

| Fractional coordinates of Mo <sub>2</sub> FeB <sub>2</sub> under different pressures |        |                                 |          |          |
|--|--------|---------------------------------|----------|----------|
| Element  | Atom   | Fractional coordinates of atoms |          |          |
|  | Number | u                               | v        | w        |
| 0 GPa  |        |                                 |          |          |
| B  | 1      | 0.387479                        | 0.887479 | 0.000000 |
| B  | 2      | 0.612521                        | 0.112521 | 0.000000 |
| B  | 3      | 0.112521                        | 0.387478 | 0.000000 |
| B  | 4      | 0.887479                        | 0.612522 | 0.000000 |
| Fe   | 1      | 0.000000                        | 0.000000 | 0.000000 |
| Fe   | 2      | 0.500000                        | 0.500000 | 0.000000 |
| Mo   | 1      | 0.177493                        | 0.677491 | 0.500000 |
| Mo   | 2      | 0.822507                        | 0.322509 | 0.500000 |
| Mo   | 3      | 0.322509                        | 0.177493 | 0.500000 |
| Mo   | 4      | 0.677491                        | 0.822507 | 0.500000 |
| 10 GPa   |        |                                 |          |          |
| B  | 1      | 0.387020                        | 0.887021 | 0.000000 |
| B  | 2      | 0.612980                        | 0.112980 | 0.000000 |
| B  | 3      | 0.112980                        | 0.387020 | 0.000000 |
| B  | 4      | 0.887021                        | 0.612980 | 0.000000 |
| Fe   | 1      | 0.000000                        | 0.000000 | 0.000000 |
| Fe   | 2      | 0.500000                        | 0.500000 | 0.000000 |
| Mo   | 1      | 0.177677                        | 0.677677 | 0.500000 |
| Mo   | 2      | 0.822323                        | 0.322323 | 0.500000 |
| Mo   | 3      | 0.322323                        | 0.177677 | 0.500000 |
| Mo   | 4      | 0.677677                        | 0.822323 | 0.500000 |
| 20 GPa   |        |                                 |          |          |
| B  | 1      | 0.387020                        | 0.887021 | 0.000000 |
| B  | 2      | 0.612980                        | 0.112980 | 0.000000 |
| B  | 3      | 0.112980                        | 0.387020 | 0.000000 |
| B  | 4      | 0.887021                        | 0.612980 | 0.000000 |
| Fe   | 1      | 0.000000                        | 0.000000 | 0.000000 |
| Fe   | 2      | 0.500000                        | 0.500000 | 0.000000 |
| Mo   | 1      | 0.177677                        | 0.677677 | 0.500000 |
| Mo   | 2      | 0.822323                        | 0.322323 | 0.500000 |
| Mo   | 3      | 0.322323                        | 0.177677 | 0.500000 |
| Mo   | 4      | 0.677677                        | 0.822323 | 0.500000 |
| 30 GPa   |        |                                 |          |          |
| B  | 1      | 0.386277                        | 0.886277 | 0.000000 |
| B  | 2      | 0.613723                        | 0.113723 | 0.000000 |
| B  | 3      | 0.113723                        | 0.386277 | 0.000000 |
| B  | 4      | 0.886277                        | 0.613723 | 0.000000 |
| Fe   | 1      | 0.000000                        | 0.000000 | 0.000000 |
| Fe   | 2      | 0.500000                        | 0.500000 | 0.000000 |

