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Supporting Information on the Paper

Molybdenum Tricarbonyl Complex Functionalised with a Molecular Triazatriangulene Platform on Au(111): Surface Spectroscopic Characterization

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Content

1. Synthesis/NMR Spectroscopy 2

2. Vibrational Spectra 12

3. NEXAFS-Spectra 13

4. Theoretical Calculations 14

5. XPS Fitting Parameter 15

6. Detailed Vibrational Analysis 15

1. Synthesis/NMR Spectroscopy

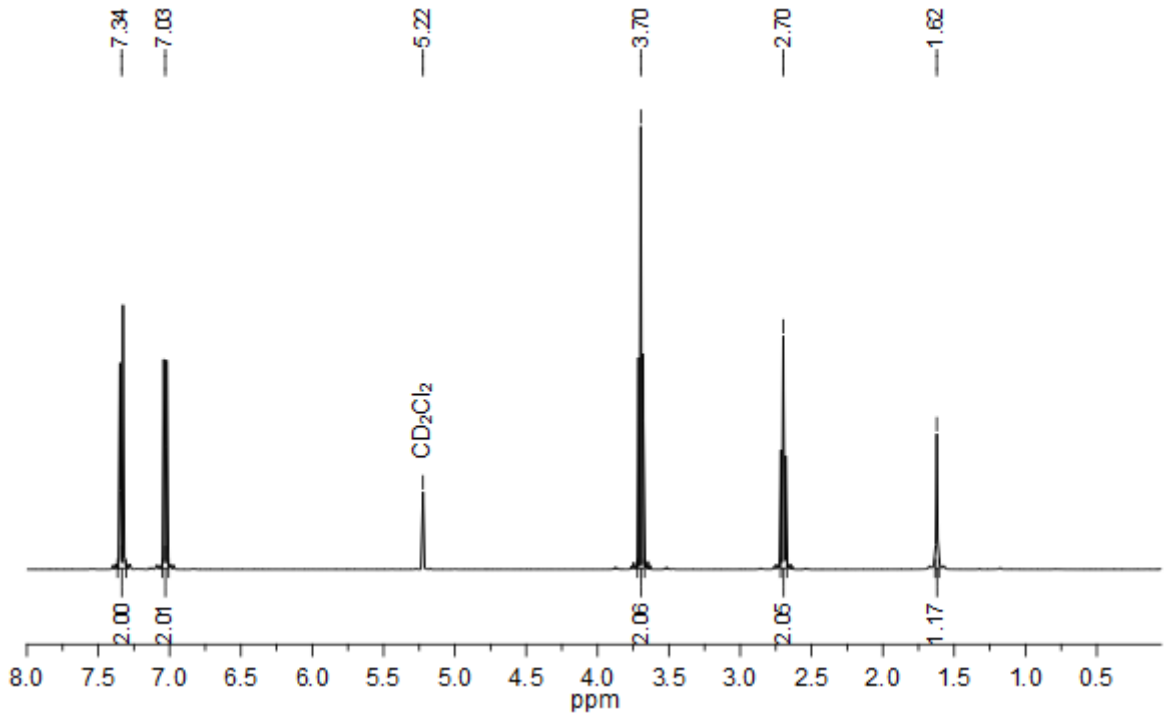

Figure S1. ^{1}H NMR spectrum of 2-(4-bromophenyl)ethanol (**3**).

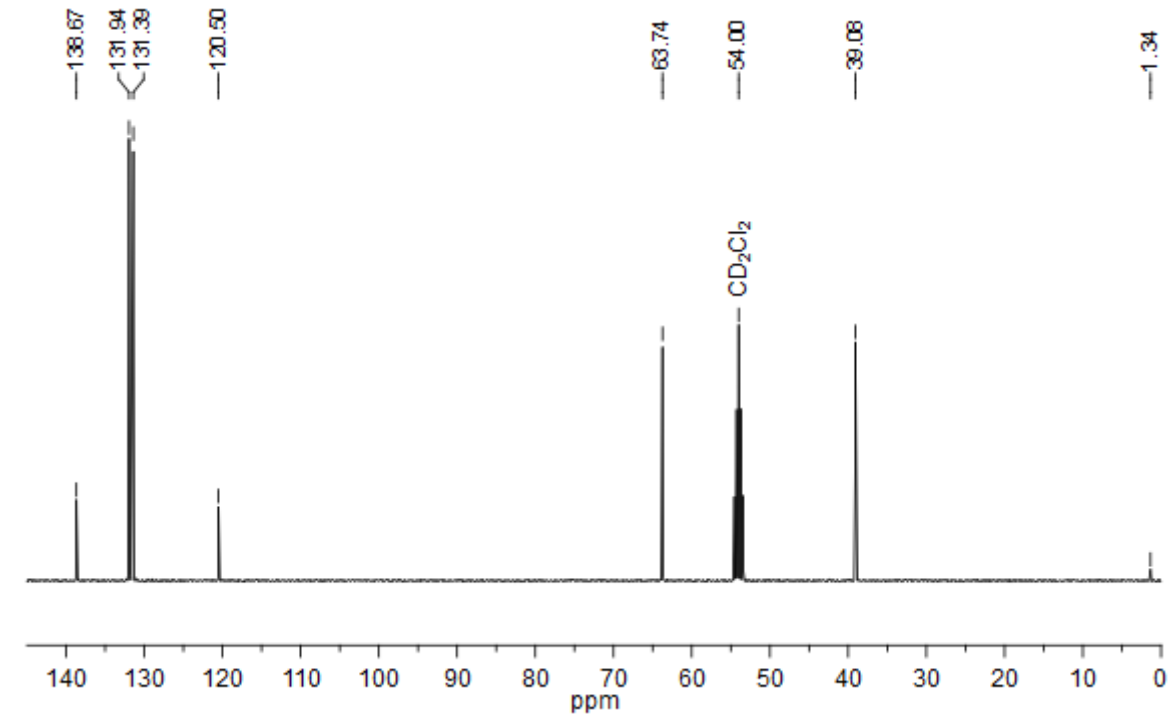

Figure S2. ^{13}C NMR spectrum of 2-(4-bromophenyl)ethanol (**3**).

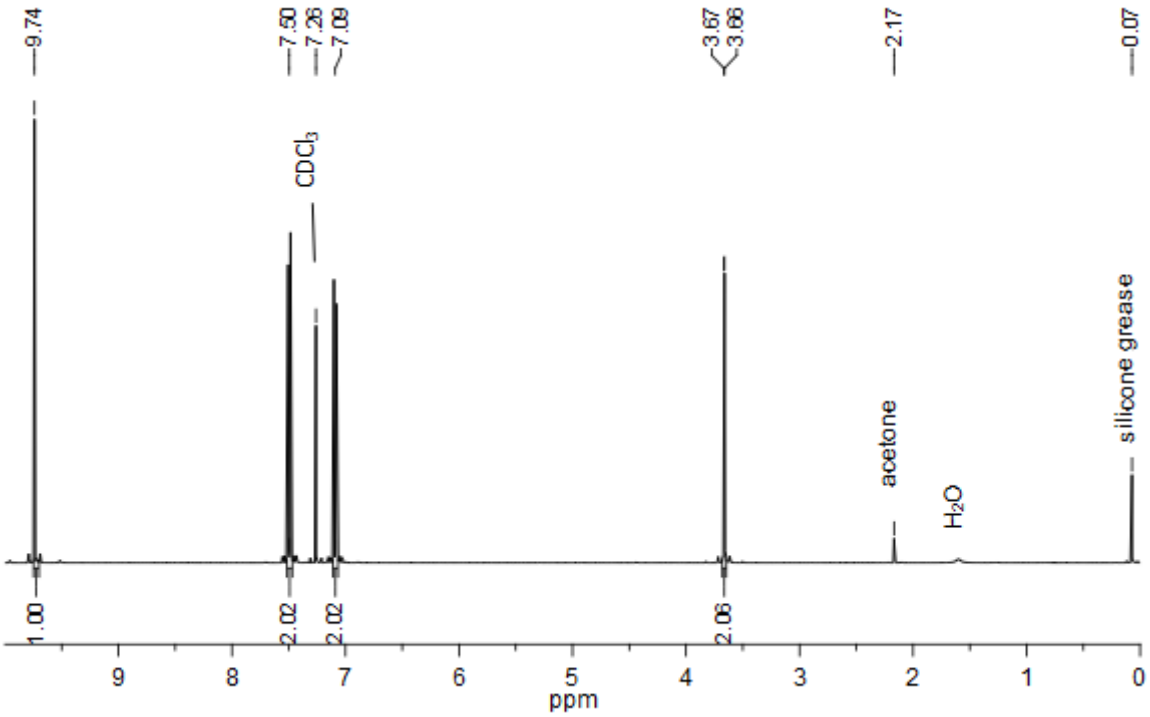

Figure S3. ^{1}H NMR spectrum of 2-(4-bromophenyl)acetaldehyde (**4**).

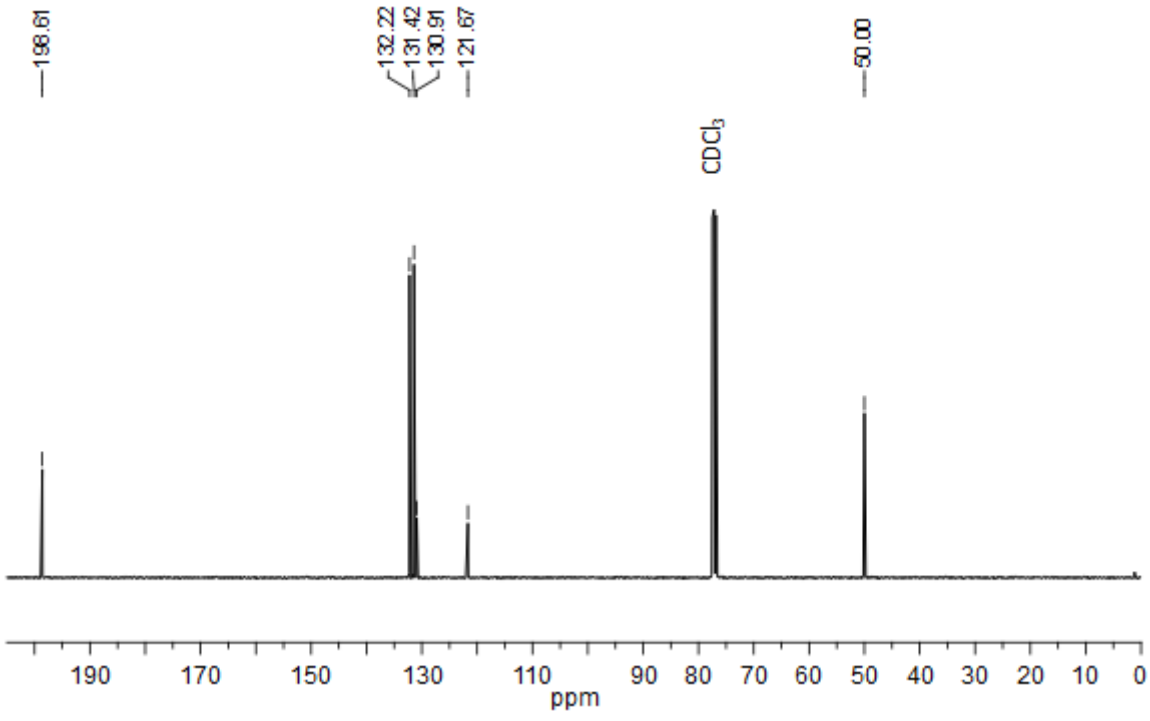

Figure S4. ^{13}C NMR spectrum of 2-(4-bromophenyl)acetaldehyde (**4**).

