**Table S1.** Symmetry Components

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Interaction** | **Space rank,**  **l** | **Space component,**  **m** | **Spin Rank,**  **** | **Spin Component,**  **** |
| Isotropic chemical shift | 0 | 0 | 1 | {-1,0,1} |
| Chemical shift anisotropy/Heteronuclear dipole-dipole | 2 | {-2, -1,1,2} | 1 | {-1,0,1} |
| J-coupling | 0 | 0 | 0 | 0 |
| Homonuclear dipole-dipole | 2 | {-2, -1,1,2} | 2 | {-2, -1,0,1,2} |