **12c** in C_6D_6.

Figure 44. ^{1}H NMR spectrum of **12d** and **13d** (2.5 : 1) in C_6D_6.

Figure 45. ^{1}H - ^{1}H NOESY spectrum of **12d** and **13d** (2.5 : 1) in C_6D_6.

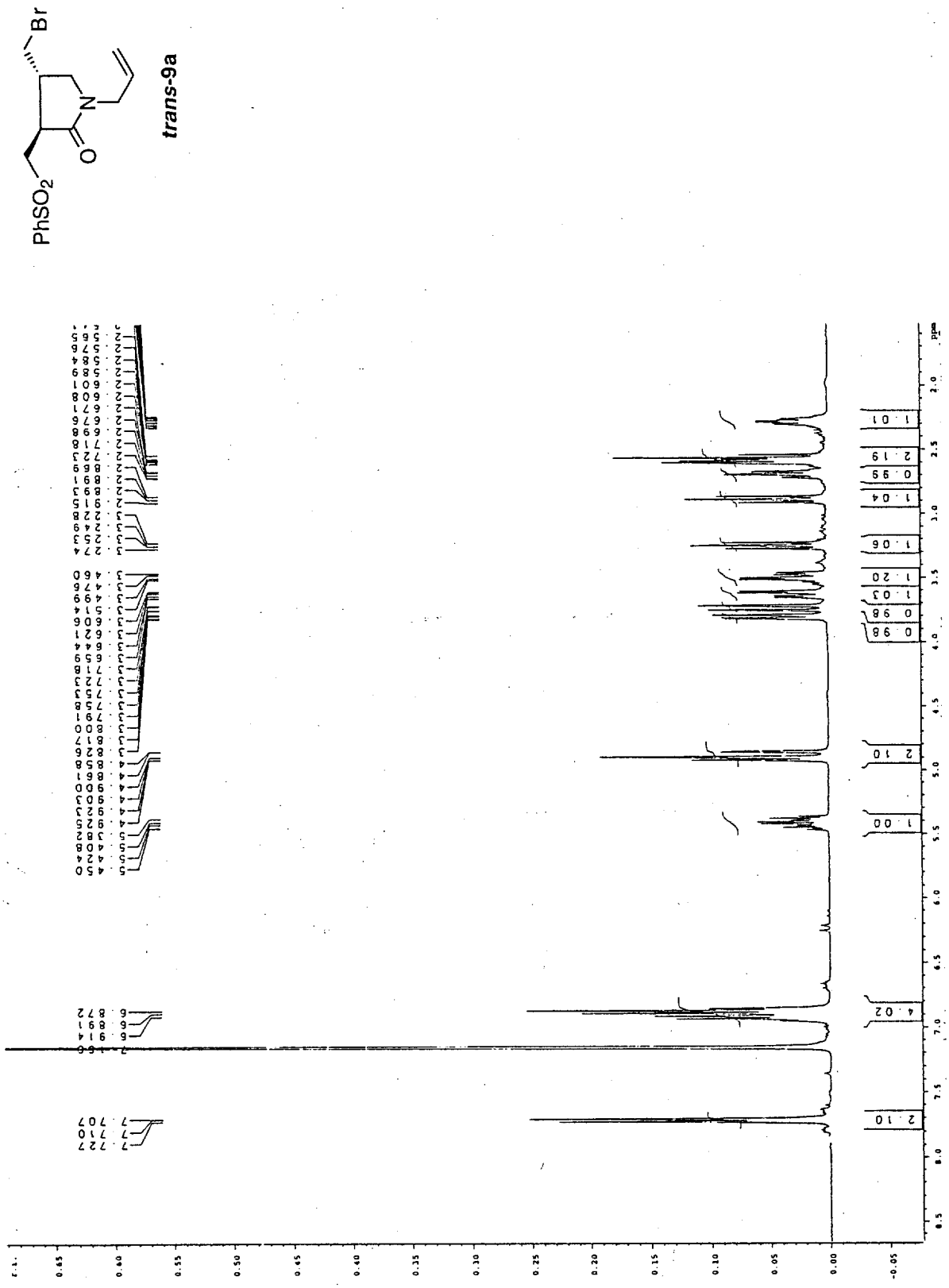

Figure 1. ^{1}H NMR spectrum of ***trans*-9a** in C_6D_6 (3 - 1).

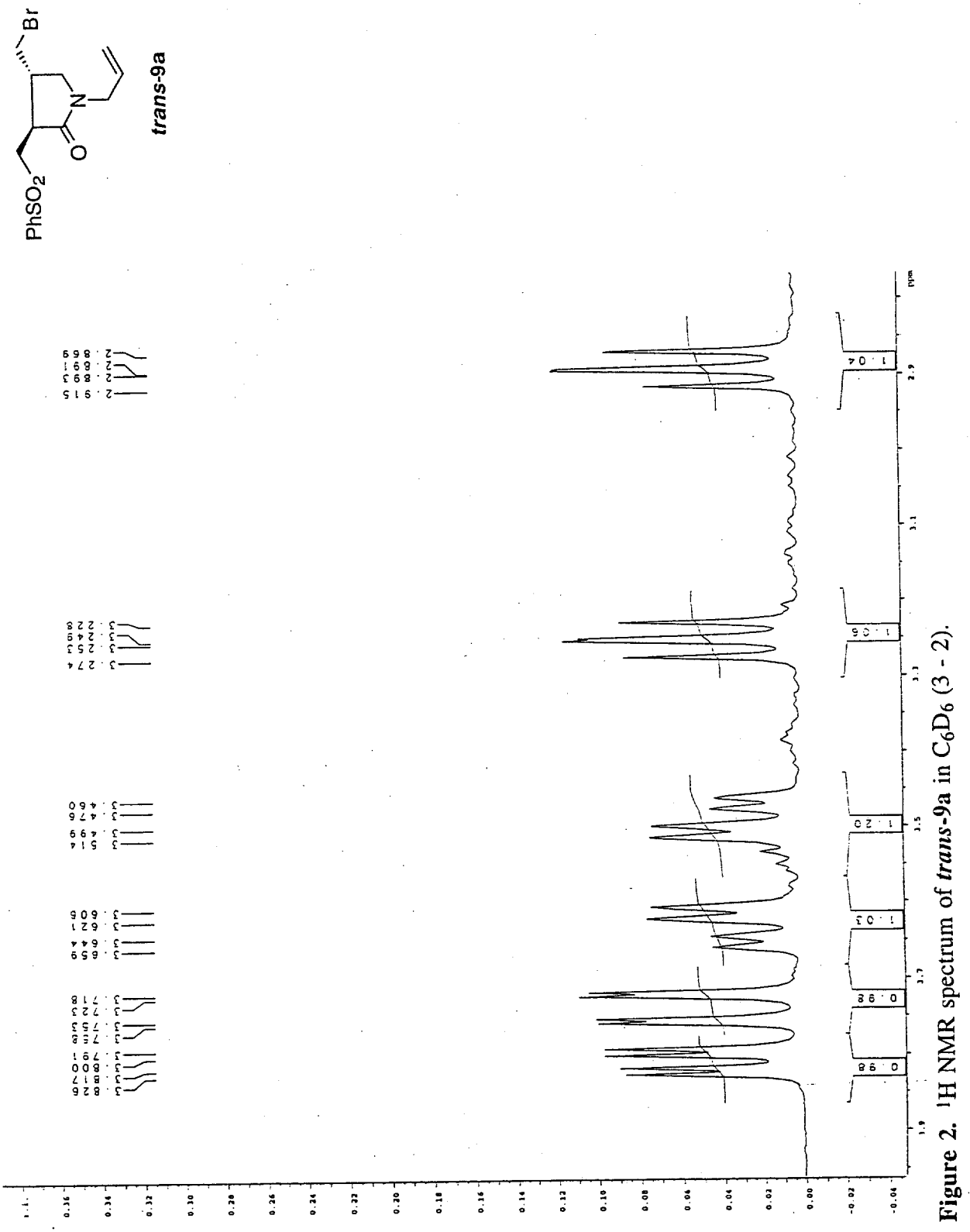

Figure 2. ^{1}H NMR spectrum of ***trans*-9a** in C_6D_6 (3 - 2).

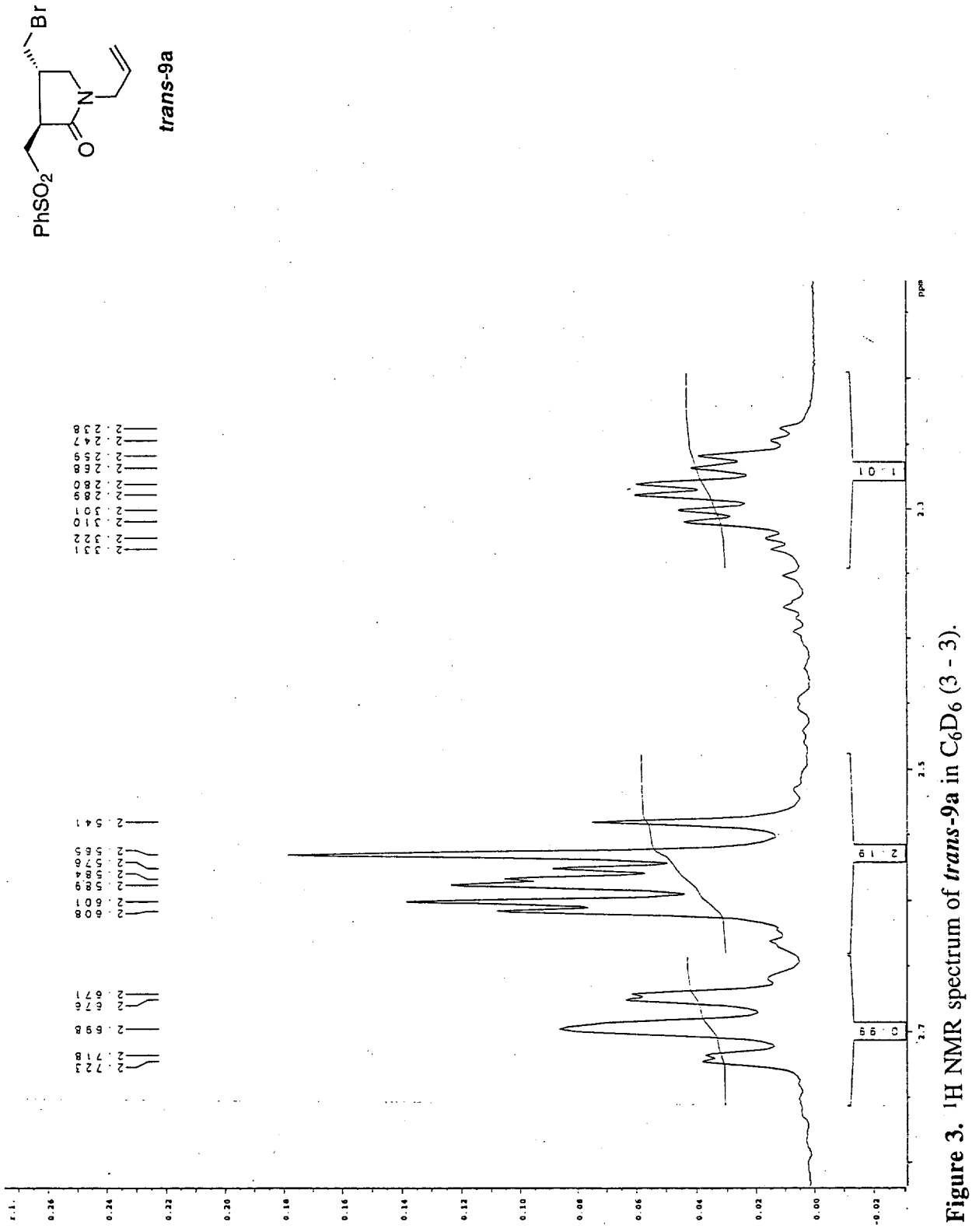

Figure 3. ^{1}H NMR spectrum of ***trans*-9a** in C_6D_6 (3 - 3).

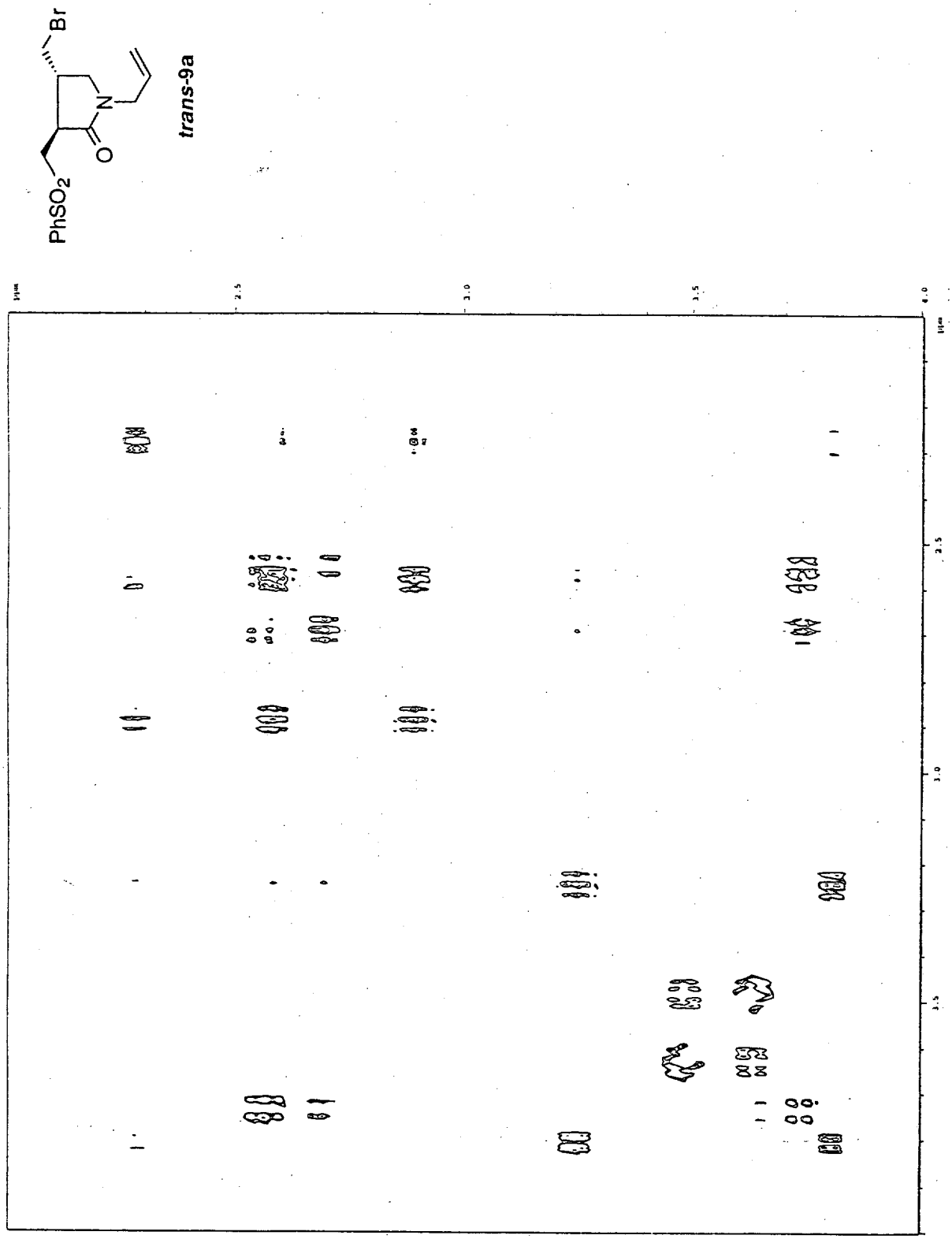

Figure 4. ^1H - ^1H NOESY spectrum of ***trans*-9a** in C_6D_6.

