

Supporting Information

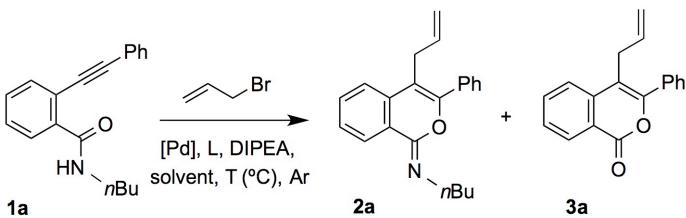
On the Regiochemical Differences between Pd-Catalyzed Heterocyclization-Allylation and -Arylation Reactions of Alkynylbenzamides: Preparation of 4-Allyl-isochromen-1-imines and Computational Study

Rosana Álvarez, Unai Vilar, Youssef Madich and José M. Aurrecoechea

Table of contents

	<u>Page</u>
- Table S1. Survey of reaction conditions for Pd-catalyzed heterocyclization-allylation of alkynylbenzamides	S2
- Figure S1. Energy reaction profiles for the allylation pathway	S3
- Figure S2. Energy reaction profile for the arylation pathway	S4
- Fig. S3. ORTEP diagram of 2a	S5
- Copies of ^1H NMR and ^{13}C NMR spectra for new compounds	S6-S24
- Computational data	S25-S69

Table S1. Survey of reaction conditions for Pd-catalyzed heterocyclization-allylation of alkynylbenzamides^a



Entry	[Pd], L	Solvent	T (°C) ^b	t (h)	2a (%)	3a (%)
1	PdCl ₂	DMF	120	16	24	28
2	PdCl ₂ (PPh ₃) ₂	DMF	120	16	13	36
3	Pd(OAc) ₂	DMF	120	16	14	34
4	Pd(OAc) ₂ , PPh ₃	DMF	120	16	10	45
5	Pd(PPh ₃) ₄	DMF	120	16	14	49
6 ^c	Pd(PPh ₃) ₄	1,4-dioxane	100	16	43	5
7	Pd(PPh ₃) ₄	MeCN	100	16	^d	^d
8 ^e	Pd(PPh ₃) ₄	Toluene	120	16	40	1.5
9 ^f	PdCl ₂ (PPh ₃) ₂	Toluene	120	16	29	-
10	Pd ₂ (dba) ₃ , PPh ₃	Toluene	120	23	62 ^g	-
11 ^h	Pd ₂ (dba) ₃ , PPh ₃	Toluene	120	20	58	-
12	Pd ₂ (dba) ₃	Toluene	120	19	73 ^g	-
13 ⁱ	Pd ₂ (dba) ₃	Toluene	120	20	66	-
14 ^j	Pd ₂ (dba) ₃	Toluene	120	26	47	-
15 ^k	Pd ₂ (dba) ₃	Toluene	120	19	39 ^g	-

^a Unless otherwise indicated, reactions were run using a Pd complex [Pd] (5 mol%), PPh₃ (where indicated, 10 mol%), DIPEA (1 equiv) and allyl bromide (5 equiv) under an Ar atmosphere. Yields were determined in the crude product by ¹H NMR using an internal standard. ^b Oil bath temperature. ^c 31% recovered starting material. ^d 91% recovered starting material. ^e Formation of Pd black, 40% recovered starting material. ^f Formation of Pd black, 49% recovered starting material. ^g Isolated yield. ^h Reaction run with 2,6-lutidine (1 equiv) instead of DIPEA. ⁱ Reaction run in the presence of ⁷Bu₄NBr (1 equiv). ^j Reaction run with 2 equiv of allyl bromide. ^k Reaction run under an air atmosphere.

The formation of lactone **3a**¹ was particularly prominent in DMF (entries 1-5), but this was minimized with the use of toluene as solvent (entries 8-15). Pd₂(dba)₃ as catalyst in toluene provided the best yield of the allylated isochromenimine **2a** (entry 12), while the use of a Pd(II) precatalyst or running the reaction under an air atmosphere led to poor results (entries 9 and 15, respectively). A gradual deposition of Pd black was generally observed in toluene, which was avoided with the use of ⁷Bu₄NBr as additive, albeit with some loss of yield (entry 13). Decreasing the amount of allyl bromide from the standard five to two equivalents had a negative impact on the yield of **2a** (entry 14).

¹ Y. L. Shi, K. E. Roth, S. D. Ramgren, S. A. Blum, *J. Am. Chem. Soc.* 2009, **131**, 18022-18023.

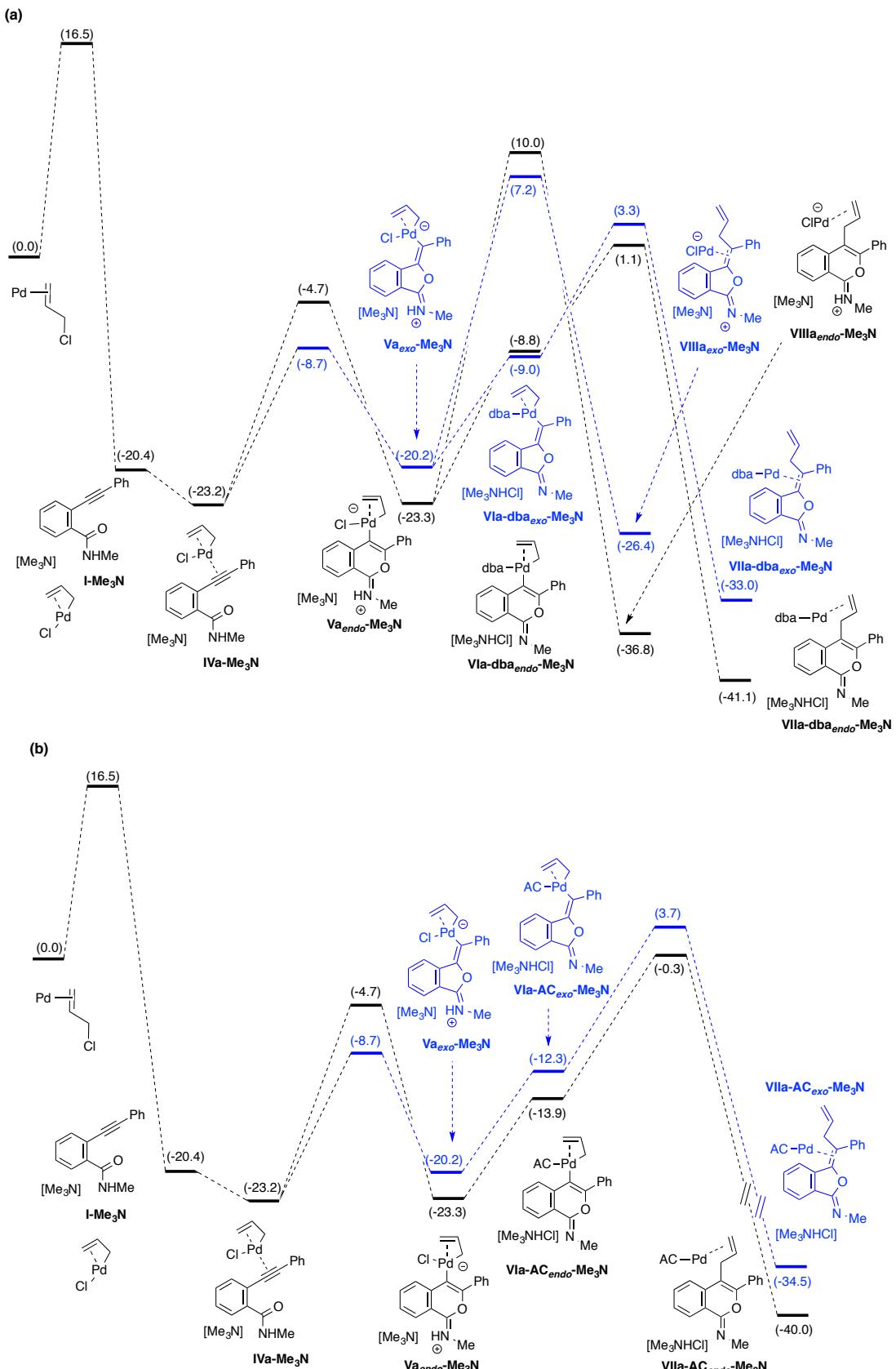


Figure S1. (a) Energy reaction profile (toluene) for the **I** to **VIIa-dba** allylation pathway in the presence of Me_3N . (b) Energy reaction profile (toluene) for the **I** to **VIIa-AC** ($\text{AC} = \text{allyl chloride}$) allylation pathway in the presence of Me_3N . Relative Gibbs free energies are given in kcal/mol (wB97XD/LANL2DZ/6-31G*(SMD, toluene)//wB97XD/LANL2DZ/6-31G* energies)

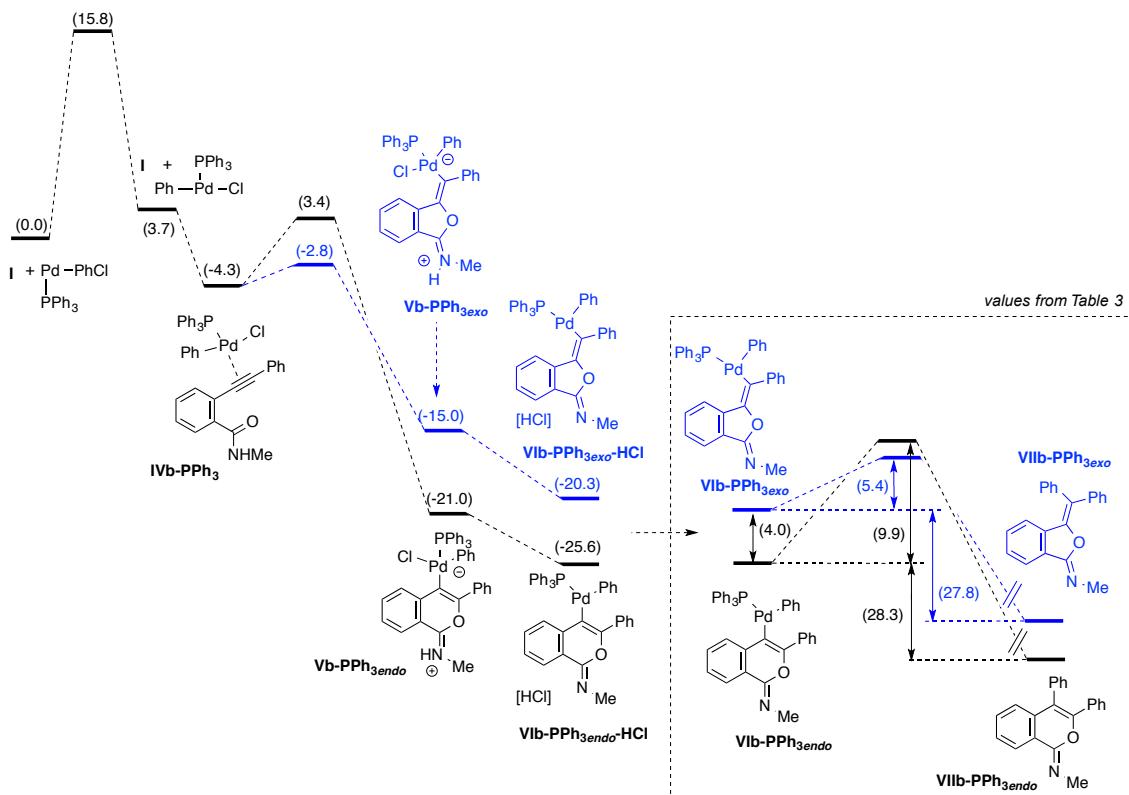


Figure S2. Energy reaction profile (acetonitrile) for the **I** to **VIIb-PPh₃** arylation pathway. Relative Gibbs free energies are given in kcal/mol (wB97XD/LANL2DZ/6-31G*(SMD, CH₃CN)/wB97XD/LANL2DZ/6-31G* energies)

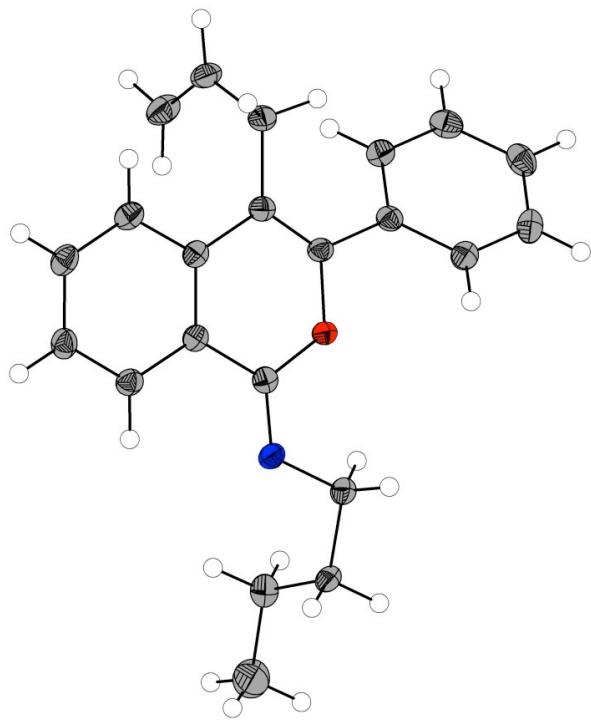
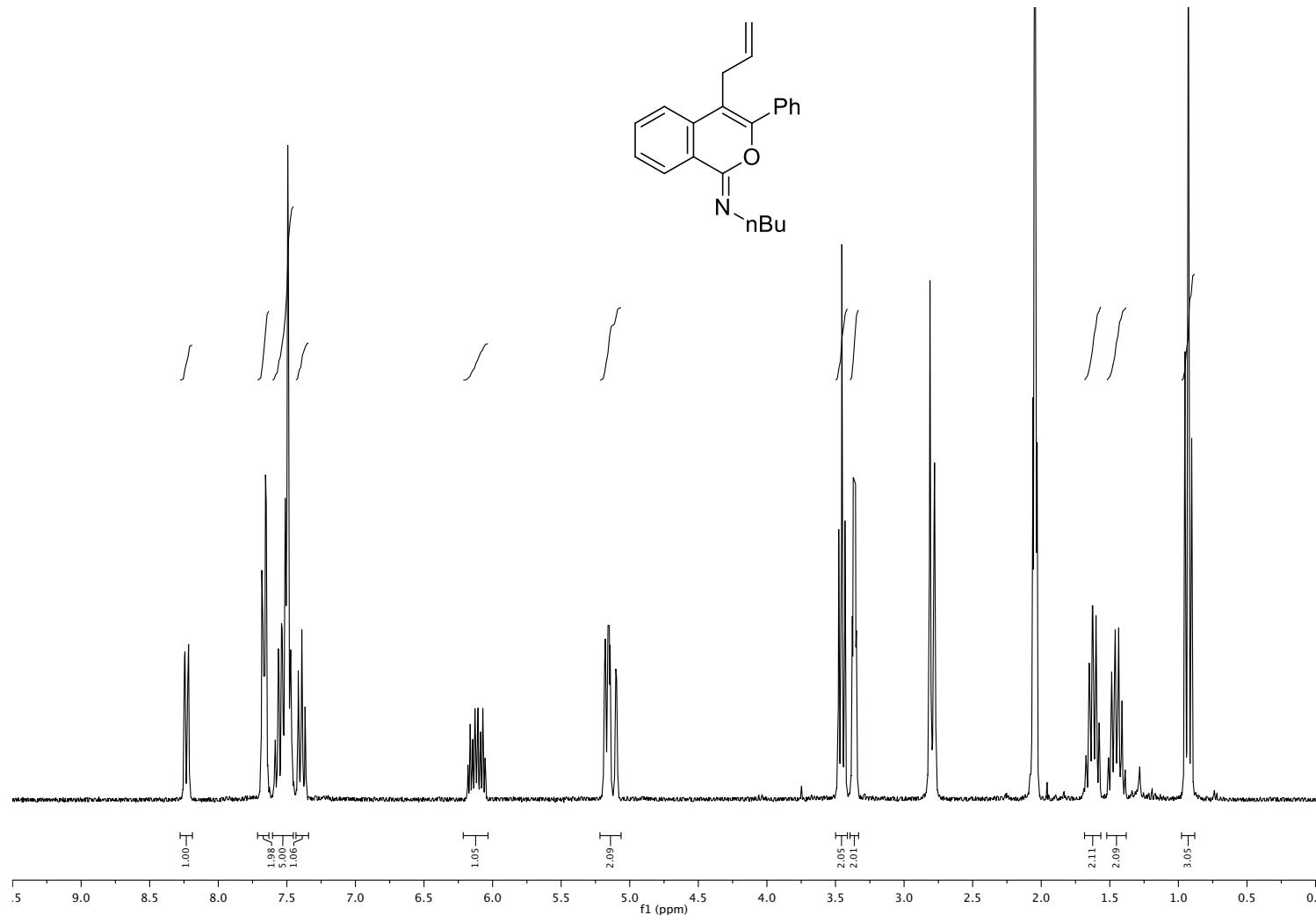


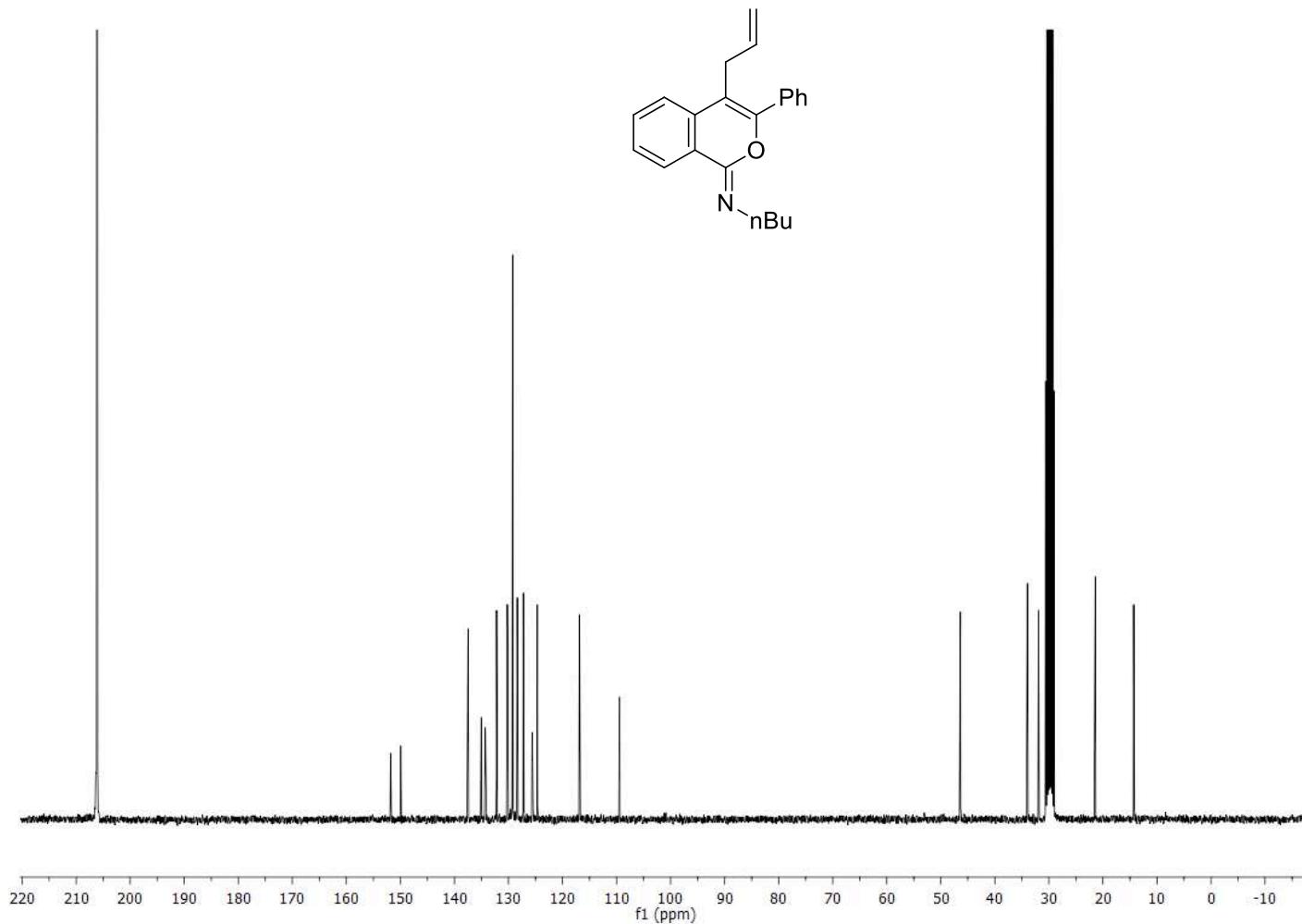
Figure S3. ORTEP diagram of **2a** with thermal ellipsoids at 50% probability. CCDC 1545290 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Copies of ^1H NMR and ^{13}C NMR spectra

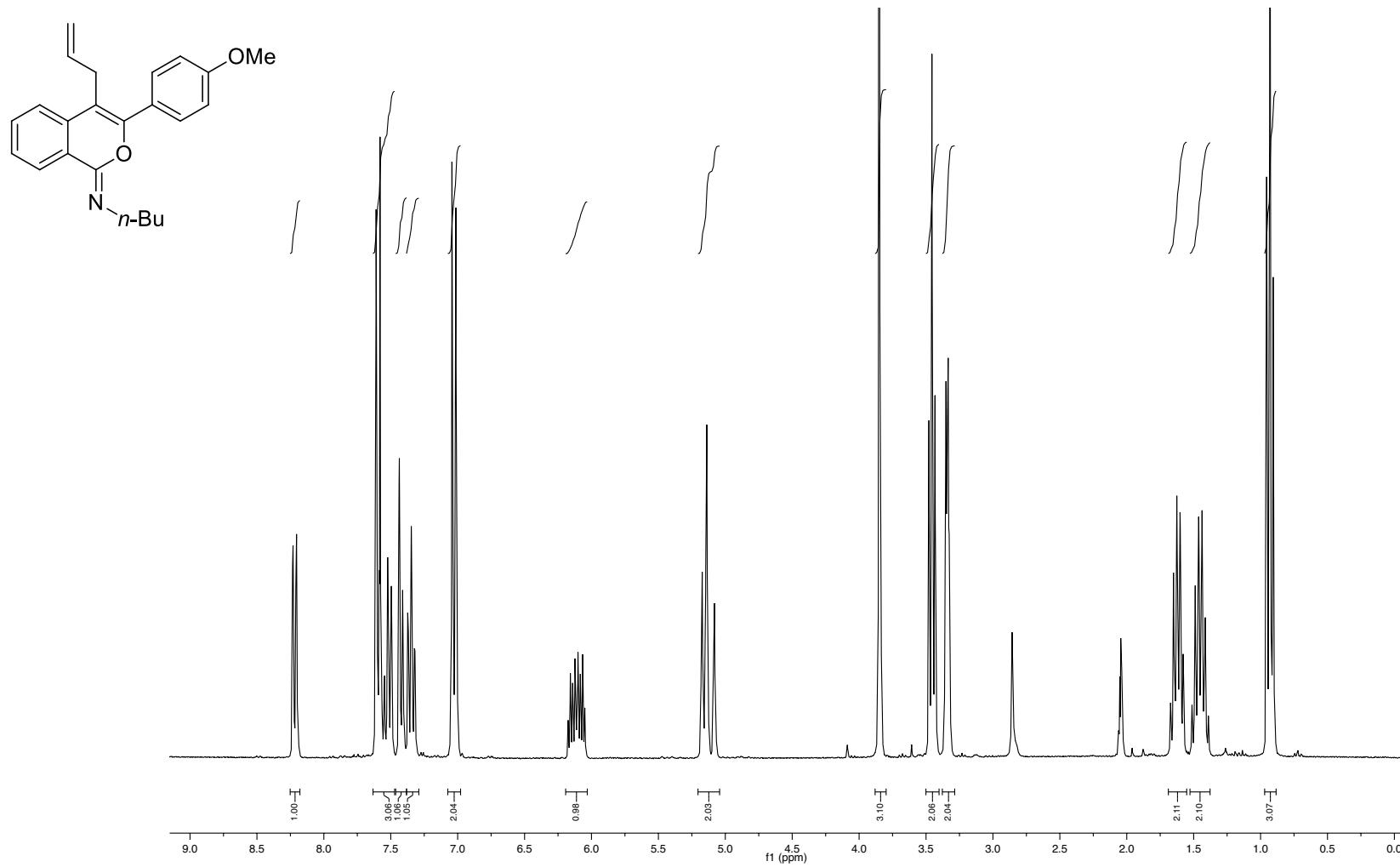
¹H NMR (300.13 MHz, acetone-d₆) spectrum of 2a



