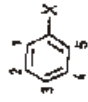


source: Gunther, NMR spectroscopy



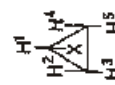
$J_{HH}$  in selected organic compounds

Tab. 10.2

| X                             | $J_{cis}$ | $J_{trans}$ | $2J$ | Ref. | X   | $J$  | Ref. |
|-------------------------------|-----------|-------------|------|------|---|------|------|
| H                             | 11.6      | 19.1        | 2.5  | 2    | Li  | 8.90 | 2    |
| Li                            | 19.3      | 23.9        | 7.1  | 2    | Si(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> | 8.0  | 2    |
| COOH                          | 10.2      | 17.2        | 1.7  | 2    | H   | ~7.5 | 2    |
| CN                            | 11.75     | 17.92       | 0.91 | 2    | C <sub>6</sub> H <sub>6</sub>                   | 7.82 | 2    |
| C <sub>6</sub> H <sub>6</sub> | 11.48     | 16.59       | 1.08 | 2    | CN  | 7.80 | 2    |
| CH <sub>3</sub>               | 10.02     | 16.81       | 2.08 | 2    | I   | 7.45 | 2    |
| OCH <sub>3</sub>              | 7.0       | 14.1        | -2.0 | 2    | Br  | 7.33 | 2    |
| Cl                            | 7.1       | 14.8        | -1.4 | 2    | CH <sub>3</sub>                                 | 7.26 | 2    |
| Br                            | 7.1       | 15.2        | -1.8 | 2    | N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>  | 7.13 | 2    |
| F                             | 4.65      | 12.75       | -3.2 | 2    | OC <sub>2</sub> H <sub>5</sub>                  | 6.97 | 2    |
|                               |           |             |      | 2    | O(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>  | 4.7  | 2    |



H<sub>3</sub>C-CH<sub>2</sub>-X



| X                 | $J(1,2)$ | $J(1,3)$ | $J(2,4)$ | $J(3,5)$ | $J(2,3)$ | Ref. |
|-------------------|----------|----------|----------|----------|----------|------|
| H                 | 8.97     | 5.58     | 8.97     | 5.58     | -4.34    | 3    |
| Cl                | 7.01     | 3.58     | 10.26    | 10.58    | -6.01    | 4    |
| Br                | 7.13     | 3.80     | 10.16    | 10.45    | -8.12    | 4    |
| I                 | 7.51     | 4.37     | 9.89     | 9.97     | -5.94    | 4    |
| NH <sub>2</sub>   | 6.63     | 3.66     | 9.65     | 9.89     | -4.29    | 4    |
| CN                | 8.43     | 5.12     | 9.18     | 9.49     | -4.72    | 4    |
| COOH              | 8.04     | 4.57     | 9.26     | 9.66     | -4.00    | 4    |
| COCl              | 7.88     | 4.43     | 9.19     | 9.99     | -4.46    | 4    |
| COCH <sub>3</sub> | 7.96     | 4.55     | 8.76     | 9.60     | -3.41    | 4    |

| X                                | $J(1,2)$ | $J(1,3)$ | $J(1,4)$ | $J(1,5)$ | $J(2,3)$ | $J(2,4)$ | Ref. |
|----------------------------------|----------|----------|----------|----------|----------|----------|------|
| H                                | 7.54     | 1.37     | 0.66     | 1.37     | 7.54     | 1.37     | 8    |
| Li                               | 6.73     | 1.54     | 0.77     | 0.74     | 7.42     | 1.29     | 8    |
| CH <sub>3</sub>                  | 7.64     | 1.25     | 0.60     | 1.87     | 7.52     | 1.61*    | 7    |
| COOCH <sub>3</sub>               | 7.86     | 1.35     | 0.63     | 1.79     | 7.49     | 1.31     | 8    |
| I                                | 7.93     | 1.14     | 0.47     | 1.88     | 7.47     | 1.76     | 8    |
| Br                               | 8.05     | 1.12     | 0.46     | 2.1      | 7.44     | 1.78     | 8    |
| Cl                               | 8.05     | 1.13     | 0.48     | 2.27     | 7.51     | 1.72     | 8    |
| NH <sub>2</sub>                  | 8.02     | 1.11     | 0.47     | 2.53     | 7.39     | 1.60     | 8    |
| N(CH <sub>3</sub> ) <sub>2</sub> | 8.40     | 1.01     | 0.43     | 2.76     | 7.29     | 1.76     | 8    |
| N(CH <sub>3</sub> ) <sub>3</sub> | 8.55     | 0.92     | 0.48     | 3.05     | 7.46     | 1.69     | 8    |
| NO <sub>2</sub>                  | 8.36     | 1.18     | 0.55     | 2.40     | 7.47     | 1.48     | 8    |
| OH                               | 8.17     | 1.09     | 0.49     | 2.71     | 7.40     | 1.74     | 8    |
| OCH <sub>3</sub>                 | 8.30     | 1.03     | 0.44     | 2.94     | 7.36     | 1.76     | 8    |
| F                                | 8.36     | 1.07     | 0.43     | 2.74     | 7.47     | 1.82**   | 8    |

