Article

29Si NMR Chemical Shifts in Crystalline and Amorphous Silicon Nitrides

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Supporting information

**Table S1.** Results of NMR calculations of hypothetical Si3N4 structures

|  |  |  |  |
| --- | --- | --- | --- |
| **Structure** | **Site** | **Coordination number of Si** | **isocomp [ppm]** |
| CaSi2O4 | 1 | 4 | −42.3 |
| 2 | 4 | −50.7 |
| 3 | 5 | −120.3 |
| CaAl2O4 | 1 | 4 | −52.4 |
| 2 | 5 | −121.3 |
| 3 | 3 | 43.1 |
| 4 | 4 | −44.2 |
| 5 | 4 | −42.6 |
| 6 | 4 | −45.0 |
| 7 | 4 | −44.7 |
| 8 | 4 | −50.2 |
| 9 | 4 | −37.6 |
| CaFe2O4 | 1 | 6 | −202.5 |
| 2 | 4 | −46.1 |
| 3 | 5 | −116.6 |
| CaTi2O4 | 1 | 6 | −226.3 |
| 2 | 6 | −220.2 |
| Fe2CaO4 | 1 | 5 | −172.7 |
| 2 | 6 | −124.8 |
| 3 | 6 | −185.2 |
| Distorted Nb3Te4 | 1 | 6 | −163.5 |
| Nb3Te4 | 1 | 6 | −163.4 |
| Ni3Si4 | 1 | 6 | −210.8 |
| 2 | 6 | −165.2 |
| Olevine | 1 | 6 | −206.8 |
| 2 | 6 | −191.9 |
| 3 | 4 | −26.5 |
| phaseIII | 1 | 6 | −228.9 |
| 2 | 6 | −219.4 |
| 3 | 6 | −217.4 |
| 4 | 4 | −49.7 |
| SrPb2O4 | 1 | 6 | −218.0 |
| 2 | 4 | −41.4 |
| Th3N4 | 1 | 6 | −221.6 |
| 2 | 5 | −76.4 |
| Yb3S4 | 1 | 7 | −232.3 |
| 2 | 6 | −201.6 |
| 3 | 6 | −186.3 |
| antibeta | 1 | 4 | −53.8 |
| d-CaGeO | 1 | 4 | −55.8 |
| 2 | 4 | −40.6 |
| d-CrB4 | 1 | 4 | −47.3 |
| 2 | 4 | −44.7 |
| d-gamma | 1 | 4 | −49.0 |
| d-NiAs | 1 | 6 | −204.1 |
| 2 | 6 | −175.3 |
| d-Sphalerite | 1 | 4 | −39.8 |
| d-Sphalerite 2 | 1 | 4 | −54.3 |
| 2 | 4 | −52.1 |
| d-Wurtzite | 1 | 4 | −44.9 |
| 2 | 4 | −40.6 |
| FeGa2O4 | 1 | 6 | −194.9 |
| 2 | 4 | −49.0 |
| 3 | 4 | −30.2 |
| 4 | 5 | −148.8 |
| 5 | 6 | −194.3 |
| In2ZnS4 | 1 | 4 | −37.7 |
| 2 | 6 | −218.3 |
| mapo | 1 | 4 | −57.5 |
| 2 | 4 | −53.0 |
| sj | 1 | 4 | −51.2 |
| 2 | 5 | −98.7 |
| 3 | 5 | −115.3 |
| 4 | 4 | −50.5 |
| 5 | 4 | −45.0 |
| 6 | 4 | −50.9 |
| wll | 1 | 4 | −45.5 |