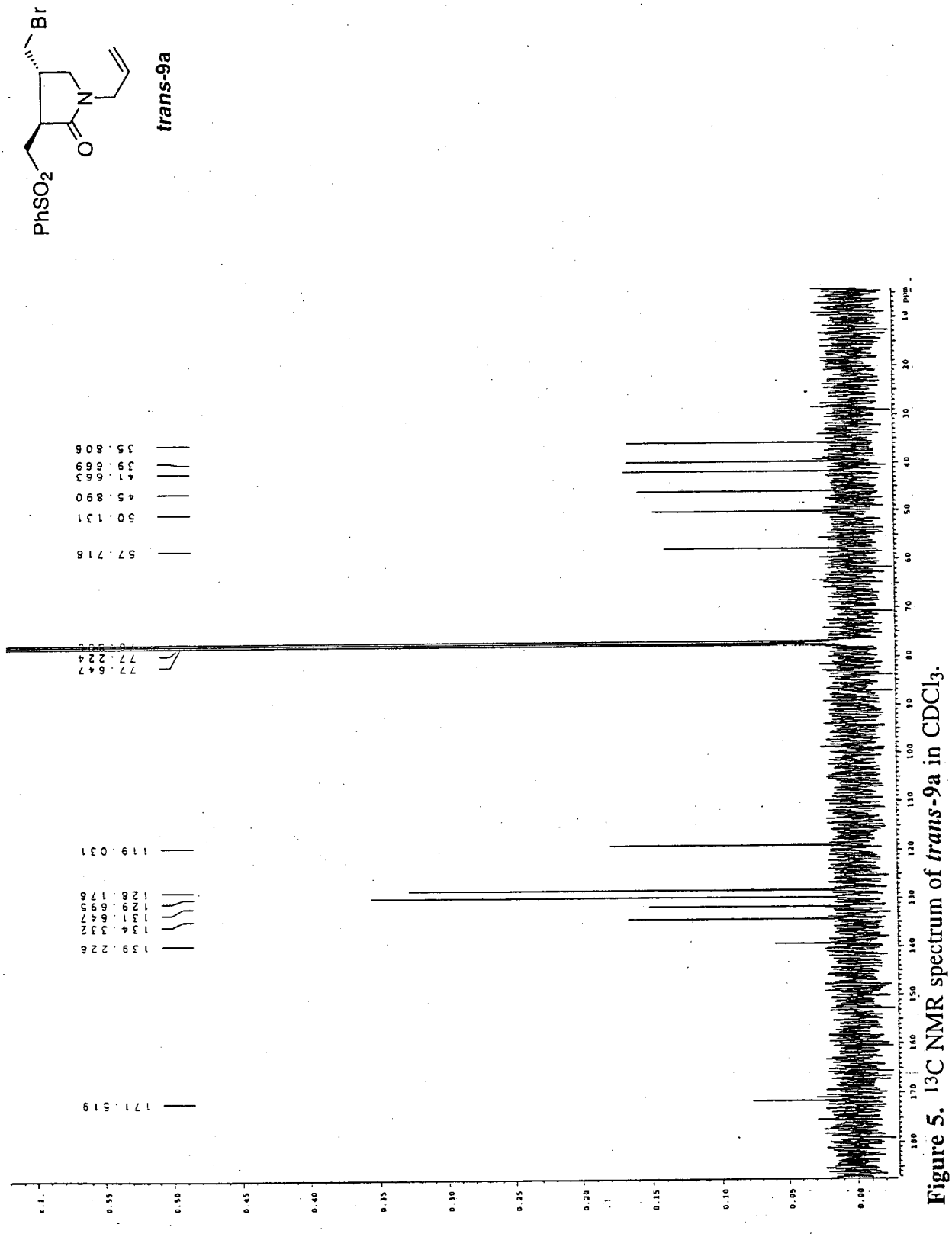

Figure 5. ^{13}C NMR spectrum of ***trans*-9a** in $CDCl_3$.

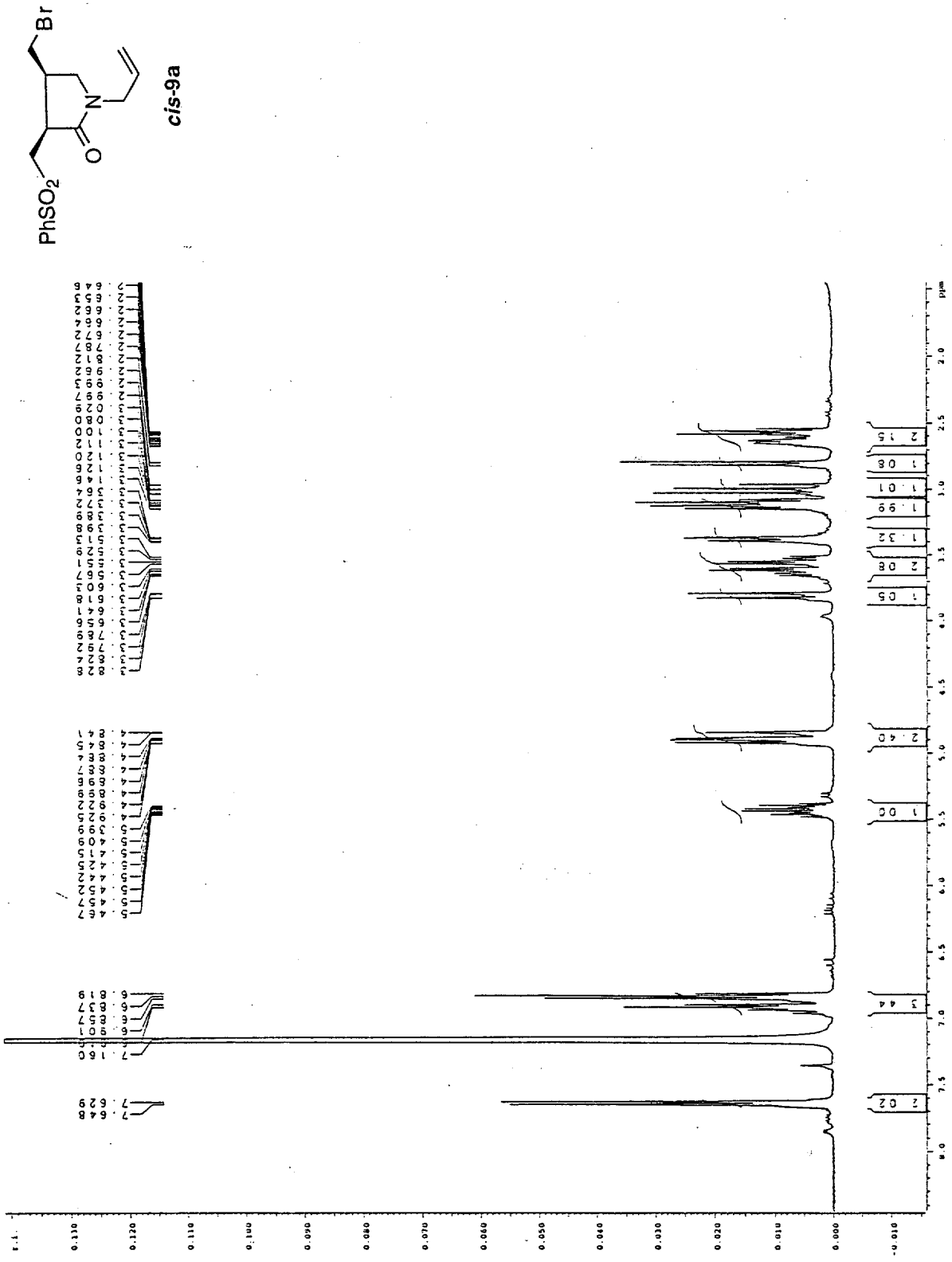

Figure 6. ^{1}H NMR spectrum of ***cis*-9a** in C_6D_6 (3 - 1).

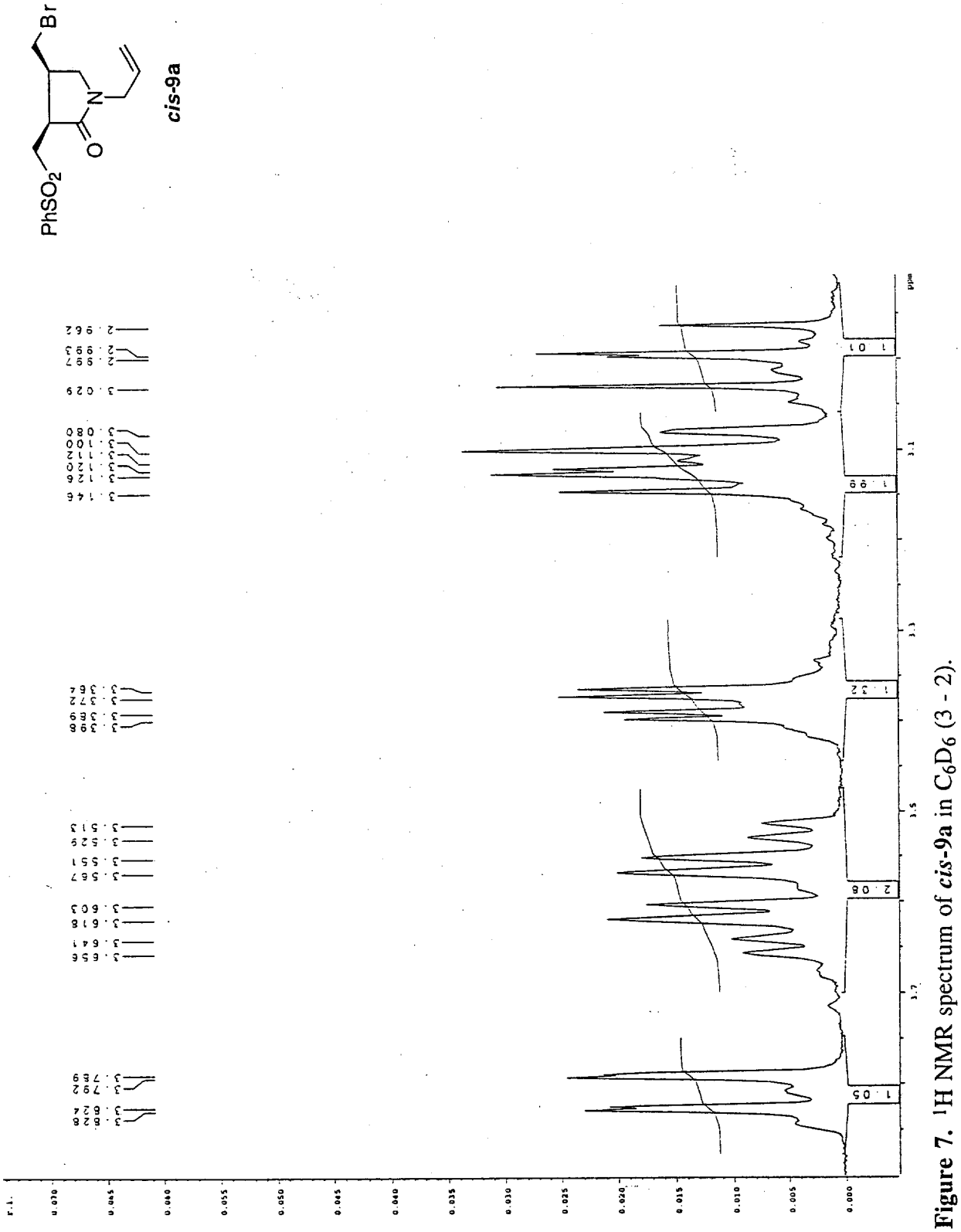

Figure 7. ^{1}H NMR spectrum of ***cis*-9a** in C_6D_6 (3 - 2).

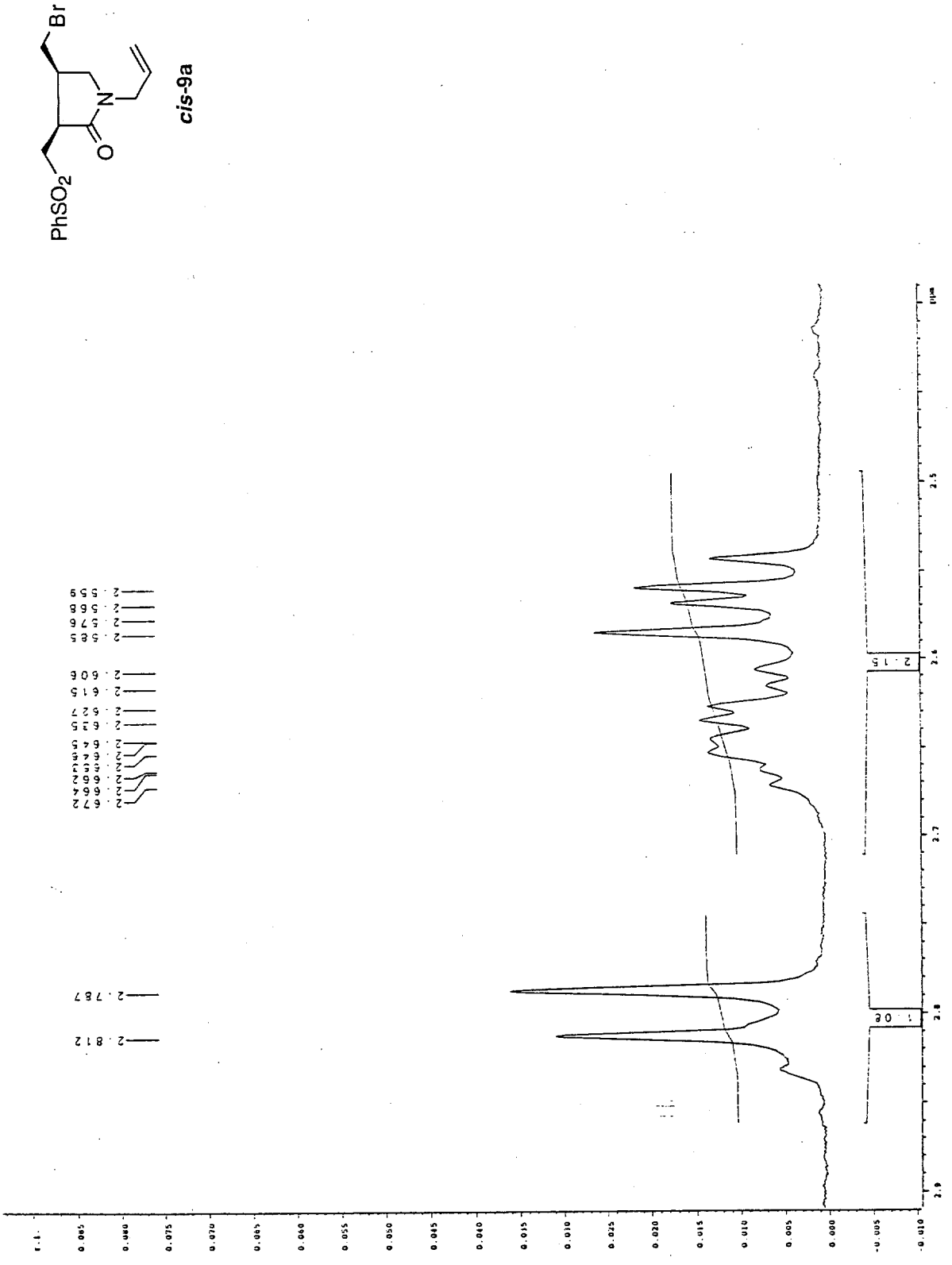

Figure 8. ^{1}H NMR spectrum of ***cis*-9a** in C_6D_6 (3 - 3).

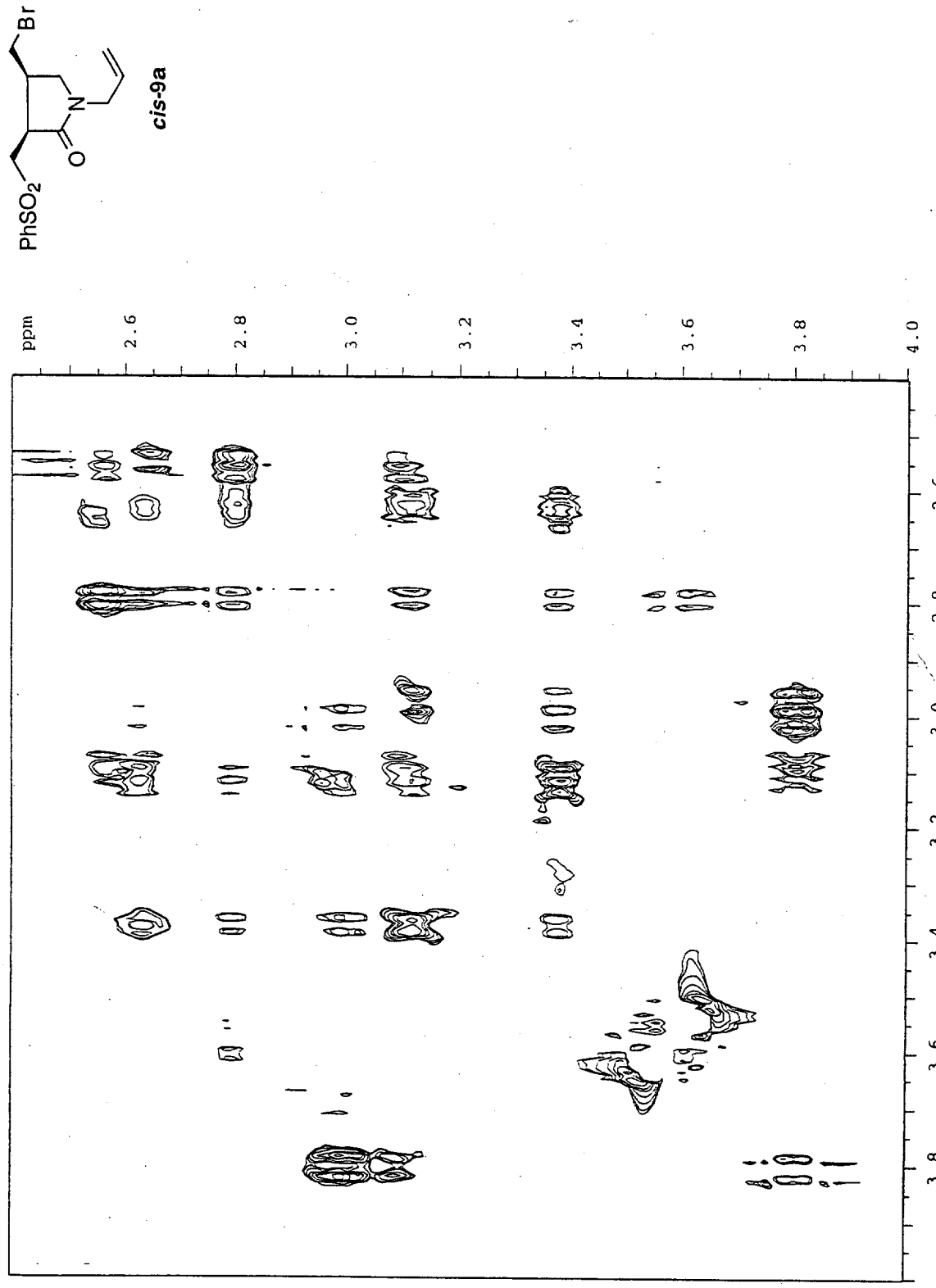

Figure 9. ^1H - ^1H NOESY spectrum of ***cis*-9a** in C_6D_6.