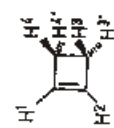
Substituent effects for  $J_{ij}$  in substituted benzene

|             |       |          |      |
|-------------|-------|----------|------|
| $J(1,CH_3)$ | -0.75 | $J(1,F)$ | 8.91 |
| $J(2,CH_3)$ | 0.36  | $J(2,F)$ | 5.69 |
| $J(3,CH_3)$ | -0.62 | $J(3,F)$ | 0.22 |

| $J_{ij}$ | F     | Cl    | Br    | I     | NO <sub>2</sub> | OCH <sub>3</sub> |
|----------|-------|-------|-------|-------|-----------------|------------------|
| 12       | +0.81 | +0.61 | +0.53 | +0.39 | +0.77           | +0.79            |
| 13       | -0.34 | -0.23 | -0.27 | -0.25 | -0.20           | -0.32            |
| 14       | -0.24 | -0.16 | -0.20 | -0.19 | -0.16           | -0.22            |
| 15       | +1.21 | +0.87 | +0.71 | +0.51 | +1.02           | +1.33            |
| 23       | -0.04 | +0.03 | -0.06 | -0.04 | -0.07           | -0.16            |
| 24       | +0.39 | +0.34 | +0.36 | +0.37 | +0.06           | +0.38            |



Ref.



|          |       |           |      |
|----------|-------|-----------|------|
| $J(1,2)$ | 1.3   | $J(1,3)$  | 1.75 |
| $J(1,2)$ | 2.85  | $J(1,4)$  | 1.0  |
|          | -0.35 | $J(3,4)$  | 4.65 |
|          |       | $J(3,4')$ | 1.75 |

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J(HH) values Part 2

Tab. 10.2

|      | J(1,2)        | J(1,3)      | J(1,4) | J(2,3) | J(1,6) | J(2,6) | Ref.     |
|------|---------------|-------------|--------|--------|--------|--------|----------|
|      | 5.05          | 1.09        | 1.98   | 1.81   | 1.33   | -1.51  | 12       |
|      | J(1,2)        | J(1,3)      | J(1,4) | J(2,3) |        |        | 13       |
|      | 9.64          | 1.02        | 1.12   | 5.04   |        |        |          |
|      | J(1,2)        | J(1,3)      | J(1,4) | J(2,3) | J(CO)2 | J(CO)2 | Mol(CO)2 |
|      | 8.9           | 8.75        | 10.14  | 8.2    | 8.4    | 8.4    | 8,4      |
|      | 1.48          | 1.50        | -0.25  | 1.27   | 1.38   | 1.38   | 1,38     |
|      | -             | -           | 0.22   | -      | -      | -      | -        |
|      | 5.51          | 5.59        | -      | 6.97   | 6.81   | 6.81   | 6,81     |
|      | 0.72          | 0.54        | -      | 0.73   | 0.77   | 0.77   | 0,77     |
|      | 0.89          | 0.76        | 0.57   | 0.51   | 0.34   | 0.34   | 0,34     |
|      | 11.17         | 10.96       | -      | 8.45   | 8.43   | 8.43   | 8,43     |
|      | 6.7           | 5.89        | 6.47   | 3.17   | 2.75   | 2.75   | 2,75     |
|      | -1.42         | -           | -      | 8.80   | 8.70   | 8.70   | 8,70     |
|      | 0.4           | -           | 0.74   | -1.07  | -1.22  | -1.22  | -1,22    |
|      | -13.0         | 0.32        | -      | 0.92   | 0.94   | 0.94   | 0,94     |
|      | -             | -           | -      | -      | -      | -      | -        |
|      | -             | 15          | 16     | 17     | 14,05  | -14.14 | 14       |
| Ref. | 14            | 15          | 16     | 17     | 17     | 14     | 14       |
|      | $^3J_{trans}$ | $^3J_{cis}$ | $^3J$  |        |        |        | Ref.     |
|      | 4.45          | 3.1         | 5.5    |        |        |        | 18       |
|      | 7.15          | 5.65        | <0.4   |        |        |        | 18       |
|      | 6.3           | 3.8         | 2.0    |        |        |        | 18       |
|      | J(1,2)        | J(1,3)      | J(1,4) | J(2,3) |        |        | 18       |
|      | -14.53        | 2.21        | 10.81  | 5.58   |        |        |          |

|                 | J(1,2) | J(1,3) | J(1,4) | J(2,4) | Ref.   |        |
|-----------------|--------|--------|--------|--------|--------|--------|
|                 | 10.2   | 1.9    | 0.1    | 3.0    | 3      |        |
|                 | J(1,2) | J(1,3) | J(1,4) | J(2,3) | J(2,4) | J(3,4) |
|                 | 9.76   | 0.90   | 0.88   | 5.78   | 1.80   | 9.45   |
|                 | J(1,2) | J(1,3) | J(1,4) | J(1,5) | J(1,6) |        |
|                 | 1.74   | 10.17  | -0.86  | 0.60   | 1.30   |        |
|                 | J(2,3) | J(2,4) | J(2,5) | J(3,4) |        |        |
|                 | 17.05  | -0.83  | 0.60   | 10.41  |        |        |
|                 | J(1,2) | J(1,3) | J(1,4) | J(2,3) |        |        |
|                 | 7.54   | 1.37   | 0.66   | 7.54   |        |        |
|                 | 8.28   | 1.24   | 0.74   | 6.85   |        |        |
|                 | 8.55   | 1.20   | 0.82   | 6.59   |        |        |
|                 | 6.87   | 0.82   | 1.04   | 8.34   |        |        |
|                 | 1.75   | 0.85   | 1.4    | 3.3    |        |        |
|                 | 5.00   | 1.06   | 2.60   | 3.60   |        |        |
|                 | 4.88   | 1.24   | 1.00   | 7.67   |        |        |
|                 | J(1,5) | J(2,4) |        |        |        |        |
|                 | -0.13  | 1.97   |        |        |        |        |
| X               | J(1,2) | J(1,3) | J(1,4) | J(2,3) |        |        |
| CH <sub>2</sub> | 8.97   | -0.02  | 1.46   | 9.19   |        |        |
| O               | 8.77   | 0.28   | 1.13   | 9.28   |        |        |
| NH              | 8.82   | 0.08   | 1.50   | 9.31   |        |        |