LAMMPS data file for 500w\_25h202\_5pnp\_sci\_npt\_100ps2 (force field SciPCFF.frc+ )

1824 atoms

1422 bonds

1482 angles

2683 dihedrals

35 impropers

10 atom types

9 bond types

11 angle types

14 dihedral types

4 improper types

16.724545 43.275455 xlo xhi

16.724545 43.275455 ylo yhi

16.724545 43.275455 zlo zhi

Masses

1 55.847 # Fe (fe,iron in magnetite= atom id )

8 12.0112 # C

3 15.9994 # O

4 1.00797 # H

7 14.0067 # N

5 15.9994 # O

9 1.00797 # H

2 15.9994 # O (

6 1.00797 # H

10 15.9994 # O

Total Molecules Id = 531

Total atom id type = 10

Number of items/atoms = 1824

Number of items 1 to 149 present atoms in the magnetite which represent by Molecules Id is 1 for magnetite. The two atom id type considered in magnetite : 1 is for fe,iron atom in magnetite and 2 is for ox, oxygen atom in the magnetite.

Number of items 150 to 1649 present atoms in the water which represent by Molecules Id is 2 to 501 for water molecules. The two atom id type is considered in water : 1 is for o\*,oxygen atom in water and 2 is for hw,hydrogen atom in water.

So the items 150,151,152 represent one water molecule whose molecule id is 2 and next items in the sequence 153,154,155 represent second water molecule whose molecule id is 3 and this process is considered numbering for water atoms upto items for water is 1649

Number of items 1650 to 1749 present atoms in the H2O2 which represent by Molecules Id is 502 to 526 for H2O2 1749.The two atom type id is considered in H2O2 : 5 is for oh,oxygen atom in H2O2 and 6 is for ho,hydrogen atom in H2O2. So the items 1650,1651,1652,1653 represent one H2O2 molecule whose molecule id is 502 and next items in the sequence 1654,1655,1656,1657 represent second H2O2 molecule whose molecule id is 503 and this process is considered for numbering H2O2 atoms upto items for water is 1749

Number of items 1750 to 1824 present atoms in the PNP which represent by Molecules Id is 527 to 531 for PNP. The four atom id type is considered in PNP : 7 is for n3o,nitrogen atom in PNP,8 is for cp,carbon atom in PNP,9 is for hc,hydrogen atom in PNP and 10 is for o12, oxygen atom in PNP.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Number of atoms= Items column in dump file | Molecule Id | Atom Id  (according to masses) | Charge on each atom | X | y | z |

Atoms

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Bonds

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13 1 16 5 # fex ox (1)

14 1 8 5 # fex ox (1)

15 1 7 6 # fex ox (1)

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17 1 109 6 # fex ox (1)

18 1 7 11 # fex ox (1)

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22 1 46 10 # fex ox (1)

23 1 16 10 # fex ox (1)

24 1 26 11 # fex ox (1)

25 1 109 11 # fex ox (1)

26 1 12 75 # fex ox (1)

27 1 12 13 # fex ox (1)

28 1 19 13 # fex ox (1)

29 1 14 141 # fex ox (1)

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33 1 17 43 # fex ox (1)

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1216 2 1565 1563 # hw o\* (1)

1217 2 1567 1566 # hw o\* (1)

1218 2 1568 1566 # hw o\* (1)

1219 2 1570 1569 # hw o\* (1)

1220 2 1571 1569 # hw o\* (1)

1221 2 1573 1572 # hw o\* (1)

1222 2 1574 1572 # hw o\* (1)

1223 2 1576 1575 # hw o\* (1)

1224 2 1577 1575 # hw o\* (1)

1225 2 1579 1578 # hw o\* (1)

1226 2 1580 1578 # hw o\* (1)

1227 2 1582 1581 # hw o\* (1)

1228 2 1583 1581 # hw o\* (1)

1229 2 1585 1584 # hw o\* (1)

1230 2 1586 1584 # hw o\* (1)

1231 2 1588 1587 # hw o\* (1)

1232 2 1589 1587 # hw o\* (1)

1233 2 1591 1590 # hw o\* (1)

1234 2 1592 1590 # hw o\* (1)

1235 2 1594 1593 # hw o\* (1)

1236 2 1595 1593 # hw o\* (1)

1237 2 1597 1596 # hw o\* (1)

1238 2 1598 1596 # hw o\* (1)

1239 2 1600 1599 # hw o\* (1)

1240 2 1601 1599 # hw o\* (1)

1241 2 1603 1602 # hw o\* (1)

1242 2 1604 1602 # hw o\* (1)

