Table 1. Calculated 57 vibrational frequencies (cm^{-1}) of the diequatorial chair conformer of *trans*-4-methylcyclohexoxy radical (C$_s$ symmetry) in its ground state and $\tilde{B}$ excited state.[a]

assignment	symmetry	CASSCF(9,7)[b] $\tilde{B}$	CASSCF(9,7)[b] $\tilde{X}$	B3LYP[c] $\tilde{X}$
ν_{32}	a′	108	109	106
ν_{57}	a″	214	219	211
ν_{56}	a″	240	241	228
ν_{31}	a′	245	250	244
ν_{55}	a″	267	256	252
ν_{54}	a″	331	336	328
ν_{30}	a′	355	377	364
ν_{29}	a′	426	426	411
ν_{28}	a′	456	455	431
ν_{53}	a″	463	465	450
ν_{27}	a′	536	596	579
ν_{26}	a′	694	781	749
ν_{25}	a′	797	814	769
ν_{52}	a″	817	851	795
ν_{24}	a′	884	914	808
ν_{51}	a″	908	951	882
ν_{50}	a″	975	960	933
ν_{23}	a′	989	991	948
ν_{22}	a′	999	1024	951
ν_{21}	a′	1009	1032	1001
ν_{49}	a″	1030	1045	1017
ν_{48}	a″	1097	1094	1039
ν_{20}	a′	1104	1117	1057
ν_{47}	a″	1140	1133	1066
ν_{19}	a′	1164	1200	1112
ν_{46}	a″	1220	1205	1148
ν_{18}	a′	1237	1282	1181
ν_{45}	a″	1264	1286	1198
ν_{17}	a′	1316	1317	1222
ν_{16}	a′	1324	1321	1254
ν_{44}	a″	1371	1351	1272
ν_{43}	a″	1382	1387	1315
ν_{15}	a′	1383	1388	1316
ν_{14}	a′	1414	1419	1322
ν_{42}	a″	1442	1445	1351
ν_{13}	a′	1463	1451	1360

Table 1.-continued

assignment	symmetry	CASSCF(9,7)[b] $\widetilde{B}$	CASSCF(9,7)[b] $\widetilde{X}$	B3LYP[c] $\widetilde{X}$
ν_{41}	a″	1476	1469	1382
ν_{12}	a′	1484	1482	1405
ν_{40}	a″	1542	1541	1471
ν_{11}	a′	1555	1549	1475
ν_{39}	a″	1556	1554	1482
ν_{38}	a″	1557	1556	1489
ν_{10}	a′	1558	1557	1491
ν_{9}	a′	1570	1564	1492
ν_{8}	a′	3010	2997	2777
ν_{37}	a″	3022	3003	2928
ν_{7}	a′	3029	3009	2943
ν_{6}	a′	3037	3018	2951
ν_{36}	a″	3074	3031	2970
ν_{5}	a′	3075	3032	2972
ν_{4}	a′	3090	3038	2977
ν_{35}	a″	3092	3062	2998
ν_{34}	a″	3096	3066	3002
ν_{3}	a′	3097	3083	3027
ν_{2}	a′	3138	3085	3029
ν_{33}	a″	3139	3088	3030
ν_{1}	a′	3198	3089	3035

[a] All calculations employed the 6-31+G(d) basis set. [b] A uniform scale factor of 0.95 was used. [c] The calculated B3LYP frequencies are scaled by 0.98.

Table 2. Calculated 57 vibrational frequencies (cm^{-1}) of the diequatorial chair conformer of *cis*-3-methylcyclohexoxy radical (C$_1$ symmetry) in its ground state and $\tilde{B}$ excited state.[a]

assignment	CASSCF(9,7)[b] $\tilde{B}$	CASSCF(9,7)[b] $\tilde{X}$	B3LYP[c] $\tilde{X}$
ν_{57}	146	147	144
ν_{56}	150	152	146
ν_{55}	239	239	228
ν_{54}	244	243	234
ν_{53}	278	283	279
ν_{52}	349	348	339
ν_{51}	380	399	383
ν_{50}	405	419	408
ν_{49}	454	449	431
ν_{48}	463	475	457
ν_{47}	525	550	535
ν_{46}	680	794	756
ν_{45}	796	851	775
ν_{44}	868	884	820
ν_{43}	882	896	854
ν_{42}	907	914	861
ν_{41}	935	957	914
ν_{40}	967	997	933
ν_{39}	1001	1003	961
ν_{38}	1013	1014	984
ν_{37}	1058	1070	1016
ν_{36}	1106	1098	1037
ν_{35}	1113	1125	1070
ν_{34}	1139	1131	1076
ν_{33}	1163	1192	1117
ν_{32}	1207	1210	1155
ν_{31}	1240	1269	1165
ν_{30}	1272	1289	1191
ν_{29}	1322	1312	1230
ν_{28}	1326	1335	1263
ν_{27}	1348	1349	1275
ν_{26}	1386	1380	1289
ν_{25}	1402	1390	1319
ν_{24}	1425	1434	1342
ν_{23}	1428	1436	1355
ν_{22}	1459	1449	1360