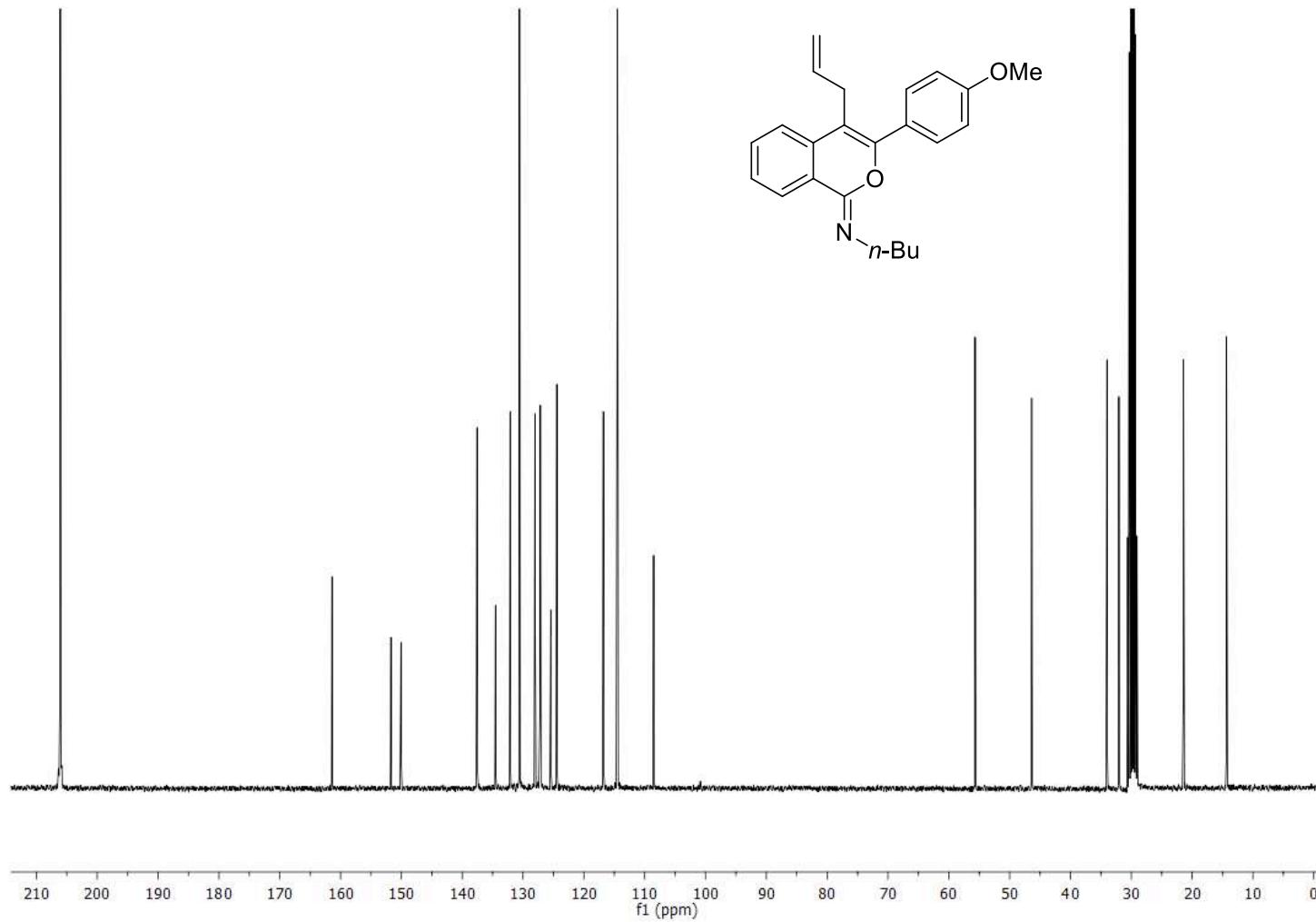
¹³C NMR (77 MHz, acetone-d₆) spectrum of 2a



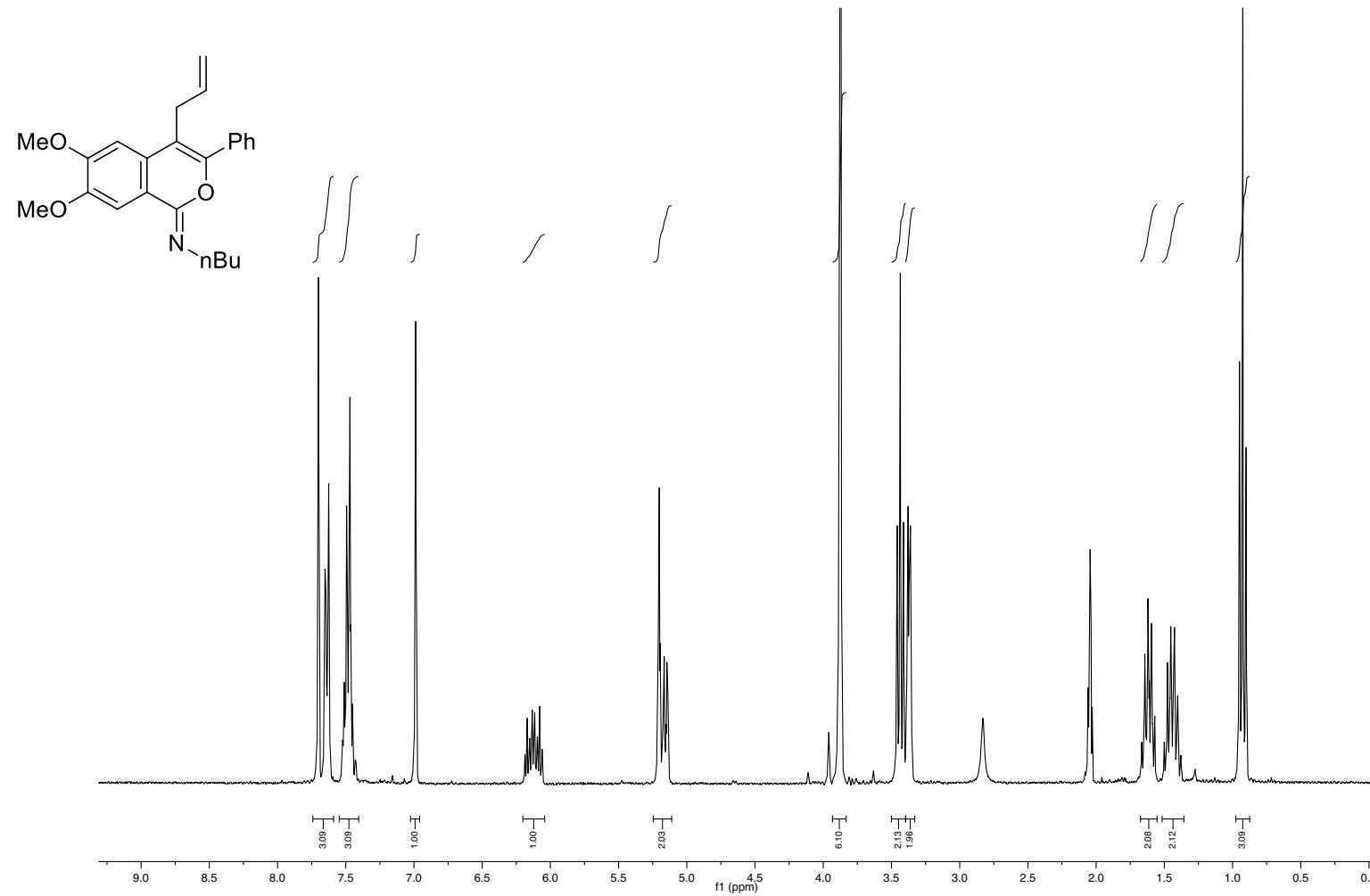
¹H NMR (300.13 MHz, acetone-d₆) spectrum of 2b



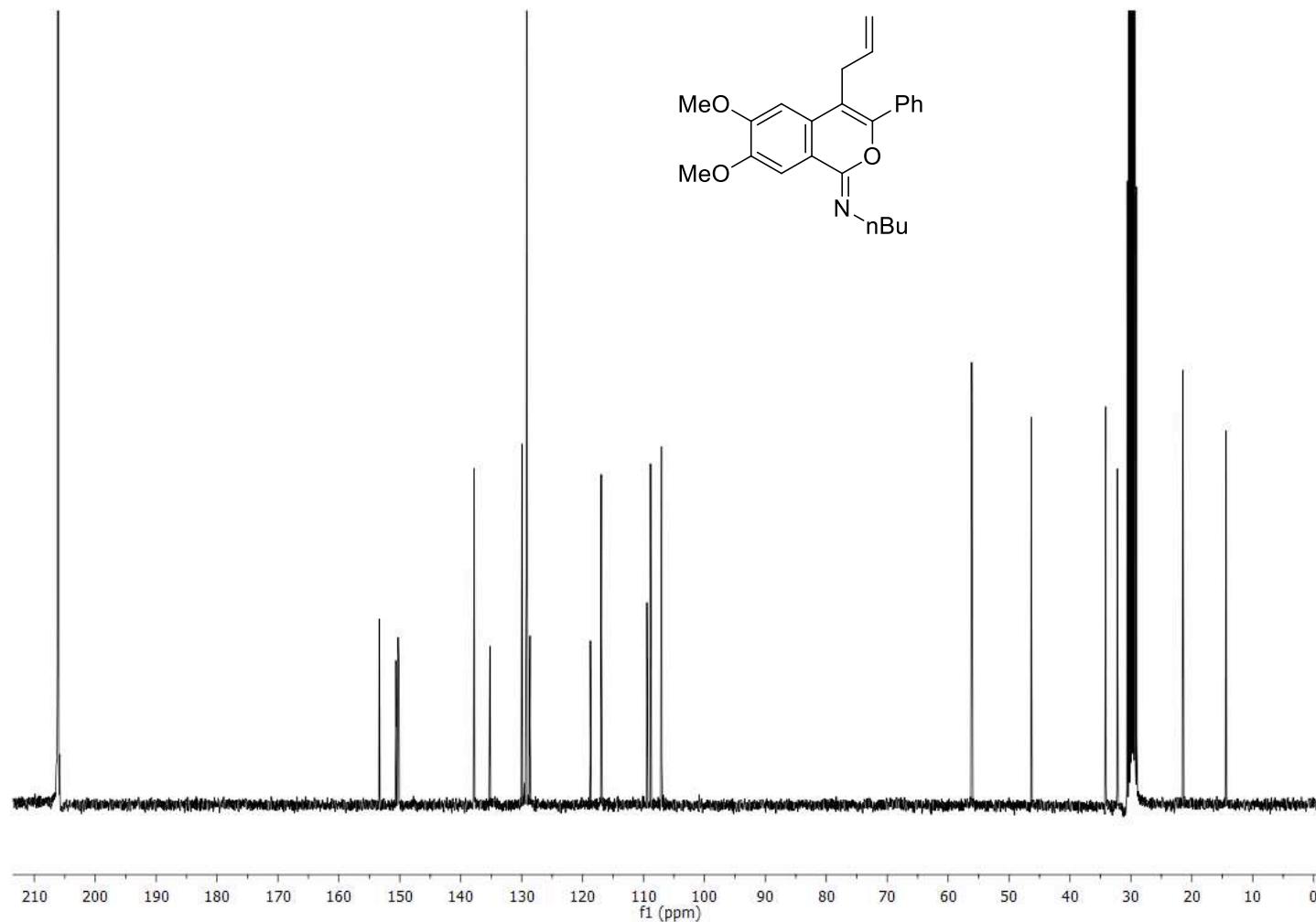
¹³C NMR (77 MHz, acetone-d₆) spectrum of 2b



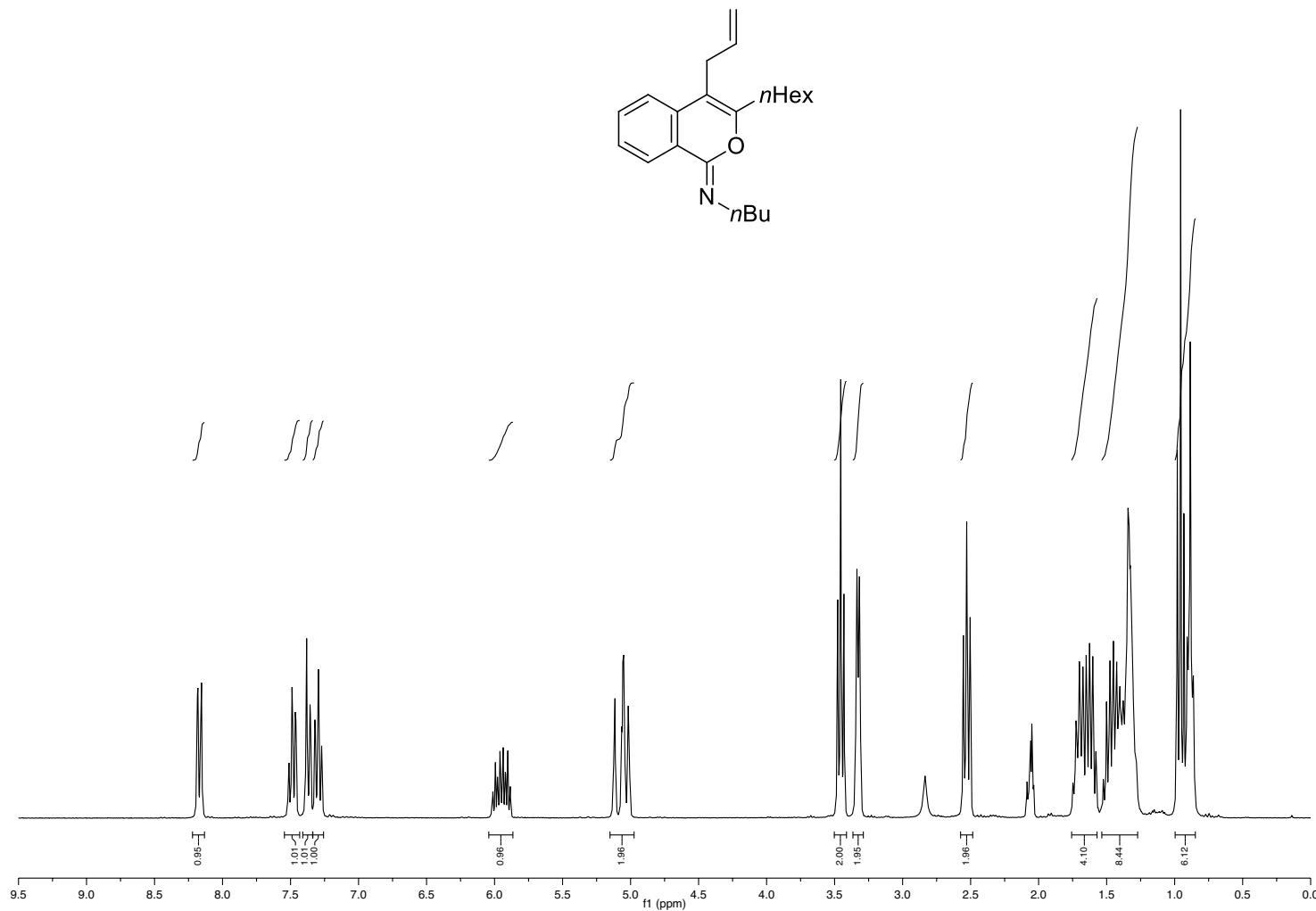
¹H NMR (300.13 MHz, acetone-d₆) spectrum of 2c



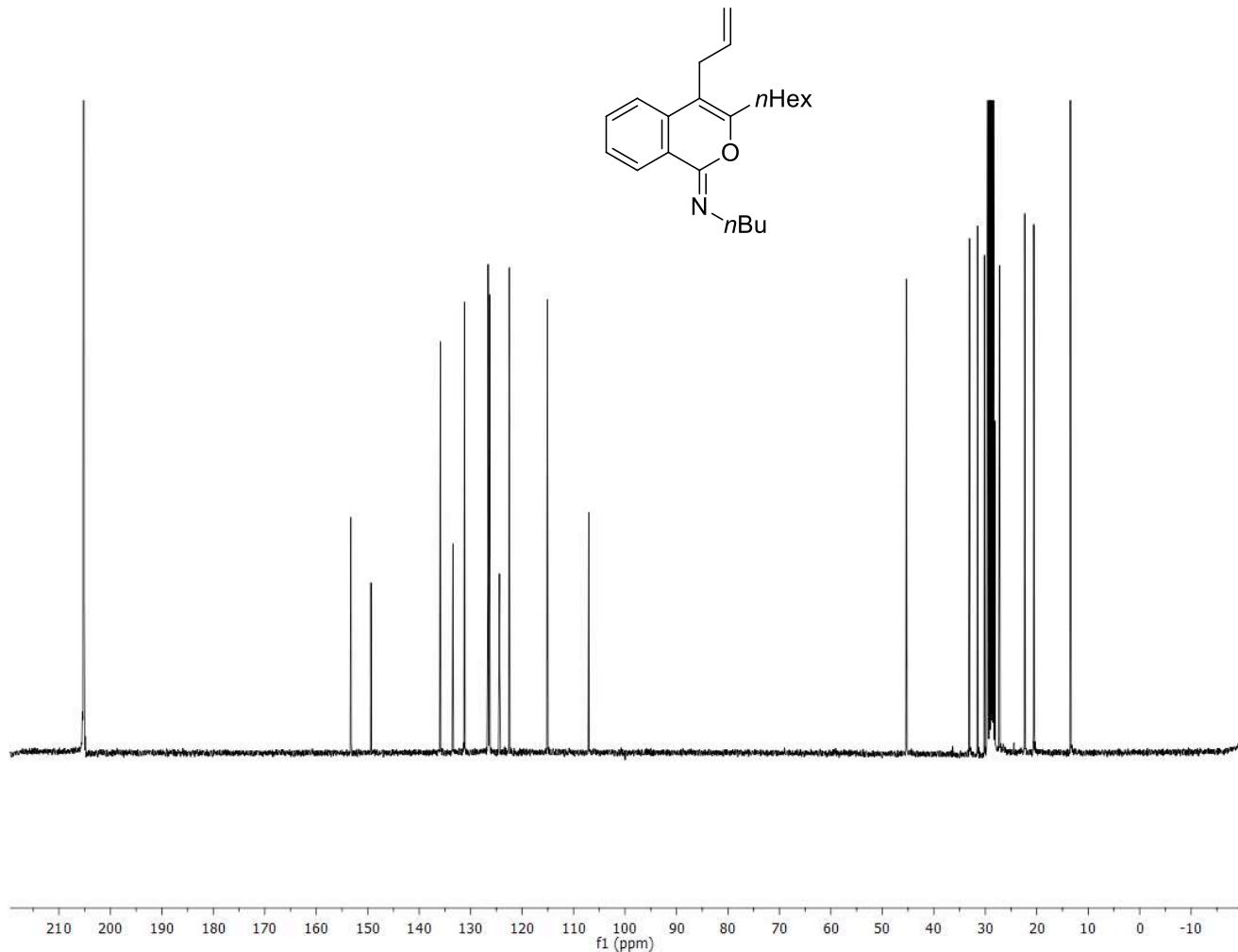
¹³C NMR (77 MHz, acetone-d₆) spectrum of 2c



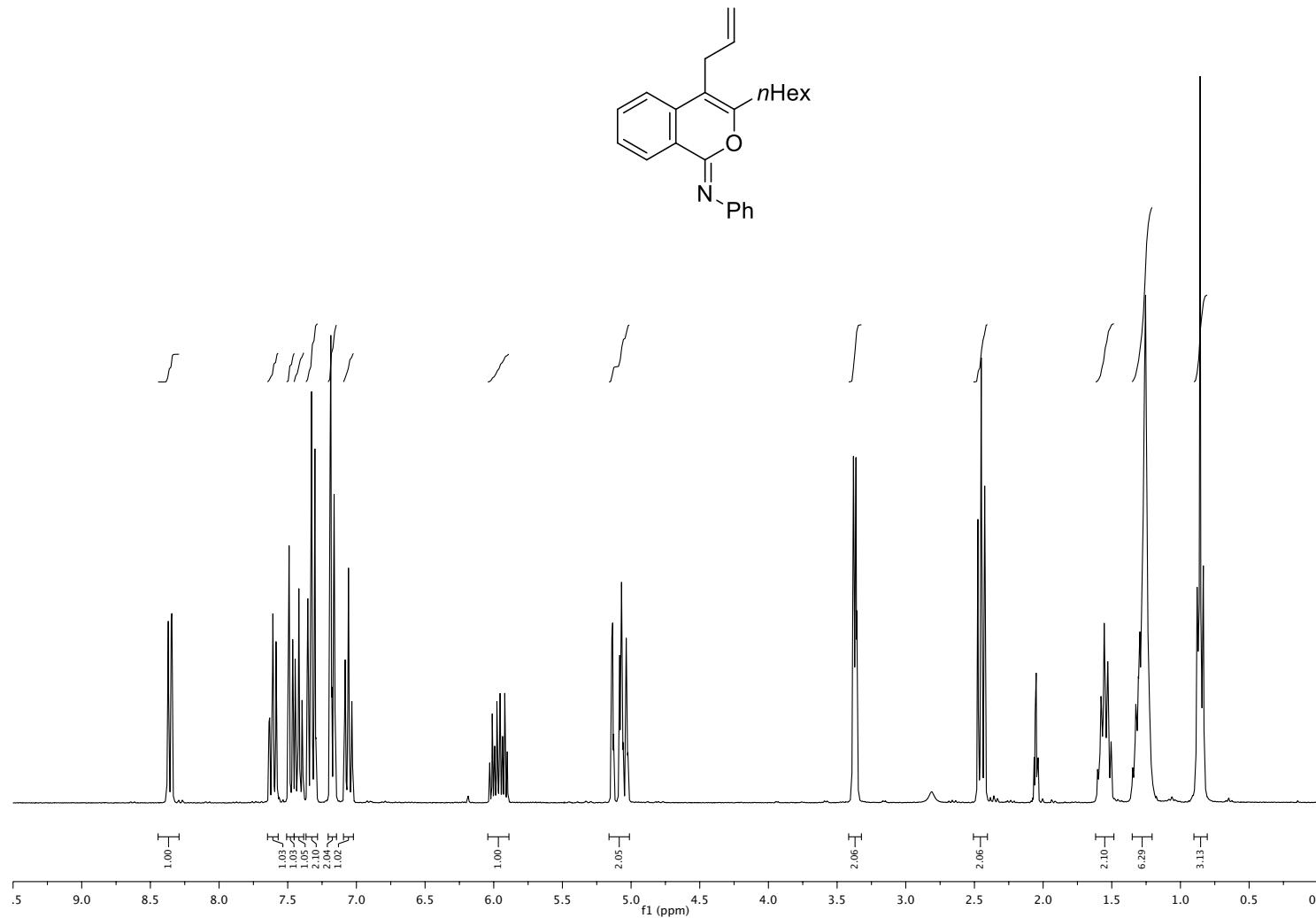
¹H NMR (300.13 MHz, acetone-d₆) spectrum of 2d



