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Table 4. Number of internal coordinates

Internal coordinate	Molecule			
	1	2	3	4
R_i	15	17	14	16
K_i	4	4	6	6
L_i	10	8	10	8
H_i	-	6	-	6
Σ_i	5	4	5	4
P_i	5	4	5	4
Ψ_i	5	4	5	4
T_i	5	4	5	4
A_i	12	12	18	18
Γ_i'	4	4	6	6
Γ_i''	4	4	6	6
Γ_i'''	4	4	6	6
E_i	6	6	-	-
Θ_i	-	1	-	1
X_i	-	1	-	1
Φ_i	-	1	-	1
Ω_i	-	1	-	1

Internal coordinate	Molecule			
	1	2	3	4
Δ_i'	-	2	-	2
Δ_i''	-	2	-	2
Δ_i'''	-	2	-	2
Λ_i'	-	2	-	2
Λ_i''	-	2	-	2
Z_i	-	2	-	2
Total	$69 + 10^a$	$87 + 10$	$75 + 11$	$93 + 11$

^a The second figure denotes the number of redundant coordinates.

**Table 7. Observed and calculated frequencies (cm^{-1}) for
2,2-(dimethylmetano)-2,4-didehydroadamantane (2)**

Mode	Calc.	Obs.		Potential energy distribution (P.E.D.)
		Raman	Infrared	
A' ν_1	3003	3027 m	3025 m	CH ₃ stretch.
ν_2	2991		3010 m	CH ₂ stretch., CH ₃ stretch.
ν_3	2988	3002 m		CH stretch.
ν_4	2986	2980 m	2980 m	CH ₂ stretch., CH ₃ stretch.
ν_5	2959			CH stretch.
ν_6	2948			CH ₂ stretch.
ν_7	2942		2925 s,bd	CH ₂ stretch.
ν_8	2910	2919 s,bd		CH ₃ stretch.
ν_9	2905			CH ₂ stretch.
ν_{10}	2900			CH stretch.
ν_{11}	2891			CH ₃ stretch.
ν_{12}	2882	2878 m,sh	2880 s	CH ₂ stretch.
ν_{13}	1532	1494 w	1495 w	CH ₂ sciss.
ν_{14}	1465	1465 w,sh	1470 m	CH ₂ sciss.
ν_{15}	1449	1444 m		CH ₂ sciss., CH bend.
ν_{16}	1439	1418 vw	1420 vw	CH ₂ sciss., CH bend.
ν_{17}	1374	1375 vw		CH ₃ sym. def.

Mode	Calc.	Obs.	Potential energy distribution (P.E.D.)	
		Raman	Infrared	
ν_{18}	1364	1369 vw		CH ₃ sym. def., CH ₂ wagg.
ν_{19}	1343		1350 w	CH ₂ wagg., CH ₃ sym. def., CH bend., CC stretch.
ν_{20}	1339	1343 vw		CH ₂ wagg., CH bend., CH ₃ sym. def.
ν_{21}	1315	1325 w		CH ₃ asym. def., CH ₃ symm. def.
ν_{22}	1308		1310 vw	CH ₂ twist., CH ₂ wagg., CC stretch.
ν_{23}	1300			CH ₃ asym. def., CH ₃ rock.
ν_{24}	1291	1293 vw	1295 w	CC stretch., CH ₃ asym. def., CC ₂ sciss.
ν_{25}	1269	1275 w		CH bend., CC stretch., CH ₂ wagg.
ν_{26}	1247	1265 w	1265 vw	CC stretch., CC ₂ rock., (CCC) _s def.
ν_{27}	1229	1239 w		CH bend., CC stretch., CH ₂ wagg.
ν_{28}	1220	1217 w		CC stretch., CH bend.
ν_{29}	1154	1147 m	1150 w	CC stretch., CH bend., CH ₂ twist.
ν_{30}	1108		1115 w	CC stretch., CH ₃ rock.
ν_{31}	1073	1079 w	1085 w	CH ₂ rock., CC stretch.
ν_{32}	1054	1068 w	1070 w	CH ₂ rock., CC stretch., CCC def.
ν_{33}	1014		1015 w	CH ₃ rock., CC stretch.
ν_{34}	1010	1014 vw		CH ₃ rock., CC stretch.
ν_{35}	988	986 vw	972 w	CC stretch., CCC def., CH ₂ rock.

