# Supporting Information

## A Hierarchy of Homodesmotic Reactions for Thermochemistry

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| | Molecule | | Molecule |
|---|---|---|---|
| **1** | 1,3-cyclohexadiene | **35** | 1,3-pentadiene |
| **2** | 1,3-hexadiene | **36** | 1,3-pentadiyne |
| **3** | 1,3-hexadiyne | **37** | 1,4-pentadiene |
| **5** | 1,4-hexadiene | **38** | 1,4-pentadiyne |
| **6** | 1,4-hexadiyne | **39** | penta-1-ene-3-yne |
| **7** | 2-butene | **40** | penta-1-ene-4-yne |
| **8** | 2-pentene | **41** | penta-1-yne-3-ene |
| **9** | 2-pentyne | **42** | 2,4-hexadiene |
| **10** | hexa-1-ene-3-yne | **43** | 2,4-hexadiyne |
| **11** | hexa-1-ene-4-yne | **44** | hexa-2-ene-4-yne |
| **12** | hexa-1-yne-3-ene | **45** | 1,2,3-hexatriene |
| **13** | hexa-1-yne-4-ene | **46** | 1,2,3-pentatriene |
| **14** | propane | **47** | E-2,3,4-hexatriene |
| **15** | propene | **48** | Z-2,3,4-hexatriene |
| **16** | propyne | **49** | 1,5-hexadiene |
| **17** | ethane | **50** | 1,5-hexadiyne |
| **18** | 1,3-butadiene | **51** | Hexa-1-ene-5-yne |
| **19** | 1,3-butadiyne | **52** | cyclopentadiene |
| **20** | allene | **53** | 2-ethyl-1-butene |
| **21** | butatriene | **54** | 2-methyl-1-pentene |
| **22** | ethene | **55** | 2-methyl-2-pentene |
| **23** | vinylacetylene | **56** | 2-methylpentane |
| **24** | methane | **57** | 3-methylpentane |
| **25** | butane | **58** | E-3-methyl-2-pentene |
| **26** | acetylene | **59** | Z-3-methyl-2-pentene |
| **29** | pentane | **60** | 2-methylpropene |
| **30** | 2-butyne | **61** | 2-methyl-1-butene |
| **31** | 1-butyne | **62** | 2-methyl-2-butene |
| **32** | 1-butene | **63** | Isobutene |
| **33** | 1-pentene | **64** | Isopentane |
| **34** | 1-pentyne | **65** | $H_2$ |

**Table S1**. Reaction energies (kcal mol$^{-1}$) for prototype hypohomodesmotic reactions.

| Reaction | | B3LYP 6-31G(d) | M05-2X 6-31G(d) | M06 6-31G(d) | M06-2X 6-31G(d) | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit | MP2 cc-pVDZ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **18+17** → 2(**15**) | (17) | 4.66 | 3.85 | 4.04 | 3.71 | 3.00 | 2.91 | 2.83 | 2.80 | 2.78 | 4.04 |
| **19+17** → 2(**16**) | (18) | 3.46 | 0.70 | 2.03 | 0.80 | −3.30 | −3.60 | −3.86 | −3.94 | −3.96 | 1.23 |
| **23+17** → **15+16** | (19) | 2.12 | 0.96 | 1.18 | 0.92 | −0.41 | −0.59 | −0.74 | −0.79 | −0.81 | 1.18 |
| **18+16** → **23+15** | (20) | 2.54 | 2.89 | 2.87 | 2.78 | 3.40 | 3.51 | 3.57 | 3.58 | 3.59 | 2.86 |
| **21+22** → 2(**20**) | (21) | 1.80 | 0.21 | 0.96 | 0.27 | −0.63 | −0.65 | −0.67 | −0.65 | −0.64 | 2.35 |
| **18+19** → 2(**23**) | (22) | 3.88 | 2.63 | 3.71 | 2.66 | 0.51 | 0.50 | 0.45 | 0.43 | 0.44 | 2.92 |
| **19+15** → **23+16** | (23) | 1.34 | −0.26 | 0.85 | −0.12 | −2.89 | −3.01 | −3.12 | −3.15 | −3.15 | 0.06 |

| Reaction | | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (No ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **18+17** → 2(**15**) | (17) | 3.86 | 3.74 | 3.71 | 3.69 | 3.23 | 3.03 | 3.68 | 3.46 | 3.28 |
| **19+17** → 2(**16**) | (18) | 1.25 | 0.81 | 0.67 | 0.58 | −1.09 | −1.15 | −0.05 | 0.00 | −0.69 |
| **23+17** → **15+16** | (19) | 0.97 | 0.73 | 0.65 | 0.60 | 0.35 | 0.10 | 0.83 | 0.60 | 0.19 |
| **18+16** → **23+15** | (20) | 2.89 | 3.01 | 3.06 | 3.10 | 2.88 | 2.93 | 2.84 | 2.86 | 3.09 |
| **21+22** → 2(**20**) | (21) | 2.13 | 2.01 | 1.99 | 1.96 | 1.09 | 0.77 | 2.17 | 1.88 | 1.66 |
| **18+19** → 2(**23**) | (22) | 3.17 | 3.09 | 3.08 | 3.08 | 1.44 | 1.68 | 1.96 | 2.27 | 2.21 |
| **19+15** → **23+16** | (23) | 0.28 | 0.09 | 0.02 | −0.01 | −1.44 | −1.25 | −0.88 | −0.59 | −0.88 |

**Table S2**. Atomization energies (kcal mol$^{-1}$) for conjugated hydrocarbons (Set A).

| Molecule | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| 1,3-pentadiene | 1304.39 | 1232.96 | 1302.65 | 1307.22 | 1307.56 | 985.13 | 1001.96 | 1004.06 | 1004.61 | 1004.77 |
| 1,3-pentadiyne | 989.93 | 948.09 | 987.73 | 997.53 | 995.54 | 720.51 | 738.29 | 740.28 | 740.71 | 740.81 |
| penta-1-ene-3-yne | 1146.82 | 1090.32 | 1145.02 | 1152.07 | 1151.47 | 853.68 | 870.96 | 873.04 | 873.55 | 873.69 |
| penta-1-yne-3-ene | 1143.10 | 1086.95 | 1142.24 | 1148.52 | 1148.61 | 850.84 | 868.18 | 870.27 | 870.75 | 870.87 |
| 1,3-hexadiene | 1597.22 | 1507.69 | 1596.53 | 1601.64 | 1602.30 | 1208.60 | 1228.55 | 1230.99 | 1231.62 | 1231.80 |
| 1,3-hexadiyne | 1282.87 | 1222.74 | 1281.58 | 1291.83 | 1290.36 | 944.14 | 965.07 | 967.40 | 967.92 | 968.04 |
| hexa-1-ene-3-yne | 1439.69 | 1365.00 | 1438.82 | 1446.35 | 1446.25 | 1077.24 | 1097.66 | 1100.08 | 1100.67 | 1100.83 |
| hexa-1-yne-3-ene | 1435.94 | 1361.68 | 1436.16 | 1443.01 | 1443.54 | 1074.31 | 1094.78 | 1097.20 | 1097.77 | 1097.91 |
| 2,4-hexadiene | 1601.17 | 1512.01 | 1599.87 | 1605.75 | 1605.75 | 1211.38 | 1231.04 | 1233.46 | 1234.08 | 1234.25 |
| 2,4-hexadiyne | 1291.56 | 1231.64 | 1289.05 | 1300.77 | 1297.89 | 951.24 | 971.82 | 974.11 | 974.64 | 974.77 |
| hexa-2-ene-4-yne | 1444.02 | 1369.80 | 1442.72 | 1451.09 | 1450.19 | 1080.55 | 1100.69 | 1103.09 | 1103.67 | 1103.81 |
| 1,2,3-hexatriene | 1433.54 | 1359.26 | 1430.28 | 1438.69 | 1437.24 | 1063.26 | 1083.50 | 1085.90 | 1086.48 | 1086.64 |
| 1,2,3-pentatriene | 1140.53 | 1084.39 | 1136.25 | 1143.96 | 1142.22 | 839.64 | 856.77 | 858.83 | 859.33 | 859.47 |
| E-2,3,4-hexatriene | 1437.02 | 1362.92 | 1433.09 | 1442.12 | 1440.38 | 1065.96 | 1086.01 | 1088.40 | 1088.98 | 1089.13 |

| Molecule | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1,3-pentadiene | 1241.10 | 1301.20 | 1318.44 | 1324.27 | 1329.96 | 1206.05 | 1260.15 | 1219.84 | 1278.60 | 1310.67 |
| 1,3-pentadiyne | 952.74 | 1006.10 | 1021.24 | 1026.27 | 1031.19 | 899.49 | 947.72 | 915.26 | 968.23 | 996.80 |
| penta-1-ene-3-yne | 1096.25 | 1152.73 | 1169.00 | 1174.41 | 1179.69 | 1052.86 | 1103.79 | 1067.33 | 1122.90 | 1153.25 |
| penta-1-yne-3-ene | 1094.05 | 1150.57 | 1166.88 | 1172.34 | 1177.69 | 1050.74 | 1101.71 | 1065.30 | 1120.95 | 1151.42 |
| 1,3-hexadiene | 1520.79 | 1593.55 | 1614.37 | 1621.40 | 1628.30 | 1479.21 | 1544.80 | 1495.56 | 1566.73 | 1605.44 |
| 1,3-hexadiyne | 1232.33 | 1298.44 | 1317.13 | 1323.37 | 1329.50 | 1172.55 | 1232.33 | 1190.88 | 1256.32 | 1291.52 |
| hexa-1-ene-3-yne | 1375.75 | 1444.97 | 1464.80 | 1471.42 | 1477.90 | 1325.88 | 1388.34 | 1342.90 | 1410.92 | 1447.91 |
| hexa-1-yne-3-ene | 1373.68 | 1442.88 | 1462.77 | 1469.45 | 1475.99 | 1323.86 | 1386.33 | 1340.96 | 1409.05 | 1446.18 |
| 2,4-hexadiene | 1523.63 | 1596.38 | 1617.23 | 1624.24 | 1631.11 | 1481.73 | 1547.29 | 1498.09 | 1569.26 | 1608.01 |
| 2,4-hexadiyne | 1238.65 | 1304.70 | 1323.32 | 1329.50 | 1335.55 | 1178.43 | 1238.18 | 1196.69 | 1262.06 | 1297.16 |
| hexa-2-ene-4-yne | 1379.15 | 1448.28 | 1468.14 | 1474.74 | 1481.20 | 1328.94 | 1391.34 | 1345.97 | 1413.96 | 1450.99 |
| 1,2,3-hexatriene | 1362.22 | 1431.54 | 1451.35 | 1457.93 | 1464.37 | 1314.51 | 1376.83 | 1332.60 | 1400.59 | 1437.47 |
| 1,2,3-pentatriene | 1082.33 | 1138.98 | 1155.22 | 1160.58 | 1165.82 | 1041.22 | 1092.06 | 1056.75 | 1112.32 | 1142.54 |
| E-2,3,4-hexatriene | 1364.94 | 1434.36 | 1454.17 | 1460.73 | 1467.16 | 1316.75 | 1379.14 | 1334.89 | 1402.95 | 1439.84 |

**Table S3**. Atomization energies (kcal mol$^{-1}$) for non-conjugated hydrocarbons (Set B).

| Molecule | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| pentane | 1592.06 | 1490.69 | 1591.65 | 1597.24 | 1597.38 | 1219.77 | 1236.88 | 1238.67 | 1239.14 | 1239.26 |
| 1-pentene | 1443.81 | 1357.40 | 1443.59 | 1447.69 | 1448.57 | 1099.35 | 1116.53 | 1118.52 | 1119.05 | 1119.20 |
| 1-pentyne | 1284.78 | 1213.54 | 1285.44 | 1291.48 | 1292.09 | 968.00 | 985.80 | 987.84 | 988.32 | 988.44 |
| 2-pentene | 1447.24 | 1361.03 | 1446.28 | 1450.94 | 1451.39 | 1101.74 | 1118.72 | 1120.68 | 1121.20 | 1121.33 |
| 2-pentyne | 1292.01 | 1220.60 | 1291.02 | 1298.44 | 1297.88 | 973.59 | 991.15 | 993.17 | 993.66 | 993.78 |
| 1,4-pentadiene | 1295.30 | 1223.83 | 1295.31 | 1298.13 | 1299.87 | 978.74 | 995.89 | 998.04 | 998.61 | 998.78 |
| 1,4-pentadiyne | 972.88 | 931.89 | 974.43 | 981.42 | 982.17 | 711.47 | 729.77 | 731.98 | 732.43 | 732.53 |
| penta-1-ene-4-yne | 1134.95 | 1078.73 | 1135.80 | 1140.58 | 1141.94 | 846.07 | 863.82 | 866.01 | 866.52 | 866.65 |
| 1,4-hexadiene | 1591.92 | 1502.65 | 1592.21 | 1596.70 | 1598.00 | 1204.98 | 1224.98 | 1227.45 | 1228.09 | 1228.27 |
| 1,4-hexadiyne | 1273.88 | 1214.80 | 1274.97 | 1284.17 | 1283.81 | 941.49 | 962.65 | 965.20 | 965.76 | 965.89 |
| hexa-1-ene-4-yne | 1435.60 | 1361.27 | 1435.94 | 1442.93 | 1443.09 | 1075.68 | 1096.26 | 1098.79 | 1099.40 | 1099.56 |
| hexa-1-yne-4-ene | 1431.68 | 1357.68 | 1432.86 | 1439.30 | 1440.36 | 1072.46 | 1093.09 | 1095.61 | 1096.20 | 1096.35 |
| 1,5-hexadiene | 1588.47 | 1499.05 | 1589.64 | 1593.23 | 1595.21 | 1202.49 | 1222.75 | 1225.26 | 1225.93 | 1226.12 |
| 1,5-hexadiyne | 1269.95 | 1210.75 | 1272.76 | 1280.15 | 1281.45 | 939.11 | 960.53 | 963.11 | 963.66 | 963.79 |
| hexa-1-ene-5-yne | 1429.27 | 1354.98 | 1431.25 | 1436.85 | 1438.52 | 1070.93 | 1091.78 | 1094.33 | 1094.94 | 1095.10 |
| 2-ethyl-1-butene | 1738.78 | 1634.35 | 1740.52 | 1746.11 | 1746.77 | 1323.38 | 1343.53 | 1345.83 | 1346.41 | 1346.56 |
| 2-methyl-1-pentene | 1739.68 | 1635.41 | 1741.13 | 1747.22 | 1747.74 | 1324.57 | 1344.68 | 1347.00 | 1347.59 | 1347.74 |
| 2-methyl-2-pentene | 1741.94 | 1637.96 | 1742.52 | 1748.47 | 1748.81 | 1325.43 | 1345.42 | 1347.71 | 1348.29 | 1348.44 |
| 2-methylpentane | 1884.58 | 1765.46 | 1886.55 | 1893.23 | 1893.43 | 1442.43 | 1462.53 | 1464.65 | 1465.20 | 1465.33 |
| 3-methylpentane | 1883.63 | 1764.45 | 1885.90 | 1892.77 | 1892.88 | 1441.14 | 1461.19 | 1463.31 | 1463.86 | 1463.99 |
| E-3-methyl-2-pentene | 1741.24 | 1637.25 | 1742.03 | 1748.30 | 1748.41 | 1324.48 | 1344.41 | 1346.69 | 1347.27 | 1347.41 |
| Z-3-methyl-2-pentene | 1741.12 | 1637.08 | 1741.98 | 1748.39 | 1748.63 | 1324.45 | 1344.38 | 1346.66 | 1347.24 | 1347.39 |

| Molecule | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| pentane | 1509.49 | 1578.29 | 1597.17 | 1603.50 | 1609.76 | 1485.20 | 1547.69 | 1496.67 | 1563.80 | 1598.60 |
| 1-pentene | 1371.81 | 1436.37 | 1454.45 | 1460.54 | 1466.53 | 1342.60 | 1401.02 | 1355.02 | 1418.10 | 1451.56 |
| 1-pentyne | 1227.08 | 1288.20 | 1305.46 | 1311.24 | 1316.91 | 1189.61 | 1245.03 | 1202.74 | 1262.82 | 1294.89 |
| 2-pentene | 1374.29 | 1438.81 | 1456.87 | 1462.94 | 1468.91 | 1344.73 | 1403.10 | 1357.20 | 1420.22 | 1453.66 |
| 2-pentyne | 1231.81 | 1292.75 | 1309.99 | 1315.70 | 1321.30 | 1194.00 | 1249.24 | 1207.08 | 1266.91 | 1298.89 |
| 1,4-pentadiene | 1234.04 | 1294.19 | 1311.43 | 1317.28 | 1322.98 | 1199.92 | 1254.13 | 1213.32 | 1272.18 | 1304.22 |
| 1,4-pentadiyne | 940.71 | 993.85 | 1009.40 | 1014.58 | 1019.64 | 890.18 | 938.21 | 904.99 | 957.68 | 986.83 |
| penta-1-ene-4-yne | 1088.12 | 1144.80 | 1161.21 | 1166.73 | 1172.11 | 1045.86 | 1097.01 | 1059.96 | 1115.77 | 1146.39 |
| 1,4-hexadiene | 1516.40 | 1589.20 | 1610.05 | 1617.08 | 1623.97 | 1475.57 | 1541.22 | 1491.53 | 1562.78 | 1601.51 |
| 1,4-hexadiyne | 1225.74 | 1291.47 | 1310.64 | 1316.97 | 1323.16 | 1168.50 | 1227.93 | 1185.75 | 1250.74 | 1286.56 |
| hexa-1-ene-4-yne | 1372.86 | 1442.07 | 1462.11 | 1468.77 | 1475.29 | 1323.87 | 1386.37 | 1340.42 | 1408.47 | 1445.74 |
| hexa-1-yne-4-ene | 1370.56 | 1439.90 | 1459.93 | 1466.65 | 1473.22 | 1321.59 | 1384.21 | 1338.25 | 1406.47 | 1443.81 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 1,5-hexadiene | 1513.72 | 1586.68 | 1607.57 | 1614.64 | 1621.55 | 1473.28 | 1539.09 | 1489.19 | 1560.60 | 1599.39 |
| 1,5-hexadiyne | 1223.70 | 1289.75 | 1308.96 | 1315.37 | 1321.65 | 1166.69 | 1226.47 | 1184.02 | 1249.41 | 1285.35 |
| hexa-1-ene-5-yne | 1368.80 | 1438.30 | 1458.36 | 1465.10 | 1471.70 | 1320.09 | 1382.88 | 1336.71 | 1405.11 | 1442.48 |
| 2-ethyl-1-butene | 1654.11 | 1731.74 | 1753.44 | 1760.72 | 1767.90 | 1617.65 | 1687.82 | 1632.92 | 1708.75 | 1748.92 |
| 2-methyl-1-pentene | 1654.57 | 1732.12 | 1753.90 | 1761.19 | 1768.37 | 1618.39 | 1688.50 | 1633.56 | 1709.31 | 1749.59 |
| 2-methyl-2-pentene | 1655.92 | 1733.46 | 1755.18 | 1762.46 | 1769.64 | 1619.22 | 1689.31 | 1634.49 | 1710.22 | 1750.45 |
| 2-methylpentane | 1790.26 | 1871.86 | 1894.37 | 1901.89 | 1909.34 | 1759.08 | 1833.09 | 1773.33 | 1852.96 | 1894.46 |
| 3-methylpentane | 1789.53 | 1871.27 | 1893.77 | 1901.30 | 1908.75 | 1758.24 | 1832.36 | 1772.56 | 1852.34 | 1893.84 |
| E-3-methyl-2-pentene | 1655.46 | 1733.06 | 1754.77 | 1762.04 | 1769.21 | 1618.68 | 1688.82 | 1634.01 | 1709.82 | 1750.01 |
| Z-3-methyl-2-pentene | 1655.48 | 1733.12 | 1754.81 | 1762.07 | 1769.23 | 1618.69 | 1688.84 | 1634.03 | 1709.86 | 1750.01 |

**Table S4**. Isogyric bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+6(**65**) → 5(**24**) | −142.30 | −110.05 | −149.30 | −143.21 | −142.00 | −153.67 | −150.15 | −149.29 | −149.17 | −149.16 |
| **36**+8(**65**) → 5(**24**) | −237.21 | −188.11 | −253.54 | −238.13 | −240.21 | −254.92 | −246.50 | −245.47 | −245.40 | −245.44 |
| **39**+7(**65**) → 5(**24**) | −190.09 | −149.28 | −201.60 | −190.97 | −191.18 | −203.44 | −197.50 | −196.52 | −196.40 | −196.41 |
| **41**+7(**65**) → 5(**24**) | −193.81 | −152.66 | −204.37 | −194.52 | −194.04 | −206.28 | −200.28 | −199.29 | −199.20 | −199.22 |
| **2**+7(**65**) → 6(**24**) | −160.75 | −124.60 | −166.89 | −160.35 | −158.55 | −174.29 | −170.71 | −169.80 | −169.68 | −169.69 |
| **3**+9(**65**) → 6(**24**) | −255.56 | −202.74 | −271.14 | −255.39 | −256.69 | −275.39 | −266.88 | −265.78 | −265.72 | −265.77 |
| **10**+8(**65**) → 6(**24**) | −208.51 | −163.89 | −219.25 | −208.25 | −207.69 | −223.97 | −217.95 | −216.90 | −216.80 | −216.81 |
| **12**+8(**65**) → 6(**24**) | −212.26 | −167.21 | −221.91 | −211.59 | −210.40 | −226.91 | −220.83 | −219.78 | −219.70 | −219.74 |
| **42**+7(**65**) → 6(**24**) | −156.81 | −120.29 | −163.55 | −156.24 | −155.10 | −171.51 | −168.22 | −167.32 | −167.23 | −167.24 |
| **43**+9(**65**) → 6(**24**) | −246.86 | −193.83 | −263.68 | −246.45 | −249.15 | −268.29 | −260.12 | −259.07 | −259.00 | −259.04 |
| **44**+8(**65**) → 6(**24**) | −204.18 | −159.08 | −215.35 | −203.51 | −203.75 | −220.66 | −214.91 | −213.89 | −213.81 | −213.83 |
| **45**+8(**65**) → 6(**24**) | −214.67 | −169.62 | −227.80 | −215.92 | −216.70 | −237.96 | −232.11 | −231.08 | −230.99 | −231.01 |
| **46**+9(**65**) → 5(**24**) | −196.38 | −155.21 | −210.36 | −199.08 | −200.43 | −217.47 | −211.69 | −210.72 | −210.61 | −210.62 |
| **47**+8(**65**) → 6(**24**) | −211.18 | −165.96 | −224.98 | −212.49 | −213.56 | −235.25 | −229.60 | −228.59 | −228.49 | −228.52 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+6(**65**) → 5(**24**) | −135.00 | −135.14 | −133.94 | −133.14 | −132.42 | −140.82 | −141.34 | −135.66 | −135.99 | −133.34 |
| **36**+8(**65**) → 5(**24**) | −226.86 | −223.15 | −221.97 | −221.23 | −220.56 | −240.44 | −237.01 | −233.29 | −229.59 | −226.90 |
| **39**+7(**65**) → 5(**24**) | −181.60 | −180.06 | −178.80 | −178.05 | −177.38 | −190.54 | −189.32 | −184.69 | −183.31 | −180.61 |
| **41**+7(**65**) → 5(**24**) | −183.80 | −182.23 | −180.92 | −180.11 | −179.38 | −192.66 | −191.40 | −186.73 | −185.26 | −182.44 |
| **2**+**7(65)** → 6(**24**) | −150.18 | −150.76 | −149.41 | −148.48 | −147.62 | −157.73 | −158.67 | −151.74 | −152.45 | −149.40 |
| **3**+9(**65**) → 6(**24**) | −242.15 | −238.79 | −237.48 | −236.59 | −235.78 | −257.44 | −254.38 | −249.47 | −246.10 | −243.02 |
| **10**+8(**65**) → 6(**24**) | −196.97 | −195.80 | −194.39 | −193.50 | −192.70 | −207.59 | −206.75 | −200.93 | −199.88 | −196.79 |
| **12**+8(**65**) → 6(**24**) | −199.04 | −197.89 | −196.42 | −195.48 | −194.61 | −209.62 | −208.75 | −202.87 | −201.75 | −198.51 |
| **42**+7(**65**) → 6(**24**) | −147.34 | −147.94 | −146.55 | −145.64 | −144.81 | −155.21 | −156.18 | −149.20 | −149.93 | −146.84 |
| **43**+9(**65**) → 6(**24**) | −235.83 | −232.53 | −231.29 | −230.47 | −229.73 | −251.57 | −248.52 | −243.66 | −240.36 | −237.37 |
| **44**+8(**65**) → 6(**24**) | −193.57 | −192.49 | −191.05 | −190.19 | −189.40 | −204.53 | −203.74 | −197.85 | −196.85 | −193.70 |
| **45**+8(**65**) → 6(**24**) | −210.50 | −209.24 | −207.84 | −206.99 | −206.23 | −218.96 | −218.26 | −211.22 | −210.21 | −207.23 |
| **46**+9(**65**) → 5(**24**) | −195.53 | −193.82 | −192.58 | −191.87 | −191.24 | −202.18 | −201.05 | −195.28 | −193.89 | −191.32 |
| **47**+8(**65**) → 6(**24**) | −207.78 | −206.42 | −205.03 | −204.19 | −203.44 | −216.72 | −215.95 | −208.94 | −207.85 | −204.85 |

**Table S5**. Isogyric bond separation reaction energies (kcal mol$^{-1}$) for non-conjugated species (Set B).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **29**+4(**65**) → 5(**24**) | −74.17 | −59.14 | −71.00 | −67.94 | −65.97 | −82.40 | −82.55 | −82.29 | −82.31 | −82.34 |
| **33**+5(**65**) → 5(**24**) | −112.65 | −89.02 | −113.71 | −110.11 | −107.89 | −121.13 | −119.24 | −118.63 | −118.56 | −118.57 |
| **34**+6(**65**) → 5(**24**) | −161.90 | −129.47 | −166.52 | −158.94 | −157.46 | −170.80 | −166.31 | −165.51 | −165.46 | −165.50 |
| **8**+5(**65**) → 5(**24**) | −109.22 | −85.39 | −111.02 | −106.87 | −105.07 | −118.74 | −117.05 | −116.47 | −116.42 | −116.43 |
| **9**+6(**65**) → 5(**24**) | −154.67 | −122.42 | −160.94 | −151.98 | −151.68 | −165.21 | −160.96 | −160.19 | −160.12 | −160.15 |
| **37**+6(**65**) → 5(**24**) | −151.39 | −119.18 | −156.65 | −152.29 | −149.69 | −160.06 | −156.22 | −155.31 | −155.17 | −155.15 |
| **38**+8(**65**) → 5(**24**) | −254.25 | −204.30 | −266.83 | −254.24 | −253.58 | −263.96 | −255.02 | −253.78 | −253.68 | −253.72 |
| **40**+7(**65**) → 5(**24**) | −201.96 | −160.87 | −210.81 | −202.46 | −200.71 | −211.05 | −204.63 | −203.54 | −203.43 | −203.44 |
| **5**+7(**65**) → 6(**24**) | −166.06 | −129.64 | −171.20 | −165.28 | −162.85 | −177.92 | −174.28 | −173.33 | −173.21 | −173.22 |
| **6**+9(**65**) → 6(**24**) | −264.54 | −210.68 | −277.75 | −263.06 | −263.23 | −278.04 | −269.29 | −267.98 | −267.87 | −267.91 |
| **11**+8(**65**) → 6(**24**) | −212.61 | −167.62 | −222.13 | −211.67 | −210.86 | −225.53 | −219.34 | −218.20 | −218.07 | −218.09 |
| **13**+8(**65**) → 6(**24**) | −216.52 | −171.21 | −225.21 | −215.30 | −213.59 | −228.75 | −222.51 | −221.37 | −221.27 | −221.30 |
| **49**+7(**65**) → 6(**24**) | −169.51 | −133.24 | −173.78 | −168.76 | −165.64 | −180.41 | −176.51 | −175.52 | −175.38 | −175.37 |
| **50**+9(**65**) → 6(**24**) | −268.48 | −214.73 | −279.97 | −267.07 | −265.59 | −280.43 | −271.42 | −270.07 | −269.97 | −270.02 |
| **51**+8(**65**) → 6(**24**) | −218.93 | −173.91 | −226.83 | −217.75 | −215.43 | −230.29 | −223.83 | −222.65 | −222.53 | −222.55 |
| **53**+6(**65**) → 6(**24**) | −128.97 | −101.35 | −128.25 | −123.26 | −120.98 | −141.20 | −139.39 | −138.76 | −138.73 | −138.77 |
| **54**+6(**65**) → 6(**24**) | −128.07 | −100.29 | −127.64 | −122.15 | −120.00 | −140.01 | −138.25 | −137.59 | −137.55 | −137.59 |
| **55**+6(**65**) → 6(**24**) | −125.81 | −97.75 | −126.25 | −120.89 | −118.93 | −139.15 | −137.51 | −136.87 | −136.85 | −136.88 |
| **56**+5(**65**) → 6(**24**) | −92.95 | −73.66 | −87.56 | −83.52 | −81.22 | −103.83 | −104.05 | −103.73 | −103.77 | −103.83 |
| **57**+5(**65**) → 6(**24**) | −93.90 | −74.67 | −88.21 | −83.98 | −81.77 | −105.12 | −105.39 | −105.08 | −105.11 | −105.17 |
| **58**+6(**65**) → 6(**24**) | −126.51 | −98.45 | −126.74 | −121.07 | −119.33 | −140.10 | −138.51 | −137.89 | −137.87 | −137.91 |
| **59**+6(**65**) → 6(**24**) | −126.63 | −98.62 | −126.78 | −120.98 | −119.12 | −140.13 | −138.54 | −137.92 | −137.90 | −137.94 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **29**+4(**65**) → 5(**24**) | −63.10 | −65.13 | −64.38 | −63.82 | −63.25 | −68.62 | −70.56 | −65.78 | −67.55 | −65.72 |
| **33**+5(**65**) → 5(**24**) | −102.54 | −103.52 | −102.52 | −101.82 | −101.17 | −107.75 | −108.85 | −103.95 | −104.87 | −102.61 |
| **34**+6(**65**) → 5(**24**) | −149.02 | −148.14 | −146.92 | −146.17 | −145.47 | −157.27 | −156.46 | −152.76 | −151.76 | −149.13 |
| **8**+5(**65**) → 5(**24**) | −100.06 | −101.08 | −100.10 | −99.42 | −98.79 | −105.62 | −106.77 | −101.77 | −102.75 | −100.51 |
| **9**+6(**65**) → 5(**24**) | −144.29 | −143.59 | −142.39 | −141.71 | −141.08 | −152.88 | −152.25 | −148.43 | −147.68 | −145.12 |
| **37**+6(**65**) → 5(**24**) | −142.06 | −142.15 | −140.95 | −140.13 | −139.40 | −146.95 | −147.36 | −142.18 | −142.41 | −139.80 |
| **38**+8(**65**) → 5(**24**) | −238.90 | −235.40 | −233.82 | −232.92 | −232.11 | −249.75 | −246.52 | −243.57 | −240.14 | −236.87 |
| **40**+7(**65**) → 5(**24**) | −189.73 | −188.00 | −186.59 | −185.72 | −184.95 | −197.54 | −196.10 | −192.07 | −190.44 | −187.47 |
| **5**+7(**65**) → 6(**24**) | −154.57 | −155.12 | −153.73 | −152.80 | −151.95 | −161.37 | −162.25 | −155.76 | −156.40 | −153.34 |
| **6**+9(**65**) → 6(**24**) | −248.73 | −245.76 | −243.97 | −243.00 | −242.12 | −261.50 | −258.77 | −254.60 | −251.68 | −247.98 |
| **11**+8(**65**) → 6(**24**) | −199.86 | −198.70 | −197.08 | −196.15 | −195.32 | −209.60 | −208.71 | −203.40 | −202.33 | −198.95 |
| **13**+8(**65**) → 6(**24**) | −202.16 | −200.87 | −199.26 | −198.28 | −197.39 | −211.88 | −210.87 | −205.57 | −204.33 | −200.89 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **49**+7(**65**) → 6(**24**) | −157.25 | −157.64 | −156.21 | −155.24 | −154.37 | −163.66 | −164.38 | −158.11 | −158.58 | −155.46 |
| **50**+9(**65**) → 6(**24**) | −250.78 | −247.48 | −245.65 | −244.60 | −243.64 | −263.30 | −260.24 | −256.33 | −253.01 | −249.18 |
| **51**+8(**65**) → 6(**24**) | −203.92 | −202.47 | −200.83 | −199.82 | −198.91 | −213.38 | −212.21 | −207.12 | −205.70 | −202.21 |
| **53**+6(**65**) → 6(**24**) | −115.11 | −116.12 | −114.92 | −114.12 | −113.34 | −122.76 | −124.03 | −117.85 | −118.81 | −116.09 |
| **54**+6(**65**) → 6(**24**) | −114.65 | −115.74 | −114.47 | −113.65 | −112.86 | −122.02 | −123.35 | −117.21 | −118.26 | −115.42 |
| **55**+6(**65**) → 6(**24**) | −113.30 | −114.40 | −113.18 | −112.37 | −111.60 | −121.20 | −122.54 | −116.28 | −117.34 | −114.56 |
| **56**+5(**65**) → 6(**24**) | −77.21 | −79.54 | −78.58 | −77.90 | −77.21 | −84.81 | −87.14 | −80.91 | −82.98 | −80.70 |
| **57**+5(**65**) → 6(**24**) | −77.93 | −80.14 | −79.18 | −78.50 | −77.80 | −85.65 | −87.87 | −81.68 | −83.61 | −81.32 |
| **58**+6(**65**) → 6(**24**) | −113.76 | −114.80 | −113.59 | −112.80 | −112.03 | −121.74 | −123.03 | −116.76 | −117.74 | −114.99 |
| **59**+6(**65**) → 6(**24**) | −113.74 | −114.74 | −113.55 | −112.77 | −112.01 | −121.73 | −123.00 | −116.74 | −117.71 | −115.00 |

**Table S6**. Isodesmic bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+3(**24**) → 2(**17**)+2(**22**) | 19.86 | 22.03 | 18.66 | 20.98 | 19.10 | 14.18 | 13.91 | 13.80 | 13.72 | 13.67 |
| **36**+3(**24**) → 2(**17**)+2(**26**) | 33.30 | 34.18 | 27.70 | 33.40 | 28.06 | 20.38 | 19.96 | 19.73 | 19.68 | 19.67 |
| **39**+3(**24**) → 2(**17**)+**22**+**26** | 26.25 | 27.90 | 23.00 | 26.88 | 23.50 | 18.14 | 17.77 | 17.63 | 17.59 | 17.57 |
| **41**+3(**24**) → 2(**17**)+**22**+**26** | 22.52 | 24.53 | 20.23 | 23.33 | 20.64 | 15.30 | 14.99 | 14.86 | 14.79 | 14.75 |
| **2**+4(**24**) → 3(**17**)+2(**22**) | 20.77 | 23.67 | 20.16 | 22.23 | 20.45 | 14.76 | 14.62 | 14.49 | 14.40 | 14.34 |
| **3**+4(**24**) → 3(**17**)+2(**26**) | 34.32 | 35.75 | 29.18 | 34.53 | 29.49 | 21.11 | 20.86 | 20.62 | 20.56 | 20.54 |
| **10**+4(**24**) → 3(**17**)+**22**+**26** | 27.19 | 29.49 | 24.43 | 28.00 | 24.90 | 18.80 | 18.59 | 18.44 | 18.38 | 18.36 |
| **12**+4(**24**) → 3(**17**)+**22**+**26** | 23.44 | 26.17 | 21.77 | 24.66 | 22.19 | 15.87 | 15.71 | 15.56 | 15.48 | 15.43 |
| **42**+4(**24**) → 3(**17**)+2(**22**) | 24.72 | 27.99 | 23.49 | 26.34 | 23.91 | 17.54 | 17.11 | 16.97 | 16.85 | 16.79 |
| **43**+4(**24**) → 3(**17**)+2(**26**) | 43.01 | 44.66 | 36.65 | 43.47 | 37.02 | 28.22 | 27.61 | 27.33 | 27.28 | 27.27 |
| **44**+4(**24**) → 3(**17**)+**22**+**26** | 31.52 | 34.30 | 28.33 | 32.74 | 28.84 | 22.11 | 21.62 | 21.45 | 21.37 | 21.34 |
| **45**+4(**24**) → 2(**17**)+3(**22**) | 9.20 | 12.30 | 5.06 | 11.97 | 7.04 | −7.39 | −7.27 | −7.64 | −7.85 | −7.96 |
| **46**+3(**24**) → **17**+3(**22**) | 8.12 | 10.51 | 3.41 | 10.41 | 5.39 | −8.10 | −8.12 | −8.47 | −8.67 | −8.77 |
| **47**+4(**24**) → 2(**17**)+3(**22**) | 12.69 | 15.96 | 7.87 | 15.40 | 10.17 | −4.68 | −4.76 | −5.14 | −5.36 | −5.47 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+3(**24**) → 2(**17**)+2(**22**) | 19.04 | 19.69 | 19.84 | 19.72 | 19.64 | 15.58 | 16.08 | 16.72 | 17.30 | 17.45 |
| **36**+3(**24**) → 2(**17**)+2(**26**) | 25.46 | 26.34 | 26.06 | 25.68 | 25.33 | 20.35 | 21.07 | 21.81 | 22.54 | 21.89 |
| **39**+3(**24**) → 2(**17**)+**22**+**26** | 21.58 | 22.10 | 22.10 | 21.84 | 21.59 | 18.06 | 18.43 | 19.04 | 19.40 | 19.18 |
| **41**+3(**24**) → 2(**17**)+**22**+**26** | 19.38 | 19.93 | 19.99 | 19.78 | 19.59 | 15.94 | 16.36 | 17.00 | 17.45 | 17.36 |
| **2**+4(**24**) → 3(**17**)+2(**22**) | 21.25 | 22.11 | 22.27 | 22.13 | 22.02 | 17.12 | 17.77 | 18.52 | 19.28 | 19.42 |
| **3**+4(**24**) → 3(**17**)+2(**26**) | 27.57 | 28.73 | 28.46 | 28.06 | 27.69 | 21.78 | 22.73 | 23.52 | 24.48 | 23.81 |
| **10**+4(**24**) → 3(**17**)+**22**+**26** | 23.60 | 24.40 | 24.42 | 24.13 | 23.86 | 19.45 | 20.03 | 20.69 | 21.28 | 21.04 |
| **12**+4(**24**) → 3(**17**)+**22**+**26** | 21.53 | 22.30 | 22.39 | 22.15 | 21.95 | 17.42 | 18.02 | 18.76 | 19.41 | 19.31 |
| **42**+4(**24**) → 3(**17**)+2(**22**) | 24.09 | 24.93 | 25.14 | 24.96 | 24.83 | 19.63 | 20.26 | 21.06 | 21.81 | 21.98 |
| **43**+4(**24**) → 3(**17**)+2(**26**) | 33.89 | 35.00 | 34.65 | 34.18 | 33.74 | 27.66 | 28.58 | 29.32 | 30.22 | 29.46 |
| **44**+4(**24**) → 3(**17**)+**22**+**26** | 27.01 | 27.70 | 27.76 | 27.44 | 27.16 | 22.50 | 23.03 | 23.77 | 24.31 | 24.13 |
| **45**+4(**24**) → 2(**17**)+3(**22**) | 3.17 | 4.98 | 4.93 | 4.55 | 4.26 | −2.78 | −1.15 | −0.55 | 1.26 | 0.93 |
| **46**+3(**24**) → **17**+3(**22**) | 0.75 | 2.36 | 2.29 | 1.93 | 1.65 | −4.44 | −2.96 | −2.49 | −0.86 | −1.20 |
| **47**+4(**24**) → 2(**17**)+3(**22**) | 5.89 | 7.80 | 7.75 | 7.35 | 7.05 | −0.54 | 1.16 | 1.74 | 3.63 | 3.30 |