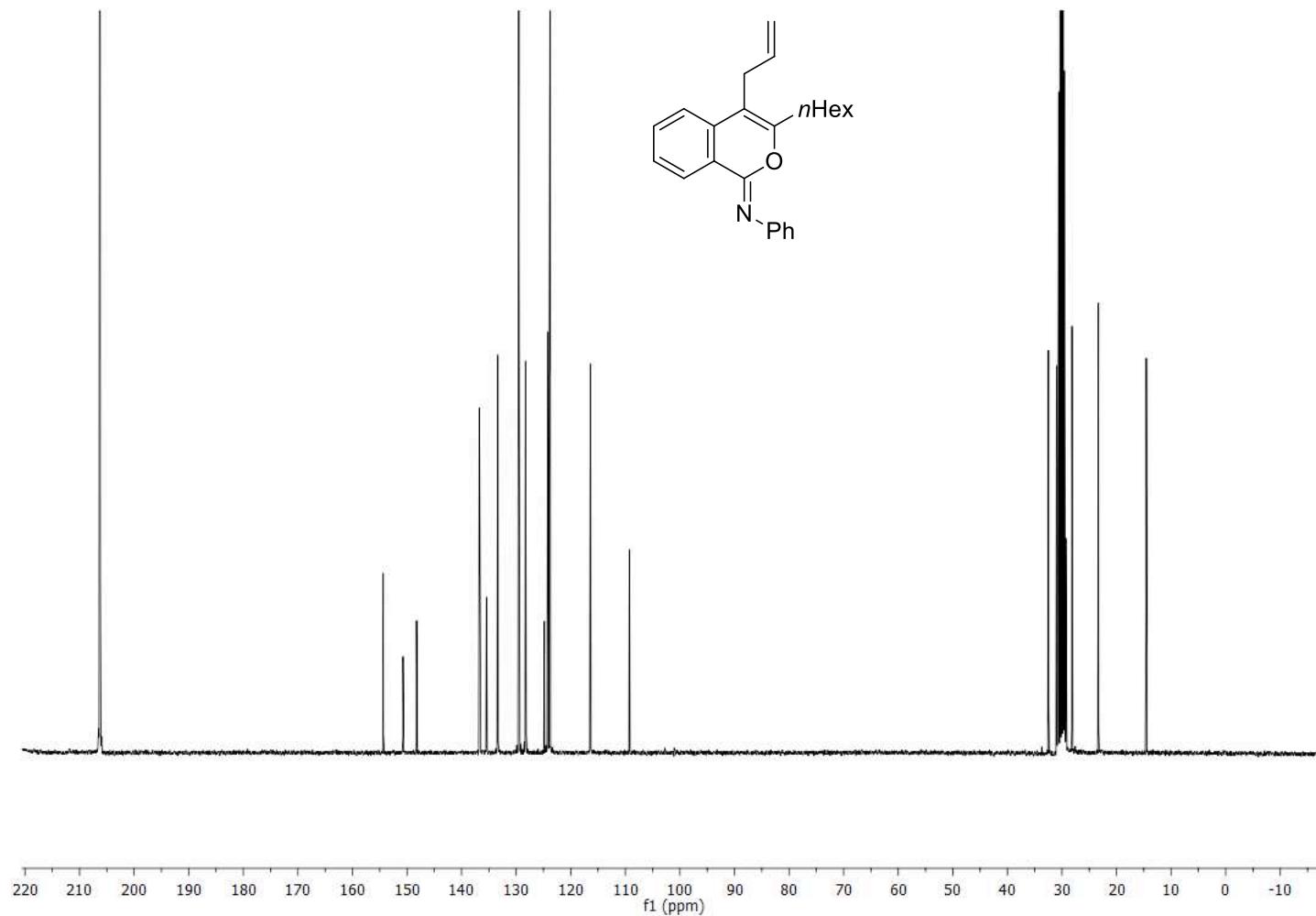
¹³C NMR (77 MHz, acetone-d₆) spectrum of 2d



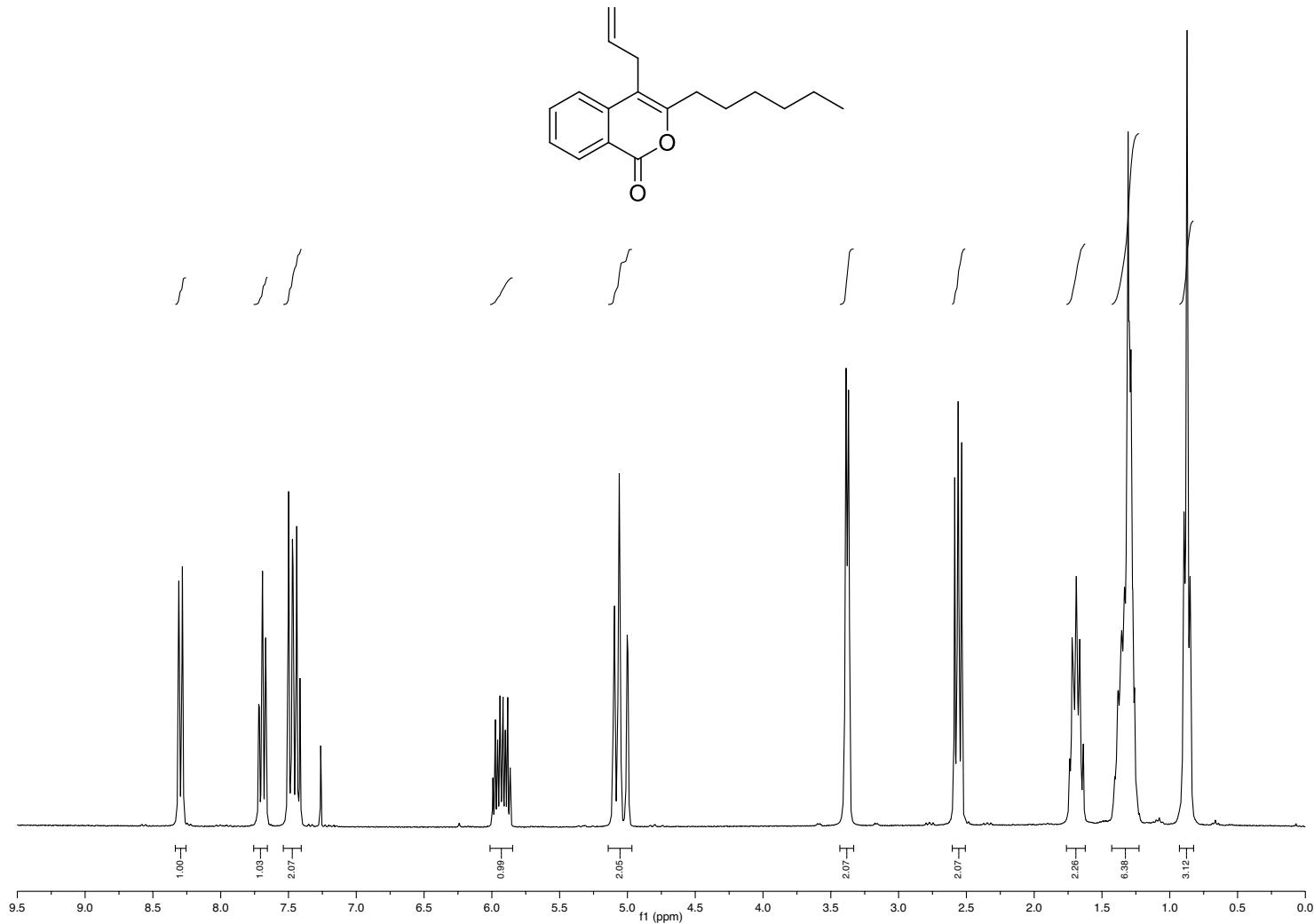
¹H NMR (300.13 MHz, acetone-d₆) spectrum of 2e



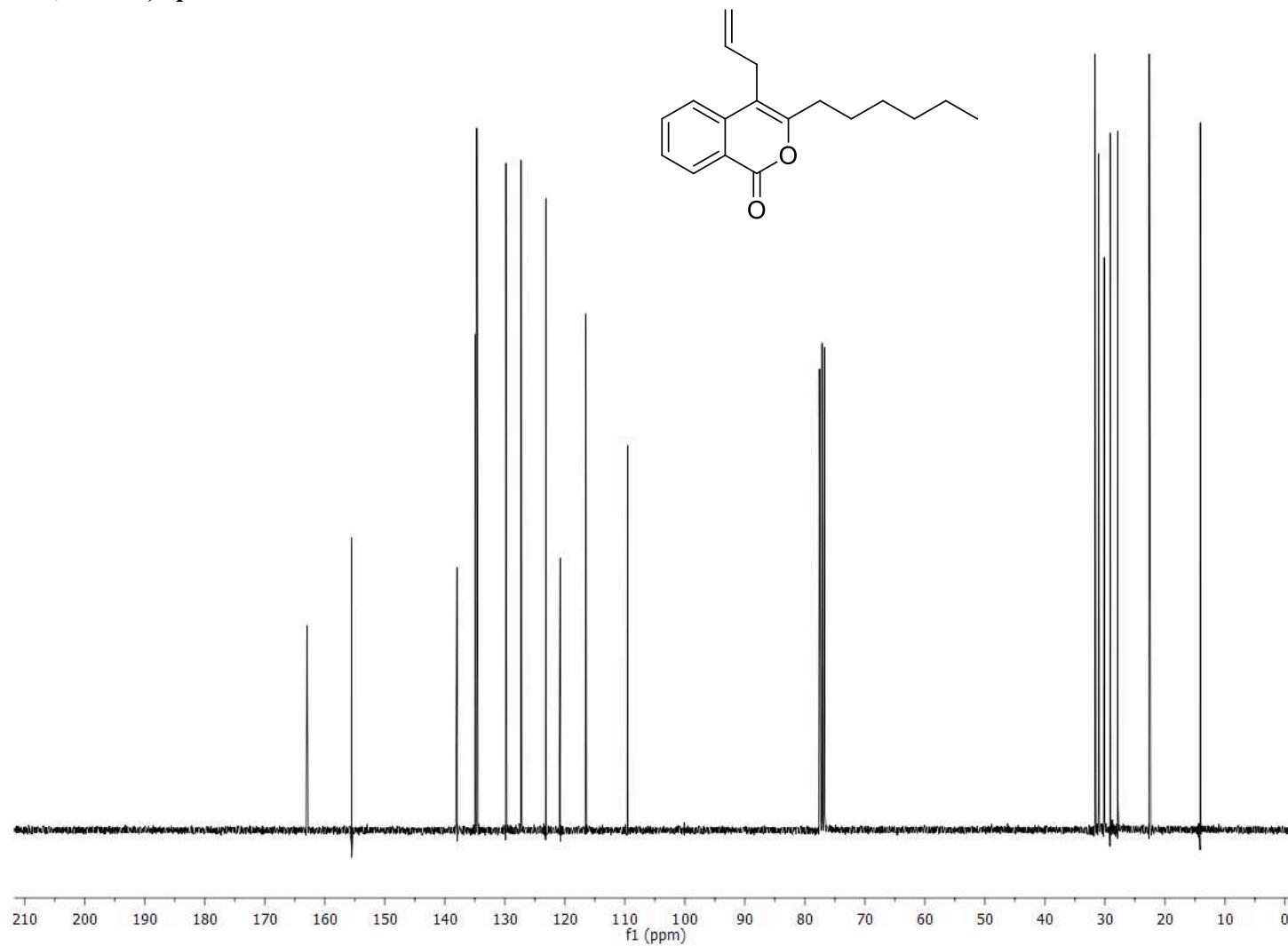
¹³C NMR (77 MHz, acetone-d₆) spectrum of 2e



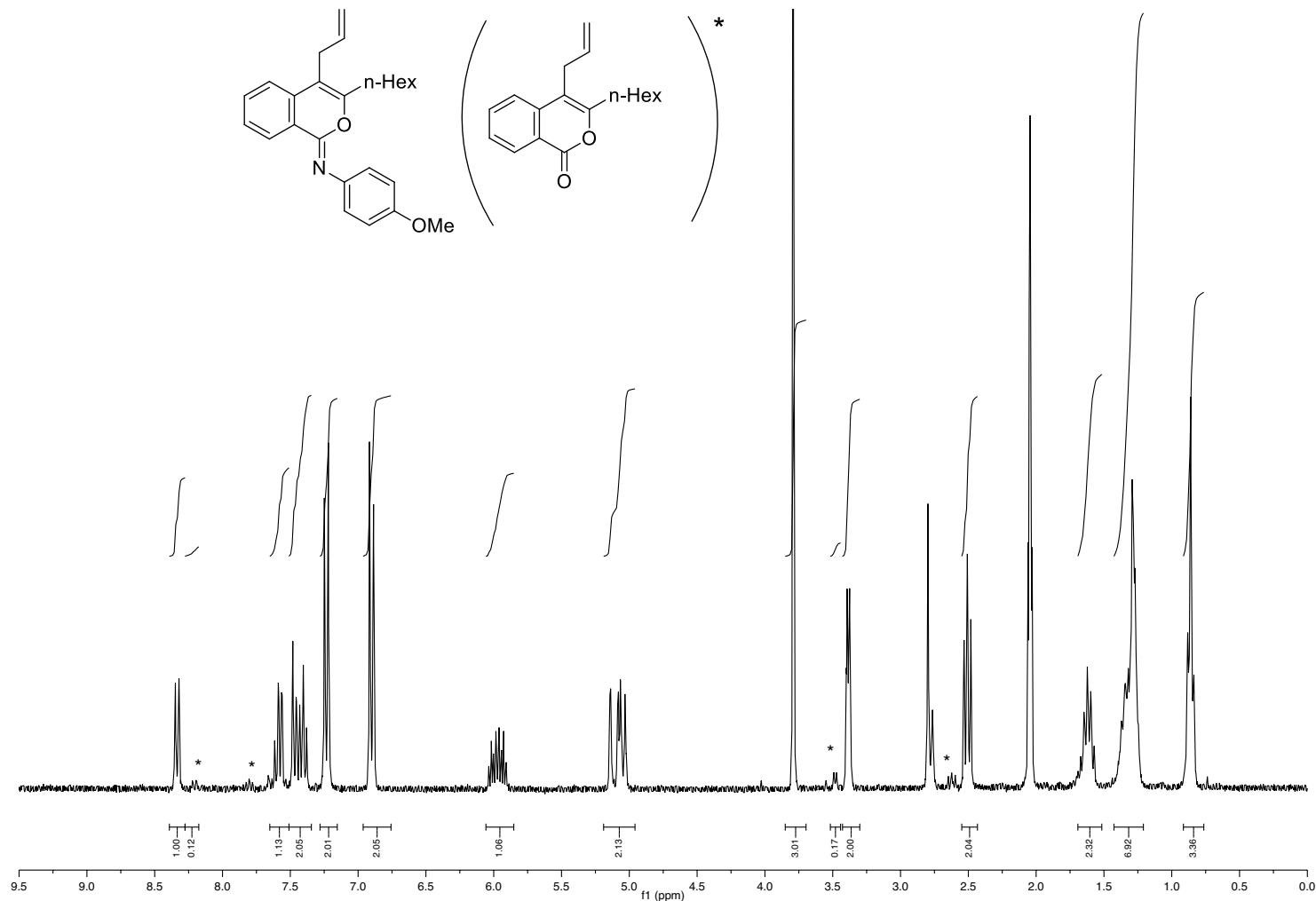
¹H NMR (300.13 MHz, CDCl₃) spectrum of 3b