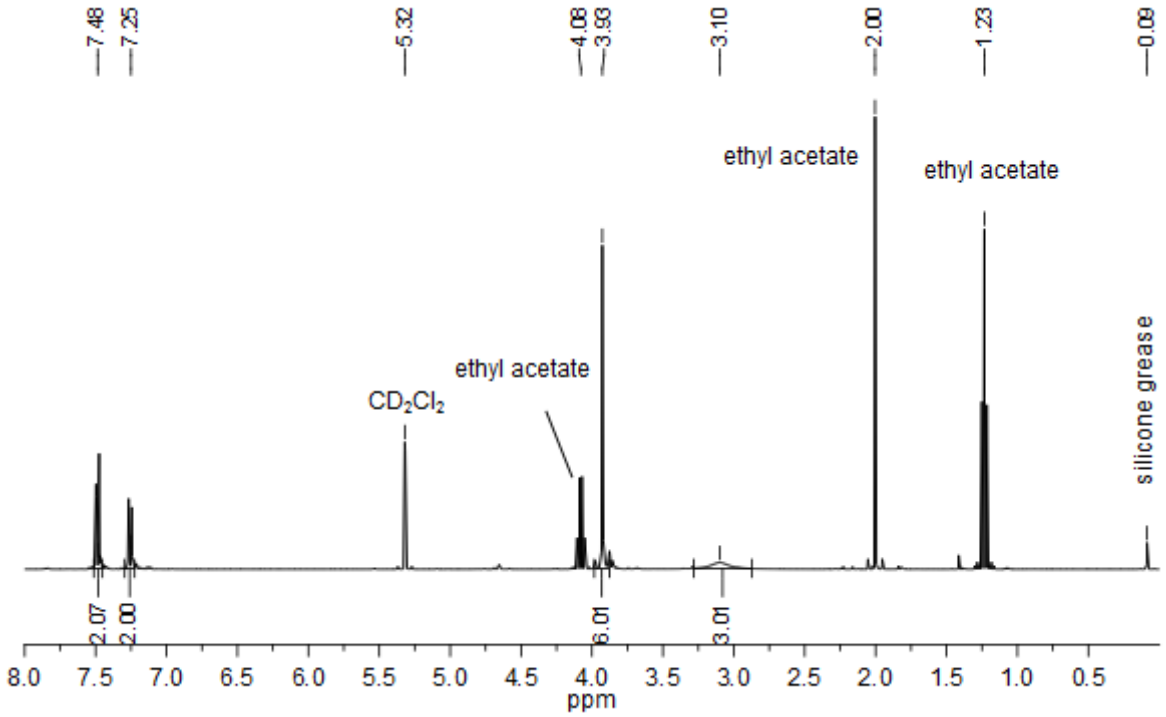

Figure S5. ^{1}H NMR spectrum of 2-(4-bromophenyl)-2-(hydroxymethyl)propane-1,3-diol (**5**).

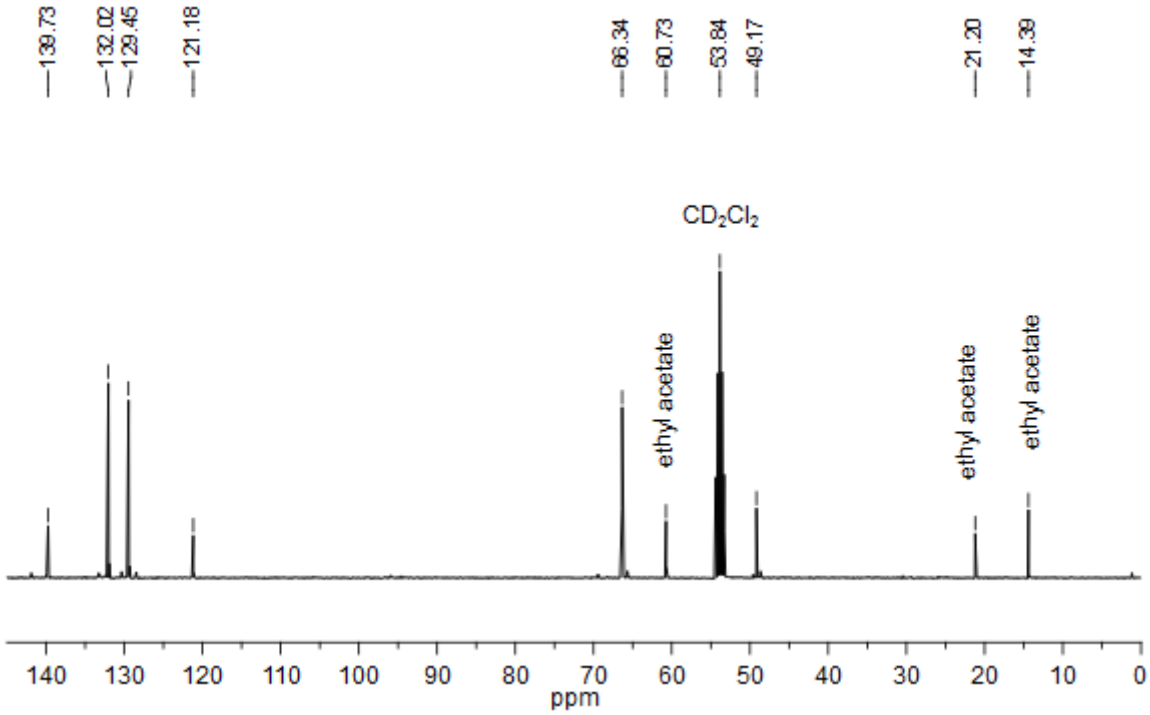

Figure S6. ^{13}C NMR spectrum of 2-(4-bromophenyl)-2-(hydroxymethyl)propane-1,3-diol (**5**).

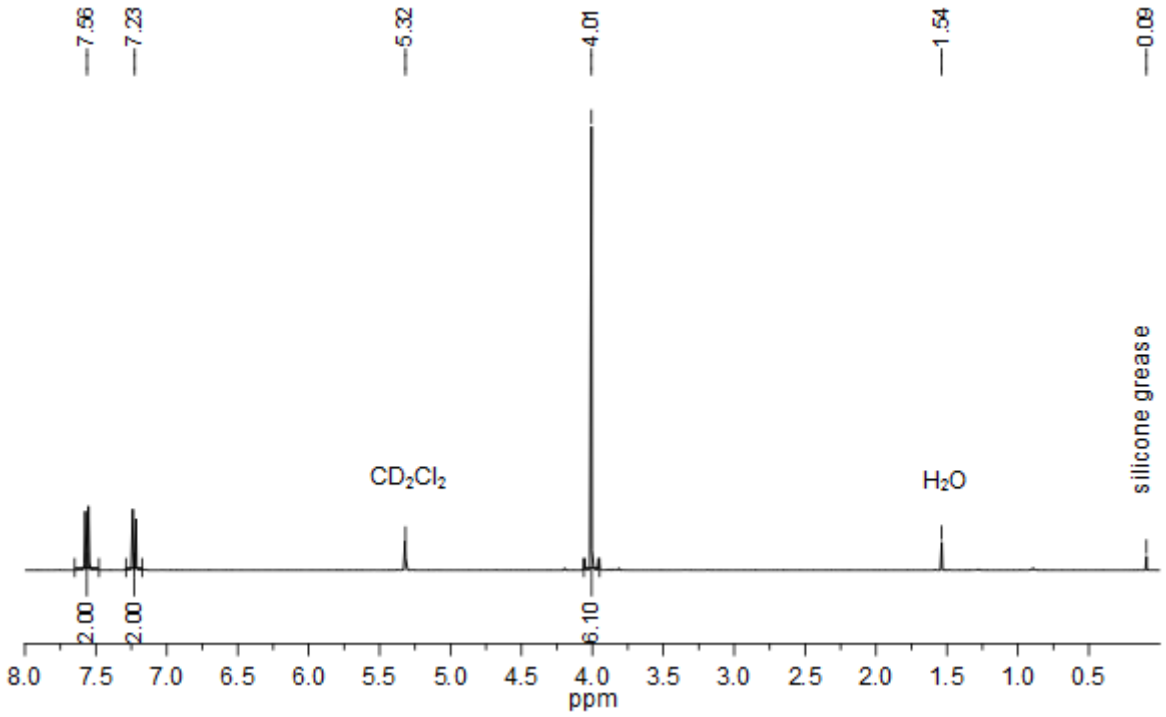

Figure S7. ^{1}H NMR spectrum of 1,3-dichloro-2-chloromethyl-2-(4-bromophenyl)propane (**6**).

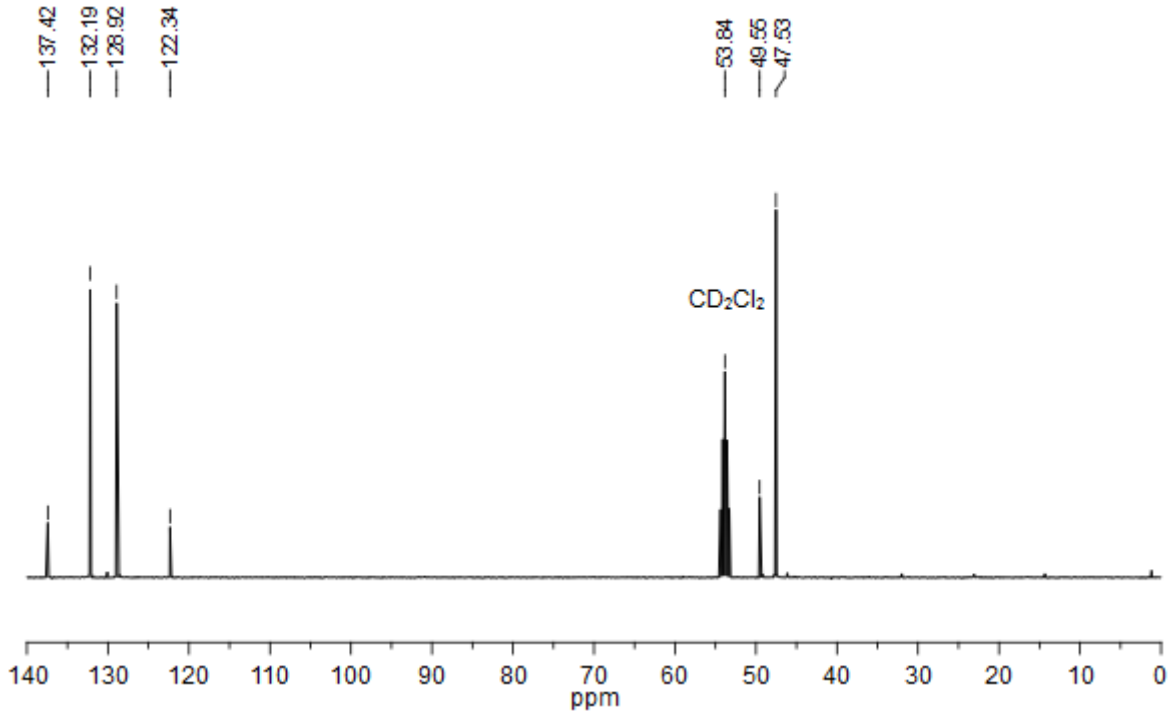

Figure S8. ^{13}C NMR spectrum of 1,3-dichloro-2-chloromethyl-2-(4-bromophenyl)propane (**6**).

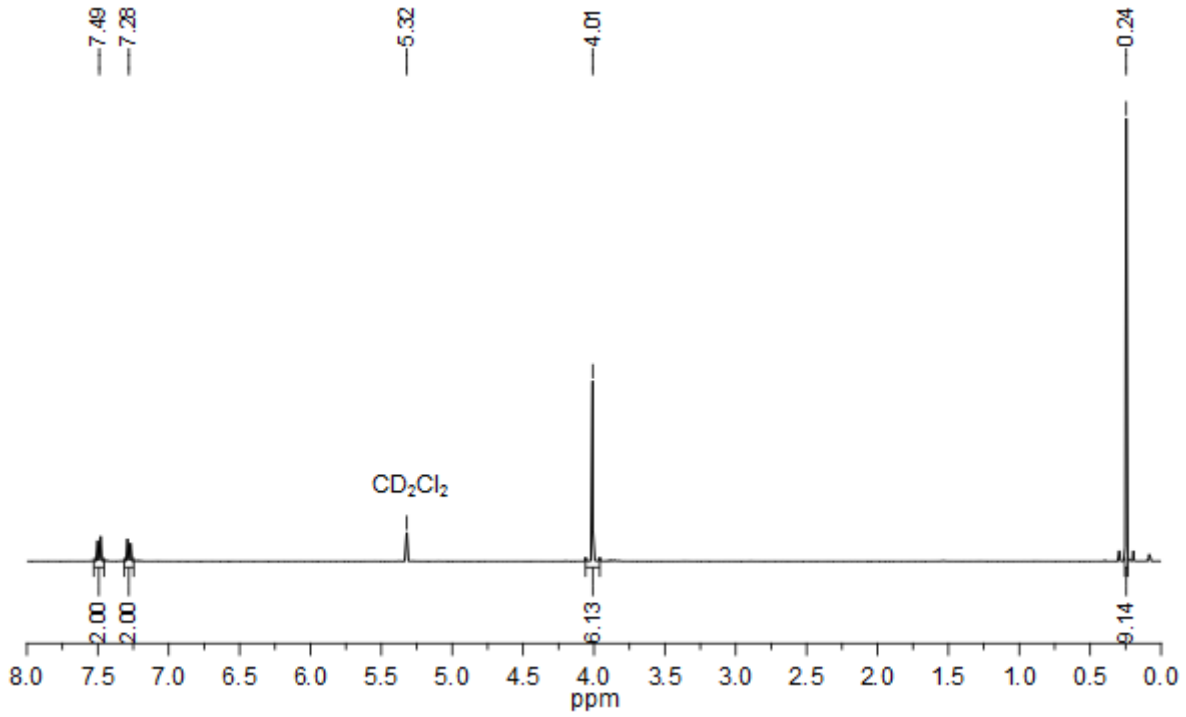

Figure S9. ^{1}H NMR spectrum of ((4-(1,3-dichloro-2-(chloromethyl)prop-2-yl)phenyl)ethynyl)trimethylsilane (**7**).