**Table S7**. Isodesmic bond separation reaction energies (kcal mol$^{-1}$) for non-conjugated species (Set B).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **29**+3(**24**) → 4(**17**) | 3.30 | 5.65 | 5.34 | 5.63 | 5.66 | 2.41 | 2.52 | 2.50 | 2.46 | 2.44 |
| **33**+3(**24**) → **22**+3(**17**) | 7.16 | 9.42 | 8.44 | 8.77 | 8.48 | 5.19 | 5.33 | 5.30 | 5.27 | 5.24 |
| **34**+3(**24**) → **26**+3(**17**) | 12.09 | 14.07 | 12.27 | 13.61 | 12.49 | 9.25 | 9.46 | 9.48 | 9.47 | 9.46 |
| **8**+3(**24**) → 3(**17**)+**22** | 10.59 | 13.04 | 11.13 | 12.01 | 11.29 | 7.59 | 7.52 | 7.47 | 7.41 | 7.37 |
| **9**+3(**24**) → 3(**17**)+**26** | 19.32 | 21.12 | 17.85 | 20.57 | 18.27 | 14.85 | 14.80 | 14.81 | 14.81 | 14.80 |
| **37**+3(**24**) → 2(**22**)+2(**17**) | 10.77 | 12.89 | 11.31 | 11.89 | 11.41 | 7.79 | 7.85 | 7.78 | 7.72 | 7.68 |
| **38**+3(**24**) → 2(**26**)+2(**17**) | 16.25 | 17.99 | 14.41 | 17.29 | 14.69 | 11.34 | 11.45 | 11.43 | 11.41 | 11.39 |
| **40**+3(**24**) → **22**+**26**+2(**17**) | 14.37 | 16.31 | 13.79 | 15.40 | 13.97 | 10.53 | 10.64 | 10.60 | 10.56 | 10.53 |
| **5**+4(**24**) → 3(**17**)+**2(22)** | 15.47 | 18.63 | 15.84 | 17.30 | 16.16 | 11.13 | 11.05 | 10.96 | 10.87 | 10.81 |
| **6**+4(**24**) → 3(**17**)+**2(26)** | 25.33 | 27.81 | 22.57 | 26.87 | 22.94 | 18.47 | 18.44 | 18.42 | 18.40 | 18.40 |
| **11**+4(**24**) → 3(**17**)+**22**+**26** | 23.09 | 25.77 | 21.55 | 24.58 | 21.73 | 17.25 | 17.19 | 17.15 | 17.11 | 17.08 |
| **13**+4(**24**) → 3(**17**)+**22**+**26** | 19.18 | 22.18 | 18.47 | 20.95 | 19.00 | 14.03 | 14.02 | 13.98 | 13.91 | 13.87 |
| **49**+4(**24**) → 2(**22**)+3(**17**) | 12.02 | 15.03 | 13.26 | 13.82 | 13.36 | 8.64 | 8.82 | 8.77 | 8.70 | 8.66 |
| **50**+4(**24**) → 2(**26**)+3(**17**) | 21.39 | 23.76 | 20.36 | 22.85 | 20.59 | 16.08 | 16.32 | 16.33 | 16.30 | 16.29 |
| **51**+4(**24**) → **22**+**26**+3(**17**) | 16.77 | 19.47 | 16.86 | 18.50 | 17.16 | 12.49 | 12.71 | 12.69 | 12.65 | 12.62 |
| **53**+4(**24**) → 4(**17**)+**22** | 10.21 | 13.28 | 12.99 | 14.01 | 13.29 | 6.33 | 6.44 | 6.38 | 6.29 | 6.24 |
| **54**+4(**24**) → 4(**17**)+**22** | 11.11 | 14.34 | 13.60 | 15.12 | 14.27 | 7.52 | 7.59 | 7.55 | 7.47 | 7.42 |
| **55**+4(**24**) → 4(**17**)+**22** | 13.37 | 16.88 | 14.99 | 16.38 | 15.34 | 8.37 | 8.33 | 8.26 | 8.18 | 8.12 |
| **56**+4(**24**) → 5(**17**) | 3.89 | 7.33 | 7.86 | 8.45 | 8.31 | 2.17 | 2.28 | 2.25 | 2.19 | 2.16 |
| **57**+4(**24**) → 5(**17**) | 2.95 | 6.32 | 7.22 | 7.99 | 7.77 | 0.88 | 0.95 | 0.91 | 0.85 | 0.81 |
| **58**+4(**24**) → 4(**17**)+**22** | 12.67 | 16.18 | 14.50 | 16.20 | 14.94 | 7.42 | 7.32 | 7.24 | 7.15 | 7.09 |
| **59**+4(**24**) → 4(**17**)+**22** | 12.55 | 16.01 | 14.45 | 16.29 | 15.15 | 7.39 | 7.29 | 7.21 | 7.12 | 7.07 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **29**+3(**24**) → 4(**17**) | 6.46 | 7.01 | 7.22 | 7.16 | 7.11 | 5.12 | 5.52 | 5.77 | 6.24 | 6.96 |
| **33**+3(**24**) → **22**+3(**17**) | 9.26 | 9.97 | 10.17 | 10.10 | 10.04 | 7.33 | 7.90 | 8.01 | 8.67 | 9.42 |
| **34**+3(**24**) → **26**+3(**17**) | 11.93 | 12.67 | 12.89 | 12.77 | 12.65 | 10.00 | 10.62 | 10.56 | 11.20 | 12.22 |
| **8**+3(**24**) → 3(**17**)+**22** | 11.75 | 12.41 | 12.59 | 12.50 | 12.42 | 9.46 | 9.98 | 10.19 | 10.79 | 11.62 |
| **9**+3(**24**) → 3(**17**)+**26** | 16.65 | 17.22 | 17.43 | 17.24 | 17.04 | 14.39 | 14.83 | 14.90 | 15.28 | 16.64 |
| **37**+3(**24**) → 2(**22**)+2(**17**) | 11.98 | 12.69 | 12.83 | 12.73 | 12.65 | 9.46 | 10.06 | 10.20 | 10.88 | 11.65 |
| **38**+3(**24**) → 2(**26**)+2(**17**) | 13.43 | 14.09 | 14.22 | 13.99 | 13.78 | 11.04 | 11.56 | 11.53 | 11.99 | 13.31 |
| **40**+3(**24**) → **22**+**26**+2(**17**) | 13.45 | 14.16 | 14.32 | 14.16 | 14.02 | 11.06 | 11.65 | 11.67 | 12.27 | 13.30 |
| **5**+4(**24**) → 3(**17**)+**2(22)** | 16.86 | 17.75 | 17.95 | 17.80 | 17.69 | 13.47 | 14.19 | 14.50 | 15.33 | 16.44 |
| **6**+4(**24**) → 3(**17**)+**2(26)** | 20.99 | 21.76 | 21.96 | 21.66 | 21.35 | 17.73 | 18.33 | 18.38 | 18.90 | 20.77 |
| **11**+4(**24**) → 3(**17**)+**22**+**26** | 20.72 | 21.50 | 21.73 | 21.48 | 21.24 | 17.44 | 18.06 | 18.22 | 18.82 | 20.48 |
| **13**+4(**24**) → 3(**17**)+**22**+**26** | 18.41 | 19.32 | 19.55 | 19.35 | 19.17 | 15.16 | 15.90 | 16.05 | 16.83 | 18.22 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **49**+4(**24**) → 2(**22**)+3(**17**) | 14.18 | 15.23 | 15.47 | 15.36 | 15.27 | 11.18 | 12.06 | 12.15 | 13.15 | 14.19 |
| **50**+4(**24**) → 2(**26**)+3(**17**) | 18.94 | 20.04 | 20.28 | 20.06 | 19.84 | 15.92 | 16.87 | 16.66 | 17.57 | 19.09 |
| **51**+4(**24**) → **22**+**26**+3(**17**) | 16.65 | 17.72 | 17.98 | 17.81 | 17.65 | 13.66 | 14.57 | 14.50 | 15.46 | 16.75 |
| **53**+4(**24**) → 4(**17**)+**22** | 14.09 | 15.41 | 15.67 | 15.55 | 15.45 | 10.75 | 11.75 | 12.00 | 13.17 | 14.43 |
| **54**+4(**24**) → 4(**17**)+**22** | 14.55 | 15.78 | 16.13 | 16.02 | 15.93 | 11.49 | 12.43 | 12.64 | 13.73 | 15.01 |
| **55**+4(**24**) → 4(**17**)+**22** | 15.89 | 17.12 | 17.41 | 17.29 | 17.19 | 12.31 | 13.23 | 13.56 | 14.65 | 16.02 |
| **56**+4(**24**) → 5(**17**) | 9.75 | 10.63 | 10.93 | 10.82 | 10.74 | 7.37 | 7.96 | 8.52 | 9.26 | 10.45 |
| **57**+4(**24**) → 5(**17**) | 9.02 | 10.04 | 10.33 | 10.23 | 10.15 | 6.53 | 7.23 | 7.75 | 8.63 | 9.86 |
| **58**+4(**24**) → 4(**17**)+**22** | 15.43 | 16.73 | 17.00 | 16.87 | 16.77 | 11.77 | 12.74 | 13.09 | 14.24 | 15.62 |
| **59**+4(**24**) → 4(**17**)+**22** | 15.45 | 16.78 | 17.04 | 16.90 | 16.79 | 11.78 | 12.77 | 13.10 | 14.28 | 15.70 |

**Table S8**. Hypohomodesmotic bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+**17**+**22** → 3(**15**) | 4.67 | 4.68 | 3.81 | 4.37 | 3.95 | 2.81 | 2.64 | 2.55 | 2.50 | 2.48 |
| **36**+**17**+**26** → 3(**16**) | 3.95 | 3.07 | 1.27 | 2.53 | 1.36 | −2.57 | −2.97 | −3.30 | −3.39 | −3.41 |
| **39**+**17**+**26** → **15**+2(**16**) | 1.62 | 1.38 | 0.43 | 0.77 | 0.65 | −0.95 | −1.28 | −1.47 | −1.53 | −1.56 |
| **41**+**17**+**22** → 2(**15**)+**16** | 2.62 | 2.59 | 1.52 | 1.97 | 1.64 | 0.07 | −0.17 | −0.32 | −0.38 | −0.41 |
| **2**+2(**17**)+**22** → 3(**15**)+**14** | 4.46 | 4.49 | 3.50 | 3.90 | 3.55 | 2.54 | 2.44 | 2.34 | 2.29 | 2.26 |
| **3**+2(**17**)+**26** → 3(**16**)+**14** | 3.84 | 2.80 | 0.94 | 1.94 | 1.04 | −2.68 | −2.99 | −3.32 | −3.41 | −3.43 |
| **10**+2(**17**)+**26** → **15**+2(**16**)+**14** | 1.44 | 1.13 | 0.05 | 0.16 | 0.30 | −1.13 | −1.37 | −1.57 | −1.63 | −1.66 |
| **12**+2(**17**)+**22** → 2(**15**)+**16**+**14** | 2.40 | 2.40 | 1.25 | 1.57 | 1.43 | −0.20 | −0.37 | −0.52 | −0.59 | −0.62 |
| **42**+**17**+2(**22**) → 4(**15**) | 4.47 | 4.85 | 3.69 | 4.20 | 3.71 | 2.38 | 2.08 | 1.97 | 1.90 | 1.86 |
| **43**+**17**+2(**26**) → 4(**16**) | 3.88 | 3.17 | 1.41 | 2.31 | 1.43 | −2.38 | −2.97 | −3.39 | −3.49 | −3.51 |
| **44**+**17**+**22**+**26** → 2(**15**)+**2**(**16**) | 1.83 | 1.99 | 0.81 | 1.08 | 0.94 | −0.77 | −1.19 | −1.41 | −1.49 | −1.52 |
| **45**+2(**22**)+**17** → 2(**20**)+**15**+**14** | 1.58 | 1.04 | −0.05 | 0.41 | 0.00 | −0.78 | −0.73 | −0.75 | −0.74 | −0.72 |
| **46**+2(**22**) → 2(**20**)+**15** | 1.63 | 1.09 | 0.11 | 0.58 | 0.12 | −0.65 | −0.66 | −0.68 | −0.66 | −0.65 |
| **47**+3(**22**) → 2(**20**)+2(**15**) | 1.14 | 0.75 | −0.37 | 0.03 | −0.15 | −1.02 | −1.06 | −1.10 | −1.09 | −1.08 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+**17**+**22** → 3(**15**) | 4.32 | 4.07 | 3.91 | 3.86 | 3.83 | 3.31 | 3.02 | 3.84 | 3.53 | 3.30 |
| **36**+**17**+**26** → 3(**16**) | 2.37 | 2.53 | 1.90 | 1.73 | 1.63 | −0.29 | −0.21 | 0.86 | 1.06 | 0.14 |
| **39**+**17**+**26** → **15**+2(**16**) | 1.28 | 1.02 | 0.69 | 0.59 | 0.52 | 0.20 | −0.12 | 0.78 | 0.49 | −0.04 |
| **41**+**17**+**22** → 2(**15**)+**16** | 1.87 | 1.58 | 1.32 | 1.22 | 1.15 | 0.87 | 0.55 | 1.44 | 1.11 | 0.67 |
| **2**+2(**17**)+**22** → 3(**15**)+**14** | 4.42 | 4.19 | 3.99 | 3.93 | 3.89 | 3.16 | 2.90 | 3.78 | 3.49 | 3.18 |
| **3**+2(**17**)+**26** → 3(**16**)+**14** | 2.36 | 2.64 | 1.94 | 1.77 | 1.66 | −0.54 | −0.37 | 0.69 | 0.97 | −0.03 |
| **10**+2(**17**)+**26** → **15**+2(**16**)+**14** | 1.19 | 1.03 | 0.64 | 0.53 | 0.46 | −0.09 | −0.33 | 0.57 | 0.34 | −0.27 |
| **12**+2(**17**)+**22** → 2(**15**)+**16**+**14** | 1.91 | 1.67 | 1.36 | 1.25 | 1.18 | 0.67 | 0.40 | 1.32 | 1.04 | 0.54 |
| **42**+**17**+2(**22**) → 4(**15**) | 4.46 | 4.10 | 3.90 | 3.81 | 3.76 | 3.26 | 2.85 | 3.89 | 3.45 | 3.11 |
| **43**+**17**+2(**26**) → 4(**16**) | 3.10 | 3.26 | 2.43 | 2.25 | 2.14 | 0.13 | 0.20 | 1.38 | 1.57 | 0.45 |
| **44**+**17**+**22**+**26** → 2(**15**)+**2**(**16**) | 1.79 | 1.42 | 1.03 | 0.90 | 0.82 | 0.56 | 0.13 | 1.22 | 0.81 | 0.19 |
| **45**+2(**22**)+**17** → 2(**20**)+**15**+**14** | 3.09 | 2.95 | 2.72 | 2.69 | 2.67 | 1.05 | 0.77 | 2.35 | 2.09 | 1.75 |
| **46**+2(**22**) → 2(**20**)+**15** | 2.78 | 2.62 | 2.43 | 2.41 | 2.39 | 1.07 | 0.77 | 2.27 | 2.00 | 1.71 |
| **47**+3(**22**) → 2(**20**)+2(**15**) | 3.01 | 2.85 | 2.58 | 2.55 | 2.52 | 0.87 | 0.54 | 2.21 | 1.90 | 1.50 |

**Table S9**. Homodesmotic bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+**22** → **18**+**15** | 0.01 | 0.34 | −0.04 | 0.33 | 0.25 | −0.19 | −0.27 | −0.28 | −0.30 | −0.30 |
| **36**+**26** → **19**+**16** | 0.48 | 0.80 | 0.57 | 0.50 | 0.56 | 0.73 | 0.63 | 0.55 | 0.55 | 0.55 |
| **39**+**26** → **23**+**16** | −0.51 | −0.37 | −0.52 | −0.41 | −0.27 | −0.55 | −0.68 | −0.74 | −0.75 | −0.75 |
| **41**+**22** → **23**+**15** | 0.49 | 0.84 | 0.56 | 0.79 | 0.72 | 0.48 | 0.42 | 0.42 | 0.41 | 0.40 |
| **2**+**22**+**17** → **18**+**14**+**15** | −0.21 | 0.15 | −0.35 | −0.15 | −0.16 | −0.45 | −0.48 | −0.49 | −0.51 | −0.52 |
| **3**+**26**+**17** → **19**+**14**+**16** | 0.38 | 0.53 | 0.24 | −0.09 | 0.24 | 0.62 | 0.61 | 0.53 | 0.53 | 0.53 |
| **10**+**26**+**17** → **23**+**14**+**16** | −0.69 | −0.62 | −0.91 | −1.02 | −0.63 | −0.72 | −0.78 | −0.83 | −0.85 | −0.85 |
| **12**+**22**+**17** → **23**+**14**+**15** | 0.28 | 0.65 | 0.29 | 0.39 | 0.51 | 0.21 | 0.23 | 0.22 | 0.20 | 0.19 |
| **42**+2(**22**) → 2(**15**)+**18** | −0.20 | 0.52 | −0.15 | 0.15 | 0.00 | −0.62 | −0.83 | −0.87 | −0.90 | −0.92 |
| **43**+2(**26**) → 2(**16**)+**19** | 0.41 | 0.90 | 0.71 | 0.28 | 0.63 | 0.92 | 0.63 | 0.47 | 0.45 | 0.45 |
| **44**+**22**+**26** → **15**+**16**+**23** | −0.30 | 0.24 | −0.14 | −0.09 | 0.02 | −0.36 | −0.59 | −0.67 | −0.70 | −0.71 |
| **45**+**22**+**17** → **21**+**15**+**14** | −0.21 | −0.20 | −0.26 | −0.55 | −0.26 | −0.15 | −0.07 | −0.08 | −0.08 | −0.08 |
| **46**+**22** → **21**+**15** | −0.17 | −0.15 | −0.10 | −0.38 | −0.15 | −0.03 | −0.01 | −0.01 | −0.01 | −0.01 |
| **47**+2(**22**) → **21**+2(**15**) | −0.66 | −0.49 | −0.59 | −0.92 | −0.42 | −0.39 | −0.41 | −0.43 | −0.44 | −0.44 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+**22** → **18**+**15** | 0.28 | 0.21 | 0.18 | 0.15 | 0.14 | 0.07 | −0.01 | 0.28 | 0.21 | 0.35 |
| **36**+**26** → **19**+**16** | 1.14 | 1.28 | 1.09 | 1.06 | 1.05 | 0.80 | 0.94 | 1.14 | 1.28 | 1.14 |
| **39**+**26** → **23**+**16** | 0.10 | 0.05 | −0.04 | −0.06 | −0.07 | −0.15 | −0.22 | 0.10 | 0.05 | −0.09 |
| **41**+**22** → **23**+**15** | 0.69 | 0.61 | 0.59 | 0.57 | 0.56 | 0.52 | 0.45 | 0.69 | 0.61 | 0.83 |
| **2**+**22**+**17** → **18**+**14**+**15** | 0.38 | 0.33 | 0.25 | 0.22 | 0.19 | −0.08 | −0.13 | 0.38 | 0.33 | 0.25 |
| **3**+**26**+**17** → **19**+**14**+**16** | 1.13 | 1.39 | 1.13 | 1.10 | 1.08 | 0.55 | 0.78 | 1.13 | 1.39 | 0.80 |
| **10**+**26**+**17** → **23**+**14**+**16** | 0.01 | 0.06 | −0.08 | −0.11 | −0.13 | −0.44 | −0.43 | 0.01 | 0.06 | −0.40 |
| **12**+**22**+**17** → **23**+**14**+**15** | 0.73 | 0.70 | 0.63 | 0.61 | 0.59 | 0.32 | 0.30 | 0.73 | 0.70 | 0.71 |
| **42**+2(**22**) → 2(**15**)+**18** | 0.42 | 0.24 | 0.16 | 0.11 | 0.06 | 0.03 | −0.18 | 0.42 | 0.24 | 0.54 |
| **43**+2(**26**) → 2(**16**)+**19** | 1.86 | 2.01 | 1.62 | 1.58 | 1.56 | 1.22 | 1.35 | 1.86 | 2.01 | 1.62 |
| **44**+**22**+**26** → **15**+**16**+**23** | 0.61 | 0.45 | 0.30 | 0.26 | 0.23 | 0.21 | 0.03 | 0.61 | 0.45 | 0.54 |
| **45**+**22**+**17** → **21**+**15**+**14** | 0.74 | 0.82 | 0.71 | 0.71 | 0.71 | −0.05 | 0.00 | 0.74 | 0.82 | 0.10 |
| **46**+**22** → **21**+**15** | 0.43 | 0.49 | 0.43 | 0.43 | 0.43 | −0.03 | 0.00 | 0.43 | 0.49 | 0.07 |
| **47**+2(**22**) → **21**+2(**15**) | 0.66 | 0.71 | 0.57 | 0.56 | 0.55 | −0.22 | −0.23 | 0.66 | 0.71 | 0.01 |

**Table S10**. Homodesmotic bond separation reaction energies (kcal mol$^{-1}$) for non-conjugated species (Set B).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **29**+2(**17**) → 3(**14**) | −0.08 | 0.14 | −0.10 | 0.45 | 0.39 | −0.12 | −0.22 | −0.21 | −0.22 | −0.22 |
| **33**+2(**17**) → **15**+2(**14**) | −0.15 | −0.04 | −0.13 | −0.22 | −0.08 | −0.28 | −0.25 | −0.25 | −0.26 | −0.27 |
| **34**+2(**17**) → **16**+2(**14**) | 0.05 | 0.03 | −0.16 | −0.13 | 0.08 | −0.08 | −0.01 | 0.00 | −0.01 | −0.02 |
| **8**+**17**+**22** → 2(**15**)+**14** | −0.66 | −0.36 | −0.58 | −0.79 | −0.56 | −0.84 | −0.91 | −0.94 | −0.96 | −0.98 |
| **9**+**26**+**17** → 2(**16**)+**14** | −1.37 | −1.45 | −1.58 | −1.74 | −1.28 | −1.30 | −1.40 | −1.45 | −1.47 | −1.48 |
| **37**+2(**17**) → 2(**15**)+**14** | −0.48 | −0.51 | −0.40 | −0.91 | −0.44 | −0.63 | −0.58 | −0.63 | −0.66 | −0.68 |
| **38**+2(**17**) → 2(**16**)+**14** | −4.44 | −4.58 | −5.02 | −5.02 | −4.87 | −4.80 | −4.76 | −4.83 | −4.87 | −4.89 |
| **40**+2(**17**) → **15**+**16**+**14** | −1.60 | −1.68 | −1.78 | −2.16 | −1.73 | −1.76 | −1.68 | −1.73 | −1.76 | −1.78 |
| **5**+2(**17**)+**22** → 3(**15**)+**14** | −0.85 | −0.55 | −0.82 | −1.04 | −0.74 | −1.08 | −1.14 | −1.20 | −1.25 | −1.27 |
| **6**+2(**17**)+**26** → 3(**16**)+**14** | −5.14 | −5.13 | −5.67 | −5.73 | −5.51 | −5.33 | −5.41 | −5.52 | −5.56 | −5.58 |
| **11**+2(**17**)+**26** → 2(**16**)+**15**+**14** | −2.66 | −2.59 | −2.83 | −3.26 | −2.87 | −2.69 | −2.77 | −2.86 | −2.91 | −2.93 |
| **13**+2(**17**)+**22** → **16**+2(**15**)+**14** | −1.86 | −1.60 | −2.05 | −2.14 | −1.75 | −2.05 | −2.05 | −2.11 | −2.15 | −2.18 |
| **49**+3(**17**) → 2(**15**)+2(**14**) | −0.36 | −0.21 | −0.26 | −0.71 | −0.24 | −0.63 | −0.51 | −0.54 | −0.57 | −0.58 |
| **50**+3(**17**) → 2(**16**)+2(**14**) | −0.43 | −0.65 | −0.89 | −1.18 | −0.72 | −0.91 | −0.80 | −0.84 | −0.87 | −0.88 |
| **51**+3(**17**) → **15**+**16**+2(**14**) | −0.33 | −0.35 | −0.52 | −0.78 | −0.30 | −0.64 | −0.52 | −0.54 | −0.57 | −0.59 |
| **53**+2(**17**) → 2(**14**)+**60** | −1.93 | −2.01 | −1.16 | −1.02 | −0.89 | −2.58 | −2.64 | −2.69 | −2.72 | −2.74 |
| **54**+2(**17**) → 2(**14**)+**60** | −1.03 | −0.96 | −0.55 | 0.09 | 0.08 | −1.40 | −1.50 | −1.52 | −1.54 | −1.56 |
| **55**+**17**+**22** → **14**+**15**+**60** | −2.71 | −2.36 | −2.30 | −2.46 | −2.14 | −3.49 | −3.60 | −3.65 | −3.68 | −3.70 |
| **56**+2(**17**) → **63**+2(**14**) | −1.07 | −0.91 | −0.75 | 0.05 | −0.10 | −1.46 | −1.59 | −1.60 | −1.61 | −1.61 |
| **57**+2(**17**) → **63**+2(**14**) | −2.02 | −1.92 | −1.40 | −0.41 | −0.65 | −2.75 | −2.93 | −2.94 | −2.95 | −2.96 |
| **58**+**17**+**22** → **14**+**15**+**60** | −3.41 | −3.06 | −2.79 | −2.64 | −2.54 | −4.44 | −4.61 | −4.67 | −4.71 | −4.72 |
| **59**+**17**+**22** → **14**+**15**+**60** | −3.53 | −3.23 | −2.84 | −2.55 | −2.32 | −4.47 | −4.64 | −4.70 | −4.73 | −4.75 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **29**+2(**17**) → 3(**14**) | 0.14 | 0.15 | 0.15 | 0.14 | 0.12 | 0.08 | 0.08 | 0.16 | 0.16 | 0.13 |
| **33**+2(**17**) → **15**+2(**14**) | 0.14 | 0.19 | 0.15 | 0.13 | 0.11 | −0.13 | −0.08 | −0.02 | 0.03 | −0.05 |
| **34**+2(**17**) → **16**+2(**14**) | 0.01 | 0.17 | 0.13 | 0.11 | 0.09 | −0.25 | −0.10 | −0.16 | −0.02 | −0.10 |
| **8**+**17**+**22** → 2(**15**)+**14** | −0.18 | −0.29 | −0.38 | −0.42 | −0.45 | −0.41 | −0.54 | −0.27 | −0.41 | −0.58 |
| **9**+**26**+**17** → 2(**16**)+**14** | −0.85 | −0.93 | −1.04 | −1.07 | −1.09 | −1.05 | −1.17 | −0.94 | −1.07 | −1.25 |
| **37**+2(**17**) → 2(**15**)+**14** | 0.05 | −0.02 | −0.15 | −0.19 | −0.21 | −0.41 | −0.46 | −0.26 | −0.33 | −0.53 |
| **38**+2(**17**) → 2(**16**)+**14** | −4.08 | −4.07 | −4.25 | −4.31 | −4.35 | −4.40 | −4.44 | −4.31 | −4.36 | −4.67 |
| **40**+2(**17**) → **15**+**16**+**14** | −1.26 | −1.27 | −1.40 | −1.45 | −1.48 | −1.60 | −1.62 | −1.47 | −1.51 | −1.74 |
| **5**+2(**17**)+**22** → 3(**15**)+**14** | 0.03 | −0.16 | −0.33 | −0.40 | −0.45 | −0.49 | −0.68 | −0.25 | −0.46 | −0.76 |
| **6**+2(**17**)+**26** → 3(**16**)+**14** | −4.22 | −4.33 | −4.56 | −4.63 | −4.68 | −4.60 | −4.77 | −4.44 | −4.62 | −5.00 |
| **11**+2(**17**)+**26** → 2(**16**)+**15**+**14** | −1.70 | −1.87 | −2.05 | −2.11 | −2.16 | −2.10 | −2.30 | −1.91 | −2.12 | −2.43 |
| **13**+2(**17**)+**22** → **16**+2(**15**)+**14** | −1.21 | −1.32 | −1.48 | −1.55 | −1.59 | −1.59 | −1.72 | −1.38 | −1.54 | −1.84 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **49**+3(**17**) → 2(**15**)+2(**14**) | 0.15 | 0.24 | 0.14 | 0.11 | 0.08 | −0.37 | −0.28 | −0.17 | −0.08 | −0.26 |
| **50**+3(**17**) → 2(**16**)+2(**14**) | −0.67 | −0.40 | −0.54 | −0.59 | −0.62 | −1.20 | −0.95 | −1.05 | −0.81 | −1.04 |
| **51**+3(**17**) → **15**+**16**+2(**14**) | −0.17 | 0.01 | −0.10 | −0.14 | −0.17 | −0.68 | −0.51 | −0.51 | −0.35 | −0.54 |
| **53**+2(**17**) → 2(**14**)+**60** | −0.76 | −0.53 | −0.63 | −0.67 | −0.70 | −1.32 | −1.17 | −1.02 | −0.82 | −0.99 |
| **54**+2(**17**) → 2(**14**)+**60** | −0.30 | −0.15 | −0.17 | −0.20 | −0.22 | −0.57 | −0.49 | −0.38 | −0.26 | −0.32 |
| **55**+**17**+**22** → **14**+**15**+**60** | −1.75 | −1.74 | −1.84 | −1.88 | −1.90 | −2.16 | −2.22 | −1.88 | −1.90 | −2.08 |
| **56**+2(**17**) → **63**+2(**14**) | −0.42 | −0.31 | −0.34 | −0.36 | −0.38 | −0.63 | −0.57 | −0.44 | −0.35 | −0.41 |
| **57**+2(**17**) → **63**+2(**14**) | −1.15 | −0.90 | −0.94 | −0.96 | −0.97 | −1.47 | −1.30 | −1.21 | −0.97 | −1.04 |
| **58**+**17**+**22** → **14**+**15**+**60** | −2.21 | −2.13 | −2.25 | −2.30 | −2.33 | −2.70 | −2.71 | −2.35 | −2.31 | −2.52 |
| **59**+**17**+**22** → **14**+**15**+**60** | −2.19 | −2.08 | −2.21 | −2.27 | −2.31 | −2.69 | −2.68 | −2.34 | −2.27 | −2.52 |

**Table S11**. Hyperhomodesmotic bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+**15** → **18**+**7** | 0.48 | 0.54 | 0.28 | 0.74 | 0.56 | 0.40 | 0.43 | 0.44 | 0.45 | 0.45 |
| **36**+**16** → **19**+**30** | 1.70 | 1.88 | 1.71 | 1.77 | 1.60 | 1.85 | 1.93 | 1.90 | 1.91 | 1.91 |
| **39**+**16** → **23**+**30** | 0.71 | 0.72 | 0.62 | 0.86 | 0.77 | 0.57 | 0.61 | 0.61 | 0.61 | 0.62 |
| **41**+**15** → **23**+**7** | 0.96 | 1.04 | 0.88 | 1.21 | 1.03 | 1.07 | 1.13 | 1.15 | 1.15 | 1.16 |
| **2**+2(**15**) → **18**+**7**+**32** | 0.47 | 0.57 | 0.16 | 0.70 | 0.38 | 0.41 | 0.45 | 0.45 | 0.46 | 0.47 |
| **3**+2(**16**) → **19**+**30**+**31** | 1.73 | 1.96 | 1.73 | 1.83 | 1.66 | 1.92 | 2.00 | 1.97 | 1.98 | 1.99 |
| **10**+2(**16**) → **23**+**30**+**31** | 0.66 | 0.82 | 0.59 | 0.90 | 0.80 | 0.58 | 0.61 | 0.60 | 0.61 | 0.61 |
| **12**+2(**15**) → **23**+**7**+**32** | 0.96 | 1.07 | 0.80 | 1.24 | 1.04 | 1.07 | 1.15 | 1.17 | 1.17 | 1.18 |
| **42**+2(**15**) → 2(**7**)+**18** | 0.75 | 0.91 | 0.48 | 0.99 | 0.63 | 0.56 | 0.58 | 0.59 | 0.59 | 0.59 |
| **43**+2(**16**) → 2(**30**)+**19** | 2.84 | 3.07 | 2.99 | 2.82 | 2.70 | 3.16 | 3.22 | 3.16 | 3.17 | 3.18 |
| **44**+**15**+**16** → **7**+**30**+**23** | 1.39 | 1.53 | 1.32 | 1.59 | 1.37 | 1.35 | 1.41 | 1.40 | 1.41 | 1.41 |
| **45**+**15**+**14** → **21**+**7**+**25** | 0.27 | −0.09 | 0.00 | −0.26 | −0.07 | 0.47 | 0.72 | 0.73 | 0.75 | 0.76 |
| **46**+**15** → **21**+**7** | 0.30 | 0.05 | 0.21 | 0.04 | 0.16 | 0.56 | 0.70 | 0.72 | 0.74 | 0.75 |
| **47**+2(**15**) → **21**+2(**7**) | 0.28 | −0.09 | 0.05 | −0.09 | 0.21 | 0.79 | 1.01 | 1.02 | 1.06 | 1.08 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **35**+**15** → **18**+**7** | 0.51 | 0.57 | 0.58 | 0.59 | 0.59 | 0.33 | 0.40 | 0.48 | 0.42 | 0.45 |
| **36**+**16** → **19**+**30** | 1.87 | 2.18 | 2.03 | 1.97 | 1.90 | 1.56 | 1.88 | 1.62 | 1.94 | 1.69 |
| **39**+**16** → **23**+**30** | 0.83 | 0.95 | 0.91 | 0.85 | 0.78 | 0.61 | 0.72 | 0.67 | 0.79 | 0.63 |
| **41**+**15** → **23**+**7** | 0.93 | 0.98 | 0.99 | 1.00 | 1.01 | 0.78 | 0.86 | 0.92 | 0.86 | 0.91 |
| **2**+2(**15**) → **18**+**7**+**32** | 0.66 | 0.72 | 0.72 | 0.63 | 0.54 | 0.41 | 0.48 | 0.59 | 0.53 | 0.37 |
| **3**+2(**16**) → **19**+**30**+**31** | 2.10 | 2.42 | 2.25 | 2.18 | 2.11 | 1.69 | 2.02 | 1.79 | 2.13 | 1.84 |
| **10**+2(**16**) → **23**+**30**+**31** | 0.97 | 1.10 | 1.04 | 0.97 | 0.89 | 0.71 | 0.81 | 0.78 | 0.91 | 0.72 |
| **12**+2(**15**) → **23**+**7**+**32** | 1.01 | 1.08 | 1.09 | 1.02 | 0.94 | 0.81 | 0.92 | 0.97 | 0.94 | 0.82 |
| **42**+2(**15**) → 2(**7**)+**18** | 0.90 | 0.97 | 0.97 | 0.97 | 0.97 | 0.54 | 0.63 | 0.85 | 0.69 | 0.70 |
| **43**+2(**16**) → 2(**30**)+**19** | 3.33 | 3.80 | 3.51 | 3.40 | 3.28 | 2.74 | 3.23 | 2.87 | 3.35 | 2.86 |
| **44**+**15**+**16** → **7**+**30**+**23** | 1.59 | 1.72 | 1.65 | 1.60 | 1.54 | 1.22 | 1.37 | 1.42 | 1.45 | 1.29 |
| **45**+**15**+**14** → **21**+**7**+**25** | 0.90 | 1.10 | 1.03 | 1.06 | 1.09 | 0.15 | 0.36 | 0.40 | 0.47 | 0.45 |
| **46**+**15** → **21**+**7** | 0.67 | 0.85 | 0.83 | 0.86 | 0.88 | 0.23 | 0.40 | 0.42 | 0.46 | 0.49 |
| **47**+2(**15**) → **21**+2(**7**) | 1.14 | 1.45 | 1.38 | 1.43 | 1.46 | 0.29 | 0.58 | 0.67 | 0.71 | 0.71 |

**Table S12**. Hyperhomodesmotic bond separation reaction energies (kcal mol$^{-1}$) for non-conjugated species (Set B).

| Reaction | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **29**+**14** → 2(**25**) | −0.05 | −0.03 | −0.20 | 0.20 | 0.16 | −0.06 | −0.05 | −0.05 | −0.05 | −0.05 |
| **33**+**14** → **32**+**25** | 0.07 | 0.09 | 0.01 | 0.08 | 0.03 | 0.02 | 0.05 | 0.05 | 0.05 | 0.05 |
| **34**+**14** → **31**+**25** | 0.20 | 0.29 | 0.14 | 0.39 | 0.35 | 0.13 | 0.16 | 0.17 | 0.16 | 0.16 |
| **8**+**15** → **7**+**32** | 0.01 | 0.05 | −0.07 | 0.06 | −0.03 | 0.02 | 0.02 | 0.01 | 0.01 | 0.01 |
| **9**+**16** → **30**+**31** | −0.02 | −0.02 | −0.09 | 0.19 | 0.14 | 0.00 | −0.01 | −0.02 | −0.02 | −0.02 |
| **37**+**14** → 2(**32**) | −0.07 | −0.07 | −0.01 | −0.04 | 0.00 | −0.09 | −0.15 | −0.18 | −0.20 | −0.21 |
| **38**+**14** → 2(**31**) | −4.17 | −3.89 | −4.32 | −3.71 | −4.10 | −4.44 | −4.58 | −4.66 | −4.69 | −4.69 |
| **40**+**14** → **32**+**31** | −1.26 | −1.11 | −1.24 | −1.07 | −1.13 | −1.31 | −1.37 | −1.42 | −1.45 | −1.46 |
| **5**+**14**+**15** → 2(**32**)+**7** | 0.03 | 0.08 | −0.11 | 0.24 | 0.01 | 0.05 | 0.00 | −0.03 | −0.05 | −0.05 |
| **6**+**14**+**16** → 2(**31**)+**30** | −3.66 | −3.35 | −3.83 | −3.15 | −3.70 | −3.85 | −3.93 | −4.00 | −4.02 | −4.02 |
| **11**+**14**+**16** → **31**+**32**+**30** | −1.11 | −0.94 | −1.14 | −0.91 | −1.23 | −1.12 | −1.17 | −1.21 | −1.23 | −1.24 |
| **13**+**14**+**15** → **31**+**32**+**7** | −1.05 | −0.83 | −1.19 | −0.64 | −0.83 | −1.01 | −1.04 | −1.07 | −1.09 | −1.10 |
| **49**+2(**14**) → 2(**32**)+**25** | 0.06 | 0.15 | 0.08 | 0.03 | 0.08 | −0.05 | 0.00 | −0.02 | −0.03 | −0.03 |
| **50**+2(**14**) → 2(**31**)+**25** | −0.14 | −0.04 | −0.24 | 0.00 | −0.06 | −0.52 | −0.53 | −0.58 | −0.60 | −0.60 |
| **51**+2(**14**) → **31**+**32**+**25** | 0.03 | 0.13 | −0.03 | 0.18 | 0.20 | −0.15 | −0.13 | −0.15 | −0.17 | −0.17 |
| **53**+**60** → 2(**61**) | −0.23 | −0.18 | −0.55 | −0.59 | −0.67 | −0.31 | −0.30 | −0.29 | −0.29 | −0.29 |
| **54**+**14** → **61**+**25** | −0.16 | −0.12 | −0.30 | 0.18 | 0.08 | −0.23 | −0.24 | −0.24 | −0.24 | −0.25 |
| **55**+**15** → **62**+**32** | −0.12 | −0.04 | −0.06 | −0.10 | −0.02 | −0.10 | −0.12 | −0.12 | −0.12 | −0.12 |
| **56**+**14** → **64**+**25** | −0.10 | −0.11 | −0.28 | 0.21 | 0.16 | −0.16 | −0.15 | −0.15 | −0.15 | −0.16 |
| **57**+**63** → 2(**64**) | −0.11 | −0.15 | −0.35 | 0.16 | 0.11 | −0.21 | −0.22 | −0.22 | −0.22 | −0.22 |
| **58**+**60** → **62**+**61** | −0.17 | −0.05 | −0.44 | −0.50 | −0.53 | −0.19 | −0.16 | −0.17 | −0.16 | −0.16 |
| **59**+**60** → **62**+**61** | −0.29 | −0.22 | −0.48 | −0.41 | −0.32 | −0.22 | −0.20 | −0.20 | −0.19 | −0.19 |

| Reaction | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| **29**+**14** → 2(**25**) | −0.03 | −0.02 | −0.02 | −0.02 | −0.03 | −0.03 | −0.02 | −0.02 | −0.01 | −0.03 |
| **33**+**14** → **32**+**25** | 0.09 | 0.12 | 0.12 | 0.03 | −0.06 | 0.04 | 0.08 | 0.06 | 0.10 | 0.09 |
| **34**+**14** → **31**+**25** | 0.16 | 0.21 | 0.22 | 0.20 | 0.19 | 0.09 | 0.16 | 0.09 | 0.17 | 0.16 |
| **8**+**15** → **7**+**32** | 0.10 | 0.09 | 0.08 | 0.00 | −0.09 | 0.08 | 0.07 | 0.22 | 0.09 | 0.10 |
| **9**+**16** → **30**+**31** | 0.11 | 0.10 | 0.09 | 0.01 | −0.06 | 0.09 | 0.07 | 0.11 | 0.10 | 0.11 |
| **37**+**14** → 2(**32**) | 0.13 | 0.02 | −0.03 | −0.22 | −0.41 | 0.05 | −0.05 | 0.08 | −0.02 | 0.13 |
| **38**+**14** → 2(**31**) | −3.62 | −3.80 | −3.90 | −3.96 | −4.01 | −3.63 | −3.83 | −3.64 | −3.81 | −3.62 |
| **40**+**14** → **32**+**31** | −0.99 | −1.12 | −1.16 | −1.29 | −1.41 | −0.98 | −1.10 | −0.97 | −1.08 | −0.99 |
| **5**+**14**+**15** → 2(**32**)+**7** | 0.35 | 0.24 | 0.19 | 0.00 | −0.19 | 0.22 | 0.14 | 0.41 | 0.19 | 0.35 |
| **6**+**14**+**16** → 2(**31**)+**30** | −3.02 | −3.17 | −3.26 | −3.37 | −3.48 | −3.07 | −3.22 | −3.05 | −3.18 | −3.02 |
| **11**+**14**+**16** → **31**+**32**+**30** | −0.69 | −0.82 | −0.87 | −1.05 | −1.23 | −0.72 | −0.84 | −0.68 | −0.80 | −0.69 |
| **13**+**14**+**15** → **31**+**32**+**7** | −0.70 | −0.80 | −0.84 | −0.96 | −1.07 | −0.72 | −0.80 | −0.56 | −0.77 | −0.70 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **49**+2(**14**) → 2(**32**)+**25** | 0.15 | 0.19 | 0.17 | −0.01 | −0.20 | 0.03 | 0.09 | 0.08 | 0.14 | 0.15 |
| **50**+2(**14**) → 2(**31**)+**25** | −0.30 | −0.22 | −0.27 | −0.32 | −0.35 | −0.48 | −0.38 | −0.47 | −0.34 | −0.30 |
| **51**+2(**14**) → **31**+**32**+**25** | 0.02 | 0.07 | 0.05 | −0.07 | −0.18 | −0.12 | −0.04 | −0.09 | 0.00 | 0.02 |
| **53**+**60** → 2(**61**) | −0.16 | −0.27 | −0.33 | −0.34 | −0.35 | −0.26 | −0.35 | −0.22 | −0.32 | −0.16 |
| **54**+**14** → **61**+**25** | −0.08 | −0.11 | −0.11 | −0.12 | −0.12 | −0.11 | −0.13 | −0.07 | −0.09 | −0.08 |
| **55**+**15** → **62**+**32** | 0.16 | 0.13 | 0.12 | 0.03 | −0.07 | 0.09 | 0.06 | 0.14 | 0.11 | 0.16 |
| **56**+**14** → **64**+**25** | 0.00 | 0.00 | −0.02 | −0.02 | −0.03 | −0.02 | −0.03 | 0.01 | 0.00 | 0.00 |
| **57**+**63** → 2(**64**) | −0.13 | −0.11 | −0.12 | −0.12 | −0.12 | −0.14 | −0.13 | −0.12 | −0.11 | −0.13 |
| **58**+**60** → **62**+**61** | −0.04 | −0.15 | −0.21 | −0.21 | −0.22 | −0.15 | −0.23 | −0.10 | −0.20 | −0.04 |
| **59**+**60** → **62**+**61** | −0.02 | −0.09 | −0.17 | −0.18 | −0.20 | −0.14 | −0.21 | −0.09 | −0.17 | −0.02 |

**Table S13**. Atomization energies and isogyric, isodesmic, hypohomodesmotic, homodesmotic, and hyperhomodesmotic bond separation reaction energies (kcal mol$^{-1}$) for cyclopentadiene and 1,3-cyclohexadiene.