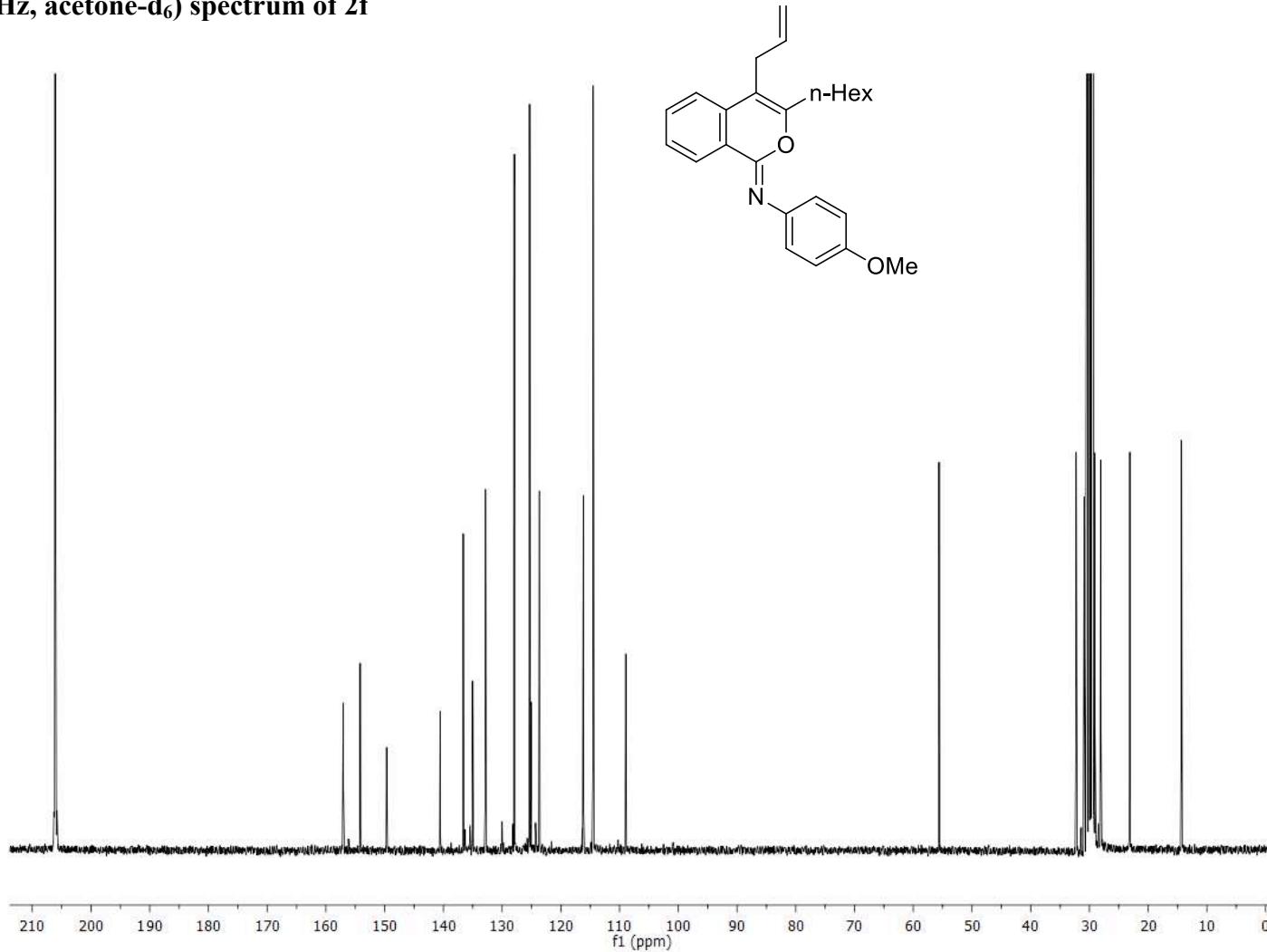
¹³C NMR (77 MHz, CDCl₃) spectrum of 3b

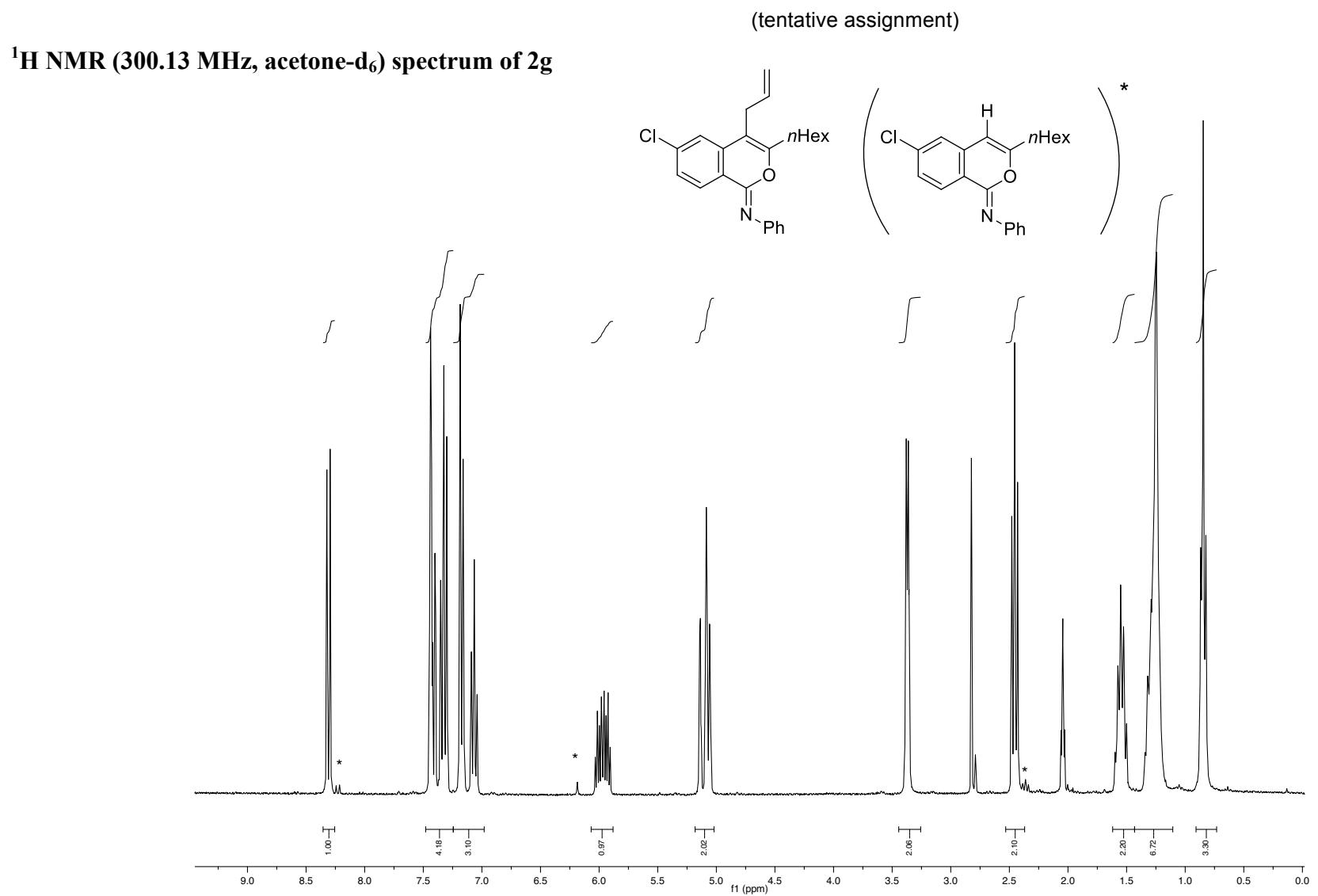


¹H NMR (300.13 MHz, acetone-d₆) spectrum of 2f

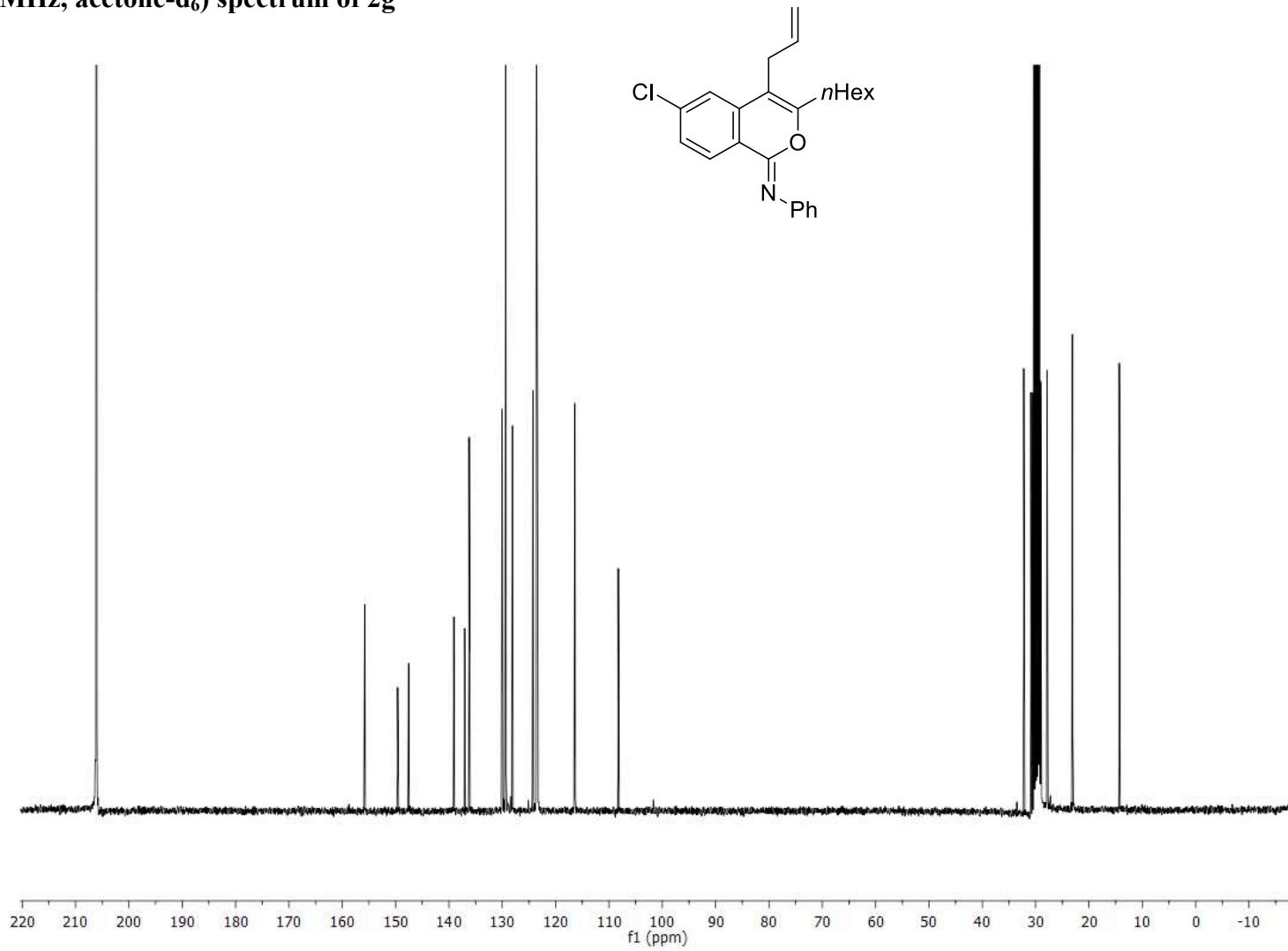


¹³C NMR (77 MHz, acetone-d₆) spectrum of 2f



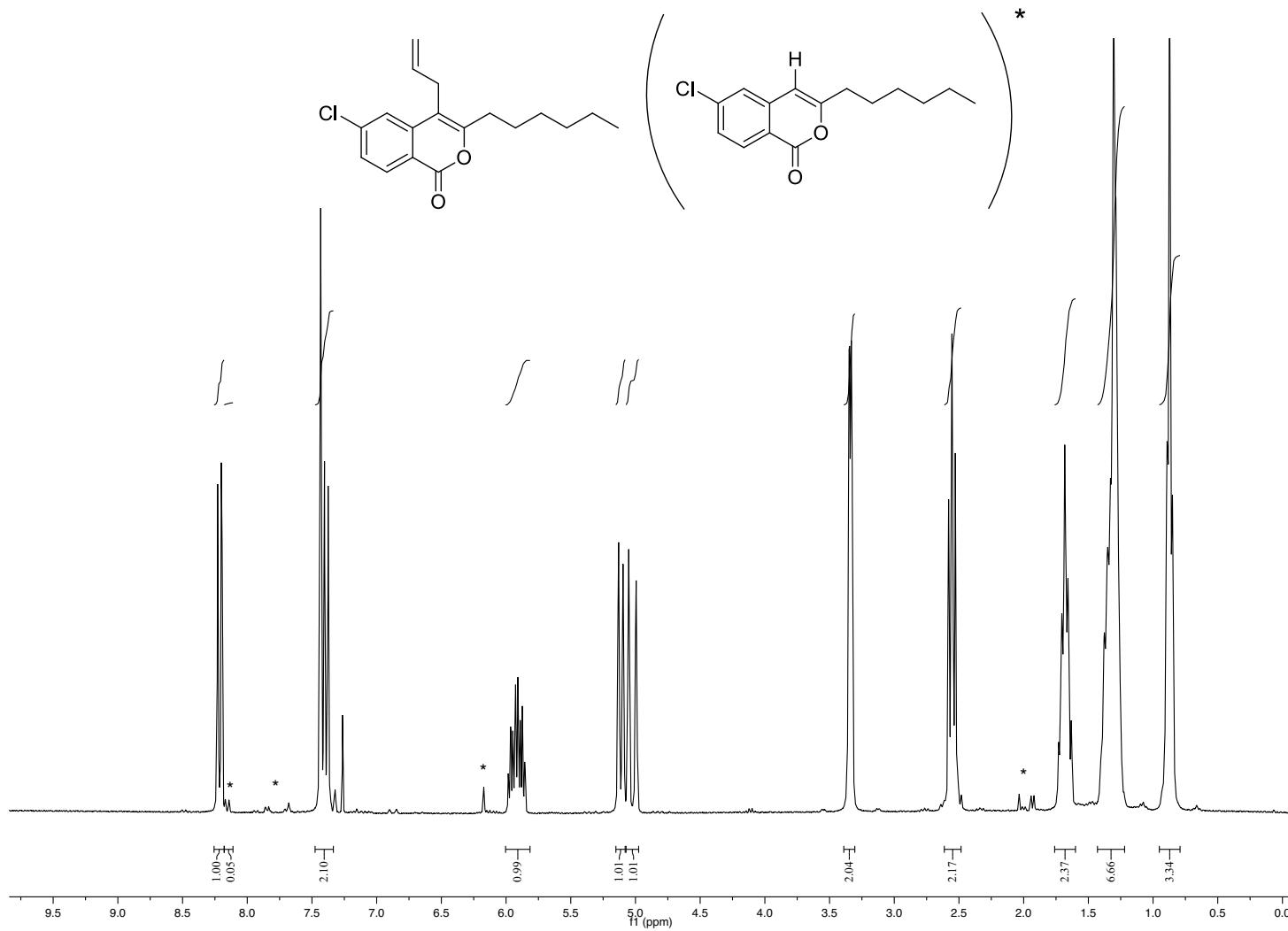


¹³C NMR (77 MHz, acetone-d₆) spectrum of 2g

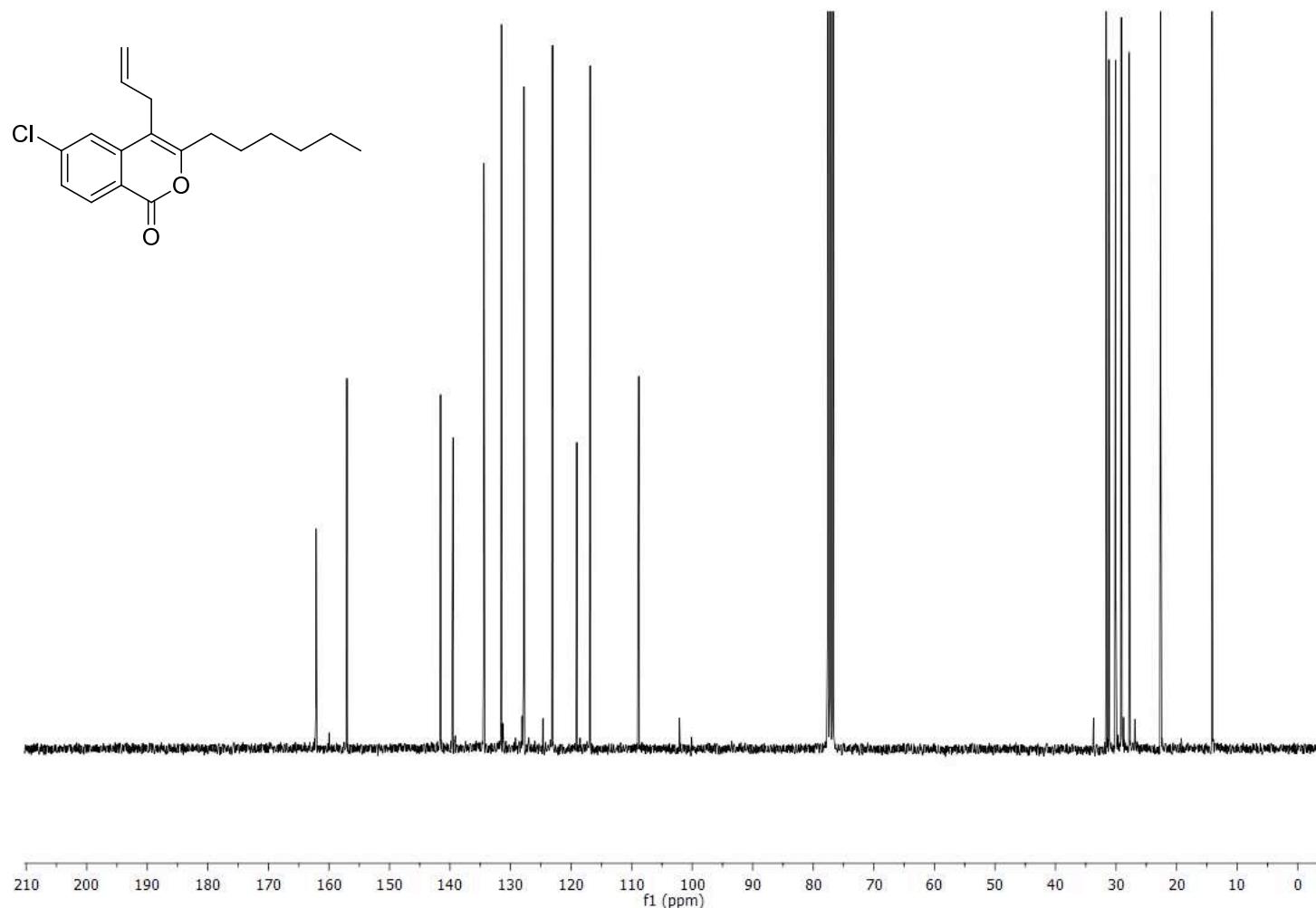


(tentative assignment)

¹H NMR (300.13 MHz, CDCl₃) spectrum of 3c



¹³C NMR (77 MHz, CDCl₃) spectrum of 3c



Computational Data

	SCF	SCF+zpve	Enthalpy	TS	Free energy
Pd-allylC1	-441883,0	-441836,7	-441832,3	24,6	-441856,8
TSC1Pdallyl	-441865,3	-441819,9	-441815,7	23,7	-441839,4
C1Pdallyl	-441898,4	-441852,7	-441848,1	24,6	-441872,7
IVa	-910802,3	-910598,7	-910583,2	51,2	-910634,4
TSIVa-Va_{endo}	-910786,8	-910583,4	-910568,6	50,0	-910618,5
Va_{endo}	-910802,2	-910597,4	-910582,7	48,7	-910631,4
VI_{endo}	-621631,1	-621434,8	-621421,8	43,8	-621465,7
VIIa_{endo}	-621646,2	-621448,1	-621435,4	44,4	-621479,8
VIIa-dba_{endo}	1080478,9	-1080116,7	-1080094,1	65,8	-1080159,9
-	-	-	-	-	-
TSVIIa-VIIa-dba_{endo}	1080469,8	-1080107,4	-1080084,7	66,3	-1080151,0
-	-	-	-	-	-
VIIa-dba_{endo}	1080508,6	-1080145,0	-1080122,0	67,9	-1080189,9
TSIVa-Va_{exo}	-910787,4	-910584,4	-910569,4	50,1	-910619,5
Va_{exo}	-910797,0	-910592,5	-910577,7	49,8	-910627,5
VIIa_{exo}	-621624,0	-621428,2	-621415,0	45,3	-621460,2
TSVIIa-VIIa_{exo}	-621599,9	-621404,5	-621391,5	44,7	-621436,2
VIIa_{exo}	-621634,9	-621437,7	-621424,5	45,1	-621469,6
VIIa-dba_{exo}	1080476,4	-1080114,1	-1080090,9	67,7	-1080158,6
-	-	-	-	-	-
TSVIIa-VIIa-dba_{exo}	1080466,5	-1080104,5	-1080081,7	67,0	-1080148,6
-	-	-	-	-	-
VIIa-dba_{exo}	1080503,3	-1080140,1	-1080117,0	68,2	-1080185,2
ClPh_Pd-PPh₃	1163759,3	-1163526,2	-1163509,8	55,4	-1163565,2
I	-468882,7	-468725,9	-468715,3	39,9	-468755,2
TSC1PdAr-PPh₃	1163742,3	-1163509,5	-1163493,5	53,5	-1163547,0
PdAr-PPh₃	1163749,6	-1163516,3	-1163500,4	52,9	-1163553,3
IVb-PPh₃	1632665,8	-1632272,9	-1632246,4	75,5	-1632321,9
TSIVb-Vb-PPh_{3endo}	1632655,2	-1632262,9	-1632236,9	73,5	-1632310,4
Vb-PPh_{3endo}	1632671,7	-1632278,3	-1632252,3	73,8	-1632326,1
VIIb-PPh_{3endo}	1343499,0	-1343115,0	-1343090,2	71,8	-1343162,0
-	-	-	-	-	-
TSVIIb-VIIb-PPh_{3endo}	1343494,7	-1343110,6	-1343086,4	69,8	-1343156,2
-	-	-	-	-	-
VIIb-PPh_{3endo}	1343536,9	-1343151,4	-1343127,0	70,4	-1343197,4
TSIVb-Vb-PPh_{3exo}	1632655,7	-1632264,4	-1632238,0	75,4	-1632313,5
Vb-PPh_{3-exo}	1632664,4	-1632271,1	-1632244,9	75,2	-1632320,1
VIIb-PPh_{3exo}	1343497,3	-1343112,8	-1343088,0	71,6	-1343159,6
-	-	-	-	-	-
TSVIIb-VIIb-PPh_{3exo}	1343492,0	-1343108,6	-1343084,0	71,8	-1343155,8
VIIb-PPh_{3exo}	1343535,4	-1343150,2	-1343125,7	71,0	-1343196,7

	SCF	SCF+zpve	Enthalpy	TS	Free energy
dba	-458826,8	-458662,3	-458652,1	39,0	-458691,1
AC	-362351,0	-362305,4	-362301,8	21,2	-362323,0
I-Me₃N	-578346,4	-578111,0	-578096,2	49,4	-578145,6
Pd-allylCl	-441883,0	-441836,7	-441832,3	24,6	-441856,8
TSClPdallyl	-441865,3	-441819,9	-441815,7	23,7	-441839,4
I-Me₃N + ClPdallyl	-441898,4	-441852,7	-441848,1	24,6	-441872,7
IVa-Me₃N	-1020268,4	-1019986,3	-1019966,7	59,9	-1020026,6
TSIVa-Va_{endo}-Me₃N	-1020251,1	-1019969,1	-1019950,3	58,2	-1020008,5
Va_{endo}-Me₃N	-1020266,3	-1019982,8	-1019964,2	58,5	-1020022,7
TSVa-VIIIA_{endo}-Me₃N	-1020233,5	-1019950,9	-1019932,4	57,1	-1019989,5
VIIIA_{endo}-Me₃N	-1020289,9	-1020003,9	-1019986,1	54,4	-1020040,5
VIa-AC_{endo}-Me₃N	-1382623,3	-1382292,9	-1382270,4	67,6	-1382338,0
TSVIa-VIIA-AC_{endo}-Me₃N	-1382612,0	-1382282,0	-1382260,0	65,9	-1382325,9
VIIA-AC_{endo}-Me₃N	-1382651,7	-1382320,3	-1382298,0	67,1	-1382365,1
VIa-dba_{endo}-Me₃N	-1479101,2	-1478652,1	-1478623,0	81,6	-1478704,7
TSVIa-VIIA-dba_{endo}-Me₃N	-1479091,4	-1478642,7	-1478614,1	81,2	-1478695,3
VIIA-dba_{endo}-Me₃N	-1479138,8	-1478688,0	-1478659,4	80,1	-1478739,6
TSIVa-Va_{exo}-Me₃N	-1020249,4	-1019967,9	-1019948,8	60,1	-1020008,9
Va_{exo}-Me₃N	-1020259,6	-1019977,0	-1019957,9	60,5	-1020018,4
TSVa-VIIIA_{exo}-Me₃N	-1020232,9	-1019950,8	-1019931,8	59,7	-1019991,6
VIIIA_{exo}-Me₃N	-1020278,7	-1019993,8	-1019975,6	55,9	-1020031,5
VIa-AC_{exo}-Me₃N	-1382619,7	-1382289,9	-1382267,2	68,9	-1382336,0
TSVIa-VIIA-AC_{exo}-Me₃N	-1382607,6	-1382277,8	-1382255,6	66,0	-1382321,6
VIIA-AC_{exo}-Me₃N	-1382645,9	-1382314,7	-1382292,3	67.2	-1382359,4
VIa-dba_{exo}-Me₃N	-1479100,0	-1478651,2	-1478622,0	82,7	-1478704,8
TSVIa-VIIA-dba_{exo}-Me₃N	-1479089,5	-1478640,6	-1478612,0	80,5	-1478692,5
VIIA-dba_{exo}-Me₃N	-1479120,8	-1478671,3	-1478642,2	85,3	-1478727,4

AC

Num. Imaginary Frequencies: 0

C	1.133482	-0.136949	-0.448664
C	2.223218	-0.190024	0.311118
H	1.059152	-0.738504	-1.352114
H	3.067340	-0.819841	0.047917
H	2.312562	0.393961	1.224244
C	-0.036993	0.738308	-0.142409
C1	-1.542026	-0.237638	0.115401
H	0.121253	1.320900	0.766513
H	-0.264109	1.415322	-0.968642

I

Num. Imaginary Frequencies: 0

C	-1.191949	-0.813082	-0.039419
C	-2.583554	-0.487619	-0.034716
C	-2.974335	0.808735	0.333769
C	-4.320587	1.149815	0.346668
C	-5.286770	0.209177	-0.005307
C	-4.903206	-1.079156	-0.370599
C	-3.558558	-1.429681	-0.386511
C	0.006605	-0.968931	-0.004531
C	1.421849	-1.153014	0.036585
C	1.954952	-2.445941	-0.056588
C	3.327587	-2.654551	-0.033392
C	4.194826	-1.572100	0.076800
C	3.678484	-0.282740	0.155268
C	2.302430	-0.056551	0.136923
C	1.770067	1.348505	0.249639
N	2.417825	2.253496	-0.543107
C	1.990291	3.635077	-0.602030
H	1.164230	3.781227	-1.308784
H	2.832258	4.265213	-0.899479
H	1.648826	3.933387	0.390009
O	0.864892	1.662604	1.004221
H	3.000847	1.898906	-1.285349
H	4.352626	0.563164	0.257395
H	5.268474	-1.729476	0.107016
H	3.720320	-3.664581	-0.099767
H	1.272004	-3.284534	-0.145127
H	-2.208458	1.526629	0.609971
H	-4.617697	2.154153	0.633690
H	-6.338661	0.479092	0.006672
H	-5.654310	-1.813871	-0.644486
H	-3.253172	-2.432263	-0.669136

C1Ph_PdL

Num. Imaginary Frequencies: 0

C	1.208879	2.769680	-0.212266
C	1.782044	1.525689	-0.497495
C	3.029760	1.481902	-1.127534
C	3.695518	2.660564	-1.453947
C	3.122544	3.893812	-1.154867
C	1.877591	3.946847	-0.532828
P	0.841906	0.024958	-0.004448
C	1.541313	-1.273147	-1.103771
C	2.685054	-2.014284	-0.791498
C	3.177193	-2.960445	-1.687376
C	2.534331	-3.173982	-2.903613
C	1.390287	-2.444571	-3.219586
C	0.893118	-1.506147	-2.321235
Pd	-1.425839	0.245809	-0.029887
C1	-3.798413	2.289979	0.101326
C	-3.594473	0.539393	0.012422
C	-3.665656	-0.102955	-1.243406
C	-3.840506	-1.488501	-1.290839
C	-3.936027	-2.235234	-0.118531
C	-3.803458	-1.607236	1.117618
C	-3.625934	-0.223365	1.201199
C	1.564206	-0.403998	1.631490
C	2.793512	0.079047	2.089131
C	3.286546	-0.315663	3.330948
C	2.559240	-1.197677	4.125140
C	1.330920	-1.680074	3.678429
C	0.833215	-1.278494	2.443602
H	-3.603709	0.279670	2.161401
H	-3.854783	-2.185393	2.035033
H	-4.094635	-3.307405	-0.169803
H	-3.920478	-1.975041	-2.257793
H	-3.674195	0.492031	-2.149871
H	3.368080	0.768678	1.477643
H	4.239920	0.071337	3.679075
H	2.945766	-1.503118	5.093162
H	0.753923	-2.360269	4.298103
H	-0.135904	-1.634706	2.101078
H	3.191151	-1.858256	0.156860
H	4.064772	-3.532362	-1.432233
H	2.918770	-3.912740	-3.600913

H	0.879582	-2.613042	-4.163168
H	-0.014076	-0.952620	-2.552597
H	3.482652	0.525094	-1.370617
H	4.662297	2.613556	-1.946704
H	3.641699	4.812295	-1.412968
H	1.420043	4.905567	-0.307597
H	0.226829	2.808546	0.253768

dba

Num. Imaginary Frequencies: 0

C	3.775767	-0.133330	0.007286
C	4.902793	-0.964745	0.031493
C	6.186263	-0.433710	-0.032234
C	6.364847	0.942995	-0.121291
C	5.252793	1.784087	-0.144778
C	3.972729	1.252404	-0.081196
H	4.765168	-2.040644	0.101280
H	7.046198	-1.096416	-0.013425
H	7.365061	1.362433	-0.173277
H	5.386823	2.859333	-0.215202
H	3.118705	1.922592	-0.101344
C	2.446762	-0.748863	0.070121
C	1.256222	-0.132934	0.053866
H	2.421605	-1.836458	0.133476
C	-0.000571	-0.921664	0.108995
H	1.167043	0.948946	-0.008357
O	0.003422	-2.143907	0.167570
C	-1.263316	-0.140725	0.080462
C	-2.449631	-0.764615	0.068711
H	-1.184273	0.943433	0.048455
C	-3.778832	-0.147063	0.029079
H	-2.420101	-1.853937	0.070203
C	-4.889204	-0.953660	-0.250891
C	-6.167491	-0.411443	-0.322224
C	-6.358843	0.949056	-0.102668
C	-5.265025	1.762085	0.191624
C	-3.988942	1.220307	0.257616
H	-4.741676	-2.016818	-0.421948
H	-7.014249	-1.052590	-0.547940
H	-7.355728	1.376260	-0.155078
H	-5.410386	2.822506	0.374580
H	-3.149498	1.863522	0.504191

I_Me3N_ClPdallyl

Num. Imaginary Frequencies: 0

C	-1.106771	1.458419	0.234471
C	-1.943812	0.487325	-0.395711
C	-2.103635	-0.726637	0.276051
Pd	0.019171	-0.259490	-0.036831
Cl	2.281795	0.145883	0.020598
H	-0.757016	2.315168	-0.333983
H	-1.144072	1.595415	1.314100
H	-2.201644	0.580908	-1.447250
H	-2.527821	-1.582304	-0.241300
H	-2.116507	-0.767294	1.363599

I_Me3N

Num. Imaginary Frequencies: 0

C	1.545354	0.918399	-0.980414
C	0.783675	1.724346	-0.112031
C	1.403996	2.785405	0.559952
C	2.754669	3.049770	0.366513
C	3.506233	2.250361	-0.490035
C	2.901047	1.185207	-1.151225
C	-0.593239	1.416360	0.110240
C	-1.740192	1.057717	0.247776
C	-3.075621	0.549849	0.276755
C	-3.459464	-0.374246	-0.707391
C	-4.747758	-0.892732	-0.704653
C	-5.661679	-0.497383	0.270625
C	-5.284595	0.421751	1.246884
C	-3.997469	0.945743	1.253652
C	0.899039	-0.225634	-1.725666
O	-0.030269	-0.065006	-2.504014
N	1.473775	-1.427933	-1.469651
C	0.890116	-2.629032	-2.026279
H	-0.082088	-2.861869	-1.571793
H	1.573653	-3.465196	-1.859793
H	0.735331	-2.499611	-3.099513
H	2.005480	-1.508023	-0.595410
H	3.482662	0.551362	-1.813806
H	4.561908	2.453130	-0.642176
H	3.220387	3.880999	0.887137
H	0.812951	3.397854	1.233272
H	-2.734676	-0.662783	-1.462898
H	-5.041936	-1.606435	-1.468281
H	-6.667925	-0.905914	0.269021
H	-5.996864	0.732590	2.005245

H	-3.696903	1.662978	2.010773
N	2.379554	-1.672059	1.325475
C	3.084461	-0.554672	1.936529
C	0.995272	-1.729780	1.776578
C	3.069666	-2.927517	1.573880
H	3.183647	-0.674440	3.030953
H	4.085864	-0.468920	1.503922
H	2.547391	0.375954	1.735265
H	0.914041	-1.886488	2.867054
H	0.481879	-0.798767	1.517849
H	0.478650	-2.552212	1.270953
H	3.129722	-3.171335	2.650406
H	2.546411	-3.744495	1.066084
H	4.088203	-2.871853	1.176953