Mode	Calc.	Obs.	Potential energy distribution (P.E.D.)	
		Raman	Infrared	
ν_{36}	950	928 m		CC stretch., CCC def., CH ₂ rock.
ν_{37}	896	912 vw	916 w	CCC def., CH ₂ rock., CC stretch.
ν_{38}	848	853 vw	846 w	CC stretch., (CCC) _s def. (CC) _{inv} stretch., CCC def.,
ν_{39}	826	840 m		CC stretch., (CC) _{inv} stretch.
ν_{40}	800	782 w	785 vw	CC stretch.,
ν_{41}	756	764 s	765 w	CC stretch., (CC) _{inv} stretch.
ν_{42}	717	708 w	710 vw	CCC def., CC stretch.
ν_{43}	641	647 m		CC stretch., CCC def.,
ν_{44}	578	570 w		CCC def., CC stretch.
ν_{45}	549	543 w		CC ₂ sciss., CCC def., (CCC) _s def.
ν_{46}	467			CCC def., CC ₂ sciss.
ν_{47}	421	425 w	420 vw	CC ₂ rock., (CCC) _s def.
ν_{48}	359	391 w	390 vw	CCC def., (CCC) _s def., CC ₂ sciss., CC stretch.
ν_{49}	327	327 w		CCC def.
ν_{50}	219	231 vw		(CCC) _s def., CC ₂ rock.
A" ν_{51}	2958			CH stretch.
ν_{52}	2948			CH ₂ stretch.

Mode	Calc.	Obs.	Potential energy distribution (P.E.D.)	
		Raman	Infrared	
ν_{53}	2901			CH ₃ stretch.
ν_{54}	2898			CH ₃ stretch.
ν_{55}	2882			CH ₂ stretch.
ν_{56}	2875	2859 m	2860 s	CH ₂ stretch.
ν_{57}	1461		1460 m	CH ₂ sciss.
ν_{58}	1372	1386 vw	1370 m	CH ₂ wagg., CC stretch., CH bend.
ν_{59}	1352	1355 vw	1360 vw	CH bend., CH ₂ wagg.
ν_{60}	1322		1330 m	CH ₃ asym. def.
ν_{61}	1312			CH ₃ asym. def.
ν_{62}	1299			CH ₂ wagg., CH bend., CC stretch.
ν_{63}	1270		1280 w	CH ₂ twist., CH ₂ wagg., CC stretch.
ν_{64}	1234		1235 w	CH ₂ twist., CH ₂ wagg., CC stretch.
ν_{65}	1216			CH bend., CH ₂ twist.
ν_{66}	1196	1192 m	1195 w,sh	CH ₂ twist., CH bend.
ν_{67}	1163		1175 m	CH ₂ twist., CH bend.
ν_{68}	1156	1165 vw		CH bend., CH ₂ wagg., CH ₂ twist.
ν_{69}	1127	1123 vw		CH ₃ rock.
ν_{70}	1089	1101 w	1100 vw	CH ₂ rock., CH bend., CC stretch.
ν_{71}	1045	1042 w	1045 w	CC stretch., CH bend., CH ₂ twist.

Mode	Calc.	Obs.	Potential energy distribution (P.E.D.)	
		Raman	Infrared	
ν_{72}	1015			CH bend., CH ₃ rock., CH ₂ rock., CC stretch.
ν_{73}	1004	1006 w		CC ₂ rock., CH ₂ rock.
ν_{74}	956	944 w	950 w	CC stretch., CCC def., CH ₂ rock.
ν_{75}	891	888 vw	885vw	CH ₂ rock., CH bend., CC stretch.
ν_{76}	837	870 vw	860 w	CC stretch., (CCC) _s def., CCC def.
ν_{77}	796	820 vw	830 vw	CC stretch.
ν_{78}	705	717 vw	720 w	CC stretch., CCC def.
ν_{79}	630		590 s	CC stretch., CC ₂ wagg., (CCC) _s def.
ν_{80}	489	510 w	515 w	CCC def., CC stretch.
ν_{81}	459	452 w	460 vw	CC ₂ wagg., CCC def.
ν_{82}	425		435 w	CCC def.
ν_{83}	290	310 vw,sh		CCC def., CH ₃ tors.
ν_{84}	259			CH ₃ tors.
ν_{85}	203	216 vw		CC ₂ wagg., (CCC) _s def., CC stretch.
ν_{86}	153	152 vw		CC ₂ twist., CH ₃ tors.
ν_{87}	63			CH ₃ tors.