1243 2 1606 1605 # hw o\* (1)

1244 2 1607 1605 # hw o\* (1)

1245 2 1609 1608 # hw o\* (1)

1246 2 1610 1608 # hw o\* (1)

1247 2 1612 1611 # hw o\* (1)

1248 2 1613 1611 # hw o\* (1)

1249 2 1615 1614 # hw o\* (1)

1250 2 1616 1614 # hw o\* (1)

1251 2 1618 1617 # hw o\* (1)

1252 2 1619 1617 # hw o\* (1)

1253 2 1621 1620 # hw o\* (1)

1254 2 1622 1620 # hw o\* (1)

1255 2 1624 1623 # hw o\* (1)

1256 2 1625 1623 # hw o\* (1)

1257 2 1627 1626 # hw o\* (1)

1258 2 1628 1626 # hw o\* (1)

1259 2 1630 1629 # hw o\* (1)

1260 2 1631 1629 # hw o\* (1)

1261 2 1633 1632 # hw o\* (1)

1262 2 1634 1632 # hw o\* (1)

1263 2 1636 1635 # hw o\* (1)

1264 2 1637 1635 # hw o\* (1)

1265 2 1639 1638 # hw o\* (1)

1266 2 1640 1638 # hw o\* (1)

1267 2 1642 1641 # hw o\* (1)

1268 2 1643 1641 # hw o\* (1)

1269 2 1645 1644 # hw o\* (1)

1270 2 1646 1644 # hw o\* (1)

1271 2 1648 1647 # hw o\* (1)

1272 2 1649 1647 # hw o\* (1)

1273 3 1650 1651 # oh oh (1)

1274 4 1652 1650 # ho oh (1)

1275 4 1653 1651 # ho oh (1)

1276 3 1654 1655 # oh oh (1)

1277 4 1656 1654 # ho oh (1)

1278 4 1657 1655 # ho oh (1)

1279 3 1658 1659 # oh oh (1)

1280 4 1660 1658 # ho oh (1)

1281 4 1661 1659 # ho oh (1)

1282 3 1662 1663 # oh oh (1)

1283 4 1664 1662 # ho oh (1)

1284 4 1665 1663 # ho oh (1)

1285 3 1666 1667 # oh oh (1)

1286 4 1668 1666 # ho oh (1)

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1290 4 1673 1671 # ho oh (1)

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1294 3 1678 1679 # oh oh (1)

1295 4 1680 1678 # ho oh (1)

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1297 3 1682 1683 # oh oh (1)

1298 4 1684 1682 # ho oh (1)

1299 4 1685 1683 # ho oh (1)

1300 3 1686 1687 # oh oh (1)

1301 4 1688 1686 # ho oh (1)

1302 4 1689 1687 # ho oh (1)

1303 3 1690 1691 # oh oh (1)

1304 4 1692 1690 # ho oh (1)

1305 4 1693 1691 # ho oh (1)

1306 3 1694 1695 # oh oh (1)

1307 4 1696 1694 # ho oh (1)

1308 4 1697 1695 # ho oh (1)

1309 3 1698 1699 # oh oh (1)

1310 4 1700 1698 # ho oh (1)

1311 4 1701 1699 # ho oh (1)

1312 3 1702 1703 # oh oh (1)

1313 4 1704 1702 # ho oh (1)

1314 4 1705 1703 # ho oh (1)

1315 3 1706 1707 # oh oh (1)

1316 4 1708 1706 # ho oh (1)

1317 4 1709 1707 # ho oh (1)

1318 3 1710 1711 # oh oh (1)

1319 4 1712 1710 # ho oh (1)

1320 4 1713 1711 # ho oh (1)

1321 3 1714 1715 # oh oh (1)

1322 4 1716 1714 # ho oh (1)

1323 4 1717 1715 # ho oh (1)

1324 3 1718 1719 # oh oh (1)

1325 4 1720 1718 # ho oh (1)

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1327 3 1722 1723 # oh oh (1)

1328 4 1724 1722 # ho oh (1)

1329 4 1725 1723 # ho oh (1)

1330 3 1726 1727 # oh oh (1)

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1335 4 1733 1731 # ho oh (1)

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1342 3 1742 1743 # oh oh (1)

1343 4 1744 1742 # ho oh (1)

1344 4 1745 1743 # ho oh (1)

1345 3 1746 1747 # oh oh (1)

1346 4 1748 1746 # ho oh (1)

1347 4 1749 1747 # ho oh (1)

1348 5 1751 1750 # cp n3o (-2)

1349 6 1750 1763 # n3o o12 (-2)

1350 6 1750 1764 # n3o o12 (-2)