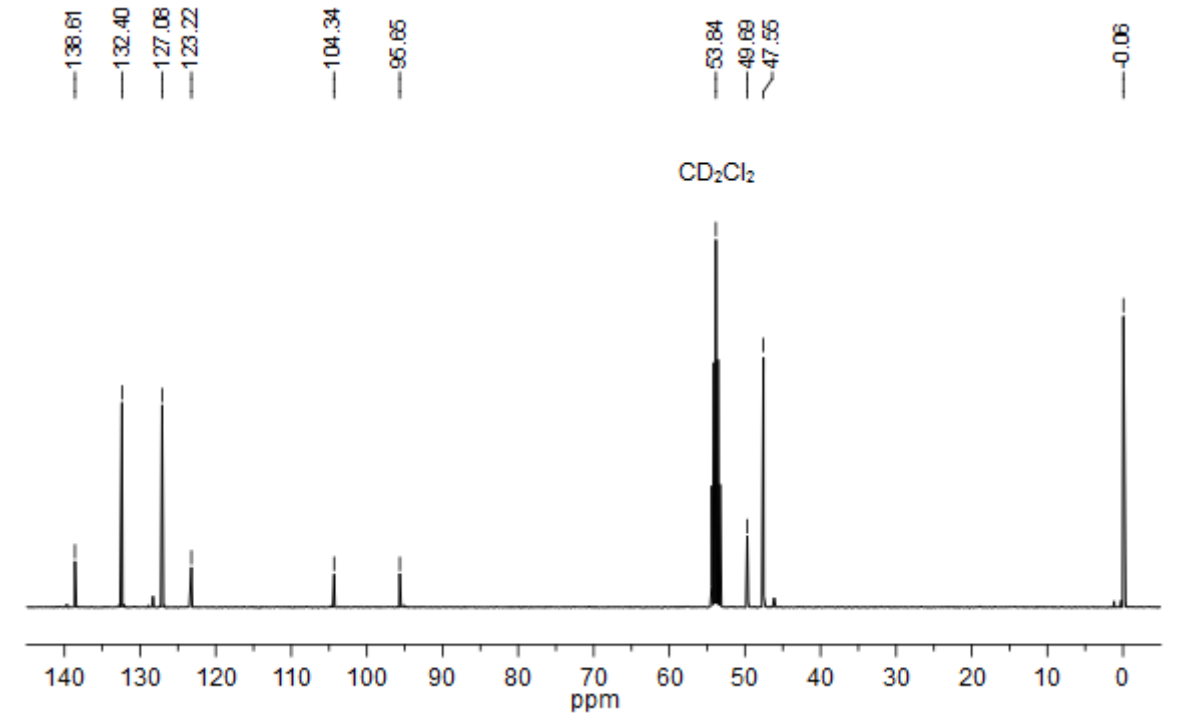

Figure S10. ^{13}C NMR spectrum of ((4-(1,3-dichloro-2-(chloromethyl)prop-2-yl)phenyl)ethynyl)trimethylsilane (**7**).

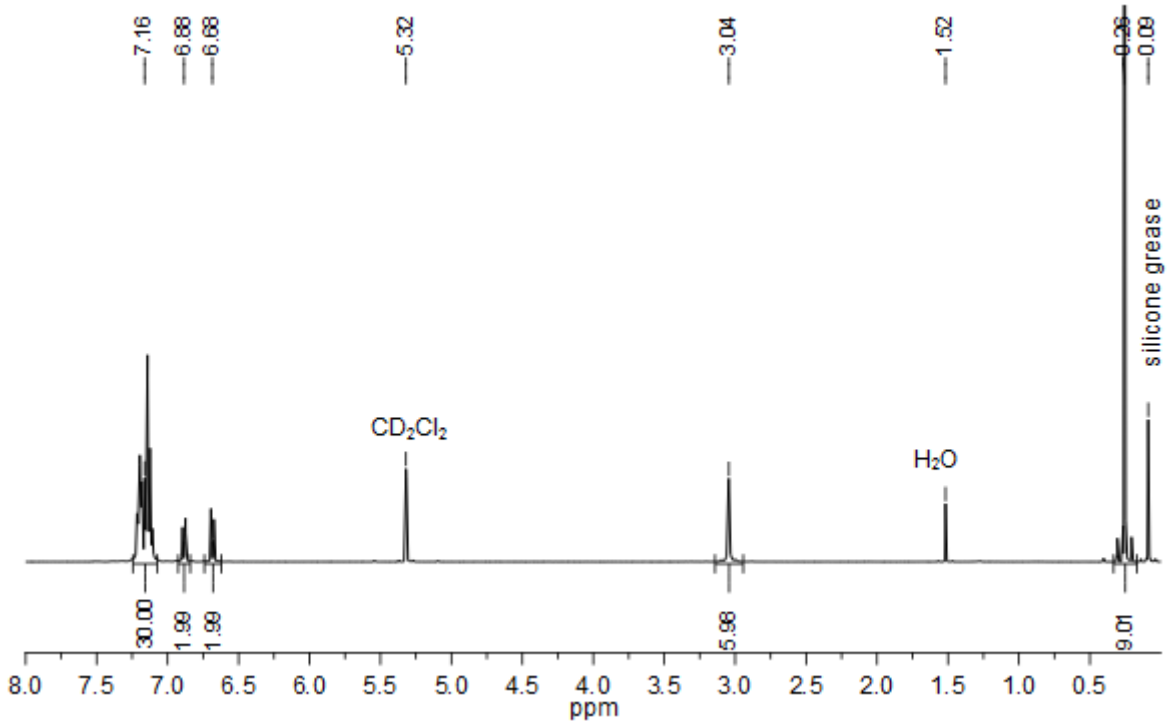

Figure S11. ^{1}H NMR spectrum of TMS-alk-tpd (**8**).

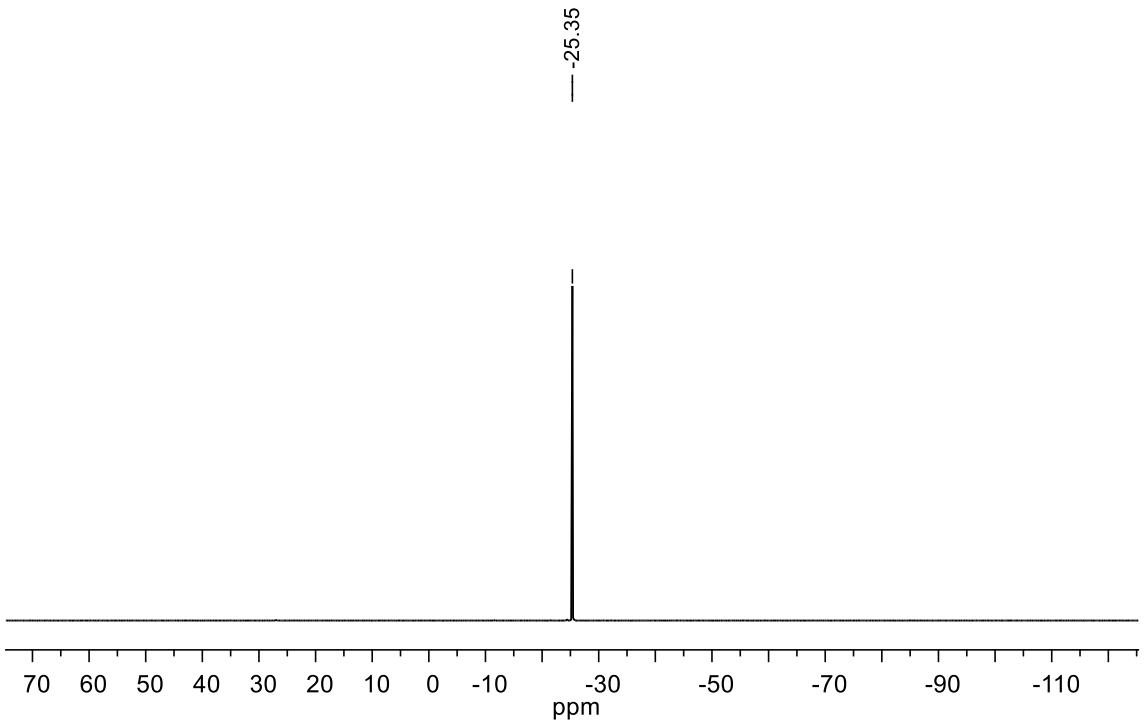

Figure S12. ^{31}P NMR spectrum of TMS-alk-tpd (**8**).

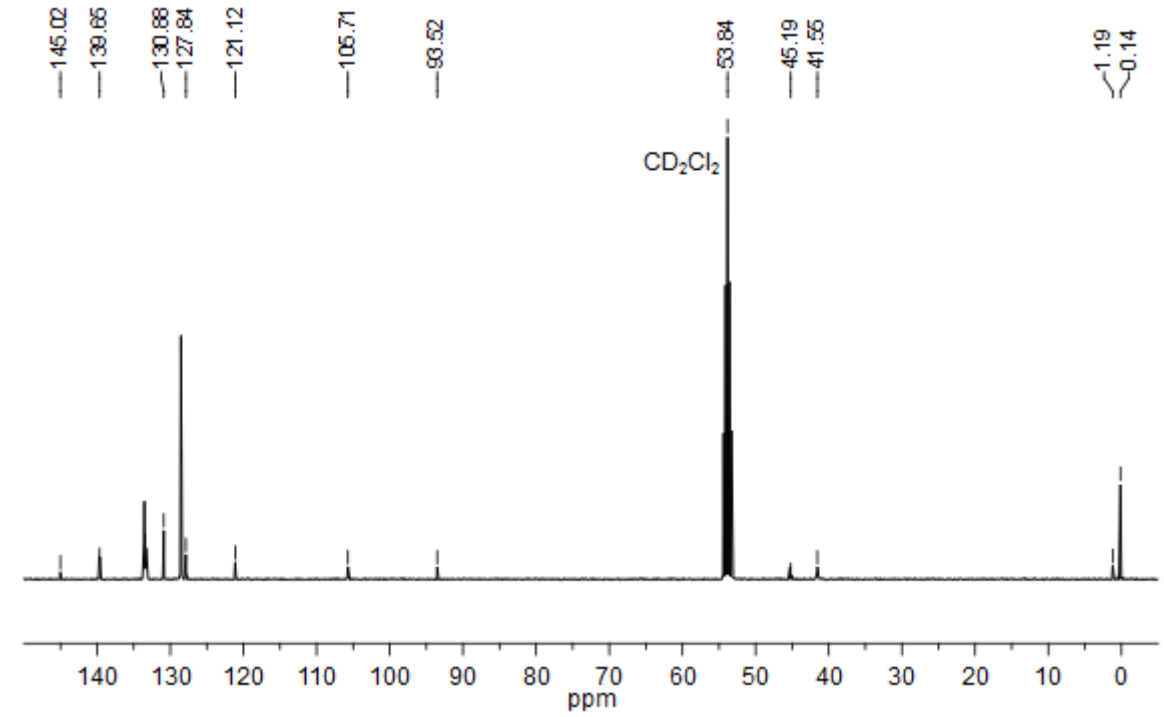

Figure S13. ^{13}C NMR spectrum of TMS-alk-tpd (**9**).