IVa-Me3N

Num. Imaginary Frequencies: 0

C	-3.920907	0.535156	1.053806
C	-3.207112	0.916526	-0.090716
C	-3.863308	1.044082	-1.321808
C	-5.228696	0.798229	-1.402286
C	-5.940367	0.424340	-0.263569
C	-5.286305	0.293594	0.960395
C	-1.792249	1.152564	-0.011000
Pd	-0.740719	-0.915351	0.370693
C	-0.735273	-3.043393	0.312084
C	-0.339721	-2.561404	-0.956393
C	-1.190974	-1.653859	-1.612958
C	-0.604645	1.445586	-0.011850
C	0.699881	2.038812	0.073204
C	1.707008	1.734093	-0.854470
C	2.948774	2.355863	-0.740603
C	3.193628	3.273703	0.276719
C	2.204094	3.546889	1.217594
C	0.964785	2.926820	1.122418
C	1.469057	0.753561	-1.973522
O	0.590199	0.907225	-2.814769
C1	-0.388058	-0.614520	2.710597
N	2.343537	-0.278145	-1.973928
C	2.336389	-1.245988	-3.047406
H	2.866292	-0.470894	-1.105429
H	2.586964	-0.768572	-4.000152
H	1.357010	-1.722292	-3.171015
H	3.082363	-2.014162	-2.829906
H	3.724498	2.116725	-1.461752
H	4.161090	3.761897	0.344459
H	2.396331	4.243280	2.027607
H	0.191598	3.113425	1.859474
H	-3.390434	0.418996	1.994438
H	-5.840497	-0.001283	1.846105
H	-7.007212	0.233360	-0.331364
H	-5.738371	0.899358	-2.355476
H	-3.293707	1.332090	-2.199908
H	-0.819829	-1.057356	-2.442737
H	-2.272230	-1.759731	-1.533258
H	0.705231	-2.630821	-1.248509
H	-0.023691	-3.561365	0.947036
H	-1.784441	-3.247223	0.520512
N	3.612062	-1.023205	0.562775
C	3.338104	-0.139152	1.693481
C	3.004128	-2.328089	0.784166
C	5.041456	-1.142480	0.321355
H	3.770917	-0.532530	2.630270
H	3.764826	0.847756	1.497730
H	2.258256	-0.034039	1.833054
H	5.579080	-1.576032	1.183868
H	5.219874	-1.781720	-0.550500
H	5.461950	-0.153059	0.115201
H	3.458457	-2.861627	1.637816
H	1.940200	-2.191574	0.996492
H	3.118256	-2.950685	-0.111670

IVa

Num. Imaginary Frequencies: 0

C	2.604782	-0.111318	1.109944
C	1.566844	-1.060434	1.096733
C	1.873763	-2.425657	1.111826
C	3.195715	-2.845386	1.188200
C	4.223519	-1.908414	1.239272
C	3.926380	-0.549957	1.187114
C	0.187245	-0.672578	1.018046
C	-1.016992	-0.468067	1.053256
Pd	-0.395338	-0.071149	-1.206587
C1	-0.556680	-2.348627	-1.871905
C	2.290268	1.354894	1.023313
N	3.080559	2.044562	0.150314
C	2.932278	3.469819	-0.051240
C	-2.412081	-0.182742	1.232813

C	-2.797222	0.939349	1.978341
C	-4.147504	1.222472	2.144591
C	-5.111205	0.395573	1.569457
C	-4.726373	-0.715951	0.821219
C	-3.379498	-1.009426	0.645928
C	-0.529654	2.090576	-1.033942
C	0.198592	1.747967	-2.184191
C	-0.405008	0.859538	-3.110590
O	1.404138	1.891031	1.673232
H	3.691675	1.522723	-0.458272
H	2.498358	3.896736	0.853982
H	2.267829	3.701493	-0.893364
H	3.909443	3.923800	-0.234924
H	4.728975	0.181059	1.230466
H	5.256770	-2.232977	1.313161
H	3.421047	-3.906857	1.204396
H	1.064068	-3.142838	1.038052
H	-3.057503	-1.858072	0.049342
H	-5.478205	-1.355499	0.369394
H	-6.165479	0.618894	1.703516
H	-4.448974	2.089761	2.724131
H	-2.031664	1.573038	2.415271
H	-0.034082	2.551054	-0.183819
H	-1.612244	2.201239	-1.080511
H	1.276338	1.895991	-2.202688
H	0.194330	0.389325	-3.883406
H	-1.471699	0.928925	-3.317937

IVb-PPh3

Num. Imaginary Frequencies: 0

C	1.598165	2.625729	2.487490
C	1.309794	1.268972	2.273451
C	0.833398	0.478926	3.328088
C	0.639801	1.043607	4.583490
C	0.916721	2.392153	4.794424
C	1.397948	3.176851	3.746872
C	1.455894	0.735896	0.945917
C	1.680729	0.588511	-0.262430
C	1.883284	0.801477	-1.670792
C	2.133919	-0.268322	-2.535887
C	2.187948	-0.063410	-3.909748
C	1.968884	1.205359	-4.436824
C	1.733564	2.279310	-3.580830
C	1.708145	2.094896	-2.200739
C	1.625352	3.288544	-1.290863
N	0.578048	4.124587	-1.501379
C	0.444069	5.315627	-0.687822
Pd	0.742828	-1.295098	0.406278
Cl	-0.130407	-3.485997	0.413437
C	2.599339	-2.065855	0.615801
C	3.035564	-3.064165	-0.258227
C	4.330392	-3.571358	-0.158360
C	5.194839	-3.105540	0.828183
C	4.757471	-2.123662	1.711618
C	3.469821	-1.598478	1.600708
O	2.498561	3.519700	-0.464504
H	1.595601	3.278775	-3.982766
H	1.997683	1.365594	-5.510141
H	2.388149	-0.903178	-4.567502
H	2.271708	-1.260025	-2.119961
H	0.617444	-0.571558	3.153796
H	0.270004	0.427114	5.396782
H	0.760777	2.831685	5.775046
H	1.620344	4.226849	3.912008
H	1.969602	3.224467	1.661023
H	-0.244816	3.754942	-1.957014
H	0.248507	5.070397	0.362083
H	1.368958	5.894342	-0.740263
H	-0.381497	5.915724	-1.074779
H	3.163013	-0.820958	2.293934
H	5.421574	-1.753454	2.488355
H	6.199954	-3.509192	0.911556
H	4.656243	-4.345234	-0.848580
H	2.357989	-3.471833	-1.002554
P	-1.580533	-0.507541	-0.066346
C	-2.037662	-1.217327	-1.685003
C	-2.924217	-0.980218	1.082695
C	-1.918273	1.293614	-0.245244
C	-3.013780	-2.204871	-1.820038
C	-3.254065	-2.782866	-3.064392
C	-2.525061	-2.381789	-4.179557
C	-1.545170	-1.399441	-4.049472
C	-1.298134	-0.826967	-2.808120
H	-3.575719	-2.536108	-0.952939
H	-4.010561	-3.556102	-3.157705
H	-2.712839	-2.839361	-5.146318
H	-0.962314	-1.084441	-4.910158
H	-0.522504	-0.072178	-2.715164

C	-2.466257	1.882558	-1.387755
C	-2.798136	3.238338	-1.393555
C	-2.586800	4.016821	-0.259017
C	-2.023879	3.440372	0.878128
C	-1.690023	2.091899	0.882612
H	-2.663566	1.281898	-2.269693
H	-3.245337	3.676860	-2.281400
H	-2.859768	5.068177	-0.259192
H	-1.847371	4.037390	1.767753
H	-1.273507	1.651332	1.783598
C	-4.214149	-0.455431	0.930324
C	-5.222684	-0.803346	1.820261
C	-4.951279	-1.675086	2.874182
C	-3.672423	-2.198564	3.031251
C	-2.658803	-1.854150	2.139200
H	-4.427863	0.233564	0.117728
H	-6.219337	-0.390775	1.694612
H	-5.738762	-1.945608	3.571596
H	-3.457800	-2.883562	3.845800
H	-1.669492	-2.287362	2.243971

IVb

Num. Imaginary Frequencies: 0

C	-1.526343	-1.660578	1.730591
C	-1.989839	-0.691967	0.853014
C	-2.876078	0.300291	1.245308
C	-3.310845	0.316448	2.570628
C	-2.862543	-0.645225	3.471881
C	-1.973454	-1.629924	3.051884
Pd	-1.343628	-0.684773	-1.004430
C1	-3.251741	-1.659422	-1.852760
C	0.701816	-0.339739	-0.441341
C	1.675898	-1.389788	-0.264784
C	1.350351	-2.719652	-0.558399
C	2.297514	-3.728269	-0.427481
C	3.590168	-3.421987	-0.015648
C	3.928467	-2.101730	0.269015
C	2.983894	-1.084070	0.159702
C	3.360545	0.319418	0.546075
O	2.790931	0.926862	1.441371
C	0.170444	0.784106	-0.531667
C	-0.121380	2.193737	-0.458903
C	-1.183454	2.751491	-1.183593
C	-1.446888	4.112090	-1.091328
C	-0.656798	4.922963	-0.279102
C	0.397288	4.369120	0.444378
C	0.670352	3.009052	0.363050
N	4.401708	0.843119	-0.150324
C	4.833753	2.207863	0.078022
H	4.932759	-1.856659	0.602953
H	4.333748	-4.205903	0.087103
H	2.023099	-4.753719	-0.652915
H	0.345206	-2.956269	-0.896979
H	-1.798843	2.114551	-1.813204
H	-2.271787	4.538926	-1.653043
H	-0.865156	5.986239	-0.206865
H	1.008566	4.998709	1.083848
H	1.480175	2.562504	0.931231
H	4.724453	0.354240	-0.970787
H	4.108592	2.931039	-0.313300
H	4.942164	2.377575	1.151185
H	5.797592	2.362994	-0.410263
H	-3.231144	1.044961	0.541054
H	-4.008332	1.084488	2.891767
H	-3.206394	-0.626544	4.501596
H	-1.617909	-2.380668	3.751562
H	-0.826917	-2.425384	1.409244

VIA-ACendo-Me3N

Num. Imaginary Frequencies: 0

C	1.618948	3.396892	0.064060
C	1.868704	2.182520	-0.589435
C	3.129628	1.984951	-1.164314
C	4.122954	2.952796	-1.057579
C	3.870243	4.145548	-0.385779
C	2.611511	4.364581	0.169235
C	0.821103	1.139663	-0.630922
O	-0.425388	1.744810	-0.727582
C	-1.589127	1.048326	-0.718508
C	-1.499692	-0.412452	-0.628746
C	-0.230805	-1.014858	-0.508922
C	0.978923	-0.191821	-0.516072
C	-2.661692	-1.190990	-0.638661
C	-2.589448	-2.566859	-0.501473
C	-1.340505	-3.175602	-0.355214
C	-0.183569	-2.411916	-0.362062
N	-2.695377	1.685184	-0.772464
C	-2.630240	3.131788	-0.840604

Pd	2.844504	-1.100811	-0.338502
C	2.764441	-0.224722	1.751251
C	1.651979	-0.892403	2.503820
C	4.682425	-2.191131	-1.109026
C	3.515359	-2.668237	-1.708958
C	2.627537	-1.768602	-2.357016
C	3.995052	-0.812274	1.576886
H	4.854181	-0.215244	1.285793
C	-6.019443	1.497325	-0.873716
N	-6.196341	0.701812	0.359861
C	-5.173007	1.000450	1.384317
C	-7.569420	0.783857	0.894892
Cl	-6.162052	-2.091373	-0.374316
H	5.274850	-2.844073	-0.476627
H	5.196387	-1.321845	-1.514709
H	3.151431	-3.657566	-1.437540
H	1.650837	-2.123438	-2.669496
H	0.785971	-2.889551	-0.245075
H	-1.272451	-4.253224	-0.235028
H	-3.512265	-3.138496	-0.500571
H	-3.633024	-0.725892	-0.759181
H	-3.646828	3.531235	-0.915314
H	-2.157063	3.566774	0.051346
H	3.324158	1.071071	-1.715598
H	5.092210	2.780720	-1.516943
H	4.644022	4.902861	-0.304155
H	2.401465	5.294417	0.689550
H	0.641806	3.572780	0.500876
H	-2.057957	3.482583	-1.709643
H	3.026890	-0.939183	-2.937581
H	4.200177	-1.804147	1.971902
H	2.656157	0.844427	1.591536
H	-6.084196	-0.361358	0.069986
H	-5.366938	1.984818	1.821865
H	-5.224719	0.227884	2.153848
H	-4.191190	0.996654	0.905443
H	-6.238547	2.549758	-0.667227
H	-4.983818	1.388175	-1.205904
H	-6.703782	1.109064	-1.630395
H	-7.794802	1.814510	1.184067
H	-8.262250	0.439787	0.125400
H	-7.645861	0.118551	1.756360
Cl	1.668534	-0.347950	4.233586
H	0.674314	-0.626491	2.106596
H	1.757390	-1.978208	2.514090

VIIa-AC_{exo}-Me3N

	Num. Imaginary Frequencies: 0		
C	1.868339	2.895352	0.495134
C	2.170750	1.915591	-0.464259
C	3.113762	2.238416	-1.451692
C	3.710422	3.493167	-1.498597
C	3.395685	4.454123	-0.541086
C	2.475060	4.146236	0.457307
C	1.583758	0.561525	-0.395939
Pd	2.904663	-1.013735	-0.700777
C	4.426764	-1.457003	0.888132
H	5.383995	-1.276722	0.408775
C	0.281605	0.360009	-0.160942
C	-0.516214	-0.857180	0.006983
C	-1.854234	-0.476814	0.129725
C	-1.898442	0.984602	0.065385
O	-0.622223	1.440418	-0.074917
C	-2.877286	-1.400911	0.291298
C	-2.534785	-2.747987	0.334025
C	-1.195395	-3.141451	0.234845
C	-0.174709	-2.206906	0.075681
N	-2.915220	1.744286	0.120445
C	-2.688953	3.176213	0.031310
C	3.661496	-0.409366	1.346286
C	2.569600	-0.590979	2.358532
C	4.007060	-2.547826	-1.973760
C	2.652071	-2.495475	-2.301366
C	2.045418	-1.255629	-2.638388
C	-5.841871	1.045677	-1.403942
N	-6.588528	0.695949	-0.176707
C	-6.134555	1.463429	1.003192
C	-8.050944	0.762832	-0.366718
Cl	-6.334885	-2.137274	0.351594
H	3.378088	1.489791	-2.193361
H	4.430114	3.718612	-2.280517
H	3.868317	5.431313	-0.569295
H	2.226813	4.884318	1.214682
H	1.147593	2.669795	1.274293
H	-3.652149	3.680364	-0.094426
H	-2.035392	3.447903	-0.807492
H	-2.220351	3.562528	0.946047
H	-3.919831	-1.113679	0.386099

H	-3.324060	-3.483212	0.453771
H	-0.945401	-4.197325	0.291116
H	0.863192	-2.522953	0.020835
H	0.964750	-1.202743	-2.718523
H	2.010936	-3.330066	-2.024031
H	2.593945	-0.534361	-3.241513
H	4.430970	-3.454555	-1.554761
H	4.712512	-1.849577	-2.420500
H	-6.436300	2.510205	0.896927
H	-6.592831	1.025280	1.891859
H	-5.045042	1.395098	1.060550
H	-6.131629	2.047074	-1.737431
H	-4.773531	1.027273	-1.176114
H	-6.081545	0.306823	-2.171003
H	-8.352217	1.793862	-0.573264
H	-8.323320	0.109281	-1.196949
H	-8.534138	0.395352	0.539870
H	4.239663	-2.472097	1.230518
H	4.012900	0.610554	1.208470
H	-6.395802	-0.372110	0.032740
H	2.141908	-1.594069	2.328714
C1	3.235145	-0.349553	4.027475
H	1.776538	0.143040	2.231801

Pd_allylC1

Num. Imaginary Frequencies: 0			
C	1.613859	0.951422	0.279158
C	0.325284	1.075472	-0.483416
C	-0.802412	1.676978	0.083382
Pd	-1.096705	-0.427616	0.021735
C1	2.455955	-0.618946	-0.035533
H	2.325890	1.725275	-0.020681
H	1.450534	1.012015	1.356117
H	0.433904	1.062735	-1.567831
H	-1.549087	2.145211	-0.554336
H	-0.784407	2.023928	1.116211

PdallylC1

Num. Imaginary Frequencies: 0			
C	-1.107164	1.458478	0.234443
Pd	0.019236	-0.259366	-0.036880
C1	2.281806	0.145818	0.020657
H	-0.757671	2.315453	-0.333855
C	-1.943896	0.487017	-0.395668
H	-1.144559	1.595357	1.314072
C	-2.103507	-0.727008	0.276139
H	-2.202089	0.580523	-1.447180
H	-2.527803	-1.582812	-0.240905
H	-2.116027	-0.767512	1.363706

PdArC1_L

Num. Imaginary Frequencies: 0			
C	-4.206037	0.546315	1.030696
C	-3.421577	0.030935	0.001820
C	-3.956790	-0.833158	-0.952331
C	-5.279350	-1.259172	-0.818021
C	-6.059330	-0.788993	0.234970
C	-5.525831	0.114605	1.153145
Pd	-1.466943	0.119014	0.015707
C1	-1.702043	2.352089	-0.601519
H	-3.359248	-1.172917	-1.795941
H	-5.701038	-1.944179	-1.548334
H	-7.091633	-1.112399	0.331391
H	-6.142849	0.494888	1.962547
H	-3.795218	1.272912	1.724761
P	0.977959	-0.087789	0.056557
C	1.882771	1.252844	0.900490
C	1.551259	-1.635341	0.850312
C	1.723078	-0.143222	-1.612977
C	1.191932	2.050956	1.815517
C	1.854167	3.071157	2.493143
C	3.205433	3.302884	2.255429
C	3.897841	2.517328	1.335207
C	3.239059	1.497903	0.656945
H	0.129964	1.890313	1.977000
H	1.307890	3.693275	3.195232
H	3.718925	4.104577	2.778169
H	4.949774	2.703791	1.140899
H	3.776944	0.895427	-0.070047
C	2.761316	-1.012263	-1.959795
C	3.299217	-0.978993	-3.243962
C	2.806983	-0.078181	-4.184549
C	1.771064	0.788490	-3.842840
C	1.224451	0.755233	-2.564249
H	3.146898	-1.719261	-1.230501
H	4.102813	-1.659754	-3.509081
H	3.229292	-0.053558	-5.184828
H	1.382423	1.490187	-4.574572

H	0.410916	1.427223	-2.299438
C	2.552279	-1.685191	1.822653
C	2.913493	-2.902979	2.395720
C	2.284167	-4.079105	2.000382
C	1.283959	-4.038178	1.030634
C	0.915516	-2.823165	0.465609
H	3.049494	-0.773475	2.138756
H	3.689699	-2.929213	3.154524
H	2.567288	-5.026027	2.450014
H	0.785996	-4.951714	0.720285
H	0.131979	-2.797680	-0.289600

TSC1Pdally1

Num. Imaginary Frequencies: 1			
C	0.526853	1.626297	0.165701
Pd	-0.417966	-0.669877	-0.016278
Cl	2.098289	0.004524	0.017272
H	1.213393	2.268961	-0.371098
C	-0.758371	1.369741	-0.445899
H	0.567441	1.719779	1.246649
C	-1.872329	0.893367	0.273241
H	-0.852807	1.573515	-1.510312
H	-2.835568	0.847229	-0.226211
H	-1.913868	0.991530	1.357871

TSC1PdAr-PPh₃

Num. Imaginary Frequencies: 1			
C	-3.961902	0.098860	-1.253821
C	-3.394352	0.328031	0.001521
C	-3.921702	-0.228020	1.169448
C	-4.995957	-1.107833	1.054583
C	-5.551622	-1.385472	-0.193326
C	-5.036589	-0.783713	-1.340366
Pd	-1.405688	0.283179	-0.022641
Cl	-2.604378	2.395278	0.262824
H	-3.504539	0.030096	2.137148
H	-5.408567	-1.565649	1.948981
H	-6.397638	-2.061450	-0.270059
H	-5.481407	-0.988575	-2.309858
H	-3.575402	0.605242	-2.131938
P	0.950296	-0.052415	-0.022035
C	1.940916	1.412438	-0.503221
C	1.615858	-0.526084	1.619764
C	1.580999	-1.375094	-1.125502
C	2.834824	-0.061532	2.120612
C	3.287844	-0.485219	3.367900
C	2.530747	-1.376127	4.123169
C	1.312349	-1.840677	3.632417
C	0.854679	-1.411372	2.391566
H	3.431299	0.635028	1.539242
H	4.233562	-0.113424	3.751185
H	2.886466	-1.703832	5.095586
H	0.712760	-2.528296	4.221257
H	-0.104178	-1.762722	2.016013
C	2.661448	-2.197134	-0.792303
C	3.109900	-3.165013	-1.687431
C	2.485167	-3.319485	-2.921915
C	1.404210	-2.507968	-3.259053
C	0.950785	-1.545658	-2.362798
H	3.151149	-2.084694	0.170667
H	3.947591	-3.801272	-1.417195
H	2.835391	-4.075248	-3.618700
H	0.908555	-2.629893	-4.217436
H	0.097954	-0.921570	-2.620895
C	3.207689	1.313195	-1.088673
C	3.923322	2.462875	-1.409274
C	3.379667	3.718945	-1.149896
C	2.116808	3.824450	-0.573308
C	1.396264	2.676704	-0.255398
H	3.634612	0.337032	-1.300410
H	4.904075	2.376480	-1.867655
H	3.937338	4.615489	-1.404809
H	1.683223	4.800920	-0.380469
H	0.401296	2.762030	0.175192

TSIVa_Va_{endo}-Me3N

Num. Imaginary Frequencies: 1			
C	2.155956	2.914332	-1.338856
C	1.678455	1.968728	-0.424708
C	2.095483	2.011360	0.913210
C	3.009528	2.978022	1.317862
C	3.489231	3.913941	0.404282
C	3.056479	3.885504	-0.921254
C	0.771684	0.923685	-0.832865
C	0.433609	-0.304999	-0.895444
Pd	1.837049	-1.423304	0.230677
Cl	0.276583	-1.409171	2.069329
C	-0.829549	-0.863076	-1.364347

C	-0.970630	-2.225511	-1.639706
C	-2.177001	-2.733368	-2.104667
C	-3.268519	-1.887704	-2.295912
C	-3.154497	-0.537707	-1.990346
C	-1.945609	-0.023297	-1.517235
C	-1.831368	1.407837	-1.143286
N	-2.917874	1.974367	-0.603349
C	-2.844260	3.338186	-0.111865
C	3.552130	-1.456388	-1.029995
C	3.597086	-2.596523	-0.187430
C	3.523699	-2.417702	1.201745
O	-0.770939	2.054879	-1.304694
H	-4.000780	0.128793	-2.126424
H	-4.207385	-2.281860	-2.672362
H	-2.267782	-3.793825	-2.319019
H	-0.118649	-2.877635	-1.476631
H	1.807875	2.881676	-2.365931
H	3.426527	4.619030	-1.631081
H	4.199728	4.670005	0.725331
H	3.340229	3.004916	2.351664
H	1.702427	1.278966	1.613821
H	-3.522130	1.314514	-0.082148
H	-2.057290	3.448910	0.643086
H	-2.627625	4.025090	-0.933154
H	-3.809753	3.598385	0.326073
H	3.975038	-1.548075	1.675220
H	3.322955	-3.263318	1.850858
H	3.385085	-3.576894	-0.609510
H	3.419408	-1.592854	-2.099152
H	4.060837	-0.538632	-0.736895
N	-3.916665	0.176819	1.428668
C	-3.707371	-1.259528	1.255081
C	-2.927865	0.713977	2.362118
C	-5.270321	0.449203	1.889417
H	-3.879722	-1.809358	2.196570
H	-4.391488	-1.642675	0.492131
H	-2.678446	-1.449055	0.937214
H	-5.482964	-0.022581	2.865572
H	-5.417896	1.529765	1.993421
H	-5.993026	0.070025	1.159556
H	-3.022861	0.264608	3.365152
H	-1.918372	0.500766	1.996772
H	-3.058952	1.798036	2.455647

TSIVa_Va_{ando}

	Imaginary Frequencies: 1		
C	-1.528359	-2.530188	-0.347020
C	-1.600225	-1.135342	-0.244873
C	-2.867935	-0.517467	-0.242343
C	-4.015750	-1.299963	-0.428803
C	-3.923635	-2.676732	-0.562454
C	-2.674953	-3.294257	-0.497530
C	-0.380222	-0.345070	-0.177506
Pd	1.599818	-1.147263	-0.030970
C	2.489112	-0.466555	-1.859400
C	3.126096	-1.665419	-1.462133
C	3.683256	-1.742926	-0.173966
C	-2.982821	0.946650	-0.015113
O	-2.039146	1.745691	-0.169381
C	-0.226509	0.915980	-0.161881
C	0.570714	2.112306	-0.068325
C	1.552272	2.191631	0.930478
C	2.382097	3.305509	0.992950
C	2.225996	4.347746	0.081758
C	1.236766	4.277777	-0.898408
C	0.412479	3.163252	-0.978851
C1	1.166956	-1.924797	2.187805
N	-4.175088	1.431929	0.390285
C	-4.339158	2.840380	0.700322
H	-4.991880	-0.831398	-0.516164
H	-4.822212	-3.265654	-0.716487
H	-2.595374	-4.373703	-0.579455
H	-0.550750	-2.997017	-0.293529
H	-0.360176	3.096678	-1.736733
H	1.114438	5.090864	-1.607487
H	2.874211	5.217421	0.136380
H	3.146616	3.361103	1.761579
H	1.656033	1.373008	1.637649
H	-4.864929	0.782931	0.731928
H	-3.743688	3.129453	1.572915
H	-4.018038	3.445808	-0.149707
H	-5.394936	3.031571	0.898756
H	4.148111	-0.871401	0.282745
H	3.967945	-2.704173	0.240110
H	2.919741	-2.584106	-2.007608
H	1.892518	-0.455529	-2.766966
H	2.895971	0.496897	-1.554362