**Table 9. Observed and calculated frequencies (cm^{-1}) for
2,4-(dimethylmetano)adamantane (4)**

Mode	Calc.	Obs.		Potential energy distribution (P.E.D.)
		Raman	Infrared	
A' ν_1	3003	3045 w	3050 w	CH ₃ stretch.
ν_2	3001	2996 w		CH stretch.
ν_3	2991			CH ₂ stretch., CH ₃ stretch.
ν_4	2982	2968 m		CH ₂ stretch., CH ₃ stretch.
ν_5	2947			CH ₂ stretch.
ν_6	2944			CH ₂ stretch.
ν_7	2920			CH stretch.
ν_8	2913			CH stretch.
ν_9	2910	2910 s,bd		CH ₃ stretch.
ν_{10}	2906			CH stretch.
ν_{11}	2881			CH ₂ stretch.
ν_{12}	2873			CH ₃ stretch.
ν_{13}	2861	2852 s		CH ₂ stretch.
ν_{14}	1570		1560 vw	CH ₂ sciss.
ν_{15}	1476	1498 w	1500 w	CH ₂ sciss., CH bend.
ν_{16}	1468		1460 s	CH ₂ sciss., CH bend.
ν_{17}	1450	1454 w		CH ₂ sciss.
ν_{18}	1392	1400 vw	1405 vw	CH ₃ sym. def., CH ₃ asym. def.
ν_{19}	1367	1364 vw	1370 m	CH ₃ sym.def., CH ₂ wagg.

Mode	Calc.	Obs.	Potential energy distribution (P.E.D.)	
			Raman	Infrared
ν_{20}	1353	1354 vw		CH ₂ wagg., CH ₃ sym. def., CC stretch.
ν_{21}	1342	1340 vw		CH ₂ wagg., CH bend., CH ₂ twist.
ν_{22}	1337		1330 vw	CH bend., CH ₂ wagg., CH ₂ twist.
ν_{23}	1324			CH ₃ asym. def., CH ₃ sym. def.
ν_{24}	1304			CH ₃ asym. def., CH ₃ sym. def.
ν_{25}	1300		1300 vw	CH bend., CC stretch., CH ₂ wagg.
ν_{26}	1283	1284 vw		CH bend., CC stretch., CCC def., CC ₂ rock.
ν_{27}	1271	1270 w	1272 w	CH bend., CC stretch., CH ₂ twist., CH ₂ wagg.
ν_{28}	1245	1246 vw		CH ₃ rock., CC stretch., CC ₂ sciss.
ν_{29}	1226			CH bend., CH ₂ twist., CC stretch.
ν_{30}	1190	1178 m	1180 w	CH bend., CH ₃ rock., CC stretch.
ν_{31}	1155	1160 w		CC stretch., CH bend., CH ₃ rock., CC ₂ rock.
ν_{32}	1127		1135 w	CH bend., CC stretch.
ν_{33}	1097	1100 w		CH ₂ rock., CC stretch., CCC def.
ν_{34}	1063		1065 vw	CC stretch., CH ₂ rock., CH bend.
ν_{35}	1024	1020 w		CCC def., CH ₃ rock.
ν_{36}	1016			CH ₃ rock., CC stretch., CCC def.
ν_{37}	985	997 w		CC stretch., CH ₃ rock., CCC def.
ν_{38}	964	971 vw		CC stretch., CCC def., CH ₂ rock.
ν_{39}	951	947 m		CC stretch., CH ₂ rock., CCC def.
ν_{40}	934	943 w,sh		CC stretch., CCC def., CH ₂ rock.