1351 7 1751 1752 # cp cp (-2)

1352 7 1751 1756 # cp cp (-2)

1353 7 1752 1753 # cp cp (-2)

1354 8 1752 1757 # cp hc (1)

1355 7 1753 1754 # cp cp (-2)

1356 8 1753 1758 # cp hc (1)

1357 7 1754 1755 # cp cp (-2)

1358 9 1754 1759 # cp oh (1)

1359 7 1755 1756 # cp cp (-2)

1360 8 1755 1760 # cp hc (1)

1361 8 1756 1761 # cp hc (1)

1362 4 1762 1759 # ho oh (1)

1363 5 1766 1765 # cp n3o (-2)

1364 6 1765 1778 # n3o o12 (-2)

1365 6 1765 1779 # n3o o12 (-2)

1366 7 1766 1767 # cp cp (-2)

1367 7 1766 1771 # cp cp (-2)

1368 7 1767 1768 # cp cp (-2)

1369 8 1767 1772 # cp hc (1)

1370 7 1768 1769 # cp cp (-2)

1371 8 1768 1773 # cp hc (1)

1372 7 1769 1770 # cp cp (-2)

1373 9 1769 1774 # cp oh (1)

1374 7 1770 1771 # cp cp (-2)

1375 8 1770 1775 # cp hc (1)

1376 8 1771 1776 # cp hc (1)

1377 4 1777 1774 # ho oh (1)

1378 5 1781 1780 # cp n3o (-2)

1379 6 1780 1793 # n3o o12 (-2)

1380 6 1780 1794 # n3o o12 (-2)

1381 7 1781 1782 # cp cp (-2)

1382 7 1781 1786 # cp cp (-2)

1383 7 1782 1783 # cp cp (-2)

1384 8 1782 1787 # cp hc (1)

1385 7 1783 1784 # cp cp (-2)

1386 8 1783 1788 # cp hc (1)

1387 7 1784 1785 # cp cp (-2)

1388 9 1784 1789 # cp oh (1)

1389 7 1785 1786 # cp cp (-2)

1390 8 1785 1790 # cp hc (1)

1391 8 1786 1791 # cp hc (1)

1392 4 1792 1789 # ho oh (1)

1393 5 1796 1795 # cp n3o (-2)

1394 6 1795 1808 # n3o o12 (-2)

1395 6 1795 1809 # n3o o12 (-2)

1396 7 1796 1797 # cp cp (-2)

1397 7 1796 1801 # cp cp (-2)

1398 7 1797 1798 # cp cp (-2)

1399 8 1797 1802 # cp hc (1)

1400 7 1798 1799 # cp cp (-2)

1401 8 1798 1803 # cp hc (1)

1402 7 1799 1800 # cp cp (-2)

1403 9 1799 1804 # cp oh (1)

1404 7 1800 1801 # cp cp (-2)

1405 8 1800 1805 # cp hc (1)

1406 8 1801 1806 # cp hc (1)

1407 4 1807 1804 # ho oh (1)

1408 5 1811 1810 # cp n3o (-2)

1409 6 1810 1823 # n3o o12 (-2)

1410 6 1810 1824 # n3o o12 (-2)

1411 7 1811 1812 # cp cp (-2)

1412 7 1811 1816 # cp cp (-2)

1413 7 1812 1813 # cp cp (-2)

1414 8 1812 1817 # cp hc (1)

1415 7 1813 1814 # cp cp (-2)

1416 8 1813 1818 # cp hc (1)

1417 7 1814 1815 # cp cp (-2)

1418 9 1814 1819 # cp oh (1)

1419 7 1815 1816 # cp cp (-2)

1420 8 1815 1820 # cp hc (1)

1421 8 1816 1821 # cp hc (1)

1422 4 1822 1819 # ho oh (1)