| | 6-31G(d) B3LYP | B3LYP ZPVE | 6-31G(d) M05-2X | 6-31G(d) M06 | 6-31G(d) M06-2X | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ | HF cc-pV5Z | HF CBS limit |
|---|---|---|---|---|---|---|---|---|---|---|
| **Atomization** | | | | | | | | | | |
| cyclopentadiene | 1172.20 | 1113.91 | 1176.17 | 1178.67 | 1179.70 | 878.79 | 894.07 | 896.16 | 896.73 | 896.91 |
| 1,3-cyclohexadiene | 1467.79 | 1390.71 | 1472.53 | 1476.12 | 1477.40 | 1105.26 | 1123.48 | 1125.89 | 1126.53 | 1126.72 |
| **Isogyric Reactions** | | | | | | | | | | |
| **52**+7(**65**) → 5(**24**) | −164.71 | −125.69 | −170.44 | −164.37 | −162.95 | −178.33 | −174.38 | −173.39 | −173.22 | −173.18 |
| **1**+8(**65**) → 6(**24**) | −180.41 | −138.17 | −185.54 | −178.48 | −176.55 | −195.96 | −192.13 | −191.10 | −190.94 | −190.92 |
| **Isodesmic Reactions** | | | | | | | | | | |
| **52**+5(**24**) → 3(**17**)+2(**22**) | 16.82 | 22.58 | 16.60 | 18.21 | 16.05 | 10.72 | 10.95 | 10.90 | 10.86 | 10.85 |
| **1**+6(**24**) → 4(**17**)+2(**22**) | 20.49 | 26.30 | 20.59 | 22.49 | 20.36 | 14.29 | 14.48 | 14.39 | 14.33 | 14.30 |
| **Hypohomodesmotic Reactions** | | | | | | | | | | |
| **52**+3(**17**)+2(**22**) → 4(**15**)+**14** | −4.56 | −2.39 | −5.01 | −5.66 | −5.90 | −5.28 | −4.99 | −5.01 | −4.99 | −4.97 |
| **1**+4(**17**)+2(**22**) → 4(**15**)+2(**14**) | −2.02 | −0.51 | −2.83 | −3.11 | −3.34 | −2.55 | −2.38 | −2.42 | −2.42 | −2.41 |
| **Homodesmotic Reactions** | | | | | | | | | | |
| **52**+2(**17**)+2(**22**) → 2(**15**)+**14**+**18** | −9.22 | −6.73 | −8.85 | −9.71 | −9.61 | −8.28 | −7.90 | −7.84 | −7.79 | −7.75 |
| **1**+3(**17**)+2(**22**) → 2(**15**)+2(**14**)+**18** | −6.68 | −4.84 | −6.68 | −7.15 | −7.05 | −5.55 | −5.29 | −5.25 | −5.21 | −5.18 |
| **Hyperhomodesmotic Reactions** | | | | | | | | | | |
| **52**+2(**15**)+3(**14**) → 2(**7**)+2(**25**)+**18** | −8.25 | −6.50 | −8.33 | −9.13 | −9.21 | −7.03 | −6.32 | −6.22 | −6.12 | −6.06 |
| **1**+2(**15**)+4(**14**) → **18**+2(**7**)+3(**25**) | −5.70 | −4.71 | −6.20 | −6.70 | −6.77 | −4.27 | −3.63 | −3.55 | −3.47 | −3.41 |

| **Atomization** | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | $E_{FPA}$ (no ZPVE) |
|---|---|---|---|---|---|---|---|---|---|---|
| cyclopentadiene | 1125.91 | 1180.85 | 1197.42 | 1203.14 | 1208.72 | 1081.78 | 1131.03 | 1096.60 | 1150.63 | 1181.88 |
| 1,3-cyclohexadiene | 1406.56 | 1474.00 | 1494.08 | 1500.95 | 1507.68 | 1357.44 | 1418.03 | 1374.59 | 1440.86 | 1478.57 |
| **Isogyric Reactions** | | | | | | | | | | |
| **52**+7(**65**) → 5(**24**) | −151.95 | −151.95 | −150.38 | −149.31 | −148.34 | −161.62 | −162.08 | −155.43 | −155.58 | −151.98 |
| **1**+8(**65**) → 6(**24**) | −166.16 | −166.77 | −165.11 | −163.98 | −162.93 | −176.03 | −177.05 | −169.23 | −169.94 | −166.13 |
| **Isodesmic Reactions** | | | | | | | | | | |
| **52**+5(**24**) → 3(**17**)+2(**22**) | 19.49 | 20.92 | 21.31 | 21.29 | 21.30 | 13.22 | 14.36 | 14.83 | 16.15 | 16.84 |
| **1**+6(**24**) → 4(**17**)+2(**22**) | 22.66 | 24.13 | 24.47 | 24.37 | 24.30 | 17.25 | 18.41 | 18.91 | 20.24 | 20.73 |
| **Hypohomodesmotic Reactions** | | | | | | | | | | |
| **52**+3(**17**)+2(**22**) → 4(**15**)+**14** | −2.26 | −2.20 | −2.29 | −2.20 | −2.10 | −4.82 | −4.86 | −4.21 | −4.23 | −4.12 |
| **1**+4(**17**)+2(**22**) → 4(**15**)+2(**14**) | −1.19 | −1.27 | −1.48 | −1.46 | −1.43 | −2.48 | −2.63 | −1.99 | −2.17 | −2.32 |
| **Homodesmotic Reactions** | | | | | | | | | | |
| **52**+2(**17**)+2(**22**) → 2(**15**)+**14**+**18** | −6.30 | −6.07 | −6.02 | −5.90 | −5.80 | −8.06 | −7.89 | −7.89 | −7.68 | −7.40 |
| **1**+3(**17**)+2(**22**) → 2(**15**)+2(**14**)+**18** | −5.23 | −5.14 | −5.22 | −5.16 | −5.12 | −5.71 | −5.66 | −5.67 | −5.63 | −5.61 |
| **Hyperhomodesmotic Reactions** | | | | | | | | | | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **52**+2(**15**)+3(**14**) → 2(**7**)+2(**25**)+**18** | −5.99 | −5.50 | −5.39 | −5.20 | −5.04 | −7.66 | −7.18 | −7.43 | −7.16 | −6.68 |
| **1**+2(**15**)+4(**14**) → **18**+2(**7**)+3(**25**) | −5.00 | −4.65 | −4.67 | −4.54 | −4.43 | −5.37 | −5.00 | −5.31 | −5.19 | −4.96 |

**Table S14**. Comparison of reaction energies (kcal mol$^{-1}$) for prototype hypohomodesmotic reactions.

| Reaction | | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|---|
| **18+17** → 2(**15**) | (17) | 2.96 | 3.18 | 3.20 |
| **19+17** → 2(**16**) | (18) | −1.88 | −1.29 | −1.11 |
| **23+17** → **15+16** | (19) | −0.18 | 0.19 | 0.08 |
| **18+16** → **23+15** | (20) | 3.14 | 3.00 | 3.12 |
| **21+22** → 2(**20**) | (21) | −1.70 | −1.47 | −1.20 |
| **18+19** → 2(**23**) | (22) | 1.44 | 1.53 | 1.92 |
| **19+15** → **23+16** | (23) | 1.10 | 1.29 | 1.23 |

**Table S15**. Comparison of atomization energies (kcal mol$^{-1}$) for conjugated hydrocarbons (Set A).

| Molecule | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| 1,3-pentadiene | 1239.70 | 1258.54 | 1237.34 |
| 1,3-pentadiyne | 955.41 | 969.40 | 954.29 |
| penta-1-ene-3-yne | 1097.19 | 1113.86 | 1095.40 |
| penta-1-yne-3-ene | 1095.72 | 1111.88 | 1093.56 |
| 1,3-hexadiene | 1516.45 | 1539.62 | 1513.63 |
| 1,3-hexadiyne | 1231.93 | 1250.26 | 1230.33 |
| hexa-1-ene-3-yne | 1373.75 | 1394.70 | 1371.62 |
| hexa-1-yne-3-ene | 1372.46 | 1392.92 | 1369.80 |
| 2,4-hexadiene | 1519.38 | 1542.54 | 1516.65 |
| 2,4-hexadiyne | 1237.78 | 1256.41 | 1236.70 |
| hexa-2-ene-4-yne | 1377.32 | 1398.21 | 1375.19 |
| 1,2,3-hexatriene | 1363.73 | 1385.30 | 1362.04 |
| 1,2,3-pentatriene | 1086.85 | 1104.11 | 1085.66 |
| E-2,3,4-hexatriene | 1366.28 | 1387.83 | 1364.69 |

**Table S16**. Comparison of atomization energies (kcal mol$^{-1}$) for non-conjugated hydrocarbons (Set B).

| Molecule | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| pentane | 1497.68 | 1521.89 | 1495.05 |
| 1-pentene | 1365.60 | 1387.06 | 1362.98 |
| 1-pentyne | 1224.10 | 1242.75 | 1221.61 |
| 2-pentene | 1367.90 | 1389.43 | 1365.43 |
| 2-pentyne | 1227.92 | 1247.15 | 1226.05 |
| 1,4-pentadiene | 1233.20 | 1251.96 | 1230.64 |
| 1,4-pentadiyne | 946.29 | 959.44 | 944.10 |
| penta-1-ene-4-yne | 1090.62 | 1106.56 | 1088.19 |
| 1,4-hexadiene | 1512.79 | 1535.91 | 1509.85 |
| 1,4-hexadiyne | 1228.02 | 1245.86 | 1225.86 |
| hexa-1-ene-4-yne | 1371.96 | 1392.65 | 1369.65 |
| hexa-1-yne-4-ene | 1370.35 | 1390.61 | 1367.54 |
| 1,5-hexadiene | 1510.51 | 1533.50 | 1507.40 |
| 1,5-hexadiyne | 1226.70 | 1244.21 | 1223.91 |
| hexa-1-ene-5-yne | 1368.72 | 1388.96 | 1365.77 |
| 2-ethyl-1-butene | 1645.03 | 1671.03 | 1642.22 |
| 2-methyl-1-pentene | 1645.85 | 1671.75 | 1642.95 |
| 2-methyl-2-pentene | 1647.00 | 1672.95 | 1644.31 |
| 2-methylpentane | 1775.88 | 1804.64 | 1772.97 |
| 3-methylpentane | 1775.19 | 1804.01 | 1772.34 |
| E-3-methyl-2-pentene | 1646.56 | 1672.58 | 1643.92 |
| Z-3-methyl-2-pentene | 1646.51 | 1672.65 | 1643.91 |

**Table S17**. Comarison of Isogyric bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **35**+6(**65**) → 5(**24**) | −101.09 | −101.85 | −98.07 |
| **36**+8(**65**) → 5(**24**) | −177.80 | −177.51 | −172.22 |
| **39**+7(**65**) → 5(**24**) | −139.81 | −139.79 | −135.56 |
| **41**+7(**65**) → 5(**24**) | −141.29 | −141.77 | −137.40 |
| **2**+7(**65**) → 6(**24**) | −113.25 | −114.19 | −109.74 |
| **3**+9(**65**) → 6(**24**) | −190.20 | −190.07 | −184.15 |
| **10**+8(**65**) → 6(**24**) | −152.17 | −152.38 | −147.31 |
| **12**+8(**65**) → 6(**24**) | −153.46 | −154.15 | −149.13 |
| **42**+7(**65**) → 6(**24**) | −110.32 | −111.27 | −106.73 |
| **43**+9(**65**) → 6(**24**) | −184.34 | −183.93 | −177.78 |
| **44**+8(**65**) → 6(**24**) | −148.60 | −148.86 | −143.74 |
| **45**+8(**65**) → 6(**24**) | −162.18 | −161.77 | −156.89 |
| **46**+9(**65**) → 5(**24**) | −150.15 | −149.54 | −145.30 |
| **47**+8(**65**) → 6(**24**) | −159.64 | −159.24 | −154.24 |

**Table S18**. Comparison of isogyric bond separation reaction energies (kcal mol$^{-1}$) for non-conjugated species (Set B).

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **29**+4(**65**) → 5(**24**) | −50.69 | −51.98 | −49.25 |
| **33**+5(**65**) → 5(**24**) | −78.98 | −80.07 | −76.87 |
| **34**+6(**65**) → 5(**24**) | −116.69 | −117.63 | −113.80 |
| **8**+5(**65**) → 5(**24**) | −76.68 | −77.70 | −74.43 |
| **9**+6(**65**) → 5(**24**) | −112.87 | −113.24 | −109.35 |
| **37**+6(**65**) → 5(**24**) | −107.59 | −108.43 | −104.77 |
| **38**+8(**65**) → 5(**24**) | −186.92 | −187.47 | −182.42 |
| **40**+7(**65**) → 5(**24**) | −146.38 | −147.09 | −142.77 |
| **5**+7(**65**) → 6(**24**) | −116.92 | −117.90 | −113.52 |
| **6**+9(**65**) → 6(**24**) | −194.11 | −194.48 | −188.62 |
| **11**+8(**65**) → 6(**24**) | −153.96 | −154.42 | −149.28 |
| **13**+8(**65**) → 6(**24**) | −155.57 | −156.46 | −151.39 |
| **49**+7(**65**) → 6(**24**) | −119.19 | −120.32 | −115.98 |
| **50**+9(**65**) → 6(**24**) | −195.43 | −196.13 | −190.57 |
| **51**+8(**65**) → 6(**24**) | −157.19 | −158.12 | −153.16 |
| **53**+6(**65**) → 6(**24**) | −88.46 | −89.53 | −85.60 |
| **54**+6(**65**) → 6(**24**) | −87.64 | −88.80 | −84.88 |
| **55**+6(**65**) → 6(**24**) | −86.49 | −87.60 | −83.52 |
| **56**+5(**65**) → 6(**24**) | −61.41 | −62.65 | −59.30 |
| **57**+5(**65**) → 6(**24**) | −62.09 | −63.28 | −59.93 |
| **58**+6(**65**) → 6(**24**) | −86.94 | −87.97 | −83.91 |
| **59**+6(**65**) → 6(**24**) | −86.99 | −87.90 | −83.91 |

**Table S19**. Comparison of isodesmic bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **35**+3(**24**) → 2(**17**)+2(**22**) | 19.62 | 20.57 | 20.61 |
| **36**+3(**24**) → 2(**17**)+2(**26**) | 22.78 | 25.31 | 25.69 |
| **39**+3(**24**) → 2(**17**)+**22**+**26** | 20.84 | 22.83 | 22.73 |
| **41**+3(**24**) → 2(**17**)+**22**+**26** | 19.36 | 20.86 | 20.90 |
| **2**+4(**24**) → 3(**17**)+2(**22**) | 22.32 | 23.59 | 23.60 |
| **3**+4(**24**) → 3(**17**)+2(**26**) | 25.25 | 28.10 | 28.41 |
| **10**+4(**24**) → 3(**17**)+**22**+**26** | 23.34 | 25.60 | 25.64 |
| **12**+4(**24**) → 3(**17**)+**22**+**26** | 22.05 | 23.83 | 23.83 |
| **42**+4(**24**) → 3(**17**)+2(**22**) | 25.25 | 26.51 | 26.61 |
| **43**+4(**24**) → 3(**17**)+2(**26**) | 31.10 | 34.25 | 34.78 |
| **44**+4(**24**) → 3(**17**)+**22**+**26** | 26.91 | 29.11 | 29.21 |
| **45**+4(**24**) → 2(**17**)+3(**22**) | 4.02 | 6.50 | 6.47 |
| **46**+3(**24**) → **17**+3(**22**) | 1.18 | 3.38 | 3.40 |
| **47**+4(**24**) → 2(**17**)+3(**22**) | 6.56 | 9.03 | 9.12 |

**Table S20**. Comparison of isodesmic bond separation reaction energies (kcal mol$^{-1}$) for non-conjugated species (Set B).

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **29**+3(**24**) → 4(**17**) | 8.77 | 9.45 | 9.38 |
| **33**+3(**24**) → **22**+3(**17**) | 11.11 | 11.86 | 11.78 |
| **34**+3(**24**) → **26**+3(**17**) | 13.32 | 14.49 | 14.47 |
| **8**+3(**24**) → 3(**17**)+**22** | 13.40 | 14.23 | 14.23 |
| **9**+3(**24**) → 3(**17**)+**26** | 17.15 | 18.88 | 18.92 |
| **37**+3(**24**) → 2(**22**)+2(**17**) | 13.11 | 13.99 | 13.91 |
| **38**+3(**24**) → 2(**26**)+2(**17**) | 13.67 | 15.36 | 15.49 |
| **40**+3(**24**) → **22**+**26**+2(**17**) | 14.26 | 15.53 | 15.53 |
| **5**+4(**24**) → 3(**17**)+**2(22)** | 18.65 | 19.88 | 19.81 |
| **6**+4(**24**) → 3(**17**)+**2(26)** | 21.33 | 23.70 | 23.94 |
| **11**+4(**24**) → 3(**17**)+**22**+**26** | 21.55 | 23.56 | 23.67 |
| **13**+4(**24**) → 3(**17**)+**22**+**26** | 19.94 | 21.52 | 21.56 |
| **49**+4(**24**) → 2(**22**)+3(**17**) | 16.38 | 17.46 | 17.36 |
| **50**+4(**24**) → 2(**26**)+3(**17**) | 20.02 | 22.05 | 21.99 |
| **51**+4(**24**) → **22**+**26**+3(**17**) | 18.32 | 19.86 | 19.79 |
| **53**+4(**24**) → 4(**17**)+**22** | 16.48 | 17.75 | 17.71 |
| **54**+4(**24**) → 4(**17**)+**22** | 17.30 | 18.48 | 18.44 |
| **55**+4(**24**) → 4(**17**)+**22** | 18.45 | 19.68 | 19.80 |
| **56**+4(**24**) → 5(**17**) | 12.91 | 14.13 | 13.99 |
| **57**+4(**24**) → 5(**17**) | 12.22 | 13.50 | 13.36 |
| **58**+4(**24**) → 4(**17**)+**22** | 18.01 | 19.31 | 19.41 |
| **59**+4(**24**) → 4(**17**)+**22** | 17.96 | 19.37 | 19.40 |

**Table S21**. Comparison of hypohomodesmotic bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **35**+**17**+**22** → 3(**15**) | 3.30 | 3.62 | 3.66 |
| **36**+**17**+**26** → 3(**16**) | −0.74 | −0.32 | −0.18 |
| **39**+**17**+**26** → **15**+2(**16**) | −0.28 | 0.09 | −0.17 |
| **41**+**17**+**22** → 2(**15**)+**16** | 0.65 | 1.01 | 0.97 |
| **2**+2(**17**)+**22** → 3(**15**)+**14** | 3.20 | 3.67 | 3.67 |
| **3**+2(**17**)+**26** → 3(**16**)+**14** | −1.07 | −0.50 | −0.42 |
| **10**+2(**17**)+**26** → **15**+2(**16**)+**14** | −0.58 | −0.11 | −0.22 |
| **12**+2(**17**)+**22** → 2(**15**)+**16**+**14** | 0.53 | 1.02 | 0.93 |
| **42**+**17**+2(**22**) → 4(**15**) | 3.50 | 3.91 | 4.00 |
| **43**+**17**+2(**26**) → 4(**16**) | −0.25 | 0.07 | 0.29 |
| **44**+**17**+**22**+**26** → 2(**15**)+**2(16**) | 0.36 | 0.73 | 0.66 |
| **45**+2(**22**)+**17** → 2(**20**)+**15**+**14** | 1.20 | 1.58 | 1.51 |
| **46**+2(**22**) → 2(**20**)+**15** | 1.17 | 1.42 | 1.41 |
| **47**+3(**22**) → 2(**20**)+2(**15**) | 1.11 | 1.43 | 1.48 |

**Table S22**. Comparison of homodesmotic bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **35**+**22** → **18**+**15** | 0.35 | 0.44 | 0.46 |
| **36**+**26** → **19**+**16** | 1.14 | 0.96 | 0.93 |
| **39**+**26** → **23**+**16** | −0.09 | −0.09 | −0.25 |
| **41**+**22** → **23**+**15** | 0.83 | 0.83 | 0.89 |
| **2**+**22**+**17** → **18**+**14**+**15** | 0.25 | 0.49 | 0.47 |
| **3**+**26**+**17** → **19**+**14**+**16** | 0.80 | 0.79 | 0.69 |
| **10**+**26**+**17** → **23**+**14**+**16** | −0.40 | −0.29 | −0.30 |
| **12**+**22**+**17** → **23**+**14**+**15** | 0.71 | 0.83 | 0.85 |
| **42**+2(**22**) → 2(**15**)+**18** | 0.54 | 0.72 | 0.81 |
| **43**+2(**26**) → 2(**16**)+**19** | 1.62 | 1.36 | 1.41 |
| **44**+**22**+**26** → **15**+**16**+**23** | 0.54 | 0.54 | 0.58 |
| **45**+**22**+**17** → **21**+**15**+**14** | 0.10 | 0.29 | 0.29 |
| **46**+**22** → **21**+**15** | 0.07 | 0.14 | 0.18 |
| **47**+2(**22**) → **21**+2(**15**) | 0.01 | 0.14 | 0.25 |

**Table S23**. Comparison of homodesmotic bond separation reaction energies (kcal mol$^{-1}$) for non-conjugated species (Set B).

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **29**+2(**17**) → 3(**14**) | 0.36 | 0.55 | 0.47 |
| **33**+2(**17**) → **15**+2(**14**) | 0.06 | 0.27 | 0.19 |
| **34**+2(**17**) → **16**+2(**14**) | −0.12 | 0.01 | −0.09 |
| **8**+**17**+**22** → 2(**15**)+**14** | −0.28 | −0.04 | −0.04 |
| **9**+**26**+**17** → 2(**16**)+**14** | −1.33 | −1.17 | −1.30 |
| **37**+2(**17**) → 2(**15**)+**14** | −0.56 | −0.27 | −0.36 |
| **38**+2(**17**) → 2(**16**)+**14** | −4.81 | −4.70 | −4.72 |
| **40**+2(**17**) → **15**+**16**+**14** | −1.82 | −1.63 | −1.72 |
| **5**+2(**17**)+**22** → 3(**15**)+**14** | −0.46 | −0.04 | −0.11 |
| **6**+2(**17**)+**26** → 3(**16**)+**14** | −4.99 | −4.90 | −4.90 |
| **11**+2(**17**)+**26** → 2(**16**)+**15**+**14** | −2.37 | −2.15 | −2.20 |
| **13**+2(**17**)+**22** → **16**+2(**15**)+**14** | −1.58 | −1.29 | −1.33 |
| **49**+3(**17**) → 2(**15**)+2(**14**) | −0.10 | 0.23 | 0.12 |
| **50**+3(**17**) → 2(**16**)+2(**14**) | −1.27 | −0.97 | −1.19 |
| **51**+3(**17**) → **15**+**16**+2(**14**) | −0.57 | −0.27 | −0.42 |
| **53**+2(**17**) → 2(**14**)+**60** | −1.06 | −0.70 | −0.83 |
| **54**+2(**17**) → 2(**14**)+**60** | −0.24 | 0.02 | −0.11 |
| **55**+**17**+**22** → **14**+**15**+**60** | −1.73 | −1.46 | −1.43 |
| **56**+2(**17**) → **63**+2(**14**) | −0.25 | 0.13 | −0.04 |
| **57**+2(**17**) → **63**+2(**14**) | −0.94 | −0.50 | −0.67 |
| **58**+**17**+**22** → **14**+**15**+**60** | −2.17 | −1.83 | −1.82 |
| **59**+**17**+**22** → **14**+**15**+**60** | −2.22 | −1.76 | −1.82 |

**Table S24**. Comparison of hyperhomodesmotic bond separation reaction energies (kcal mol$^{-1}$) for conjugated species (Set A).

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **35**+**15** → **18**+**7** | 0.51 | 0.50 | 0.48 |
| **36**+**16** → **19**+**30** | 1.87 | 1.83 | 1.75 |
| **39**+**16** → **23**+**30** | 0.64 | 0.77 | 0.57 |
| **41**+**15** → **23**+**7** | 0.99 | 0.89 | 0.91 |
| **2**+2(**15**) → **18**+**7**+**32** | 0.47 | 0.67 | 0.65 |
| **3**+2(**16**) → **19**+**30**+**31** | 2.07 | 2.07 | 2.05 |
| **10**+2(**16**) → **23**+**30**+**31** | 0.87 | 0.99 | 1.05 |
| **12**+2(**15**) → **23**+**7**+**32** | 0.93 | 1.01 | 1.02 |
| **42**+2(**15**) → 2(**7**)+**18** | 0.87 | 0.84 | 0.86 |
| **43**+2(**16**) → 2(**30**)+**19** | 3.09 | 3.09 | 3.03 |
| **44**+**15**+**16** → **7**+**30**+**23** | 1.44 | 1.46 | 1.42 |
| **45**+**15**+**14** → **21**+**7**+**25** | 0.09 | 0.08 | 0.08 |
| **46**+**15** → **21**+**7** | 0.24 | 0.19 | 0.21 |
| **47**+2(**15**) → **21**+2(**7**) | 0.34 | 0.25 | 0.30 |

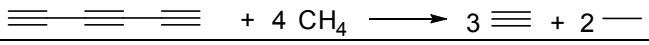
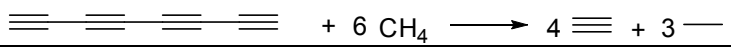
**Table S25**. Comparison of hyperhomodesmotic bond separation reaction energies (kcal mol$^{-1}$) for non-conjugated species (Set B).

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **29**+**14** → 2(**25**) | 0.00 | 0.00 | 0.02 |
| **33**+**14** → **32**+**25** | −0.06 | 0.12 | 0.11 |
| **34**+**14** → **31**+**25** | 0.24 | 0.15 | 0.22 |
| **8**+**15** → **7**+**32** | −0.06 | 0.14 | 0.13 |
| **9**+**16** → **30**+**31** | −0.06 | 0.11 | 0.06 |
| **37**+**14** → 2(**32**) | −0.45 | −0.03 | −0.06 |
| **38**+**14** → 2(**31**) | −3.74 | −3.87 | −3.64 |
| **40**+**14** → **32**+**31** | −1.22 | −1.09 | −1.03 |
| **5**+**14**+**15** → 2(**32**)+**7** | −0.19 | 0.26 | 0.22 |
| **6**+**14**+**16** → 2(**31**)+**30** | −3.18 | −3.20 | −3.00 |
| **11**+**14**+**16** → **31**+**32**+**30** | −1.04 | −0.75 | −0.69 |
| **13**+**14**+**15** → **31**+**32**+**7** | −0.82 | −0.70 | −0.62 |
| **49**+2(**14**) → 2(**32**)+**25** | −0.16 | 0.20 | 0.18 |
| **50**+2(**14**) → 2(**31**)+**25** | −0.38 | −0.41 | −0.33 |
| **51**+2(**14**) → **31**+**32**+**25** | −0.15 | −0.01 | 0.04 |
| **53**+**60** → 2(**61**) | −0.37 | −0.23 | −0.27 |
| **54**+**14** → **61**+**25** | −0.07 | −0.02 | −0.06 |
| **55**+**15** → **62**+**32** | −0.02 | 0.20 | 0.18 |
| **56**+**14** → **64**+**25** | −0.04 | 0.07 | 0.00 |
| **57**+**63** → 2(**64**) | −0.15 | −0.07 | −0.13 |
| **58**+**60** → **62**+**61** | −0.17 | −0.06 | −0.08 |
| **59**+**60** → **62**+**61** | −0.22 | 0.01 | −0.08 |

**Table S26**. Comparison of atomization energies and isogyric, isodesmic, hypohomodesmotic, homodesmotic, and hyperhomodesmotic bond separation reaction energies (kcal $mol^{-1}$) for cyclopentadiene and 1,3-cyclohexadiene.

| Reaction | $E_{FPA}$ | G3 | CBS-QB3 |
|---|---|---|---|
| **Atomization** | | | |
| cyclopentadiene | 1123.58 | 1139.02 | 1121.33 |
| 1,3-cyclohexadiene | 1401.49 | 1421.77 | 1398.99 |
| **Isogyric Reactions** | | | |
| **52**+7(**65**) → 5(**24**) | −112.97 | −114.63 | −109.63 |
| **1**+8(**65**) → 6(**24**) | −123.89 | −125.30 | −119.94 |
| **Isodesmic Reactions** | | | |
| **52**+5(**24**) → 3(**17**)+2(**22**) | 22.61 | 23.15 | 23.71 |
| **1**+6(**24**) → 4(**17**)+2(**22**) | 26.55 | 27.83 | 28.06 |
| **Hypohomodesmotic Reactions** | | | |
| **52**+3(**17**)+2(**22**) → 4(**15**)+**14** | −1.95 | −2.42 | −1.86 |
| **1**+4(**17**)+2(**22**) → 4(**15**)+2(**14**) | −0.81 | −0.70 | −0.49 |
| **Homodesmotic Reactions** | | | |
| **52**+2(**17**)+2(**22**) → 2(**15**)+**14**+**18** | −4.90 | −5.60 | −5.06 |
| **1**+3(**17**)+2(**22**) → 2(**15**)+2(**14**)+**18** | −3.77 | −3.88 | −3.69 |
| **Hyperhomodesmotic Reactions** | | | |
| **52**+2(**15**)+3(**14**) → 2(**7**)+2(**25**)+**18** | −4.93 | −6.03 | −5.47 |
| **1**+2(**15**)+4(**14**) → **18**+2(**7**)+3(**25**) | −3.97 | −4.59 | −4.32 |

**Table S27**. Incremental valence focal point table (kcal mol$^{-1}$) for the isodesmic bond separation reactions of 1,3,5-hexatriyne and 1,3,5,7-octatetrayne.[a]

| Basis Set | $\Delta E_e$[RHF] | +δ[MP2] | +δ[CCSD] | +δ[CCSD(T)] | +δ[CCSDT] | ΔE(V) |
|---|---|---|---|---|---|---|
|  | | | | | | |
| cc-pVDZ | 25.1 | +10.29 | −9.01 | +2.83 | −0.46 | [+28.75] |
| cc-pVTZ | 24.37 | +12.24 | −9.32 | +2.91 | [−0.46] | [+29.74] |
| cc-pVQZ | 23.95 | +12.05 | −9.28 | +2.98 | [−0.46] | [+29.23] |
| cc-pV5Z | 23.85 | +11.57 | [−8.86] | [+3.01] | [−0.46] | [+29.10] |
| CBS Limit | [+23.82] | [+11.07] | [−8.42] | [+3.03] | [−0.46] | [+29.03] |
| $\Delta E^{FPA}$ = ΔE(V) + ΔE(core) + ΔE(ZPVE) = 29.03 + 2.23 + 0.43 = 31.69 kcal mol$^{-1}$; | | | | | | |
| $\Delta H_f^{0K}$ ($C_6H_2$)= **163.4 ± 2.1** kcal mol$^{-1}$; $\Delta H_f^{298K}$ ($C_6H_2$)= **164.9 ± 2.1** kcal mol$^{-1}$ | | | | | | |
|  | | | | | | |
| cc-pVDZ | 37.93 | +17.10 | −14.8 | +4.64 | −0.78 | [+44.08] |
| cc-pVTZ | 36.71 | +20.13 | −15.28 | +4.78 | [−0.78] | [+45.56] |
| cc-pVQZ | 36.08 | +19.82 | −15.22 | +4.88 | [−0.78] | [+44.78] |
| cc-pV5Z | 35.93 | +19.09 | [−14.59] | [+4.92] | [−0.78] | [+44.57] |
| CBS Limit | [+35.88] | [+18.32] | [−13.92] | [+4.96] | [−0.78] | [+44.46] |
| $\Delta E^{FPA}$ = ΔE(V) + ΔE(core) + ΔE(ZPVE) = 44.46 + 0.65 + 3.49 = 48.62 kcal mol$^{-1}$; | | | | | | |
| $\Delta H_f^{0K}$ ($C_8H_2$)= **216.6 ± 4.0** kcal mol$^{-1}$; $\Delta H_f^{298K}$ ($C_8H_2$)= **219.4 ± 4.0** kcal mol$^{-1}$ | | | | | | |
| Fit | $a+be^{-cX}$ | $a+bX^{-3}$ | $a+bX^{-3}$ | $a+bX^{-3}$ | additive | |
| Points (X=) | 3,4,5 | 4,5 | 3,4 | 3,4 | | |

[a] The symbol δ denotes the increment in the energy difference (ΔE) with respect to the previous level of theory. Bracketed numbers are the result of basis set extrapolations (using the fits denoted in the table), while unbracketed numbers were explicitly computed. All energies evaluated at frozen-core CCSD(T)/TZ(2d1f,2p1d) optimized geometries.

[b] Reference enthalpies of formation (kcal mol$^{-1}$, from Gurvich, L. V.; Veyts, I. V.; Alcock, C. B. *Thermodynamic Properties of Individual Substances*; Fourth ed.; Hemisphere Pub. Co.: New York, 1989.) were as follows: $\Delta H_f^{0K}$ (methane) = -15.92; $\Delta H_f^{298K}$ (methane) = -17.83; $\Delta H_f^{0K}$ (ethane) = -16.34; $\Delta H_f^{298K}$ (ethane) = -20.08.

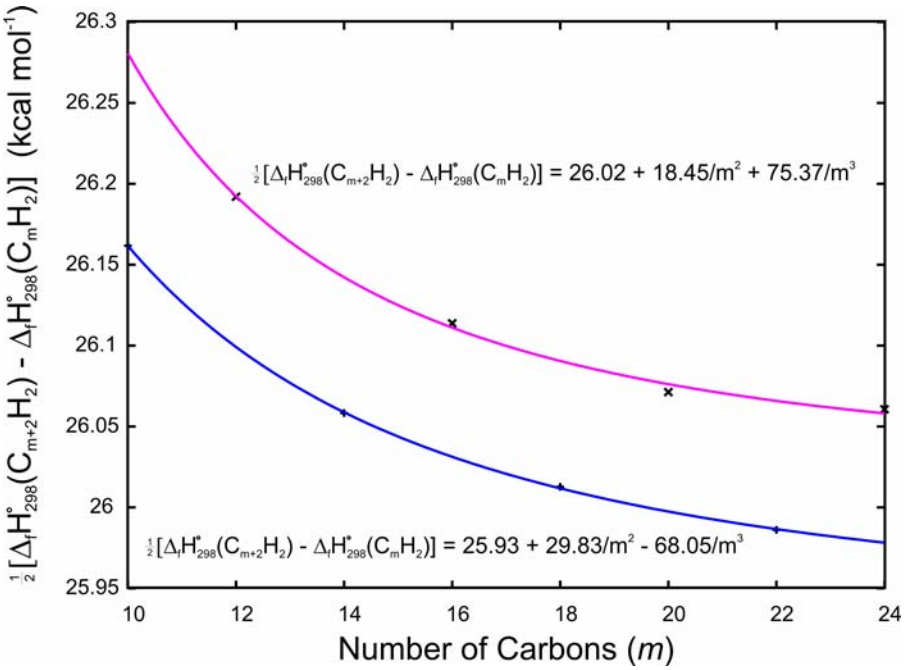



**Figure S1**. Extrapolation of differences in polyyne enthalpies of formation.

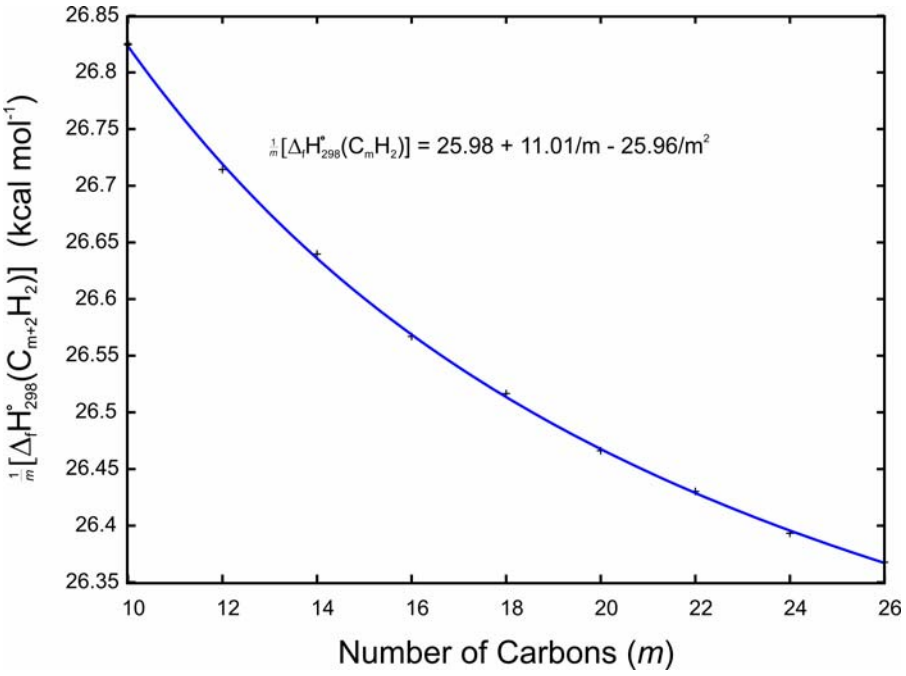



**Figure S2**. Extrapolation of polyyne enthalpies of formation.

**Table S28**. Collection A of absolute energies (hartree). All energies computed at B3LYP/6-31G(d) optimized geometries.

| | Molecule | B3LYP 6-31G(d) | B3LYP ZPVE | M05-2X 6-31G(d) | M06 6-31G(d) | M06-2X 6-31G(d) | HF cc-pVDZ | HF cc-pVTZ | HF cc-pVQZ |
|---|---|---|---|---|---|---|---|---|---|
| **1** | 1,3-cyclohexadiene | −233.418936 | 77.08 | −233.382209 | −233.223872 | −233.301303 | −231.850073 | −231.909103 | −231.923566 |
| **2** | 1,3-hexadiene | −234.625745 | 89.53 | −234.575626 | −234.419731 | −234.493673 | −233.013322 | −233.076169 | −233.090950 |
| **3** | 1,3-hexadiyne | −232.123700 | 60.13 | −232.082098 | −231.934348 | −232.009904 | −230.594759 | −230.657041 | −230.671111 |
| **5** | 1,4-hexadiene | −234.617288 | 89.26 | −234.568744 | −234.411866 | −234.486827 | −233.007549 | −233.070476 | −233.085312 |
| **6** | 1,4-hexadiyne | −232.109379 | 59.08 | −232.071561 | −231.922129 | −231.999471 | −230.590541 | −230.653189 | −230.667611 |
| **7** | 2-butene | −157.226916 | 68.11 | −157.187872 | −157.084994 | −157.132046 | −156.123479 | −156.167000 | −156.177045 |
| **8** | 2-pentene | −196.540443 | 86.21 | −196.494129 | −196.364874 | −196.424251 | −195.160610 | −195.214436 | −195.226870 |
| **9** | 2-pentyne | −195.292535 | 71.42 | −195.250893 | −195.126026 | −195.186290 | −193.957835 | −194.011510 | −194.023770 |
| **10** | hexa-1-ene-3-yne | −233.374159 | 74.69 | −233.328479 | −233.176428 | −233.251670 | −231.805426 | −231.867958 | −231.882442 |
| **11** | hexa-1-ene-4-yne | −233.367630 | 74.33 | −233.323893 | −233.170979 | −233.246623 | −231.802943 | −231.865730 | −231.880379 |
| **12** | hexa-1-yne-3-ene | −233.368181 | 74.26 | −233.324242 | −233.171105 | −233.247348 | −231.800755 | −231.863363 | −231.877857 |
| **13** | hexa-1-yne-4-ene | −233.361386 | 74.00 | −233.318981 | −233.165195 | −233.242277 | −231.797811 | −231.860683 | −231.875326 |
| **14** | propane | −119.144248 | 65.34 | −119.108383 | −119.032201 | −119.064425 | −118.272401 | −118.307186 | −118.314807 |
| **15** | propene | −117.907562 | 50.26 | −117.876690 | −117.799110 | −117.834699 | −117.082199 | −117.115839 | −117.123510 |
| **16** | propyne | −116.653270 | 34.96 | −116.628888 | −116.554193 | −116.591749 | −115.874005 | −115.907501 | −115.914972 |
| **17** | ethane | −79.830418 | 47.21 | −79.801700 | −79.751724 | −79.771828 | −79.234876 | −79.259434 | −79.264650 |
| **18** | 1,3-butadiene | −155.992138 | 53.64 | −155.957812 | −155.852940 | −155.903477 | −154.934300 | −154.976885 | −154.986885 |
| **19** | 1,3-butadiyne | −153.481644 | 23.91 | −153.457196 | −153.359891 | −153.412945 | −152.507875 | −152.549829 | −152.559149 |
| **20** | allene | −116.657673 | 34.81 | −116.630792 | −116.554548 | −116.591860 | −115.872306 | −115.905027 | −115.912501 |
| **21** | butatriene | −154.730753 | 38.04 | −154.696919 | −154.598058 | −154.647292 | −153.703637 | −153.745466 | −153.755123 |
| **22** | ethene | −78.587458 | 32.15 | −78.565005 | −78.512563 | −78.536852 | −78.039978 | −78.063548 | −78.068817 |
| **23** | vinylacetylene | −154.733801 | 38.39 | −154.705405 | −154.603457 | −154.656091 | −153.720680 | −153.762960 | −153.772660 |
| **24** | methane | −40.518383 | 28.37 | −40.497902 | −40.473999 | −40.482027 | −40.198694 | −40.213133 | −40.215933 |
| **25** | butane | −158.458056 | 83.36 | −158.415148 | −158.312880 | −158.357204 | −157.309876 | −157.354806 | −157.364833 |
| **26** | acetylene | −77.325646 | 16.71 | −77.311050 | −77.260069 | −77.287767 | −76.825632 | −76.849016 | −76.854017 |
| **29** | pentane | −197.771782 | 59.93 | −197.721597 | −197.593871 | −197.650245 | −196.347254 | −196.402347 | −196.414780 |
| **30** | 2-butyne | −155.978959 | 44.23 | −155.944904 | −155.846292 | −155.894076 | −154.920590 | −154.963920 | −154.973780 |
| **31** | 1-butyne | −155.966883 | 101.37 | −155.935014 | −155.833629 | −155.883732 | −154.911244 | −154.955110 | −154.964991 |
| **32** | 1-butene | −157.221067 | 53.09 | −157.183062 | −157.078896 | −157.126944 | −156.119294 | −156.163249 | −156.173316 |
| **33** | 1-pentene | −196.534980 | 53.30 | −196.489845 | −196.359706 | −196.419763 | −195.156798 | −195.210946 | −195.223422 |
| **34** | 1-pentyne | −195.281016 | 68.41 | −195.241999 | −195.114934 | −195.177069 | −193.948924 | −194.002992 | −194.015281 |
| **35** | 1,3-pentadiene | −195.312252 | 86.40 | −195.269434 | −195.140009 | −195.201715 | −193.976214 | −194.028737 | −194.041126 |
| **36** | 1,3-pentadiyne | −192.810039 | 71.24 | −192.775944 | −192.654811 | −192.717825 | −191.557413 | −191.609315 | −191.620983 |
| **37** | 1,4-pentadiene | −195.297771 | 71.42 | −195.257726 | −195.125526 | −195.189459 | −193.966041 | −194.019075 | −194.031532 |
| **38** | 1,4-pentadiyne | −192.782878 | 41.84 | −192.754753 | −192.629142 | −192.696512 | −191.543007 | −191.595740 | −191.607750 |
| **39** | penta-1-ene-3-yne | −194.060617 | 71.47 | −194.022410 | −193.896927 | −193.959644 | −192.768179 | −192.820353 | −192.832437 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **40** | penta-1-ene-4-yne | −194.041694 | 40.99 | −194.007717 | −193.878619 | −193.944456 | −192.756053 | −192.808984 | −192.821235 |
| **41** | penta-1-yne-3-ene | −194.054687 | 56.50 | −194.017989 | −193.891270 | −193.955086 | −192.763658 | −192.815923 | −192.828021 |
| **42** | 2,4-hexadiene | −234.632033 | 56.22 | −234.580936 | −234.426279 | −234.499175 | −233.017752 | −233.080139 | −233.094892 |
| **43** | 2,4-hexadiyne | −232.137552 | 56.16 | −232.093999 | −231.948585 | −232.021907 | −230.606081 | −230.667804 | −230.681805 |
| **44** | hexa-2-ene-4-yne | −233.381051 | 89.16 | −233.334700 | −233.183977 | −233.257950 | −231.810700 | −231.872788 | −231.887238 |
| **45** | 1,2,3-hexatriene | −233.364347 | 59.92 | −233.314868 | −233.164212 | −233.237315 | −231.783139 | −231.845390 | −231.859845 |
| **46** | 1,2,3-pentatriene | −194.050585 | 74.21 | −194.008442 | −193.884006 | −193.944898 | −192.745816 | −192.797741 | −192.809798 |
| **47** | E-2,3,4-hexatriene | −233.369905 | 74.27 | −233.319357 | −233.169678 | −233.242316 | −231.787452 | −231.849393 | −231.863824 |
| **48** | Z-2,3,4-hexatriene | −233.369901 | 56.14 | −233.319348 | −233.169515 | −233.241974 | −231.787448 | −231.849376 | −231.863803 |
| **49** | 1,5-hexadiene | −234.611790 | 74.10 | −234.564637 | −234.406324 | −234.482374 | −233.003575 | −233.066927 | −233.081826 |
| **50** | 1,5-hexadiyne | −232.103102 | 74.10 | −232.068033 | −231.915730 | −231.995715 | −230.586736 | −230.649804 | −230.664274 |
| **51** | Hexa-1-ene-5-yne | −233.357551 | 89.42 | −233.316414 | −233.161285 | −233.239341 | −231.795365 | −231.858588 | −231.873282 |
| **52** | cyclopentadiene | −194.101058 | 59.20 | −194.072055 | −193.939319 | −194.004633 | −192.808199 | −192.857189 | −192.869287 |
| **53** | 2-ethyl-1-butene | −235.851868 | 74.29 | −235.800893 | −235.645789 | −235.717232 | −234.194792 | −234.259019 | −234.273851 |
| **54** | 2-methyl-1-pentene | −235.853309 | 58.29 | −235.801864 | −235.647564 | −235.718790 | −234.196685 | −234.260846 | −234.275717 |
| **55** | 2-methyl-2-pentene | −235.856908 | 104.42 | −235.804078 | −235.649566 | −235.720494 | −234.198050 | −234.262025 | −234.276851 |
| **56** | 2-methylpentane | −237.084759 | 104.27 | −237.029426 | −236.876091 | −236.944281 | −235.383066 | −235.448276 | −235.463100 |
| **57** | 3-methylpentane | −237.083253 | 103.98 | −237.028391 | −236.875354 | −236.943410 | −235.381009 | −235.446144 | −235.460960 |
| **58** | E-3-methyl-2-pentene | −235.855791 | 119.12 | −235.803298 | −235.649279 | −235.719857 | −234.196536 | −234.260423 | −234.275226 |
| **59** | Z-3-methyl-2-pentene | −235.855600 | 119.18 | −235.803222 | −235.649427 | −235.720201 | −234.196486 | −234.260371 | −234.275178 |
| **60** | 2-methylpropene | −157.227288 | 103.99 | −157.189382 | −157.086461 | −157.133461 | −156.123860 | −156.167727 | −156.177822 |
| **61** | 2-methyl-1-butene | −196.539764 | 104.04 | −196.495573 | −196.366597 | −196.425884 | −195.159573 | −195.213609 | −195.226072 |
| **62** | 2-methyl-2-butene | −196.543587 | 68.09 | −196.497801 | −196.369941 | −196.428287 | −195.161122 | −195.214804 | −195.227241 |
| **63** | Isobutene | −158.458808 | 86.29 | −158.417263 | −158.315056 | −158.359253 | −157.310346 | −157.355306 | −157.365329 |
| **64** | Isopentane | −197.771116 | 85.91 | −197.723104 | −197.595082 | −197.651244 | −196.345847 | −196.400899 | −196.413317 |
| **65** | $H_2$ | −1.175482 | 83.03 | −1.163691 | −1.166962 | −1.163690 | −1.128727 | −1.132940 | −1.133437 |
| | H | −0.500273 | 101.08 | −0.497906 | −0.497919 | −0.496666 | −0.499278 | −0.499810 | −0.499946 |
| | C | −37.846280 | 6.37 | −37.842055 | −37.814695 | −37.828932 | −37.682418 | −37.686708 | −37.688298 |