TSIVa-Va_{exo}-Me3N

Num. Imaginary Frequencies: 1

C	0.369181	-2.310732	-0.611452
C	0.759794	-0.967305	-0.524500
C	2.114122	-0.639073	-0.655508
C	3.081472	-1.617466	-0.874224
C	2.692477	-2.947730	-0.935578
C	1.340050	-3.282906	-0.804662
C	-0.144686	0.136314	-0.350316
C	-1.318289	0.607282	-0.188335
Pd	-2.645323	-0.975218	0.345163
Cl	-3.137089	-1.661187	-1.890588
C	2.295905	0.818438	-0.601191
N	3.503373	1.384477	-0.609468
C	3.646950	2.827059	-0.564397
C	-1.913425	1.941759	-0.178888
C	-3.151656	2.152629	-0.801459
C	-3.731643	3.416083	-0.791339
C	-3.100563	4.474192	-0.140724
C	-1.874446	4.267221	0.487571
C	-1.277284	3.011862	0.464102
C	-4.170179	-2.146846	1.362068
C	-3.096094	-1.911433	2.235941
C	-2.672460	-0.577243	2.449389
O	1.239315	1.490615	-0.552913
H	-3.636163	1.319663	-1.304062
H	-4.685281	3.571489	-1.287106
H	-3.563050	5.456826	-0.122881
H	-1.377596	5.089952	0.994272
H	-0.314977	2.848729	0.936454
H	2.920702	3.288894	-1.236228
H	4.656120	3.088300	-0.888905
H	3.479436	3.221683	0.444961
H	4.332592	0.803901	-0.430269
H	4.120163	-1.337512	-1.019973
H	3.430968	-3.723642	-1.110939
H	1.035576	-4.322203	-0.881039
H	-0.684265	-2.567747	-0.568103
H	-1.733581	-0.392470	2.963413
H	-2.426478	-2.729719	2.493289
H	-3.404794	0.226742	2.508147
H	-4.369849	-3.149363	0.999049
H	-4.998030	-1.443301	1.299021
N	5.862171	0.044686	0.538701
C	6.768880	-0.934136	-0.048348
C	6.575382	1.275501	0.861243
C	5.206259	-0.494859	1.725712
H	7.590997	-1.204011	0.637463
H	6.220681	-1.848530	-0.295576
H	7.203128	-0.531273	-0.968240
H	7.375322	1.113809	1.604830
H	7.026106	1.690650	-0.045745
H	5.874070	2.011352	1.268195
H	5.926962	-0.738512	2.525233
H	4.490508	0.237701	2.112400
H	4.654275	-1.401951	1.462886

TSIVa_Va_{exo}

Num. Imaginary Frequencies: 1

C	1.848929	2.225627	1.062700
C	0.833132	1.942134	0.139860
C	0.370147	2.956479	-0.707557
C	0.918628	4.232186	-0.633207
C	1.917794	4.514076	0.295643
C	2.374376	3.509961	1.146968
C	0.289310	0.587922	0.058783
Pd	1.756171	-0.940737	-0.157681
C	3.527025	-2.028501	-0.789416
C	2.693633	-1.808093	-1.899142
C	2.278696	-0.485484	-2.185170
C	-0.885276	0.094045	0.007347
C	-1.783578	-1.026821	0.023913
C	-3.149355	-0.722026	-0.041495
C	-4.117425	-1.725494	-0.031216
C	-3.714022	-3.049390	0.051904
C	-2.351673	-3.357661	0.141855
C	-1.383021	-2.365379	0.132226
C	-3.337793	0.734064	-0.070023
O	-2.291800	1.417177	-0.024950
N	-4.549717	1.299354	-0.125395
C	-4.745751	2.737662	-0.140756
Cl	1.719237	-1.652959	2.121863
H	2.202562	1.433398	1.717067
H	3.150513	3.724285	1.875635
H	2.341607	5.512365	0.354823
H	0.560997	5.010356	-1.301649
H	-0.416909	2.733943	-1.420141
H	-3.869138	3.210828	0.302672

H	-5.629978	2.990730	0.448519
H	-4.871829	3.112094	-1.162114
H	-5.356117	0.699234	-0.196152
H	-5.177515	-1.489662	-0.078168
H	-4.453887	-3.842764	0.064126
H	-2.042574	-4.394016	0.235653
H	-0.330450	-2.602461	0.246652
H	1.490036	-0.320672	-2.913770
H	2.145527	-2.643638	-2.329885
H	2.967630	0.346535	-2.045494
H	3.674369	-3.033018	-0.407261
H	4.284008	-1.298057	-0.510790

TSIVb-Vb-PPh₃endo

Num. Imaginary Frequencies: 1

C	-0.062745	2.255992	2.596824
C	0.574292	1.029530	2.364285
C	0.481475	0.006403	3.322239
C	-0.251050	0.210335	4.484539
C	-0.887798	1.429474	4.707068
C	-0.789135	2.449982	3.763727
C	1.262175	0.776911	1.124428
C	1.561811	0.096910	0.088496
C	2.548444	0.345896	-0.950234
C	2.898424	-0.670027	-1.847544
C	3.846312	-0.449757	-2.835492
C	4.467494	0.793601	-2.946648
C	4.121563	1.814367	-2.073471
C	3.154267	1.611652	-1.081670
C	2.767902	2.714168	-0.166035
N	2.996395	3.982819	-0.564268
C	2.570481	5.100626	0.256063
Pd	0.234169	-1.501090	0.252671
Cl	-1.227576	-3.348204	0.669030
C	1.856837	-2.628147	0.744000
C	1.981782	-3.885762	0.137745
C	3.105305	-4.681316	0.357370
C	4.123021	-4.249863	1.204413
C	4.008284	-3.009344	1.821713
C	2.893060	-2.205124	1.583731
O	2.260488	2.518201	0.953382
H	4.645815	2.763451	-2.140468
H	5.226997	0.962792	-3.703306
H	4.113268	-1.254357	-3.513333
H	2.429825	-1.641303	-1.732146
H	0.950352	-0.953262	3.131630
H	-0.327502	-0.589626	5.213918
H	-1.461119	1.584175	5.616281
H	-1.286866	3.399482	3.934798
H	0.020599	3.040574	1.855446
H	3.185392	4.148097	-1.539329
H	1.478151	5.134290	0.338777
H	2.992030	5.004125	1.258454
H	2.932549	6.024543	-0.198013
H	2.858905	-1.226894	2.054903
H	4.792207	-2.655442	2.487200
H	4.993678	-4.875133	1.382642
H	3.176833	-5.651760	-0.127909
H	1.185149	-4.260378	-0.497209
P	-1.661326	-0.174646	-0.585930
C	-2.426333	-0.757728	-2.149160
C	-3.058797	0.052292	0.568976
C	-1.190829	1.550347	-1.022517
C	-2.969771	0.125577	-3.090732
C	-3.560475	-0.360241	-4.252984
C	-3.615263	-1.732020	-4.486755
C	-3.077718	-2.614805	-3.554531
C	-2.482796	-2.134586	-2.390712
H	-2.923859	1.197900	-2.924573
H	-3.975319	0.335259	-4.976980
H	-4.074858	-2.111337	-5.394969
H	-3.118483	-3.685647	-3.729855
H	-2.071105	-2.825184	-1.659387
C	-0.255510	1.730359	-2.050787
C	0.184570	3.000632	-2.398215
C	-0.297439	4.117350	-1.714970
C	-1.219995	3.949282	-0.687912
C	-1.666138	2.672521	-0.343526
H	0.131333	0.865572	-2.583570
H	0.906333	3.116009	-3.202214
H	0.038693	5.114027	-1.988453
H	-1.606942	4.813941	-0.155748
H	-2.388249	2.555348	0.458405
C	-4.301371	0.547108	0.157489
C	-5.305445	0.777707	1.090933
C	-5.077012	0.516509	2.441525
C	-3.848161	0.011869	2.854039
C	-2.844409	-0.227292	1.919688

H	-4.485728	0.746899	-0.894317
H	-6.268634	1.158884	0.764330
H	-5.863037	0.697450	3.169198
H	-3.666348	-0.206137	3.901933
H	-1.897702	-0.650766	2.236887

TSIVb_Vb-PPh_{3endo}

Num.	Imaginary Frequencies:	1
C	0.072338	3.030245
C	-0.089425	2.121641
C	-0.949022	2.424811
C	-1.657498	3.619729
C	-1.500584	4.517565
C	-0.633486	4.225004
C	0.617766	0.869131
C	0.683933	-0.408892
Pd	-1.122384	-1.155482
Cl	-2.879736	-2.242742
C	1.810394	-1.259670
C	1.611854	-2.637222
C	2.639624	-3.462378
C	3.896699	-2.926151
C	4.118010	-1.569873
C	3.093764	-0.727815
C	3.343283	0.716462
N	4.615217	1.130632
C	4.928252	2.524897
C	-2.036951	-0.707535
O	2.426339	1.560997
H	5.089741	-1.160712
H	4.697645	-3.562208
H	2.457548	-4.523872
H	0.623682	-3.042588
H	0.747823	2.785594
H	-0.514755	4.928107
H	-2.056399	5.450645
H	-2.336925	3.844638
H	-1.068077	1.715343
H	5.329802	0.440687
H	4.677049	2.809620
H	4.356467	3.155798
H	5.994723	2.681904
C	-3.237571	-0.003618
C	-3.868803	0.428360
C	-3.317355	0.151502
C	-2.133346	-0.577109
C	-1.488897	-1.008805
H	-3.680183	0.203234
H	-4.802531	0.979170
H	-3.812479	0.491791
H	-1.698014	-0.806275
H	-0.555056	-1.556162
		1.985845

TSIVb-Vb-PPh_{3exo}

Num.	Imaginary Frequencies:	1
C	3.766770	0.247849
C	2.508894	-0.335711
C	2.079499	-1.347112
C	2.878927	-1.743310
C	4.128587	-1.159109
C	4.571782	-0.169647
C	1.651430	0.096578
C	1.420327	1.209340
C	0.658449	2.048810
C	-0.185559	1.573517
C	-0.958762	2.472835
C	-0.888741	3.846820
C	-0.031280	4.327219
C	0.734772	3.427914
C	1.659660	3.710791
N	1.821773	4.944119
C	2.631584	5.176150
Pd	0.378638	-1.262457
Cl	-0.783797	-3.090292
C	2.082213	-1.920671
C	2.681382	-1.255578
C	3.870056	-1.733227
C	4.477617	-2.872213
C	3.886796	-3.534061
C	2.694579	-3.063150
O	2.283687	2.733171
H	0.037764	5.397544
H	-1.494551	4.535610
H	-1.627874	2.096253
H	-0.235607	0.507008
H	1.114192	-1.818337
H	2.529207	-2.519911
H	4.760622	-1.480520
		4.160010

H	5.550873	0.279852	2.599493
H	4.105337	1.018777	0.727162
H	1.180452	5.662987	0.187612
H	3.593417	4.673658	1.549549
H	2.796642	6.248877	1.775237
H	2.141504	4.785602	2.563285
H	2.237792	-3.597697	-0.323751
H	4.351791	-4.425967	-1.285384
H	5.404259	-3.243171	-3.201170
H	4.321919	-1.209761	-4.131020
H	2.229543	-0.355500	-3.149382
P	-1.654123	-0.486168	0.336632
C	-3.238214	-0.468959	-0.577420
C	-1.989326	-1.516728	1.815500
C	-1.551700	1.221030	1.008614
C	-4.460470	-0.280229	0.077736
C	-5.643317	-0.214943	-0.648911
C	-5.615929	-0.341505	-2.037440
C	-4.405896	-0.541120	-2.693419
C	-3.219228	-0.608011	-1.966721
H	-4.487328	-0.185520	1.159896
H	-6.588163	-0.071094	-0.133207
H	-6.541832	-0.296422	-2.603675
H	-4.382281	-0.665450	-3.771895
H	-2.281602	-0.815194	-2.471415
C	-2.285805	2.280288	0.467662
C	-2.099905	3.580473	0.932172
C	-1.177379	3.838990	1.941394
C	-0.433830	2.790598	2.480894
C	-0.613850	1.494542	2.012421
H	-3.005517	2.093441	-0.322764
H	-2.681483	4.390299	0.501288
H	-1.040298	4.851313	2.312813
H	0.295096	2.978295	3.263790
H	-0.015359	0.689969	2.431079
C	-2.498953	-1.006312	3.014074
C	-2.738625	-1.853557	4.092200
C	-2.475702	-3.216498	3.981645
C	-1.972714	-3.731266	2.789608
C	-1.726245	-2.888515	1.709658
H	-2.699174	0.056428	3.114514
H	-3.131928	-1.446471	5.019213
H	-2.663036	-3.876536	4.823755
H	-1.769437	-4.793642	2.694820
H	-1.339139	-3.292281	0.776371

TSIVb-Vb-PPh₃exo

Num. Imaginary Frequencies: 1			
C	-0.559118	-2.282083	-1.248584
C	-1.379557	-1.259002	-0.755168
C	-2.724576	-1.542697	-0.478298
C	-3.252846	-2.817550	-0.671202
C	-2.429388	-3.826554	-1.147848
C	-1.089244	-3.550541	-1.432695
C	-0.948953	0.093891	-0.514000
C	-0.069370	1.020775	-0.437328
Pd	1.780620	0.107944	-0.777499
Cl	3.913209	-0.564707	-1.422619
C	-3.414415	-0.339605	0.006511
N	-4.688220	-0.366401	0.415249
C	-5.377504	0.795615	0.946892
C	-0.098768	2.463205	-0.187696
C	1.009338	3.104116	0.385617
C	0.985371	4.471794	0.633043
C	-0.132567	5.225276	0.286291
C	-1.228695	4.602592	-0.307370
C	-1.217822	3.233114	-0.540088
C	1.691713	-0.837964	0.948945
O	-2.731783	0.705973	0.017370
H	-5.161773	-1.255937	0.440903
H	-5.530689	0.696107	2.025899
H	-6.344843	0.916402	0.452384
H	-4.762237	1.674408	0.755990
H	-4.299030	-3.030503	-0.468473
H	-2.827077	-4.823441	-1.305767
H	-0.445317	-4.338728	-1.809547
H	0.480884	-2.076025	-1.476031
H	1.891021	2.520567	0.636002
H	1.848843	4.949287	1.085625
H	-0.146615	6.295868	0.468032
H	-2.098171	5.187821	-0.592528
H	-2.071457	2.750075	-0.999533
C	2.112153	-2.167494	0.999417
C	2.051246	-2.863533	2.205763
C	1.587286	-2.239846	3.360509
C	1.182459	-0.910124	3.305336
C	1.227705	-0.206222	2.101662
H	2.510985	-2.650371	0.114615

H	2.385227	-3.897087	2.239972
H	1.548001	-2.784759	4.299290
H	0.821686	-0.410325	4.200330
H	0.892618	0.825291	2.078362

TSVIIa-VIIa-AC_{endo}-Me3N

Num. Imaginary Frequencies:	1		
C	2.609315	3.464405	-0.168294
C	2.503065	2.083052	0.055112
C	3.553950	1.435497	0.716847
C	4.685679	2.138022	1.116928
C	4.786845	3.504195	0.874034
C	3.740357	4.163710	0.233140
C	1.303341	1.365107	-0.421642
O	0.230056	2.236480	-0.466525
C	-1.042953	1.833514	-0.742133
C	-1.201126	0.507675	-1.349777
C	-0.089858	-0.354414	-1.393902
C	1.189399	0.085036	-0.836665
C	-2.445957	0.093234	-1.832885
C	-2.604273	-1.177737	-2.362875
C	-1.505582	-2.037378	-2.424541
C	-0.267364	-1.631284	-1.948923
N	-2.020514	2.601607	-0.471997
C	-1.737209	3.891328	0.126456
Pd	2.362912	-1.532445	-0.036761
C	1.292113	-1.562794	1.852921
C	-0.168109	-1.791115	1.616130
C	4.375719	-2.247986	-0.986592
C	3.429049	-1.868959	-1.915865
C	2.841515	-0.533388	-1.971871
C	2.227801	-2.595217	1.838508
H	3.175474	-2.485794	2.358308
C	-5.010732	1.931277	0.878010
N	-4.996082	0.458086	1.013131
C	-3.682776	-0.061045	1.448367
C	-6.100808	-0.040307	1.857668
C1	-5.953939	-0.505166	-1.542461
H	4.705948	-3.280074	-0.938585
H	4.994600	-1.513394	-0.476027
H	2.968920	-2.643084	-2.527915
H	2.214325	-0.357024	-2.840530
H	0.576654	-2.314446	-1.982961
H	-1.620160	-3.033603	-2.841810
H	-3.589821	-1.483080	-2.699160
H	-3.297924	0.763726	-1.786901
H	-2.668425	4.314679	0.514121
H	-1.005967	3.831480	0.943250
H	3.474595	0.374305	0.935999
H	5.485786	1.614590	1.632379
H	5.669873	4.052503	1.187891
H	3.805979	5.230776	0.042668
H	1.799142	3.985837	-0.665401
H	-1.337056	4.591437	-0.619014
H	3.498605	0.300071	-1.733377
H	1.914695	-3.617845	1.637517
H	1.532359	-0.634650	2.368695
H	-5.230397	0.064509	0.007933
H	-3.513451	0.183842	2.500575
H	-3.670900	-1.144086	1.313719
H	-2.908886	0.394911	0.831371
H	-4.897048	2.392022	1.864235
H	-4.184324	2.225007	0.224269
H	-5.962486	2.219228	0.427937
H	-6.008880	0.369502	2.867507
H	-7.044070	0.260944	1.399860
H	-6.055069	-1.130103	1.883645
C1	-1.065354	-1.981278	3.195159
H	-0.640763	-0.946957	1.116425
H	-0.359984	-2.699443	1.043832

TSVIIa-VIIa-AC_{exo}-Me3N

Num. Imaginary Frequencies:	1		
C	3.766706	1.496512	0.826583
C	2.796299	1.657799	-0.173137
C	2.684833	2.917862	-0.782057
C	3.489014	3.978285	-0.380933
C	4.431148	3.806732	0.630082
C	4.568182	2.558509	1.230755
C	1.971830	0.513144	-0.617730
Pd	2.500746	-1.462864	0.116189
C	2.101293	-2.475606	1.977865
H	3.047979	-2.659889	2.477998
C	0.679134	0.643640	-0.968383
C	-0.314805	-0.314097	-1.456574
C	-1.538938	0.354361	-1.535204
C	-1.322152	1.725781	-1.072762
O	0.016472	1.865405	-0.801711

C	-2.710637	-0.282587	-1.919334
C	-2.642323	-1.637703	-2.227584
C	-1.421379	-2.316717	-2.158587
C	-0.248906	-1.670242	-1.772769
N	-2.182695	2.635184	-0.888337
C	-1.736319	3.919708	-0.380060
C	1.503916	-1.218795	2.040370
C	0.036707	-1.010144	1.831771
C	4.208994	-2.707061	-0.862947
C	3.399155	-2.077523	-1.785508
C	3.210225	-0.629458	-1.842221
C	-5.101041	1.911277	0.619345
N	-5.063172	0.487258	1.019866
C	-3.734687	0.066600	1.511678
C	-6.141041	0.144822	1.970915
C1	-6.034416	-1.030436	-1.250371
H	1.958073	3.065819	-1.572580
H	3.380986	4.944060	-0.866063
H	5.059349	4.636155	0.940878
H	5.305596	2.407568	2.013848
H	3.891407	0.520749	1.289057
H	-0.896176	3.841797	0.321295
H	-2.575847	4.412957	0.118521
H	-1.420817	4.563912	-1.210354
H	-3.664155	0.234579	-1.958612
H	-3.558137	-2.156519	-2.490920
H	-1.386901	-3.376118	-2.395596
H	0.679974	-2.223256	-1.689741
H	2.648265	-0.284673	-2.703856
H	2.746778	-2.692320	-2.402929
H	4.085478	-0.019608	-1.629828
H	4.239679	-3.790556	-0.818288
H	5.012486	-2.177159	-0.356045
H	-3.514941	0.559246	2.462562
H	-3.735621	-1.016216	1.646150
H	-2.984575	0.339317	0.769977
H	-4.997541	2.542857	1.507173
H	-4.281843	2.110538	-0.078698
H	-6.058749	2.097600	0.129835
H	-6.008584	0.704432	2.901107
H	-7.098129	0.385046	1.506010
H	-6.105517	-0.928571	2.162657
H	1.502457	-3.358001	1.759576
H	2.006149	-0.417457	2.578694
H	-5.313574	-0.098315	0.117927
H	-0.407152	-1.771036	1.188564
C1	-0.873569	-1.086871	3.414015
H	-0.176940	-0.021888	1.426602

TSVIA-VIIa-dba_{endo}

Num. Imaginary Frequencies: 1			
C	2.238104	-0.705727	-2.392105
C	1.124152	-1.343604	-1.833367
C	1.218485	-2.706190	-1.528031
C	2.394825	-3.404305	-1.768059
C	3.499221	-2.755775	-2.317146
C	3.416155	-1.403208	-2.633009
C	-0.062761	-0.523449	-1.528275
C	-1.337682	-0.961558	-1.163641
C	-2.491307	-0.026334	-1.245343
C	-3.805172	-0.576573	-0.819211
Pd	-0.353549	-0.279488	0.644527
C	-2.025992	0.180411	2.199257
C	-0.808344	-0.113674	2.781059
C	0.420321	0.631552	2.519948
C	1.716031	0.210240	0.916198
C	2.554811	-0.962968	1.156591
C	3.902995	-0.940998	0.766447
C	4.448777	0.264138	0.132155
O	3.622210	1.351797	0.059126
C	2.285603	1.319096	0.397703
C	2.063731	-2.131366	1.762718
C	2.882366	-3.230561	1.963367
C	4.218890	-3.196610	1.558426
C	4.724130	-2.054018	0.960932
C	1.684342	2.651108	0.168390
C	2.504862	3.787447	0.254215
C	1.978843	5.059929	0.072626
C	0.625077	5.229656	-0.209975
C	-0.194782	4.111046	-0.315459
C	0.328047	2.835353	-0.130245
N	5.630457	0.333886	-0.323502
C	6.053477	1.579671	-0.930009
O	-2.371463	1.136201	-1.617854
H	-2.877023	-0.473309	2.358732
H	-2.241539	1.163509	1.786068
H	-0.712672	-1.051235	3.326444
H	1.254883	0.351121	3.155119

H	1.019122	-2.176724	2.055892
H	2.477428	-4.123634	2.430649
H	4.858987	-4.060171	1.710845
H	5.755340	-1.992263	0.630566
H	6.152270	2.377844	-0.180726
H	7.029568	1.433398	-1.399741
H	-0.333215	1.985212	-0.258197
H	-1.246481	4.217431	-0.562741
H	0.216343	6.224836	-0.357941
H	2.632138	5.924176	0.150177
H	3.560813	3.664633	0.466497
H	5.344818	1.938148	-1.689475
H	0.326489	1.705041	2.371066
H	-1.562804	-2.020256	-1.053121
H	-0.012695	0.499775	-1.898198
H	0.376827	-3.217361	-1.068906
H	2.458129	-4.456584	-1.507456
H	4.424518	-3.298371	-2.483875
H	4.277331	-0.885302	-3.043201
H	2.181926	0.356548	-2.616547
C	-4.899718	0.195887	-0.847109
H	-3.830118	-1.610639	-0.483601
C	-6.266699	-0.163324	-0.455786
H	-4.755274	1.213640	-1.208752
C	-7.283547	0.784452	-0.629708
C	-8.598149	0.498905	-0.277061
C	-8.918173	-0.743723	0.261234
C	-7.916494	-1.696950	0.443550
C	-6.604952	-1.410585	0.089665
H	-7.036098	1.755245	-1.051420
H	-9.371339	1.247404	-0.421844
H	-9.943409	-0.970547	0.537922
H	-8.160163	-2.667239	0.865913
H	-5.836864	-2.163410	0.240267