Angles

1 1 2 1 10 # ox fex ox

2 1 2 1 4 # ox fex ox

3 1 4 1 10 # ox fex ox

4 2 1 2 46 # fex ox fex

5 2 1 2 26 # fex ox fex

6 2 26 2 46 # fex ox fex

7 1 51 3 74 # ox fex ox

8 1 51 3 104 # ox fex ox

9 1 74 3 104 # ox fex ox

10 1 4 3 51 # ox fex ox

11 1 4 3 74 # ox fex ox

12 1 4 3 104 # ox fex ox

13 2 1 4 3 # fex ox fex

14 2 1 4 7 # fex ox fex

15 2 1 4 8 # fex ox fex

16 2 3 4 7 # fex ox fex

17 2 3 4 8 # fex ox fex

18 2 7 4 8 # fex ox fex

19 2 16 5 87 # fex ox fex

20 2 8 5 87 # fex ox fex

21 2 8 5 16 # fex ox fex

22 2 7 6 63 # fex ox fex

23 2 7 6 109 # fex ox fex

24 2 63 6 109 # fex ox fex

25 1 4 7 6 # ox fex ox

26 1 4 7 11 # ox fex ox

27 1 6 7 11 # ox fex ox

28 1 4 8 5 # ox fex ox

29 1 4 8 9 # ox fex ox

30 1 5 8 9 # ox fex ox

31 2 8 9 87 # fex ox fex

32 2 8 9 63 # fex ox fex

33 2 63 9 87 # fex ox fex

34 2 1 10 46 # fex ox fex

35 2 1 10 16 # fex ox fex

36 2 16 10 46 # fex ox fex

37 2 7 11 26 # fex ox fex

38 2 7 11 109 # fex ox fex

39 2 26 11 109 # fex ox fex

40 1 13 12 75 # ox fex ox

41 2 12 13 19 # fex ox fex

42 1 15 14 141 # ox fex ox

43 2 14 15 19 # fex ox fex

44 1 5 16 10 # ox fex ox

45 1 5 16 23 # ox fex ox

46 1 10 16 23 # ox fex ox

47 1 21 17 43 # ox fex ox

48 2 81 18 148 # fex ox fex

49 2 19 18 81 # fex ox fex

50 2 19 18 78 # fex ox fex

51 2 19 18 148 # fex ox fex

52 2 78 18 81 # fex ox fex

53 2 78 18 148 # fex ox fex

54 1 13 19 15 # ox fex ox

55 1 13 19 18 # ox fex ox

56 1 13 19 22 # ox fex ox

57 1 13 19 23 # ox fex ox

58 1 13 19 21 # ox fex ox

59 1 15 19 18 # ox fex ox

60 1 15 19 22 # ox fex ox

61 1 15 19 23 # ox fex ox

62 1 15 19 21 # ox fex ox

63 1 18 19 22 # ox fex ox

64 1 18 19 23 # ox fex ox

65 1 18 19 21 # ox fex ox

66 1 22 19 23 # ox fex ox

67 1 21 19 22 # ox fex ox

68 1 21 19 23 # ox fex ox

69 2 111 20 148 # fex ox fex

70 2 44 20 111 # fex ox fex

71 2 44 20 81 # fex ox fex

72 2 44 20 148 # fex ox fex

73 2 81 20 111 # fex ox fex

74 2 81 20 148 # fex ox fex

75 2 17 21 19 # fex ox fex

76 2 19 22 44 # fex ox fex

77 2 19 22 39 # fex ox fex

78 2 19 22 148 # fex ox fex

79 2 44 22 148 # fex ox fex

80 2 39 22 44 # fex ox fex

81 2 39 22 148 # fex ox fex

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83 2 16 23 44 # fex ox fex

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85 2 19 23 44 # fex ox fex

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87 2 44 23 81 # fex ox fex

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89 2 24 25 30 # fex ox fex

90 1 2 26 11 # ox fex ox

91 1 2 26 35 # ox fex ox

92 1 11 26 35 # ox fex ox

93 1 28 27 119 # ox fex ox

94 2 27 28 30 # fex ox fex

95 2 42 29 146 # fex ox fex

96 2 41 29 146 # fex ox fex

97 2 41 29 42 # fex ox fex

98 2 30 29 146 # fex ox fex

99 2 30 29 42 # fex ox fex

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104 1 25 30 35 # ox fex ox

105 1 25 30 34 # ox fex ox

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109 1 28 30 34 # ox fex ox

110 1 29 30 33 # ox fex ox

111 1 29 30 35 # ox fex ox

112 1 29 30 34 # ox fex ox

113 1 33 30 35 # ox fex ox

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122 2 94 32 146 # fex ox fex