**Table S29**. Collection B of absolute energies (hartree). All energies computed at B3LYP/6-31G(d) optimized geometries.

| | Molecule | HF cc-pV5Z | HF CBS limit | MP2 cc-pVDZ | MP2 cc-pVTZ | MP2 cc-pVQZ | MP2 cc-pV5Z | MP2 CBS limit | CCSD cc-pVDZ |
|---|---|---|---|---|---|---|---|---|---|
| **1** | 1,3-cyclohexadiene | −231.927048 | −231.928152 | −232.654670 | −232.886253 | −232.960965 | −232.987284 | −233.012349 | −232.713640 |
| **2** | 1,3-hexadiene | −233.094514 | −233.095646 | −233.835261 | −234.076388 | −234.152549 | −234.179230 | −234.204617 | −233.906251 |
| **3** | 1,3-hexadiyne | −230.674297 | −230.675230 | −231.378453 | −231.606852 | −231.679090 | −231.704312 | −231.728365 | −231.420442 |
| **5** | 1,4-hexadiene | −233.088887 | −233.090021 | −233.828267 | −234.069447 | −234.145663 | −234.172340 | −234.197714 | −233.900443 |
| **6** | 1,4-hexadiyne | −230.670864 | −230.671810 | −231.367964 | −231.595740 | −231.668737 | −231.694108 | −231.718261 | −231.413976 |
| **7** | 2-butene | −156.179505 | −156.180303 | −156.684616 | −156.851418 | −156.903352 | −156.921479 | −156.938713 | −156.739334 |
| **8** | 2-pentene | −195.229897 | −195.230871 | −195.865310 | −196.073315 | −196.138152 | −196.160800 | −196.182360 | −195.932570 |
| **9** | 2-pentyne | −194.026664 | −194.027559 | −194.639694 | −194.840937 | −194.904198 | −194.926169 | −194.947079 | −194.693807 |
| **10** | hexa-1-ene-3-yne | −231.885848 | −231.886895 | −232.605567 | −232.839991 | −232.914306 | −232.940230 | −232.964904 | −232.663343 |
| **11** | hexa-1-ene-4-yne | −231.883813 | −231.884864 | −232.600971 | −232.835371 | −232.910019 | −232.936011 | −232.960731 | −232.660144 |
| **12** | hexa-1-yne-3-ene | −231.881217 | −231.882232 | −232.602274 | −232.836658 | −232.911069 | −232.937081 | −232.961860 | −232.660114 |
| **13** | hexa-1-yne-4-ene | −231.878720 | −231.879743 | −232.597298 | −232.831904 | −232.906550 | −232.932619 | −232.957433 | −232.656508 |
| **14** | propane | −118.316720 | −118.317361 | −118.717911 | −118.851421 | −118.891861 | −118.905967 | −118.919400 | −118.767900 |
| **15** | propene | −117.125423 | −117.126058 | −117.499938 | −117.625567 | −117.664530 | −117.678172 | −117.691113 | −117.542424 |
| **16** | propyne | −115.916702 | −115.917224 | −116.270947 | −116.389861 | −116.427247 | −116.440281 | −116.452663 | −116.300246 |
| **17** | ethane | −79.265982 | −79.266439 | −79.537313 | −79.629642 | −79.657100 | −79.666666 | −79.675763 | −79.574424 |
| **18** | 1,3-butadiene | −154.989321 | −154.990105 | −155.469000 | −155.627643 | −155.677915 | −155.695584 | −155.712351 | −155.515579 |
| **19** | 1,3-butadiyne | −152.561151 | −152.561698 | −153.006546 | −153.152075 | −153.198689 | −153.214965 | −153.230489 | −153.024331 |
| **20** | allene | −115.914277 | −115.914831 | −116.264154 | −116.382395 | −116.419684 | −116.432658 | −116.444960 | −116.298935 |
| **21** | butatriene | −153.757359 | −153.758033 | −154.217174 | −154.369058 | −154.417507 | −154.434305 | −154.450257 | −154.254509 |
| **22** | ethene | −78.070152 | −78.070606 | −78.314878 | −78.399128 | −78.425061 | −78.434176 | −78.442791 | −78.345106 |
| **23** | vinylacetylene | −153.774889 | −153.775555 | −154.235447 | −154.387329 | −154.435836 | −154.452819 | −154.468963 | −154.268805 |
| **24** | methane | −40.216670 | −40.216934 | −40.360076 | −40.411505 | −40.426092 | −40.431096 | −40.435836 | −40.383627 |
| **25** | butane | −157.367322 | −157.368144 | −157.898644 | −158.073336 | −158.126763 | −158.145396 | −158.163155 | −157.961468 |
| **26** | acetylene | −76.855135 | −76.855456 | −77.081441 | −77.159080 | −77.183404 | −77.191990 | −77.200147 | −77.098481 |
| **29** | pentane | −196.417845 | −196.418848 | −197.079325 | −197.295223 | −197.361629 | −197.384786 | −197.406869 | −197.154983 |
| **30** | 2-butyne | −154.976101 | −154.976815 | −155.459284 | −155.619210 | −155.669580 | −155.687126 | −155.703814 | −155.500801 |
| **31** | 1-butyne | −154.967294 | −154.967994 | −155.451176 | −155.611429 | −155.661729 | −155.679304 | −155.696027 | −155.493104 |
| **32** | 1-butene | −156.175798 | −156.176610 | −156.680471 | −156.847319 | −156.899197 | −156.917500 | −156.934912 | −156.735537 |
| **33** | 1-pentene | −195.226478 | −195.227470 | −195.861349 | −196.069427 | −196.134289 | −196.156977 | −196.178566 | −195.929171 |
| **34** | 1-pentyne | −194.018159 | −194.019039 | −194.632161 | −194.833685 | −194.896976 | −194.919058 | −194.940087 | −194.686808 |
| **35** | 1,3-pentadiene | −194.044120 | −194.045075 | −194.654499 | −194.854409 | −194.917667 | −194.939827 | −194.960890 | −194.713015 |
| **36** | 1,3-pentadiyne | −191.623590 | −191.624341 | −192.197863 | −192.384901 | −192.444261 | −192.464951 | −192.484672 | −192.227364 |
| **37** | 1,4-pentadiene | −194.034553 | −194.035519 | −194.643246 | −194.843242 | −194.906490 | −194.928682 | −194.949763 | −194.703252 |
| **38** | 1,4-pentadiyne | −191.610398 | −191.611147 | −192.178681 | −192.365380 | −192.425386 | −192.446326 | −192.466268 | −192.212526 |
| **39** | penta-1-ene-3-yne | −192.835267 | −192.836132 | −193.425115 | −193.618190 | −193.679612 | −193.701014 | −193.721364 | −193.470336 |
| **40** | penta-1-ene-4-yne | −192.824070 | −192.824923 | −193.412160 | −193.605547 | −193.667209 | −193.688783 | −193.709297 | −193.459180 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **41** | penta-1-yne-3-ene | −192.830810 | −192.831646 | −193.421608 | −193.614737 | −193.676242 | −193.697726 | −193.718176 | −193.466953 |
| **42** | 2,4-hexadiene | −233.098428 | −233.099543 | −233.839787 | −234.080895 | −234.157112 | −234.183746 | −234.209095 | −233.910259 |
| **43** | 2,4-hexadiyne | −230.685003 | −230.685949 | −231.388529 | −231.616835 | −231.688953 | −231.714068 | −231.738011 | −231.429810 |
| **44** | hexa-2-ene-4-yne | −231.890614 | −231.891643 | −232.610993 | −232.845264 | −232.919627 | −232.945515 | −232.970163 | −232.668215 |
| **45** | 1,2,3-hexatriene | −231.863235 | −231.864274 | −232.584013 | −232.818576 | −232.892874 | −232.918731 | −232.943342 | −232.645226 |
| **46** | 1,2,3-pentatriene | −192.812614 | −192.813472 | −193.402923 | −193.596271 | −193.657657 | −193.678984 | −193.699265 | −193.451783 |
| **47** | E-2,3,4-hexatriene | −231.867206 | −231.868241 | −232.588344 | −232.823074 | −232.897357 | −232.923193 | −232.947785 | −232.648792 |
| **48** | Z-2,3,4-hexatriene | −231.867183 | −231.868216 | −232.588370 | −232.823074 | −232.897352 | −232.923194 | −232.947795 | −232.648813 |
| **49** | 1,5-hexadiene | −233.085437 | −233.086592 | −233.823998 | −234.065437 | −234.141711 | −234.168446 | −234.193863 | −233.896794 |
| **50** | 1,5-hexadiyne | −230.667517 | −230.668453 | −231.364702 | −231.592999 | −231.666061 | −231.691561 | −231.715849 | −231.411106 |
| **51** | Hexa-1-ene-5-yne | −231.876708 | −231.877750 | −232.594496 | −232.829358 | −232.904044 | −232.930161 | −232.955010 | −232.654115 |
| **52** | cyclopentadiene | −192.872211 | −192.873143 | −193.472370 | −193.662991 | −193.724915 | −193.746804 | −193.767633 | −193.516424 |
| **53** | 2-ethyl-1-butene | −234.277430 | −234.278568 | −235.046278 | −235.296227 | −235.374069 | −235.401236 | −235.427122 | −235.125421 |
| **54** | 2-methyl-1-pentene | −234.279307 | −234.280449 | −235.047012 | −235.296830 | −235.374792 | −235.401982 | −235.427886 | −235.126603 |
| **55** | 2-methyl-2-pentene | −234.280429 | −234.281567 | −235.049155 | −235.298958 | −235.376843 | −235.404011 | −235.429899 | −235.127914 |
| **56** | 2-methylpentane | −235.466722 | −235.467894 | −236.261799 | −236.519135 | −236.598544 | −236.626196 | −236.652579 | −236.349351 |
| **57** | 3-methylpentane | −235.464581 | −235.465751 | −236.260644 | −236.518194 | −236.597587 | −236.625247 | −236.651639 | −236.348014 |
| **58** | E-3-methyl-2-pentene | −234.278796 | −234.279931 | −235.048423 | −235.298331 | −235.376183 | −235.403338 | −235.429218 | −235.127054 |
| **59** | Z-3-methyl-2-pentene | −234.278752 | −234.279889 | −235.048453 | −235.298419 | −235.376248 | −235.403387 | −235.429249 | −235.127072 |
| **60** | 2-methylpropene | −156.180288 | −156.181085 | −156.686290 | −156.853513 | −156.905543 | −156.923703 | −156.940966 | −156.740566 |
| **61** | 2-methyl-1-butene | −195.229091 | −195.230056 | −195.866414 | −196.075083 | −196.140072 | −196.162743 | −196.184326 | −195.933203 |
| **62** | 2-methyl-2-butene | −195.230252 | −195.231213 | −195.868363 | −196.076995 | −196.141985 | −196.164638 | −196.186207 | −195.934651 |
| **63** | Isobutene | −157.367806 | −157.368619 | −157.901279 | −158.076072 | −158.129562 | −158.148173 | −158.165915 | −157.963406 |
| **64** | Isopentane | −196.416366 | −196.417358 | −197.081064 | −197.297224 | −197.363668 | −197.386804 | −197.408871 | −197.155823 |
| **65** | $H_2$ | −1.133586 | −1.133649 | −1.155124 | −1.164627 | −1.166558 | −1.167247 | −1.167878 | −1.163450 |
| | H | −0.499995 | −0.500022 | | | | | | |
| | C | −37.688643 | −37.688738 | −37.736491 | −37.756467 | −37.763406 | −37.765903 | −37.768256 | −37.759365 |

**Table S30**. Collection C of absolute energies (hartree). All energies computed at B3LYP/6-31G(d) optimized geometries.

| | Molecule | CCSD cc-pVTZ | CCSD(T) cc-pVDZ | CCSD(T) cc-pVTZ | MP2(fc) cc-pCVTZ | MP2(all) cc-pCVTZ | Focal Point $E_{FPA}$ (No ZPVE) | G3 | CBS-QB3 |
|---|---|---|---|---|---|---|---|---|---|
| **1** | 1,3-cyclohexadiene | −232.929610 | −232.746817 | −232.978802 | −232.893942 | −233.17931 | −233.390271 | −233.324554 | −232.940235 |
| **2** | 1,3-hexadiene | −234.131236 | −233.938145 | −234.179013 | −234.083923 | −234.36919 | −234.592508 | −234.528175 | −234.122568 |
| **3** | 1,3-hexadiyne | −231.634048 | −231.455499 | −231.685101 | −231.614980 | −231.90051 | −232.092150 | −232.028596 | −231.671828 |
| **5** | 1,4-hexadiene | −234.125537 | −233.931729 | −234.172712 | −234.077044 | −234.36230 | −234.586238 | −234.521961 | −234.116544 |
| **6** | 1,4-hexadiyne | −231.627038 | −231.447323 | −231.676204 | −231.604487 | −231.89000 | −232.084241 | −232.020266 | −231.664703 |
| **7** | 2-butene | −156.895108 | −156.758863 | −156.925398 | −156.856363 | −157.04658 | −157.202909 | −157.160161 | −156.875739 |
| **8** | 2-pentene | −196.126873 | −195.957321 | −196.164838 | −196.079435 | −196.31720 | −196.511645 | −196.458128 | −196.101009 |
| **9** | 2-pentyne | −194.882062 | −194.719523 | −194.920901 | −194.847731 | −195.08565 | −195.264967 | −195.211911 | −194.879267 |
| **10** | hexa-1-ene-3-yne | −232.882286 | −232.696307 | −232.931096 | −232.848077 | −233.13348 | −233.341410 | −233.277725 | −232.896622 |
| **11** | hexa-1-ene-4-yne | −232.879157 | −232.692366 | −232.927184 | −232.843634 | −233.12905 | −233.337965 | −233.274078 | −232.893477 |
| **12** | hexa-1-yne-3-ene | −232.879092 | −232.693216 | −232.928110 | −232.844648 | −233.12999 | −233.338660 | −233.274472 | −232.893726 |
| **13** | hexa-1-yne-4-ene | −232.875709 | −232.688908 | −232.923998 | −232.839997 | −233.12535 | −233.334879 | −233.270583 | −232.890115 |
| **14** | propane | −118.892822 | −118.781126 | −118.913918 | −118.854863 | −118.99750 | −119.124538 | −119.092627 | −118.855864 |
| **15** | propene | −117.659720 | −117.557131 | −117.682322 | −117.629315 | −117.77191 | −117.890461 | −117.858489 | −117.646210 |
| **16** | propyne | −116.411546 | −116.316119 | −116.435324 | −116.394136 | −116.53683 | −116.640820 | −116.609017 | −116.421736 |
| **17** | ethane | −79.660835 | −79.582749 | −79.674369 | −79.631913 | −79.72700 | −79.815578 | −79.794610 | −79.630569 |
| **18** | 1,3-butadiene | −155.663431 | −155.537374 | −155.695787 | −155.632798 | −155.82288 | −155.970577 | −155.927780 | −155.666948 |
| **19** | 1,3-butadiyne | −153.160423 | −153.049415 | −153.196287 | −153.157959 | −153.34823 | −153.464968 | −153.422768 | −153.211127 |
| **20** | allene | −116.409193 | −116.315222 | −116.433404 | −116.386539 | −116.52917 | −116.638600 | −116.607337 | −116.420359 |
| **21** | butatriene | −154.395926 | −154.279010 | −154.431117 | −154.374706 | −154.56492 | −154.702525 | −154.661152 | −154.426033 |
| **22** | ethene | −78.423690 | −78.354893 | −78.438695 | −78.401681 | −78.496642 | −78.577319 | −78.556320 | −78.416640 |
| **23** | vinylacetylene | −154.410590 | −154.291831 | −154.444226 | −154.392962 | −154.58312 | −154.716014 | −154.673509 | −154.437507 |
| **24** | methane | −40.431742 | −40.387351 | −40.438052 | −40.412622 | −40.46019 | −40.509953 | −40.500284 | −40.410005 |
| **25** | butane | −158.124884 | −157.979646 | −158.153601 | −158.077955 | −158.26816 | −158.433621 | −158.390869 | −158.081525 |
| **26** | acetylene | −77.171144 | −77.109592 | −77.187594 | −77.162013 | −77.25699 | −77.323640 | −77.302255 | −77.187430 |
| **29** | pentane | −197.356914 | −197.178132 | −197.393268 | −197.301015 | −197.53877 | −197.742672 | −197.689092 | −197.307210 |
| **30** | 2-butyne | −155.650451 | −155.521502 | −155.681634 | −155.624858 | −155.81525 | −155.956627 | −155.914230 | −155.654745 |
| **31** | 1-butyne | −155.643039 | −155.513961 | −155.674437 | −155.616861 | −155.80709 | −155.949266 | −155.906552 | −155.646166 |
| **32** | 1-butene | −156.891375 | −156.755238 | −156.921625 | −156.852239 | −157.04238 | −157.199356 | −157.156310 | −156.871268 |
| **33** | 1-pentene | −196.123563 | −195.953851 | −196.161464 | −196.075520 | −196.31322 | −196.508301 | −196.454717 | −196.097107 |
| **34** | 1-pentyne | −194.875352 | −194.712621 | −194.914390 | −194.840288 | −195.07808 | −195.258586 | −195.204985 | −194.872182 |
| **35** | 1,3-pentadiene | −194.899452 | −194.739871 | −194.939536 | −194.860759 | −195.09848 | −195.283739 | −195.230155 | −194.897249 |
| **36** | 1,3-pentadiyne | −192.402317 | −192.257380 | −192.445691 | −192.391891 | −192.62989 | −192.783463 | −192.730733 | −192.446920 |
| **37** | 1,4-pentadiene | −194.889853 | −194.729478 | −194.929303 | −194.849635 | −195.08727 | −195.273455 | −195.219921 | −194.886574 |
| **38** | 1,4-pentadiyne | −192.387159 | −192.241001 | −192.428877 | −192.372764 | −192.61058 | −192.767581 | −192.714032 | −192.430672 |
| **39** | penta-1-ene-3-yne | −193.650646 | −193.498275 | −193.691788 | −193.625125 | −193.86299 | −194.032827 | −193.979913 | −193.671417 |
| **40** | penta-1-ene-4-yne | −193.639842 | −193.486527 | −193.680418 | −193.612444 | −193.85017 | −194.021891 | −193.968360 | −193.659936 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **41** | penta-1-yne-3-ene | −193.647342 | −193.495025 | −193.688676 | −193.621558 | −193.85936 | −194.029917 | −193.976501 | −193.668493 |
| **42** | 2,4-hexadiene | −234.135204 | −233.942189 | −234.183035 | −234.088445 | −234.37380 | −234.596591 | −234.532245 | −234.127371 |
| **43** | 2,4-hexadiyne | −231.643374 | −231.464751 | −231.694248 | −231.625003 | −231.91072 | −232.101142 | −232.037891 | −231.681980 |
| **44** | hexa-2-ene-4-yne | −232.887071 | −232.701213 | −232.935926 | −232.853381 | −233.13889 | −233.346332 | −233.282564 | −232.902307 |
| **45** | 1,2,3-hexatriene | −232.863945 | −232.679904 | −232.914628 | −232.826557 | −233.11194 | −233.324774 | −233.261800 | −232.881353 |
| **46** | 1,2,3-pentatriene | −193.631956 | −193.481403 | −193.674928 | −193.603086 | −193.84092 | −194.015755 | −193.963560 | −193.655895 |
| **47** | E-2,3,4-hexatriene | −232.867622 | −232.683542 | −232.918394 | −232.831047 | −233.11650 | −233.328554 | −233.265535 | −232.885574 |
| **48** | Z-2,3,4-hexatriene | −232.867621 | −232.683570 | −232.918399 | −232.831056 | −233.11650 | −233.328569 | −233.265536 | −232.885544 |
| **49** | 1,5-hexadiene | −234.122139 | −233.927992 | −234.169241 | −234.073003 | −234.35819 | −234.582859 | −234.518476 | −234.112627 |
| **50** | 1,5-hexadiyne | −231.624710 | −231.444570 | −231.674090 | −231.601571 | −231.88695 | −232.082321 | −232.017916 | −231.661598 |
| **51** | Hexa-1-ene-5-yne | −232.873588 | −232.686443 | −232.921823 | −232.837434 | −233.12272 | −233.332761 | −233.268366 | −232.887297 |
| **52** | cyclopentadiene | −193.694066 | −193.544905 | −193.735977 | −193.669475 | −193.90730 | −194.078447 | −194.022818 | −193.712750 |
| **53** | 2-ethyl-1-butene | −235.358784 | −235.155608 | −235.404955 | −235.303511 | −235.58885 | −235.821190 | −235.757124 | −235.327120 |
| **54** | 2-methyl-1-pentene | −235.359865 | −235.156621 | −235.405842 | −235.304125 | −235.58948 | −235.822256 | −235.758010 | −235.328276 |
| **55** | 2-methyl-2-pentene | −235.361150 | −235.158102 | −235.407300 | −235.306303 | −235.59169 | −235.823629 | −235.759510 | −235.330447 |
| **56** | 2-methylpentane | −236.589897 | −236.377916 | −236.634386 | −236.526122 | −236.81146 | −237.053170 | −236.989298 | −236.535123 |
| **57** | 3-methylpentane | −236.588736 | −236.376693 | −236.633392 | −236.525177 | −236.81052 | −237.052177 | −236.988361 | −236.534121 |
| **58** | E-3-methyl-2-pentene | −235.360370 | −235.157345 | −235.406657 | −235.305675 | −235.59106 | −235.822932 | −235.758885 | −235.329824 |
| **59** | Z-3-methyl-2-pentene | −235.360411 | −235.157366 | −235.406712 | −235.305749 | −235.59113 | −235.822926 | −235.759106 | −235.329814 |
| **60** | 2-methylpropene | −156.896668 | −156.760478 | −156.927159 | −156.858479 | −157.04871 | −157.204841 | −157.162185 | −156.877856 |
| **61** | 2-methyl-1-butene | −196.128004 | −195.958215 | −196.166310 | −196.081206 | −196.31900 | −196.513352 | −196.459891 | −196.102705 |
| **62** | 2-methyl-2-butene | −196.129402 | −195.959771 | −196.167829 | −196.083169 | −196.32101 | −196.514885 | −196.461415 | −196.105099 |
| **63** | Isobutene | −158.126830 | −157.981869 | −158.155845 | −158.080716 | −158.27094 | −158.435911 | −158.393483 | −158.084603 |
| **64** | Isopentane | −197.357886 | −197.179377 | −197.394703 | −197.303039 | −197.54082 | −197.744133 | −197.691005 | −197.309468 |
| **65** | $H_2$ | −1.172337 | −1.163450 | −1.172337 | −1.164627 | −1.16463 | −1.175588 | −1.176829 | −1.166082 |
| | H | | | | | −0.49981 | −0.500022 | −0.498642 | −0.499818 |
| | C | −37.778559 | −37.760340 | −37.780695 | −37.757799 | −37.80415 | −37.838975 | −37.825356 | −37.785377 |

**Table S31**. Polyyne absolute energies (hartree). All energies computed at B3LYP/6-31G(d) optimized geometries.

| Molecule | B3LYP | M05-2X | M06-2X | M06 |
|---|---|---|---|---|
| $C_6H_2$ | −229.640061 | −229.604597 | −229.539274 | −229.461376 |
| $C_8H_2$ | −305.799631 | −305.752236 | −305.665917 | −305.563400 |
| $C_{10}H_2$ | −381.959661 | −381.899953 | −381.792635 | −381.665746 |
| $C_{12}H_2$ | −458.119921 | −458.048131 | −457.919709 | −457.768577 |
| $C_{14}H_2$ | −534.280297 | −534.195878 | −534.046433 | −533.871149 |
| $C_{16}H_2$ | −610.440737 | −610.343935 | −610.173377 | −609.974007 |
| $C_{18}H_2$ | −686.601212 | −686.491464 | −686.299864 | −686.076562 |
| $C_{20}H_2$ | −762.761708 | −762.639442 | −762.426724 | −762.179405 |
| $C_{22}H_2$ | −838.922215 | −838.787035 | −838.553276 | −838.282008 |
| $C_{24}H_2$ | −915.082728 | −914.935178 | −914.680314 | −914.384912 |
| $C_{26}H_2$ | −991.243246 | −991.082715 | −990.806805 | −990.487503 |

## Cartesian Coordinates

**B3LYP/6-31G(d) Optimized Structures**

1,3-cyclohexadiene (**1**)

| | | | |
|---|---|---|---|
| C | 1.2602580 | 0.7262900 | 0.1038860 |
| C | 1.2603170 | -0.7261910 | -0.1038850 |
| C | 0.1138130 | -1.4250640 | -0.0643900 |
| C | -1.1953550 | -0.7319220 | 0.2392260 |
| C | -1.1954150 | 0.7318290 | -0.2392230 |
| C | 0.1137000 | 1.4250740 | 0.0643820 |
| H | 2.2110390 | 1.2273920 | 0.2715840 |
| H | 2.2111390 | -1.2272220 | -0.2715670 |
| H | 0.1161000 | -2.5063380 | -0.1842240 |
| H | -2.0367100 | -1.2722020 | -0.2104630 |
| H | -1.3622490 | -0.7637420 | 1.3297120 |
| H | -1.3623160 | 0.7636340 | -1.3297070 |
| H | -2.0368120 | 1.2720410 | 0.2104700 |
| H | 0.1159020 | 2.5063470 | 0.1842250 |

1,3-hexadiene (**2**)

| | | | |
|---|---|---|---|
| C | -3.1325550 | -0.1646500 | 0.2681550 |
| C | -1.9605260 | 0.4048360 | -0.0491400 |
| C | -0.6830920 | -0.2933920 | -0.0791350 |
| C | 0.4880470 | 0.2821480 | -0.3984960 |
| C | 1.8198740 | -0.4116370 | -0.4273890 |
| C | 2.8346260 | 0.2019020 | 0.5540900 |
| H | -4.0596300 | 0.4004960 | 0.2763660 |
| H | -3.2012390 | -1.2181590 | 0.5307830 |
| H | -1.9361480 | 1.4644900 | -0.3065460 |
| H | -0.7023360 | -1.3542930 | 0.1766280 |
| H | 0.4968410 | 1.3454860 | -0.6490760 |
| H | 1.6860750 | -1.4779660 | -0.2052740 |
| H | 2.2380140 | -0.3549420 | -1.4441110 |
| H | 3.8045360 | -0.3032130 | 0.4818890 |
| H | 2.9950450 | 1.2660860 | 0.3435160 |
| H | 2.4805990 | 0.1167740 | 1.5873190 |

1,3-hexadiyne (**3**)

| | | | |
|---|---|---|---|
| C | -3.3466050 | 0.2463760 | 0.0000700 |
| C | -2.1500690 | 0.0457610 | -0.0000400 |
| C | -0.8006310 | -0.1805240 | -0.0001340 |
| C | 0.3978910 | -0.3857900 | -0.0000360 |
| C | 1.8417070 | -0.6076240 | 0.0000650 |
| C | 2.6557540 | 0.7014170 | 0.0000040 |
| H | -4.3980130 | 0.4221300 | 0.0001930 |
| H | 2.1130620 | -1.2106430 | 0.8777780 |
| H | 2.1131760 | -1.2107960 | -0.8775070 |
| H | 3.7277440 | 0.4773600 | 0.0000900 |
| H | 2.4279310 | 1.3020480 | -0.8858530 |
| H | 2.4278160 | 1.3022050 | 0.8857250 |

1,4-hexadiene (**5**)

| | | | |
|---|---|---|---|
| C | -2.9909600 | -0.4286970 | -0.1142690 |
| C | -1.8255530 | -0.1307320 | 0.4607770 |
| C | -0.7574520 | 0.7487770 | -0.1456800 |
| C | 0.5392260 | 0.0061290 | -0.3673430 |
| C | 1.7063090 | 0.3102230 | 0.2063680 |
| C | 2.9957530 | -0.4304130 | -0.0062490 |
| H | -3.7199170 | -1.0746670 | 0.3679700 |
| H | -3.2634420 | -0.0332420 | -1.0911530 |
| H | -1.5861810 | -0.5524580 | 1.4378720 |
| H | -1.1277430 | 1.1519380 | -1.0993470 |
| H | -0.5690610 | 1.6091810 | 0.5126550 |
| H | 0.4838760 | -0.8503530 | -1.0418350 |
| H | 1.7497940 | 1.1648040 | 0.8850560 |
| H | 2.8664070 | -1.2732650 | -0.6936780 |
| H | 3.7711030 | 0.2288740 | -0.4198850 |
| H | 3.3912230 | -0.8225310 | 0.9407160 |

1,4-hexadiyne (**6**)

| | | | |
|---|---|---|---|
| C | -2.8141380 | -0.9007520 | 0.0000050 |
| C | -1.9546220 | -0.0543980 | -0.0000040 |
| C | -0.9199930 | 0.9902930 | 0.0000050 |
| C | 0.4519920 | 0.4628200 | -0.0000110 |
| C | 1.5820290 | 0.0355050 | -0.0000030 |
| C | 2.9458150 | -0.4880880 | 0.0000070 |
| H | -3.5658160 | -1.6569210 | -0.0000080 |
| H | -1.0653300 | 1.6401330 | 0.8758540 |
| H | -1.0653380 | 1.6401460 | -0.8758340 |
| H | 2.9475340 | -1.5848010 | -0.0001930 |
| H | 3.5012760 | -0.1552700 | -0.8852080 |
| H | 3.5011730 | -0.1555710 | 0.8853950 |

2-butene (**7**)

| | | | |
|---|---|---|---|
| C | 1.9635030 | 0.0792220 | 0.0001310 |
| C | 0.5381140 | -0.3953330 | -0.0002090 |
| C | -0.5381160 | 0.3953540 | -0.0002160 |
| C | -1.9634920 | -0.0792390 | 0.0001280 |
| H | 2.5074790 | -0.2886270 | 0.8809840 |
| H | 2.5081760 | -0.2895990 | -0.8798660 |
| H | 2.0228530 | 1.1731430 | -0.0004560 |
| H | 0.3924600 | -1.4777080 | -0.0001820 |
| H | -0.3925090 | 1.4777470 | -0.0001420 |
| H | -2.0227660 | -1.1731560 | -0.0015650 |
| H | -2.5072640 | 0.2876580 | 0.8815070 |
| H | -2.5084870 | 0.2905190 | -0.8792920 |

2-pentene (**8**)

| | | | |
|---|---|---|---|
| C | -2.3403300 | -0.4626960 | 0.2712860 |
| C | -1.3021940 | 0.5617090 | -0.2178340 |
| C | 0.0653560 | -0.0372130 | -0.4088150 |
| C | 1.1718420 | 0.3365440 | 0.2392340 |
| C | 2.5342550 | -0.2691560 | 0.0542550 |
| H | -3.3315020 | -0.0049260 | 0.3688450 |
| H | -2.4277940 | -1.3022270 | -0.4291370 |
| H | -2.0557970 | -0.8728880 | 1.2466540 |
| H | -1.2424140 | 1.3969320 | 0.4918920 |
| H | -1.6517060 | 0.9879620 | -1.1704850 |
| H | 0.1307930 | -0.8527190 | -1.1337580 |
| H | 1.1033190 | 1.1491160 | 0.9657980 |
| H | 2.5189910 | -1.0737410 | -0.6889640 |
| H | 3.2645810 | 0.4824870 | -0.2756150 |
| H | 2.9179560 | -0.6851300 | 0.9960100 |

2-pentyne (**9**)

| | | | |
|---|---|---|---|
| C | 2.6538890 | 0.2270990 | 0.0005910 |
| C | 1.2257510 | -0.0831520 | -0.0011500 |
| C | 0.0449580 | -0.3466880 | -0.0008790 |
| C | -1.3910800 | -0.6386280 | 0.0005240 |
| C | -2.2661360 | 0.6290790 | 0.0000320 |
| H | 2.8318590 | 1.2915090 | -0.1968620 |
| H | 3.1139800 | -0.0102030 | 0.9678720 |
| H | 3.1885490 | -0.3444400 | -0.7682470 |
| H | -1.6410160 | -1.2535470 | -0.8754060 |
| H | -1.6394050 | -1.2517810 | 0.8781650 |
| H | -3.3284330 | 0.3606350 | 0.0014670 |
| H | -2.0639300 | 1.2417230 | 0.8844140 |
| H | -2.0658890 | 1.2398380 | -0.8861070 |

hexa1ene-3-yne (**10**)

| | | | |
|---|---|---|---|
| C | 3.1190670 | -0.2625630 | 0.1034600 |
| C | 2.0503950 | 0.5311100 | -0.0655960 |
| C | 0.6973320 | 0.0877550 | -0.0611880 |
| C | -0.4673770 | -0.2538820 | -0.0669800 |
| C | -1.8724120 | -0.6625220 | -0.0662790 |
| C | -2.8485050 | 0.5163110 | 0.1056290 |
| H | 4.1246610 | 0.1464780 | 0.0873950 |
| H | 3.0180710 | -1.3323180 | 0.2604200 |
| H | 2.2040790 | 1.5996780 | -0.2200330 |
| H | -2.0972910 | -1.1902070 | -1.0041840 |
| H | -2.0369930 | -1.3956260 | 0.7359080 |
| H | -3.8833850 | 0.1571440 | 0.0991430 |
| H | -2.6697340 | 1.0356570 | 1.0524380 |
| H | -2.7304150 | 1.2419380 | -0.7053630 |

hexa1ene-4-yne (**11**)

| | | | |
|---|---|---|---|
| C | -2.8394310 | -0.5889790 | 0.2929030 |
| C | -1.7825610 | -0.2121030 | -0.4244600 |
| C | -0.8211780 | 0.8874010 | -0.0231290 |
| C | 0.5751560 | 0.4354890 | 0.0154380 |
| C | 1.7196150 | 0.0447350 | 0.0330080 |
| C | 3.1031250 | -0.4245420 | 0.0625020 |
| H | -3.5069100 | -1.3769300 | -0.0453470 |
| H | -3.0795480 | -0.1248380 | 1.2475060 |
| H | -1.5628720 | -0.7040910 | -1.3713960 |
| H | -0.9071530 | 1.7216160 | -0.7373770 |
| H | -1.1150240 | 1.2923440 | 0.9546480 |
| H | 3.1554470 | -1.5162480 | -0.0314320 |
| H | 3.6908920 | 0.0067290 | -0.7572110 |
| H | 3.5968160 | -0.1505880 | 1.0030320 |

hexa-1-yne-3-ene (**12**)

| | | | |
|---|---|---|---|
| C | 3.2230130 | -0.3686990 | -0.0061580 |
| C | 2.0801110 | 0.0215970 | -0.0971880 |
| C | 0.7503300 | 0.5115000 | -0.2324010 |
| C | -0.3176000 | -0.0053280 | 0.4001790 |
| C | -1.7232900 | 0.5003760 | 0.2549020 |
| C | -2.6868470 | -0.5703980 | -0.2878190 |
| H | 4.2235550 | -0.7243390 | 0.0874920 |
| H | 0.6143740 | 1.3653620 | -0.8974820 |
| H | -0.1722300 | -0.8607960 | 1.0602370 |
| H | -2.0882920 | 0.8365730 | 1.2371750 |
| H | -1.7342210 | 1.3802310 | -0.4006110 |
| H | -3.7084770 | -0.1794270 | -0.3503250 |
| H | -2.3842700 | -0.8988930 | -1.2879740 |
| H | -2.7047430 | -1.4530040 | 0.3623940 |

hexa-1-yne-4-ene (**13**)

| | | | |
|---|---|---|---|
| C | 2.9521510 | -0.7403200 | -0.1421140 |
| C | 2.0047720 | 0.0017440 | -0.0424760 |
| C | 0.8444120 | 0.8907910 | 0.0900910 |
| C | -0.4345370 | 0.1455790 | 0.4102120 |
| C | -1.5487530 | 0.2131520 | -0.3202720 |
| C | -2.8302180 | -0.5062370 | -0.0109030 |
| H | 3.7869070 | -1.3970550 | -0.2341750 |
| H | 1.0539500 | 1.6248210 | 0.8838690 |
| H | 0.7141050 | 1.4696540 | -0.8339590 |
| H | -0.4078200 | -0.4772950 | 1.3044630 |
| H | -1.5513320 | 0.8340690 | -1.2184360 |
| H | -2.7453620 | -1.1060780 | 0.9013580 |
| H | -3.6609570 | 0.1998520 | 0.1224510 |
| H | -3.1164570 | -1.1762290 | -0.8327980 |

propane (**14**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2775210 | -0.2599370 |
| C | 0.0000000 | -1.2775210 | -0.2599370 |
| C | 0.0000000 | 0.0000000 | 0.5862770 |
| H | 0.0000000 | 2.1757500 | 0.3684760 |
| H | 0.0000000 | -2.1757500 | 0.3684760 |
| H | -0.8847390 | 1.3229590 | -0.9072490 |
| H | 0.8847390 | 1.3229590 | -0.9072490 |
| H | 0.8847390 | -1.3229590 | -0.9072490 |
| H | -0.8847390 | -1.3229590 | -0.9072490 |
| H | -0.8777430 | 0.0000000 | 1.2468100 |
| H | 0.8777430 | 0.0000000 | 1.2468100 |

propene (**15**)

| | | | |
|---|---|---|---|
| C | 1.2933320 | 0.1504100 | 0.0000000 |
| C | 0.0000000 | 0.4744930 | 0.0000000 |
| C | -1.1391340 | -0.5044980 | 0.0000000 |
| H | 2.0737110 | 0.9068500 | 0.0000000 |
| H | 1.6223610 | -0.8871920 | 0.0000000 |
| H | -0.2788420 | 1.5294860 | 0.0000000 |
| H | -0.7800120 | -1.5391840 | 0.0000000 |
| H | -1.7812050 | -0.3661940 | 0.8804630 |
| H | -1.7812050 | -0.3661940 | -0.8804630 |

propyne (**16**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.2189320 |
| C | 0.0000000 | 0.0000000 | 1.4260340 |
| C | 0.0000000 | 0.0000000 | -1.2413640 |
| H | 0.0000000 | 1.0223780 | -1.6379110 |
| H | -0.8854060 | -0.5111890 | -1.6379110 |
| H | 0.8854060 | -0.5111890 | -1.6379110 |
| H | 0.0000000 | 0.0000000 | 2.4921200 |

ethane (**17**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.7654190 | 0.0000000 |
| C | 0.0000000 | -0.7654190 | 0.0000000 |
| H | -0.5106150 | 1.1641590 | 0.8842520 |
| H | 0.5106150 | -1.1641590 | -0.8842520 |
| H | -0.5106150 | 1.1641590 | -0.8842520 |
| H | 0.5106150 | -1.1641590 | 0.8842520 |
| H | 1.0210400 | 1.1642630 | 0.0000000 |
| H | -1.0210400 | -1.1642630 | 0.0000000 |

