

## Supporting Information

**Table S1.** A selection of the calculated and measured vibrational frequencies, IR and Raman intensities for pure DMSO.

| Calculated                                    |                                     |   |   | Experimental                  |       |     |
|---|-------------------------------------|---|---|-------------------------------|-------|-----|
| Intensities                                   |                                     |   |   | Intensities                   |       |     |
| $\nu_{\text{scaled}}$<br>( $\text{cm}^{-1}$ ) | $\Delta\nu$<br>( $\text{cm}^{-1}$ ) | Raman<br>( $\text{A}^4 \cdot \text{AMU}^{-1}$ ) | Infrared<br>( $\text{km} \cdot \text{mol}^{-1}$ ) | $\nu$<br>( $\text{cm}^{-1}$ ) | Raman | IR  |
| 269   | -37                                 | 2.2   | 0.76  | 306                           | 8.2   | -   |
| 306   | -28                                 | 3.0   | 15  | 334                           | 10    | -   |
| 347   | -36                                 | 1.4   | 11  | 383                           | 3.4   | -   |
| 660   | -8                                  | 36  | 1.1   | 668                           | 24    | 10  |
| 699   | 0                                   | 16  | 6.8   | 699                           | 10    | 28  |
|   |                                     |   |   | 896                           | 0.1   | 4.0 |
| 872   | -58                                 | 0.12  | 46  | 930                           | 0.4   | 21  |
| 917   | -36                                 | 0.64  | 8.9   | 953                           | 1.9   | 52  |
| 931   | -95                                 | 3.5   | 37  | 1026                          | 2.7   | 110 |
| 1004  | -39                                 | 3.6   | 97  | 1043                          | 5.4   | 240 |
| 1005  | -54                                 | 3.3   | 35  | 1059                          | 3.1   | 52  |
| 1297  | +7                                  | 1.4   | 0.012   | 1290                          | 0.2   | 2.1 |
| 1317  | +8                                  | 4.5   | 4.1   | 1309                          | 0.8   | 12  |

|      |     |     |      |      |     |     |
|------|-----|-----|------|------|-----|-----|
|      |     |     |      | 1330 | 0.2 | 17  |
| 1387 | -20 | 1.3 | 7.6  | 1407 | 1.3 | 35  |
| 1399 | -17 | 7.5 | 4.6  | 1416 | 4.4 | 5.6 |
| 1403 | -19 | 8.0 | 0.19 | 1422 | 4.7 | 3.7 |
| 1418 | -19 | 1.0 | 16   | 1437 | 1.2 | 29  |