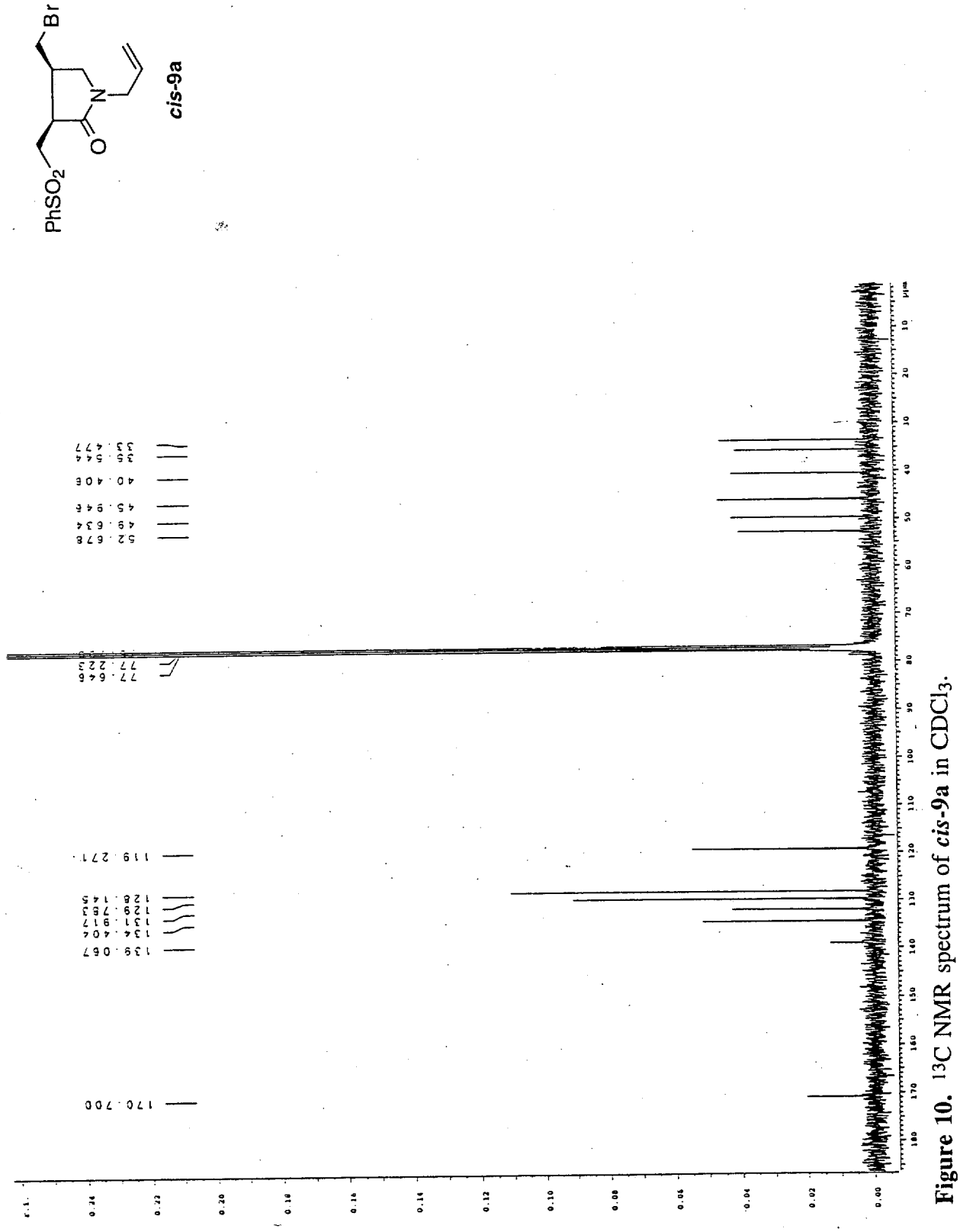

Figure 10. ^{13}C NMR spectrum of ***cis*-9a** in $CDCl_3$.

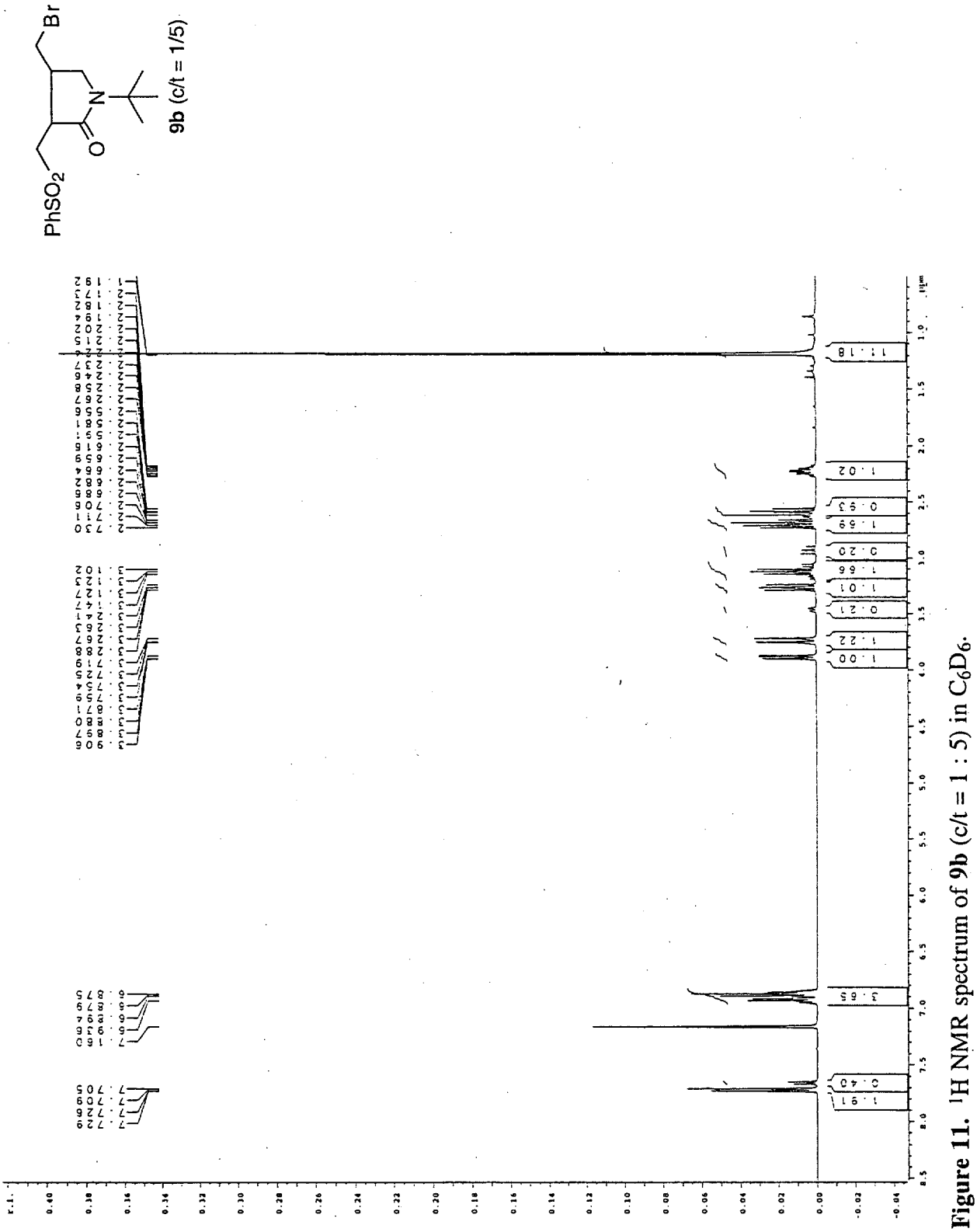

Figure 11. ^{1}H NMR spectrum of **9b** (*c*/*t* = 1 : 5) in C_6D_6.

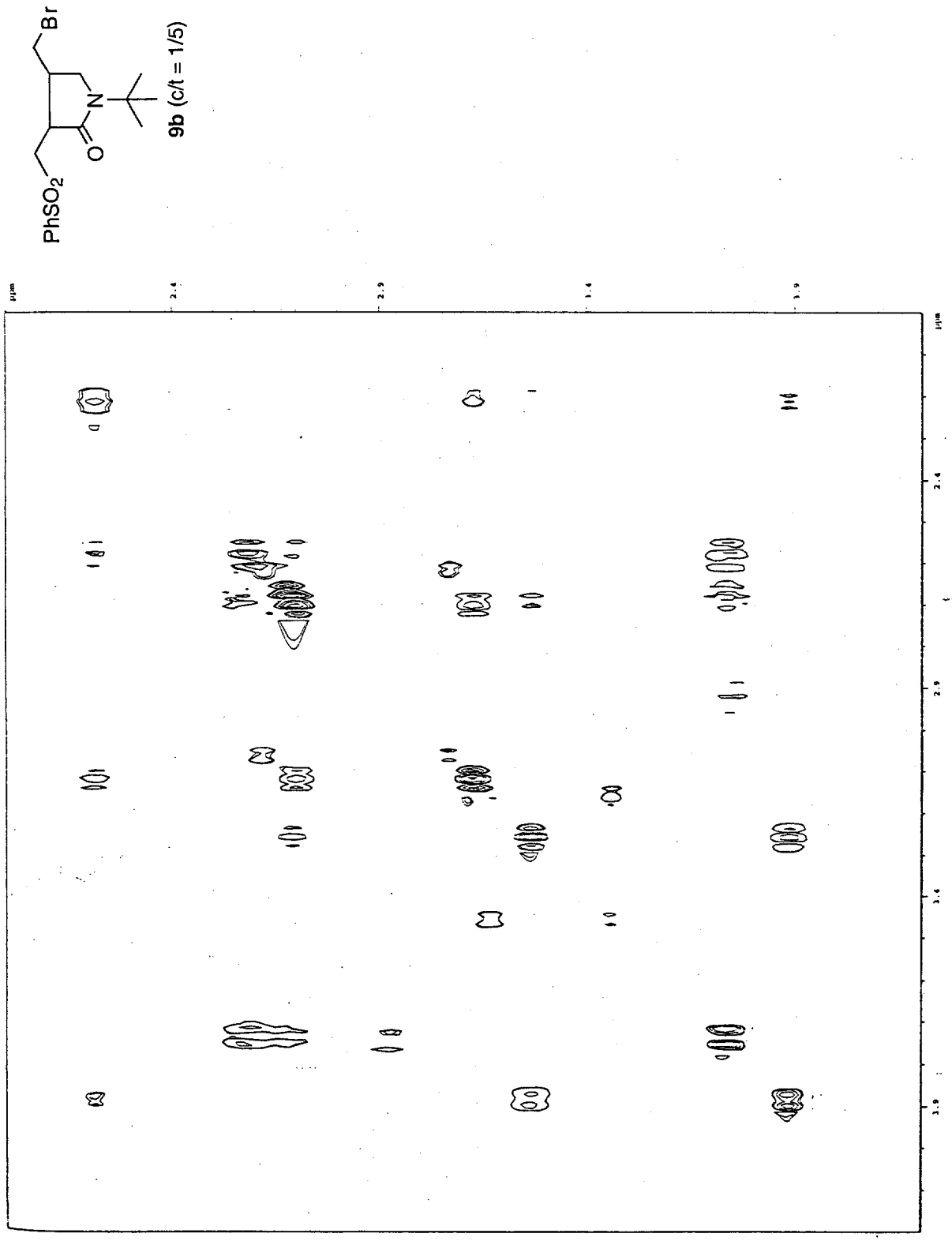

Figure 12. ^1H - ^1H NOESY spectrum of **9b** (c/t = 1 : 5) in C_6D_6.

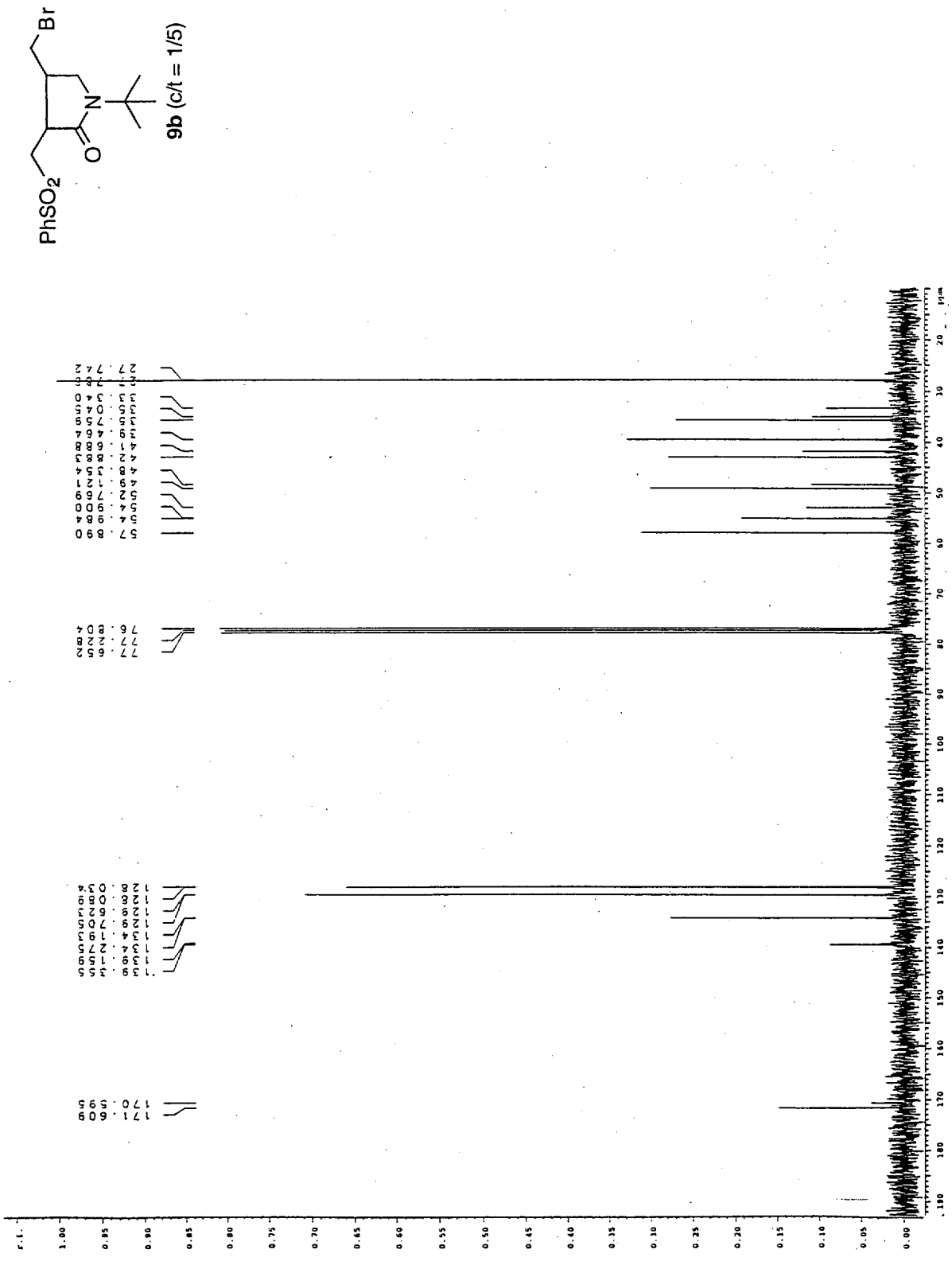

Figure 13. ^{13}C NMR spectrum of **9b** (c/t = 1 : 5) in $CDCl_3$.