1,3-butadiene (**18**)

| | | | |
|---|---|---|---|
| C | 0.6016940 | 1.7516380 | 0.0000000 |
| C | 0.6016940 | 0.4109560 | 0.0000000 |
| H | -0.3254550 | 2.3208860 | 0.0000000 |
| H | 1.5241810 | 2.3243690 | 0.0000000 |
| H | 1.5517350 | -0.1243970 | 0.0000000 |
| C | -0.6016940 | -0.4109560 | 0.0000000 |
| C | -0.6016940 | -1.7516380 | 0.0000000 |
| H | -1.5517350 | 0.1243970 | 0.0000000 |
| H | -1.5241810 | -2.3243690 | 0.0000000 |
| H | 0.3254550 | -2.3208860 | 0.0000000 |

1,3-butadiyne (**19**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 2.9630080 |
| C | 0.0000000 | 0.0000000 | 1.8966890 |
| C | 0.0000000 | 0.0000000 | 0.6843940 |
| C | 0.0000000 | 0.0000000 | -0.6843940 |
| C | 0.0000000 | 0.0000000 | -1.8966890 |
| H | 0.0000000 | 0.0000000 | -2.9630080 |

allene (**20**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 1.3071140 |
| C | 0.0000000 | 0.0000000 | 0.0000000 |
| C | 0.0000000 | 0.0000000 | -1.3071140 |
| H | -0.9273170 | 0.0000000 | -1.8768140 |
| H | 0.9273170 | 0.0000000 | -1.8768140 |
| H | 0.0000000 | 0.9273170 | 1.8768140 |
| H | 0.0000000 | -0.9273170 | 1.8768140 |

butatriene (**21**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6355080 |
| C | 0.0000000 | 0.0000000 | -0.6355080 |
| C | 0.0000000 | 0.0000000 | 1.9531260 |
| C | 0.0000000 | 0.0000000 | -1.9531260 |
| H | 0.0000000 | 0.9265290 | -2.5242220 |
| H | 0.0000000 | -0.9265290 | -2.5242220 |
| H | 0.0000000 | 0.9265290 | 2.5242220 |
| H | 0.0000000 | -0.9265290 | 2.5242220 |

ethene (**22**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6654520 |
| C | 0.0000000 | 0.0000000 | -0.6654520 |
| H | 0.0000000 | 0.9236000 | -1.2395730 |
| H | 0.0000000 | -0.9236000 | -1.2395730 |
| H | 0.0000000 | -0.9236000 | 1.2395730 |
| H | 0.0000000 | 0.9236000 | 1.2395730 |

vinylacetylene (**23**)

| | | | |
|---|---|---|---|
| C | -0.4529000 | 1.8667200 | 0.0000000 |
| C | 0.0000000 | 0.7439130 | 0.0000000 |
| H | -0.8689870 | 2.8483760 | 0.0000000 |
| C | 0.5793790 | -0.5574440 | 0.0000000 |
| H | 1.6685300 | -0.5967850 | 0.0000000 |
| C | -0.1220030 | -1.7005320 | 0.0000000 |
| H | 0.3813940 | -2.6624010 | 0.0000000 |
| H | -1.2077950 | -1.7051310 | 0.0000000 |

methane (**24**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000450 | 0.0000000 |
| H | -1.0462850 | 0.3173120 | 0.0000000 |
| H | 0.0494960 | -1.0922230 | 0.0000000 |
| H | 0.4983950 | 0.3873210 | 0.8927360 |
| H | 0.4983950 | 0.3873210 | -0.8927360 |

butane (**25**)

| | | | |
|---|---|---|---|
| C | -0.4215840 | 0.6409070 | 0.0000000 |
| C | 0.4215840 | -0.6409070 | 0.0000000 |
| C | 0.4215840 | 1.9202470 | 0.0000000 |
| C | -0.4215840 | -1.9202470 | 0.0000000 |
| H | -1.0832740 | 0.6374700 | 0.8781320 |
| H | -1.0832740 | 0.6374700 | -0.8781320 |
| H | 1.0832740 | -0.6374700 | 0.8781320 |
| H | 1.0832740 | -0.6374700 | -0.8781320 |
| H | 0.2093690 | -2.8165600 | 0.0000000 |
| H | -0.2093690 | 2.8165600 | 0.0000000 |
| H | -1.0685810 | -1.9683430 | -0.8847400 |
| H | -1.0685810 | -1.9683430 | 0.8847400 |
| H | 1.0685810 | 1.9683430 | -0.8847400 |
| H | 1.0685810 | 1.9683430 | 0.8847400 |

acetylene (**26**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 1.6693820 |
| C | 0.0000000 | 0.0000000 | 0.6025580 |
| C | 0.0000000 | 0.0000000 | -0.6025580 |
| H | 0.0000000 | 0.0000000 | -1.6693820 |

hexadieneyne (**27**)

| | | | |
|---|---|---|---|
| C | -0.1698920 | 3.0086620 | 0.0000000 |
| C | 0.1698920 | -3.0086620 | 0.0000000 |
| C | 0.6282330 | 1.9278200 | 0.0000000 |
| C | -0.6282330 | -1.9278200 | 0.0000000 |
| C | 0.1698920 | 0.5847080 | 0.0000000 |
| C | -0.1698920 | -0.5847080 | 0.0000000 |
| H | -1.2521650 | 2.9204310 | 0.0000000 |
| H | 1.2521650 | -2.9204310 | 0.0000000 |
| H | 0.2497010 | 4.0098890 | 0.0000000 |
| H | -0.2497010 | -4.0098890 | 0.0000000 |
| H | 1.7097150 | 2.0666130 | 0.0000000 |
| H | -1.7097150 | -2.0666130 | 0.0000000 |

hexadiyneene (**28**)

| | | | |
|---|---|---|---|
| C | 0.5058830 | 3.0217880 | 0.0000000 |
| C | -0.5058830 | -3.0217880 | 0.0000000 |
| C | 0.5058830 | 1.8102860 | 0.0000000 |
| C | -0.5058830 | -1.8102860 | 0.0000000 |
| C | 0.5509210 | 0.3935590 | 0.0000000 |
| C | -0.5509210 | -0.3935590 | 0.0000000 |
| H | 0.4949640 | 4.0880730 | 0.0000000 |
| H | -0.4949640 | -4.0880730 | 0.0000000 |
| H | 1.5357080 | -0.0703780 | 0.0000000 |
| H | -1.5357080 | 0.0703780 | 0.0000000 |

pentane (**29**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2838390 | -0.5232230 |
| C | 0.0000000 | -1.2838390 | -0.5232230 |
| C | 0.0000000 | 0.0000000 | 0.3165430 |
| C | 0.0000000 | 2.5607530 | 0.3238470 |
| C | 0.0000000 | -2.5607530 | 0.3238470 |
| H | 0.8781440 | 1.2834790 | -1.1847360 |
| H | -0.8781440 | 1.2834790 | -1.1847360 |
| H | 0.8781440 | -1.2834790 | -1.1847360 |
| H | -0.8781440 | -1.2834790 | -1.1847360 |
| H | 0.8785650 | 0.0000000 | 0.9793410 |
| H | -0.8785650 | 0.0000000 | 0.9793410 |
| H | 0.0000000 | -3.4585730 | -0.3050300 |
| H | 0.0000000 | 3.4585730 | -0.3050300 |
| H | -0.8847320 | -2.6071820 | 0.9708950 |
| H | 0.8847320 | -2.6071820 | 0.9708950 |
| H | -0.8847320 | 2.6071820 | 0.9708950 |
| H | 0.8847320 | 2.6071820 | 0.9708950 |

2-butyne (**30**)

| | | | |
|---|---|---|---|
| C | 2.0659480 | 0.0000200 | 0.0000090 |
| C | 0.6045930 | 0.0001990 | 0.0000710 |
| H | 2.4664550 | -0.9672740 | -0.3281000 |
| H | 2.4666390 | 0.1994680 | 1.0016990 |
| H | 2.4665860 | 0.7677490 | -0.6736570 |
| H | -2.4661480 | 0.9675060 | 0.3282290 |
| C | -0.6045920 | -0.0004390 | -0.0001530 |
| H | -2.4667290 | -0.7675750 | 0.6736640 |
| C | -2.0659520 | 0.0001140 | 0.0000360 |
| H | -2.4667830 | -0.1992330 | -1.0016160 |

1-butyne (**31**)

| | | | |
|---|---|---|---|
| C | -1.3354630 | -1.4669780 | 0.0000000 |
| C | -0.7390580 | -0.4166850 | 0.0000000 |
| H | -1.8616040 | -2.3941990 | 0.0000000 |
| C | 0.0000000 | 0.8474770 | 0.0000000 |
| C | 1.5277240 | 0.6529000 | 0.0000000 |
| H | -0.2953480 | 1.4393260 | 0.8771740 |
| H | -0.2953480 | 1.4393260 | -0.8771740 |
| H | 2.0341500 | 1.6241200 | 0.0000000 |
| H | 1.8494660 | 0.0955720 | -0.8853320 |
| H | 1.8494660 | 0.0955720 | 0.8853320 |

1-butene (**32**)

| | | | |
|---|---|---|---|
| C | -1.8618690 | 0.0180780 | -0.2792180 |
| H | -0.6720780 | -1.2243730 | 0.9136020 |
| C | -0.7234730 | -0.2963630 | 0.3399780 |
| H | -2.7407430 | -0.6190220 | -0.2241690 |
| C | 0.5401930 | 0.5204510 | 0.3082500 |
| C | 1.7294290 | -0.2462660 | -0.2946650 |
| H | 0.3661690 | 1.4444330 | -0.2577630 |
| H | 0.8003900 | 0.8255570 | 1.3330220 |
| H | 2.6410310 | 0.3616710 | -0.2733530 |
| H | 1.9301560 | -1.1687840 | 0.2636210 |
| H | 1.5289120 | -0.5247390 | -1.3351760 |
| H | -1.9595150 | 0.9298570 | -0.8658550 |

1-pentene (**33**)

| | | | |
|---|---|---|---|
| C | -2.4849490 | -0.2165920 | -0.3042250 |
| C | -1.4194630 | 0.3413530 | 0.2718000 |
| C | -0.0744200 | -0.3127730 | 0.4336200 |
| C | 1.0572400 | 0.4486630 | -0.2830580 |
| C | 2.4314140 | -0.1965640 | -0.0793040 |
| H | -0.1176620 | -1.3449710 | 0.0608080 |
| H | 0.1736540 | -0.3775490 | 1.5048460 |
| H | -1.4991330 | 1.3609400 | 0.6547390 |
| H | -3.4300380 | 0.3119480 | -0.3979180 |
| H | -2.4537720 | -1.2291430 | -0.7025650 |
| H | 0.8260780 | 0.5039780 | -1.3549180 |
| H | 1.0804750 | 1.4861850 | 0.0787870 |
| H | 3.2161570 | 0.3632160 | -0.6006680 |
| H | 2.6985410 | -0.2339860 | 0.9840990 |
| H | 2.4467580 | -1.2251350 | -0.4602090 |

1-pentyne (**34**)

| | | | |
|---|---|---|---|
| C | 2.6470330 | -0.2416250 | 0.0003560 |
| C | 1.5076070 | 0.1589610 | -0.0004620 |
| C | 0.1202400 | 0.6247610 | -0.0000240 |
| C | -0.9089710 | -0.5258120 | -0.0001970 |
| C | -2.3510650 | -0.0126000 | 0.0001940 |
| H | -0.0507080 | 1.2647820 | -0.8774890 |
| H | -0.0501890 | 1.2641380 | 0.8780080 |
| H | 3.6528540 | -0.5952730 | 0.0002360 |
| H | -0.7332020 | -1.1584160 | -0.8787240 |
| H | -0.7329370 | -1.1589050 | 0.8779240 |
| H | -3.0652910 | -0.8432520 | 0.0000350 |
| H | -2.5546490 | 0.6021480 | 0.8856290 |
| H | -2.5549420 | 0.6026690 | -0.8848190 |

1,3-pentadiene (**35**)

| | | | |
|---|---|---|---|
| C | -1.3605810 | 0.3955840 | 0.0000660 |
| H | -1.3621610 | 1.4863510 | -0.0000030 |
| C | -2.5304130 | -0.2602080 | 0.0000260 |
| H | -3.4806570 | 0.2650880 | -0.0001120 |
| H | -2.5741030 | -1.3472530 | -0.0000810 |
| C | -0.0530300 | -0.2448440 | -0.0000340 |
| H | -0.0449470 | -1.3362060 | -0.0000180 |
| C | 1.1145400 | 0.4192990 | -0.0000710 |
| H | 1.0929500 | 1.5106240 | -0.0000440 |
| C | 2.4718260 | -0.2171430 | 0.0000330 |
| H | 3.0552030 | 0.0878260 | -0.8798710 |
| H | 3.0550500 | 0.0876880 | 0.8801050 |
| H | 2.4046130 | -1.3102450 | -0.0000940 |

1,3-pentadiyne (**36**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 1.5205070 |
| C | 0.0000000 | 0.0000000 | 2.7336780 |
| H | 0.0000000 | 0.0000000 | 3.7996930 |
| C | 0.0000000 | 0.0000000 | 0.1524010 |
| C | 0.0000000 | 0.0000000 | -1.0628540 |
| C | 0.0000000 | 0.0000000 | -2.5194050 |
| H | 0.0000000 | 1.0231360 | -2.9152200 |
| H | 0.8860620 | -0.5115680 | -2.9152200 |
| H | -0.8860620 | -0.5115680 | -2.9152200 |

1,4-pentadiene (**37**)

| | | | |
|---|---|---|---|
| C | -0.0000260 | 0.6639300 | -0.0008750 |
| H | 0.3136240 | 1.3168250 | -0.8279110 |
| H | -0.3137910 | 1.3190190 | 0.8244160 |
| C | 1.1766960 | -0.1779190 | 0.4335050 |
| H | 0.9928620 | -0.8381740 | 1.2819160 |
| C | 2.3760660 | -0.1759370 | -0.1486830 |
| H | 2.5967350 | 0.4640360 | -1.0011170 |
| H | 3.1855890 | -0.8089960 | 0.2049180 |
| C | -1.1766470 | -0.1792090 | -0.4329690 |
| H | -0.9925780 | -0.8422290 | -1.2791690 |
| C | -2.3760960 | -0.1754890 | 0.1490380 |
| H | -2.5969280 | 0.4670750 | 0.9994780 |
| H | -3.1854710 | -0.8098160 | -0.2026260 |

1,4-pentadiyne (**38**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2299970 | 0.0726910 |
| C | 0.0000000 | 2.2470300 | -0.5753130 |
| H | 0.0000000 | 3.1419950 | -1.1550340 |
| C | 0.0000000 | 0.0000000 | 0.8764870 |
| H | 0.8762800 | 0.0000000 | 1.5413050 |
| H | -0.8762800 | 0.0000000 | 1.5413050 |
| C | 0.0000000 | -1.2299970 | 0.0726910 |
| C | 0.0000000 | -2.2470300 | -0.5753130 |
| H | 0.0000000 | -3.1419950 | -1.1550340 |

penta-1-ene-3-yne (**39**)

| | | | |
|---|---|---|---|
| C | 1.2712350 | 0.8807090 | 0.0000000 |
| H | 1.2580610 | 1.9711660 | 0.0000000 |
| C | 2.4520430 | 0.2432870 | 0.0000000 |
| H | 3.3851280 | 0.7984460 | 0.0000000 |
| H | 2.5160950 | -0.8407530 | 0.0000000 |
| C | 0.0000000 | 0.2391920 | 0.0000000 |
| C | -1.1038960 | -0.2639620 | 0.0000000 |
| C | -2.4219350 | -0.8898450 | 0.0000000 |
| H | -2.5616530 | -1.5234760 | 0.8848630 |
| H | -3.2206650 | -0.1381930 | 0.0000000 |
| H | -2.5616530 | -1.5234760 | -0.8848630 |

penta-1-ene-4-yne (**40**)

| | | | |
|---|---|---|---|
| C | -0.0374580 | 0.7744880 | 0.0941420 |
| H | -0.1065810 | 1.5279270 | 0.8942620 |
| H | 0.2016480 | 1.3247260 | -0.8254620 |
| C | 1.0810980 | -0.1959320 | 0.4129200 |
| H | 0.9261920 | -0.8185240 | 1.2931250 |
| C | 2.1989080 | -0.3136160 | -0.3010170 |
| H | 2.3770920 | 0.2871810 | -1.1906430 |
| H | 2.9804930 | -1.0156600 | -0.0239380 |
| C | -1.3405150 | 0.1146680 | -0.0435800 |
| C | -2.4070530 | -0.4417960 | -0.1466160 |
| H | -3.3487270 | -0.9325160 | -0.2424410 |

penta-1-yne-3-ene (**41**)

| | | | |
|---|---|---|---|
| C | -0.0927460 | 0.4793060 | -0.0003470 |
| H | 0.1222550 | 1.5486510 | -0.0001720 |
| C | 0.9271980 | -0.3964670 | -0.0003960 |
| H | 0.7006610 | -1.4619650 | 0.0000460 |
| C | -1.4676280 | 0.1109010 | 0.0004230 |
| C | -2.6469410 | -0.1648570 | 0.0000480 |
| H | -3.6806030 | -0.4254620 | -0.0004080 |
| C | 2.3750670 | -0.0120190 | 0.0001610 |
| H | 2.8909670 | -0.4176560 | 0.8811690 |
| H | 2.8922930 | -0.4199430 | -0.8789540 |
| H | 2.5047290 | 1.0751940 | -0.0010180 |

2,4-hexadiene (**42**)

| | | | |
|---|---|---|---|
| C | 3.1901850 | 0.1400900 | 0.0001190 |
| H | 3.7596360 | -0.1895560 | 0.8804520 |
| H | 3.7601680 | -0.1903150 | -0.8795880 |
| H | 3.1729840 | 1.2353200 | -0.0003660 |
| C | 1.8045230 | -0.4330960 | -0.0000190 |
| H | 1.7325690 | -1.5222620 | 0.0000650 |
| C | 0.6692390 | 0.2852900 | -0.0001600 |
| H | 0.7332360 | 1.3751060 | -0.0002230 |
| C | -0.6692410 | -0.2853170 | -0.0001580 |
| H | -0.7332320 | -1.3751340 | -0.0002160 |
| C | -1.8045110 | 0.4331130 | -0.0000070 |
| H | -1.7325110 | 1.5222750 | 0.0000810 |
| C | -3.1901980 | -0.1400800 | 0.0001200 |
| H | -3.7599810 | 0.1899340 | -0.8798650 |
| H | -3.1729960 | -1.2353100 | 0.0001230 |
| H | -3.7598600 | 0.1899350 | 0.8801680 |

2,4-hexadiyne (**43**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6840090 |
| C | 0.0000000 | 0.0000000 | 1.8998700 |
| C | 0.0000000 | 0.0000000 | 3.3570240 |
| H | -0.5109570 | 0.8859220 | 3.7547810 |
| H | -0.5117520 | -0.8854630 | 3.7547810 |
| H | 1.0227090 | -0.0004590 | 3.7547810 |
| C | 0.0000000 | 0.0000000 | -0.6840090 |
| C | 0.0000000 | 0.0000000 | -1.8998700 |
| C | 0.0000000 | 0.0000000 | -3.3570240 |
| H | 0.5117520 | -0.8854630 | -3.7547810 |
| H | -1.0227090 | -0.0004590 | -3.7547810 |
| H | 0.5109570 | 0.8859220 | -3.7547810 |

hexa-2-ene-4-yne (**44**)

| | | | |
|---|---|---|---|
| C | 0.7161490 | 0.5278040 | 0.0003960 |
| H | 1.0004430 | 1.5815860 | 0.0008380 |
| C | 1.6845880 | -0.4052490 | 0.0004210 |
| H | 1.3976580 | -1.4562260 | 0.0003560 |
| C | 3.1526630 | -0.1040970 | -0.0001200 |
| H | 3.6481650 | -0.5390690 | 0.8787560 |
| H | 3.6462150 | -0.5368070 | -0.8813900 |
| H | 3.3430930 | 0.9743690 | 0.0006430 |
| C | -0.6794820 | 0.2493020 | -0.0002250 |
| C | -1.8773230 | 0.0556830 | -0.0008270 |
| C | -3.3149360 | -0.1953110 | 0.0002000 |
| H | -3.8826320 | 0.7398290 | -0.0799490 |
| H | -3.6100270 | -0.8350700 | -0.8411470 |
| H | -3.6328700 | -0.6974040 | 0.9228300 |

1,2,3-hexatriene (**45**)

| | | | |
|---|---|---|---|
| C | 0.7300080 | 0.3666350 | -0.0354490 |
| C | 1.9487300 | 0.0068310 | -0.0447990 |
| C | -0.5379990 | 0.7353090 | -0.0211050 |
| C | 3.2137740 | -0.3647000 | -0.0550970 |
| H | 3.5406740 | -1.2918830 | 0.4116950 |
| H | -0.8184650 | 1.6729410 | -0.5069810 |
| C | -1.6632350 | -0.0519550 | 0.6053770 |
| H | -2.1309410 | 0.5632110 | 1.3885600 |
| H | -1.2575830 | -0.9416820 | 1.0984260 |
| H | 3.9829250 | 0.2405830 | -0.5309870 |
| C | -2.7379330 | -0.4543990 | -0.4191300 |
| H | -3.5586520 | -0.9914070 | 0.0695690 |
| H | -3.1617890 | 0.4264140 | -0.9158320 |
| H | -2.3162330 | -1.1045020 | -1.1932400 |

1,2,3-pentatriene (**46**)

| | | | |
|---|---|---|---|
| C | -1.3244320 | -0.0410930 | -0.0005950 |
| C | -0.0798850 | -0.2971910 | 0.0004020 |
| C | -2.6161760 | 0.2230770 | 0.0002210 |
| H | -2.9903170 | 1.2450300 | 0.0000240 |
| H | -3.3611050 | -0.5702900 | 0.0001430 |
| C | 1.2135740 | -0.5634310 | -0.0000420 |
| H | 1.5319230 | -1.6078780 | -0.0000530 |
| C | 2.3086720 | 0.4696060 | -0.0000440 |
| H | 2.9543420 | 0.3508390 | -0.8806430 |
| H | 1.9018650 | 1.4840570 | -0.0011160 |
| H | 2.9527690 | 0.3524350 | 0.8819950 |

E-2,3,4-hexatriene (**47**)

| | | | |
|---|---|---|---|
| C | -0.6050850 | -0.1938510 | 0.0012850 |
| C | 0.6050430 | 0.1933830 | -0.0013020 |
| C | -1.8646960 | -0.5925570 | -0.0002700 |
| C | 1.8645440 | 0.5924660 | 0.0000840 |
| H | 2.0734490 | 1.6640250 | 0.0003460 |
| C | 3.0602560 | -0.3232970 | 0.0001120 |
| H | 3.6898270 | -0.1428820 | 0.8821120 |
| H | 2.7584300 | -1.3740520 | -0.0006070 |
| H | 3.6909570 | -0.1419490 | -0.8808440 |
| H | -2.0740050 | -1.6640310 | -0.0008270 |
| C | -3.0600960 | 0.3236330 | 0.0000370 |
| H | -2.7578750 | 1.3742680 | 0.0007450 |
| H | -3.6899710 | 0.1434470 | -0.8817820 |
| H | -3.6906060 | 0.1425080 | 0.8811780 |

Z-2,3,4-hexatriene (**48**)

| | | | |
|---|---|---|---|
| C | -0.6353110 | -0.5039010 | -0.0003140 |
| C | 0.6352120 | -0.5038200 | -0.0005910 |
| C | -1.9564940 | -0.5043400 | 0.0001680 |
| H | -2.4788020 | -1.4630290 | 0.0008670 |
| C | 1.9563770 | -0.5042500 | 0.0002530 |
| H | 2.4787580 | -1.4629150 | 0.0008300 |
| C | 2.8203450 | 0.7294670 | 0.0000870 |
| H | 3.4756340 | 0.7473220 | 0.8815980 |
| H | 3.4759540 | 0.7469810 | -0.8812310 |
| H | 2.2156490 | 1.6402080 | -0.0002680 |
| C | -2.8202530 | 0.7295970 | 0.0000760 |
| H | -3.4759330 | 0.7471610 | -0.8811530 |
| H | -3.4753580 | 0.7476950 | 0.8817020 |
| H | -2.2151550 | 1.6400670 | -0.0004300 |

1,5-hexadiene (**49**)

| | | | |
|---|---|---|---|
| C | -0.5730780 | -0.2964960 | -0.5198690 |
| H | -0.4838000 | 0.5901110 | -1.1594740 |
| H | -0.4489460 | -1.1718100 | -1.1761520 |
| C | 0.5732010 | -0.2971770 | 0.5200300 |
| H | 0.4840690 | 0.5887440 | 1.1606140 |
| H | 0.4490580 | -1.1732420 | 1.1752230 |
| C | -1.9346740 | -0.3375250 | 0.1178530 |
| H | -2.1393520 | -1.2094620 | 0.7425870 |
| C | -2.8745840 | 0.5992790 | -0.0130430 |
| H | -2.7152360 | 1.4864500 | -0.6231290 |
| H | -3.8403180 | 0.5159200 | 0.4784740 |
| C | 1.9345820 | -0.3374080 | -0.1182680 |
| H | 2.1391780 | -1.2087110 | -0.7439000 |
| C | 2.8745090 | 0.5992940 | 0.0132730 |
| H | 2.7155310 | 1.4856860 | 0.6245910 |
| H | 3.8400730 | 0.5165060 | -0.4786850 |

1,5-hexadiyne (**50**)

| | | | |
|---|---|---|---|
| C | 0.4822490 | 0.6086770 | 0.0000000 |
| H | 0.2710160 | 1.2312730 | -0.8781860 |
| H | 0.2710160 | 1.2312730 | 0.8781870 |
| C | -0.4822490 | -0.6086770 | 0.0000000 |
| H | -0.2710160 | -1.2312730 | -0.8781870 |
| H | -0.2710160 | -1.2312730 | 0.8781870 |
| C | 1.8863540 | 0.2006470 | 0.0000000 |
| C | 3.0403060 | -0.1546220 | -0.0000010 |
| H | 4.0611300 | -0.4626670 | -0.0000010 |
| C | -1.8863540 | -0.2006470 | 0.0000000 |
| C | -3.0403060 | 0.1546220 | 0.0000010 |
| H | -4.0611300 | 0.4626670 | 0.0000010 |

hexa-1-ene-5-yne (**51**)

| | | | |
|---|---|---|---|
| C | 0.6306670 | 0.6146190 | -0.2579790 |
| H | 0.3775870 | 0.7360110 | -1.3195180 |
| H | 0.5725630 | 1.6182800 | 0.1861770 |
| C | -0.4238250 | -0.3046980 | 0.4111630 |
| H | -0.3827490 | -1.2975140 | -0.0510440 |
| H | -0.1461480 | -0.4322630 | 1.4663760 |
| C | 1.9947890 | 0.1020070 | -0.1294360 |
| C | 3.1116800 | -0.3425430 | -0.0132350 |
| H | 4.1013110 | -0.7266940 | 0.0854470 |
| C | -1.8131410 | 0.2612330 | 0.3079290 |
| H | -1.9681800 | 1.2324840 | 0.7820280 |
| C | -2.8348680 | -0.3256240 | -0.3160920 |
| H | -2.7269170 | -1.2929060 | -0.8031720 |
| H | -3.8192790 | 0.1326440 | -0.3603930 |

cyclopentadiene (**52**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.1811960 | 0.2817040 |
| C | 0.0000000 | -1.1811960 | 0.2817040 |
| C | 0.0000000 | 0.7349470 | -0.9912320 |
| C | 0.0000000 | -0.7349470 | -0.9912320 |
| H | 0.0000000 | 2.2140510 | 0.6109470 |
| H | 0.0000000 | -2.2140510 | 0.6109470 |
| H | 0.0000000 | 1.3473910 | -1.8872770 |
| H | 0.0000000 | -1.3473910 | -1.8872770 |
| C | 0.0000000 | 0.0000000 | 1.2172810 |
| H | 0.8780920 | 0.0000000 | 1.8816520 |
| H | -0.8780920 | 0.0000000 | 1.8816520 |

2-ethyl-1-butene (**53**)

| | | | |
|---|---|---|---|
| C | -2.3811100 | -0.5269700 | -0.1488100 |
| H | -2.4771560 | -0.1740230 | -1.1817100 |
| H | -2.8432280 | 0.2206740 | 0.5054890 |
| C | -0.9174320 | -0.7700000 | 0.2254750 |
| H | -0.8674040 | -1.1818700 | 1.2457840 |
| H | -0.5123670 | -1.5658360 | -0.4168600 |
| C | 1.4520310 | 0.1695410 | 0.5490870 |
| H | 1.9658950 | 1.1283410 | 0.6868310 |
| H | 1.4802860 | -0.3425060 | 1.5227200 |
| C | 0.0083730 | 0.4295780 | 0.1604670 |
| C | -0.3942720 | 1.6508220 | -0.2068640 |
| H | -1.4173270 | 1.8678130 | -0.4983130 |
| H | 0.2982270 | 2.4890800 | -0.2289060 |
| H | -2.9579240 | -1.4537300 | -0.0577360 |
| C | 2.2347520 | -0.6738090 | -0.4743050 |
| H | 3.2721780 | -0.8114550 | -0.1487060 |
| H | 1.7960910 | -1.6691560 | -0.6053160 |
| H | 2.2486810 | -0.1823080 | -1.4535790 |

2-methyl-1-pentene (**54**)

| | | | |
|---|---|---|---|
| C | 2.7795670 | -0.2812390 | 0.0000890 |
| H | 2.8882850 | -0.9209810 | -0.8844510 |
| H | 2.8882140 | -0.9201120 | 0.8852660 |
| H | 3.6128470 | 0.4304880 | -0.0002290 |
| C | 1.4297350 | 0.4438900 | -0.0003230 |
| H | 1.3666140 | 1.0994680 | 0.8781010 |
| H | 1.3666410 | 1.0985590 | -0.8794330 |
| C | 0.2426440 | -0.5243340 | 0.0001760 |
| H | 0.3247870 | -1.1941530 | -0.8715210 |
| H | 0.3249930 | -1.1935700 | 0.8723110 |
| C | -2.2755420 | -0.9169200 | -0.0001230 |
| H | -2.2237560 | -1.5730770 | 0.8799450 |
| H | -3.2537180 | -0.4262230 | -0.0003440 |
| H | -2.2233600 | -1.5730650 | -0.8801820 |
| C | -1.1451910 | 0.0848460 | 0.0001140 |
| C | -1.3802490 | 1.4010530 | 0.0001090 |
| H | -0.5824280 | 2.1372250 | 0.0002060 |
| H | -2.3949000 | 1.7916650 | 0.0000790 |

2-methyl-2-pentene (**55**)

| | | | |
|---|---|---|---|
| C | 2.6038190 | -0.1847260 | 0.4941320 |
| H | 2.7986310 | -1.2635770 | 0.4628070 |
| H | 2.2850290 | 0.0643580 | 1.5124680 |
| C | 1.5284010 | 0.2145430 | -0.5320380 |
| H | 1.3742200 | 1.2981790 | -0.4939730 |
| H | 1.9106200 | -0.0030460 | -1.5410450 |
| H | 3.5502410 | 0.3318880 | 0.2961390 |
| C | 0.2355030 | -0.5301170 | -0.3291740 |
| C | -0.9824490 | -0.0445490 | -0.0428890 |
| C | -2.1613470 | -0.9730680 | 0.1340610 |
| H | -2.6063130 | -0.8636760 | 1.1334450 |
| H | -2.9594060 | -0.7431270 | -0.5863410 |
| H | -1.8788350 | -2.0224070 | 0.0022760 |
| H | 0.3288410 | -1.6149290 | -0.4187370 |
| C | -1.3133520 | 1.4185940 | 0.1267940 |
| H | -1.7428340 | 1.6051370 | 1.1211310 |
| H | -0.4488760 | 2.0758400 | 0.0081340 |
| H | -2.0747710 | 1.7312980 | -0.6016150 |

2-methylpentane (**56**)

| | | | |
|---|---|---|---|
| C | 2.8461150 | -0.2121150 | 0.1508480 |
| H | 2.9979440 | -1.2275250 | -0.2358810 |
| H | 2.9048970 | -0.2643950 | 1.2451150 |
| H | 3.6817960 | 0.4054540 | -0.1979530 |
| C | 1.4988220 | 0.3591680 | -0.3046030 |
| H | 1.4022090 | 1.3883370 | 0.0646970 |
| H | 1.4828600 | 0.4255270 | -1.4021720 |
| C | 0.3051820 | -0.4827680 | 0.1669070 |
| H | 0.2943890 | -0.5136520 | 1.2677760 |
| H | 0.4600820 | -1.5211570 | -0.1619600 |
| C | -1.0751890 | -0.0130270 | -0.3338440 |
| H | -1.0277620 | 0.0452460 | -1.4327450 |
| C | -2.1586950 | -1.0381840 | 0.0334820 |
| H | -2.2493260 | -1.1391510 | 1.1230820 |
| H | -3.1396960 | -0.7378530 | -0.3537540 |
| H | -1.9259300 | -2.0295750 | -0.3734950 |
| C | -1.4521210 | 1.3795380 | 0.1954420 |
| H | -1.4850610 | 1.3832480 | 1.2932620 |
| H | -0.7385990 | 2.1485250 | -0.1193920 |
| H | -2.4424860 | 1.6813000 | -0.1659750 |

3-methylpentane (**57**)

| | | | |
|---|---|---|---|
| C | -2.5865380 | -0.1694240 | -0.2874970 |
| H | -2.5732850 | -0.1957530 | -1.3844630 |
| H | -2.7986160 | 0.8611740 | 0.0170630 |
| H | -3.4267410 | -0.7881600 | 0.0481510 |
| C | -1.2640900 | -0.6837390 | 0.2935330 |
| H | -1.3012890 | -0.6292010 | 1.3919490 |
| H | -1.1640860 | -1.7502330 | 0.0476510 |
| C | 0.0000010 | 0.0501950 | -0.2010450 |
| H | 0.0000030 | 0.0027520 | -1.3026270 |
| C | 1.2640920 | -0.6837340 | 0.2935430 |
| H | 1.1640960 | -1.7502320 | 0.0476710 |
| C | 2.5865370 | -0.1694240 | -0.2875000 |
| H | 2.7986140 | 0.8611840 | 0.0170310 |
| H | 3.4267460 | -0.7881460 | 0.0481620 |
| H | 2.5732810 | -0.1957820 | -1.3844650 |
| H | 1.3012910 | -0.6291840 | 1.3919580 |
| C | -0.0000020 | 1.5316590 | 0.2075010 |
| H | -0.8808700 | 2.0575400 | -0.1752890 |
| H | -0.0000070 | 1.6333040 | 1.3012770 |
| H | 0.8808670 | 2.0575420 | -0.1752830 |

E-3-methyl-2-pentene (**58**)

| | | | |
|---|---|---|---|
| C | -2.3552780 | -0.3447720 | 0.5450020 |
| H | -2.5603570 | 0.7025370 | 0.7928220 |
| H | -2.0136880 | -0.8446840 | 1.4586230 |
| C | -1.3067380 | -0.4749390 | -0.5746410 |
| H | -1.1933290 | -1.5346400 | -0.8340980 |
| H | -1.6937480 | 0.0260090 | -1.4754550 |
| H | -3.3040380 | -0.8027290 | 0.2423780 |
| C | 0.0921900 | 1.6041420 | -0.0524350 |
| H | -0.3209510 | 2.1054740 | -0.9387940 |
| H | -0.5206840 | 1.9259540 | 0.8000030 |
| H | 1.1016060 | 1.9899810 | 0.1071400 |
| C | 0.0520200 | 0.1040090 | -0.2255530 |
| C | 1.1154220 | -0.7047740 | -0.0951920 |
| H | 0.9487980 | -1.7716780 | -0.2552380 |
| C | 2.5345730 | -0.3478970 | 0.2491250 |
| H | 2.8505120 | -0.8531190 | 1.1724110 |
| H | 3.2233950 | -0.6826840 | -0.5388180 |
| H | 2.6893520 | 0.7249620 | 0.3911940 |

Z-3-methyl-2-pentene (**59**)

| | | | |
|---|---|---|---|
| C | 1.7222130 | -1.2654670 | -0.4377580 |
| H | 2.4030110 | -0.5403970 | -0.8977860 |
| H | 1.1032930 | -1.6916850 | -1.2351250 |
| C | 0.8451220 | -0.6130980 | 0.6476100 |
| H | 0.2123570 | -1.3829060 | 1.1011010 |
| H | 1.4970870 | -0.2423580 | 1.4519170 |
| H | 2.3329710 | -2.0709010 | -0.0136620 |
| C | 0.7434010 | 1.8416920 | -0.0628780 |
| H | 1.1580840 | 2.2046520 | 0.8884020 |
| H | 1.5944210 | 1.7275460 | -0.7481180 |
| H | 0.0920310 | 2.6228670 | -0.4676380 |
| C | 0.0031550 | 0.5378140 | 0.1307780 |
| C | -1.3049380 | 0.4479570 | -0.1565280 |
| H | -1.7967710 | 1.3479960 | -0.5300890 |
| C | -2.2089250 | -0.7479460 | -0.0385700 |
| H | -3.0654360 | -0.5293610 | 0.6141490 |
| H | -2.6268810 | -1.0183890 | -1.0181070 |
| H | -1.7043400 | -1.6327700 | 0.3590300 |

2-methylpropene (**60**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2780500 | -0.6789490 |
| H | 0.8800490 | 1.3322870 | -1.3350580 |
| H | -0.8800490 | 1.3322870 | -1.3350580 |
| H | 0.0000000 | 2.1632770 | -0.0355860 |
| C | 0.0000000 | 0.0000000 | 0.1229670 |
| C | 0.0000000 | 0.0000000 | 1.4595870 |
| H | 0.0000000 | -0.9246540 | 2.0317330 |
| H | 0.0000000 | 0.9246540 | 2.0317330 |
| C | 0.0000000 | -1.2780500 | -0.6789490 |
| H | -0.8800490 | -1.3322870 | -1.3350580 |
| H | 0.8800490 | -1.3322870 | -1.3350580 |
| H | 0.0000000 | -2.1632770 | -0.0355860 |

2-methyl1butene (**61**)

| | | | |
|---|---|---|---|
| C | -2.0466790 | -0.0374600 | -0.0000170 |
| H | -2.1625420 | 0.5973670 | 0.8855120 |
| H | -2.1625600 | 0.5972500 | -0.8856270 |
| H | -2.8666550 | -0.7637560 | 0.0000350 |
| C | -0.6958450 | -0.7558220 | 0.0000210 |
| H | -0.6409040 | -1.4270190 | 0.8715620 |
| H | -0.6408800 | -1.4270580 | -0.8714890 |
| C | 0.5407970 | 0.1199630 | 0.0000080 |
| C | 0.5042760 | 1.4562640 | 0.0000040 |
| H | -0.4265780 | 2.0150420 | 0.0000360 |
| H | 1.4180550 | 2.0453500 | -0.0000170 |
| C | 1.8495130 | -0.6339490 | -0.0000140 |
| H | 1.9302640 | -1.2869130 | 0.8802440 |
| H | 1.9300770 | -1.2872260 | -0.8800530 |
| H | 2.7093490 | 0.0429860 | -0.0002200 |

2-methyl-2-butene (**62**)

| | | | |
|---|---|---|---|
| C | 0.6299770 | 1.4581460 | -0.0000020 |
| H | 1.2053410 | 1.7797630 | -0.8795410 |
| H | 1.2052540 | 1.7797710 | 0.8795950 |
| H | -0.3137780 | 2.0083300 | -0.0000470 |
| C | 0.4496580 | -0.0403270 | -0.0000050 |
| C | -0.7343490 | -0.6715470 | -0.0000080 |
| H | -0.7141070 | -1.7628070 | -0.0000110 |
| C | -2.1152160 | -0.0778570 | 0.0000030 |
| H | -2.6836190 | -0.4103590 | -0.8796890 |
| H | -2.6834530 | -0.4099870 | 0.8799440 |
| H | -2.1152700 | 1.0154470 | -0.0002260 |
| C | 1.7412900 | -0.8241830 | 0.0000040 |
| H | 2.3537860 | -0.5805900 | -0.8799270 |
| H | 2.3537890 | -0.5805610 | 0.8799250 |
| H | 1.5638950 | -1.9044010 | 0.0000240 |

isobutane (**63**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.3723860 |
| H | 0.0000000 | 0.0000000 | 1.4729970 |
| C | 0.0000000 | 1.4622620 | -0.0957830 |
| H | 0.0000000 | 1.5214110 | -1.1923030 |
| H | -0.8863010 | 1.9976790 | 0.2656140 |
| H | 0.8863010 | 1.9976790 | 0.2656140 |
| C | -1.2663560 | -0.7311310 | -0.0957830 |
| H | -1.3175810 | -0.7607060 | -1.1923030 |
| H | -1.2868900 | -1.7663990 | 0.2656140 |
| H | -2.1731910 | -0.2312800 | 0.2656140 |
| C | 1.2663560 | -0.7311310 | -0.0957830 |
| H | 2.1731910 | -0.2312800 | 0.2656140 |
| H | 1.2868900 | -1.7663990 | 0.2656140 |
| H | 1.3175810 | -0.7607060 | -1.1923030 |

isopentane (**64**)

| | | | |
|---|---|---|---|
| C | 1.7410720 | -0.8232940 | -0.0114140 |
| H | 1.9212420 | -0.8597470 | 1.0712190 |
| H | 1.6465490 | -1.8562880 | -0.3673220 |
| H | 2.6310880 | -0.3868020 | -0.4802890 |
| C | 0.4821530 | -0.0028120 | -0.3296630 |
| H | 0.3476610 | -0.0032400 | -1.4229870 |
| C | -0.7651880 | -0.6629650 | 0.2912360 |
| H | -0.7745820 | -1.7243560 | 0.0058720 |
| H | -0.6681250 | -0.6451320 | 1.3872590 |
| C | -2.1021100 | -0.0320760 | -0.1145020 |
| H | -2.2223770 | -0.0278380 | -1.2052910 |
| H | -2.9438410 | -0.5921930 | 0.3087900 |
| H | -2.1910650 | 1.0031950 | 0.2328150 |
| C | 0.6621650 | 1.4545360 | 0.1217720 |
| H | -0.1902630 | 2.0825280 | -0.1588170 |
| H | 0.7760070 | 1.5131820 | 1.2126110 |
| H | 1.5591590 | 1.8963550 | -0.3284320 |