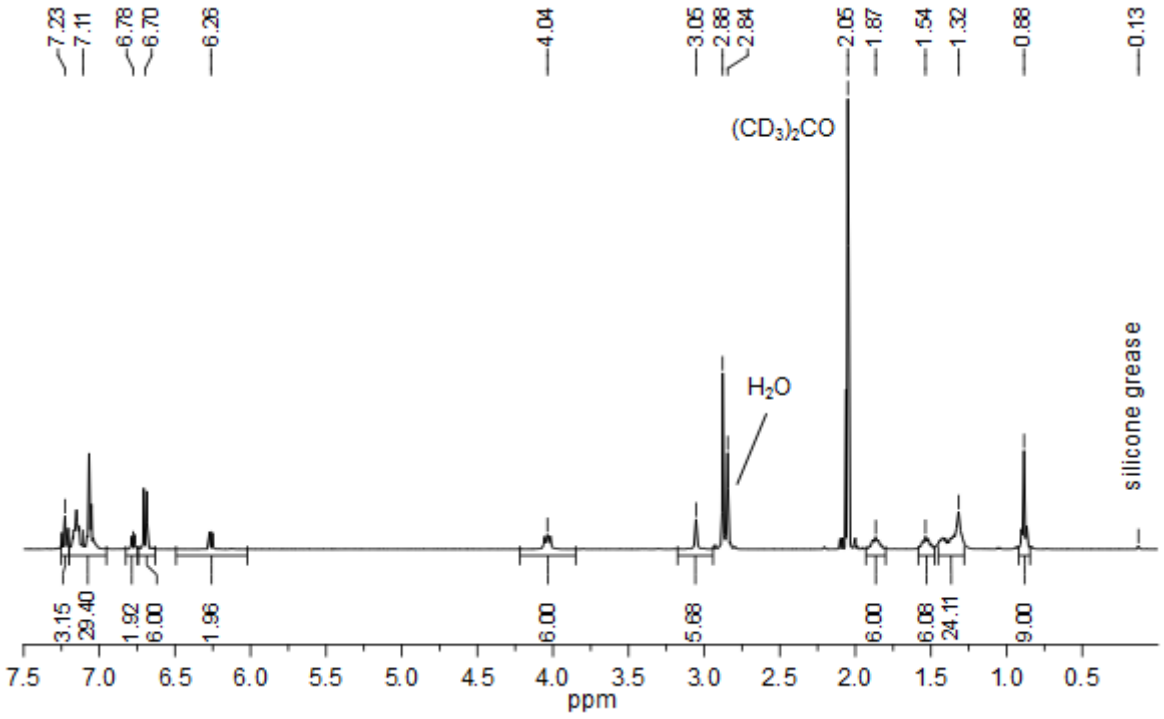

Figure S14. ^{1}H NMR spectrum of *octyl*-TATA-P_3 (**9**).

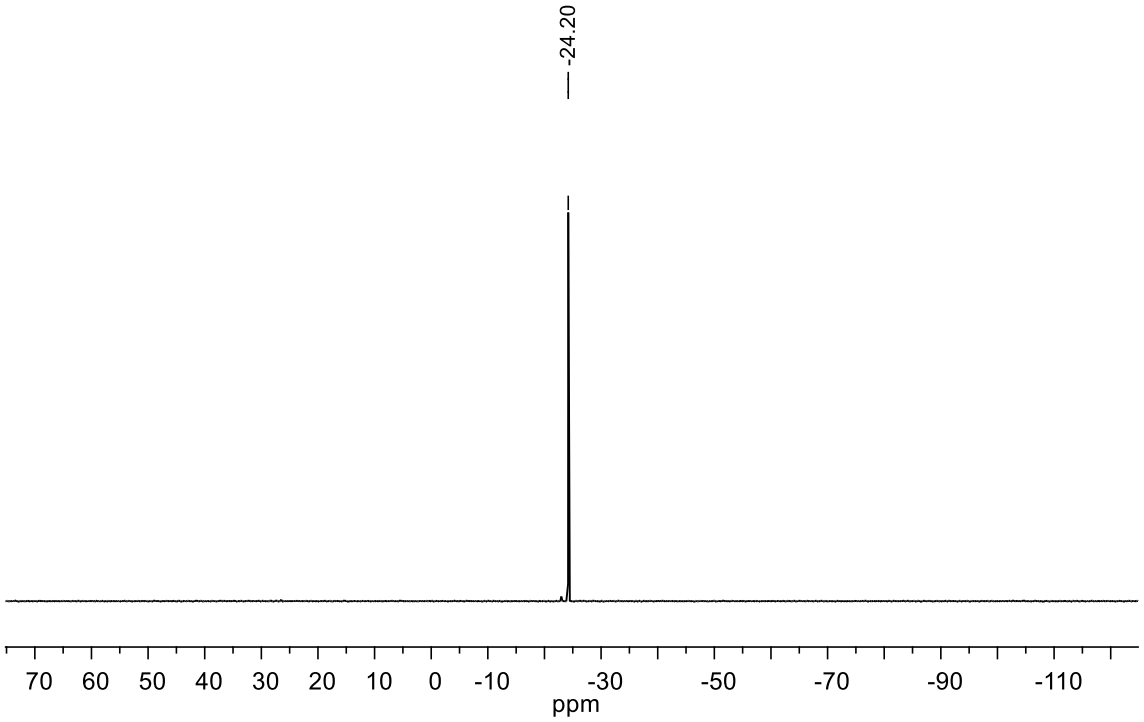

Figure S15. ^{31}P NMR spectrum of *octyl*-TATA-P_3 (**9**).

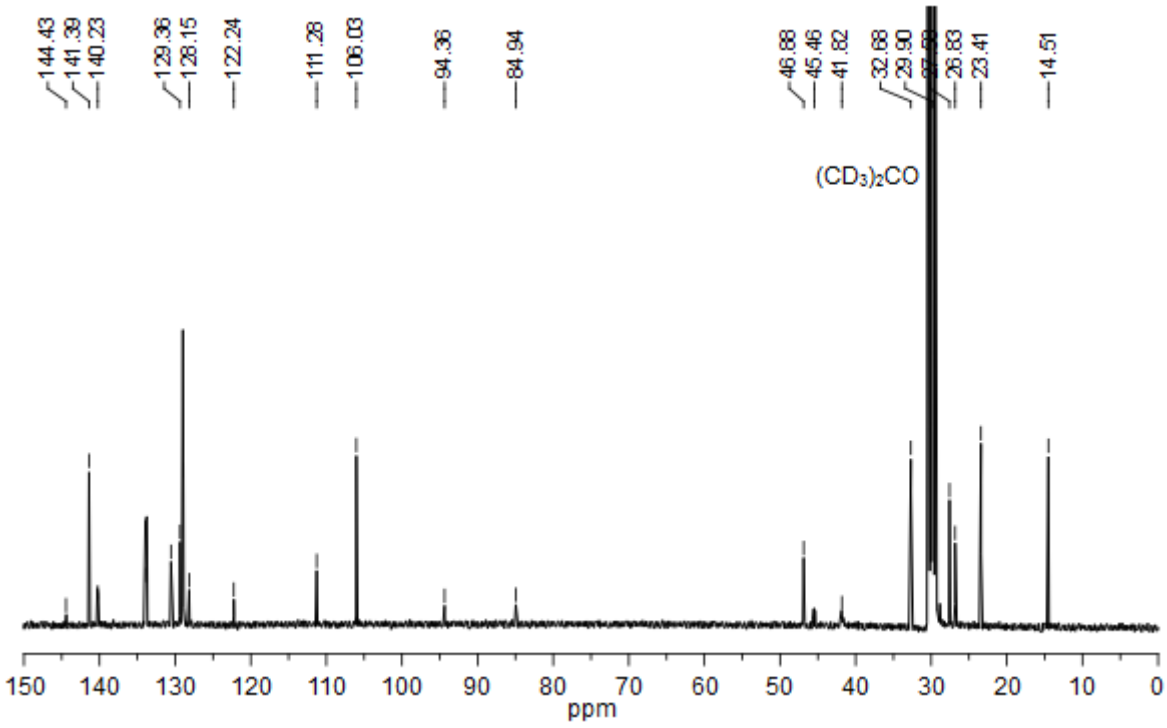

Figure S16. ^{13}C NMR spectrum of *octyl*-TATA-P_3 (**9**).

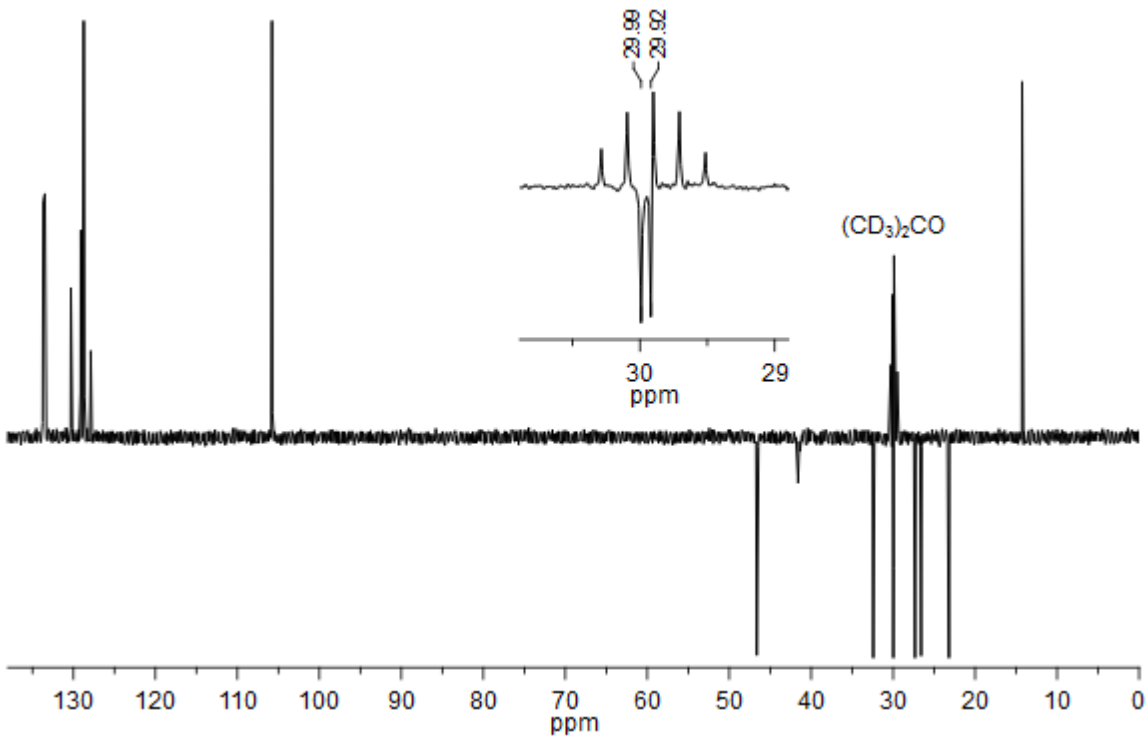

Figure S17. ^{13}C-DEPT135 NMR spectrum of *octyl*-TATA-P$_3$ (**9**).

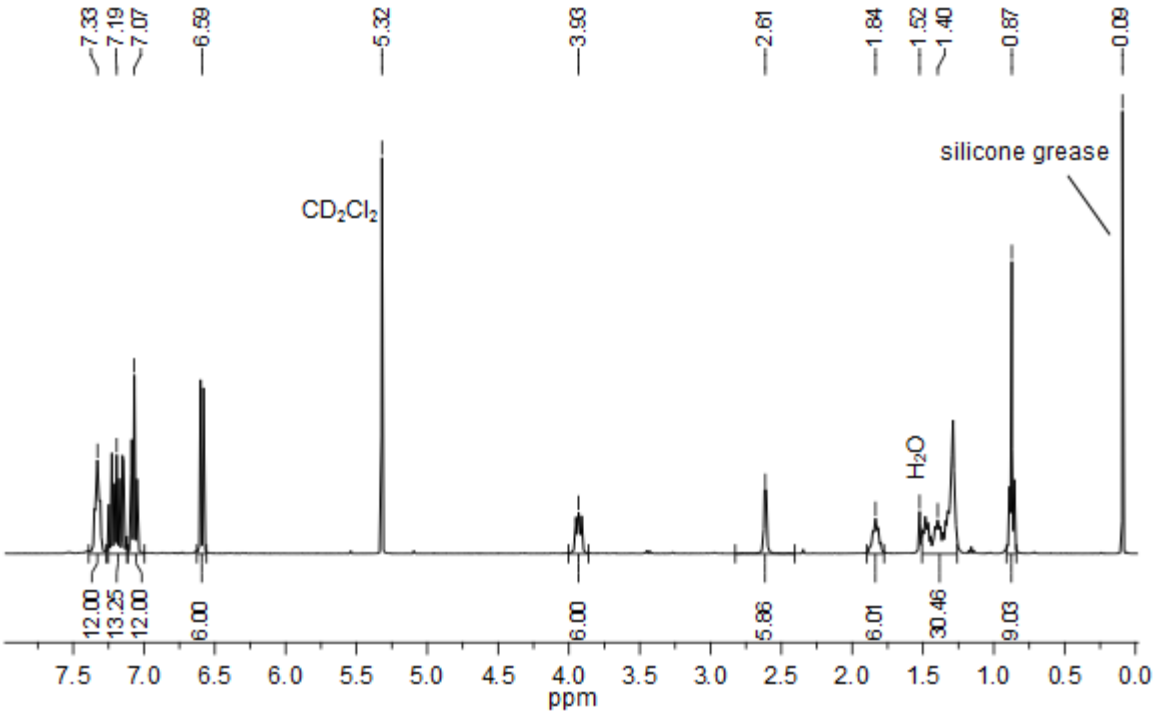

Figure S18. ^{1}H NMR spectrum of [Mo(CO)$_3$(TATA-P$_3$)] (**1**).