Mode	Calc.	Obs.	Potential energy distribution (P.E.D.)	
		Raman	Infrared	
ν_{41}	856		865 vw	CCC def., CC stretch.
ν_{42}	804	809 w	815 w	CC stretch., CCC def.
ν_{43}	795	781 m	785 vw	CC stretch., CCC def.
ν_{44}	729	737 m	740 vw	CC stretch.
ν_{45}	677		670 vw	CCC def., CC stretch.
ν_{46}	669	665 m		CC stretch., CCC def.
ν_{47}	595			CCC def., CC ₂ rock.
ν_{48}	579	571 vw	575 vw	CC ₂ sciss., CCC def.
ν_{49}	464			CCC def., CC ₂ sciss., CC ₂ rock.
ν_{50}	440	451 w		CC ₂ rock., CCC def., CC stretch.
ν_{51}	383	389 vw	390 vw	CCC def.
ν_{52}	338	338 vw		CCC def., CC ₂ sciss.
ν_{53}	264	268 vw		CCC def., CC ₂ rock.
A" ν_{54}	2999	2996 w	3000 m	CH stretch.
ν_{55}	2947			CH ₂ stretch.
ν_{56}	2913		2915 s, br	CH stretch.
ν_{57}	2903			CH ₃ stretch.
ν_{58}	2901			CH ₃ stretch.
ν_{59}	2880			CH ₂ stretch.
ν_{60}	2875		2858 s	CH ₂ stretch.
ν_{61}	1466		1470 s	CH ₂ sciss.

Mode	Calc.	Obs.	Potential energy distribution (P.E.D.)	
		Raman	Infrared	
ν_{62}	1390	1380 vw	1382 w	CH ₂ wagg., CH bend., CC stretch.
ν_{63}	1355			CH ₂ wagg., CH bend.
ν_{64}	1345		1345 w	CH ₃ asym. def.
ν_{65}	1317		1315 vw	CH ₃ asym. def.
ν_{66}	1312			CH ₂ wagg., CH bend., CC stretch.
ν_{67}	1299			CH bend., CC stretch., CH ₂ twist.
ν_{68}	1279		1265 vw	CH ₂ twist., CC stretch., CH bend.
ν_{69}	1252		1250 m	CH bend., CH ₂ wagg., CC stretch.
ν_{70}	1237			CH ₂ twist., CC stretch.
ν_{71}	1212	1214 vw		CH ₂ twist., CH bend.
ν_{72}	1196	1200 vw	1200 vw	CH bend., CH ₃ rock.
ν_{73}	1175		1165 w	CH bend., CH ₂ twist., CH ₂ wagg.
ν_{74}	1155		1140 vw	CH bend., CH ₂ twist., CH ₂ wagg.
ν_{75}	1098		1105 m	CH bend., CC stretch.
ν_{76}	1078	1084 vw	1085 w	CC stretch., CH ₂ twist.
ν_{77}	1055	1058 w		CC stretch., CH ₂ rock.
ν_{78}	1042	1040 w	1045 w	CC stretch., CH ₃ rock.
ν_{79}	1008		1000 w	CH ₃ rock.
ν_{80}	965		952 w	CH ₂ rock., CC stretch.
ν_{81}	913			CC stretch., CCC def.
ν_{82}	902	881 w	885 vw	CH ₂ rock.

Mode	Calc.	Obs.	Potential energy distribution (P.E.D.)	
		Raman	Infrared	
ν_{83}	801	821 vw	815 w	CC stretch.
ν_{84}	769			CC stretch.
ν_{85}	652	633 vw	640 vw	CCC def., CC stretch.
ν_{86}	484	487 vw		CCC def., CC ₂ wagg.
ν_{87}	457	451 vw		CCC def., CC ₂ wagg.
ν_{88}	435	435 vw		CCC def., CC ₂ wagg.
ν_{89}	353		365 vw	CH ₃ tors.
ν_{90}	279	286 vw		CCC def.
ν_{91}	231	230 vw		CCC def., CC ₂ wagg.
ν_{92}	169			CC ₂ twist., CH ₃ tors.
ν_{93}	87			CH ₃ tors., CC ₂ twist.