$H_2$ (**65**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 0.3713970 |
| H | 0.0000000 | 0.0000000 | -0.3713970 |

## B3LYP/6-311G(d,p) Optimized Structures (CBS-QB3)

1,3-cyclohexadiene (**1**)

| | | | |
|---|---|---|---|
| C | 1.2566190 | -0.7253100 | -0.1069590 |
| C | 1.2566170 | 0.7253130 | 0.1069590 |
| C | 0.1134820 | 1.4227270 | 0.0640640 |
| C | -1.1927440 | 0.7293230 | -0.2435350 |
| C | -1.1927420 | -0.7293260 | 0.2435350 |
| C | 0.1134850 | -1.4227260 | -0.0640640 |
| H | 2.2038480 | -1.2256060 | -0.2801740 |
| H | 2.2038450 | 1.2256110 | 0.2801740 |
| H | 0.1160780 | 2.5011340 | 0.1863340 |
| H | -2.0342210 | 1.2718070 | 0.1963650 |
| H | -1.3498610 | 0.7543750 | -1.3333060 |
| H | -1.3498590 | -0.7543780 | 1.3333060 |
| H | -2.0342180 | -1.2718120 | -0.1963650 |
| H | 0.1160840 | -2.5011330 | -0.1863340 |

1,3-hexadiene (**2**)

| | | | |
|---|---|---|---|
| C | -3.1272380 | -0.1663410 | 0.2676120 |
| C | -1.9589160 | 0.4036220 | -0.0473060 |
| C | -0.6815770 | -0.2916810 | -0.0797030 |
| C | 0.4860110 | 0.2841730 | -0.3964090 |
| C | 1.8166040 | -0.4079010 | -0.4296120 |
| C | 2.8321390 | 0.1980000 | 0.5544960 |
| H | -4.0517570 | 0.3981730 | 0.2771550 |
| H | -3.1928810 | -1.2185740 | 0.5264080 |
| H | -1.9369220 | 1.4618810 | -0.3009800 |
| H | -0.6985680 | -1.3513970 | 0.1720680 |
| H | 0.4926320 | 1.3461270 | -0.6433900 |
| H | 1.6824780 | -1.4731600 | -0.2160800 |
| H | 2.2309920 | -0.3427930 | -1.4444530 |
| H | 3.7986960 | -0.3076390 | 0.4800970 |
| H | 2.9947150 | 1.2603770 | 0.3499220 |
| H | 2.4784750 | 0.1077750 | 1.5847850 |

1,3-hexadiyne (**3**)

| | | | |
|---|---|---|---|
| C | -3.3352630 | 0.2461520 | 0.0000230 |
| C | -2.1442930 | 0.0464500 | -0.0000170 |
| C | -0.7985150 | -0.1791550 | -0.0000530 |
| C | 0.3942370 | -0.3841030 | 0.0000030 |
| C | 1.8340790 | -0.6067940 | 0.0000480 |
| C | 2.6517110 | 0.6987790 | -0.0000260 |
| H | -4.3826380 | 0.4214220 | 0.0000700 |
| H | 2.0993900 | -1.2096560 | 0.8763910 |
| H | 2.0994290 | -1.2097800 | -0.8761990 |
| H | 3.7207610 | 0.4731960 | 0.0000140 |
| H | 2.4256820 | 1.2983610 | -0.8838790 |
| H | 2.4256410 | 1.2984870 | 0.8837300 |

1,4-hexadiene (**5**)

| | | | |
|---|---|---|---|
| C | -2.9847470 | -0.4297410 | -0.1138150 |
| C | -1.8228440 | -0.1310540 | 0.4592340 |
| C | -0.7567180 | 0.7489000 | -0.1455580 |
| C | 0.5395860 | 0.0095500 | -0.3694230 |
| C | 1.7015380 | 0.3069250 | 0.2090800 |
| C | 2.9909700 | -0.4299260 | -0.0065520 |
| H | -3.7096580 | -1.0748880 | 0.3698720 |
| H | -3.2551930 | -0.0356330 | -1.0892170 |
| H | -1.5847930 | -0.5506220 | 1.4351050 |
| H | -1.1254940 | 1.1519390 | -1.0966640 |
| H | -0.5701410 | 1.6047940 | 0.5145050 |
| H | 0.4871230 | -0.8379560 | -1.0521300 |
| H | 1.7412860 | 1.1531760 | 0.8948950 |
| H | 2.8649810 | -1.2631890 | -0.7019280 |
| H | 3.7643110 | 0.2344210 | -0.4084450 |
| H | 3.3808650 | -0.8299650 | 0.9362180 |

1,4-hexadiyne (**6**)

| | | | |
|---|---|---|---|
| C | -2.8135620 | -0.8903700 | 0.0000040 |
| C | -1.9520700 | -0.0550030 | -0.0000030 |
| C | -0.9150880 | 0.9823960 | 0.0000040 |
| C | 0.4534100 | 0.4554950 | -0.0000070 |
| C | 1.5793520 | 0.0349960 | -0.0000020 |
| C | 2.9416170 | -0.4845770 | 0.0000000 |
| H | -3.5708330 | -1.6352190 | -0.0000010 |
| H | -1.0585560 | 1.6280290 | 0.8754070 |
| H | -1.0585630 | 1.6280490 | -0.8753840 |
| H | 2.9419600 | -1.5783900 | -0.0001870 |
| H | 3.4920810 | -0.1498950 | -0.8839950 |
| H | 3.4919610 | -0.1502000 | 0.8841860 |

2-butene (**7**)

| | | | |
|---|---|---|---|
| C | 1.9608200 | 0.0790650 | 0.0000320 |
| C | 0.5364480 | -0.3941760 | -0.0001350 |
| C | -0.5364490 | 0.3941800 | 0.0000040 |
| C | -1.9608180 | -0.0790680 | 0.0000460 |
| H | 2.5021190 | -0.2898590 | 0.8786780 |
| H | 2.5023920 | -0.2900360 | -0.8783650 |
| H | 2.0205280 | 1.1702310 | -0.0000570 |
| H | 0.3899720 | -1.4742440 | -0.0003490 |
| H | -0.3899770 | 1.4742480 | 0.0001790 |
| H | -2.0205210 | -1.1702330 | -0.0009080 |
| H | -2.5019590 | 0.2891400 | 0.8790940 |
| H | -2.5025560 | 0.2907450 | -0.8779460 |

2-pentene (**8**)

| | | | |
|---|---|---|---|
| C | -2.3388900 | -0.4617880 | 0.2703160 |
| C | -1.2996680 | 0.5609590 | -0.2173350 |
| C | 0.0666350 | -0.0367990 | -0.4081270 |
| C | 1.1694150 | 0.3342220 | 0.2398060 |
| C | 2.5314290 | -0.2685800 | 0.0540010 |
| H | -3.3269860 | -0.0036710 | 0.3687010 |
| H | -2.4279330 | -1.2981380 | -0.4297090 |
| H | -2.0552860 | -0.8722340 | 1.2430730 |
| H | -1.2387420 | 1.3940920 | 0.4905680 |
| H | -1.6452570 | 0.9860490 | -1.1687840 |
| H | 0.1335690 | -0.8480400 | -1.1345350 |
| H | 1.0987780 | 1.1429980 | 0.9671210 |
| H | 2.5175660 | -1.0690900 | -0.6896200 |
| H | 3.2577730 | 0.4845600 | -0.2721700 |
| H | 2.9129920 | -0.6846080 | 0.9933870 |

2-pentyne (**9**)

| | | | |
|---|---|---|---|
| C | 2.6476410 | 0.2275000 | 0.0004250 |
| C | 1.2222460 | -0.0821890 | -0.0007650 |
| C | 0.0474380 | -0.3447540 | -0.0006260 |
| C | -1.3854580 | -0.6374710 | 0.0003630 |
| C | -2.2641980 | 0.6262830 | 0.0000230 |
| H | 2.8217190 | 1.2897200 | -0.1959290 |
| H | 3.1042040 | -0.0109920 | 0.9657710 |
| H | 3.1776430 | -0.3431680 | -0.7681330 |
| H | -1.6287140 | -1.2515320 | -0.8744870 |
| H | -1.6275500 | -1.2502510 | 0.8764330 |
| H | -3.3235150 | 0.3562070 | 0.0010380 |
| H | -2.0642030 | 1.2375780 | 0.8826820 |
| H | -2.0656010 | 1.2362190 | -0.8838930 |

hexa-1-ene-3-yne (**10**)

| | | | |
|---|---|---|---|
| C | 3.1142850 | -0.2616060 | 0.0720300 |
| C | 2.0441570 | 0.5327830 | -0.0455710 |
| C | 0.6936970 | 0.0878480 | -0.0432190 |
| C | -0.4640390 | -0.2563690 | -0.0459500 |
| C | -1.8659440 | -0.6643130 | -0.0460410 |
| C | -2.8453190 | 0.5170200 | 0.0734170 |
| H | 4.1159820 | 0.1506130 | 0.0613600 |
| H | 3.0155650 | -1.3352290 | 0.1807500 |
| H | 2.1903090 | 1.6055970 | -0.1528600 |
| H | -2.0749580 | -1.2237300 | -0.9657330 |
| H | -2.0338970 | -1.3671250 | 0.7784760 |
| H | -3.8774760 | 0.1577080 | 0.0689510 |
| H | -2.6770760 | 1.0683770 | 1.0008870 |
| H | -2.7194740 | 1.2116070 | -0.7598280 |

hexa-1-ene-4-yne (**11**)

| | | | |
|---|---|---|---|
| C | -2.8326490 | -0.5879540 | 0.2926650 |
| C | -1.7827760 | -0.2066430 | -0.4253230 |
| C | -0.8168020 | 0.8845460 | -0.0198550 |
| C | 0.5756410 | 0.4306470 | 0.0148680 |
| C | 1.7148570 | 0.0435410 | 0.0320190 |
| C | 3.0961980 | -0.4236720 | 0.0615290 |
| H | -3.5000980 | -1.3701390 | -0.0507060 |
| H | -3.0636570 | -0.1338110 | 1.2516600 |
| H | -1.5707600 | -0.6889410 | -1.3764230 |
| H | -0.8984480 | 1.7185980 | -0.7302510 |
| H | -1.1038970 | 1.2840790 | 0.9588800 |
| H | 3.1458060 | -1.5122510 | -0.0358300 |
| H | 3.6801390 | 0.0113660 | -0.7549730 |
| H | 3.5841050 | -0.1516960 | 1.0022310 |

hexa-1-yne-3-ene (**12**)

| | | | |
|---|---|---|---|
| C | 3.2157340 | -0.3674710 | -0.0052990 |
| C | 2.0782130 | 0.0198050 | -0.0961820 |
| C | 0.7499490 | 0.5078700 | -0.2322800 |
| C | -0.3158660 | -0.0050450 | 0.3983730 |
| C | -1.7195590 | 0.5005240 | 0.2536200 |
| C | -2.6851970 | -0.5684880 | -0.2863970 |
| H | 4.2150710 | -0.7163040 | 0.0821470 |
| H | 0.6179890 | 1.3584270 | -0.8984860 |
| H | -0.1699660 | -0.8572970 | 1.0591040 |
| H | -2.0794920 | 0.8355240 | 1.2352320 |
| H | -1.7302350 | 1.3784860 | -0.3999620 |
| H | -3.7035710 | -0.1762890 | -0.3489030 |
| H | -2.3846580 | -0.8979900 | -1.2841320 |
| H | -2.7047720 | -1.4477260 | 0.3639910 |

hexa-1-yne-4-ene (**13**)

| | | | |
|---|---|---|---|
| C | 2.9433960 | -0.7393160 | -0.1402580 |
| C | 2.0011460 | -0.0004090 | -0.0427610 |
| C | 0.8444080 | 0.8881120 | 0.0878710 |
| C | -0.4352100 | 0.1492680 | 0.4114330 |
| C | -1.5437620 | 0.2106400 | -0.3207340 |
| C | -2.8256590 | -0.5042410 | -0.0102150 |
| H | 3.7761990 | -1.3922450 | -0.2311040 |
| H | 1.0579850 | 1.6197940 | 0.8785660 |
| H | 0.7180530 | 1.4608550 | -0.8370040 |
| H | -0.4113580 | -0.4642290 | 1.3097070 |
| H | -1.5415360 | 0.8213150 | -1.2232840 |
| H | -2.7451300 | -1.0940240 | 0.9057040 |
| H | -3.6533500 | 0.2032730 | 0.1116580 |
| H | -3.1067810 | -1.1790690 | -0.8262630 |

propane (**14**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2769660 | -0.2595640 |
| C | 0.0000000 | -1.2769660 | -0.2595640 |
| C | 0.0000000 | 0.0000000 | 0.5855420 |
| H | 0.0000000 | 2.1733910 | 0.3667780 |
| H | 0.0000000 | -2.1733910 | 0.3667780 |
| H | -0.8827400 | 1.3223730 | -0.9053690 |
| H | 0.8827400 | 1.3223730 | -0.9053690 |
| H | 0.8827400 | -1.3223730 | -0.9053690 |
| H | -0.8827400 | -1.3223730 | -0.9053690 |
| H | -0.8755120 | 0.0000000 | 1.2447210 |
| H | 0.8755120 | 0.0000000 | 1.2447210 |

propene (**15**)

| | | | |
|---|---|---|---|
| C | 1.2903420 | 0.1533120 | 0.0000000 |
| C | 0.0000000 | 0.4729620 | 0.0000000 |
| C | -1.1363990 | -0.5067200 | 0.0000000 |
| H | 2.0647520 | 0.9120640 | 0.0000000 |
| H | 1.6205040 | -0.8815130 | 0.0000000 |
| H | -0.2791550 | 1.5254200 | 0.0000000 |
| H | -0.7771370 | -1.5384800 | 0.0000000 |
| H | -1.7763130 | -0.3674090 | 0.8784580 |
| H | -1.7763130 | -0.3674090 | -0.8784580 |

propyne (**16**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.2191710 |
| C | 0.0000000 | 0.0000000 | 1.4200720 |
| C | 0.0000000 | 0.0000000 | -1.2379520 |
| H | 0.0000000 | 1.0209490 | -1.6299500 |
| H | -0.8841680 | -0.5104740 | -1.6299500 |
| H | 0.8841680 | -0.5104740 | -1.6299500 |
| H | 0.0000000 | 0.0000000 | 2.4821030 |

ethane (**17**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.7651740 | 0.0000000 |
| C | 0.0000000 | -0.7651740 | 0.0000000 |
| H | -0.5092270 | 1.1636760 | 0.8819200 |
| H | 0.5092270 | -1.1636760 | -0.8819200 |
| H | -0.5092270 | 1.1636760 | -0.8819200 |
| H | 0.5092270 | -1.1636760 | 0.8819200 |
| H | 1.0183490 | 1.1637400 | 0.0000000 |
| H | -1.0183490 | -1.1637400 | 0.0000000 |

1,3-butadiene (**18**)

| | | | |
|---|---|---|---|
| C | 0.6010020 | 1.7477170 | 0.0000000 |
| C | 0.6010020 | 0.4108460 | 0.0000000 |
| H | -0.3251110 | 2.3141120 | 0.0000000 |
| H | 1.5224870 | 2.3173360 | 0.0000000 |
| H | 1.5495400 | -0.1225190 | 0.0000000 |
| C | -0.6010020 | -0.4108460 | 0.0000000 |
| C | -0.6010020 | -1.7477170 | 0.0000000 |
| H | -1.5495400 | 0.1225190 | 0.0000000 |
| H | -1.5224870 | -2.3173360 | 0.0000000 |
| H | 0.3251110 | -2.3141120 | 0.0000000 |

1,3-butadiyne (**19**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 2.9515080 |
| C | 0.0000000 | 0.0000000 | 1.8891200 |
| C | 0.0000000 | 0.0000000 | 0.6826060 |
| C | 0.0000000 | 0.0000000 | -0.6826060 |
| C | 0.0000000 | 0.0000000 | -1.8891200 |
| H | 0.0000000 | 0.0000000 | -2.9515080 |

allene (**20**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 1.3023510 |
| C | 0.0000000 | 0.0000000 | 0.0000000 |
| C | 0.0000000 | 0.0000000 | -1.3023510 |
| H | -0.9270000 | 0.0000000 | -1.8672660 |
| H | 0.9270000 | 0.0000000 | -1.8672660 |
| H | 0.0000000 | 0.9270000 | 1.8672660 |
| H | 0.0000000 | -0.9270000 | 1.8672660 |

butatriene (**21**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6326720 |
| C | 0.0000000 | 0.0000000 | -0.6326720 |
| C | 0.0000000 | 0.0000000 | 1.9465820 |
| C | 0.0000000 | 0.0000000 | -1.9465820 |
| H | 0.0000000 | 0.9262230 | -2.5132960 |
| H | 0.0000000 | -0.9262230 | -2.5132960 |
| H | 0.0000000 | 0.9262230 | 2.5132960 |
| H | 0.0000000 | -0.9262230 | 2.5132960 |

ethene (**22**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6634640 |
| C | 0.0000000 | 0.0000000 | -0.6634640 |
| H | 0.0000000 | 0.9224650 | -1.2347260 |
| H | 0.0000000 | -0.9224650 | -1.2347260 |
| H | 0.0000000 | -0.9224650 | 1.2347260 |
| H | 0.0000000 | 0.9224650 | 1.2347260 |

vinylacetylene (**23**)

| | | | |
|---|---|---|---|
| C | -0.4499720 | 1.8608130 | 0.0000000 |
| C | 0.0000000 | 0.7434700 | 0.0000000 |
| H | -0.8614940 | 2.8401040 | 0.0000000 |
| C | 0.5768330 | -0.5568020 | 0.0000000 |
| H | 1.6634870 | -0.5939350 | 0.0000000 |
| C | -0.1227200 | -1.6962490 | 0.0000000 |
| H | 0.3793390 | -2.6560350 | 0.0000000 |
| H | -1.2061770 | -1.6975230 | 0.0000000 |

methane (**24**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000110 | 0.0000000 |
| H | -1.0471500 | 0.3052210 | 0.0000000 |
| H | 0.0612580 | -1.0890010 | 0.0000000 |
| H | 0.4929460 | 0.3918570 | 0.8905750 |
| H | 0.4929460 | 0.3918570 | -0.8905750 |

butane (**25**)

| | | | |
|---|---|---|---|
| C | -0.4207410 | 0.6407730 | 0.0000000 |
| C | 0.4207410 | -0.6407730 | 0.0000000 |
| C | 0.4207410 | 1.9200650 | 0.0000000 |
| C | -0.4207410 | -1.9200650 | 0.0000000 |
| H | -1.0807790 | 0.6374690 | 0.8762790 |
| H | -1.0807790 | 0.6374690 | -0.8762790 |
| H | 1.0807790 | -0.6374690 | 0.8762790 |
| H | 1.0807790 | -0.6374690 | -0.8762790 |
| H | 0.2093130 | -2.8138420 | 0.0000000 |
| H | -0.2093130 | 2.8138420 | 0.0000000 |
| H | -1.0659160 | -1.9692190 | -0.8829220 |
| H | -1.0659160 | -1.9692190 | 0.8829220 |
| H | 1.0659160 | 1.9692190 | -0.8829220 |
| H | 1.0659160 | 1.9692190 | 0.8829220 |

acetylene (**26**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 1.6619260 |
| C | 0.0000000 | 0.0000000 | 0.5990750 |
| C | 0.0000000 | 0.0000000 | -0.5990750 |
| H | 0.0000000 | 0.0000000 | -1.6619260 |

hexadieneyne (**27**)

| | | | |
|---|---|---|---|
| C | -0.1695360 | 3.0011880 | 0.0000000 |
| C | 0.1695360 | -3.0011880 | 0.0000000 |
| C | 0.6260040 | 1.9232590 | 0.0000000 |
| C | -0.6260040 | -1.9232590 | 0.0000000 |
| C | 0.1695360 | 0.5816510 | 0.0000000 |
| C | -0.1695360 | -0.5816510 | 0.0000000 |
| H | -1.2491750 | 2.9102160 | 0.0000000 |
| H | 1.2491750 | -2.9102160 | 0.0000000 |
| H | 0.2490540 | 4.0001460 | 0.0000000 |
| H | -0.2490540 | -4.0001460 | 0.0000000 |
| H | 1.7051890 | 2.0593030 | 0.0000000 |
| H | -1.7051890 | -2.0593030 | 0.0000000 |

hexadiyneene (**28**)

| | | | |
|---|---|---|---|
| C | 0.5038690 | 3.0133170 | 0.0000000 |
| C | -0.5038690 | -3.0133170 | 0.0000000 |
| C | 0.5038690 | 1.8079170 | 0.0000000 |
| C | -0.5038690 | -1.8079170 | 0.0000000 |
| C | 0.5485950 | 0.3930900 | 0.0000000 |
| C | -0.5485950 | -0.3930900 | 0.0000000 |
| H | 0.4937130 | 4.0756410 | 0.0000000 |
| H | -0.4937130 | -4.0756410 | 0.0000000 |
| H | 1.5324680 | -0.0670820 | 0.0000000 |
| H | -1.5324680 | 0.0670820 | 0.0000000 |

pentane (**29**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2836440 | -0.5224810 |
| C | 0.0000000 | -1.2836440 | -0.5224810 |
| C | 0.0000000 | 0.0000000 | 0.3149950 |
| C | 0.0000000 | 2.5598460 | 0.3237730 |
| C | 0.0000000 | -2.5598460 | 0.3237730 |
| H | 0.8761330 | 1.2829440 | -1.1823580 |
| H | -0.8761330 | 1.2829440 | -1.1823580 |
| H | 0.8761330 | -1.2829440 | -1.1823580 |
| H | -0.8761330 | -1.2829440 | -1.1823580 |
| H | 0.8767240 | 0.0000000 | 0.9760470 |
| H | -0.8767240 | 0.0000000 | 0.9760470 |
| H | 0.0000000 | -3.4561500 | -0.3026530 |
| H | 0.0000000 | 3.4561500 | -0.3026530 |
| H | -0.8827320 | -2.6060150 | 0.9692930 |
| H | 0.8827320 | -2.6060150 | 0.9692930 |
| H | -0.8827320 | 2.6060150 | 0.9692930 |
| H | 0.8827320 | 2.6060150 | 0.9692930 |

2-butyne (**30**)

| | | | |
|---|---|---|---|
| C | -2.0601790 | -0.0000060 | 0.0000010 |
| C | -0.6014780 | 0.0001420 | 0.0000820 |
| H | -2.4562370 | -0.8856810 | -0.5058990 |
| H | -2.4563550 | 0.8808940 | -0.5140940 |
| H | -2.4564050 | 0.0047000 | 1.0198990 |
| H | 2.4561120 | 0.8857890 | 0.5059060 |
| C | 0.6014770 | -0.0002260 | -0.0001300 |
| H | 2.4564660 | -0.0046680 | -1.0198510 |
| C | 2.0601800 | 0.0000490 | 0.0000230 |
| H | 2.4564160 | -0.8807890 | 0.5141790 |

1-butyne (**31**)

| | | | |
|---|---|---|---|
| C | -1.3327800 | -1.4608640 | 0.0000000 |
| C | -0.7397090 | -0.4157120 | 0.0000000 |
| H | -1.8587130 | -2.3836090 | 0.0000000 |
| C | 0.0000000 | 0.8443820 | 0.0000000 |
| C | 1.5268410 | 0.6507600 | 0.0000000 |
| H | -0.2976930 | 1.4314130 | 0.8760210 |
| H | -0.2976930 | 1.4314130 | -0.8760210 |
| H | 2.0325780 | 1.6195210 | 0.0000000 |
| H | 1.8477050 | 0.0949340 | -0.8833990 |
| H | 1.8477050 | 0.0949340 | 0.8833990 |

1-butene (**32**)

| | | | |
|---|---|---|---|
| C | -1.8578460 | 0.0172280 | -0.2807720 |
| H | -0.6767910 | -1.2166870 | 0.9186960 |
| C | -0.7241440 | -0.2940710 | 0.3404130 |
| H | -2.7341240 | -0.6186610 | -0.2217080 |
| C | 0.5390070 | 0.5199660 | 0.3080690 |
| C | 1.7277010 | -0.2467940 | -0.2942200 |
| H | 0.3653880 | 1.4420560 | -0.2559900 |
| H | 0.7965620 | 0.8221270 | 1.3314780 |
| H | 2.6368760 | 0.3601460 | -0.2742090 |
| H | 1.9287060 | -1.1663370 | 0.2637520 |
| H | 1.5268620 | -0.5250010 | -1.3321080 |
| H | -1.9517870 | 0.9243770 | -0.8708530 |

1-pentene (**33**)

| | | | |
|---|---|---|---|
| C | -2.4813130 | -0.2177080 | -0.3037620 |
| C | -1.4194260 | 0.3409440 | 0.2694980 |
| C | -0.0754350 | -0.3104320 | 0.4336660 |
| C | 1.0566790 | 0.4481420 | -0.2828250 |
| C | 2.4298320 | -0.1971640 | -0.0786180 |
| H | -0.1183700 | -1.3414900 | 0.0652610 |
| H | 0.1686490 | -0.3698090 | 1.5033930 |
| H | -1.5018110 | 1.3586940 | 0.6501610 |
| H | -3.4238230 | 0.3102700 | -0.3969020 |
| H | -2.4472990 | -1.2288750 | -0.6990840 |
| H | 0.8260300 | 0.5014950 | -1.3523270 |
| H | 1.0802400 | 1.4835500 | 0.0769630 |
| H | 3.2128570 | 0.3601410 | -0.5997160 |
| H | 2.6968500 | -0.2329670 | 0.9822460 |
| H | 2.4446510 | -1.2237010 | -0.4577450 |

1-pentyne (**34**)

| | | | |
|---|---|---|---|
| C | 2.6400510 | -0.2422150 | 0.0003260 |
| C | 1.5071850 | 0.1588180 | -0.0003890 |
| C | 0.1226270 | 0.6230590 | -0.0000490 |
| C | -0.9079840 | -0.5247180 | -0.0002300 |
| C | -2.3492240 | -0.0114750 | 0.0002160 |
| H | -0.0426220 | 1.2610580 | -0.8765780 |
| H | -0.0422500 | 1.2604960 | 0.8769560 |
| H | 3.6421040 | -0.5942740 | 0.0003210 |
| H | -0.7328480 | -1.1555450 | -0.8768900 |
| H | -0.7325060 | -1.1561200 | 0.8759460 |
| H | -3.0620650 | -0.8398000 | 0.0000980 |
| H | -2.5526950 | 0.6014060 | 0.8838910 |
| H | -2.5530480 | 0.6019620 | -0.8829920 |

1,3-pentadiene (**35**)

| | | | |
|---|---|---|---|
| C | -1.3592000 | 0.3942400 | -0.0000030 |
| H | -1.3623340 | 1.4827180 | -0.0000020 |
| C | -2.5258230 | -0.2599520 | -0.0000270 |
| H | -3.4730500 | 0.2656280 | -0.0000540 |
| H | -2.5673200 | -1.3447340 | -0.0000570 |
| C | -0.0523050 | -0.2442700 | -0.0000120 |
| H | -0.0430210 | -1.3335150 | -0.0000190 |
| C | 1.1119520 | 0.4181840 | 0.0000030 |
| H | 1.0886020 | 1.5072200 | 0.0000130 |
| C | 2.4682500 | -0.2165100 | 0.0000360 |
| H | 3.0487450 | 0.0898160 | -0.8779370 |
| H | 3.0486510 | 0.0896940 | 0.8781150 |
| H | 2.4024790 | -1.3069730 | -0.0000430 |

1,3-pentadiyne (**36**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 1.5156950 |
| C | 0.0000000 | 0.0000000 | 2.7232080 |
| H | 0.0000000 | 0.0000000 | 3.7851620 |
| C | 0.0000000 | 0.0000000 | 0.1510430 |
| C | 0.0000000 | 0.0000000 | -1.0583090 |
| C | 0.0000000 | 0.0000000 | -2.5110940 |
| H | 0.0000000 | 1.0216230 | -2.9028070 |
| H | 0.8847510 | -0.5108110 | -2.9028070 |
| H | -0.8847510 | -0.5108110 | -2.9028070 |

1,4-pentadiene (**37**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.6660240 | -0.0000170 |
| H | -0.3123320 | 1.3172230 | 0.8252040 |
| H | 0.3123320 | 1.3171830 | -0.8252710 |
| C | -1.1752180 | -0.1749810 | -0.4341220 |
| H | -0.9942180 | -0.8274810 | -1.2862930 |
| C | -2.3693260 | -0.1798110 | 0.1501950 |
| H | -2.5864780 | 0.4532270 | 1.0057170 |
| H | -3.1746780 | -0.8123340 | -0.2060240 |
| C | 1.1752200 | -0.1749540 | 0.4341340 |
| H | 0.9942160 | -0.8274150 | 1.2863350 |
| C | 2.3693260 | -0.1798180 | -0.1501860 |
| H | 2.5864740 | 0.4531680 | -1.0057480 |
| H | 3.1746740 | -0.8123330 | 0.2060570 |

1,4-pentadiyne (**38**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2282990 | 0.0697450 |
| C | 0.0000000 | 2.2435150 | -0.5693320 |
| H | 0.0000000 | 3.1387750 | -1.1411780 |
| C | 0.0000000 | 0.0000000 | 0.8696810 |
| H | 0.8760560 | 0.0000000 | 1.5296580 |
| H | -0.8760560 | 0.0000000 | 1.5296580 |
| C | 0.0000000 | -1.2282990 | 0.0697450 |
| C | 0.0000000 | -2.2435150 | -0.5693320 |
| H | 0.0000000 | -3.1387750 | -1.1411780 |

penta-1-ene-3-yne (**39**)

| | | | |
|---|---|---|---|
| C | 1.2757570 | 0.8661820 | 0.0000000 |
| H | 1.2700400 | 1.9541530 | 0.0000000 |
| C | 2.4480240 | 0.2213510 | 0.0000000 |
| H | 3.3831510 | 0.7681870 | 0.0000000 |
| H | 2.5008960 | -0.8609670 | 0.0000000 |
| C | 0.0000000 | 0.2380920 | 0.0000000 |
| C | -1.1024810 | -0.2532040 | 0.0000000 |
| C | -2.4233370 | -0.8660020 | 0.0000000 |
| H | -2.5652320 | -1.4962400 | 0.8833480 |
| H | -3.2114010 | -0.1074010 | 0.0000000 |
| H | -2.5652320 | -1.4962400 | -0.8833480 |

penta-1-ene-4-yne (**40**)

| | | | |
|---|---|---|---|
| C | -0.0390610 | 0.7725660 | 0.0920760 |
| H | -0.1127200 | 1.5235330 | 0.8900310 |
| H | 0.1945770 | 1.3185180 | -0.8279870 |
| C | 1.0813020 | -0.1917910 | 0.4138200 |
| H | 0.9311090 | -0.8066170 | 1.2974850 |
| C | 2.1932210 | -0.3134130 | -0.3012350 |
| H | 2.3652230 | 0.2793530 | -1.1945860 |
| H | 2.9731450 | -1.0117910 | -0.0203620 |
| C | -1.3384170 | 0.1123480 | -0.0437020 |
| C | -2.3993150 | -0.4418200 | -0.1450630 |
| H | -3.3377120 | -0.9303350 | -0.2399610 |

penta-1-yne-3-ene (**41**)

| | | | |
|---|---|---|---|
| C | 0.0930520 | 0.4769300 | -0.0001970 |
| H | -0.1169950 | 1.5448360 | 0.0001790 |
| C | -0.9251990 | -0.3943550 | -0.0001970 |
| H | -0.6983240 | -1.4576510 | -0.0004460 |
| C | 1.4662600 | 0.1090300 | -0.0003530 |
| C | 2.6398840 | -0.1645600 | 0.0003060 |
| H | 3.6712640 | -0.4180900 | 0.0006430 |
| C | -2.3713710 | -0.0110360 | 0.0002230 |
| H | -2.8846900 | -0.4186630 | -0.8779730 |
| H | -2.8845100 | -0.4197480 | 0.8780130 |
| H | -2.5025030 | 1.0732660 | 0.0008930 |

2,4-hexadiene (**42**)

| | | | |
|---|---|---|---|
| C | 3.1858120 | 0.1398440 | 0.0000290 |
| H | 3.7526430 | -0.1908910 | 0.8782590 |
| H | 3.7528520 | -0.1913390 | -0.8778940 |
| H | 3.1695720 | 1.2323750 | -0.0002460 |
| C | 1.8011660 | -0.4319790 | 0.0000170 |
| H | 1.7279340 | -1.5188160 | 0.0000740 |
| C | 0.6689470 | 0.2843360 | -0.0000380 |
| H | 0.7338320 | 1.3719630 | -0.0001060 |
| C | -0.6689480 | -0.2843370 | -0.0000150 |
| H | -0.7338340 | -1.3719650 | 0.0000190 |
| C | -1.8011650 | 0.4319810 | -0.0000220 |
| H | -1.7279300 | 1.5188170 | -0.0000530 |
| C | -3.1858120 | -0.1398440 | 0.0000110 |
| H | -3.7527440 | 0.1910570 | -0.8780890 |
| H | -3.1695670 | -1.2323740 | 0.0000810 |
| H | -3.7527510 | 0.1911710 | 0.8780640 |

2,4-hexadiyne (**43**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6824130 |
| C | 0.0000000 | 0.0000000 | 1.8923780 |
| C | 0.0000000 | 0.0000000 | 3.3460090 |
| H | 0.5104040 | 0.8843980 | 3.7397760 |
| H | -1.0211130 | -0.0001760 | 3.7397760 |
| H | 0.5107090 | -0.8842220 | 3.7397760 |
| C | 0.0000000 | 0.0000000 | -0.6824130 |
| C | 0.0000000 | 0.0000000 | -1.8923780 |
| C | 0.0000000 | 0.0000000 | -3.3460090 |
| H | -0.5107090 | -0.8842220 | -3.7397760 |
| H | -0.5104040 | 0.8843980 | -3.7397760 |
| H | 1.0211130 | -0.0001760 | -3.7397760 |

hexa-2-ene-4-yne (**44**)

| | | | |
|---|---|---|---|
| C | 0.7136980 | 0.5255670 | 0.0000300 |
| H | 0.9941710 | 1.5778630 | 0.0001630 |
| C | 1.6804720 | -0.4032770 | -0.0000900 |
| H | 1.3931890 | -1.4519430 | -0.0001900 |
| C | 3.1469850 | -0.1031220 | -0.0002320 |
| H | 3.6387160 | -0.5386620 | 0.8771820 |
| H | 3.6381000 | -0.5368330 | -0.8789280 |
| H | 3.3386010 | 0.9724040 | 0.0007610 |
| C | -0.6804930 | 0.2479650 | -0.0000210 |
| C | -1.8722560 | 0.0552140 | -0.0001870 |
| C | -3.3071510 | -0.1947280 | 0.0003640 |
| H | -3.8704830 | 0.7396990 | -0.0794980 |
| H | -3.5982530 | -0.8325650 | -0.8400490 |
| H | -3.6215650 | -0.6956780 | 0.9213810 |

1,2,3-hexatriene (**45**)

| | | | |
|---|---|---|---|
| C | 0.7313400 | 0.3633760 | -0.0326380 |
| C | 1.9450560 | 0.0059820 | -0.0445440 |
| C | -0.5332920 | 0.7308550 | -0.0154390 |
| C | 3.2074250 | -0.3622600 | -0.0584730 |
| H | 3.5312620 | -1.2923230 | 0.3983850 |
| H | -0.8078070 | 1.6729860 | -0.4907320 |
| C | -1.6580630 | -0.0594280 | 0.6025620 |
| H | -2.1173820 | 0.5472450 | 1.3938110 |
| H | -1.2539370 | -0.9541200 | 1.0818240 |
| H | 3.9706270 | 0.2510630 | -0.5275670 |
| C | -2.7389910 | -0.4447160 | -0.4206290 |
| H | -3.5561030 | -0.9851370 | 0.0644720 |
| H | -3.1630160 | 0.4416700 | -0.9014210 |
| H | -2.3244960 | -1.0842380 | -1.2038070 |

1,2,3-pentatriene (**46**)

| | | | |
|---|---|---|---|
| C | -1.3199030 | -0.0403420 | -0.0004590 |
| C | -0.0810040 | -0.2969440 | 0.0001470 |
| C | -2.6083280 | 0.2232510 | 0.0001560 |
| H | -2.9774430 | 1.2441710 | -0.0006050 |
| H | -3.3480670 | -0.5713640 | 0.0008910 |
| C | 1.2089090 | -0.5624920 | -0.0002020 |
| H | 1.5219010 | -1.6060580 | 0.0004450 |
| C | 2.3028820 | 0.4687440 | 0.0001310 |
| H | 2.9457860 | 0.3492130 | -0.8791570 |
| H | 1.8976250 | 1.4809630 | -0.0003970 |
| H | 2.9448530 | 0.3497710 | 0.8801820 |

E-2,3,4-hexatriene (**47**)

| | | | |
|---|---|---|---|
| C | 0.6023170 | -0.1937360 | -0.0011220 |
| C | -0.6023090 | 0.1936640 | 0.0008570 |
| C | 1.8583860 | -0.5917040 | 0.0001410 |
| C | -1.8583600 | 0.5916860 | -0.0002730 |
| H | -2.0620560 | 1.6616310 | -0.0006570 |
| C | -3.0530250 | -0.3226980 | 0.0001290 |
| H | -3.6805200 | -0.1415440 | -0.8797420 |
| H | -2.7522220 | -1.3707340 | 0.0005630 |
| H | -3.6806760 | -0.1408600 | 0.8797500 |
| H | 2.0621450 | -1.6616360 | -0.0000520 |
| C | 3.0529980 | 0.3227520 | 0.0001780 |
| H | 2.7521320 | 1.3707700 | 0.0003310 |
| H | 3.6805450 | 0.1411500 | 0.8799180 |
| H | 3.6806180 | 0.1414360 | -0.8795750 |

Z-2,3,4-hexatriene (**48**)

| | | | |
|---|---|---|---|
| C | -0.6326800 | -0.5010650 | -0.0001690 |
| C | 0.6326760 | -0.5010430 | -0.0003580 |
| C | -1.9501370 | -0.5029600 | 0.0001480 |
| H | -2.4654210 | -1.4626700 | 0.0006310 |
| C | 1.9501340 | -0.5029600 | 0.0001950 |
| H | 2.4653970 | -1.4626810 | 0.0006420 |
| C | 2.8155030 | 0.7274320 | -0.0000060 |
| H | 3.4686270 | 0.7426160 | 0.8798960 |
| H | 3.4689430 | 0.7421530 | -0.8796820 |
| H | 2.2144490 | 1.6373740 | -0.0003570 |
| C | -2.8154940 | 0.7274370 | 0.0000110 |
| H | -3.4690160 | 0.7421290 | -0.8796060 |
| H | -3.4685430 | 0.7426580 | 0.8799700 |
| H | -2.2144440 | 1.6373810 | -0.0004240 |

1,5-hexadiene (**49**)

| | | | |
|---|---|---|---|
| C | 0.5733100 | -0.2965860 | 0.5187380 |
| H | 0.4848110 | 0.5870100 | 1.1583500 |
| H | 0.4532110 | -1.1720080 | 1.1709830 |
| C | -0.5733370 | -0.2968090 | -0.5187050 |
| H | -0.4848640 | 0.5865310 | -1.1586740 |
| H | -0.4532240 | -1.1724950 | -1.1705900 |
| C | 1.9332630 | -0.3359030 | -0.1183790 |
| H | 2.1397860 | -1.2054140 | -0.7419180 |
| C | 2.8702090 | 0.5983380 | 0.0132490 |
| H | 2.7087980 | 1.4828670 | 0.6225600 |
| H | 3.8332180 | 0.5133390 | -0.4777210 |
| C | -1.9332780 | -0.3358950 | 0.1184540 |
| H | -2.1398220 | -1.2052330 | 0.7422280 |
| C | -2.8701700 | 0.5983720 | -0.0133590 |
| H | -2.7087390 | 1.4827430 | -0.6228950 |
| H | -3.8331530 | 0.5135640 | 0.4776940 |

1,5-hexadiyne (**50**)

| | | | |
|---|---|---|---|
| C | 0.4821330 | 0.6076540 | 0.0000000 |
| H | 0.2757320 | 1.2284500 | -0.8772100 |
| H | 0.2757320 | 1.2284500 | 0.8772100 |
| C | -0.4821330 | -0.6076540 | 0.0000000 |
| H | -0.2757320 | -1.2284500 | -0.8772100 |
| H | -0.2757320 | -1.2284500 | 0.8772100 |
| C | 1.8839890 | 0.2026710 | 0.0000000 |
| C | 3.0316080 | -0.1527310 | -0.0000010 |
| H | 4.0484670 | -0.4600230 | -0.0000010 |
| C | -1.8839890 | -0.2026710 | 0.0000000 |
| C | -3.0316080 | 0.1527310 | 0.0000010 |
| H | -4.0484670 | 0.4600230 | 0.0000010 |

hexa-1-ene-5-yne (**51**)

| | | | |
|---|---|---|---|
| C | 0.6321870 | 0.6126600 | -0.2577320 |
| H | 0.3860530 | 0.7336400 | -1.3181580 |
| H | 0.5788150 | 1.6132040 | 0.1869740 |
| C | -0.4234790 | -0.3051030 | 0.4080550 |
| H | -0.3834490 | -1.2950760 | -0.0539920 |
| H | -0.1491790 | -0.4325090 | 1.4614820 |
| C | 1.9935070 | 0.1014290 | -0.1287180 |
| C | 3.1045190 | -0.3412580 | -0.0118600 |
| H | 4.0899100 | -0.7249220 | 0.0879040 |
| C | -1.8115710 | 0.2602490 | 0.3070000 |
| H | -1.9678360 | 1.2270970 | 0.7844540 |
| C | -2.8315360 | -0.3231010 | -0.3150790 |
| H | -2.7230480 | -1.2865230 | -0.8045600 |
| H | -3.8130310 | 0.1358240 | -0.3541000 |

cyclopentadiene (**52**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.1795220 | 0.2809340 |
| C | 0.0000000 | -1.1795220 | 0.2809340 |
| C | 0.0000000 | 0.7341730 | -0.9889490 |
| C | 0.0000000 | -0.7341730 | -0.9889490 |
| H | 0.0000000 | 2.2101160 | 0.6081660 |
| H | 0.0000000 | -2.2101160 | 0.6081660 |
| H | 0.0000000 | 1.3463450 | -1.8817540 |
| H | 0.0000000 | -1.3463450 | -1.8817540 |
| C | 0.0000000 | 0.0000000 | 1.2149490 |
| H | 0.8768940 | 0.0000000 | 1.8768270 |
| H | -0.8768940 | 0.0000000 | 1.8768270 |