Table 2.-continued

assignment	CASSCF(9,7)[b] $\widetilde{B}$	CASSCF(9,7)[b] $\widetilde{X}$	B3LYP[c] $\widetilde{X}$
ν_{21}	1475	1467	1375
ν_{20}	1483	1482	1403
ν_{19}	1544	1542	1471
ν_{18}	1551	1547	1474
ν_{17}	1554	1552	1481
ν_{16}	1555	1556	1490
ν_{15}	1557	1557	1491
ν_{14}	1571	1566	1493
ν_{13}	3005	2993	2777
ν_{12}	3027	3002	2923
ν_{11}	3032	3015	2949
ν_{10}	3038	3020	2956
ν_9	3071	3027	2966
ν_8	3079	3033	2972
ν_7	3083	3038	2976
ν_6	3094	3060	2999
ν_5	3096	3070	3008
ν_4	3098	3078	3021
ν_3	3133	3086	3029
ν_2	3139	3089	3033
ν_1	3199	3091	3038

[a] All calculations employed the 6-31+G(d) basis set. [b] A uniform scale factor of 0.95 was used. [c] The calculated B3LYP frequencies are scaled by 0.98.

Table 3. Calculated 57 vibrational frequencies (cm^{-1}) of the diequatorial chair conformer of *trans*-2-methylcyclohexoxy radical (C$_1$ symmetry) in its ground state and $\tilde{B}$ excited state.[a]

assignment	CASSCF(9,7)[b] $\tilde{B}$	CASSCF(9,7)[b] $\tilde{X}$	B3LYP[c] $\tilde{X}$
ν_{57}	119	122	113
ν_{56}	180	189	178
ν_{55}	218	236	225
ν_{54}	267	263	254
ν_{53}	323	327	313
ν_{52}	340	344	335
ν_{51}	348	356	341
ν_{50}	399	432	416
ν_{49}	424	441	422
ν_{48}	481	479	477
ν_{47}	549	561	543
ν_{46}	676	787	745
ν_{45}	805	849	811
ν_{44}	844	875	820
ν_{43}	876	878	839
ν_{42}	885	935	882
ν_{41}	936	946	918
ν_{40}	963	1007	932
ν_{39}	1007	1013	972
ν_{38}	1028	1022	978
ν_{37}	1083	1072	1042
ν_{36}	1087	1097	1059
ν_{35}	1110	1110	1061
ν_{34}	1142	1140	1101
ν_{33}	1166	1165	1115
ν_{32}	1202	1206	1147
ν_{31}	1237	1275	1192
ν_{30}	1272	1279	1238
ν_{29}	1310	1319	1243
ν_{28}	1322	1345	1260
ν_{27}	1359	1368	1298
ν_{26}	1389	1387	1311
ν_{25}	1407	1421	1321
ν_{24}	1408	1430	1346
ν_{23}	1433	1447	1348
ν_{22}	1444	1448	1362

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Table 3.-continued

assignment	CASSCF(9,7)[b] $\widetilde{B}$	CASSCF(9,7)[b] $\widetilde{X}$	B3LYP[c] $\widetilde{X}$
ν_{21}	1480	1461	1368
ν_{20}	1503	1481	1400
ν_{19}	1543	1545	1472
ν_{18}	1549	1549	1477
ν_{17}	1551	1553	1481
ν_{16}	1557	1555	1488
ν_{15}	1564	1560	1492
ν_{14}	1567	1567	1493
ν_{13}	3024	3005	2859
ν_{12}	3030	3012	2946
ν_{11}	3034	3023	2957
ν_{10}	3039	3026	2962
ν_{9}	3069	3027	2967
ν_{8}	3075	3034	2973
ν_{7}	3079	3047	2995
ν_{6}	3081	3063	2999
ν_{5}	3093	3067	3007
ν_{4}	3098	3074	3013
ν_{3}	3139	3086	3032
ν_{2}	3150	3095	3051
ν_{1}	3187	3104	3053

[a] All calculations employed the 6-31+G(d) basis set. [b] A uniform scale factor of 0.95 was used. [c] The calculated B3LYP frequencies are scaled by 0.98.