TSVIIa-VIIa-dba_{exo}

Num.	Imaginary Frequencies:	1
C	0.240293	3.018738
C	1.366493	2.495061
C	2.409206	3.377771
C	2.339963	4.722876
C	1.225909	5.222747
C	0.176980	4.363926
C	1.420062	1.071146
C	2.546400	0.336744
C	2.836652	-1.044249
C	4.173439	-1.292894
C	4.722768	-0.080781
O	3.724017	0.865936
C	4.772509	-2.522201
C	3.994326	-3.525403
C	2.649749	-3.290140
C	2.055861	-2.056565
N	5.880661	0.106924
C	6.164459	1.404581
Pd	-0.422709	-0.057919
C	-2.081901	0.076903
C	-0.812879	-0.042437
C	0.264903	0.913622
C	-1.382504	-0.798863
C	-0.124429	-0.321489
C	1.075571	-1.131161
C	2.206518	-0.480313
C	3.384344	-1.177117
C	3.452418	-2.542662
C	2.332496	-3.204054
C	1.156018	-2.505949
C	-2.573046	0.087673
O	-2.504383	1.251041
C	-3.859404	-0.514293
C	-4.981959	0.217336
C	-6.324281	-0.207334
C	-7.332754	0.759598
C	-8.620325	0.413914
C	-8.923265	-0.911615
C	-7.931990	-1.887024
C	-6.646495	-1.539800
H	-0.597916	2.372644
H	-0.702115	4.737404
H	1.172802	6.274320
H	3.160292	5.384991
H	3.282673	3.002475
H	7.122835	1.357453
H	6.235063	2.180421
H	5.386542	1.722724
H	5.813473	-2.679833
H	4.428038	-4.501114
H	2.054111	-4.090491
		2.328944

H	1.001508	-1.904321	1.857290
H	1.162775	0.736834	3.063953
H	-0.550186	-0.970825	3.238469
H	-0.021077	1.962037	2.437641
H	-2.813617	-0.708779	2.360331
H	-2.467265	1.029070	1.844418
H	-1.569890	-1.863507	-1.087184
H	-0.099368	0.692021	-1.977910
H	2.164729	0.591605	-2.552523
H	4.257096	-0.650487	-2.994540
H	4.377667	-3.084326	-2.528919
H	2.381866	-4.266620	-1.641636
H	0.300713	-3.032513	-1.203816
H	-3.839750	-1.551183	-0.524549
H	-4.881842	1.251858	-1.169679
H	-7.099149	1.795522	-0.561130
H	-8.164656	-2.924434	0.480548
H	-5.889736	-2.313502	-0.221992
H	-9.386840	1.179303	0.141085
H	-9.928473	-1.186495	0.668751

TSV1a-VIIa-dba_{endo}-Me3N

Num. Imaginary Frequencies:	1	
C	-1.765697	-1.549525
C	-0.488617	-2.050979
C	-0.384497	-3.356792
C	-1.521425	-4.126437
C	-2.785627	-3.602632
C	-2.902111	-2.310940
C	0.681007	-1.167896
C	2.009454	-1.510221
C	3.135478	-0.718837
C	4.495174	-1.161536
Pd	1.317560	-0.293934
C	3.219619	0.101395
C	2.041717	0.121640
C	0.957112	1.060927
C	-0.511782	0.833905
C	-1.669755	0.056313
C	-2.966797	0.511538
C	-3.129428	1.772530
O	-2.004503	2.490011
C	-0.729066	2.014429
C	-1.536696	-1.158685
C	-2.650913	-1.906442
C	-3.932200	-1.458766
C	-4.086008	-0.249712
C	0.268249	3.019434
C	0.036756	4.374084
C	0.981505	5.334200
C	2.165672	4.960304
C	2.391942	3.620824
C	1.448425	2.656836
N	-4.257450	2.220360
C	-4.269840	3.481564
O	2.967961	0.252757
H	3.960163	-0.668978
H	3.548041	0.960705
H	1.836056	-0.695473
H	0.156022	1.047933
H	-0.540285	-1.534057
H	-2.522018	-2.861487
H	-4.807387	-2.061915
H	-5.076128	0.098008
H	-5.275718	3.654326
H	-3.554778	3.502835
H	1.624842	1.626337
H	3.292159	3.311217
H	2.900667	5.713280
H	0.793629	6.378983
H	-0.885414	4.667642
H	-4.017296	4.322886
H	1.259201	2.062013
H	2.262829	-2.487712
H	0.523430	-0.312279
H	0.591330	-3.780897
H	-1.417230	-5.136038
H	-3.686451	-4.173626
H	-3.896709	-1.905236
H	-1.859232	-0.530638
C	5.578602	-0.485650
H	4.562280	-2.029892
C	6.982757	-0.766747
H	5.392276	0.379725
C	7.961533	0.138589
C	9.307064	-0.074686
C	9.697968	-1.203791
C	8.735873	-2.117151

C	7.392973	-1.901700	0.308257
H	7.658570	1.020527	2.011695
H	10.049645	0.640333	1.514634
H	10.747957	-1.375921	0.243752
H	9.036056	-3.003297	-0.521220
H	6.658002	-2.628152	-0.025092
H	-6.452006	-0.920957	1.082375
N	-6.579835	-0.076587	1.782546
C	-7.540826	-0.584040	2.782486
C	-5.263883	0.240775	2.373957
C	-7.129077	1.046118	0.989936
H	-5.375690	1.035280	3.118273
H	-4.864860	-0.659849	2.844454
H	-4.600746	0.575347	1.574121
H	-7.435036	1.852620	1.663583
H	-6.351572	1.400124	0.306555
H	-7.988517	0.674336	0.428826
H	-7.748115	0.190882	3.525990
H	-8.455587	-0.875264	2.264291
H	-7.112237	-1.467472	3.258091
Cl	-6.513669	-2.395720	0.052155

TSV1a-VIIa-dba_{exo}-Me3N

Num.	Imaginary Frequencies:	1
C	-8.428856	-0.598767
C	-7.238503	-1.266238
C	-7.324657	-2.524513
C	-8.559076	-3.091510
C	-9.735201	-2.414353
C	-9.666542	-1.165314
C	-5.962803	-0.620240
C	-4.727137	-1.084847
C	-3.535723	-0.291055
O	-3.643433	0.801981
C	-2.219375	-0.901102
C	-1.035816	-0.255600
C	0.305821	-0.864831
C	1.323040	-0.152826
C	2.612878	-0.669235
C	2.915496	-1.900129
C	1.909521	-2.617240
C	0.620330	-2.108034
Pd	-1.607257	0.282573
C	-1.323263	1.658009
C	-2.229721	0.561021
C	-3.432534	0.334237
C	-0.021708	1.748409
C	1.205442	1.218228
C	1.686453	-0.021347
C	3.053518	-0.116876
C	3.432760	1.071848
O	2.320986	1.849738
C	3.805590	-1.220304
C	3.160258	-2.241625
C	1.797510	-2.143515
C	1.044162	-1.043956
N	4.567206	1.386555
C	4.647498	2.626582
C	-0.254348	3.061909
C	0.584138	4.152770
C	0.357465	5.395467
C	-0.717103	5.581476
C	-1.570730	4.515152
C	-1.351204	3.271971
C	6.346212	-0.473967
N	7.242242	-1.055480
C	8.452782	-1.663906
C	7.555469	-0.098136
Cl	6.004994	-3.440556
H	-2.040892	2.459091
H	-2.417838	4.645434
H	-0.892072	6.551909
H	1.022514	6.223033
H	1.422617	4.020621
H	5.639922	2.704508
H	4.499132	3.501586
H	3.889876	2.678400
H	4.849667	-1.322895
H	3.720650	-3.129761
H	1.308947	-2.955737
H	-0.022852	-1.011458
H	-0.480717	1.763791
H	-1.858772	-0.200249
H	-1.789933	2.606455
H	-4.017053	-0.547324
H	-3.946076	1.117213
H	6.866246	0.327075
H	6.053333	-1.263581

H	5.467667	-0.075045	-1.504420
H	8.233133	0.673065	-0.290967
H	6.621133	0.359251	0.427204
H	8.031509	-0.648481	0.902620
H	9.053487	-0.895019	-2.076355
H	9.022181	-2.140507	-0.782744
H	8.144009	-2.428523	-2.296536
H	-2.220110	-1.952932	-0.683577
H	-1.153927	0.670655	-1.885771
H	1.099434	0.821716	-2.478269
H	3.383036	-0.093700	-2.643280
H	3.924286	-2.304021	-1.572523
H	2.150527	-3.564446	-0.444656
H	-0.141940	-2.667508	-0.306356
H	-4.548216	-2.041303	-0.396990
H	-6.026880	0.350876	-1.601464
H	-8.377400	0.376227	-1.578549
H	-8.606961	-4.067197	0.589372
H	-6.419563	-3.068114	0.083662
H	6.704438	-1.905189	-0.543298

TSVIIa-VIIa_{exo}

Num. Imaginary Frequencies:	1		
C	1.980857	-1.981261	0.193830
C	1.900777	-0.596228	0.056223
C	3.066227	0.167640	0.001622
C	4.328230	-0.401768	0.094985
C	4.405805	-1.782059	0.249153
C	3.242147	-2.559922	0.295547
C	2.674255	1.570591	-0.164181
O	1.295195	1.606687	-0.195153
C	0.768619	0.329769	-0.035426
C	-0.563585	0.148903	0.077787
Pd	-1.371213	-1.619377	-0.720227
C	-1.188123	-1.232873	1.430760
C	-1.555227	-2.653148	1.179516
C	-2.763238	-3.095541	0.702905
N	3.422921	2.580173	-0.262274
C	2.814283	3.886939	-0.429913
C	-1.481713	1.312361	0.126581
C	-2.532712	1.442629	-0.788523
C	-3.419523	2.511953	-0.712936
C	-3.276366	3.468164	0.288860
C	-2.239017	3.347767	1.211003
C	-1.351035	2.280637	1.131363
H	-2.646318	0.698335	-1.574607
H	-4.222633	2.597630	-1.439097
H	-3.970495	4.300960	0.351778
H	-2.120679	4.088988	1.996276
H	-0.541790	2.192513	1.850433
H	2.671357	4.092994	-1.498173
H	3.494773	4.645851	-0.034149
H	1.838612	3.983355	0.062046
H	5.214182	0.222736	0.046760
H	5.375336	-2.264319	0.325921
H	3.326632	-3.637223	0.403186
H	1.086438	-2.596037	0.192587
H	-0.279266	-1.137961	2.019972
H	-0.772112	-3.392517	1.347927
H	-1.995292	-0.607349	1.808476
H	-2.936451	-4.155659	0.552680
H	-3.632471	-2.442994	0.660627

TSVIB-VIIB-PPh₃endo

Num. Imaginary Frequencies:	1		
C	-2.414021	-1.577949	2.419603
C	-1.789804	-0.326068	2.270240
C	-2.117244	0.689349	3.181563
C	-3.022975	0.457863	4.213713
C	-3.625152	-0.788636	4.357238
C	-3.313850	-1.804446	3.457506
Pd	0.069443	-0.442273	1.427782
C	-1.450338	0.454489	0.368982
C	-2.142312	-0.184723	-0.601181
O	-2.809917	0.484533	-1.606193
C	-2.824637	1.844446	-1.718645
C	-2.008436	2.595727	-0.758335
C	-1.325938	1.914350	0.262819
C	-0.490244	2.672037	1.102484
C	-0.363295	4.041967	0.948717
C	-1.068036	4.705803	-0.058644
C	-1.881512	3.979635	-0.910480
C	-2.351158	-1.637044	-0.771250
C	-1.292426	-2.547197	-0.697152
C	-1.515788	-3.912473	-0.842608
C	-2.803345	-4.387894	-1.073846
C	-3.862834	-3.486975	-1.172029
C	-3.638367	-2.122920	-1.031263

N	-3.495582	2.398718	-2.643274
C	-4.237178	1.540961	-3.544687
P	2.010975	-0.281407	0.069675
C	2.596432	-1.821409	-0.731368
C	2.428648	-3.023141	-0.035468
C	2.856846	-4.227082	-0.587676
C	3.449550	-4.241798	-1.847519
C	3.610654	-3.051714	-2.553574
C	3.184861	-1.848199	-2.000663
C	1.540686	0.794952	-1.336697
C	0.651283	0.299084	-2.298486
C	0.103429	1.146484	-3.253747
C	0.429418	2.500961	-3.255417
C	1.317916	2.998879	-2.308636
C	1.870533	2.151258	-1.351800
C	3.520849	0.503055	0.748198
C	4.746367	0.516065	0.073646
C	5.845770	1.160715	0.628943
C	5.731751	1.802953	1.861251
C	4.517124	1.795744	2.539316
C	3.417552	1.144229	1.985726
H	-2.425600	4.454015	-1.719969
H	-0.969520	5.780109	-0.181077
H	0.294287	4.597937	1.610889
H	0.082117	2.157059	1.869456
H	-0.286233	-2.184191	-0.517745
H	-0.676211	-4.599538	-0.785721
H	-2.980973	-5.453219	-1.187779
H	-4.869632	-3.850532	-1.355577
H	-4.463294	-1.421872	-1.106396
H	-3.573092	0.878838	-4.118648
H	-4.947095	0.893124	-3.011771
H	-4.797176	2.162711	-4.248106
H	-2.202799	-2.382616	1.724512
H	-3.776878	-2.782477	3.557617
H	-4.336550	-0.965060	5.158862
H	-3.261656	1.261097	4.905690
H	-1.684502	1.677858	3.078542
H	2.543740	2.556064	-0.602036
H	1.565371	4.055778	-2.295973
H	-0.024549	3.167296	-3.982222
H	-0.599390	0.753040	-3.981807
H	0.368895	-0.750049	-2.293323
H	3.290223	-0.926382	-2.566045
H	4.063905	-3.061308	-3.540260
H	3.778563	-5.180375	-2.283420
H	2.720473	-5.153557	-0.037905
H	1.947501	-3.013192	0.940099
H	4.845142	0.014913	-0.884608
H	6.794596	1.161877	0.100823
H	6.592845	2.304342	2.293111
H	4.424182	2.290203	3.501494
H	2.468036	1.128447	2.516024

TSVIB-VIIB-PPh₃exo

Num.	Imaginary Frequencies:	1
C	4.608472	-1.160573
C	3.319221	-1.559627
C	3.050097	-2.917671
C	4.052581	-3.867049
C	5.332586	-3.462138
C	5.609839	-2.108465
P	1.944830	-0.370088
C	2.753517	1.112332
C	2.930935	1.135609
C	3.524090	2.228998
C	3.929336	3.324164
C	3.752352	3.311367
C	3.174441	2.207601
Pd	-0.020732	-1.017240
C	-1.780696	-1.360031
C	-2.232682	-2.685167
C	-3.072544	-3.190351
C	-3.496323	-2.370146
C	-3.076768	-1.041590
C	-2.229602	-0.536121
C	-1.705102	-0.397122
C	-1.905392	0.925210
O	-2.730006	1.395334
C	-2.624439	2.755480
C	-1.744485	3.222279
C	-1.315741	2.101385
C	-0.394936	2.254727
C	0.066765	3.533509
C	-0.376386	4.650217
C	-1.291492	4.502624
N	-3.173790	3.440356
C	-3.967860	2.718653

C	-2.377899	-1.320624	0.785453
C	-3.729920	-1.643623	0.630283
C	-4.363508	-2.486713	1.536348
C	-3.655513	-3.019886	2.611379
C	-2.309536	-2.702204	2.773694
C	-1.673882	-1.861346	1.865300
C	1.497801	0.093456	1.783099
C	1.818729	-0.721340	2.871560
C	1.280736	-0.453440	4.128947
C	0.419903	0.624948	4.309889
C	0.111254	1.453956	3.232907
C	0.648348	1.189446	1.979321
H	-3.418642	1.874103	3.437148
H	-4.879381	2.306129	2.546626
H	-4.260935	3.406152	3.796283
H	-1.638915	5.347236	0.331195
H	0.008291	5.634833	-1.539532
H	0.802348	3.660730	-2.799041
H	-0.019023	1.393977	-2.262036
H	-0.627082	-1.607747	1.998757
H	-1.750106	-3.105889	3.612986
H	-4.151336	-3.678551	3.318718
H	-5.414537	-2.726520	1.402446
H	-4.276376	-1.229465	-0.211709
H	-1.938921	0.509501	-3.153474
H	-3.419618	-0.390862	-4.900701
H	-4.164839	-2.758272	-4.815950
H	-3.407977	-4.222559	-2.956789
H	-1.948770	-3.318683	-1.184013
H	2.475662	-1.575929	2.740150
H	1.532480	-1.096868	4.966894
H	-0.011346	0.819423	5.287155
H	-0.559203	2.299399	3.358810
H	0.399959	1.837086	1.145220
H	3.036675	2.209102	1.192035
H	4.063554	4.163164	0.088989
H	4.380000	4.186139	-2.371012
H	3.659421	2.232309	-3.727024
H	2.590383	0.294419	-2.630298
H	4.828072	-0.106219	0.790777
H	6.609546	-1.791721	1.106906
H	6.116944	-4.200596	0.776136
H	3.834723	-4.920046	0.121892
H	2.048972	-3.228958	-0.202206

TSVa-VIIIta_{endo}-Me3N

Num. Imaginary Frequencies: 1			
C	1.970064	3.142288	-0.980962
C	1.870486	1.898557	-0.339374
C	2.866846	1.527428	0.572119
C	3.948253	2.368705	0.811883
C	4.046018	3.594980	0.161569
C	3.048573	3.981029	-0.732147
C	0.739211	1.009450	-0.632949
O	-0.428701	1.772215	-0.781575
C	-1.600063	1.234275	-0.964813
C	-1.704760	-0.134396	-1.360516
C	-0.552286	-0.930863	-1.210148
C	0.694828	-0.351843	-0.727823
C	-0.668689	-2.302118	-1.521804
C	-1.859296	-2.827103	-1.975577
C	-2.990582	-2.008701	-2.155002
C	-2.914761	-0.670467	-1.847804
N	-2.655876	2.011659	-0.740859
C	-2.481770	3.382663	-0.286741
Pd	1.634569	-1.548443	0.639211
C	3.089004	-2.326461	-0.842216
C	4.083508	-2.250608	0.091585
C1	0.185176	-1.250854	2.547492
C	2.374525	-1.168146	-1.429344
H	4.556490	-3.150433	0.468774
H	4.519688	-1.298499	0.382227
H	2.778140	-3.316133	-1.177442
H	1.898894	-1.412724	-2.378477
H	0.192967	-2.943991	-1.374820
H	-1.924746	-3.886959	-2.201355
H	-3.912946	-2.430978	-2.540369
H	-3.770807	-0.019769	-1.994038
H	-1.940035	3.963627	-1.036820
H	-3.470914	3.820798	-0.148834
H	-3.465684	1.483714	-0.343742
H	2.767229	0.589035	1.112714
H	4.707019	2.067124	1.527553
H	4.888737	4.251915	0.355194
H	3.115151	4.937224	-1.242829
H	1.204393	3.446092	-1.688566
H	-1.925357	3.430212	0.656439
H	2.969972	-0.259481	-1.497628

N	-4.351448	0.515139	0.967906
C	-5.513526	-0.269251	0.565138
C	-3.340212	-0.340258	1.603252
C	-4.747232	1.586238	1.878537
H	-6.011866	-0.742676	1.428106
H	-6.238738	0.374486	0.056300
H	-5.199204	-1.057530	-0.124763
H	-5.207891	1.195983	2.801428
H	-3.865663	2.170190	2.162072
H	-5.466766	2.249095	1.385645
H	-3.707448	-0.768687	2.549156
H	-3.068375	-1.160716	0.935751
H	-2.428330	0.224272	1.819368

TSVa-VIIIa_{exo}-Me3N

Num.	Imaginary Frequencies:	1
C	0.239443	-2.577104
C	0.643922	-1.227543
C	2.016476	-0.915529
C	2.991417	-1.904222
C	2.575567	-3.215507
C	1.205147	-3.540677
C	-0.074168	-0.013322
O	0.897234	1.022230
C	2.093841	0.500017
C	-1.402843	0.308395
Pd	-2.573723	-0.975239
C	-4.836891	-1.689766
C	-3.551326	-1.753239
C	-2.655335	-0.582386
N	3.150266	1.304406
C	2.999319	2.735101
C	-1.743233	1.758546
C	-1.582158	2.575283
C	-1.900967	3.928106
C	-2.371870	4.482250
C	-2.525395	3.674655
C	-2.223362	2.317445
C1	-2.183203	-0.934603
N	5.511061	0.241191
C	4.818657	-0.418527
C	6.085549	1.509285
C	6.545490	-0.621978
H	-2.347687	1.681004
H	-2.892546	4.100116
H	-2.619712	5.538679
H	-1.781346	4.548471
H	-1.206035	2.142905
H	3.962433	3.212082
H	2.259591	3.138933
H	2.670649	2.964229
H	4.059126	0.867021
H	4.035422	-1.636096
H	3.297069	-4.009536
H	0.910919	-4.585675
H	-0.801883	-2.840234
H	-1.879080	-0.820064
H	-3.122129	-2.733173
H	-3.200264	0.320541
H	-5.422547	-2.592575
H	-5.333960	-0.738783
H	7.335310	-0.851257
H	7.007299	-0.136227
H	6.103661	-1.567460
H	5.498860	-0.644822
H	4.368546	-1.352188
H	4.015978	0.227793
H	6.843029	1.373024
H	5.294740	2.156219
H	6.559423	2.013602

Va_{endo}-Me3N

Num.	Imaginary Frequencies:	0
O	-0.960877	1.559825
C	0.336108	1.026668
C	0.574324	-0.301427
C	-0.570229	-1.150841
C	-1.848457	-0.604648
C	-1.998268	0.806599
C	-2.931444	-1.423674
C	-2.766501	-2.786033
C	-1.519449	-3.353558
C	-0.447279	-2.559583
C	1.288427	2.128231
C	1.237110	3.293187
C	2.171786	4.305554
C	3.162550	4.169326
C	3.204919	3.021610

C	2.270634	2.007850	0.972365
Pd	2.458042	-1.085342	0.059767
C	4.644001	-1.533328	0.103037
C	4.173943	-1.455730	-1.208713
C	3.459221	-0.300335	-1.637489
N	-3.166713	1.445791	-0.694480
C	-3.249343	2.883540	-0.501705
Cl	1.804054	-1.997889	2.192814
H	-3.878931	-0.975184	-1.478130
H	-3.588361	-3.423474	-1.567153
H	-1.399223	-4.432408	-0.946585
H	0.514584	-2.991226	-0.329112
H	0.475184	3.396073	-1.558679
H	2.132004	5.198693	-1.219273
H	3.895748	4.957617	0.511271
H	3.963159	2.916367	1.926106
H	2.288443	1.120029	1.598802
H	-4.013812	0.893378	-0.474312
H	-2.931680	3.179860	0.504769
H	-2.617732	3.402337	-1.226570
H	-4.286174	3.184148	-0.658311
H	4.957535	-0.638894	0.637285
H	4.992342	-2.478247	0.505837
H	4.091685	-2.371723	-1.791442
H	2.966326	-0.320605	-2.605482
H	3.779591	0.686921	-1.305930
N	-5.404377	0.137807	0.582738
C	-6.146229	1.315805	1.021371
C	-6.309592	-0.852336	0.009743
C	-4.643568	-0.434317	1.692941
H	-7.074818	-1.181327	0.733442
H	-6.816388	-0.429463	-0.863253
H	-5.740744	-1.731199	-0.307221
H	-5.297014	-0.746961	2.524433
H	-4.078234	-1.302529	1.343596
H	-3.931732	0.306386	2.071071
H	-6.889294	1.073977	1.800352
H	-5.451789	2.056820	1.430565
H	-6.670874	1.761334	0.169983