2-ethyl-1-butene (**53**)

| | | | |
|---|---|---|---|
| C | -2.3811860 | -0.5220040 | -0.1568520 |
| H | -2.4679400 | -0.1787980 | -1.1912170 |
| H | -2.8474120 | 0.2292860 | 0.4860710 |
| C | -0.9225500 | -0.7647340 | 0.2318200 |
| H | -0.8806400 | -1.1635550 | 1.2548350 |
| H | -0.5130780 | -1.5645070 | -0.3979990 |
| C | 1.4487930 | 0.1576910 | 0.5536170 |
| H | 1.9609700 | 1.1114370 | 0.7093610 |
| H | 1.4684340 | -0.3685990 | 1.5166730 |
| C | 0.0088170 | 0.4281280 | 0.1642500 |
| C | -0.3842720 | 1.6482130 | -0.2050620 |
| H | -1.4036810 | 1.8692980 | -0.4970830 |
| H | 0.3145330 | 2.4780900 | -0.2260670 |
| H | -2.9590990 | -1.4449310 | -0.0632740 |
| C | 2.2329910 | -0.6694110 | -0.4807400 |
| H | 3.2658040 | -0.8170430 | -0.1533580 |
| H | 1.7924300 | -1.6580490 | -0.6323530 |
| H | 2.2541170 | -0.1599260 | -1.4477890 |

2-methyl-1-pentene (**54**)

| | | | |
|---|---|---|---|
| C | 2.7775800 | -0.2819270 | 0.0000630 |
| H | 2.8854250 | -0.9197860 | -0.8828150 |
| H | 2.8854370 | -0.9194560 | 0.8831790 |
| H | 3.6100750 | 0.4266810 | -0.0000740 |
| C | 1.4293760 | 0.4448290 | -0.0000620 |
| H | 1.3678590 | 1.0983840 | 0.8767210 |
| H | 1.3678360 | 1.0980600 | -0.8770860 |
| C | 0.2418450 | -0.5202800 | 0.0001320 |
| H | 0.3211960 | -1.1879020 | -0.8702090 |
| H | 0.3211720 | -1.1875250 | 0.8707660 |
| C | -2.2709690 | -0.9185920 | 0.0000350 |
| H | -2.2145830 | -1.5715290 | 0.8788090 |
| H | -3.2476550 | -0.4314070 | -0.0000650 |
| H | -2.2144930 | -1.5717090 | -0.8786000 |
| C | -1.1451830 | 0.0859730 | -0.0000080 |
| C | -1.3824470 | 1.3982600 | -0.0001780 |
| H | -0.5868880 | 2.1332580 | -0.0002390 |
| H | -2.3965960 | 1.7833520 | -0.0002840 |

2-methyl-2-pentene (**55**)

| | | | |
|---|---|---|---|
| C | 2.6001880 | -0.1816500 | 0.4948630 |
| H | 2.7975750 | -1.2575830 | 0.4705640 |
| H | 2.2804190 | 0.0730620 | 1.5088380 |
| C | 1.5247590 | 0.2077350 | -0.5340450 |
| H | 1.3697650 | 1.2887670 | -0.5058570 |
| H | 1.9049000 | -0.0186240 | -1.5389520 |
| H | 3.5431840 | 0.3350240 | 0.2948150 |
| C | 0.2326090 | -0.5339870 | -0.3273630 |
| C | -0.9802690 | -0.0451920 | -0.0423880 |
| C | -2.1626970 | -0.9667820 | 0.1362050 |
| H | -2.6049290 | -0.8511590 | 1.1330710 |
| H | -2.9554190 | -0.7337230 | -0.5849410 |
| H | -1.8839090 | -2.0144400 | 0.0074960 |
| H | 0.3213230 | -1.6171310 | -0.4148160 |
| C | -1.3044230 | 1.4183920 | 0.1246520 |
| H | -1.7366250 | 1.6045290 | 1.1148620 |
| H | -0.4381320 | 2.0691420 | 0.0101000 |
| H | -2.0591490 | 1.7310410 | -0.6067230 |

2-methylpentane (**56**)

| | | | |
|---|---|---|---|
| C | 2.8452150 | -0.2116330 | 0.1505850 |
| H | 2.9959950 | -1.2264020 | -0.2310360 |
| H | 2.9048560 | -0.2583450 | 1.2425270 |
| H | 3.6789350 | 0.4024250 | -0.2009630 |
| C | 1.4984380 | 0.3579590 | -0.3060200 |
| H | 1.4031510 | 1.3863680 | 0.0577180 |
| H | 1.4811650 | 0.4181660 | -1.4013450 |
| C | 0.3049680 | -0.4796490 | 0.1696290 |
| H | 0.2933080 | -0.5040070 | 1.2682710 |
| H | 0.4585070 | -1.5173110 | -0.1531720 |
| C | -1.0744810 | -0.0130030 | -0.3327350 |
| H | -1.0249650 | 0.0447230 | -1.4290270 |
| C | -2.1562670 | -1.0392810 | 0.0322700 |
| H | -2.2485450 | -1.1388620 | 1.1194030 |
| H | -3.1343820 | -0.7416260 | -0.3569540 |
| H | -1.9209510 | -2.0278600 | -0.3729600 |
| C | -1.4536820 | 1.3784380 | 0.1950900 |
| H | -1.4869490 | 1.3816340 | 1.2904840 |
| H | -0.7433090 | 2.1466700 | -0.1194310 |
| H | -2.4419550 | 1.6774400 | -0.1664270 |

3-methylpentane (**57**)

| | | | |
|---|---|---|---|
| C | -2.5846000 | -0.1722880 | -0.2904960 |
| H | -2.5688100 | -0.2063800 | -1.3847080 |
| H | -2.7985940 | 0.8574000 | 0.0064080 |
| H | -3.4227240 | -0.7884490 | 0.0466510 |
| C | -1.2634680 | -0.6810400 | 0.2962920 |
| H | -1.3020720 | -0.6201200 | 1.3918440 |
| H | -1.1607300 | -1.7458920 | 0.0567420 |
| C | -0.0000030 | 0.0510050 | -0.1986850 |
| H | -0.0000220 | 0.0010740 | -1.2977190 |
| C | 1.2634450 | -0.6810930 | 0.2962400 |
| H | 1.1606910 | -1.7459220 | 0.0565930 |
| C | 2.5845870 | -0.1722960 | -0.2904770 |
| H | 2.7985800 | 0.8573620 | 0.0065340 |
| H | 3.4226980 | -0.7885000 | 0.0466250 |
| H | 2.5688170 | -0.2062790 | -1.3846930 |
| H | 1.3020360 | -0.6202700 | 1.3917980 |
| C | 0.0000370 | 1.5322390 | 0.2068610 |
| H | -0.8784830 | 2.0562510 | -0.1762670 |
| H | 0.0001090 | 1.6343220 | 1.2981640 |
| H | 0.8785150 | 2.0562390 | -0.1763820 |

E-3-methyl-2-pentene (**58**)

| | | | |
|---|---|---|---|
| C | -2.3532200 | -0.3442140 | 0.5449990 |
| H | -2.5593010 | 0.6995420 | 0.7954240 |
| H | -2.0103070 | -0.8460450 | 1.4541120 |
| C | -1.3062710 | -0.4702910 | -0.5755490 |
| H | -1.1919920 | -1.5257770 | -0.8396850 |
| H | -1.6888650 | 0.0356030 | -1.4722510 |
| H | -3.2995710 | -0.8014620 | 0.2429240 |
| C | 0.0968860 | 1.6020630 | -0.0511420 |
| H | -0.3201790 | 2.1013330 | -0.9335400 |
| H | -0.5088480 | 1.9212990 | 0.8038620 |
| H | 1.1058290 | 1.9839500 | 0.1016660 |
| C | 0.0527530 | 0.1034190 | -0.2253260 |
| C | 1.1116170 | -0.7052450 | -0.0957140 |
| H | 0.9424040 | -1.7691220 | -0.2579030 |
| C | 2.5295260 | -0.3493280 | 0.2493590 |
| H | 2.8437520 | -0.8573430 | 1.1685540 |
| H | 3.2158830 | -0.6807480 | -0.5384350 |
| H | 2.6834550 | 0.7203480 | 0.3955100 |

Z-3-methyl-2-pentene (**59**)

| | | | |
|---|---|---|---|
| C | 1.6963370 | -1.2850160 | -0.4381590 |
| H | 2.3714390 | -0.5755470 | -0.9239960 |
| H | 1.0600160 | -1.7209990 | -1.2127050 |
| C | 0.8458150 | -0.6049330 | 0.6504420 |
| H | 0.2140590 | -1.3564590 | 1.1292530 |
| H | 1.5126470 | -0.2249430 | 1.4340740 |
| H | 2.3082630 | -2.0848790 | -0.0115970 |
| C | 0.7480760 | 1.8448760 | -0.0678190 |
| H | 1.1504060 | 2.2131160 | 0.8836090 |
| H | 1.6034320 | 1.7220500 | -0.7417430 |
| H | 0.1013730 | 2.6192120 | -0.4852620 |
| C | 0.0064570 | 0.5438560 | 0.1290960 |
| C | -1.2976360 | 0.4520460 | -0.1578250 |
| H | -1.7889160 | 1.3484370 | -0.5341420 |
| C | -2.1959800 | -0.7455740 | -0.0340740 |
| H | -3.0444630 | -0.5306650 | 0.6258810 |
| H | -2.6212970 | -1.0134280 | -1.0082510 |
| H | -1.6853760 | -1.6274200 | 0.3549190 |

2-methylpropene (**60**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2760720 | -0.6781250 |
| H | 0.8785880 | 1.3270510 | -1.3317800 |
| H | -0.8785880 | 1.3270510 | -1.3317800 |
| H | 0.0000000 | 2.1586540 | -0.0360830 |
| C | 0.0000000 | 0.0000000 | 0.1239730 |
| C | 0.0000000 | 0.0000000 | 1.4569370 |
| H | 0.0000000 | -0.9238350 | 2.0256620 |
| H | 0.0000000 | 0.9238350 | 2.0256620 |
| C | 0.0000000 | -1.2760720 | -0.6781250 |
| H | -0.8785880 | -1.3270510 | -1.3317800 |
| H | 0.8785880 | -1.3270510 | -1.3317800 |
| H | 0.0000000 | -2.1586540 | -0.0360830 |

2-methyl-1-butene (**61**)

| | | | |
|---|---|---|---|
| C | -2.0460390 | -0.0375450 | 0.0000200 |
| H | -2.1638370 | 0.5949670 | 0.8838020 |
| H | -2.1638550 | 0.5949530 | -0.8837700 |
| H | -2.8623270 | -0.7642570 | 0.0000340 |
| C | -0.6951410 | -0.7525980 | 0.0000120 |
| H | -0.6370020 | -1.4210010 | 0.8701000 |
| H | -0.6370210 | -1.4210160 | -0.8700650 |
| C | 0.5410760 | 0.1211070 | -0.0000100 |
| C | 0.5061540 | 1.4540070 | -0.0000470 |
| H | -0.4227500 | 2.0111530 | -0.0000590 |
| H | 1.4199680 | 2.0385870 | -0.0000710 |
| C | 1.8466000 | -0.6351160 | 0.0000150 |
| H | 1.9231490 | -1.2858150 | 0.8788690 |
| H | 1.9230790 | -1.2860100 | -0.8786990 |
| H | 2.7046950 | 0.0393130 | -0.0000910 |

2-methyl-2-butene (**62**)

| | | | |
|---|---|---|---|
| C | 0.6253880 | 1.4564900 | -0.0000110 |
| H | 1.1990400 | 1.7761330 | -0.8780400 |
| H | 1.1989700 | 1.7761490 | 0.8780580 |
| H | -0.3170500 | 2.0030780 | -0.0000500 |
| C | 0.4483340 | -0.0409190 | -0.0000030 |
| C | -0.7314340 | -0.6719850 | 0.0000010 |
| H | -0.7086380 | -1.7608540 | 0.0000150 |
| C | -2.1111700 | -0.0788960 | 0.0000030 |
| H | -2.6773520 | -0.4114030 | -0.8777440 |
| H | -2.6772300 | -0.4111050 | 0.8779450 |
| H | -2.1116500 | 1.0115750 | -0.0001800 |
| C | 1.7406910 | -0.8206760 | 0.0000050 |
| H | 2.3492350 | -0.5747840 | -0.8786350 |
| H | 2.3492400 | -0.5747600 | 0.8786350 |
| H | 1.5645780 | -1.8981100 | 0.0000210 |

isobutane (**63**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.3718180 |
| H | 0.0000000 | 0.0000000 | 1.4698600 |
| C | 0.0000000 | 1.4611630 | -0.0956940 |
| H | 0.0000000 | 1.5198980 | -1.1898300 |
| H | -0.8840930 | 1.9951230 | 0.2652020 |
| H | 0.8840930 | 1.9951230 | 0.2652020 |
| C | -1.2654040 | -0.7305810 | -0.0956940 |
| H | -1.3162700 | -0.7599490 | -1.1898300 |
| H | -1.2857800 | -1.7632090 | 0.2652020 |
| H | -2.1698730 | -0.2319140 | 0.2652020 |
| C | 1.2654040 | -0.7305810 | -0.0956940 |
| H | 2.1698730 | -0.2319140 | 0.2652020 |
| H | 1.2857800 | -1.7632090 | 0.2652020 |
| H | 1.3162700 | -0.7599490 | -1.1898300 |

isopentane (**64**)

| | | | |
|---|---|---|---|
| C | 1.7389670 | -0.8248350 | -0.0124840 |
| H | 1.9200660 | -0.8604440 | 1.0675550 |
| H | 1.6419600 | -1.8551690 | -0.3672840 |
| H | 2.6264440 | -0.3909900 | -0.4825000 |
| C | 0.4817950 | -0.0028100 | -0.3284950 |
| H | 0.3456500 | -0.0038480 | -1.4190960 |
| C | -0.7652370 | -0.6598910 | 0.2934680 |
| H | -0.7730170 | -1.7198150 | 0.0131260 |
| H | -0.6681320 | -0.6370270 | 1.3869490 |
| C | -2.1015970 | -0.0322550 | -0.1158620 |
| H | -2.2204080 | -0.0332740 | -1.2042870 |
| H | -2.9410360 | -0.5903840 | 0.3078730 |
| H | -2.1924730 | 1.0016970 | 0.2266550 |
| C | 0.6641160 | 1.4536940 | 0.1214840 |
| H | -0.1859600 | 2.0811410 | -0.1570380 |
| H | 0.7803800 | 1.5115860 | 1.2096800 |
| H | 1.5582670 | 1.8931130 | -0.3302980 |

$H_2$ (**65**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 0.3720630 |
| H | 0.0000000 | 0.0000000 | -0.3720630 |

## MP2(full)/6-31G(d) Optimized Structures (G3)

1,3-cyclohexadiene (**1**)

| | | | |
|---|---|---|---|
| C | -1.2533420 | -0.7212790 | 0.1186070 |
| C | -1.2533420 | 0.7212790 | -0.1186070 |
| C | -0.1006970 | 1.4172720 | -0.0676210 |
| C | 1.1813300 | 0.7100000 | 0.2807740 |
| C | 1.1813300 | -0.7100000 | -0.2807740 |
| C | -0.1006970 | -1.4172720 | 0.0676210 |
| H | -2.1958300 | -1.2220010 | 0.3268760 |
| H | -2.1958300 | 1.2220010 | -0.3268760 |
| H | -0.0956520 | 2.4959480 | -0.2061070 |
| H | 2.0487960 | 1.2653910 | -0.0905700 |
| H | 1.2789430 | 0.6673560 | 1.3769450 |
| H | 1.2789430 | -0.6673560 | -1.3769450 |
| H | 2.0487960 | -1.2653910 | 0.0905710 |
| H | -0.0956520 | -2.4959480 | 0.2061070 |

1,3-hexadiene (**2**)

| | | | |
|---|---|---|---|
| C | -3.1122280 | -0.1806790 | 0.2716360 |
| C | -1.9466020 | 0.4094410 | -0.0401530 |
| C | -0.6724620 | -0.2889510 | -0.0946500 |
| C | 0.4946040 | 0.3013570 | -0.4099620 |
| C | 1.8193510 | -0.3922610 | -0.4498440 |
| C | 2.7955760 | 0.1777510 | 0.5818040 |
| H | -4.0429640 | 0.3748930 | 0.3019210 |
| H | -3.1659300 | -1.2401240 | 0.5057890 |
| H | -1.9316050 | 1.4748970 | -0.2696200 |
| H | -0.6847400 | -1.3557690 | 0.1349820 |
| H | 0.4980710 | 1.3699430 | -0.6354750 |
| H | 1.6749870 | -1.4643680 | -0.2739230 |
| H | 2.2575560 | -0.2934040 | -1.4514720 |
| H | 3.7657080 | -0.3243830 | 0.5267180 |
| H | 2.9591900 | 1.2463330 | 0.4150780 |
| H | 2.4002900 | 0.0520290 | 1.5930150 |

1,3-hexadiyne (**3**)

| | | | |
|---|---|---|---|
| C | 3.3530920 | 0.2499350 | 0.0000100 |
| C | 2.1467470 | 0.0412240 | -0.0000020 |
| C | 0.7943250 | -0.1843760 | -0.0000130 |
| C | -0.4125650 | -0.4054170 | -0.0000230 |
| C | -1.8592100 | -0.6077150 | -0.0000320 |
| C | -2.6316190 | 0.7147970 | 0.0000460 |
| H | 4.4059230 | 0.4200140 | 0.0000160 |
| H | -2.1371320 | -1.2025150 | -0.8778290 |
| H | -2.1371280 | -1.2026170 | 0.8776970 |
| H | -3.7083190 | 0.5249030 | 0.0000360 |
| H | -2.3839820 | 1.3047100 | 0.8848200 |
| H | -2.3839840 | 1.3048120 | -0.8846600 |

1,4-hexadiene (**5**)

| | | | |
|---|---|---|---|
| C | -2.9516140 | -0.4567530 | -0.1118590 |
| C | -1.7955690 | -0.1218990 | 0.4707550 |
| C | -0.7583040 | 0.7725050 | -0.1475730 |
| C | 0.5249750 | 0.0281760 | -0.3849960 |
| C | 1.6895320 | 0.3090750 | 0.2134240 |
| C | 2.9639390 | -0.4458000 | -0.0054910 |
| H | -3.6623810 | -1.1208780 | 0.3685140 |
| H | -3.2253020 | -0.0729740 | -1.0907270 |
| H | -1.5491260 | -0.5298600 | 1.4507070 |
| H | -1.1471900 | 1.1724430 | -1.0931090 |
| H | -0.5609780 | 1.6300850 | 0.5087320 |
| H | 0.4703380 | -0.8105460 | -1.0806330 |
| H | 1.7311530 | 1.1462040 | 0.9116310 |
| H | 2.8180320 | -1.2617170 | -0.7182460 |
| H | 3.7510420 | 0.2094020 | -0.3935560 |
| H | 3.3366630 | -0.8739800 | 0.9311190 |

1,4-hexadiyne (**6**)

| | | | |
|---|---|---|---|
| C | -2.8373700 | -0.8889790 | -0.0000020 |
| C | -1.9477410 | -0.0563930 | 0.0000290 |
| C | -0.9188840 | 0.9896460 | 0.0000640 |
| C | 0.4429260 | 0.4450130 | -0.0001060 |
| C | 1.5951050 | 0.0438800 | -0.0001770 |
| C | 2.9562070 | -0.4875570 | 0.0000870 |
| H | -3.5837680 | -1.6501290 | -0.0000290 |
| H | -1.0583830 | 1.6339480 | 0.8773900 |
| H | -1.0585210 | 1.6340800 | -0.8771430 |
| H | 2.9457450 | -1.5809210 | -0.0048150 |
| H | 3.5084230 | -0.1513990 | -0.8817740 |
| H | 3.5050450 | -0.1592400 | 0.8869950 |

2-butene (**7**)

| | | | |
|---|---|---|---|
| C | 1.9556370 | -0.0791800 | 0.0000150 |
| C | 0.5367640 | 0.3996850 | 0.0000480 |
| C | -0.5367640 | -0.3996850 | -0.0000500 |
| C | -1.9556370 | 0.0791800 | -0.0000130 |
| H | 2.4971450 | 0.2831740 | -0.8803080 |
| H | 2.4971130 | 0.2829560 | 0.8804470 |
| H | 1.9998540 | -1.1716310 | -0.0001200 |
| H | 0.3859940 | 1.4799680 | 0.0001620 |
| H | -0.3859940 | -1.4799680 | -0.0001660 |
| H | -1.9998540 | 1.1716310 | 0.0000660 |
| H | -2.4971310 | -0.2830010 | -0.8804150 |
| H | -2.4971270 | -0.2831290 | 0.8803390 |

2-pentene (**8**)

| | | | |
|---|---|---|---|
| C | -2.3091140 | -0.4773130 | 0.2688100 |
| C | -1.3014260 | 0.5693800 | -0.2096340 |
| C | 0.0597320 | -0.0177640 | -0.4257030 |
| C | 1.1597970 | 0.3316780 | 0.2531750 |
| C | 2.5156740 | -0.2708030 | 0.0504820 |
| H | -3.3025000 | -0.0395470 | 0.4030020 |
| H | -2.3960240 | -1.2938750 | -0.4539340 |
| H | -1.9910950 | -0.9063020 | 1.2225830 |
| H | -1.2343740 | 1.3829160 | 0.5217980 |
| H | -1.6640610 | 1.0163490 | -1.1442400 |
| H | 0.1344860 | -0.8009320 | -1.1831130 |
| H | 1.0807260 | 1.1121530 | 1.0111830 |
| H | 2.4898070 | -1.0405550 | -0.7254720 |
| H | 3.2469910 | 0.4881660 | -0.2473080 |
| H | 2.8880700 | -0.7294450 | 0.9727250 |

2-pentyne (**9**)

| | | | |
|---|---|---|---|
| C | -2.6540630 | 0.2252620 | 0.0000190 |
| C | -1.2250520 | -0.0822980 | -0.0000500 |
| C | -0.0345180 | -0.3534960 | 0.0000070 |
| C | 1.4011190 | -0.6392980 | 0.0000080 |
| C | 2.2500860 | 0.6344550 | 0.0000010 |
| H | -2.8227850 | 1.3058100 | -0.0110810 |
| H | -3.1473790 | -0.2001180 | -0.8784900 |
| H | -3.1432790 | -0.1813330 | 0.8896450 |
| H | 1.6508820 | -1.2481740 | 0.8767550 |
| H | 1.6508830 | -1.2481770 | -0.8767360 |
| H | 3.3153720 | 0.3870090 | 0.0000020 |
| H | 2.0354340 | 1.2386130 | -0.8841920 |
| H | 2.0354330 | 1.2386230 | 0.8841870 |

hexa-1-ene-3-yne (**10**)

| | | | |
|---|---|---|---|
| C | 2.9272270 | 0.6105800 | 0.2094120 |
| C | 2.1158760 | -0.3335870 | -0.2965290 |
| C | 0.7094710 | -0.3765290 | -0.0672670 |
| C | -0.5003770 | -0.4639940 | 0.1035530 |
| C | -1.9469910 | -0.5038960 | 0.3122870 |
| C | -2.6521210 | 0.7316540 | -0.2547800 |
| H | 3.9919120 | 0.5983610 | 0.0039210 |
| H | 2.5463570 | 1.4101610 | 0.8358570 |
| H | 2.5377140 | -1.1194890 | -0.9212680 |
| H | -2.3542980 | -1.4088700 | -0.1532080 |
| H | -2.1558000 | -0.5889480 | 1.3852570 |
| H | -3.7299100 | 0.6708250 | -0.0801640 |
| H | -2.2750650 | 1.6401860 | 0.2195980 |
| H | -2.4794210 | 0.8124090 | -1.3300510 |

hexa-1-ene-4-yne (**11**)

| | | | |
|---|---|---|---|
| C | -2.8199440 | -0.6040910 | 0.2927840 |
| C | -1.7764580 | -0.1988040 | -0.4364830 |
| C | -0.8307100 | 0.8936670 | -0.0137760 |
| C | 0.5592080 | 0.4297620 | 0.0222310 |
| C | 1.7198280 | 0.0510260 | 0.0306210 |
| C | 3.1009150 | -0.4262250 | 0.0587710 |
| H | -3.4819240 | -1.3917380 | -0.0505720 |
| H | -3.0442760 | -0.1621040 | 1.2592710 |
| H | -1.5680390 | -0.6660300 | -1.3973500 |
| H | -0.9100920 | 1.7404660 | -0.7091040 |
| H | -1.1265890 | 1.2712010 | 0.9725940 |
| H | 3.1421950 | -1.5119430 | -0.0658910 |
| H | 3.6901600 | 0.0270480 | -0.7433160 |
| H | 3.5815380 | -0.1789110 | 1.0094830 |

hexa-1-yne-3-ene (**12**)

| | | | |
|---|---|---|---|
| C | 3.2144050 | -0.3708320 | -0.0002890 |
| C | 2.0629910 | 0.0252210 | -0.1034050 |
| C | 0.7325810 | 0.5159100 | -0.2473780 |
| C | -0.3224920 | 0.0108460 | 0.4181520 |
| C | -1.7256550 | 0.5017610 | 0.2585870 |
| C | -2.6514380 | -0.5855940 | -0.2919780 |
| H | 4.2117590 | -0.7333920 | 0.1027770 |
| H | 0.5822560 | 1.3459900 | -0.9372190 |
| H | -0.1613380 | -0.8215090 | 1.1039230 |
| H | -2.1068030 | 0.8412440 | 1.2302140 |
| H | -1.7337830 | 1.3729720 | -0.4062560 |
| H | -3.6776950 | -0.2186450 | -0.3813150 |
| H | -2.3153980 | -0.9109910 | -1.2797080 |
| H | -2.6613520 | -1.4595330 | 0.3654580 |

hexa-1-yne-4-ene (**13**)

| | | | |
|---|---|---|---|
| C | 2.9386280 | -0.7512520 | -0.1349650 |
| C | 1.9814410 | -0.0012640 | -0.0453350 |
| C | 0.8367500 | 0.9050430 | 0.0829670 |
| C | -0.4305530 | 0.1653150 | 0.4177780 |
| C | -1.5396860 | 0.2084340 | -0.3292760 |
| C | -2.8091110 | -0.5164120 | -0.0067520 |
| H | 3.7603210 | -1.4243290 | -0.2252030 |
| H | 1.0562190 | 1.6468710 | 0.8625030 |
| H | 0.7007860 | 1.4636970 | -0.8507320 |
| H | -0.4115980 | -0.4345690 | 1.3273650 |
| H | -1.5355220 | 0.8059360 | -1.2416030 |
| H | -2.7106140 | -1.0859260 | 0.9209510 |
| H | -3.6450170 | 0.1815930 | 0.1078830 |
| H | -3.0793880 | -1.2124510 | -0.8076610 |

propane (**14**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2667270 | -0.2601730 |
| C | 0.0000000 | -1.2667270 | -0.2601730 |
| C | 0.0000000 | 0.0000000 | 0.5879680 |
| H | 0.0000000 | 2.1665070 | 0.3612660 |
| H | 0.0000000 | -2.1665070 | 0.3612660 |
| H | -0.8834890 | 1.3033550 | -0.9046490 |
| H | 0.8834890 | 1.3033550 | -0.9046490 |
| H | 0.8834890 | -1.3033550 | -0.9046490 |
| H | -0.8834890 | -1.3033550 | -0.9046490 |
| H | -0.8767380 | 0.0000000 | 1.2451650 |
| H | 0.8767380 | 0.0000000 | 1.2451650 |

propene (**15**)

| | | | |
|---|---|---|---|
| C | 1.2911060 | 0.1336650 | 0.0000000 |
| C | 0.0000000 | 0.4793900 | 0.0000000 |
| C | -1.1396130 | -0.4921960 | 0.0000000 |
| H | 2.0808660 | 0.8771150 | 0.0000000 |
| H | 1.5998950 | -0.9078490 | 0.0000000 |
| H | -0.2630070 | 1.5364360 | 0.0000000 |
| H | -0.7752400 | -1.5227640 | 0.0000000 |
| H | -1.7757350 | -0.3540460 | 0.8803980 |
| H | -1.7757350 | -0.3540460 | -0.8803980 |

propyne (**16**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.2147970 |
| C | 0.0000000 | 0.0000000 | 1.4328260 |
| C | 0.0000000 | 0.0000000 | -1.2460720 |
| H | 0.0000000 | 1.0214050 | -1.6360520 |
| H | -0.8845630 | -0.5107030 | -1.6360520 |
| H | 0.8845630 | -0.5107030 | -1.6360520 |
| H | 0.0000000 | 0.0000000 | 2.4988550 |

ethane (**17**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.7621890 | 0.0000000 |
| C | 0.0000000 | -0.7621890 | 0.0000000 |
| H | -0.5093450 | 1.1572660 | 0.8822110 |
| H | 0.5093450 | -1.1572660 | -0.8822110 |
| H | -0.5093450 | 1.1572660 | -0.8822110 |
| H | 0.5093450 | -1.1572660 | 0.8822110 |
| H | 1.0186900 | 1.1572650 | 0.0000000 |
| H | -1.0186900 | -1.1572650 | 0.0000000 |

1,3-butadiene (**18**)

| | | | |
|---|---|---|---|
| C | 0.6055440 | 1.7465860 | 0.0000000 |
| C | 0.6055440 | 0.4041970 | 0.0000000 |
| H | -0.3216100 | 2.3128130 | 0.0000000 |
| H | 1.5273900 | 2.3176620 | 0.0000000 |
| H | 1.5533520 | -0.1336480 | 0.0000000 |
| C | -0.6055440 | -0.4041970 | 0.0000000 |
| C | -0.6055440 | -1.7465860 | 0.0000000 |
| H | -1.5533520 | 0.1336480 | 0.0000000 |
| H | -1.5273900 | -2.3176620 | 0.0000000 |
| H | 0.3216100 | -2.3128130 | 0.0000000 |

1,3-butadiyne (**19**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 2.9763810 |
| C | 0.0000000 | 0.0000000 | 1.9095120 |
| C | 0.0000000 | 0.0000000 | 0.6863680 |
| C | 0.0000000 | 0.0000000 | -0.6863680 |
| C | 0.0000000 | 0.0000000 | -1.9095120 |
| H | 0.0000000 | 0.0000000 | -2.9763810 |

allene (**20**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 1.3111320 |
| C | 0.0000000 | 0.0000000 | 0.0000000 |
| C | 0.0000000 | 0.0000000 | -1.3111320 |
| H | -0.9267800 | 0.0000000 | -1.8766750 |
| H | 0.9267800 | 0.0000000 | -1.8766750 |
| H | 0.0000000 | 0.9267800 | 1.8766750 |
| H | 0.0000000 | -0.9267800 | 1.8766750 |

butatriene (**21**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6371320 |
| C | 0.0000000 | 0.0000000 | -0.6371320 |
| C | 0.0000000 | 0.0000000 | 1.9591780 |
| C | 0.0000000 | 0.0000000 | -1.9591780 |
| H | 0.0000000 | 0.9263470 | -2.5273580 |
| H | 0.0000000 | -0.9263470 | -2.5273580 |
| H | 0.0000000 | 0.9263470 | 2.5273580 |
| H | 0.0000000 | -0.9263470 | 2.5273580 |

ethene (**22**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6674320 |
| C | 0.0000000 | 0.0000000 | -0.6674320 |
| H | 0.0000000 | 0.9229600 | -1.2375450 |
| H | 0.0000000 | -0.9229600 | -1.2375450 |
| H | 0.0000000 | -0.9229600 | 1.2375450 |
| H | 0.0000000 | 0.9229600 | 1.2375450 |

vinylacetylene (**23**)

| | | | |
|---|---|---|---|
| C | -0.4698860 | 1.8672890 | 0.0000000 |
| C | 0.0000000 | 0.7397030 | 0.0000000 |
| H | -0.9069030 | 2.8399430 | 0.0000000 |
| C | 0.5942520 | -0.5578250 | 0.0000000 |
| H | 1.6815990 | -0.6003080 | 0.0000000 |
| C | -0.1164460 | -1.6971850 | 0.0000000 |
| H | 0.3789470 | -2.6616480 | 0.0000000 |
| H | -1.2011620 | -1.6898800 | 0.0000000 |

methane (**24**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.0000000 |
| H | -1.0529870 | 0.2794680 | 0.0000000 |
| H | 0.0875100 | -1.0859210 | 0.0000000 |
| H | 0.4827380 | 0.4032260 | 0.8895260 |
| H | 0.4827380 | 0.4032260 | -0.8895260 |

butane (**25**)

| | | | |
|---|---|---|---|
| C | -0.4214040 | 0.6355330 | 0.0000000 |
| C | 0.4214040 | -0.6355330 | 0.0000000 |
| C | 0.4214040 | 1.9060320 | 0.0000000 |
| C | -0.4214040 | -1.9060320 | 0.0000000 |
| H | -1.0794260 | 0.6300990 | 0.8772890 |
| H | -1.0794260 | 0.6300990 | -0.8772890 |
| H | 1.0794260 | -0.6300990 | 0.8772890 |
| H | 1.0794260 | -0.6300990 | -0.8772890 |
| H | 0.2046350 | -2.8022730 | 0.0000000 |
| H | -0.2046350 | 2.8022730 | 0.0000000 |
| H | -1.0651780 | -1.9468780 | -0.8833320 |
| H | -1.0651780 | -1.9468780 | 0.8833320 |
| H | 1.0651780 | 1.9468780 | -0.8833320 |
| H | 1.0651780 | 1.9468780 | 0.8833320 |

acetylene (**26**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 1.6742940 |
| C | 0.0000000 | 0.0000000 | 0.6081470 |
| C | 0.0000000 | 0.0000000 | -0.6081470 |
| H | 0.0000000 | 0.0000000 | -1.6742940 |

hexadieneyne (**27**)

| | | | |
|---|---|---|---|
| C | -0.1713990 | 3.0051020 | 0.0000000 |
| C | 0.1713990 | -3.0051020 | 0.0000000 |
| C | 0.6398960 | 1.9325850 | 0.0000000 |
| C | -0.6398960 | -1.9325850 | 0.0000000 |
| C | 0.1713990 | 0.5896470 | 0.0000000 |
| C | -0.1713990 | -0.5896470 | 0.0000000 |
| H | -1.2511860 | 2.9004520 | 0.0000000 |
| H | 1.2511860 | -2.9004520 | 0.0000000 |
| H | 0.2353950 | 4.0103110 | 0.0000000 |
| H | -0.2353950 | -4.0103110 | 0.0000000 |
| H | 1.7190140 | 2.0782140 | 0.0000000 |
| H | -1.7190140 | -2.0782140 | 0.0000000 |

hexadiyneene (**28**)

| | | | |
|---|---|---|---|
| C | 0.5274770 | 3.0227870 | 0.0000000 |
| C | -0.5274770 | -3.0227870 | 0.0000000 |
| C | 0.5274770 | 1.8003940 | 0.0000000 |
| C | -0.5274770 | -1.8003940 | 0.0000000 |
| C | 0.5601270 | 0.3798310 | 0.0000000 |
| C | -0.5601270 | -0.3798310 | 0.0000000 |
| H | 0.5149720 | 4.0893340 | 0.0000000 |
| H | -0.5149720 | -4.0893340 | 0.0000000 |
| H | 1.5336370 | -0.1070950 | 0.0000000 |
| H | -1.5336370 | 0.1070950 | 0.0000000 |

pentane (**29**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2745400 | -0.5242930 |
| C | 0.0000000 | -1.2745400 | -0.5242930 |
| C | 0.0000000 | 0.0000000 | 0.3132010 |
| C | 0.0000000 | 2.5404370 | 0.3256320 |
| C | 0.0000000 | -2.5404370 | 0.3256320 |
| H | 0.8776490 | 1.2726090 | -1.1823280 |
| H | -0.8776490 | 1.2726090 | -1.1823280 |
| H | 0.8776490 | -1.2726090 | -1.1823280 |
| H | -0.8776490 | -1.2726090 | -1.1823280 |
| H | 0.8783630 | 0.0000000 | 0.9726050 |
| H | -0.8783630 | 0.0000000 | 0.9726050 |
| H | 0.0000000 | -3.4407950 | -0.2952040 |
| H | 0.0000000 | 3.4407950 | -0.2952040 |
| H | -0.8836230 | -2.5769350 | 0.9698100 |
| H | 0.8836230 | -2.5769350 | 0.9698100 |
| H | -0.8836230 | 2.5769350 | 0.9698100 |
| H | 0.8836230 | 2.5769350 | 0.9698100 |

2-butyne (**30**)

| | | | |
|---|---|---|---|
| C | -2.0718760 | 0.0000030 | 0.0000040 |
| C | -0.6099690 | -0.0000090 | -0.0000260 |
| H | -2.4645070 | -0.4362600 | 0.9227580 |
| H | -2.4645440 | -0.5809830 | -0.8391790 |
| H | -2.4645160 | 1.0172610 | -0.0835470 |
| H | 2.4645050 | -0.5808150 | -0.8393220 |
| C | 0.6099690 | -0.0000010 | 0.0000280 |
| H | 2.4645420 | -0.4364520 | 0.9226440 |
| C | 2.0718760 | 0.0000020 | -0.0000040 |
| H | 2.4645190 | 1.0172750 | -0.0833580 |

1-butyne (**31**)

| | | | |
|---|---|---|---|
| C | -0.6414340 | 1.8767650 | 0.0000000 |
| C | 0.0000000 | 0.8401410 | 0.0000000 |
| H | -1.2004040 | 2.7846340 | 0.0000000 |
| C | 0.7474450 | -0.4174150 | 0.0000000 |
| C | -0.1722600 | -1.6409350 | 0.0000000 |
| H | 1.4040340 | -0.4471350 | 0.8770870 |
| H | 1.4040340 | -0.4471350 | -0.8770870 |
| H | 0.4165240 | -2.5623420 | 0.0000000 |
| H | -0.8133440 | -1.6396740 | -0.8843110 |
| H | -0.8133440 | -1.6396740 | 0.8843110 |

1-butene (**32**)

| | | | |
|---|---|---|---|
| C | -1.8447360 | 0.0147770 | -0.2872700 |
| H | -0.6726020 | -1.2016850 | 0.9545810 |
| C | -0.7140870 | -0.2892640 | 0.3586260 |
| H | -2.7242670 | -0.6177480 | -0.2305540 |
| C | 0.5418020 | 0.5263720 | 0.3094700 |
| C | 1.7075540 | -0.2538050 | -0.3003400 |
| H | 0.3593770 | 1.4388940 | -0.2692120 |
| H | 0.8129260 | 0.8446450 | 1.3240750 |
| H | 2.6215930 | 0.3464970 | -0.3127720 |
| H | 1.9103870 | -1.1636810 | 0.2719890 |
| H | 1.4761510 | -0.5478610 | -1.3273070 |
| H | -1.9267650 | 0.9124580 | -0.8937090 |

1-pentene (**33**)

| | | | |
|---|---|---|---|
| C | -2.4572470 | -0.2340940 | -0.3112450 |
| C | -1.4078560 | 0.3544010 | 0.2726340 |
| C | -0.0691850 | -0.2892040 | 0.4650300 |
| C | 1.0404330 | 0.4346020 | -0.3015600 |
| C | 2.4098110 | -0.1984670 | -0.0823660 |
| H | -0.1157420 | -1.3363020 | 0.1408820 |
| H | 0.1880510 | -0.3003460 | 1.5331230 |
| H | -1.5036470 | 1.3829680 | 0.6221550 |
| H | -3.4029330 | 0.2812110 | -0.4421330 |
| H | -2.4034520 | -1.2564320 | -0.6750090 |
| H | 0.7919780 | 0.4308160 | -1.3688530 |
| H | 1.0655190 | 1.4867210 | 0.0070440 |
| H | 3.1879610 | 0.3292210 | -0.6407790 |
| H | 2.6837420 | -0.1783570 | 0.9767270 |
| H | 2.4127840 | -1.2429240 | -0.4081170 |

1-pentyne (**34**)

| | | | |
|---|---|---|---|
| C | 2.6442340 | -0.2437460 | 0.0000550 |
| C | 1.4948790 | 0.1632440 | -0.0000600 |
| C | 0.1088560 | 0.6295930 | 0.0000120 |
| C | -0.9009850 | -0.5233270 | 0.0000050 |
| C | -2.3390230 | -0.0191780 | -0.0000040 |
| H | -0.0638210 | 1.2644120 | -0.8779030 |
| H | -0.0637550 | 1.2643500 | 0.8779840 |
| H | 3.6492030 | -0.5993710 | -0.0001220 |
| H | -0.7206820 | -1.1521700 | -0.8779230 |
| H | -0.7206930 | -1.1521730 | 0.8779320 |
| H | -3.0488620 | -0.8506030 | 0.0000350 |
| H | -2.5395660 | 0.5930510 | 0.8842800 |
| H | -2.5395850 | 0.5929840 | -0.8843300 |

1,3-pentadiene (**35**)

| | | | |
|---|---|---|---|
| C | -1.3558860 | 0.4010790 | -0.0000120 |
| H | -1.3625700 | 1.4911160 | 0.0000180 |
| C | -2.5223950 | -0.2643200 | -0.0000510 |
| H | -3.4749510 | 0.2539050 | -0.0000530 |
| H | -2.5552480 | -1.3502060 | -0.0000810 |
| C | -0.0527130 | -0.2442160 | -0.0000070 |
| H | -0.0428100 | -1.3353850 | -0.0000370 |
| C | 1.1139750 | 0.4242850 | 0.0000310 |
| H | 1.0909780 | 1.5148940 | 0.0000610 |
| C | 2.4634310 | -0.2198700 | 0.0000350 |
| H | 3.0441070 | 0.0768710 | -0.8801740 |
| H | 3.0440900 | 0.0768460 | 0.8802650 |
| H | 2.3779320 | -1.3097890 | 0.0000190 |

1,3-pentadiyne (**36**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 1.5247650 |
| C | 0.0000000 | 0.0000000 | 2.7487470 |
| H | 0.0000000 | 0.0000000 | 3.8153270 |
| C | 0.0000000 | 0.0000000 | 0.1532250 |
| C | 0.0000000 | 0.0000000 | -1.0723950 |
| C | 0.0000000 | 0.0000000 | -2.5308590 |
| H | 0.0000000 | 1.0224810 | -2.9187410 |
| H | 0.8854940 | -0.5112400 | -2.9187410 |
| H | -0.8854940 | -0.5112400 | -2.9187410 |