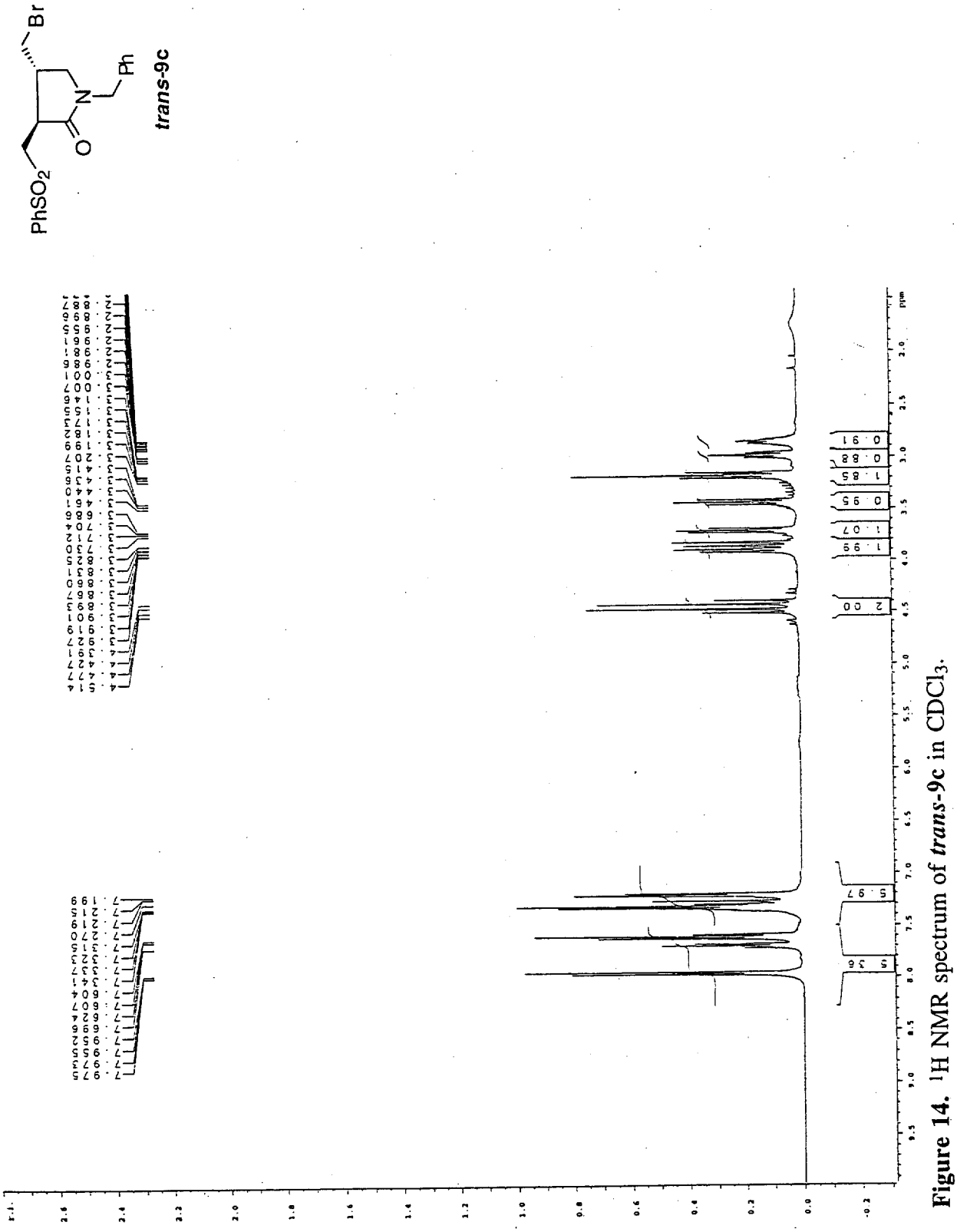

Figure 14. ^{1}H NMR spectrum of ***trans*-9c** in $CDCl_3$.

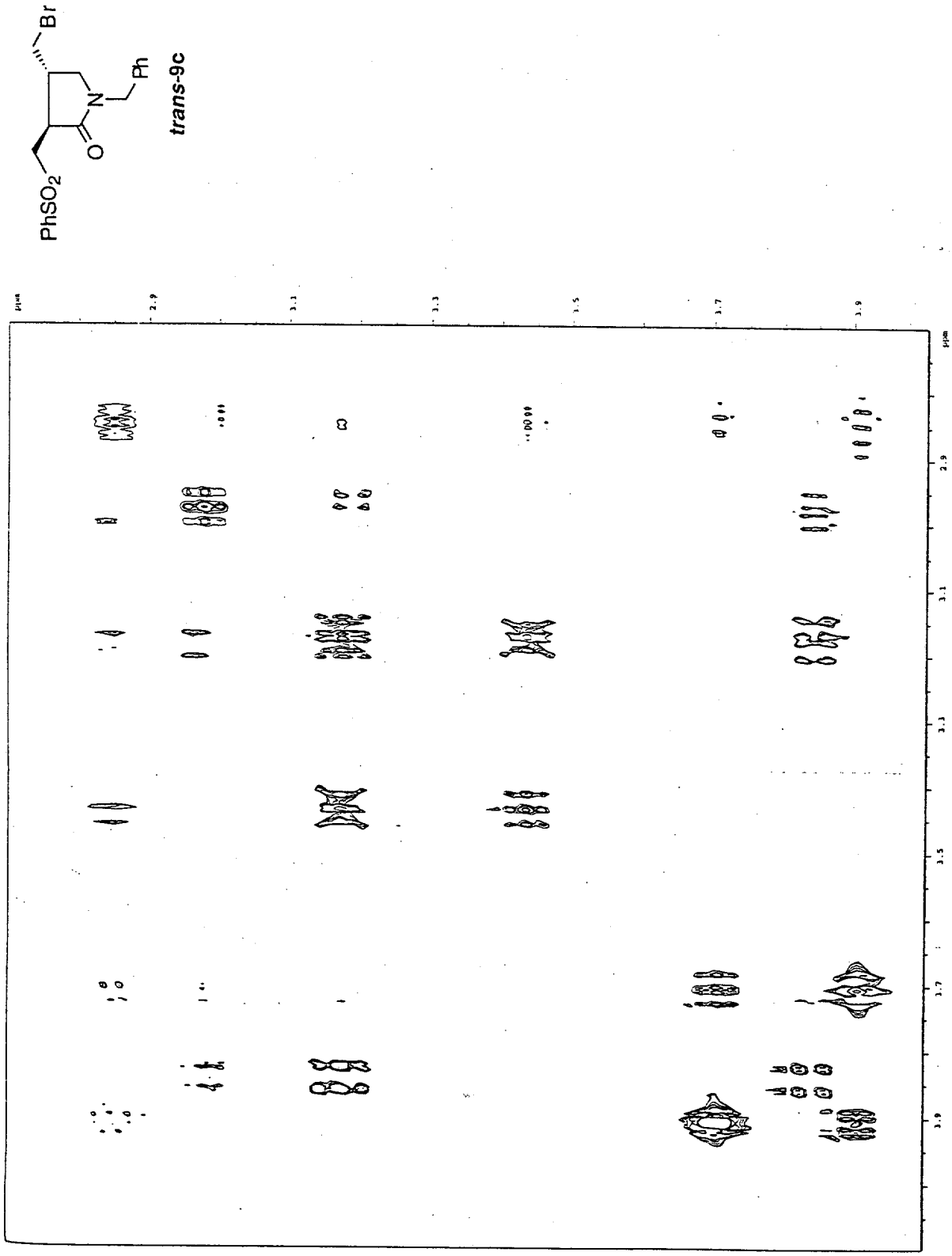

Figure 15. ^{1}H - ^{1}H NOESY spectrum of ***trans*-9c** in $CDCl_3$.

Figure 16. ^{13}C NMR spectrum of ***trans*-9c** in $CDCl_3$.

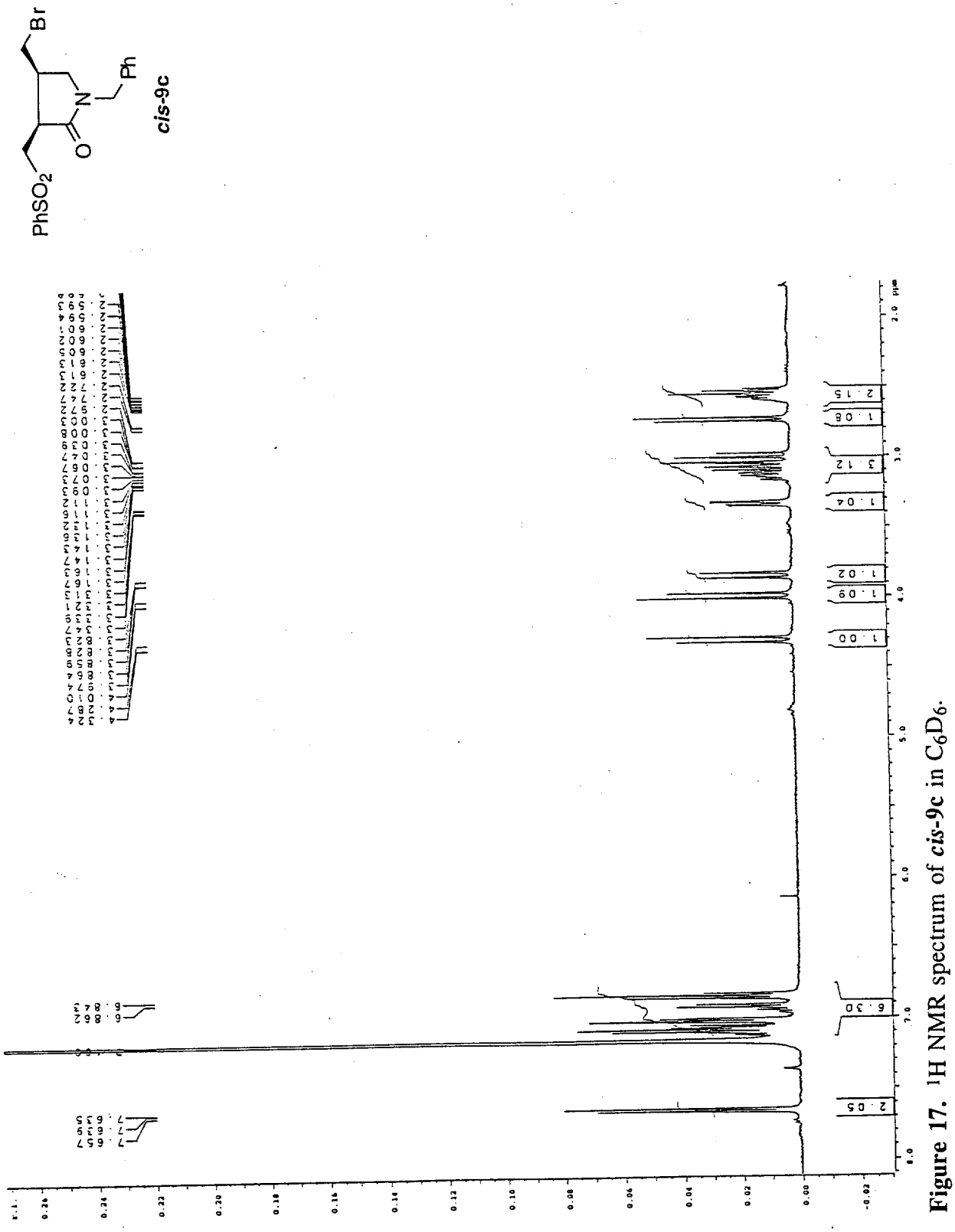

Figure 17. ^{1}H NMR spectrum of ***cis*-9c** in C_6D_6.

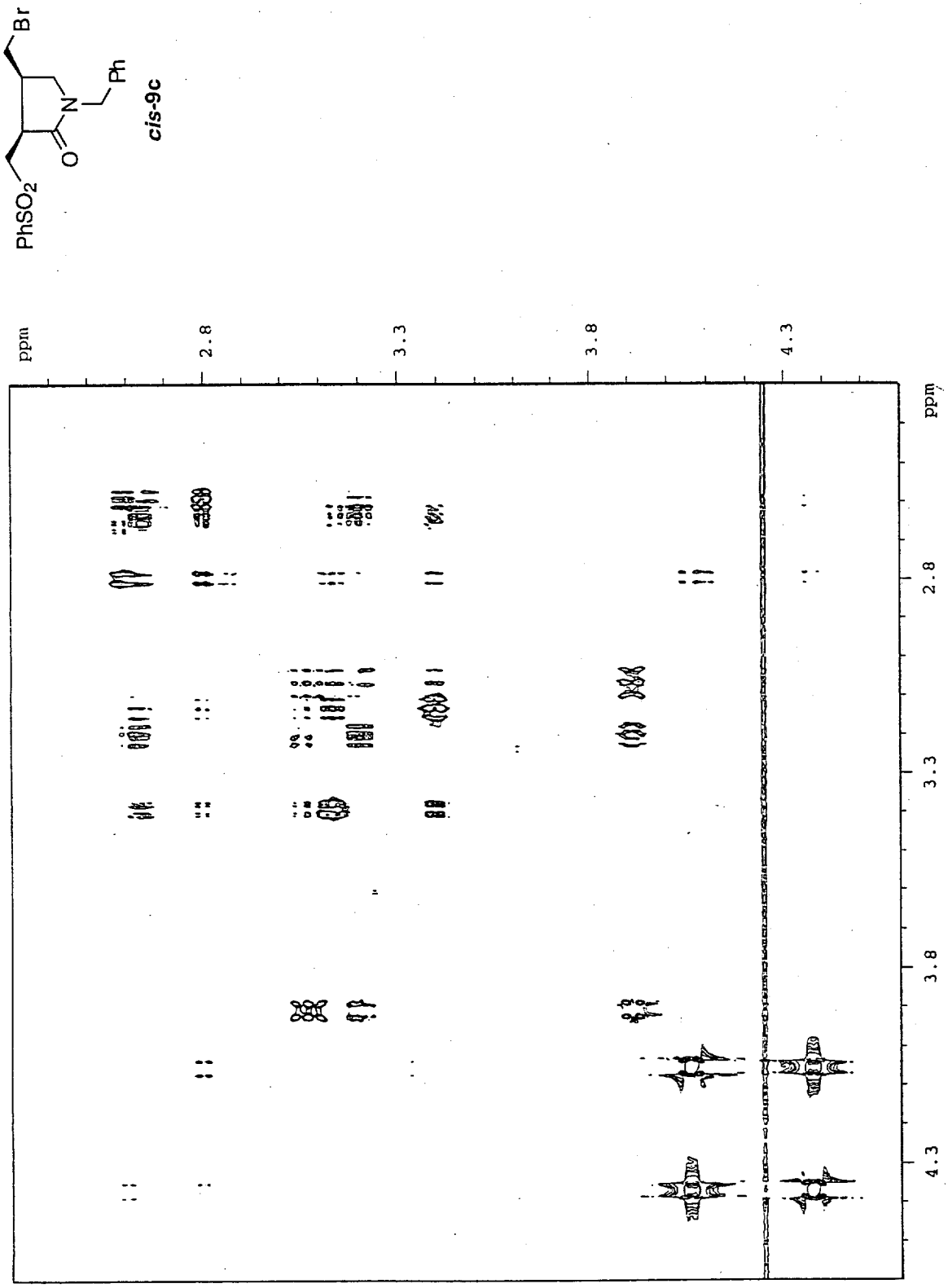

Figure 18. ^{1}H - ^{1}H NOESY spectrum of ***cis*-9c** in C_6D_6.

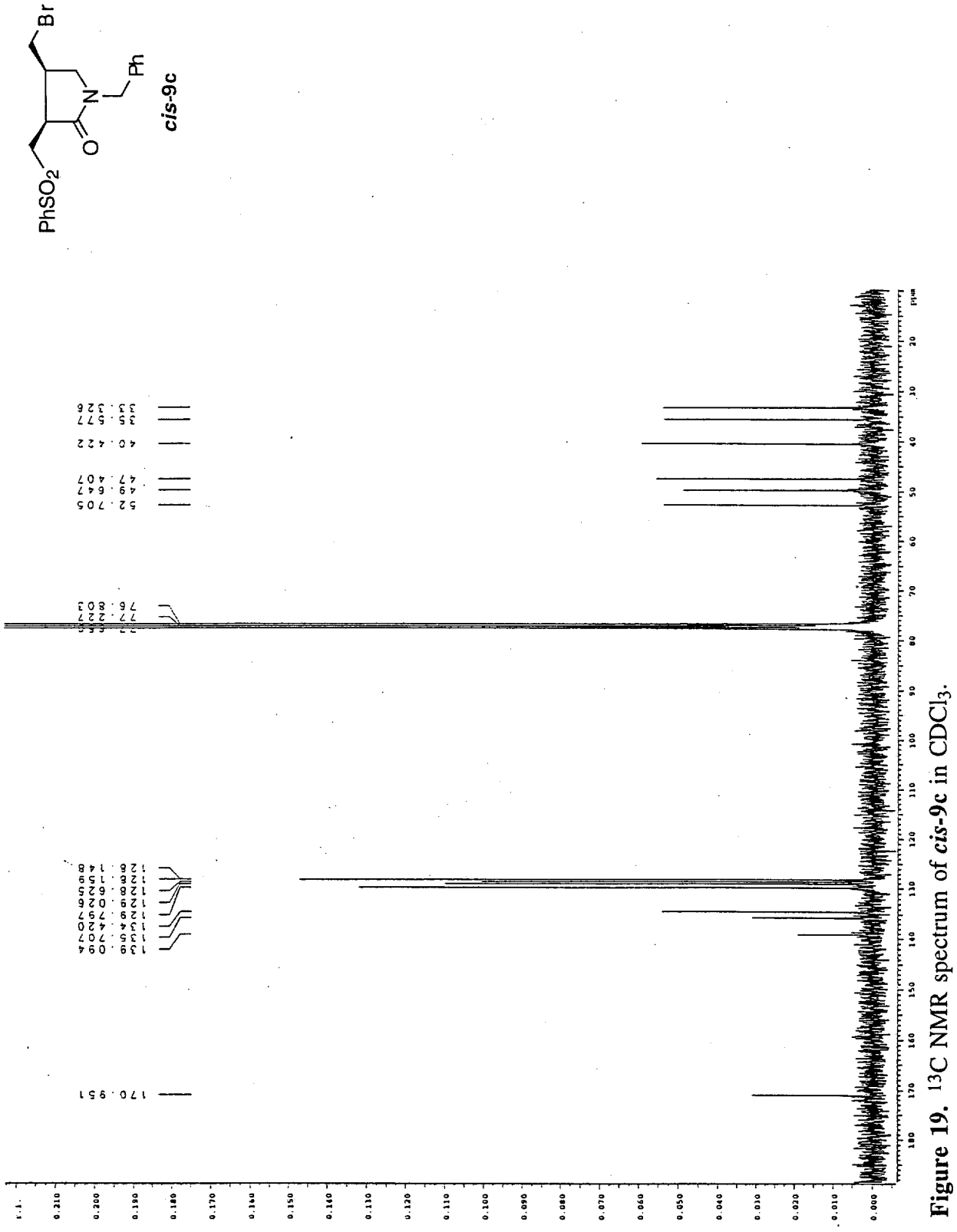

Figure 19. ^{13}C NMR spectrum of ***cis*-9c** in $CDCl_3$.