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127 2 94 33 96 # fex ox fex

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132 2 26 35 94 # fex ox fex

133 2 30 35 42 # fex ox fex

134 2 30 35 94 # fex ox fex

135 2 42 35 94 # fex ox fex

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137 1 38 36 40 # ox fex ox

138 1 38 36 53 # ox fex ox

139 1 47 37 120 # ox fex ox

140 1 47 37 139 # ox fex ox

141 1 120 37 139 # ox fex ox

142 1 38 37 47 # ox fex ox

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162 1 29 42 47 # ox fex ox

163 1 29 42 51 # ox fex ox

164 1 29 42 54 # ox fex ox

165 1 32 42 35 # ox fex ox

166 1 32 42 47 # ox fex ox

167 1 32 42 51 # ox fex ox

168 1 32 42 54 # ox fex ox

169 1 35 42 47 # ox fex ox

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171 1 35 42 54 # ox fex ox

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183 1 20 44 43 # ox fex ox

184 1 20 44 47 # ox fex ox

185 1 20 44 51 # ox fex ox

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187 1 22 44 43 # ox fex ox

188 1 22 44 47 # ox fex ox

189 1 22 44 51 # ox fex ox

190 1 23 44 43 # ox fex ox

191 1 23 44 47 # ox fex ox

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193 1 43 44 47 # ox fex ox

194 1 43 44 51 # ox fex ox

195 1 47 44 51 # ox fex ox

196 2 48 45 133 # fex ox fex

197 2 48 45 127 # fex ox fex

198 2 127 45 133 # fex ox fex

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1373 5 1751 1750 1763 # cp n3o o12

1374 5 1751 1750 1764 # cp n3o o12

1375 6 1763 1750 1764 # o12 n3o o12

1376 7 1752 1751 1750 # cp cp n3o

1377 7 1756 1751 1750 # cp cp n3o

1378 8 1752 1751 1756 # cp cp cp

1379 8 1751 1752 1753 # cp cp cp

1380 9 1751 1752 1757 # cp cp hc

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1387 10 1755 1754 1759 # cp cp oh

1388 8 1754 1755 1756 # cp cp cp

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1394 11 1754 1759 1762 # cp oh ho

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1397 6 1778 1765 1779 # o12 n3o o12

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1460 11 1799 1804 1807 # cp oh ho

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Dihedrals

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2 1 10 1 2 26 # ox fex ox fex

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4 1 4 1 2 26 # ox fex ox fex

5 1 2 1 10 46 # ox fex ox fex

6 1 2 1 10 16 # ox fex ox fex

7 1 4 1 10 46 # ox fex ox fex

8 1 4 1 10 16 # ox fex ox fex

9 1 2 1 4 3 # ox fex ox fex

10 1 2 1 4 7 # ox fex ox fex

11 1 2 1 4 8 # ox fex ox fex

12 1 10 1 4 3 # ox fex ox fex

13 1 10 1 4 7 # ox fex ox fex

14 1 10 1 4 8 # ox fex ox fex

15 1 10 46 2 1 # ox fex ox fex

16 1 10 46 2 26 # ox fex ox fex

17 1 43 46 2 1 # ox fex ox fex

18 1 43 46 2 26 # ox fex ox fex

19 1 51 46 2 1 # ox fex ox fex

20 1 51 46 2 26 # ox fex ox fex

21 1 54 46 2 1 # ox fex ox fex

22 1 54 46 2 26 # ox fex ox fex

23 1 11 26 2 1 # ox fex ox fex

24 1 11 26 2 46 # ox fex ox fex

25 1 35 26 2 1 # ox fex ox fex

26 1 35 26 2 46 # ox fex ox fex

27 1 74 3 51 42 # ox fex ox fex

28 1 74 3 51 44 # ox fex ox fex

29 1 74 3 51 46 # ox fex ox fex

30 1 104 3 51 42 # ox fex ox fex

31 1 104 3 51 44 # ox fex ox fex

32 1 104 3 51 46 # ox fex ox fex

33 1 4 3 51 42 # ox fex ox fex

34 1 4 3 51 44 # ox fex ox fex

35 1 4 3 51 46 # ox fex ox fex

36 1 51 3 74 71 # ox fex ox fex

37 1 51 3 74 87 # ox fex ox fex

38 1 51 3 74 81 # ox fex ox fex

39 1 104 3 74 71 # ox fex ox fex

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43 1 4 3 74 87 # ox fex ox fex

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46 1 51 3 104 100 # ox fex ox fex

47 1 51 3 104 109 # ox fex ox fex

48 1 74 3 104 94 # ox fex ox fex

49 1 74 3 104 100 # ox fex ox fex

50 1 74 3 104 109 # ox fex ox fex

51 1 4 3 104 94 # ox fex ox fex

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59 1 74 3 4 8 # ox fex ox fex

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2651 7 1799 1800 1801 1806 # cp cp cp hc