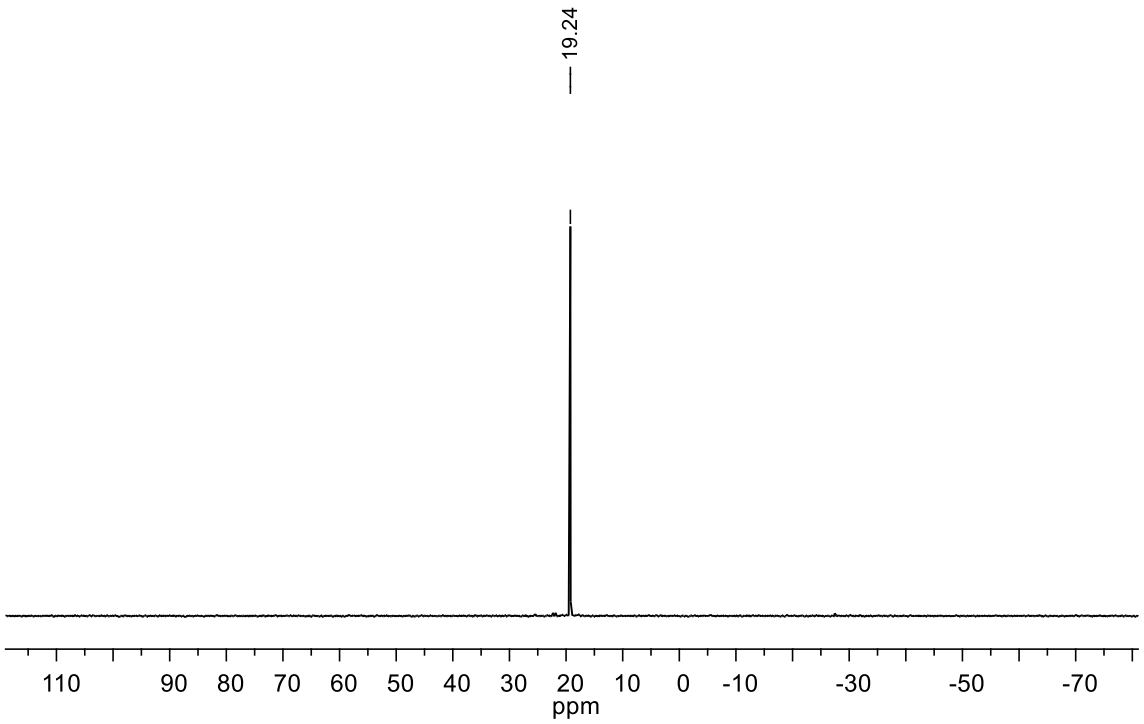

Figure S19. ^{31}P NMR spectrum of $[Mo(CO)_3(TATA\text{-}P_3)]$ (**1**).

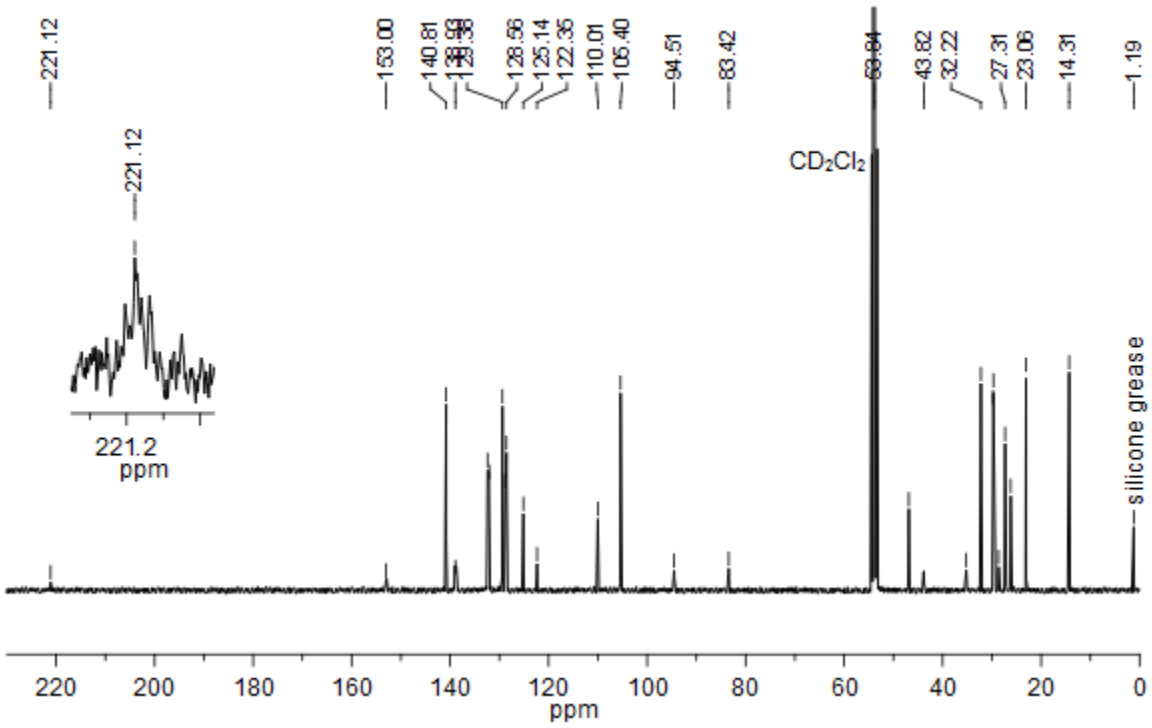

Figure S20. ^{13}C NMR spectrum of $[Mo(CO)_3(TATA\text{-}P_3)]$ (**1**).

2. Vibrational Spectra

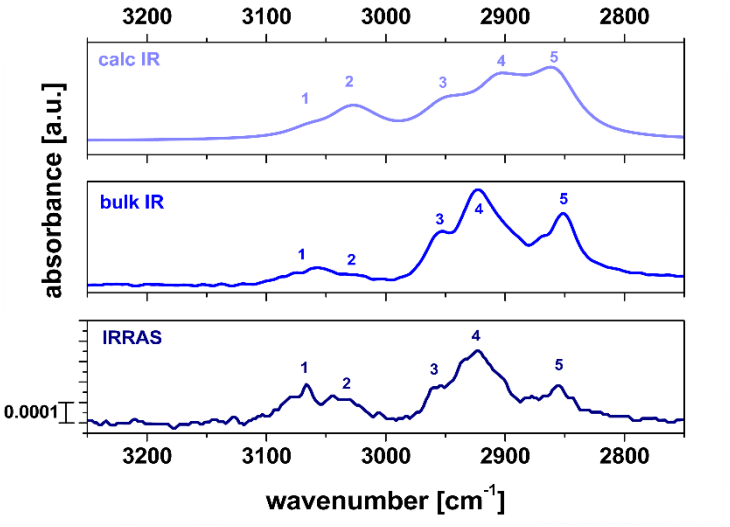

Figure S21. IR spectra of a monolayer of [Mo(CO)$_3$(TATA-P$_3$)] (**1**) on Au(111) from 3300 cm^{-1} to 2750 cm^{-1}.

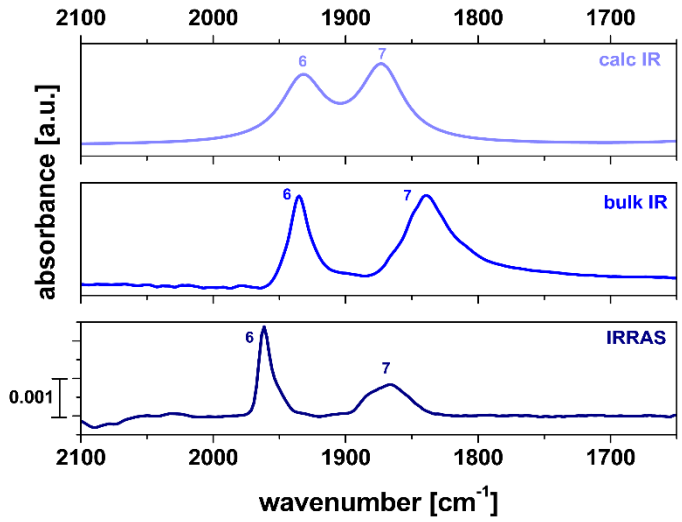

Figure S22. IR spectra of a monolayer of [Mo(CO)$_3$(TATA-P$_3$)] (**1**) on Au(111) from 2100 cm^{-1} to 1650 cm^{-1}.

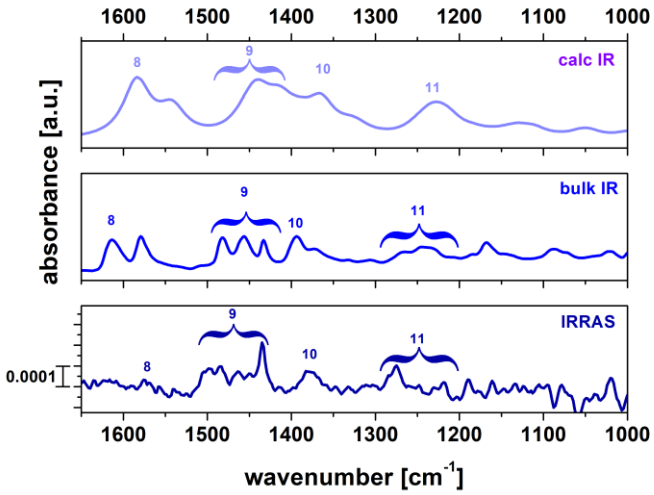

Figure S23. IR spectra of a monolayer of $[Mo(CO)_3(TATA\text{-}P_3)]$ (**1**) on Au(111) from 1650 cm^{-1} to 1000 cm^{-1}.

3. NEXAFS-Spectra

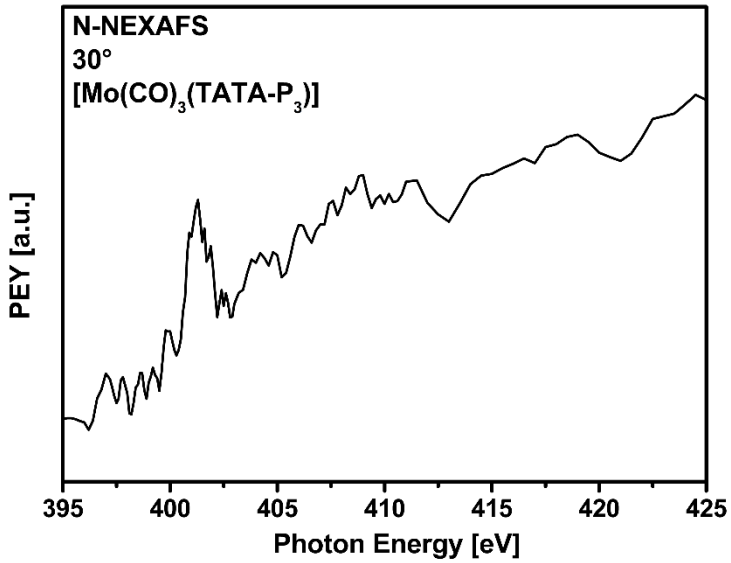

Figure S24. Original N K-edge NEXAFS spectrum of $[Mo(CO)_3(TATA\text{-}P_3)]$ (**1**) on Au(111) at 30°.