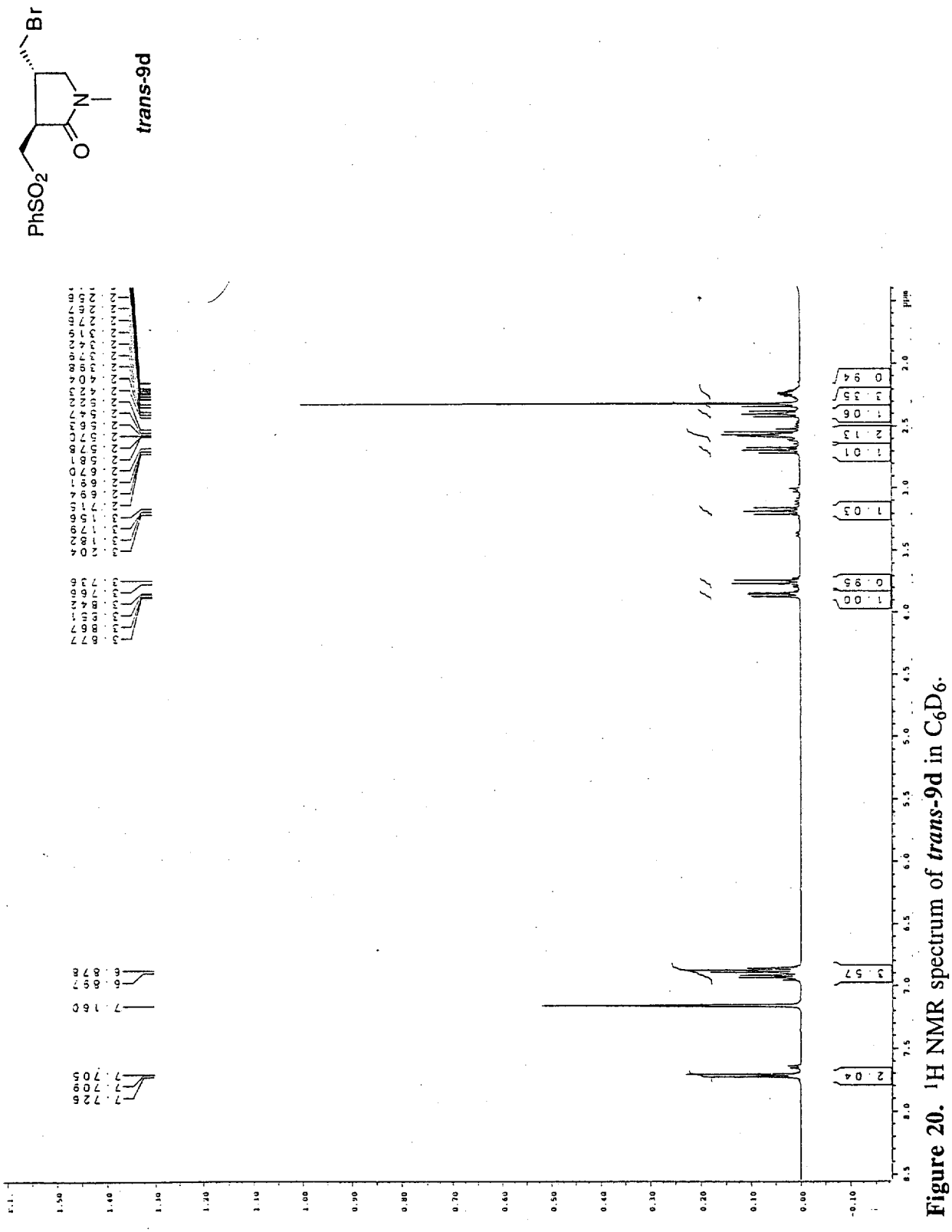

Figure 20. ^{1}H NMR spectrum of ***trans*-9d** in C_6D_6.

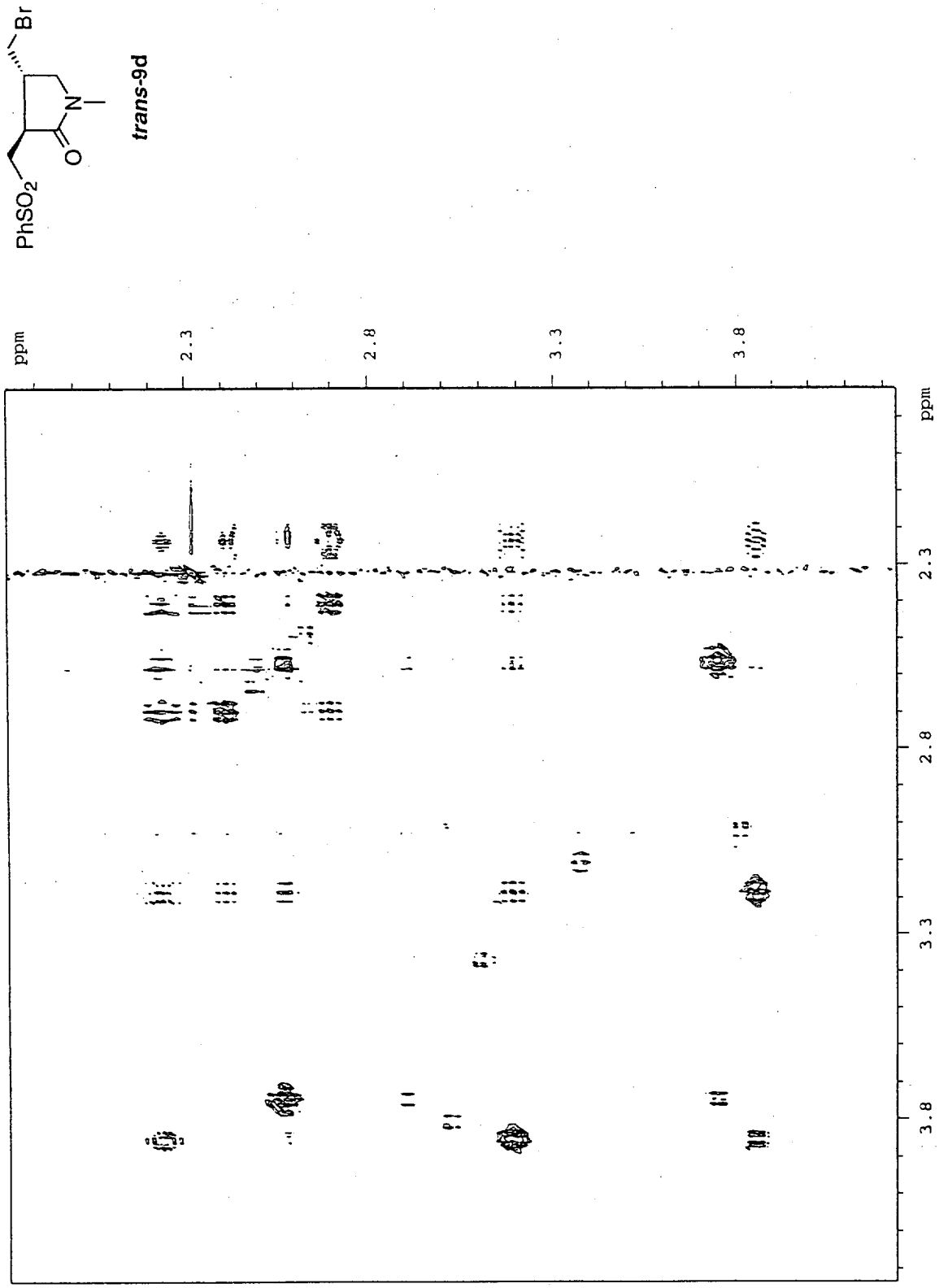

Figure 21. ^1H - ^1H NOESY spectrum of ***trans*-9d** in C_6D_6.

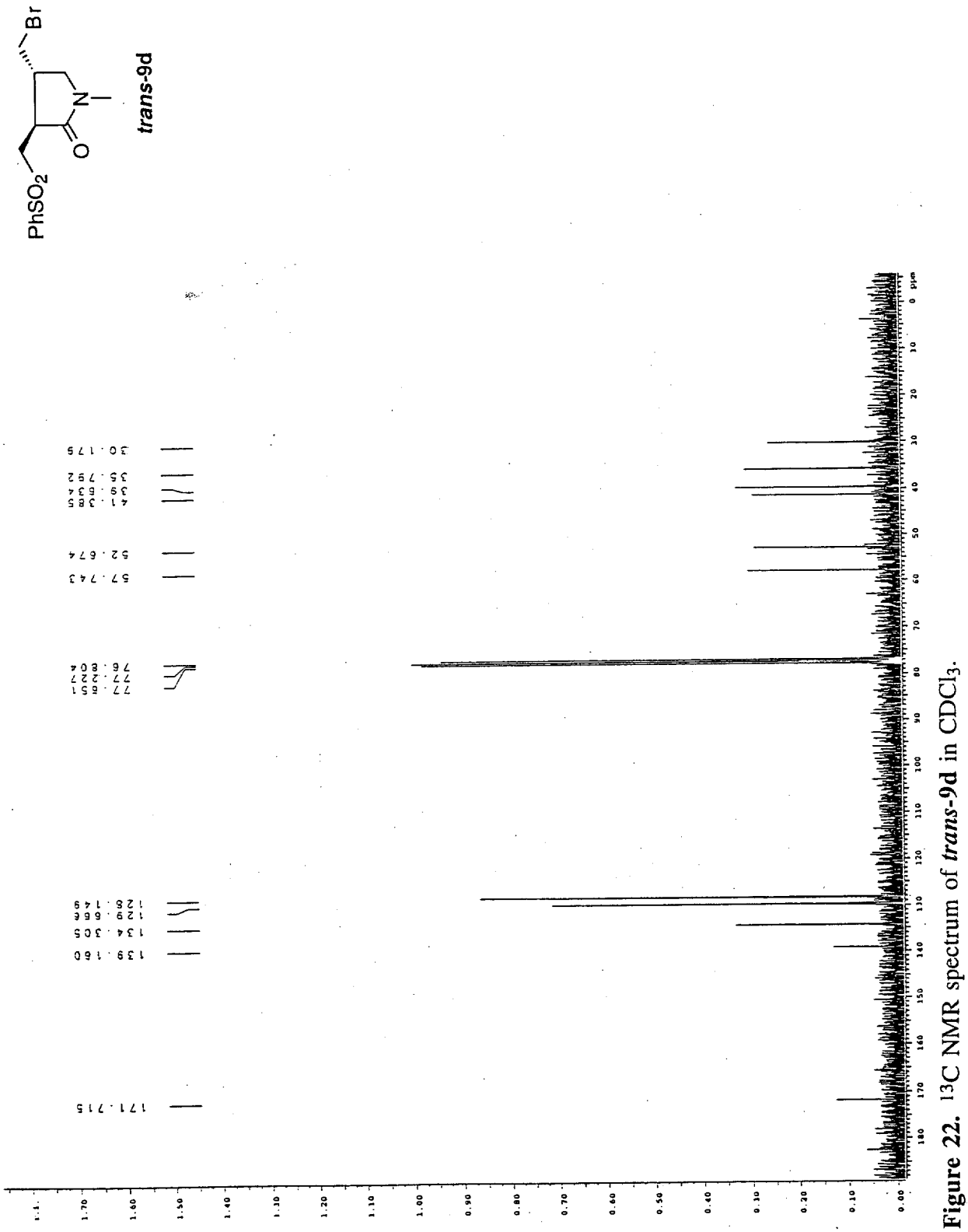

Figure 22. ^{13}C NMR spectrum of ***trans*-9d** in $CDCl_3$.

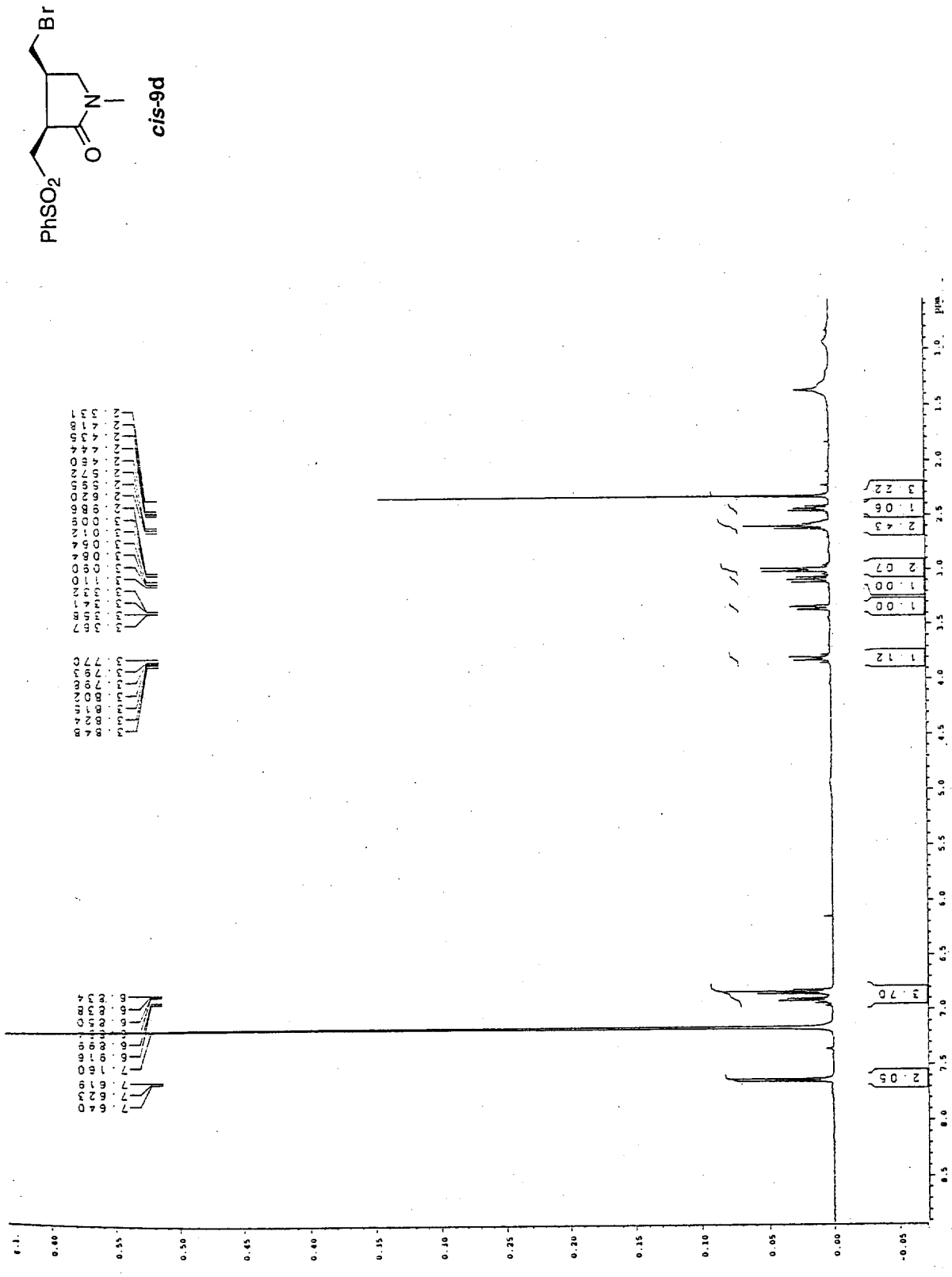

Figure 23. ^{1}H NMR spectrum of ***cis*-9d** in C_6D_6.

