

Table 20A-8-001. BiSI. Structure of phase I [73Has]. Fractional coordinates and temperature factors at RT. B [\AA^2] is defined by Eq. (e) in Introduction.

| | Bi | S | I |
|-----|-----------|-----------|-----------|
| x | 0.1318(2) | 0.8403(8) | 0.5077(3) |
| y | 0.1230(2) | 0.0500(8) | 0.8307(3) |
| z | 0.25 | 0.25 | 0.25 |
| B | 1.88(2) | 1.46(10) | 1.83(3) |

Table 20A-8-002. BiSI. Nuclear quadrupole resonance frequencies f , asymmetry parameters η , and e^2qQ/h of ^{209}Bi [75Pop].

| T [°C] | f [MHz] | ^{209}Bi transition | η | e^2qQ/h [MHz] |
|-------------|---|---|-----------|--------------------|
| 30 | $\left\{ \begin{array}{l} 19.609(9) \\ 29.992(2) \\ 46.299(2) \\ 61.959(2) \end{array} \right.$ | $\left\{ \begin{array}{l} 1/2-3/2 \\ 3/2-5/2 \\ 5/2-7/2 \\ 7/2-9/2 \end{array} \right.$ | 0.1830(3) | 372.77(1) |
| -196 | $\left\{ \begin{array}{l} 19.611(4) \\ 30.558(2) \\ 47.090(2) \\ 62.996(3) \end{array} \right.$ | $\left\{ \begin{array}{l} 1/2-3/2 \\ 3/2-5/2 \\ 5/2-7/2 \\ 7/2-9/2 \end{array} \right.$ | 0.1750(2) | 378.91(1) |