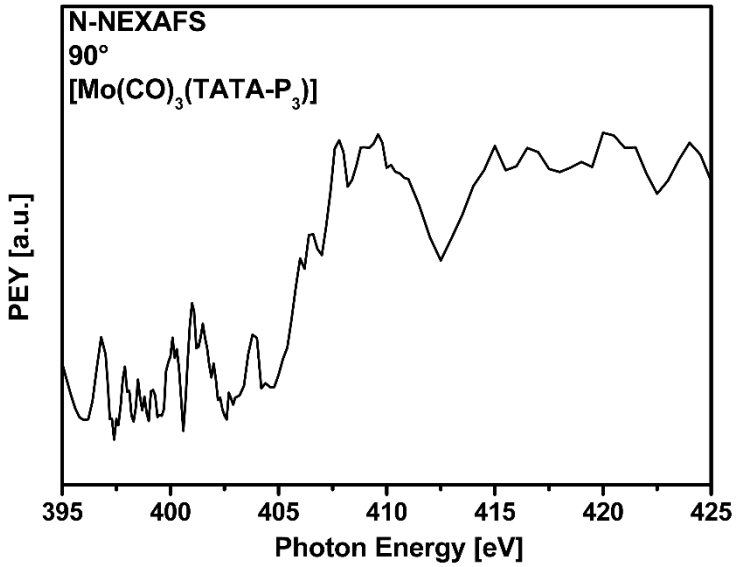

Figure S25. Original N K-edge NEXAFS spectrum of $[Mo(CO)_3(TATA\text{-}P_3)]$ (**1**) on Au(111) at 90°.

4. Theoretical Calculations

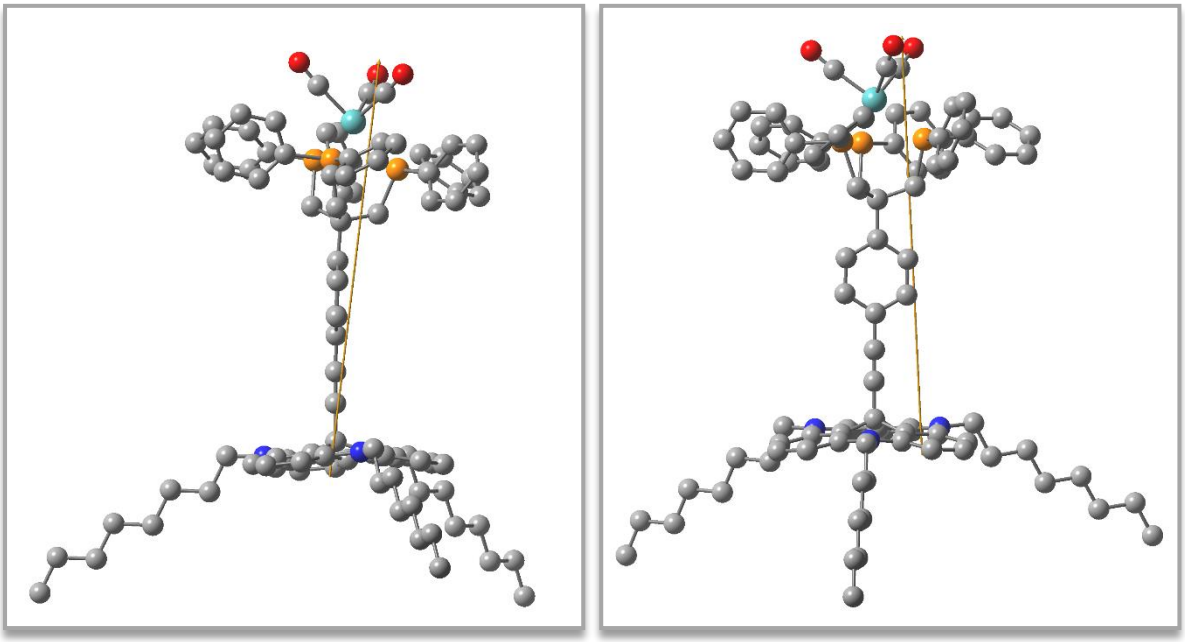

Figure S26. Resulting total TDM (yellow arrow) of the symmetric CO stretching vibration A_1 of $[Mo(CO)_3(TATA\text{-}P_3)]$ (**1**) in two different views; grey: C atoms, blue: N atoms, orange: P atoms, cyan: Mo atom and red: O atoms.

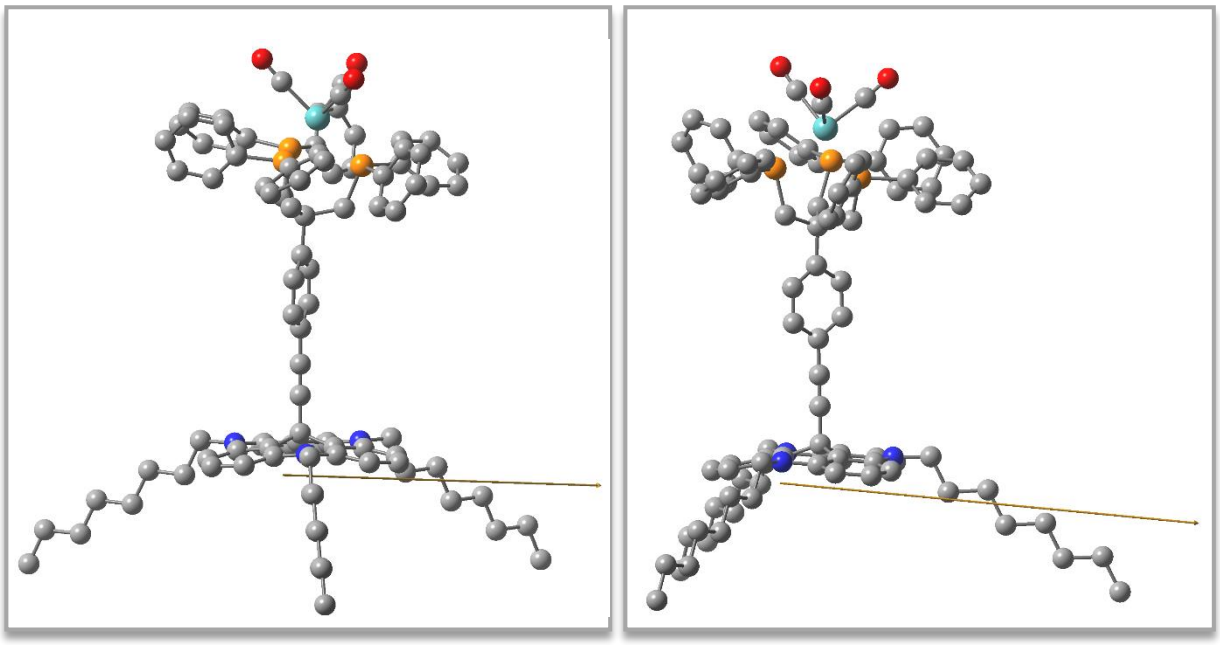

Figure S27. Resulting total TDM (yellow arrow) of the asymmetric CO stretching vibration E of [Mo(CO)$_3$(TATA-P$_3$)] (**1**) in two different views; grey: C atoms, blue: N atoms, orange: P atoms, cyan: Mo atom and red: O atoms.

5. XPS Fitting Parameter

Table S1: Fitting parameter for the XP spectra of the [Mo(CO)$_3$(TATA-P$_3$)] (**1**) monolayer on Au(111).

Component	Signal	Binding Energy (eV)	Area (%)	fwhm
Major	C 1s	284.3	77	1.1
Minor	C 1s	285.2	20	1.1
CO ligands	C 1s	286.9	3	1.1
TATA	N 1s	399.7	100	1.1
Phosphines	P 2p	131.2/132.6	100	1.9/1.9
Mo	Mo 2p	227.1/230.2	100	1.6/1.6

6. Detailed Vibrational Analysis

Table S2: A full vibrational analysis with vibration assignment is shown. The energies of calculated spectra were corrected by using the equation: $\nu_{corr.} = \nu_{calc.} \cdot 0.9788$.

Peak #	Mode No.	Calc. freq. uncorrected	Calc. freq. Corrected	Calc. Intensity	Bulk freq.	IRRAS freq.	TDM	Assignment
	1	910.0	890.7	4.87			⊥	C-H bending Ar-P
	2	911.4	892.0	4.60			⊥	C-H bending Ar-P
	3	912.2	892.8	1.00			/	C-H bending Ar-P
	4	913.9	894.5	3.44			⊥	C-H bending Ar-P
	5	921.4	901.8	0.80			∥	CH_2 bending chain
	6	922.3	902.7	1.01			/	CH_2 bending chain
	7	925.1	905.5	1.26			/	C-H bending Ar-P
	8	926.3	906.6	1.36			∥	C-H bending Ar-P
	9	926.5	906.8	0.01			∥	CH_2 bending chain
	10	927.4	907.7	1.35			∥	C-H bending Ar-P
	11	942.3	922.3	0.13			∥	CH_2 bending chain
	12	943.1	923.1	0.11			∥	CH_2 bending chain

	13	951.8	931.6	0.32			/	C-H bending Ar-TATA
	14	953.0	932.8	0.25			/	C-H bending Ar-TATA
	15	953.9	933.6	0.22			/	C-H bending Ar-TATA
	16	962.0	941.6	0.03			/	C-H bending Ar-Spacer
	17	968.0	947.4	0.42			/	C-H bending Ar-Spacer
	18	969.2	948.6	0.48			∥	C-H bending Ar-P
	19	969.6	949.0	0.14			/	C-H bending Ar-P
	20	970.3	949.7	0.46			∥	C-H bending Ar-P
	21	972.3	951.6	7.33			⊥	C-C-stretching chain
	22	976.3	955.6	0.04			∥	C-C-stretching chain
	23	976.8	956.1	0.09			∥	C-C-stretching chain
	24	976.8	956.1	1.74			∥	C-H bending Ar-P
	25	977.5	956.7	2.41			∥	C-H bending Ar-P
	26	978.1	957.3	1.45			∥	C-H bending Ar-P
	27	979.2	958.4	2.84			∥	C=C ring deformation Ar-P
	28	979.4	958.6	2.81			/	C=C ring deformation Ar-P
	29	979.8	959.0	0.23			∥	C=C ring deformation Ar-P
	30	980.9	960.1	0.57			∥	C=C ring deformation Ar-P
	31	981.0	960.2	1.68			∥	C=C ring deformation Ar-p
	32	981.3	960.5	1.14			∥	C=C ring deformation Ar-P
	33	985.3	964.4	2.40			⊥	C=C ring deformation Ar-Spacer
	34	987.6	966.6	0.82			⊥	C-C-stretching chain
	35	992.8	971.7	0.01			/	C-C-stretching chain
	36	993.0	971.9	0.01			∥	C-C-stretching chain
	37	994.4	973.3	0.00			∥	CH_2 bending chain
	38	994.9	973.8	0.14			/	C-H bend. Ar-P, C=C ring def. Ar-P
	39	995.3	974.2	0.10			/	C-H bend. Ar-P, C=C ring def. Ar-P
	40	995.9	974.7	0.11			/	C-H bend. Ar-P, C=C ring def. Ar-P
	41	1000.1	978.9	1.54			∥	C-H bend. Ar-P, C=C ring def. Ar-P
	42	1000.9	979.6	1.58			∥	C-H bend. Ar-P, C=C ring def. Ar-P
	43	1001.6	980.3	1.53			∥	C-H bend. Ar-P, C=C ring def. Ar-P
	44	1003.4	982.1	1.69			∥	CH_2 bending chain
	45	1003.5	982.2	30.93			⊥	C=C ring def. Ar-Spacer, $C_{q,TATA}$-C_{alk}-stretching
	46	1003.9	982.6	3.35			/	CH_2 bending chain
	47	1017.4	995.8	1.28			∥	C=C ring deformation Ar-P
	48	1018.4	996.8	6.32			/	CH_2-P bending, C=C ring deformation Ar-P
	49	1018.9	997.3	1.13			/	C=C ring deformation Ar-P
	50	1019.6	997.9	12.07			∥	C=C ring deformation Ar-P
	51	1020.0	998.3	7.96			∥	C=C ring deformation Ar-P
	52	1020.8	999.1	0.50			/	C=C ring deformation Ar-P
	53	1022.1	1000.4	4.85			/	CH_2-P bend., C=C ring deformation Ar-P
	54	1024.7	1002.9	0.00			∥	CH_2 bending chain
	55	1025.4	1003.6	15.27			∥	C-C_q (Tripod) stretching
	56	1026.5	1004.7	0.20			∥	C-C-stretching chain
	57	1027.7	1005.9	0.33			∥	C-C-stretching chain
	58	1028.1	1006.3	0.36			∥	C-C-stretching chain
13	59	1035.6	1013.6	2.41	1030-1010	1030-1010	⊥	C-C-stretching chain, N-C bending
	60	1035.6	1013.6	1.10			/	C-C-stretching chain, N-C bending
	61	1035.7	1013.7	1.40			/	C-C-stretching chain, N-C bending
	62	1046.8	1024.6	0.03			∥	C-C-stretching chain
13	63	1047.7	1025.4	0.07	1030-1010	1030-1010	/	C-C-stretching chain
	64	1049.2	1026.9	0.07			⊥	C-C-stretching chain
	65	1050.9	1028.6	0.24			/	C-C-stretching chain
	66	1051.5	1029.2	0.20			∥	C-C-stretching chain
13	67	1052.6	1030.2	0.15	1030-1010	1030-1010	/	C-C-stretching chain
	68	1063.3	1040.7	14.56			∥	C-H bending Ar-P
	69	1065.0	1042.4	13.19			∥	C-H bending Ar-P
	70	1067.7	1045.0	6.77			∥	C-H bending Ar-P
13	71	1071.4	1048.6	3.89	1030-1010	1030-1010	⊥	C-H bending Ar-P
	72	1072.7	1049.9	2.16			⊥	C-H bending Ar-P, C-P stretching
	73	1073.2	1050.4	12.29			∥	C-H bending Ar-P, C-P stretching
	74	1073.6	1050.8	4.10			∥	C-H bending Ar-P, C-P stretching
	75	1074.4	1051.6	3.55			/	C-H bending Ar-P
	76	1074.8	1052.0	3.40			∥	C-H bending Ar-P
	77	1076.9	1054.0	6.04			⊥	Calk-C_q TATA, C-N-stretching