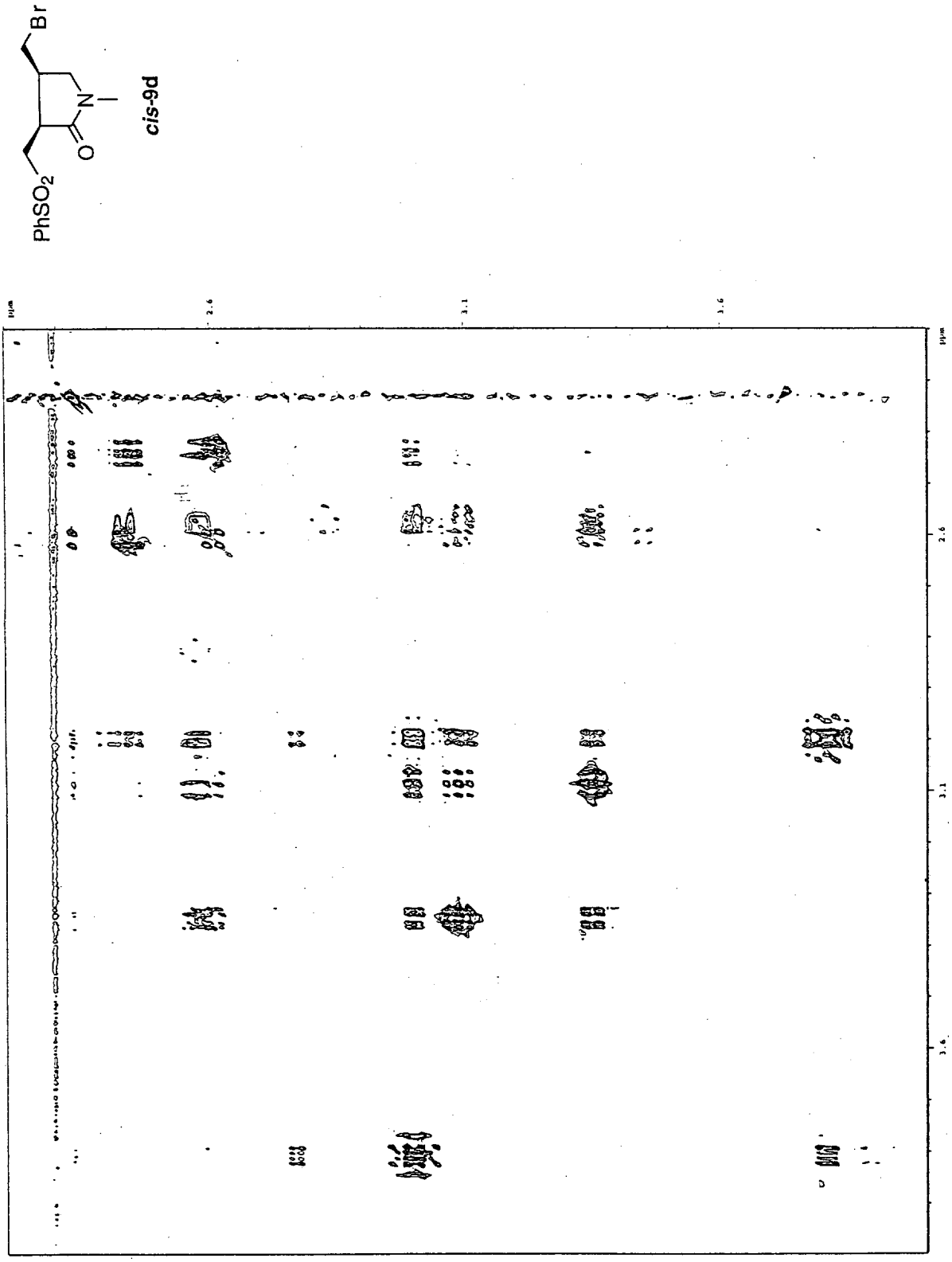

Figure 24. ^1H - ^1H NOESY spectrum of ***cis*-9d** in C_6D_6.

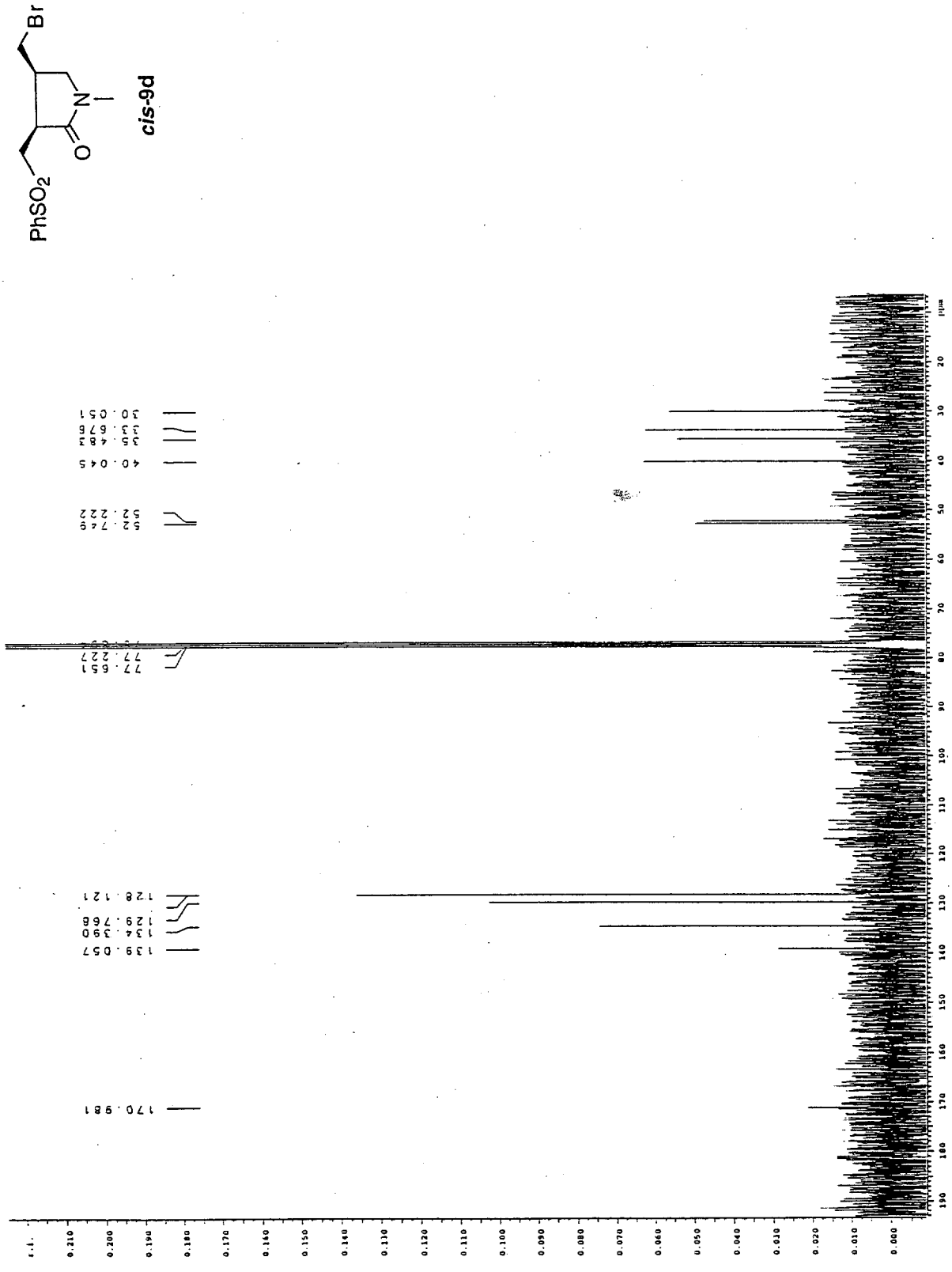

Figure 25. ^{13}C NMR spectrum of ***cis*-9d** in $CDCl_3$.

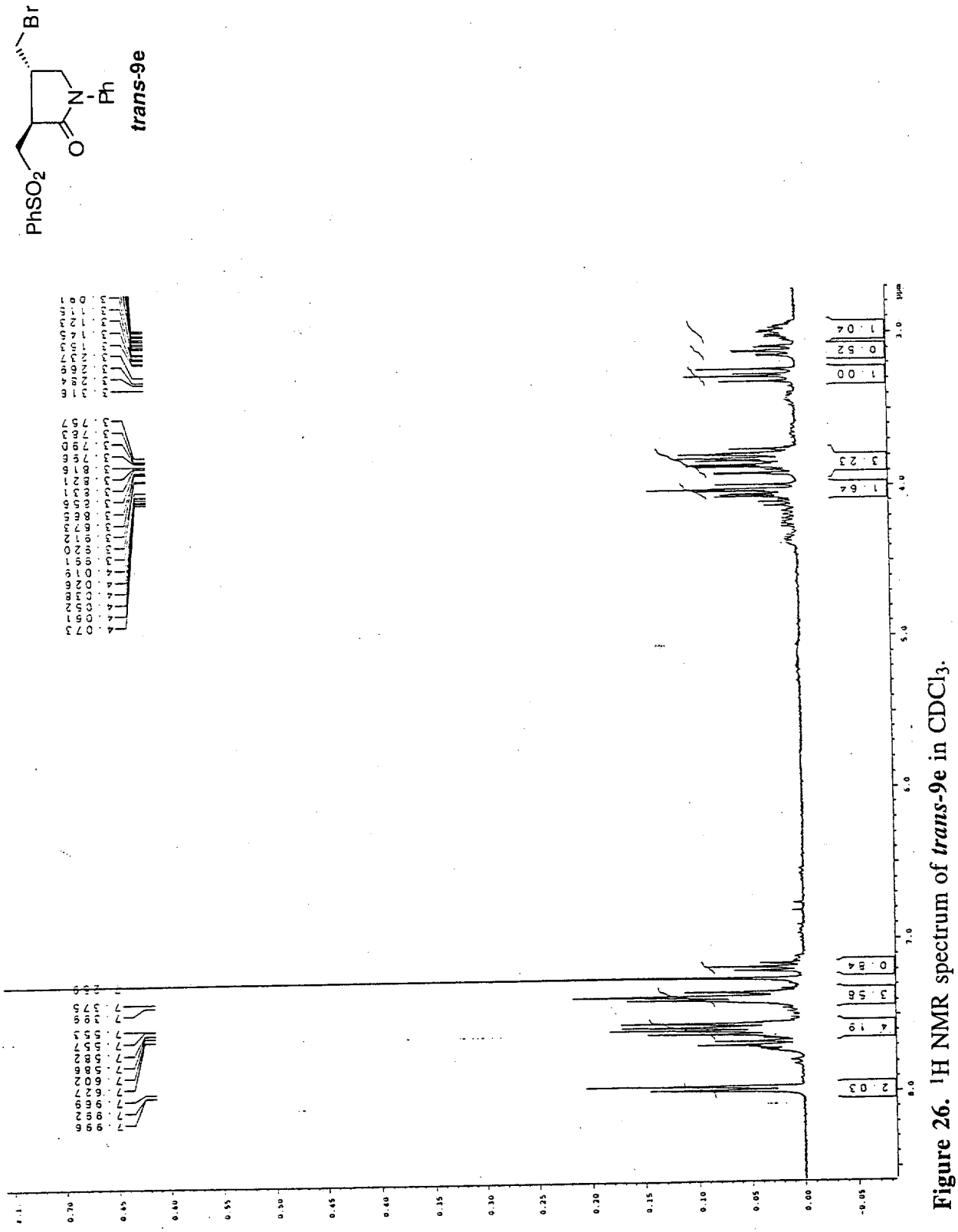

Figure 26. ^{1}H NMR spectrum of ***trans*-9e** in $CDCl_3$.

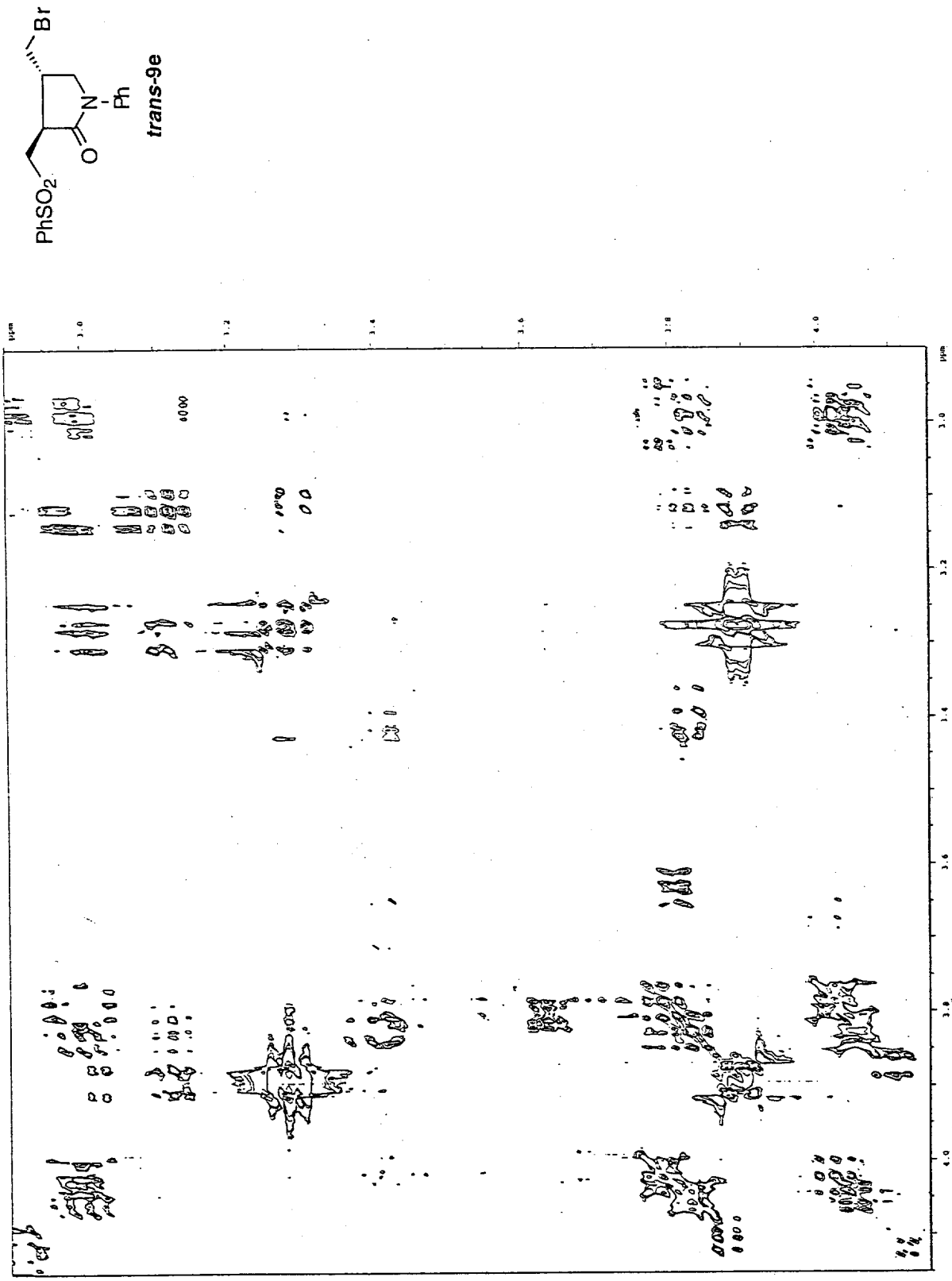

Figure 27. ^1H - ^1H NOESY spectrum of ***trans*-9e** in $CDCl_3$.

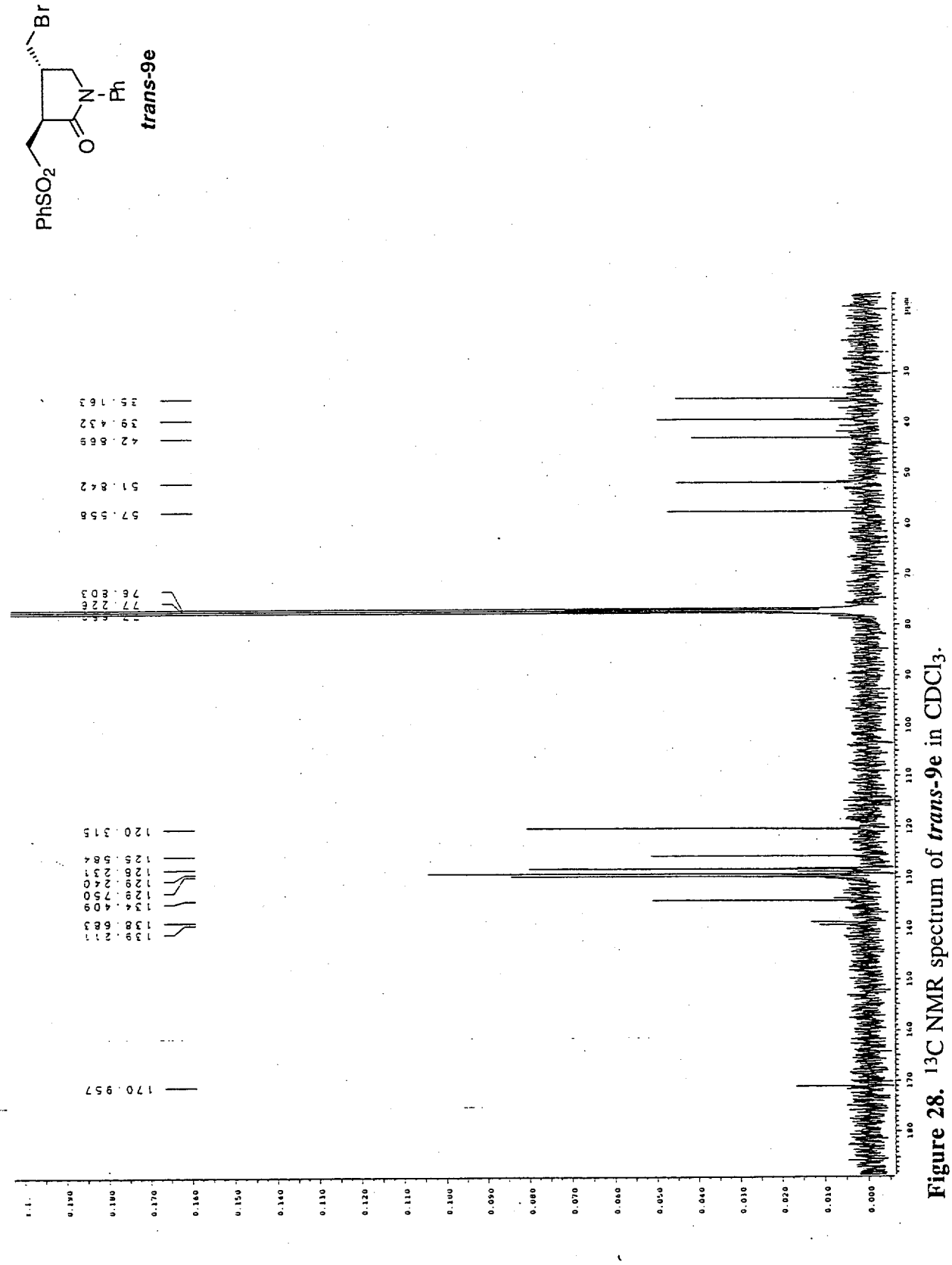

Figure 28. ^{13}C NMR spectrum of ***trans*-9e** in $CDCl_3$.

