

## Supplementary material to:

M. Venayagamoorthy and T.A. Ford, *S. Afr. J. Chem.*, 2009, **62**, 149–155.

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### CARTESIAN COORDINATES OF THE FOUR COMPLEXES

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| Atom | SO <sub>2</sub> ·CO <sub>2</sub><br>Coordinates/Angstrom |           |           |
|------|--|-----------|-----------|
|      | X  | Y         | Z         |
| C    | -2.131898  | 0.235133  | -0.014128 |
| O    | 0.481225   | -1.025630 | -0.141578 |
| O    | -1.566495  | 1.146808  | -0.483932 |
| O    | -2.707872  | -0.667710 | 0.453252  |
| S    | 1.704459   | -0.222088 | -0.273045 |
| O    | 1.983147   | 0.814359  | 0.728944  |

| Atom | SO <sub>2</sub> ·OCS<br>Coordinates/Angstrom |           |           |
|------|--|-----------|-----------|
|      | X  | Y         | Z         |
| C    | -1.618338                                    | 0.619639  | -0.155352 |
| O    | 0.894720                                     | -1.123591 | -0.224152 |
| O    | -0.816451                                    | 1.422378  | -0.450043 |
| S    | -2.678906                                    | -0.454389 | 0.236922  |
| S    | 2.065580                                     | -0.237783 | -0.278977 |
| O    | 2.362137                                     | 0.620827  | 0.874819  |

| Atom | SO <sub>2</sub> ·CS <sub>2</sub><br>Coordinates/Angstrom |           |           |
|------|--|-----------|-----------|
|      | X  | Y         | Z         |
| C    | -1.615713  | 0.192480  | 0.030935  |
| O    | 1.285772   | -1.299549 | -0.499732 |
| S    | -1.233767  | 1.699680  | -0.150959 |
| S    | -1.962724  | -1.316070 | 0.210245  |
| S    | 1.965649   | -0.006725 | -0.329509 |
| O    | 2.387695   | 0.401418  | 1.016979  |

| Atom | SO <sub>2</sub> ·N <sub>2</sub> O<br>Coordinates/Angstrom |           |           |
|------|---|-----------|-----------|
|      | X   | Y         | Z         |
| N    | -2.085788   | 0.272463  | -0.043458 |
| O    | 0.519423  | -1.076323 | -0.145251 |
| N    | -1.539761   | 1.159377  | -0.562132 |
| O    | -2.634811   | -0.628653 | 0.482311  |
| S    | 1.680822  | -0.185801 | -0.281643 |
| O    | 1.926099  | 0.823718  | 0.756119  |

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