	78	1077.6	1054.7	13.31			‖	C-P stretching
	79	1078.9	1056.0	11.42			‖	C-P stretching
	80	1079.9	1057.0	9.33			/	C-P stretching
	81	1096.1	1072.8	0.15			/	C-H bending Ar-TATA
	82	1099.3	1076.0	0.25			‖	C-H bending Ar-TATA
	83	1102.3	1078.9	0.04			/	C-H bending Ar-TATA
	84	1104.5	1081.0	5.27			‖	CH_3 bending chain
	85	1104.9	1081.4	1.02			/	C-H bending Ar-Spacer
	86	1105.0	1081.5	5.62			‖	CH_3 bending chain
	87	1106.2	1082.7	0.29			‖	CH_2-P bending
	88	1107.6	1084.1	0.21			⊥	CH bending Ar-TATA
	89	1132.9	1108.8	20.63			‖	CH_2 bending chain
	90	1134.2	1110.1	15.81			‖	CH_2 bending chain
	91	1135.1	1111.0	37.16			‖	CH_2 bending chain
	92	1140.2	1116.0	0.42			⊥	C-H bending Ar-P
	93	1140.5	1116.3	0.36			/	C-H bending Ar-P
	94	1140.7	1116.5	0.42			/	C-H bending Ar-P
	95	1142.1	1117.8	0.03			‖	C-H bending Ar-P
	96	1142.2	1117.9	0.02			⊥	C-H bending Ar-P
	97	1142.4	1118.1	0.09			/	C-H bending Ar-P
	98	1147.0	1122.6	4.10			/	C_q-C_{Ar}-Spacer stretching
	99	1153.3	1128.8	31.24			‖	C-H bending Ar-TATA
	100	1154.3	1129.8	32.89			‖	C-H bending Ar-TATA
	101	1157.9	1133.3	2.43			‖	C-H bending Ar-P
	102	1159.5	1134.9	2.55			/	C-H bending Ar-P
	103	1161.8	1137.1	3.50			/	C-H bending Ar-P
	104	1162.3	1137.6	2.17			/	C-H bending Ar-Spacer
	105	1163.3	1138.6	2.77			‖	C-H bending Ar-P
	106	1165.4	1140.6	2.25			/	C-H bending Ar-P
	107	1165.9	1141.1	1.68			/	C-H bending Ar-P
	108	1166.5	1141.7	0.47			‖	CH_2 bending chain
	109	1167.7	1142.9	6.69			‖	CH_2 bending chain
	110	1168.5	1143.7	8.26			‖	CH_2 bending chain
	111	1169.4	1144.6	4.14			⊥	C-H bending Ar-Spacer
	112	1169.9	10932.7	0.89			‖	C-H bending Ar-TATA
	113	1174.6	1149.6	6.57			/	CH_2-P bending
	114	1182.3	1157.2	2.05			‖	C-H bending Ar-TATA
	115	1182.8	1157.7	1.37			‖	C-H bending Ar-TATA
12	116	1187.4	1162.2	3.64	1167	1162.0	/	CH_2 bending chain
	117	1187.7	1162.5	10.78			/	CH_2-P bending
	118	1188.7	1163.5	3.54			/	CH_2 bending chain
	119	1189.5	1164.2	3.76			/	CH_2 bending chain
	120	1207.0	1181.4	0.87			‖	CH_2 bending chain
	121	1208.5	1182.8	21.46			‖	CH_2 bending chain
	122	1209.4	1183.7	23.68			‖	CH_2 bending chain
	123	1225.8	1199.8	0.24			‖	CH_2-P bending
11	124	1226.9	1200.8	1.30	1290-1200	1290-1200	/	CH_2-P bending
	125	1230.4	1204.3	11.00			‖	CH_2 bending chain
	126	1231.3	1205.1	13.10			‖	CH_2 bending chain
	127	1233.6	1207.4	3.17			‖	CH_2 bending chain
	128	1239.1	1212.8	40.06			‖	CH_2 bending chain, C-H bending Ar-TATA
	129	1239.9	1213.6	39.33			‖	CH_2 bending chain
	130	1244.4	1218.0	3.62			‖	CH_2 bending chain
11	131	1244.7	1218.3	16.00	1290-1200	1290-1200	⊥	CH_2-P bending
	132	1247.2	1220.7	33.02			‖	CH_2 bending chain
	133	1247.7	1221.2	41.06			‖	C_q=C stretching TATA, N-C-stretching
	134	1259.0	1232.3	84.25			‖	C_q=C stretching TATA, N-C-stretching
	135	1259.8	1233.0	84.16			‖	C_q=C stretching TATA, N-C-stretching
11	136	1268.6	1241.7	0.76	1290-1200	1290-1200	/	CH_2 bending chain
	137	1270.5	1243.5	18.63			⊥	C-H bending Ar-Spacer
	138	1271.5	1244.5	1.25			‖	CH_2 bending chain
	139	1272.3	1245.3	1.13			‖	CH_2 bending chain
	140	1272.6	1245.6	2.72			‖	C-H bending Ar-P

11	141	1273.1	1246.1	1.42			/	CH_2 bending chain
	142	1273.4	1246.4	20.53			⊥	C-H bending Ar-Spacer
	143	1274.2	1247.1	7.96	1290-1200	1290-1200	/	C-H bending Ar-P
	144	1276.1	1249.0	3.04			⊥	CH_2 bending chain
	145	1276.4	1249.3	1.42			⊥	CH_2 bending chain
	146	1277.0	1249.9	10.90			⊥	C-H bending Ar-P
	147	1277.6	1250.5	0.01			‖	CH_2 bending chain
11	148	1280.3	1253.1	0.93			/	CH_2 bending chain
	149	1280.3	1253.1	4.95	1290-1200	1290-1200	/	C-H bending Ar-P
	150	1280.6	1253.4	2.70			/	C-H bending Ar-P
	151	1280.9	1253.7	0.75			‖	CH_2 bending chain
11	152	1282.0	1254.8	1.11	1290-1200	1290-1200	/	CH_2 bending chain
	153	1282.6	1255.4	4.08			⊥	C-H bending Ar-P
	154	1282.6	1255.4	0.21			‖	CH_2 bending chain
11	155	1284.1	1256.8	0.12	1290-1200	1290-1200	/	CH_2 bending chain
	156	1284.5	1257.2	0.03			‖	CH_2 bending chain
11	157	1286.3	1259.0	0.45			/	CH_2 bending chain
	158	1287.0	1259.7	1.94	1290-1200	1290-1200	⊥	CH_2 bending chain
	159	1287.8	1260.4	0.57			/	CH_2 bending chain
	160	1320.1	1292.1	3.64			‖	C=C ring deformation Ar-Spacer
11	161	1321.5	1293.4	0.72			/	CH_2 bending chain
	162	1323.0	1294.9	0.60	1290-1200	1290-1200	/	CH_2 bending chain
	163	1324.6	1296.5	0.84			/	CH_2 bending chain
	164	1333.2	1304.9	0.02			‖	CH_2 bending chain
	165	1347.9	1319.3	16.66			‖	CH_2 bending chain
	166	1349.1	1320.4	16.41			‖	CH_2 bending chain
	167	1350.8	1322.1	8.47			‖	CH_2 bending chain
	168	1351.0	1322.3	2.33			/	C=C ring deformation Ar-P
	169	1351.1	1322.4	2.03			/	C=C ring deformation Ar-P
	170	1351.4	1322.7	2.00			/	C=C ring deformation Ar-P
	171	1354.7	1325.9	0.53			‖	C=C ring deformation Ar-P
	172	1354.9	1326.1	0.33			/	C=C ring deformation Ar-P
	173	1355.1	1326.3	7.88			/	CH_3 bending chain
	174	1355.4	1326.6	0.60			/	C=C ring deformation Ar-P
	175	1355.6	1326.8	11.52			/	CH_3 bending chain
	176	1356.8	1328.0	8.70			/	CH_3 bending chain
	177	1358.0	1329.2	20.51			‖	CH_2 bending chain
	178	1358.9	1330.0	11.63			‖	CH_2 bending chain
	179	1359.1	1330.2	3.00			‖	CH_2 bending chain
	180	1360.9	1332.0	7.14			/	CH_2 bending chain
	181	1361.4	1332.5	0.12			‖	CH_2 bending chain
	182	1362.3	1333.4	0.05			/	CH_2 bending chain
	183	1367.7	1338.7	3.32			‖	C=C stretching Ar-TATA
	184	1368.3	1339.2	3.16			‖	C=C stretching Ar-TATA
	185	1373.9	1344.7	0.26			‖	C=C stretching Ar-TATA
	186	1374.7	1345.5	1.40			/	CH_2 bending chain
	187	1380.7	1351.4	1.11			‖	CH_2 bending chain
	188	1393.6	1364.0	146.62			‖	C-N-stretching
	189	1394.5	1364.9	147.53			‖	C-N stretching
10	190	1400.8	1371.0	7.95			⊥	CH_2 bending chain
	191	1404.2	1374.4	5.23	1410-1345	1405-1350	/	C-H bending Ar-Spacer
	192	1413.1	1383.1	0.14			⊥	CH_2 bending chain
	193	1413.3	1383.3	0.16			⊥	CH_2 bending chain
	194	1413.3	1383.3	0.28			/	CH_2 bending chain
	195	1414.0	1384.0	0.40			/	CH_2 bending chain
	196	1414.3	1384.3	0.66			/	CH_2 bending chain
	197	1414.4	1384.4	0.92			/	CH_2 bending chain
10	198	1417.2	1387.1	32.06	1410-1345	1405-1350	⊥	C-H bending Ar-P
10	199	1417.5	1387.4	11.28			/	C-H bending Ar-P
	200	1417.6	1387.5	0.10			‖	CH_2 bending chain
	201	1417.6	1387.5	4.86			‖	CH_2 bending chain
	202	1417.6	1387.5	3.90			/	CH_2 bending chain
10	203	1417.6	1387.5	0.10	1410-1345	1405-1350	/	CH_2 bending chain
	204	1419.9	1389.7	8.05			‖	C-H bending Ar-P
	205	1420.0	1389.8	8.13			‖	C-H bending Ar-P
10	206	1420.7	1390.5	5.64	1410-1345	1405-1350	⊥	C-H bending Ar-P