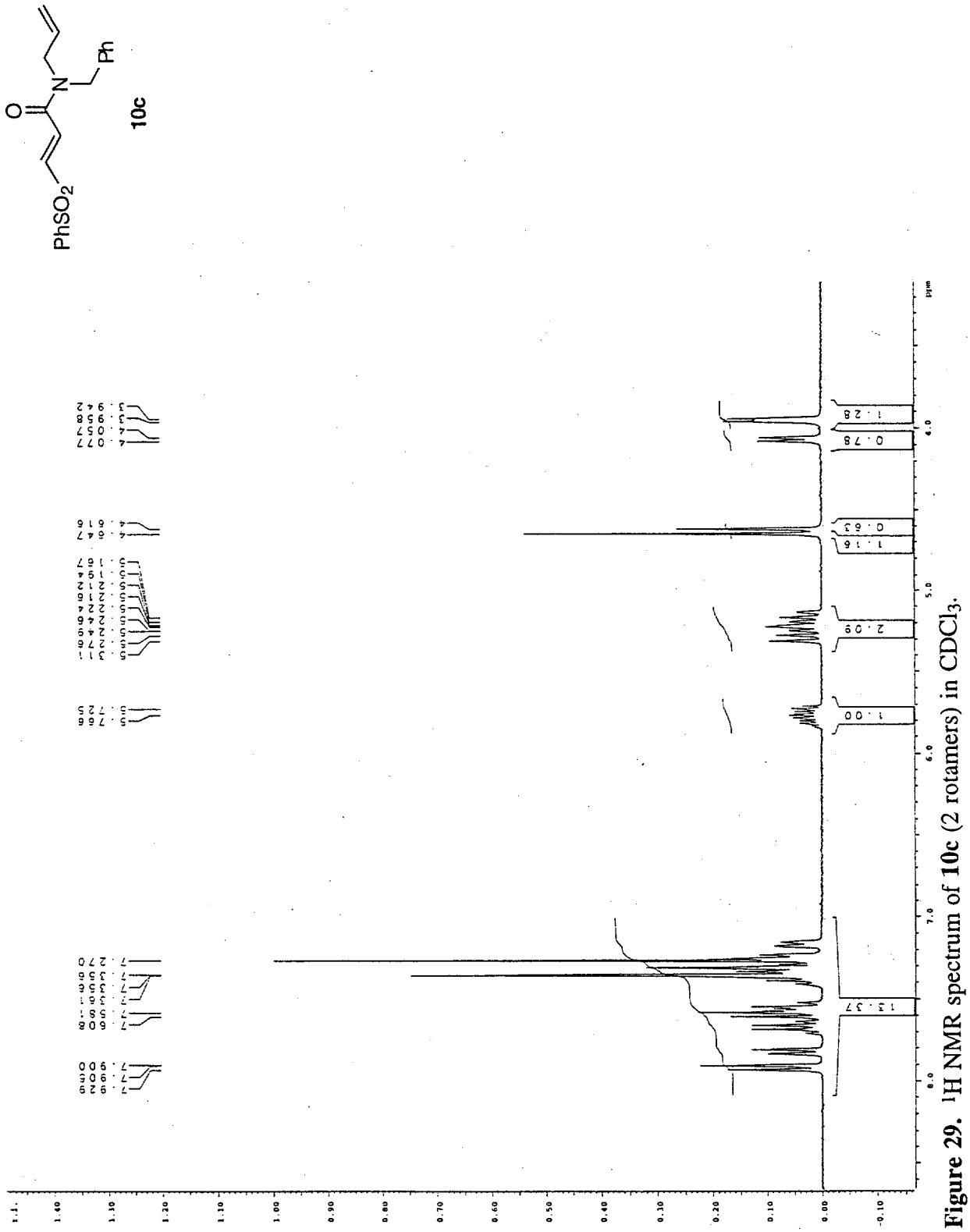

Figure 29. ^{1}H NMR spectrum of **10c** (2 rotamers) in $CDCl_3$.

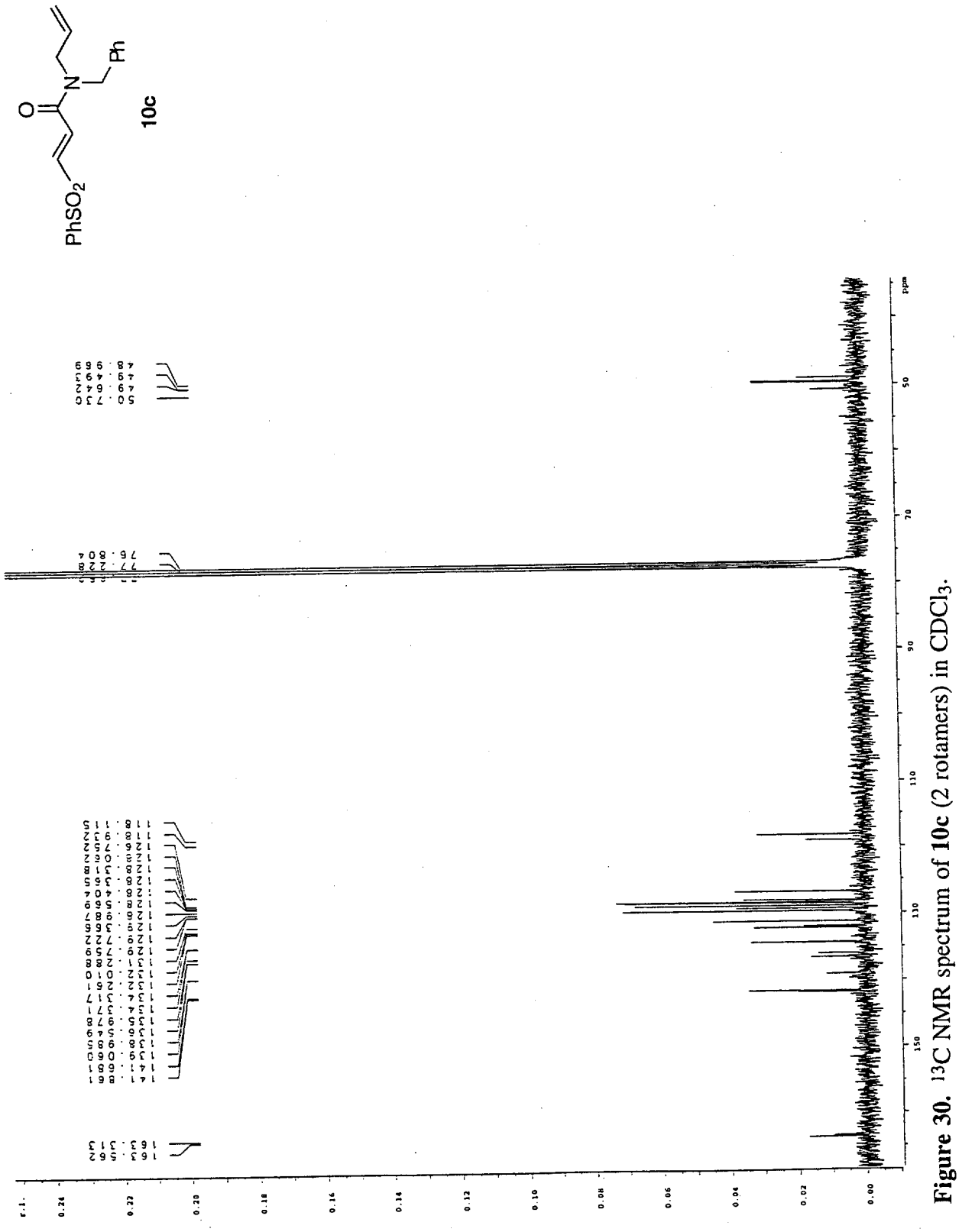

Figure 30. ^{13}C NMR spectrum of **10c** (2 rotamers) in $CDCl_3$.

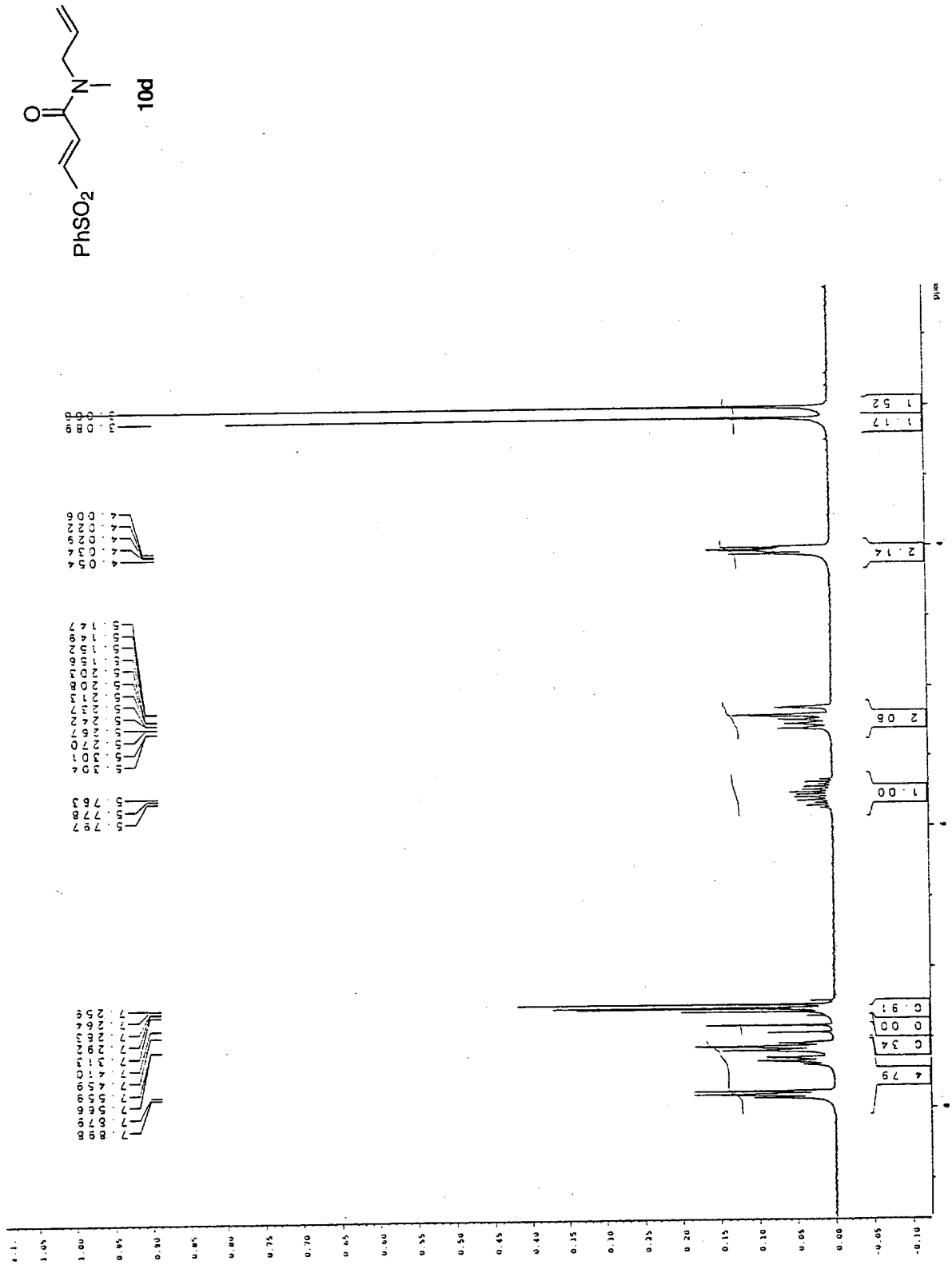

Figure 31. ^{1}H NMR spectrum of **10d** (2 rotamers) in $CDCl_3$.

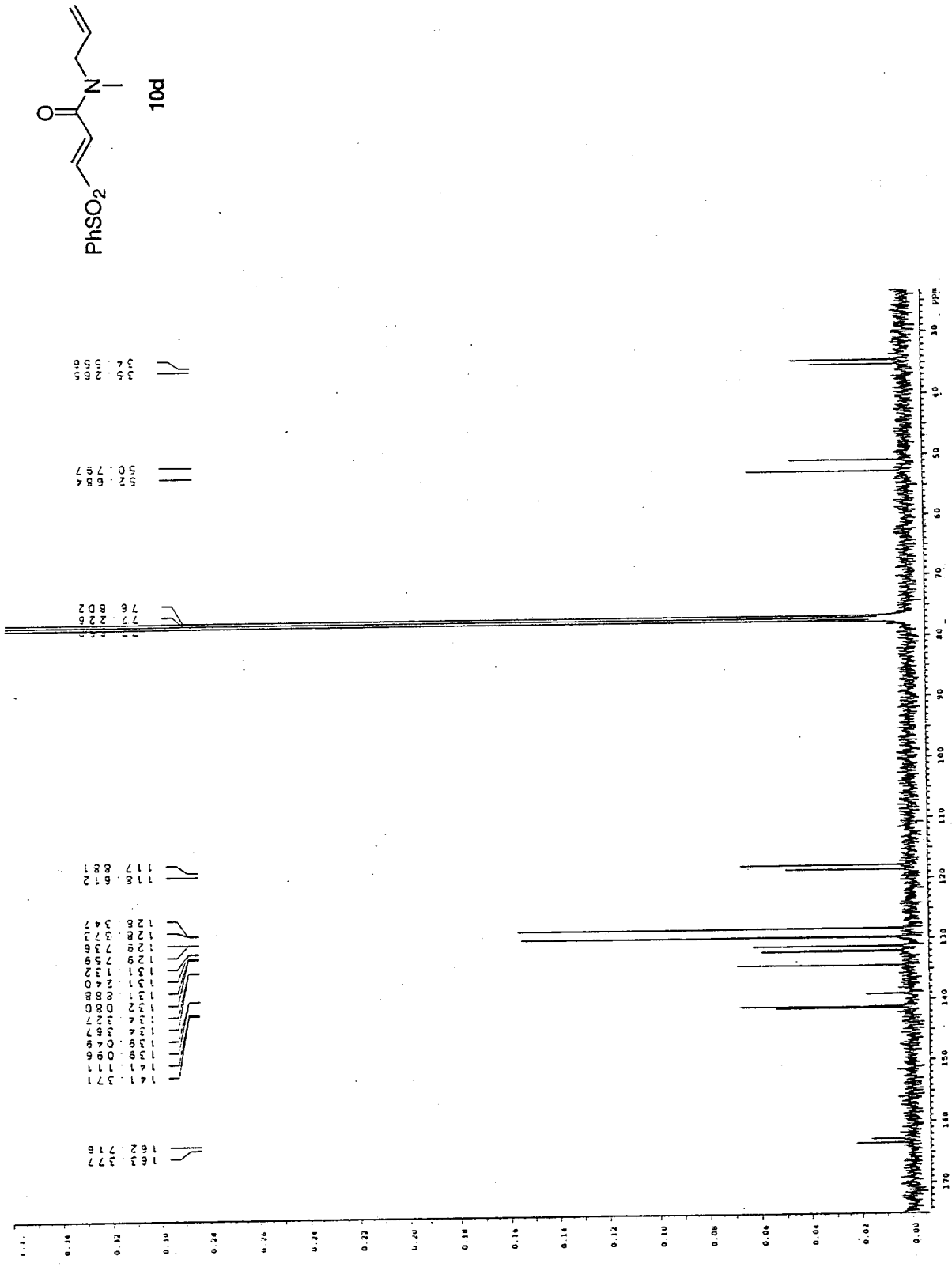

Figure 32. ^{13}C NMR spectrum of **10d** (2 rotamers) in $CDCl_3$.

