

Supplementary Material

Calculated harmonic frequencies (in wavenumbers) of cyclohexoxy radical.

Conformer: chair-equatorial
State: X2A"
Level of theory: unscaled B3LYP/6-31+G*
Symmetry: Cs (C1 in paranthesis)

a' modes:
159(159), 333(336), 393(395), 473(442), 554(546), 777(763),
841(841), 886(887), 976(961), 1017(1031), 1089(1090), 1193(1186),
1271(1269), 1275(1280), 1354(1350), 1382(1377), 1393(1394), 1507(1507),
1515(1514), 1529(1528), 2942(2929), 3021(3018), 3028(3029), 3053(3057),
3069(3070), 3075(3076), 3102(3116)

a" modes:
-522(327), 229(230), 407(437), 678(796), 801(869), 904(917),
965(1003), 1052(1060), 1085(1105), 1149(1135), 1235(1259), 1298(1304),
1339(1338), 1374(1366), 1393(1392), 1503(1503), 1508(1507), 3026(3024),
3048(3040), 3068(3069), 3099(3086)

Conformer: chair-equatorial
State: A2A'
Level of theory: unscaled B3LYP/6-31+G*
Symmetry: Cs

a' modes:
153, 328, 403, 455, 552, 778, 848, 877, 982, 1034,
1059, 1167, 1217, 1286, 1299, 1377, 1394, 1507, 1515, 1527,
2832, 3013, 3021, 3036, 3067, 3071, 3091

a" modes:
222, 287, 417, 780, 810, 903, 977, 1061, 1097, 1143,
1211, 1298, 1346, 1375, 1390, 1503, 1508, 3012, 3032, 3066,
3089

Conformer: chair-equatorial
State: A2A'
Level of theory: unscaled CASSCF(7,5)/6-31+G*
Symmetry: Cs

a' modes:
164, 348, 430, 488, 586, 843, 905, 954, 1023, 1101,
1120, 1261, 1354, 1401, 1423, 1521, 1530, 1629, 1637, 1652,
3169, 3178, 3183, 3197, 3228, 3235, 3250

a' modes:
238, 344, 462, 861, 960, 1001, 1141, 1160, 1197, 1304,
1387, 1431, 1489, 1507, 1521, 1625, 1633, 3175, 3191, 3229,
3245

Conformer: chair-equatorial
State: B2A'
Level of theory: unscaled CIS/6-31+G*

Symmetry: Cs

a' modes:

170, 347, 429, 499, 577, 826, 878, 915, 973, 1059,
1114, 1266, 1338, 1393, 1401, 1493, 1517, 1629, 1641, 1657,
3189, 3194, 3238, 3243, 3260, 3303, 3363

a" modes:

232, 363, 488, 864, 954, 1024, 1141, 1167, 1206, 1316,
1394, 1462, 1490, 1518, 1601, 1626, 1668, 3189, 3239, 3254,
3304

Conformer: chair-equatorial

State: B2A'

Level of theory: unscaled CASSCF(7,5)/6-31+G*

Symmetry: Cs

a' modes:

162, 342, 404, 480, 553, 756, 870, 911, 967, 1049,
1103, 1205, 1300, 1386, 1394, 1487, 1515, 1629, 1640, 1655,
3189, 3193, 3237, 3240, 3256, 3295, 3343

a" modes:

232, 313, 459, 863, 947, 1017, 1138, 1159, 1196, 1297,
1388, 1448, 1484, 1517, 1553, 1626, 1638, 3188, 3236, 3250,
3297

Conformer: chair-axial

State: X2A"

Level of theory: unscaled B3LYP/6-31+G*

Symmetry: Cs (C1 in paranthesis)

a' modes:

161(156), 302(300), 374(379), 484(479), 654(608), 771(841),
841(845), 865(862), 984(992), 1025(1026), 1034(1072), 1160(1162),
1274(1273), 1293(1284), 1362(1326), 1394(1384), 1422(1419), 1503(1504),
1512(1514), 1525(1525), 2958(2945), 3012(3010), 3033(3037), 3041(3041),
3066(3066), 3083(3080), 3093(3106)

a" modes:

-461(352), 211(206), 408(452), 752(752), 786(787), 878(937),
951(947), 1044(1037), 1090(1092), 1137(1135), 1215(1233), 1299(1301),
1359(1356), 1390(1395), 1397(1396), 1496(1496), 1505(1506), 3024(3022),
3041(3041), 3078(3075), 3091(3084)

Conformer: chair-axial

State: A2A'

Level of theory: unscaled B3LYP/6-31+G*

Symmetry: Cs

a' modes:

143, 298, 393, 480, 658, 770, 840, 865, 974, 1033,

1054, 1117, 1216, 1293, 1307, 1379, 1394, 1500, 1513, 1524,
2849, 3011, 3028, 3036, 3065, 3074, 3093

a" modes:

198, 378, 445, 782, 866, 902, 951, 1037, 1083, 1153,
1195, 1299, 1356, 1377, 1391, 1493, 1508, 3023, 3029, 3070,
3091

Conformer: chair-axial

State: A2A'

