

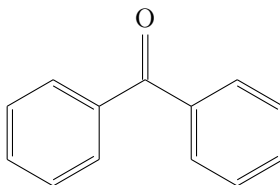
# Spectral Data for Benzophenone

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## Classification

- IUPAC name: Diphenylmethanone.
- Picture:



## Spectral Data

1.

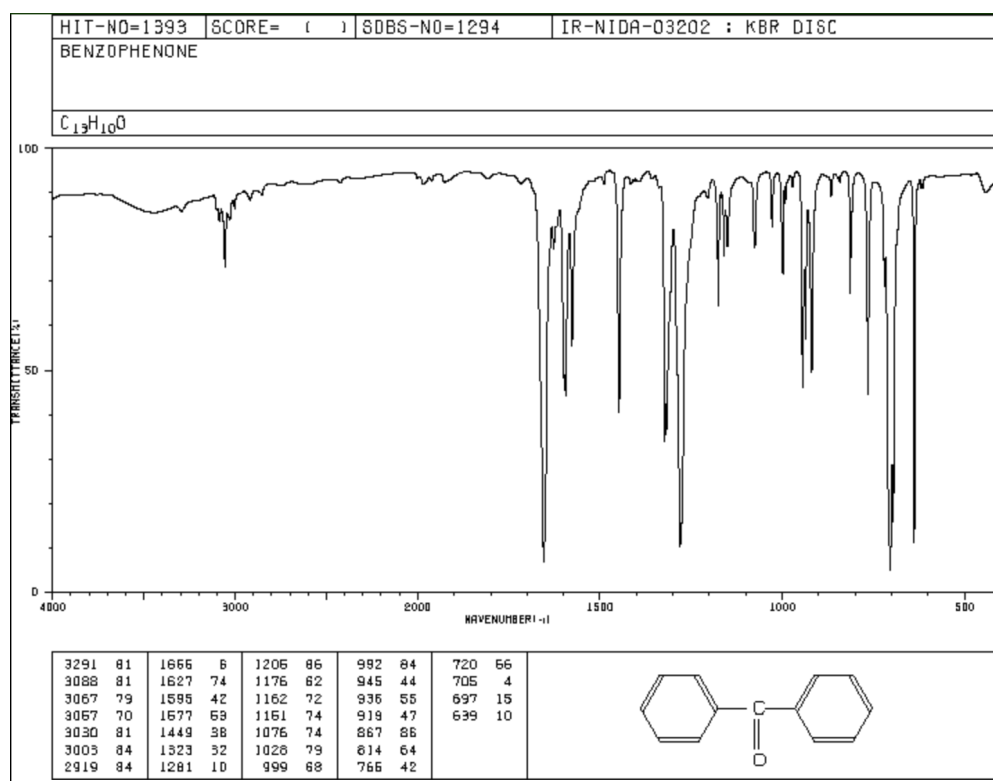
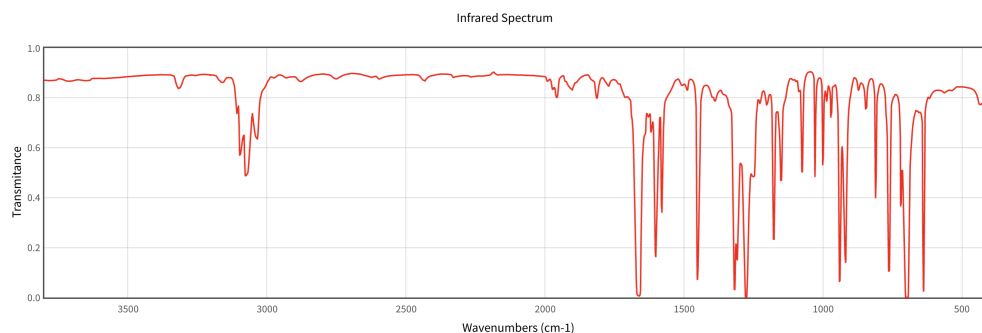


Figure 1: IR spectrum of benzophenone<sup>1</sup>.

2.

Figure 2: IR spectrum of benzophenone<sup>2</sup>.

3. Information in common:

- Molecule identifying information.
- The IR Spectrum from the SDBS database has data for much higher wavenumbers than the IR Spectrum from NIST.

4. Carbonyl data:

- Based on the IR spectra, benzophenone may have a carbonyl since we have a peak in the vicinity of  $1710\text{ cm}^{-1}$  to  $1735\text{ cm}^{-1}$  although not strictly at it. This carbonyl is part of a ketone, and the wavenumber of the peak (from Figure 1) is  $1666\text{ cm}^{-1}$ . This is consistent with the fact that benzophenone does have a carbonyl.

5. Alcohol/amine data:

- Based on the IR spectra, benzophenone has neither an alcohol nor an amine since neither spectrum shows a peak at either  $3400\text{ cm}^{-1}$  or  $3300\text{ cm}^{-1}$ , respectively. This is consistent with the fact that benzophenone has neither an alcohol nor an amine.

6. Alkyne/nitrile data:

- Based on the IR spectra, benzophenone has neither an alkyne nor a nitrile since neither spectrum shows a peak from  $2100\text{ cm}^{-1}$  to  $2300\text{ cm}^{-1}$ . This is consistent with the fact that benzophenone has neither an alkyne nor a nitrile.

7. Most prominent C–H absorption peak:

- The  $sp^2$  C–H peak, just to the left of  $3000\text{ cm}^{-1}$ , is the most prominent (and only) C–H peak. This is consistent with the fact that benzophenone has only  $sp^2$  C–H bonds (no  $sp^3$  or  $sp$  C–H) and, in fact, only  $sp^2$  hybridized carbons.

8. Other prominent stretches:

- There appears to be some aromatic activity in the vicinity of  $1500\text{ cm}^{-1}$ , owing to benzophenone's two aromatic rings. Consistent with the structure, there is not other distinguishing activity.

## References

- (1) SDBSWeb National Institute of Advanced Industrial Science and Technology <https://sdb.sdb.aist.go.jp/sdb/cgi-bin/landingpage?sdbno=1294> (accessed 10/22/2021).
- (2) Johnson, T. J.; Myers, T. L.; Su, Y.-F.; Tonkyn, R. G.; Kelly-Gorham, M. R. K.; Danby, T. O. In National Institute of Standards and Technology *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*, Linstrom, P. J., Mallard, W. G., Eds., Gaithersburg MD, 20899, (accessed 10/22/2021).