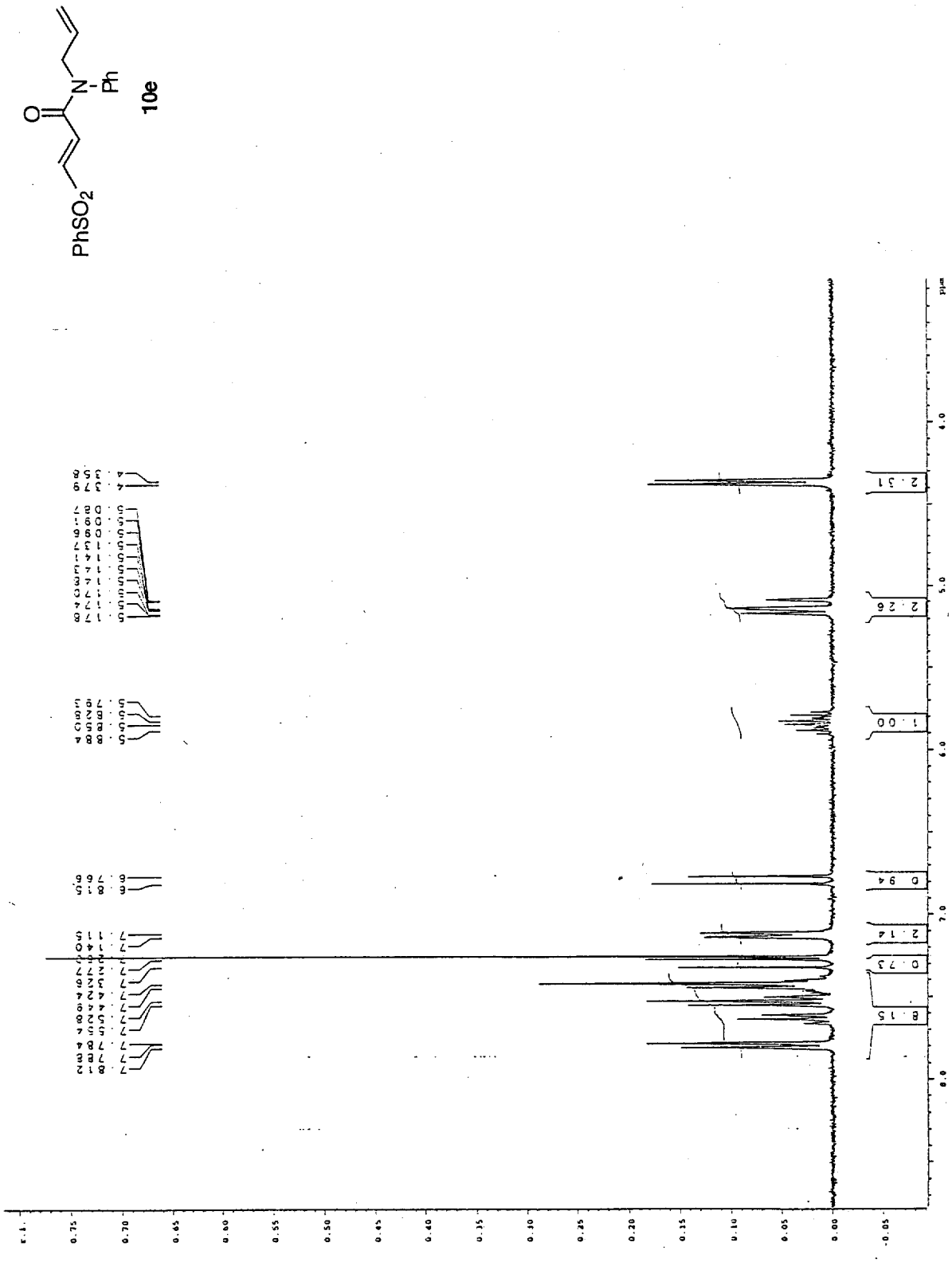

Figure 33. ^{1}H NMR spectrum of **10e** in $CDCl_3$.

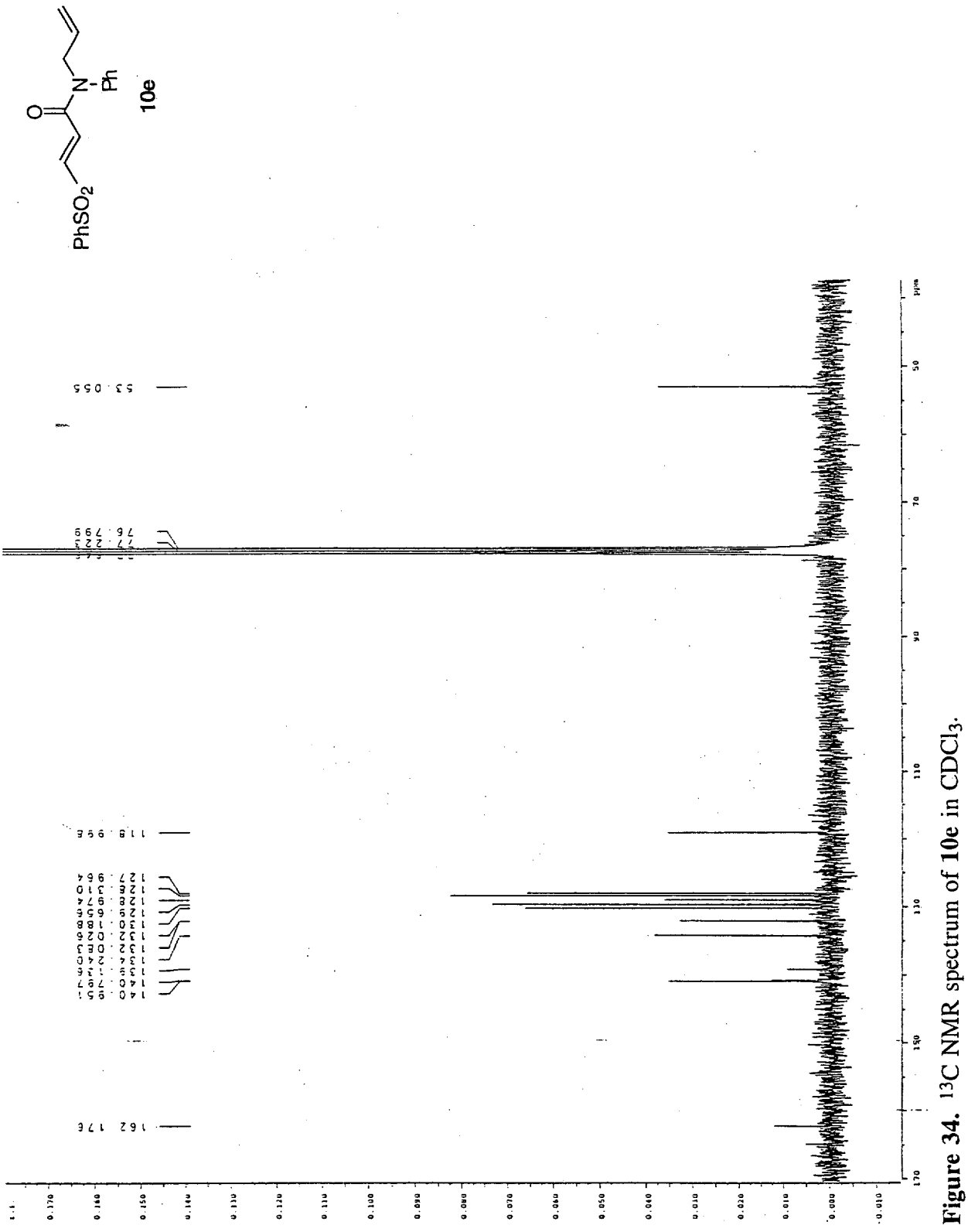

Figure 34. ^{13}C NMR spectrum of **10e** in $CDCl_3$.

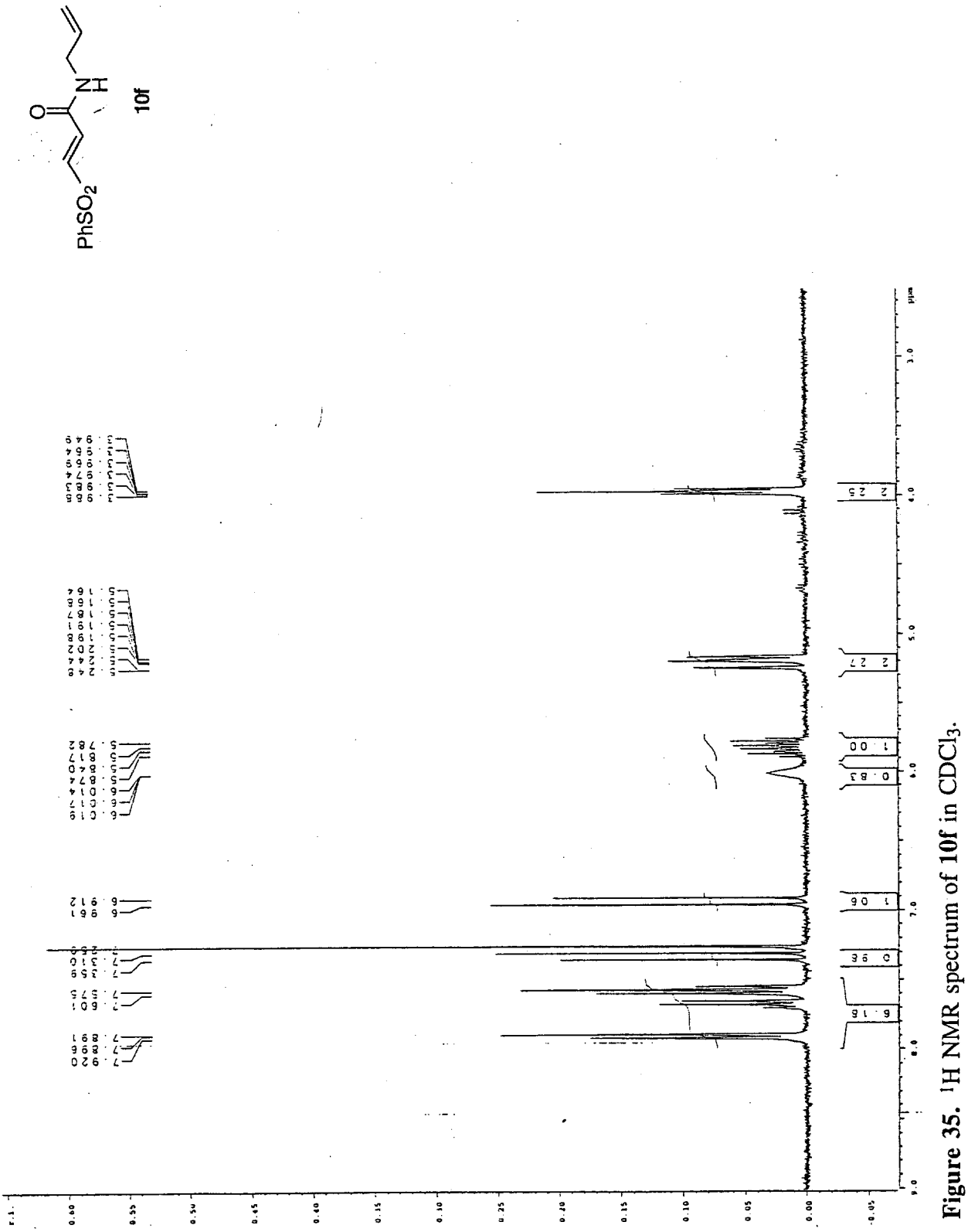

Figure 35. ^{1}H NMR spectrum of **10f** in $CDCl_3$.

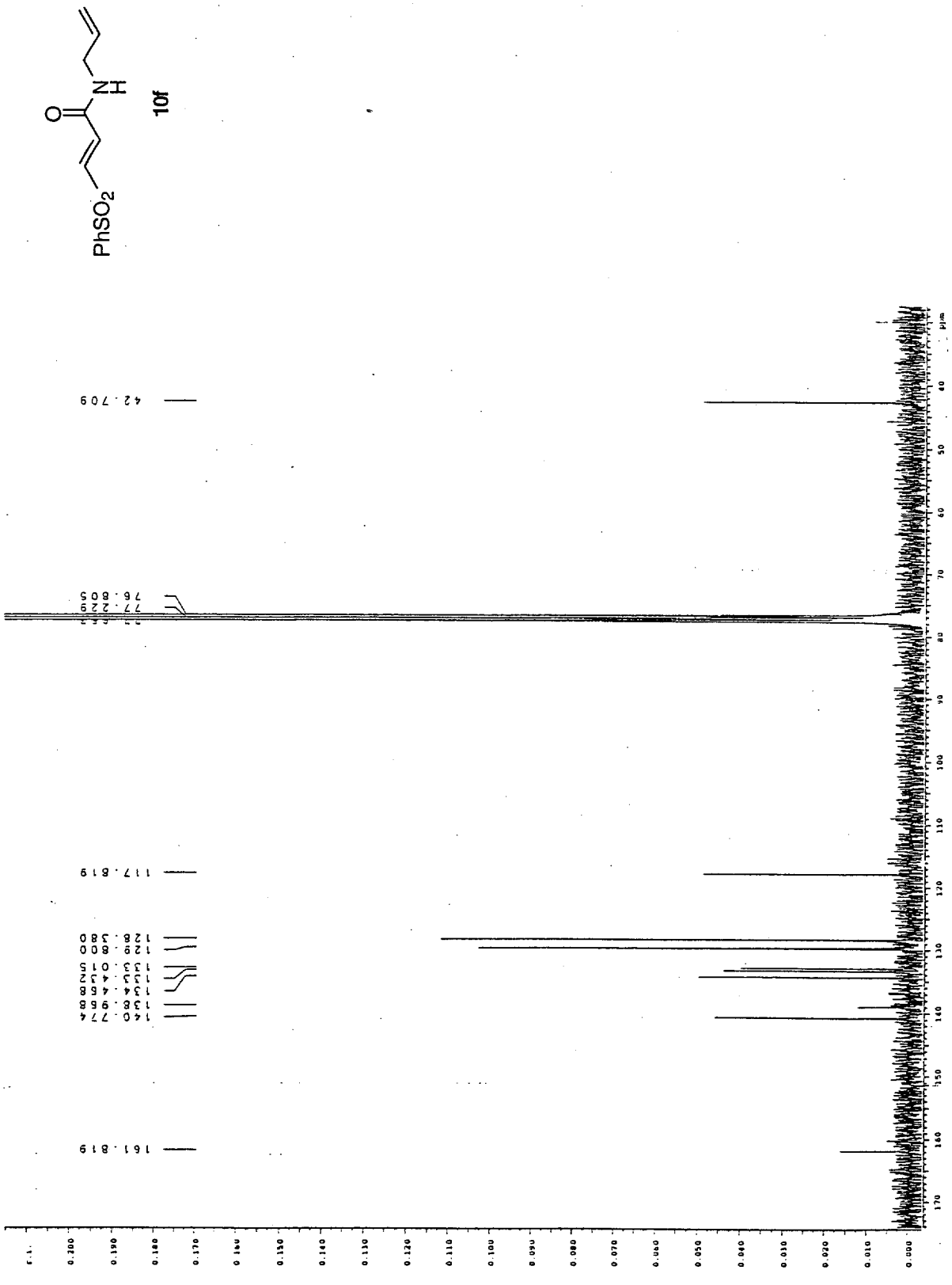

Figure 36. ^{13}C NMR spectrum of **10f** in $CDCl_3$.

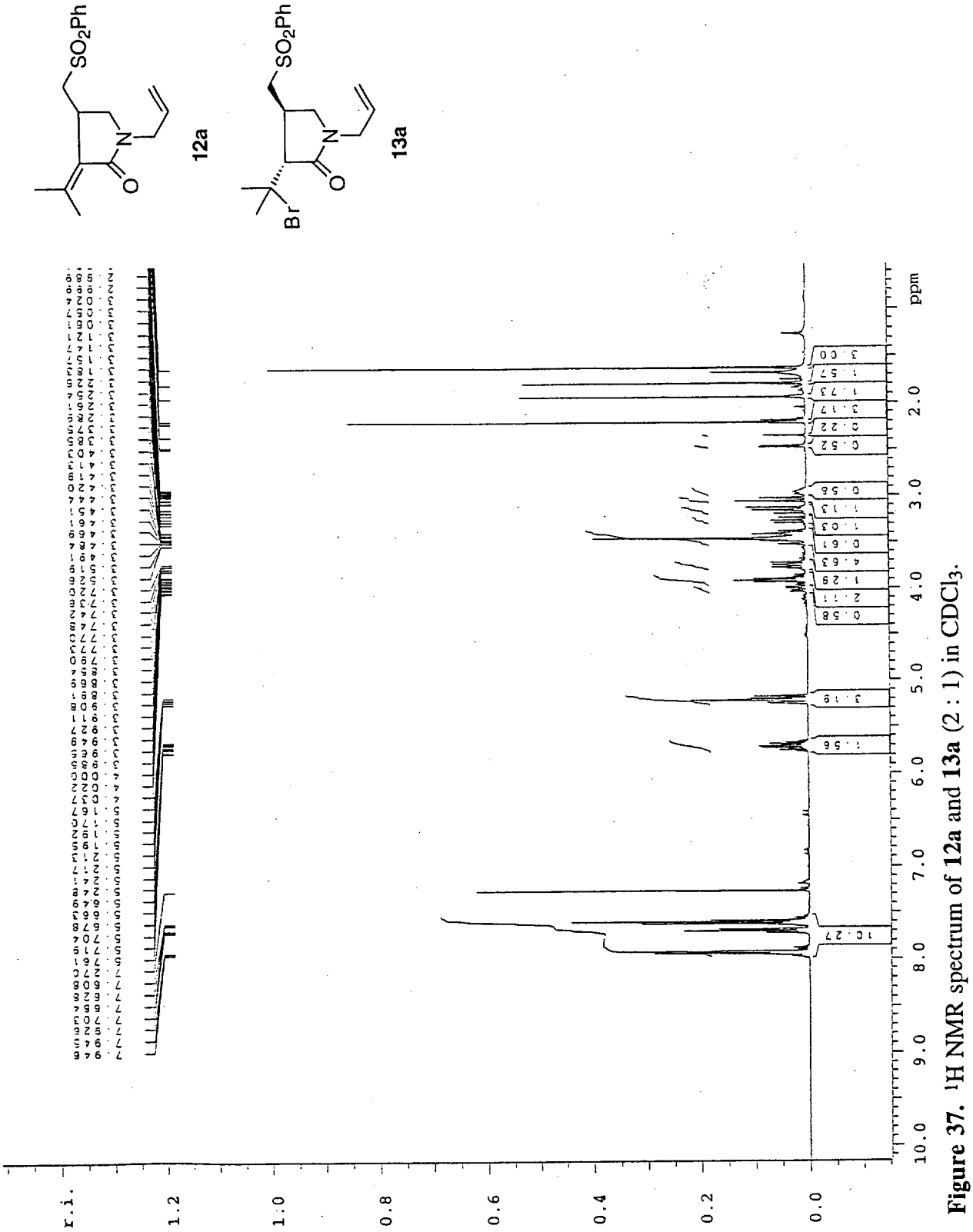

Figure 37. ^{1}H NMR spectrum of **12a** and **13a** (2 : 1) in $CDCl_3$.