2652 8 1796 1801 1800 1805 # cp cp cp hc

2653 9 1805 1800 1801 1806 # hc cp cp hc

2654 3 1812 1811 1810 1823 # cp cp n3o o12

2655 3 1812 1811 1810 1824 # cp cp n3o o12

2656 3 1816 1811 1810 1823 # cp cp n3o o12

2657 3 1816 1811 1810 1824 # cp cp n3o o12

2658 4 1813 1812 1811 1810 # cp cp cp n3o

2659 5 1817 1812 1811 1810 # hc cp cp n3o

2660 6 1816 1811 1812 1813 # cp cp cp cp

2661 7 1816 1811 1812 1817 # cp cp cp hc

2662 4 1815 1816 1811 1810 # cp cp cp n3o

2663 5 1821 1816 1811 1810 # hc cp cp n3o

2664 6 1812 1811 1816 1815 # cp cp cp cp

2665 7 1812 1811 1816 1821 # cp cp cp hc

2666 6 1811 1812 1813 1814 # cp cp cp cp

2667 7 1811 1812 1813 1818 # cp cp cp hc

2668 8 1814 1813 1812 1817 # cp cp cp hc

2669 9 1817 1812 1813 1818 # hc cp cp hc

2670 6 1812 1813 1814 1815 # cp cp cp cp

2671 10 1812 1813 1814 1819 # cp cp cp oh

2672 8 1815 1814 1813 1818 # cp cp cp hc

2673 11 1818 1813 1814 1819 # hc cp cp oh

2674 6 1813 1814 1815 1816 # cp cp cp cp

2675 7 1813 1814 1815 1820 # cp cp cp hc

2676 12 1816 1815 1814 1819 # cp cp cp oh

2677 13 1820 1815 1814 1819 # hc cp cp oh

2678 14 1813 1814 1819 1822 # cp cp oh ho

2679 14 1815 1814 1819 1822 # cp cp oh ho

2680 6 1814 1815 1816 1811 # cp cp cp cp

2681 7 1814 1815 1816 1821 # cp cp cp hc

2682 8 1811 1816 1815 1820 # cp cp cp hc

2683 9 1820 1815 1816 1821 # hc cp cp hc

Impropers

1 1 1763 1750 1751 1764 # o12 n3o cp o12

2 2 1756 1751 1752 1750 # cp cp cp n3o

3 3 1757 1752 1751 1753 # hc cp cp cp

4 3 1758 1753 1752 1754 # hc cp cp cp

5 4 1759 1754 1753 1755 # oh cp cp cp

6 3 1760 1755 1754 1756 # hc cp cp cp

7 3 1761 1756 1751 1755 # hc cp cp cp

8 1 1778 1765 1766 1779 # o12 n3o cp o12

9 2 1771 1766 1767 1765 # cp cp cp n3o

10 3 1772 1767 1766 1768 # hc cp cp cp

11 3 1773 1768 1767 1769 # hc cp cp cp

12 4 1774 1769 1768 1770 # oh cp cp cp

13 3 1775 1770 1769 1771 # hc cp cp cp

14 3 1776 1771 1766 1770 # hc cp cp cp

15 1 1793 1780 1781 1794 # o12 n3o cp o12

16 2 1786 1781 1782 1780 # cp cp cp n3o

17 3 1787 1782 1781 1783 # hc cp cp cp

18 3 1788 1783 1782 1784 # hc cp cp cp

19 4 1789 1784 1783 1785 # oh cp cp cp

20 3 1790 1785 1784 1786 # hc cp cp cp

21 3 1791 1786 1781 1785 # hc cp cp cp

22 1 1808 1795 1796 1809 # o12 n3o cp o12

23 2 1801 1796 1797 1795 # cp cp cp n3o

24 3 1802 1797 1796 1798 # hc cp cp cp

25 3 1803 1798 1797 1799 # hc cp cp cp

26 4 1804 1799 1798 1800 # oh cp cp cp

27 3 1805 1800 1799 1801 # hc cp cp cp

28 3 1806 1801 1796 1800 # hc cp cp cp

29 1 1823 1810 1811 1824 # o12 n3o cp o12

30 2 1816 1811 1812 1810 # cp cp cp n3o

31 3 1817 1812 1811 1813 # hc cp cp cp

32 3 1818 1813 1812 1814 # hc cp cp cp

33 4 1819 1814 1813 1815 # oh cp cp cp

34 3 1820 1815 1814 1816 # hc cp cp cp

35 3 1821 1816 1811 1815 # hc cp cp cp

Pair Coeffs

1 0.495580000000000 4.077000 # fex

8 0.071000000000000 3.922000 # cp

3 0.274000000000000 3.608000 # o\*

4 0.008000000000000 1.087000 # hw

7 0.048000000000000 3.760000 # n3o

5 0.096000000000000 3.580000 # oh

9 0.023000000000000 2.878000 # hc

2 0.078400000000000 3.627000 # ox

6 0.008000000000000 1.087000 # ho

10 0.048000000000000 3.400000 # o12

Angle Coeffs

1 109.5000 83.7103 -97.1839 16.9574 # ox fex ox (ox fex ox)