|        |   |          |          |          |
|--------|---|----------|----------|----------|
| Mo     | 1 | 0.177829 | 0.677828 | 0.500000 |
| Mo     | 2 | 0.822171 | 0.322172 | 0.500000 |
| Mo     | 3 | 0.322172 | 0.177829 | 0.500000 |
| Mo     | 4 | 0.677828 | 0.822171 | 0.500000 |
| 40 GPa |   |          |          |          |
| B      | 1 | 0.386026 | 0.886025 | 0.000000 |
| B      | 2 | 0.613974 | 0.113975 | 0.000000 |
| B      | 3 | 0.113975 | 0.386026 | 0.000000 |
| B      | 4 | 0.886025 | 0.613974 | 0.000000 |
| Fe     | 1 | 0.000000 | 0.000000 | 0.000000 |
| Fe     | 2 | 0.500000 | 0.500000 | 0.000000 |
| Mo     | 1 | 0.177903 | 0.677903 | 0.500000 |
| Mo     | 2 | 0.822097 | 0.322097 | 0.500000 |
| Mo     | 3 | 0.322097 | 0.177903 | 0.500000 |
| Mo     | 4 | 0.677903 | 0.822097 | 0.500000 |
| 50 GPa |   |          |          |          |
| B      | 1 | 0.385544 | 0.885546 | 0.000000 |
| B      | 2 | 0.614456 | 0.114454 | 0.000000 |
| B      | 3 | 0.114455 | 0.385544 | 0.000000 |
| B      | 4 | 0.885545 | 0.614456 | 0.000000 |
| Fe     | 1 | 0.000000 | 0.000000 | 0.000000 |
| Fe     | 2 | 0.500000 | 0.500000 | 0.000000 |
| Mo     | 1 | 0.178025 | 0.678024 | 0.500000 |
| Mo     | 2 | 0.821975 | 0.321976 | 0.500000 |
| Mo     | 3 | 0.321976 | 0.178025 | 0.500000 |
| Mo     | 4 | 0.678024 | 0.821975 | 0.500000 |
| 60 GPa |   |          |          |          |
| B      | 1 | 0.385383 | 0.885384 | 0.000000 |
| B      | 2 | 0.614617 | 0.114616 | 0.000000 |
| B      | 3 | 0.114616 | 0.385383 | 0.000000 |
| B      | 4 | 0.885384 | 0.614617 | 0.000000 |
| Fe     | 1 | 0.000000 | 0.000000 | 0.000000 |
| Fe     | 2 | 0.500000 | 0.500000 | 0.000000 |
| Mo     | 1 | 0.178144 | 0.678143 | 0.500000 |
| Mo     | 2 | 0.821856 | 0.321857 | 0.500000 |
| Mo     | 3 | 0.321857 | 0.178144 | 0.500000 |
| Mo     | 4 | 0.678143 | 0.821856 | 0.500000 |
| 70 GPa |   |          |          |          |
| B      | 1 | 0.385280 | 0.885282 | 0.000000 |
| B      | 2 | 0.614720 | 0.114718 | 0.000000 |
| B      | 3 | 0.114718 | 0.385280 | 0.000000 |
| B      | 4 | 0.885282 | 0.614720 | 0.000000 |
| Fe     | 1 | 0.000000 | 0.000000 | 0.000000 |

|         |   |          |          |          |
|---------|---|----------|----------|----------|
| Fe      | 2 | 0.500000 | 0.500000 | 0.000000 |
| Mo      | 1 | 0.178275 | 0.678274 | 0.500000 |
| Mo      | 2 | 0.821725 | 0.321726 | 0.500000 |
| Mo      | 3 | 0.321726 | 0.178275 | 0.500000 |
| Mo      | 4 | 0.678274 | 0.821725 | 0.500000 |
| 80 GPa  |   |          |          |          |
| B       | 1 | 0.385135 | 0.885135 | 0.000000 |
| B       | 2 | 0.614865 | 0.114865 | 0.000000 |
| B       | 3 | 0.114866 | 0.385134 | 0.000000 |
| B       | 4 | 0.885134 | 0.614866 | 0.000000 |
| Fe      | 1 | 0.000000 | 0.000000 | 0.000000 |
| Fe      | 2 | 0.500000 | 0.500000 | 0.000000 |
| Mo      | 1 | 0.178388 | 0.678389 | 0.500000 |
| Mo      | 2 | 0.821612 | 0.321611 | 0.500000 |
| Mo      | 3 | 0.321612 | 0.178388 | 0.500000 |
| Mo      | 4 | 0.678388 | 0.821612 | 0.500000 |
| 90 GPa  |   |          |          |          |
| B       | 1 | 0.385033 | 0.885033 | 0.000000 |
| B       | 2 | 0.614967 | 0.114967 | 0.000000 |
| B       | 3 | 0.114967 | 0.385033 | 0.000000 |
| B       | 4 | 0.885033 | 0.614967 | 0.000000 |
| Fe      | 1 | 0.000000 | 0.000000 | 0.000000 |
| Fe      | 2 | 0.500000 | 0.500000 | 0.000000 |
| Mo      | 1 | 0.178436 | 0.678436 | 0.500000 |
| Mo      | 2 | 0.821564 | 0.321564 | 0.500000 |
| Mo      | 3 | 0.321564 | 0.178436 | 0.500000 |
| Mo      | 4 | 0.678436 | 0.821564 | 0.500000 |
| 100 GPa |   |          |          |          |
| B       | 1 | 0.384958 | 0.884959 | 0.000000 |
| B       | 2 | 0.615042 | 0.115041 | 0.000000 |
| B       | 3 | 0.115041 | 0.384958 | 0.000000 |
| B       | 4 | 0.884959 | 0.615042 | 0.000000 |
| Fe      | 1 | 0.000000 | 0.000000 | 0.000000 |
| Fe      | 2 | 0.500000 | 0.500000 | 0.000000 |
| Mo      | 1 | 0.178533 | 0.678532 | 0.500000 |
| Mo      | 2 | 0.821467 | 0.321468 | 0.500000 |
| Mo      | 3 | 0.321468 | 0.178533 | 0.500000 |
| Mo      | 4 | 0.678532 | 0.821467 | 0.500000 |