Level of theory: unscaled CASSCF(7,5)/6-31+G*

Symmetry: Cs

a' modes:

156, 316, 420, 514, 704, 826, 889, 938, 1000, 1114,
1119, 1216, 1350, 1409, 1444, 1525, 1528, 1625, 1634, 1650,
3174, 3183, 3192, 3203, 3227, 3236, 3251

a" modes:

210, 382, 472, 848, 926, 1008, 1116, 1164, 1223, 1249,
1377, 1412, 1483, 1514, 1522, 1616, 1634, 3184, 3193, 3229,
3248

Conformer: chair-axial

State: B2A'

Level of theory: unscaled CIS/6-31+G*

Symmetry: Cs

a' modes:

166, 319, 417, 514, 677, 785, 860, 921, 949, 1109,
1119, 1202, 1330, 1397, 1417, 1528, 1544, 1606, 1631, 1647,
3149, 3170, 3214, 3233, 3272, 3297, 3380

a" modes:

223, 439, 686, 876, 930, 1067, 1121, 1169, 1238, 1306,
1400, 1485, 1519, 1528, 1591, 1628, 2844, 3207, 3220, 3295,
3682

Conformer: chair-axial

State: B2A'

Level of theory: unscaled CASSCF(7,5)/6-31+G*

Symmetry: Cs

a' modes:

159, 311, 403, 507, 590, 742, 858, 920, 941, 1110,
1116, 1154, 1289, 1384, 1416, 1526, 1539, 1605, 1631, 1647,
3145, 3170, 3212, 3232, 3269, 3289, 3359

a" modes:

212, 381, 501, 829, 929, 995, 1117, 1160, 1233, 1284,
1398, 1481, 1507, 1524, 1543, 1594, 1629, 3134, 3215, 3263,

Conformer: twisted-boat-equatorial
State: X
Level of theory: unscaled B3LYP/6-31+G*
Symmetry: C1

95, 175, 255, 339, 402, 421, 467, 568, 757, 771,
835, 855, 887, 930, 953, 1012, 1040, 1090, 1106, 1118,
1145, 1201, 1245, 1254, 1287, 1300, 1331, 1337, 1372, 1381,
1388, 1394, 1506, 1509, 1517, 1523, 1535, 2940, 3029, 3037,
3042, 3050, 3067, 3069, 3075, 3083, 3096, 3119

Conformer: twisted-boat-equatorial
State: B
Level of theory: unscaled CIS/6-31+G*
Symmetry: C1

88, 184, 260, 323, 427, 461, 512, 595, 799, 841,
880, 916, 951, 984, 1012, 1066, 1117, 1157, 1191, 1202,
1275, 1285, 1333, 1371, 1400, 1413, 1450, 1480, 1497, 1514,
1518, 1543, 1626, 1630, 1642, 1649, 1665, 3187, 3208, 3217,
3240, 3240, 3250, 3257, 3264, 3311, 3315, 3374

Conformer: twisted-boat-inclinal
State: X
Level of theory: unscaled B3LYP/6-31+G*
Symmetry: C1

83, 197, 258, 361, 401, 423, 522, 561, 757, 779,
829, 841, 878, 947, 964, 1004, 1032, 1052, 1105, 1122,
1154, 1184, 1233, 1258, 1282, 1303, 1335, 1341, 1362, 1380,
1392, 1405, 1501, 1510, 1511, 1523, 1535, 2946, 3027, 3033,
3040, 3047, 3059, 3067, 3078, 3088, 3091, 3123

Conformer: twisted-boat-inclinal
State: B
Level of theory: unscaled CIS/6-31+G*
Symmetry: C1

84, 197, 269, 393, 430, 456, 573, 619, 750, 832,
870, 924, 931, 956, 1031, 1076, 1100, 1152, 1185, 1197,
1245, 1278, 1312, 1381, 1390, 1408, 1469, 1496, 1505, 1521,
1533, 1540, 1596, 1629, 1634, 1647, 1659, 3161, 3192, 3206,
3227, 3232, 3248, 3259, 3266, 3307, 3314, 3382

Conformer: twisted-boat-axial

State: X
Level of theory: unscaled B3LYP/6-31+G*
Symmetry: C1

76, 161, 259, 346, 367, 472, 495, 667, 769, 776,
842, 861, 863, 892, 937, 971, 1033, 1040, 1057, 1104,
1132, 1159, 1188, 1217, 1271, 1297, 1310, 1347, 1357, 1372,
1386, 1391, 1498, 1501, 1514, 1520, 1531, 2862, 3020, 3029,
3035, 3045, 3051, 3071, 3073, 3085, 3098, 3104

Conformer: twisted-boat-axial
State: B
Level of theory: unscaled CIS/6-31+G*
Symmetry: C1

116, 180, 265, 377, 473, 504, 680, 725, 768, 837,
864, 923, 932, 962, 1028, 1096, 1124, 1148, 1191, 1227,
1255, 1325, 1373, 1384, 1411, 1425, 1480, 1500, 1516, 1528,
1542, 1591, 1599, 1631, 1643, 1654, 2719, 3154, 3183, 3203,
3242, 3274, 3291, 3297, 3375, 3793