2 109.5000 130.6992 -18.4789 0.0000 # fex ox fex (fex ox fex)

3 103.7000 49.8400 -11.6000 -8.0000 # h\* o\* h\* (hw o\* hw)

4 109.0000 58.5000 0.000000 0.000000 # \* o\_ h\_ (oh oh ho)

5 117.7000 63.9404 -18.4524 -14.3129 # cp n3o o12 (cp n3o o12)

6 128.0000 95.1035 -47.4240 -27.9164 # o12 n3o o12 (o12 n3o o12)

7 118.8000 29.2436 -8.8495 -6.6020 # cp cp n3o (n3o cp cp)

8 118.9000 61.0226 -34.9931 0.0000 # cp cp cp (cp cp cp)

9 117.9400 35.1558 -12.4682 0.0000 # cp cp h (cp cp hc)

10 123.4200 73.6781 -21.6787 0.0000 # cp cp o (cp cp oh)

11 108.1900 53.1250 -8.5016 0.0000 # cp o h\* (cp oh ho)

BondBond Coeffs

1 0.000000 2.163300 2.163300

2 0.000000 2.163300 2.163300

3 -9.500000 0.970000 0.970000

4 0.000000 0.000000 0.000000

5 93.794800 1.430000 1.210000

6 265.710600 1.210000 1.210000

7 21.049500 1.417000 1.430000

8 68.285600 1.417000 1.417000

9 1.079500 1.417000 1.098200

10 48.475400 1.417000 1.376800

11 20.657700 1.376800 0.965000

BondAngle Coeffs

1 0.000000 0.000000 0.000000 0.000000

2 0.000000 0.000000 0.000000 0.000000

3 22.350000 22.350000 0.970000 0.970000

4 0.000000 0.000000 0.000000 0.000000

5 40.375700 92.195500 1.430000 1.210000

6 95.693600 95.693600 1.210000 1.210000

7 30.521100 59.802500 1.417000 1.430000

8 28.870800 28.870800 1.417000 1.417000

9 20.003300 24.218300 1.417000 1.098200

10 58.479000 107.680600 1.417000 1.376800

11 53.861400 23.922400 1.376800 0.965000

Dihedral Coeffs

1 0.000000 0.000000 0.000000 0.000000 0.000000 -180.000000 # \* fex ox \* (ox fex ox fex)

2 0.000000 0.000000 0.000000 0.000000 1.000000 -180.000000 # \* o\_ o\_ \* (ho oh oh ho)

3 0.000000 0.000000 1.160000 0.000000 0.000000 0.000000 # cp cp n3o o12 (cp cp n3o o12)

4 0.000000 0.000000 7.212400 0.000000 0.000000 0.000000 # cp cp cp n3o (n3o cp cp cp)

5 0.000000 0.000000 2.912600 0.000000 0.000000 0.000000 # hc cp cp n3o (n3o cp cp hc)

6 8.366700 0.000000 1.193200 0.000000 0.000000 0.000000 # cp cp cp cp (cp cp cp cp)

7 0.000000 0.000000 3.966100 0.000000 0.000000 0.000000 # cp cp cp h (cp cp cp hc)

8 0.000000 0.000000 3.966100 0.000000 0.000000 0.000000 # cp cp cp h (hc cp cp cp)

9 0.000000 0.000000 1.876900 0.000000 0.000000 0.000000 # h cp cp h (hc cp cp hc)

10 0.000000 0.000000 4.849800 0.000000 0.000000 0.000000 # cp cp cp o (cp cp cp oh)

11 0.000000 0.000000 1.723400 0.000000 0.000000 0.000000 # h cp cp o (hc cp cp oh)

12 0.000000 0.000000 4.849800 0.000000 0.000000 0.000000 # cp cp cp o (oh cp cp cp)

13 0.000000 0.000000 1.723400 0.000000 0.000000 0.000000 # h cp cp o (oh cp cp hc)

14 -0.690000 0.000000 0.509700 0.000000 0.009500 0.000000 # cp cp o h\* (cp cp oh ho)