1,4-pentadiene (**37**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.6828980 | -0.0000030 |
| H | -0.3288670 | 1.3342010 | 0.8199200 |
| H | 0.3288670 | 1.3341930 | -0.8199330 |
| C | -1.1555140 | -0.1678370 | -0.4465300 |
| H | -0.9680530 | -0.8143480 | -1.3033280 |
| C | -2.3516650 | -0.1931430 | 0.1504460 |
| H | -2.5701530 | 0.4342760 | 1.0100550 |
| H | -3.1513350 | -0.8369490 | -0.2001950 |
| C | 1.1555140 | -0.1678320 | 0.4465320 |
| H | 0.9680540 | -0.8143330 | 1.3033380 |
| C | 2.3516650 | -0.1931450 | -0.1504440 |
| H | 2.5701520 | 0.4342640 | -1.0100600 |
| H | 3.1513350 | -0.8369470 | 0.2002040 |

1,4-pentadiyne (**38**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2203750 | 0.0654110 |
| C | 0.0000000 | 2.2612450 | -0.5676560 |
| H | 0.0000000 | 3.1481780 | -1.1591970 |
| C | 0.0000000 | 0.0000000 | 0.8786620 |
| H | 0.8776610 | 0.0000000 | 1.5366820 |
| H | -0.8776610 | 0.0000000 | 1.5366820 |
| C | 0.0000000 | -1.2203750 | 0.0654110 |
| C | 0.0000000 | -2.2612450 | -0.5676560 |
| H | 0.0000000 | -3.1481780 | -1.1591970 |

penta-1-ene-3-yne (**39**)

| | | | |
|---|---|---|---|
| C | 1.2597900 | 0.9145090 | 0.0000000 |
| H | 1.2398420 | 2.0032790 | 0.0000000 |
| C | 2.4434040 | 0.2785740 | 0.0000000 |
| H | 3.3743040 | 0.8347980 | 0.0000000 |
| H | 2.5061310 | -0.8044500 | 0.0000000 |
| C | 0.0000000 | 0.2463680 | 0.0000000 |
| C | -1.1060810 | -0.2772420 | 0.0000000 |
| C | -2.4064600 | -0.9414220 | 0.0000000 |
| H | -2.5226790 | -1.5744660 | 0.8844060 |
| H | -3.2188380 | -0.2094180 | 0.0000000 |
| H | -2.5226790 | -1.5744660 | -0.8844060 |

penta-1-ene-4-yne (**40**)

| | | | |
|---|---|---|---|
| C | -0.0294100 | 0.7860780 | 0.0792600 |
| H | -0.1062050 | 1.5605040 | 0.8539580 |
| H | 0.2149490 | 1.3015490 | -0.8569450 |
| C | 1.0742200 | -0.1767890 | 0.4282610 |
| H | 0.9289160 | -0.7639310 | 1.3330640 |
| C | 2.1822480 | -0.3322920 | -0.3015040 |
| H | 2.3473430 | 0.2336930 | -1.2136630 |
| H | 2.9589160 | -1.0317610 | -0.0120970 |
| C | -1.3233550 | 0.1105200 | -0.0482620 |
| C | -2.4047050 | -0.4454070 | -0.1371850 |
| H | -3.3379080 | -0.9527150 | -0.2277380 |

penta-1-yne-3-ene (**41**)

| | | | |
|---|---|---|---|
| C | 0.0848870 | 0.4897850 | -0.0000050 |
| H | -0.1399490 | 1.5559290 | 0.0000010 |
| C | -0.9246470 | -0.3993480 | -0.0000080 |
| H | -0.6855350 | -1.4619480 | -0.0000140 |
| C | 1.4607970 | 0.1171110 | -0.0000220 |
| C | 2.6486700 | -0.1690190 | 0.0000350 |
| H | 3.6797920 | -0.4402700 | -0.0000630 |
| C | -2.3696580 | -0.0185680 | 0.0000070 |
| H | -2.8823800 | -0.4207180 | -0.8802420 |
| H | -2.8823600 | -0.4206990 | 0.8802770 |
| H | -2.4898630 | 1.0679430 | -0.0000020 |

2,4-hexadiene (**42**)

| | | | |
|---|---|---|---|
| C | -3.1789400 | 0.1407790 | -0.0000140 |
| H | -3.7455950 | -0.1823060 | -0.8802420 |
| H | -3.7455840 | -0.1824180 | 0.8801800 |
| H | -3.1451950 | 1.2336500 | 0.0000550 |
| C | -1.7999000 | -0.4379040 | -0.0000590 |
| H | -1.7241640 | -1.5261190 | -0.0001630 |
| C | -0.6670200 | 0.2872990 | 0.0000190 |
| H | -0.7346950 | 1.3766990 | 0.0001210 |
| C | 0.6670200 | -0.2872990 | -0.0000240 |
| H | 0.7346950 | -1.3766990 | -0.0001320 |
| C | 1.7999000 | 0.4379040 | 0.0000600 |
| H | 1.7241640 | 1.5261190 | 0.0001680 |
| C | 3.1789400 | -0.1407790 | 0.0000180 |
| H | 3.7455820 | 0.1822790 | 0.8802640 |
| H | 3.1451950 | -1.2336500 | -0.0000860 |
| H | 3.7455970 | 0.1824450 | -0.8801590 |

2,4-hexadiyne (**43**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.6853300 |
| C | 0.0000000 | 0.0000000 | 1.9116100 |
| C | 0.0000000 | 0.0000000 | 3.3704050 |
| H | 0.0218270 | 1.0218810 | 3.7597390 |
| H | -0.8958890 | -0.4920380 | 3.7597390 |
| H | 0.8740620 | -0.5298440 | 3.7597390 |
| C | 0.0000000 | 0.0000000 | -0.6853300 |
| C | 0.0000000 | 0.0000000 | -1.9116100 |
| C | 0.0000000 | 0.0000000 | -3.3704050 |
| H | 0.8958890 | -0.4920380 | -3.7597390 |
| H | -0.8740620 | -0.5298440 | -3.7597390 |
| H | -0.0218270 | 1.0218810 | -3.7597390 |

hexa-2-ene-4-yne (**44**)

| | | | |
|---|---|---|---|
| C | 0.7251060 | 0.5401600 | -0.0000220 |
| H | 1.0214720 | 1.5894700 | 0.0000150 |
| C | 1.6799290 | -0.4084440 | -0.0000330 |
| H | 1.3775830 | -1.4548580 | -0.0000900 |
| C | 3.1455520 | -0.1147880 | 0.0000390 |
| H | 3.6349510 | -0.5455040 | 0.8802540 |
| H | 3.6350070 | -0.5453830 | -0.8802030 |
| H | 3.3291820 | 0.9629650 | 0.0001180 |
| C | -0.6716240 | 0.2600570 | -0.0001270 |
| C | -1.8798380 | 0.0639920 | 0.0001610 |
| C | -3.3152690 | -0.2041950 | -0.0000070 |
| H | -3.8865800 | 0.7283030 | -0.0022000 |
| H | -3.6069320 | -0.7796510 | -0.8834040 |
| H | -3.6078290 | -0.7760360 | 0.8854390 |

1,2,3-hexatriene (**45**)

| | | | |
|---|---|---|---|
| C | 0.7149370 | 0.3704850 | -0.0483300 |
| C | 1.9363250 | 0.0090340 | -0.0450560 |
| C | -0.5540290 | 0.7509560 | -0.0529040 |
| C | 3.2029990 | -0.3730020 | -0.0375270 |
| H | 3.5217250 | -1.2738310 | 0.4797950 |
| H | -0.8335630 | 1.6611340 | -0.5880020 |
| C | -1.6661650 | -0.0085410 | 0.6124710 |
| H | -2.1598360 | 0.6453040 | 1.3428840 |
| H | -1.2467830 | -0.8532690 | 1.1673180 |
| H | 3.9720520 | 0.1998720 | -0.5484150 |
| C | -2.6972490 | -0.5000330 | -0.4052900 |
| H | -3.5171560 | -1.0260200 | 0.0920440 |
| H | -3.1236380 | 0.3372760 | -0.9651650 |
| H | -2.2337050 | -1.1838590 | -1.1206350 |

1,2,3-pentatriene (**46**)

| | | | |
|---|---|---|---|
| C | -1.3226910 | -0.0454320 | -0.0000040 |
| C | -0.0743870 | -0.2990650 | 0.0000140 |
| C | -2.6178110 | 0.2239670 | 0.0000050 |
| H | -2.9854780 | 1.2464960 | -0.0000260 |
| H | -3.3625450 | -0.5672810 | -0.0000010 |
| C | 1.2223080 | -0.5685640 | -0.0000170 |
| H | 1.5436950 | -1.6111340 | 0.0000110 |
| C | 2.3007180 | 0.4751380 | 0.0000010 |
| H | 2.9420220 | 0.3683430 | -0.8814830 |
| H | 1.8716430 | 1.4788130 | -0.0001300 |
| H | 2.9418410 | 0.3685040 | 0.8816380 |

E-2,3,4-hexatriene (**47**)

| | | | |
|---|---|---|---|
| C | 0.6075700 | -0.1905960 | -0.0000580 |
| C | -0.6075700 | 0.1905960 | 0.0000720 |
| C | 1.8686290 | -0.5974430 | 0.0000440 |
| C | -1.8686290 | 0.5974430 | -0.0000440 |
| H | -2.0771370 | 1.6682190 | 0.0000450 |
| C | -3.0516450 | -0.3266060 | -0.0000050 |
| H | -3.6791120 | -0.1541450 | -0.8811970 |
| H | -2.7302510 | -1.3699070 | -0.0007780 |
| H | -3.6782430 | -0.1552100 | 0.8820190 |
| H | 2.0771370 | -1.6682190 | -0.0000590 |
| C | 3.0516450 | 0.3266060 | -0.0000020 |
| H | 2.7302510 | 1.3699070 | 0.0007220 |
| H | 3.6790910 | 0.1541800 | 0.8812110 |
| H | 3.6782640 | 0.1551750 | -0.8820040 |

Z-2,3,4-hexatriene (**48**)

| | | | |
|---|---|---|---|
| C | 0.6367630 | -0.5104000 | -0.0000240 |
| C | -0.6367630 | -0.5104000 | -0.0000170 |
| C | 1.9617910 | -0.5083370 | 0.0000160 |
| H | 2.4905600 | -1.4624670 | 0.0000550 |
| C | -1.9617910 | -0.5083370 | -0.0000020 |
| H | -2.4905600 | -1.4624670 | 0.0000420 |
| C | -2.8019230 | 0.7357280 | 0.0000070 |
| H | -3.4514990 | 0.7658170 | -0.8815300 |
| H | -3.4512920 | 0.7659460 | 0.8816930 |
| H | -2.1739390 | 1.6287550 | -0.0001300 |
| C | 2.8019220 | 0.7357280 | 0.0000010 |
| H | 3.4513990 | 0.7658880 | 0.8816090 |
| H | 3.4513910 | 0.7658750 | -0.8816150 |
| H | 2.1739390 | 1.6287550 | -0.0000040 |

1,5-hexadiene (**49**)

| | | | |
|---|---|---|---|
| C | -0.5599740 | -0.3165980 | -0.5259260 |
| H | -0.4619760 | 0.5746600 | -1.1562910 |
| H | -0.4314390 | -1.1872810 | -1.1830880 |
| C | 0.5599740 | -0.3165980 | 0.5259260 |
| H | 0.4619750 | 0.5746610 | 1.1562900 |
| H | 0.4314390 | -1.1872800 | 1.1830880 |
| C | -1.9189770 | -0.3488980 | 0.1025120 |
| H | -2.1525350 | -1.2277710 | 0.7044430 |
| C | -2.8283810 | 0.6253970 | -0.0079740 |
| H | -2.6338450 | 1.5178140 | -0.5962130 |
| H | -3.7954790 | 0.5631680 | 0.4796850 |
| C | 1.9189770 | -0.3488980 | -0.1025120 |
| H | 2.1525350 | -1.2277710 | -0.7044420 |
| C | 2.8283810 | 0.6253970 | 0.0079730 |
| H | 2.6338460 | 1.5178140 | 0.5962120 |
| H | 3.7954790 | 0.5631670 | -0.4796850 |

1,5-hexadiyne (**50**)

| | | | |
|---|---|---|---|
| C | 0.4706500 | 0.6094680 | 0.0000000 |
| H | 0.2570940 | 1.2281870 | -0.8784820 |
| H | 0.2570940 | 1.2281860 | 0.8784820 |
| C | -0.4706500 | -0.6094680 | 0.0000000 |
| H | -0.2570940 | -1.2281860 | -0.8784820 |
| H | -0.2570940 | -1.2281870 | 0.8784820 |
| C | 1.8742170 | 0.2033510 | 0.0000000 |
| C | 3.0377440 | -0.1601840 | -0.0000010 |
| H | 4.0582450 | -0.4697460 | -0.0000010 |
| C | -1.8742170 | -0.2033510 | 0.0000000 |
| C | -3.0377440 | 0.1601840 | 0.0000010 |
| H | -4.0582450 | 0.4697460 | 0.0000010 |

hexa-1-ene-5-yne (**51**)

| | | | |
|---|---|---|---|
| C | 0.6087300 | 0.6067470 | -0.2739260 |
| H | 0.3433910 | 0.6814990 | -1.3347250 |
| H | 0.5500320 | 1.6233180 | 0.1337710 |
| C | -0.4177920 | -0.2918990 | 0.4370840 |
| H | -0.3793780 | -1.2968090 | 0.0034370 |
| H | -0.1304190 | -0.3851620 | 1.4911170 |
| C | 1.9741490 | 0.1023140 | -0.1377200 |
| C | 3.1044600 | -0.3375220 | -0.0131070 |
| H | 4.0944250 | -0.7183370 | 0.0940590 |
| C | -1.8033370 | 0.2646760 | 0.3215970 |
| H | -1.9787630 | 1.2326970 | 0.7918900 |
| C | -2.8055720 | -0.3356640 | -0.3292330 |
| H | -2.6714230 | -1.3004260 | -0.8103660 |
| H | -3.7916850 | 0.1113090 | -0.3973590 |

cyclopentadiene (**52**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.1763860 | 0.2850850 |
| C | 0.0000000 | -1.1763860 | 0.2850850 |
| C | 0.0000000 | 0.7315150 | -0.9922410 |
| C | 0.0000000 | -0.7315150 | -0.9922410 |
| H | 0.0000000 | 2.2101320 | 0.6121130 |
| H | 0.0000000 | -2.2101320 | 0.6121130 |
| H | 0.0000000 | 1.3487320 | -1.8847570 |
| H | 0.0000000 | -1.3487320 | -1.8847570 |
| C | 0.0000000 | 0.0000000 | 1.2141440 |
| H | 0.8795600 | 0.0000000 | 1.8731490 |
| H | -0.8795600 | 0.0000000 | 1.8731490 |

2-ethyl-1-butene (**53**)

| | | | |
|---|---|---|---|
| C | -2.3635000 | -0.5182730 | -0.1357390 |
| H | -2.4678370 | -0.1440090 | -1.1573190 |
| H | -2.8035990 | 0.2175740 | 0.5420680 |
| C | -0.9031590 | -0.7786100 | 0.2092090 |
| H | -0.8388130 | -1.2127600 | 1.2168210 |
| H | -0.5092400 | -1.5525420 | -0.4619930 |
| C | 1.4453710 | 0.1711950 | 0.5532670 |
| H | 1.9543820 | 1.1324400 | 0.6842790 |
| H | 1.4739590 | -0.3356010 | 1.5270120 |
| C | 0.0104380 | 0.4212150 | 0.1619040 |
| C | -0.3961630 | 1.6438780 | -0.2089950 |
| H | -1.4156440 | 1.8570810 | -0.5094570 |
| H | 0.2942060 | 2.4823030 | -0.2197900 |
| H | -2.9446110 | -1.4408670 | -0.0557650 |
| C | 2.2117120 | -0.6675170 | -0.4728680 |
| H | 3.2575120 | -0.7853650 | -0.1747440 |
| H | 1.7830680 | -1.6669330 | -0.5791800 |
| H | 2.1884250 | -0.1826510 | -1.4526070 |

2-methyl-1-pentene (**54**)

| | | | |
|---|---|---|---|
| C | 2.7596080 | -0.2805840 | 0.0000900 |
| H | 2.8599040 | -0.9177400 | -0.8837040 |
| H | 2.8598730 | -0.9174970 | 0.8840620 |
| H | 3.5940740 | 0.4262110 | 0.0000080 |
| C | 1.4181770 | 0.4446930 | -0.0000330 |
| H | 1.3524290 | 1.0960740 | 0.8784970 |
| H | 1.3524620 | 1.0958370 | -0.8787420 |
| C | 0.2442290 | -0.5258270 | 0.0000760 |
| H | 0.3287710 | -1.1906460 | -0.8725680 |
| H | 0.3287380 | -1.1904090 | 0.8729030 |
| C | -2.2626790 | -0.9153360 | 0.0000960 |
| H | -2.2080520 | -1.5654230 | 0.8806420 |
| H | -3.2366960 | -0.4196420 | 0.0000020 |
| H | -2.2080180 | -1.5656910 | -0.8802510 |
| C | -1.1359140 | 0.0808580 | -0.0000340 |
| C | -1.3684770 | 1.4003820 | -0.0002310 |
| H | -0.5708860 | 2.1342710 | -0.0003260 |
| H | -2.3822700 | 1.7895420 | -0.0003040 |

2-methyl-2-pentene (**55**)

| | | | |
|---|---|---|---|
| C | 2.5326320 | -0.1429520 | 0.5460630 |
| H | 2.7105200 | -1.2177070 | 0.6452550 |
| H | 2.1481680 | 0.2216600 | 1.5022220 |
| C | 1.5317750 | 0.1420410 | -0.5765090 |
| H | 1.3809800 | 1.2210090 | -0.6675690 |
| H | 1.9604510 | -0.1895440 | -1.5308130 |
| H | 3.4943190 | 0.3421280 | 0.3539660 |
| C | 0.2323490 | -0.5704840 | -0.3520790 |
| C | -0.9670690 | -0.0421040 | -0.0495520 |
| C | -2.1630580 | -0.9283100 | 0.1666870 |
| H | -2.5782320 | -0.7870630 | 1.1715160 |
| H | -2.9627300 | -0.6861260 | -0.5431830 |
| H | -1.9083300 | -1.9844650 | 0.0471850 |
| H | 0.2949080 | -1.6585620 | -0.4181710 |
| C | -1.2506490 | 1.4265020 | 0.0998440 |
| H | -1.6554720 | 1.6346300 | 1.0969700 |
| H | -0.3685640 | 2.0517070 | -0.0419860 |
| H | -2.0119000 | 1.7441680 | -0.6221090 |

2-methylpentane (**56**)

| | | | |
|---|---|---|---|
| C | 2.8208430 | -0.2229530 | 0.1401900 |
| H | 2.9625390 | -1.2124420 | -0.3047120 |
| H | 2.8726830 | -0.3360950 | 1.2272760 |
| H | 3.6576720 | 0.4085700 | -0.1714490 |
| C | 1.4819360 | 0.3755560 | -0.2790210 |
| H | 1.3883040 | 1.3804070 | 0.1459690 |
| H | 1.4581190 | 0.4961580 | -1.3695300 |
| C | 0.3009970 | -0.4881630 | 0.1545930 |
| H | 0.2782910 | -0.5479510 | 1.2524920 |
| H | 0.4677620 | -1.5133830 | -0.2035910 |
| C | -1.0671330 | -0.0150350 | -0.3408890 |
| H | -1.0240790 | 0.0404980 | -1.4382960 |
| C | -2.1467230 | -1.0251410 | 0.0394960 |
| H | -2.2232750 | -1.1098090 | 1.1290030 |
| H | -3.1263870 | -0.7219240 | -0.3428170 |
| H | -1.9196350 | -2.0183920 | -0.3599400 |
| C | -1.4261870 | 1.3698040 | 0.1914780 |
| H | -1.4295540 | 1.3662790 | 1.2873750 |
| H | -0.7209530 | 2.1350180 | -0.1419360 |
| H | -2.4238960 | 1.6686590 | -0.1449280 |

3-methylpentane (**57**)

| | | | |
|---|---|---|---|
| C | -2.5668000 | -0.1531740 | -0.2795050 |
| H | -2.5452690 | -0.1500840 | -1.3738830 |
| H | -2.7724450 | 0.8660620 | 0.0552250 |
| H | -3.4076000 | -0.7777410 | 0.0357290 |
| C | -1.2536600 | -0.6864660 | 0.2857150 |
| H | -1.2780760 | -0.6407080 | 1.3829310 |
| H | -1.1620430 | -1.7485240 | 0.0256910 |
| C | 0.0000000 | 0.0418890 | -0.2078570 |
| H | 0.0000000 | -0.0030450 | -1.3081430 |
| C | 1.2536600 | -0.6864660 | 0.2857150 |
| H | 1.1620430 | -1.7485240 | 0.0256910 |
| C | 2.5668000 | -0.1531740 | -0.2795050 |
| H | 2.7724450 | 0.8660620 | 0.0552250 |
| H | 3.4076000 | -0.7777410 | 0.0357290 |
| H | 2.5452690 | -0.1500840 | -1.3738830 |
| H | 1.2780760 | -0.6407080 | 1.3829310 |
| C | 0.0000000 | 1.5102820 | 0.2099740 |
| H | -0.8795680 | 2.0378140 | -0.1667940 |
| H | 0.0000000 | 1.5920660 | 1.3031230 |
| H | 0.8795680 | 2.0378140 | -0.1667940 |

E-3-methyl-2-pentene (**58**)

| | | | |
|---|---|---|---|
| C | -2.3270690 | -0.3170380 | 0.5517690 |
| H | -2.5366130 | 0.7411460 | 0.7269560 |
| H | -1.9594590 | -0.7493380 | 1.4866620 |
| C | -1.2979440 | -0.5099180 | -0.5645070 |
| H | -1.1791500 | -1.5802860 | -0.7666210 |
| H | -1.6834350 | -0.0558550 | -1.4877800 |
| H | -3.2728300 | -0.8049150 | 0.2986230 |
| C | 0.0630980 | 1.5843340 | -0.0734780 |
| H | -0.5039940 | 2.0587910 | -0.8820890 |
| H | -0.4079030 | 1.8879710 | 0.8677000 |
| H | 1.0720030 | 1.9988340 | -0.0872700 |
| C | 0.0467550 | 0.0883440 | -0.2384980 |
| C | 1.1219730 | -0.7069460 | -0.0924690 |
| H | 0.9718970 | -1.7771770 | -0.2403590 |
| C | 2.5250960 | -0.3133650 | 0.2559210 |
| H | 2.8437780 | -0.8052310 | 1.1815590 |
| H | 3.2235760 | -0.6284300 | -0.5270340 |
| H | 2.6406750 | 0.7620240 | 0.3972220 |

Z-3-methyl-2-pentene (**59**)

| | | | |
|---|---|---|---|
| C | 1.5140550 | -1.4049490 | -0.4537980 |
| H | 2.1639220 | -0.7661510 | -1.0580520 |
| H | 0.7590940 | -1.8360710 | -1.1165330 |
| C | 0.8451480 | -0.6062150 | 0.6684570 |
| H | 0.2082270 | -1.2718520 | 1.2583490 |
| H | 1.6144510 | -0.2322350 | 1.3552210 |
| H | 2.1235390 | -2.2195410 | -0.0510910 |
| C | 0.8452750 | 1.8237980 | -0.0900000 |
| H | 1.2516350 | 2.2062710 | 0.8535740 |
| H | 1.6991860 | 1.6415430 | -0.7525130 |
| H | 0.2301650 | 2.6075990 | -0.5399220 |
| C | 0.0548530 | 0.5643020 | 0.1391730 |
| C | -1.2555570 | 0.5111820 | -0.1590160 |
| H | -1.7190210 | 1.4140280 | -0.5585200 |
| C | -2.1764060 | -0.6618190 | -0.0126690 |
| H | -3.0167830 | -0.4193930 | 0.6471350 |
| H | -2.6045830 | -0.9399040 | -0.9820550 |
| H | -1.6740370 | -1.5420950 | 0.3915240 |

2-methylpropene (**60**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 1.2726840 | -0.6788030 |
| H | 0.8802110 | 1.3235440 | -1.3295910 |
| H | -0.8802110 | 1.3235440 | -1.3295910 |
| H | 0.0000000 | 2.1530400 | -0.0315830 |
| C | 0.0000000 | 0.0000000 | 0.1195860 |
| C | 0.0000000 | 0.0000000 | 1.4588050 |
| H | 0.0000000 | -0.9243020 | 2.0284090 |
| H | 0.0000000 | 0.9243020 | 2.0284090 |
| C | 0.0000000 | -1.2726840 | -0.6788030 |
| H | -0.8802110 | -1.3235440 | -1.3295910 |
| H | 0.8802110 | -1.3235440 | -1.3295910 |
| H | 0.0000000 | -2.1530400 | -0.0315830 |

2-methyl-1-butene (**61**)

| | | | |
|---|---|---|---|
| C | 2.0311400 | -0.0375560 | -0.0000010 |
| H | 2.1381110 | 0.5950820 | -0.8848050 |
| H | 2.1381000 | 0.5951100 | 0.8847840 |
| H | 2.8535940 | -0.7577860 | 0.0000160 |
| C | 0.6911370 | -0.7603540 | 0.0000010 |
| H | 0.6352260 | -1.4266690 | -0.8721260 |
| H | 0.6352270 | -1.4266660 | 0.8721310 |
| C | -0.5358710 | 0.1156790 | 0.0000000 |
| C | -0.4927560 | 1.4546590 | 0.0000010 |
| H | 0.4388110 | 2.0086850 | 0.0000030 |
| H | -1.4046510 | 2.0441140 | -0.0000020 |
| C | -1.8427440 | -0.6283820 | -0.0000010 |
| H | -1.9225660 | -1.2761060 | -0.8803670 |
| H | -1.9225890 | -1.2760620 | 0.8803960 |
| H | -2.6946900 | 0.0560290 | -0.0000290 |

2-methyl-2-butene (**62**)

| | | | |
|---|---|---|---|
| C | -0.6343900 | 1.4515100 | 0.0000000 |
| H | -1.2092200 | 1.7634970 | -0.8796020 |
| H | 0.3063370 | 2.0028430 | -0.0000010 |
| H | -1.2092190 | 1.7634970 | 0.8796030 |
| C | -0.4489580 | -0.0400200 | 0.0000010 |
| C | 0.7371810 | -0.6726370 | -0.0000010 |
| H | 0.7177000 | -1.7630900 | 0.0000010 |
| C | 2.1096280 | -0.0714920 | 0.0000000 |
| H | 2.6748560 | -0.3983000 | 0.8796690 |
| H | 2.6748620 | -0.3983150 | -0.8796590 |
| H | 2.0952230 | 1.0191800 | -0.0000090 |
| C | -1.7336310 | -0.8226050 | 0.0000000 |
| H | -2.3402790 | -0.5789680 | 0.8801160 |
| H | -2.3402820 | -0.5789620 | -0.8801130 |
| H | -1.5489620 | -1.8999240 | -0.0000040 |

isobutane (**63**)

| | | | |
|---|---|---|---|
| C | 0.0000000 | 0.0000000 | 0.3768780 |
| H | 0.0000000 | 0.0000000 | 1.4751700 |
| C | 0.0000000 | 1.4502890 | -0.0962170 |
| H | 0.0000000 | 1.4941240 | -1.1908320 |
| H | -0.8854710 | 1.9847420 | 0.2613270 |
| H | 0.8854710 | 1.9847420 | 0.2613270 |
| C | -1.2559870 | -0.7251450 | -0.0962170 |
| H | -1.2939490 | -0.7470620 | -1.1908320 |
| H | -1.2761010 | -1.7592110 | 0.2613270 |
| H | -2.1615720 | -0.2255310 | 0.2613270 |
| C | 1.2559870 | -0.7251450 | -0.0962170 |
| H | 2.1615720 | -0.2255310 | 0.2613270 |
| H | 1.2761010 | -1.7592110 | 0.2613270 |
| H | 1.2939490 | -0.7470620 | -1.1908320 |

isopentane (**64**)

| | | | |
|---|---|---|---|
| C | 1.7403960 | -0.7972030 | -0.0034770 |
| H | 1.9039290 | -0.8182640 | 1.0795230 |
| H | 1.6616350 | -1.8316790 | -0.3518130 |
| H | 2.6250640 | -0.3500710 | -0.4672640 |
| C | 0.4797900 | -0.0032440 | -0.3357900 |
| H | 0.3529980 | -0.0057290 | -1.4281790 |
| C | -0.7502440 | -0.6778070 | 0.2751590 |
| H | -0.7601770 | -1.7299030 | -0.0362380 |
| H | -0.6405010 | -0.6827910 | 1.3681410 |
| C | -2.0807560 | -0.0354060 | -0.1046870 |
| H | -2.1898360 | 0.0173700 | -1.1925540 |
| H | -2.9204920 | -0.6165890 | 0.2868550 |
| H | -2.1703250 | 0.9788400 | 0.2912470 |
| C | 0.6295590 | 1.4451750 | 0.1217870 |
| H | -0.2198750 | 2.0628190 | -0.1800330 |
| H | 0.7118800 | 1.4921500 | 1.2135690 |
| H | 1.5332280 | 1.8947550 | -0.3012090 |

$H_2$ (**65**)

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 0.3687610 |
| H | 0.0000000 | 0.0000000 | -0.3687610 |

## B3LYP/6-31G(d) Optimized Structures (Polyynes)

$C_6H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 4.2528560 |
| C | 0.0000000 | 0.0000000 | 3.1863020 |
| C | 0.0000000 | 0.0000000 | 1.9714600 |
| C | 0.0000000 | 0.0000000 | 0.6116500 |
| C | 0.0000000 | 0.0000000 | -0.6116500 |
| C | 0.0000000 | 0.0000000 | -1.9714600 |
| C | 0.0000000 | 0.0000000 | -3.1863020 |
| H | 0.0000000 | 0.0000000 | -4.2528560 |

$C_8H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 5.5405530 |
| C | 0.0000000 | 0.0000000 | 4.4743010 |
| C | 0.0000000 | 0.0000000 | 3.2585650 |
| C | 0.0000000 | 0.0000000 | 1.9014480 |
| C | 0.0000000 | 0.0000000 | 0.6742510 |
| C | 0.0000000 | 0.0000000 | -0.6742510 |
| C | 0.0000000 | 0.0000000 | -1.9014480 |
| C | 0.0000000 | 0.0000000 | -3.2585650 |
| C | 0.0000000 | 0.0000000 | -4.4743010 |
| H | 0.0000000 | 0.0000000 | -5.5405530 |

$C_{10}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 6.8275170 |
| C | 0.0000000 | 0.0000000 | 5.7608740 |
| C | 0.0000000 | 0.0000000 | 4.5448920 |
| C | 0.0000000 | 0.0000000 | 3.1891070 |
| C | 0.0000000 | 0.0000000 | 1.9603580 |
| C | 0.0000000 | 0.0000000 | 0.6158630 |
| C | 0.0000000 | 0.0000000 | -0.6158630 |
| C | 0.0000000 | 0.0000000 | -1.9603580 |
| C | 0.0000000 | 0.0000000 | -3.1891070 |
| C | 0.0000000 | 0.0000000 | -4.5448920 |
| C | 0.0000000 | 0.0000000 | -5.7608740 |
| H | 0.0000000 | 0.0000000 | -6.8275170 |

$C_{12}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 8.1139060 |
| C | 0.0000000 | 0.0000000 | 7.0472530 |
| C | 0.0000000 | 0.0000000 | 5.8309650 |
| C | 0.0000000 | 0.0000000 | 4.4757040 |
| C | 0.0000000 | 0.0000000 | 3.2463530 |
| C | 0.0000000 | 0.0000000 | 1.9034950 |
| C | 0.0000000 | 0.0000000 | 0.6701380 |
| C | 0.0000000 | 0.0000000 | -0.6701380 |
| C | 0.0000000 | 0.0000000 | -1.9034950 |
| C | 0.0000000 | 0.0000000 | -3.2463530 |
| C | 0.0000000 | 0.0000000 | -4.4757040 |
| C | 0.0000000 | 0.0000000 | -5.8309650 |
| C | 0.0000000 | 0.0000000 | -7.0472530 |
| H | 0.0000000 | 0.0000000 | -8.1139060 |

$C_{14}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 9.3999140 |
| C | 0.0000000 | 0.0000000 | 8.3332280 |
| C | 0.0000000 | 0.0000000 | 7.1168330 |
| C | 0.0000000 | 0.0000000 | 5.7619270 |
| C | 0.0000000 | 0.0000000 | 4.5321950 |
| C | 0.0000000 | 0.0000000 | 3.1902400 |
| C | 0.0000000 | 0.0000000 | 1.9559570 |
| C | 0.0000000 | 0.0000000 | 0.6177040 |
| C | 0.0000000 | 0.0000000 | -0.6177040 |
| C | 0.0000000 | 0.0000000 | -1.9559570 |
| C | 0.0000000 | 0.0000000 | -3.1902400 |
| C | 0.0000000 | 0.0000000 | -4.5321950 |
| C | 0.0000000 | 0.0000000 | -5.7619270 |
| C | 0.0000000 | 0.0000000 | -7.1168330 |
| C | 0.0000000 | 0.0000000 | -8.3332280 |
| H | 0.0000000 | 0.0000000 | -9.3999140 |

$C_{16}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 10.6856990 |
| C | 0.0000000 | 0.0000000 | 9.6189880 |
| C | 0.0000000 | 0.0000000 | 8.4025350 |
| C | 0.0000000 | 0.0000000 | 7.0478420 |
| C | 0.0000000 | 0.0000000 | 5.8178970 |
| C | 0.0000000 | 0.0000000 | 4.4764540 |
| C | 0.0000000 | 0.0000000 | 3.2416720 |
| C | 0.0000000 | 0.0000000 | 1.9044880 |
| C | 0.0000000 | 0.0000000 | 0.6680300 |
| C | 0.0000000 | 0.0000000 | -0.6680300 |
| C | 0.0000000 | 0.0000000 | -1.9044880 |
| C | 0.0000000 | 0.0000000 | -3.2416720 |
| C | 0.0000000 | 0.0000000 | -4.4764540 |
| C | 0.0000000 | 0.0000000 | -5.8178970 |
| C | 0.0000000 | 0.0000000 | -7.0478420 |
| C | 0.0000000 | 0.0000000 | -8.4025350 |
| C | 0.0000000 | 0.0000000 | -9.6189880 |
| H | 0.0000000 | 0.0000000 | -10.6856990 |

$C_{18}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 11.9708160 |
| C | 0.0000000 | 0.0000000 | 10.9040760 |
| C | 0.0000000 | 0.0000000 | 9.6875050 |
| C | 0.0000000 | 0.0000000 | 8.3332120 |
| C | 0.0000000 | 0.0000000 | 7.1029210 |
| C | 0.0000000 | 0.0000000 | 5.7621980 |
| C | 0.0000000 | 0.0000000 | 4.5268160 |
| C | 0.0000000 | 0.0000000 | 3.1907350 |
| C | 0.0000000 | 0.0000000 | 1.9533430 |
| C | 0.0000000 | 0.0000000 | 0.6189780 |
| C | 0.0000000 | 0.0000000 | -0.6189780 |
| C | 0.0000000 | 0.0000000 | -1.9533430 |
| C | 0.0000000 | 0.0000000 | -3.1907350 |
| C | 0.0000000 | 0.0000000 | -4.5268160 |
| C | 0.0000000 | 0.0000000 | -5.7621980 |
| C | 0.0000000 | 0.0000000 | -7.1029210 |
| C | 0.0000000 | 0.0000000 | -8.3332120 |
| C | 0.0000000 | 0.0000000 | -9.6875050 |
| C | 0.0000000 | 0.0000000 | -10.9040760 |
| H | 0.0000000 | 0.0000000 | -11.9708160 |

$C_{20}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 13.2561020 |
| C | 0.0000000 | 0.0000000 | 12.1893520 |
| C | 0.0000000 | 0.0000000 | 10.9728000 |
| C | 0.0000000 | 0.0000000 | 9.6185930 |
| C | 0.0000000 | 0.0000000 | 8.3882830 |
| C | 0.0000000 | 0.0000000 | 7.0477240 |
| C | 0.0000000 | 0.0000000 | 5.8122480 |
| C | 0.0000000 | 0.0000000 | 4.4764810 |
| C | 0.0000000 | 0.0000000 | 3.2388430 |
| C | 0.0000000 | 0.0000000 | 1.9050880 |
| C | 0.0000000 | 0.0000000 | 0.6665940 |
| C | 0.0000000 | 0.0000000 | -0.6665940 |
| C | 0.0000000 | 0.0000000 | -1.9050880 |
| C | 0.0000000 | 0.0000000 | -3.2388430 |
| C | 0.0000000 | 0.0000000 | -4.4764810 |
| C | 0.0000000 | 0.0000000 | -5.8122480 |
| C | 0.0000000 | 0.0000000 | -7.0477240 |
| C | 0.0000000 | 0.0000000 | -8.3882830 |
| C | 0.0000000 | 0.0000000 | -9.6185930 |
| C | 0.0000000 | 0.0000000 | -10.9728000 |
| C | 0.0000000 | 0.0000000 | -12.1893520 |
| H | 0.0000000 | 0.0000000 | -13.2561020 |

$C_{22}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 14.5412790 |
| C | 0.0000000 | 0.0000000 | 13.4745110 |
| C | 0.0000000 | 0.0000000 | 12.2579570 |
| C | 0.0000000 | 0.0000000 | 10.9038380 |
| C | 0.0000000 | 0.0000000 | 9.6734700 |
| C | 0.0000000 | 0.0000000 | 8.3330920 |
| C | 0.0000000 | 0.0000000 | 7.0974800 |
| C | 0.0000000 | 0.0000000 | 5.7620240 |
| C | 0.0000000 | 0.0000000 | 4.5241380 |
| C | 0.0000000 | 0.0000000 | 3.1908900 |
| C | 0.0000000 | 0.0000000 | 1.9519710 |
| C | 0.0000000 | 0.0000000 | 0.6196090 |
| C | 0.0000000 | 0.0000000 | -0.6196090 |
| C | 0.0000000 | 0.0000000 | -1.9519710 |
| C | 0.0000000 | 0.0000000 | -3.1908900 |
| C | 0.0000000 | 0.0000000 | -4.5241380 |
| C | 0.0000000 | 0.0000000 | -5.7620240 |
| C | 0.0000000 | 0.0000000 | -7.0974800 |
| C | 0.0000000 | 0.0000000 | -8.3330920 |
| C | 0.0000000 | 0.0000000 | -9.6734700 |
| C | 0.0000000 | 0.0000000 | -10.9038380 |
| C | 0.0000000 | 0.0000000 | -12.2579570 |
| C | 0.0000000 | 0.0000000 | -13.4745110 |
| H | 0.0000000 | 0.0000000 | -14.5412790 |

$C_{24}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 15.8277700 |
| C | 0.0000000 | 0.0000000 | 14.7609990 |
| C | 0.0000000 | 0.0000000 | 13.5444820 |
| C | 0.0000000 | 0.0000000 | 12.1901090 |
| C | 0.0000000 | 0.0000000 | 10.9598960 |
| C | 0.0000000 | 0.0000000 | 9.6191500 |
| C | 0.0000000 | 0.0000000 | 8.3837500 |
| C | 0.0000000 | 0.0000000 | 7.0479120 |
| C | 0.0000000 | 0.0000000 | 5.8102270 |
| C | 0.0000000 | 0.0000000 | 4.4766630 |
| C | 0.0000000 | 0.0000000 | 3.2378720 |
| C | 0.0000000 | 0.0000000 | 1.9053540 |
| C | 0.0000000 | 0.0000000 | 0.6661050 |
| C | 0.0000000 | 0.0000000 | -0.6661050 |
| C | 0.0000000 | 0.0000000 | -1.9053540 |
| C | 0.0000000 | 0.0000000 | -3.2378720 |
| C | 0.0000000 | 0.0000000 | -4.4766630 |
| C | 0.0000000 | 0.0000000 | -5.8102270 |
| C | 0.0000000 | 0.0000000 | -7.0479120 |
| C | 0.0000000 | 0.0000000 | -8.3837500 |
| C | 0.0000000 | 0.0000000 | -9.6191500 |
| C | 0.0000000 | 0.0000000 | -10.9598960 |
| C | 0.0000000 | 0.0000000 | -12.1901090 |
| C | 0.0000000 | 0.0000000 | -13.5444820 |
| C | 0.0000000 | 0.0000000 | -14.7609990 |
| H | 0.0000000 | 0.0000000 | -15.8277700 |

$C_{26}H_2$

| | | | |
|---|---|---|---|
| H | 0.0000000 | 0.0000000 | 17.1126710 |
| C | 0.0000000 | 0.0000000 | 16.0458970 |
| C | 0.0000000 | 0.0000000 | 14.8294200 |
| C | 0.0000000 | 0.0000000 | 13.4751250 |
| C | 0.0000000 | 0.0000000 | 12.2448390 |
| C | 0.0000000 | 0.0000000 | 10.9043790 |
| C | 0.0000000 | 0.0000000 | 9.6687990 |
| C | 0.0000000 | 0.0000000 | 8.3332760 |
| C | 0.0000000 | 0.0000000 | 7.0954030 |
| C | 0.0000000 | 0.0000000 | 5.7621680 |
| C | 0.0000000 | 0.0000000 | 4.5231460 |
| C | 0.0000000 | 0.0000000 | 3.1910530 |
| C | 0.0000000 | 0.0000000 | 1.9514760 |
| C | 0.0000000 | 0.0000000 | 0.6198720 |
| C | 0.0000000 | 0.0000000 | -0.6198720 |
| C | 0.0000000 | 0.0000000 | -1.9514760 |
| C | 0.0000000 | 0.0000000 | -3.1910530 |
| C | 0.0000000 | 0.0000000 | -4.5231460 |
| C | 0.0000000 | 0.0000000 | -5.7621680 |
| C | 0.0000000 | 0.0000000 | -7.0954030 |
| C | 0.0000000 | 0.0000000 | -8.3332760 |
| C | 0.0000000 | 0.0000000 | -9.6687990 |
| C | 0.0000000 | 0.0000000 | -10.9043790 |
| C | 0.0000000 | 0.0000000 | -12.2448390 |
| C | 0.0000000 | 0.0000000 | -13.4751250 |
| C | 0.0000000 | 0.0000000 | -14.8294200 |
| C | 0.0000000 | 0.0000000 | -16.0458970 |
| H | 0.0000000 | 0.0000000 | -17.1126710 |