	207	1422.5	1392.3	6.42			‖	CH_3, CH_2 bending chain
10	208	1422.9	1392.7	4.67	1410-1345	1405-1350	/	CH_3, CH_2 bending chain
	209	1423.2	1393.0	7.30			‖	CH_3 bending chain
10	210	1423.3	1393.1	4.86	1410-1345	1405-1350	/	CH_2 bending chain
	211	1424.0	1393.8	6.57			‖	CH_3 bending chain
	212	1424.7	1394.4	6.58			‖	CH_3 bending chain
	213	1426.5	1396.2	1.97			‖	CH_2 bending chain
	214	1428.5	1398.2	5.48			‖	CH_2 bending chain
	215	1429.2	1398.8	2.22			/	CH_2 bending chain
	216	1431.1	1400.7	1.54			/	CH_2 bending chain
	217	1432.8	1402.4	0.07			‖	CH_2 bending chain
	218	1433.2	1402.8	1.26			/	CH_2 bending chain
	219	1433.4	1403.0	0.68			/	CH_2 bending chain
	220	1437.4	1406.9	7.98			/	CH_2 bending chain
	221	1438.7	1408.1	6.11			‖	CH_2 bending chain
	222	1439.4	1408.8	4.38			‖	CH_2 bending chain
9	223	1441.1	1410.5	7.22	1520-1415	1520-1415	⊥	CH_2 bending chain
	224	1442.4	1411.8	15.69			/	CH_2 bending chain
	225	1443.4	1412.7	19.49			/	CH_2 bending chain
	226	1444.0	1413.3	94.35			‖	C-H bending Ar-TATA
	227	1446.0	1415.3	103.16			‖	C-H bending Ar-TATA
	228	1456.9	1426.0	7.37			‖	C-H bending Ar-P
	229	1458.6	1427.6	6.95			‖	C-H bending Ar-P
	230	1459.0	1428.0	8.23			‖	C-H bending Ar-P
	231	1460.9	1429.9	13.11			‖	C-H bending Ar-P
	232	1461.4	1430.4	13.38			‖	C-H bending Ar-P
9	233	1461.7	1430.7	3.31	1520-1415	1520-1415	/	C-H bending Ar-P
	234	1473.1	1441.8	168.94			‖	C=C stretching Ar-TATA
	235	1473.2	1441.9	165.77			‖	C=C stretching Ar-TATA
9	236	1485.5	1453.9	104.93	1520-1415	1520-1415	⊥	C=C stretching Ar-C_{alkyne}-Spacer
	237	1495.2	1463.4	6.75			⊥	C=C stretching Ar-TATA
	238	1541.0	1508.3	0.93			/	C=C stretching Ar-Spacer
	239	1574.5	1541.1	125.75			‖	C=C stretching Ar-TATA
	240	1575.5	1542.0	94.67			‖	C=C stretching Ar-TATA
	241	1575.7	1542.2	34.09			‖	C=C stretching Ar-TATA
	242	1576.4	1542.9	0.58			‖	C=C stretching Ar-P
	243	1576.6	1543.1	0.52			/	C=C stretching Ar-P
	244	1577.0	1543.5	0.62			/	C=C stretching Ar-P
	245	1579.6	1546.1	1.70			‖	C=C stretching Ar-P
	246	1579.8	1546.2	1.28			‖	C=C stretching Ar-P
	247	1580.4	1546.8	1.33			‖	C=C stretching Ar-P
	248	1590.9	1557.1	0.21			/	C=C stretching Ar-P
	249	1591.1	1557.3	0.40			/	C=C stretching Ar-P
	250	1591.2	1557.4	0.18			‖	C=C stretching Ar-P
	251	1592.4	1558.6	5.99			‖	C=C stretching Ar-P
	252	1592.5	1558.7	4.63			‖	C=C stretching Ar-P
	253	1592.8	1559.0	1.19			‖	C=C stretching Ar-P
	254	1594.4	1560.5	0.21			⊥	C=C stretching Ar-TATA
8	255	1610.1	1575.9	5.84	1578	1577	⊥	C=C stretching Ar-Spacer
	256	1618.1	1583.7	267.88			‖	C=C stretching Ar-TATA
	257	1618.9	1584.5	273.40			‖	C=C stretching Ar-TATA
	258	1912.3	1871.7	704.20			‖	CO stretching asym., out of phase
7	259	1914.4	1873.7	703.02	1838	1869	‖-/	CO stretching asym., out of phase
6	260	1974.4	1932.5	1184.11	1935	1961	⊥	CO stretching sym., in phase
	261	2238.3	2190.8	11.50			⊥	CC stretching alkyne
5	262	2901.5	2839.9	5.76	2875-2830	2875-2830	/	CH_2 stretching sym. chain
	263	2901.5	2839.9	7.35			/	CH_2 stretching sym. chain
	264	2901.7	2840.1	7.76			/	CH_2 stretching sym. chain
	265	2903.3	2841.6	0.85			/	CH_2 stretching sym. chain
	266	2903.4	2841.7	0.63			/	CH_2 stretching sym. chain
	267	2903.7	2842.0	0.81			/	CH_2 stretching sym. chain
	268	2906.1	2844.4	1.12			/	CH_2 stretching sym. chain
	269	2906.3	2844.6	1.24			/	CH_2 stretching sym. chain
	270	2906.3	2844.6	1.41			/	CH_2 stretching sym. chain
	271	2913.9	2852.0	26.53			/	CH_2 stretching sym. chain
	272	2914.2	2852.3	27.90			/	CH_2 stretching sym. chain

	273	2914.4	2852.5	30.59			/	CH_2 stretching sym. chain
	274	2919.5	2857.5	42.43			/	CH_2 stretching sym. chain
	275	2919.5	2857.5	118.79			/	CH_2 stretching sym. chain
	276	2920.1	2858.1	88.10			/	CH_2 stretching sym. chain
	277	2931.7	2869.4	32.76			⊥	CH_3 stretching sym. chain
	278	2931.8	2869.5	40.59			⊥	CH_3 stretching sym. chain
	279	2931.9	2869.6	40.85			⊥	CH_3 stretching sym. chain
	280	2932.5	2870.2	0.57			‖	CH_2 stretching asym. chain
	281	2933.1	2870.8	0.58			/	CH_2 stretching asym. chain
	282	2933.4	2871.1	0.60			‖	CH_2 stretching asym. chain
	283	2936.5	2874.1	4.50			⊥	CH_2 stretching sym. chain
	284	2936.7	2874.3	1.90			/	CH_2 stretching asym. chain
	285	2937.1	2874.7	1.92			‖	CH_2 stretching asym. chain
	286	2937.2	2874.8	1.98			‖	CH_2 stretching asym. chain
	287	2938.2	2875.8	3.27			⊥	CH_2 stretching sym. chain
	288	2938.7	2876.3	2.19			/	CH_2 stretching sym. chain
	289	2947.6	2885.0	0.53			‖	CH_2 stretching asym. chain
	290	2947.6	2885.0	0.58			‖	CH_2 stretching asym. chain
	291	2947.6	2885.0	0.58			‖	CH_2 stretching asym. chain
	292	2950.7	2888.0	47.63			/	CH_2 stretching sym. chain
	293	2952.3	2889.6	45.50			/	CH_2 stretching sym. chain
	294	2952.6	2889.9	49.70			/	CH_2 stretching sym. chain
	295	2961.1	2898.2	0.19			‖	CH_2 stretching asym. chain
	296	2961.2	2898.3	0.24			‖	CH_2 stretching asym. chain
	297	2961.5	2898.6	0.25			‖	CH_2 stretching asym. chain
	298	2965.4	2902.4	4.59			‖	CH_2-P stretching sym.
4	299	2966.4	2903.40	12.97	2922	2923	⊥	CH_2-P stretching sym.
	300	2969.8	2906.7	70.44			‖	CH_2 stretching asym. chain
	301	2970.1	2907.0	73.81			‖	CH_2 stretching asym. chain
	302	2970.5	2907.4	81.81			‖	CH_2 stretching asym. chain
4	303	2978.3	2915.00	5.91	2922	2923	/	CH_2-P stretching sym.
	304	2978.6	2915.3	13.43			‖	CH_2 stretching asym. chain
	305	2979.1	2915.8	10.34			‖	CH_2 stretching asym. chain
	306	2979.5	2916.2	7.06			‖	CH_2 stretching asym. chain
	307	2996.5	2932.9	17.68			‖	CH_2 stretching asym. chain
	308	2997.2	2933.5	21.08			‖	CH_2 stretching asym. chain
	309	2997.5	2933.8	33.30			‖	CH_2 stretching asym. chain
	310	3012.2	2948.2	32.85			‖	CH_3 stretching asym. chain
	311	3012.4	2948.4	22.35			‖	CH_3 stretching asym. chain
	312	3012.4	2948.4	46.74			‖	CH_3 stretching asym. chain
3	313	3021.5	2957.3	0.81			/	CH_2-P stretching asym.
	314	3021.7	2957.5	28.14	2960	2959	/	CH_3 stretching asym. chain
	315	3022.2	2958.0	27.98			‖-/	CH_3 stretching asym. chain
	316	3022.4	2958.2	27.42			‖	CH_3 stretching asym. chain
	317	3026.2	2961.9	1.28			‖	CH_2-P stretching asym.
3	318	3028.8	2964.5	1.78	2960	2959	/	CH_2-P stretching asym.
	319	3070.1	3004.9	0.14			/	C-H stretching Ar-P
	320	3070.4	3005.2	0.13			‖	C-H stretching Ar-P
	321	3071.3	3006.1	0.07			‖	C-H stretching Ar-P
	322	3073.4	3008.1	16.00			‖	C-H stretching Ar-Spacer, Ar-P
	323	3074.5	3009.2	1.31			‖	C-H stretching Ar-P
	324	3074.6	3009.3	0.99			/	C-H stretching Ar-P
	325	3074.8	3009.5	3.98			/	C-H stretching Ar-P, Ar-spacer
	326	3079.7	3014.3	1.69			/	C-H stretching Ar-P
	327	3080.3	3014.9	1.77			/	C-H stretching Ar-P
	328	3080.9	3015.5	1.72			‖	C-H stretching Ar-P
	329	3081.5	3016.1	0.33			‖	C-H stretching Ar-P
2	330	3081.5	3016.1	0.21	3060-2997	3055-2997	/	C-H stretching Ar-P
	331	3081.7	3016.2	0.51			/	C-H stretching Ar-P
	332	3083.2	3017.7	11.94			‖	C-H stretching Ar-TATA
	333	3084.0	3018.5	12.82			‖	C-H stretching Ar-TATA
	334	3084.2	3018.7	7.93			‖	C-H stretching Ar-TATA
2	335	3087.2	3021.6	6.55	3060-2997	3055-2997	/	C-H stretching Ar-P
	336	3087.6	3022.0	5.97			/	C-H stretching Ar-P
	337	3088.0	3022.4	6.92			/	C-H stretching Ar-P
	338	3089.4	3023.8	13.76			/	C-H stretching Ar-P
	339	3089.5	3023.9	14.00			/	C-H stretching Ar-P
	340	3089.7	3024.1	13.07			/	C-H stretching Ar-P
	341	3092.6	3026.9	4.84			⊥	C-H stretching Ar-Spacer

	342	3094.7	3029.0	7.71			/	C-H stretching Ar-P
	343	3094.9	3029.2	12.90			⊥	C-H stretching Ar-P
	344	3095.2	3029.4	9.17			/-⊥	C-H stretching Ar-P
	345	3098.6	3032.8	19.31			‖	C-H stretching Ar-P
	346	3098.8	3033.0	16.89			‖	C-H stretching Ar-P
	347	3099.2	3033.4	16.11			‖	C-H stretching Ar-P
	348	3101.0	3035.1	4.93			‖	C-H stretching Ar-Spacer
	349	3102.1	3036.2	11.03			‖	C-H stretching Ar-P
	350	3102.3	3036.4	17.54			‖	C-H stretching Ar-P
	351	3102.4	3036.5	5.22			‖	C-H stretching Ar-P
	352	3109.6	3043.6	3.08			/	C-H stretching Ar-TATA
	353	3126.7	3060.3	3.28			‖	C-H stretching Ar-TATA
	354	3127.4	3061.0	15.16			‖	C-H stretching Ar-TATA
	355	3130.0	3063.5	4.54			‖	C-H stretching Ar-TATA
	356	3130.7	3064.2	11.30			‖	C-H stretching Ar-TATA
1	357	3131.0	3064.5	5.36	3100-3067	3091-3055	/	C-H stretching Ar-TATA
	358	3133.2	3066.7	5.55			/	C-H stretching Ar-TATA
	359	3133.2	3066.7	4.45			‖	C-H stretching Ar-P
	360	3136.9	3070.3	5.55			‖	C-H stretching Ar-P
	361	3137.3	3070.7	4.61			‖	C-H stretching Ar-P