MiddleBondTorsion Coeffs

1 0.000000 0.000000 0.000000 0.000000

2 0.000000 0.000000 0.000000 0.000000

3 0.000000 0.000000 0.000000 0.000000

4 0.000000 0.000000 0.000000 0.000000

5 0.000000 0.000000 0.000000 0.000000

6 27.598900 -2.312000 0.000000 1.417000

7 0.000000 -1.152100 0.000000 1.417000

8 0.000000 -1.152100 0.000000 1.417000

9 0.000000 4.822800 0.000000 1.417000

10 0.000000 4.825500 0.000000 1.417000

11 0.000000 5.543200 0.000000 1.417000

12 0.000000 4.825500 0.000000 1.417000

13 0.000000 5.543200 0.000000 1.417000

14 1.158000 3.269700 3.513200 1.376800

EndBondTorsion Coeffs

1 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

4 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

5 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 -0.118500 6.320400 0.000000 -0.118500 6.320400 0.000000 1.417000 1.417000

7 0.000000 -6.895800 0.000000 0.000000 -0.466900 0.000000 1.417000 1.098200

8 0.000000 -6.895800 0.000000 0.000000 -0.466900 0.000000 1.417000 1.098200

9 0.000000 -0.689000 0.000000 0.000000 -0.689000 0.000000 1.098200 1.098200

10 0.000000 0.265500 0.000000 0.000000 4.890500 0.000000 1.417000 1.376800

11 0.000000 -1.586700 0.000000 0.000000 4.264100 0.000000 1.098200 1.376800

12 0.000000 0.265500 0.000000 0.000000 4.890500 0.000000 1.417000 1.376800

13 0.000000 -1.586700 0.000000 0.000000 4.264100 0.000000 1.098200 1.376800

14 0.900000 -1.345600 1.190000 3.413200 0.587300 -0.132300 1.417000 0.965000

AngleTorsion Coeffs

1 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

2 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

3 0.000000 0.000000 0.000000 0.000000 -3.420700 0.000000 118.800000 117.700000

4 0.000000 7.759400 0.000000 0.000000 0.000000 0.000000 118.900000 118.800000

5 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

6 1.976700 1.023900 0.000000 1.976700 1.023900 0.000000 118.900000 118.900000

7 0.000000 2.501400 0.000000 0.000000 2.714700 0.000000 118.900000 117.940000

8 0.000000 2.501400 0.000000 0.000000 2.714700 0.000000 118.900000 117.940000

9 0.000000 2.450100 0.000000 0.000000 2.450100 0.000000 117.940000 117.940000

10 0.000000 10.015500 0.000000 0.000000 1.740400 0.000000 118.900000 123.420000

11 0.000000 1.872900 0.000000 0.000000 2.570600 0.000000 117.940000 123.420000

12 0.000000 10.015500 0.000000 0.000000 1.740400 0.000000 118.900000 123.420000

13 0.000000 1.872900 0.000000 0.000000 2.570600 0.000000 117.940000 123.420000

14 -5.136000 -1.012200 0.000000 4.685200 0.023000 -0.598000 123.420000 108.190000

AngleAngleTorsion Coeffs

1 0.000000 0.000000 0.000000

2 0.000000 0.000000 0.000000

3 -18.043600 118.800000 117.700000

4 -34.968100 118.900000 118.800000

5 0.000000 0.000000 0.000000

6 0.000000 0.000000 0.000000

7 -4.814100 118.900000 117.940000

8 -4.814100 118.900000 117.940000

9 0.359800 117.940000 117.940000

10 -21.024700 118.900000 123.420000

11 4.229600 117.940000 123.420000

12 -21.024700 118.900000 123.420000

13 4.229600 117.940000 123.420000

14 -4.607200 123.420000 108.190000

BondBond13 Coeffs

1 0.000000 0.000000 0.000000

2 0.000000 0.000000 0.000000

3 0.000000 0.000000 0.000000

4 0.000000 0.000000 0.000000

5 0.000000 0.000000 0.000000

6 53.000000 1.417000 1.417000

7 -6.274100 1.417000 1.098200

8 -6.274100 1.417000 1.098200

9 -1.707700 1.098200 1.098200

10 -2.243600 1.417000 1.376800

11 2.051700 1.098200 1.376800

12 -2.243600 1.417000 1.376800

13 2.051700 1.098200 1.376800

14 1.159000 1.417000 0.965000

Improper Coeffs

1 36.261200 0.000000 # cp n3o o12 o12

2 0.919400 0.000000 # cp cp cp n3o

3 4.891200 0.000000 # cp cp cp h

4 13.042100 0.000000 # cp cp cp o

AngleAngle Coeffs

1 0.000000 0.000000 0.000000 117.700000 128.000000 117.700000

2 0.000000 0.000000 0.000000 118.800000 118.900000 118.800000

3 0.000000 0.000000 0.000000 117.940000 117.940000 118.900000

4 0.000000 0.000000 0.000000 123.420000 123.420000 118.900000