Va_{endo}

Num.	Imaginary Frequencies:	0
C	0.258255	3.333966
C	0.426752	2.115835
C	1.564648	1.922861
C	2.530282	2.919550
C	2.366585	4.121967
C	1.224229	4.329405
C	-0.567623	1.036532
C	-0.368559	-0.294945
Pd	1.529813	-1.110800
Cl	1.322149	-2.007759
C	-1.561155	-1.118122
C	-1.467393	-2.530065
C	-2.595276	-3.315469
C	-3.881724	-2.737380
C	-4.015918	-1.372502
C	-2.862045	-0.553118
C	-2.939894	0.868549
N	-4.072503	1.579462
C	-4.094327	3.028753
C	2.179194	-0.351971
C	2.952772	-1.513482
C	3.672615	-1.588032
O	-1.865130	1.593578
H	-5.014269	-0.943183
H	-4.762580	-3.370488
H	-2.495504	-4.396484
H	-0.477094	-2.970040
H	-0.624615	3.494708
H	1.088400	5.266477
H	3.122797	4.898121
H	3.408743	2.757349
H	1.677596	0.994407
H	-4.944623	1.079908
H	-3.549569	3.355020
H	-3.640545	3.495444
H	-5.133708	3.348149
H	4.095456	-0.694041
H	4.082329	-2.534610
H	2.745378	-2.432177
H	1.502777	-0.371744
H	2.571160	0.633019

Va_{exo}-Me3N

Num.	Imaginary Frequencies:	0
O	-1.100309	0.971552
C	0.009976	0.042797

C	-0.602351	-1.258750	-0.041642
C	-1.997339	-1.104284	0.025237
C	-2.223727	0.310345	0.077155
C	-2.872903	-2.196958	0.066758
C	-2.318753	-3.459710	0.032601
C	-0.917642	-3.624294	-0.026627
C	-0.051256	-2.548332	-0.060095
C	1.275247	0.489355	-0.048178
C	1.554687	1.937550	0.020655
C	2.386461	2.428167	1.037912
C	2.672992	3.785966	1.116979
C	2.166114	4.672005	0.167414
C	1.356723	4.190152	-0.857945
C	1.044299	2.835790	-0.925741
N	-3.356691	0.982047	0.159671
C	-3.377389	2.434762	0.207020
Pd	2.899043	-0.741588	-0.116480
C	3.503478	-0.327263	-2.108834
C	4.075492	-1.582455	-1.748272
C	4.880559	-1.684933	-0.615852
Cl	2.724226	-1.360379	2.198120
H	2.790557	1.728099	1.764617
H	3.308526	4.152516	1.918151
H	2.404976	5.730170	0.224110
H	0.965450	4.871961	-1.608488
H	0.411119	2.462539	-1.725861
H	-2.613379	2.801716	0.896046
H	-4.359380	2.753251	0.560442
H	-3.191080	2.869521	-0.780871
H	-4.259111	0.478610	0.114581
H	-3.945739	-2.053581	0.136480
H	-2.959104	-4.335386	0.065773
H	-0.507767	-4.629832	-0.029490
H	1.025484	-2.679790	-0.063596
H	2.760447	-0.300744	-2.901080
H	3.650997	-2.490597	-2.173587
H	4.089649	0.584767	-2.000263
H	5.135243	-2.657714	-0.209525
H	5.494725	-0.849703	-0.286247
N	-6.108877	0.078234	-0.091179
C	-6.497376	-1.318460	-0.257828
C	-6.761434	0.652928	1.081745
C	-6.427775	0.843866	-1.293110
H	-7.582166	-1.429042	-0.427827
H	-5.969626	-1.751119	-1.113134
H	-6.233642	-1.885033	0.640579
H	-7.861510	0.624869	1.000289
H	-6.463787	0.099983	1.977314
H	-6.454919	1.696245	1.204975
H	-7.508808	0.841437	-1.513726
H	-6.105316	1.882358	-1.167742
H	-5.896723	0.420128	-2.150543

Va_{exo}

Num. Imaginary Frequencies: 0

C	-1.201304	-2.481499	-0.160663
C	-1.695402	-1.167818	-0.144903
C	-3.085566	-0.953190	-0.098559
C	-4.010364	-2.009326	-0.082044
C	-3.509327	-3.292325	-0.113308
C	-2.113865	-3.516825	-0.146672
C	-1.027256	0.102404	-0.138932
C	0.258269	0.494783	-0.106912
Pd	1.813439	-0.819707	-0.066104
Cl	1.490904	-1.313204	2.260592
C	-3.242316	0.465101	-0.041281
N	-4.348196	1.195795	0.045922
C	-4.331528	2.650288	0.102624
C	0.596026	1.929863	-0.040437
C	1.431570	2.390833	0.987793
C	1.766312	3.737392	1.068293
C	1.305894	4.638755	0.109632
C	0.494398	4.185388	-0.926929
C	0.132042	2.843736	-0.996128
C	3.756073	-1.893897	-0.403472
C	3.018422	-1.818764	-1.582819
C	2.539544	-0.558778	-2.047092
O	-2.097479	1.079500	-0.069323
H	1.796109	1.678714	1.723572
H	2.402490	4.082604	1.878235
H	1.582855	5.687447	0.167942
H	0.139717	4.879460	-1.684125
H	-0.502060	2.492684	-1.805445
H	-3.539348	2.982754	0.776450
H	-5.293963	2.993882	0.482984
H	-4.155784	3.082361	-0.887406
H	-5.230311	0.708685	0.039369
H	-5.081498	-1.831581	-0.040969

H	-4.186890	-4.139645	-0.100545
H	-1.749616	-4.539738	-0.148505
H	-0.131194	-2.658617	-0.150667
H	1.840195	-0.540163	-2.878327
H	2.565954	-2.727201	-1.977628
H	3.173509	0.323234	-1.961434
H	3.933379	-2.852268	0.072228
H	4.400388	-1.074917	-0.091032

Vb-PPh₃endo.

Num. Imaginary Frequencies:	0		
C	-1.354933	1.988725	2.087206
C	-1.511298	0.601238	2.170692
C	-1.295604	-0.034297	3.400491
C	-0.886979	0.695515	4.510609
C	-0.707016	2.072601	4.412056
C	-0.953601	2.714968	3.201865
C	-1.852359	-0.187744	0.973725
C	-1.415235	-0.051530	-0.299416
C	-1.828573	-1.075272	-1.237201
C	-2.608582	-2.185823	-0.837986
C	-3.001644	-2.223303	0.530999
O	-2.667667	-1.270206	1.347016
C	-2.939425	-3.212175	-1.752778
C	-2.509762	-3.134688	-3.053825
C	-1.737371	-2.031504	-3.470593
C	-1.403252	-1.033320	-2.587141
Pd	-0.007172	1.303527	-0.840025
Cl	1.696805	2.926994	-1.390460
N	-3.740955	-3.182638	1.095796
C	-4.022294	-3.220477	2.520819
C	-1.514237	2.580480	-1.384191
C	-2.646336	2.207702	-2.119820
C	-3.639574	3.128384	-2.457486
C	-3.536204	4.453590	-2.048694
C	-2.422485	4.845986	-1.310696
C	-1.425895	3.925425	-0.991744
H	-3.530479	-4.071170	-1.447318
H	-2.763625	-3.919059	-3.759225
H	-1.399762	-1.972125	-4.500702
H	-0.801922	-0.182819	-2.896201
H	-1.431538	-1.108618	3.485464
H	-0.701740	0.186619	5.451772
H	-0.379874	2.641802	5.277071
H	-0.831197	3.790348	3.116707
H	-1.552549	2.493192	1.148952
H	-3.988566	-3.977551	0.531583
H	-3.106502	-3.393406	3.096354
H	-4.467391	-2.277497	2.845628
H	-4.726134	-4.031304	2.709608
H	-0.549262	4.266948	-0.448815
H	-2.317861	5.880616	-0.991820
H	-4.309264	5.172858	-2.306052
H	-4.499692	2.802837	-3.038981
H	-2.775492	1.180246	-2.450175
P	1.712166	-0.249610	-0.103421
C	2.390244	0.186636	1.540923
C	1.081390	-1.965842	0.123997
C	3.141522	-0.532608	-1.213598
C	4.242030	-1.308986	-0.833373
C	5.272270	-1.555235	-1.732867
C	5.211053	-1.031784	-3.023815
C	4.121989	-0.256956	-3.407319
C	3.090648	-0.003324	-2.505303
H	4.300623	-1.721622	0.169148
H	6.124841	-2.154568	-1.426741
H	6.017243	-1.223570	-3.726229
H	4.076545	0.169154	-4.404912
H	2.262542	0.638389	-2.788473
C	2.987149	-0.740321	2.405206
C	3.451751	-0.342080	3.653677
C	3.327107	0.987289	4.052746
C	2.740718	1.914421	3.198141
C	2.271979	1.519241	1.948165
H	3.068442	-1.784803	2.117254
H	3.908572	-1.070968	4.317024
H	3.687583	1.296944	5.029700
H	2.637307	2.951481	3.502160
H	1.824071	2.246310	1.276576
C	1.054818	-2.844086	-0.964563
C	0.431325	-4.084940	-0.863913
C	-0.175140	-4.471222	0.328075
C	-0.156230	-3.604213	1.418192
C	0.462175	-2.360831	1.314826
H	1.523331	-2.556052	-1.901237
H	0.421972	-4.751450	-1.721218
H	-0.652010	-5.444172	0.409582
H	-0.612498	-3.899128	2.360329

H 0.469228 -1.692566 2.170221

Vb-PPh₃endo

Num. Imaginary Frequencies: 0

C	-1.408119	-1.482349	1.773880
C	-2.018979	-0.723783	0.773872
C	-3.240041	-0.094317	1.047826
C	-3.828696	-0.224066	2.304357
C	-3.218432	-0.984799	3.298487
C	-2.009973	-1.616665	3.025956
Pd	-1.328110	-0.471714	-1.057858
Cl	-3.264529	-0.701475	-2.383315
C	0.568545	-0.283483	-0.341093
C	1.438029	-1.447284	-0.276647
C	0.933674	-2.746058	-0.530027
C	1.749308	-3.852056	-0.473780
C	3.119523	-3.725895	-0.167979
C	3.648945	-2.484292	0.080068
C	2.817648	-1.340119	0.030432
C	3.312748	-0.025144	0.276517
O	2.520049	1.002584	0.233921
C	1.142752	0.909882	-0.064489
C	0.568303	2.267754	-0.033792
C	1.278543	3.347500	-0.573115
C	0.733166	4.625746	-0.557979
C	-0.523017	4.841699	0.004055
C	-1.226498	3.774231	0.555136
C	-0.686088	2.493679	0.540814
N	4.578299	0.282743	0.568093
C	5.025442	1.647516	0.803836
H	4.707229	-2.403078	0.312358
H	3.752883	-4.605998	-0.130775
H	1.331916	-4.835014	-0.668075
H	-0.122223	-2.840424	-0.767073
H	2.252008	3.183007	-1.025910
H	1.284966	5.453075	-0.994146
H	-0.952062	5.839168	0.011681
H	-2.202390	3.934007	1.002729
H	-1.231283	1.666492	0.978909
H	5.251509	-0.463960	0.606014
H	4.900180	2.257666	-0.095188
H	4.457564	2.103003	1.619085
H	6.081252	1.616951	1.072654
H	-3.740799	0.475991	0.272994
H	-4.779728	0.265075	2.497969
H	-3.684755	-1.088833	4.274048
H	-1.523263	-2.217331	3.790422
H	-0.462163	-1.981922	1.594089

Vb-PPh₃exo

Num. Imaginary Frequencies: 0

O	2.934113	1.715447	0.290964
C	2.093557	0.549268	0.171918
C	2.584234	-0.363998	1.161627
C	3.647382	0.248448	1.853038
C	3.799619	1.529555	1.244137
C	4.323407	-0.385821	2.907242
C	3.908430	-1.651745	3.258479
C	2.840753	-2.273364	2.571178
C	2.172180	-1.653681	1.534255
C	1.090175	0.510797	-0.725956
C	0.741874	1.688277	-1.549443
C	0.396158	1.522568	-2.900964
C	0.007841	2.611248	-3.672008
C	-0.085449	3.879511	-3.100987
C	0.225239	4.051447	-1.755420
C	0.647536	2.970330	-0.989254
N	4.658760	2.506832	1.512431
C	4.700772	3.747404	0.751711
Pd	-0.084949	-1.078471	-0.985702
Cl	-1.621173	-2.827788	-1.642577
C	1.514499	-1.995293	-1.895207
C	2.527235	-1.357378	-2.624696
C	3.613999	-2.060982	-3.144993
C	3.730854	-3.429984	-2.930602
C	2.739612	-4.084488	-2.204123
C	1.646317	-3.379403	-1.703500
H	5.376342	2.319496	2.194785
H	5.133892	3.587979	-0.240653
H	5.305522	4.468578	1.302028
H	3.689293	4.141582	0.633876
H	5.142740	0.096619	3.433211
H	4.401328	-2.179069	4.068456
H	2.539137	-3.273294	2.867463
H	1.357738	-2.138968	1.007582
H	0.428588	0.527963	-3.336197
H	-0.241087	2.463180	-4.718582
H	-0.411086	4.725240	-3.699746

H	0.128236	5.029283	-1.292052
H	0.858432	3.111260	0.065482
H	0.868557	-3.922857	-1.175663
H	2.808916	-5.156669	-2.034382
H	4.579089	-3.980664	-3.328891
H	4.373316	-1.530923	-3.716248
H	2.489126	-0.285001	-2.799055
P	-1.848896	-0.135843	0.398149
C	-2.390613	-1.170952	1.814012
C	-1.392272	1.423087	1.264131
C	-3.367062	0.320401	-0.506764
C	-1.995305	2.653941	1.005152
C	-1.549789	3.808525	1.648444
C	-0.494699	3.746233	2.552223
C	0.111699	2.518162	2.821040
C	-0.335902	1.368058	2.183303
H	-2.809931	2.718522	0.290881
H	-2.031020	4.758928	1.436950
H	-0.149555	4.646967	3.051946
H	0.927845	2.455017	3.535859
H	0.133840	0.413313	2.404032
C	-2.951695	-0.598978	2.963696
C	-3.352524	-1.401614	4.026575
C	-3.193643	-2.783973	3.954575
C	-2.638222	-3.358094	2.815387
C	-2.236920	-2.559220	1.747078
H	-3.072256	0.478265	3.033275
H	-3.787397	-0.946421	4.911716
H	-3.504879	-3.411015	4.785407
H	-2.517141	-4.435245	2.749207
H	-1.827534	-3.008415	0.846377
C	-4.648662	0.196150	0.032707
C	-5.757914	0.609947	-0.699650
C	-5.593446	1.156875	-1.969313
C	-4.317158	1.279403	-2.513414
C	-3.208222	0.853504	-1.790379
H	-4.784598	-0.235828	1.019425
H	-6.752310	0.500265	-0.276942
H	-6.460806	1.478330	-2.538745
H	-4.183230	1.694824	-3.507659
H	-2.215531	0.932041	-2.225441

Vb-PPh₃_{exo}

Num.	Imaginary Frequencies:	0
C	1.121477	-0.336140
C	1.844086	-0.487636
C	2.813552	-1.495037
C	3.041523	-2.337307
C	2.319635	-2.182694
C	1.365115	-1.175126
Pd	1.670562	0.663734
C1	3.851193	0.786289
C	-0.283564	0.841874
C	-0.754094	2.212196
C	-0.013226	3.026450
C	-0.430600	4.319087
C	-1.573418	4.840433
C	-2.298740	4.057353
C	-1.898760	2.754135
C	-1.147696	-0.192236
C	-1.047325	-1.596393
C	0.016997	-2.385770
C	-0.210868	-3.733590
C	-1.470975	-4.327553
C	-2.532722	-3.563809
C	-2.303339	-2.194975
C	-3.158475	-1.135164
O	-2.528047	0.001823
N	-4.442616	-1.170961
C	-5.201937	-0.017892
H	-4.889266	-2.075570
H	-5.342056	-0.056173
H	-6.175629	-0.003912
H	-4.657269	0.891057
H	-3.507240	-4.013176
H	-1.601384	-5.390744
H	0.605907	-4.358344
H	0.986436	-1.940983
H	0.897457	2.632918
H	0.152940	4.928822
H	-1.886371	5.858438
H	-3.175709	4.466307
H	-2.459085	2.158128
H	3.406974	-1.606070
H	3.801065	-3.110830
H	2.505619	-2.837211
H	0.801544	-1.034517
H	0.362748	0.434089

VIA-dba_{endo}

	Num. Imaginary Frequencies: 0		
C	0.486054	2.751619	1.010518
C	1.749444	2.454084	0.486622
C	2.398471	3.443450	-0.268172
C	1.789727	4.670328	-0.508878
C	0.522509	4.941130	-0.000072
C	-0.125147	3.974056	0.762770
C	2.385568	1.130438	0.665159
C	1.793126	-0.058048	0.889268
C	2.640867	-1.250352	0.894822
C	4.002687	-1.145285	0.561334
C	4.570904	0.175538	0.270487
O	3.748658	1.247932	0.441675
C	4.817209	-2.278115	0.482083
C	4.294354	-3.533220	0.743532
C	2.946034	-3.658688	1.089154
C	2.137193	-2.537157	1.160234
Pd	-0.257289	-0.391378	0.957528
C	-0.053959	-0.490871	3.068157
C	-1.181815	-1.296107	2.735078
C	-2.262177	-0.752516	2.048389
N	5.773434	0.343320	-0.104800
C	6.209128	1.696865	-0.378280
C	-0.058933	0.088174	-1.333165
C	-1.299286	-0.452017	-1.062009
C	-2.476751	0.441746	-0.847296
O	-2.361217	1.652048	-0.719806
C	1.095010	-0.596173	-1.940503
C	2.167300	0.188491	-2.380700
C	3.319158	-0.400693	-2.887463
C	3.413105	-1.787364	-2.966696
C	2.345210	-2.578001	-2.548075
C	1.195764	-1.988044	-2.039099
C	-3.799875	-0.231415	-0.814596
H	-3.043464	-1.397910	1.661654
H	-2.514082	0.302298	2.139243
H	-1.081073	-2.379218	2.779743
H	0.834172	-0.970596	3.466134
H	1.084438	-2.647413	1.403433
H	2.525791	-4.639219	1.295631
H	4.929080	-4.412290	0.683792
H	5.858882	-2.140081	0.212994
H	6.041070	2.375172	0.469607
H	7.277705	1.688017	-0.610041
H	-0.030844	2.014096	1.613629
H	-1.114811	4.165274	1.165309
H	0.044867	5.896605	-0.194936
H	2.309629	5.416670	-1.102825
H	3.384599	3.241883	-0.670402
H	5.677384	2.125798	-1.241306
H	-0.204480	0.537380	3.391155
H	-1.506503	-1.499579	-1.269058
H	-0.000495	1.175594	-1.298476
H	0.390883	-2.619555	-1.673676
H	2.420472	-3.660025	-2.592371
H	4.320725	-2.251036	-3.339962
H	4.152851	0.221544	-3.197327
H	2.103894	1.269798	-2.289923
C	-4.915818	0.482967	-0.609942
H	-3.819553	-1.309624	-0.954739
C	-6.295503	-0.006163	-0.533663
H	-4.778062	1.556152	-0.481058
C	-7.318994	0.916429	-0.281369
C	-8.645500	0.508085	-0.193631
C	-8.970556	-0.834871	-0.358424
C	-7.962835	-1.765335	-0.611705
C	-6.639288	-1.356138	-0.698839
H	-7.067561	1.965950	-0.152251
H	-9.423902	1.239000	0.002723
H	-8.211439	-2.814008	-0.743924
H	-5.867792	-2.093248	-0.900422

VIA-dba_{endo}-Me3N

	Num. Imaginary Frequencies: 0		
C	-7.467233	-1.996333	-0.409096
C	-7.052089	-0.827196	-1.063779
C	-8.030025	0.072485	-1.507300
C	-9.381344	-0.178379	-1.296383
C	-9.777513	-1.340086	-0.640627
C	-8.815886	-2.249152	-0.199812
C	-5.643171	-0.500895	-1.300117
C	-4.561666	-1.157589	-0.855898
C	-3.202010	-0.657622	-1.174078
O	-3.024161	0.307075	-1.907372
C	-2.070813	-1.407849	-0.558972
Pd	-1.316164	0.007387	1.060869

C	0.611527	0.780494	0.909588
C	1.740558	0.013681	1.428913
C	3.058668	0.455810	1.205788
C	3.268087	1.731301	0.518600
O	2.172518	2.487466	0.270237
C	0.874684	1.994865	0.391972
C	4.151107	-0.312473	1.620255
C	3.951455	-1.512938	2.277833
C	2.648820	-1.936501	2.553898
C	1.563620	-1.183918	2.139072
N	4.420939	2.158154	0.163494
C	4.486296	3.446213	-0.498081
C	-0.083782	3.033770	-0.041712
C	0.188065	4.383194	0.223179
C	-0.728902	5.370984	-0.118632
C	-1.928605	5.033632	-0.742293
C	-2.195415	3.698628	-1.032481
C	-1.279032	2.709455	-0.691219
C	-0.766330	-1.156238	-0.934745
C	0.382934	-2.057544	-0.763609
C	1.644205	-1.618358	-1.185850
C	2.772358	-2.403119	-0.991021
C	2.655483	-3.655576	-0.396293
C	1.400675	-4.122613	-0.010016
C	0.274478	-3.328057	-0.184809
C	-3.424585	0.039066	1.980399
C	-2.432341	0.240890	2.934841
C	-1.459631	1.266714	2.755148
C	7.252614	0.822678	-0.840178
N	6.693406	-0.236803	-1.709584
C	5.426759	0.169575	-2.352580
C	7.680216	-0.746502	-2.683190
C1	6.344549	-2.696186	-0.217237
H	-4.064989	-0.835088	2.036306
H	-3.789698	0.862506	1.369969
H	-2.237887	-0.541937	3.665700
H	-0.612899	1.306222	3.432105
H	0.551289	-1.534480	2.321005
H	2.484258	-2.877664	3.070219
H	4.804954	-2.125040	2.546672
H	5.156149	0.034728	1.411773
H	5.493480	3.585700	-0.904982
H	3.758645	3.544044	-1.315442
H	-1.499181	1.684259	-0.964380
H	-3.109858	3.413093	-1.543964
H	-2.642735	5.806943	-1.009976
H	-0.505893	6.410535	0.104529
H	1.120274	4.652549	0.708653
H	4.291144	4.269136	0.203255
H	-1.744559	2.217103	2.306949
H	-2.326885	-2.326230	-0.036900
H	-0.614889	-0.324297	-1.619808
H	-0.693111	-3.701748	0.138256
H	1.300215	-5.103464	0.445624
H	3.553677	-4.240900	-0.226349
H	3.763207	-2.045661	-1.249683
H	1.736718	-0.627808	-1.625122
H	-4.638061	-2.049748	-0.239414
H	-5.449550	0.390475	-1.896239
H	-7.722131	0.980040	-2.020123
H	-9.120966	-3.159990	0.306410
H	-6.731894	-2.718905	-0.068136
H	6.478298	-1.110370	-1.072271
H	5.615552	0.987495	-3.054457
H	5.015179	-0.692343	-2.881463
H	4.738907	0.504181	-1.574096
H	7.659375	1.625892	-1.462659
H	6.450401	1.213467	-0.206316
H	8.043892	0.379052	-0.232676
H	7.947465	0.044185	-3.389929
H	8.560743	-1.087115	-2.136611
H	7.242548	-1.599157	-3.204470

VIA_{endo}

Num. Imaginary Frequencies: 0

C	-1.130032	2.867839	0.506515
C	-0.876525	1.720703	-0.256066
C	-1.928663	1.162146	-1.013312
C	-3.220406	1.697015	-0.939871
C	-3.464233	2.810839	-0.149987
C	-2.409577	3.402270	0.553967
C	0.408156	1.010400	-0.222942
O	1.496272	1.840310	-0.093912
C	2.752692	1.316541	0.086181
C	2.898056	-0.146190	-0.039773
C	1.762103	-0.959297	-0.223954
C	0.445185	-0.336332	-0.262406
C	1.952664	-2.339270	-0.385795

C	3.220890	-2.895224	-0.341077
C	4.338026	-2.080686	-0.131618
C	4.175492	-0.712326	0.013879
N	3.732757	2.087223	0.319800
C	3.475626	3.509951	0.408062
Pd	-1.483269	-1.030197	-0.085293
C	-2.537486	-2.848282	0.484026
C	-3.495602	-1.849801	0.597232
C	-1.280936	-2.707997	1.156671
H	-4.367250	-1.855720	-0.049690
H	-3.563253	-1.236299	1.493609
H	-2.629004	-3.584409	-0.312340
H	-0.494846	-3.427873	0.955827
H	1.081412	-2.961039	-0.565764
H	3.347812	-3.965974	-0.473511
H	5.331385	-2.517158	-0.091014
H	5.023745	-0.053305	0.164623
H	4.415549	4.028675	0.613570
H	3.053026	3.911304	-0.523411
H	-1.693827	0.422532	-1.789956
H	-4.016228	1.252683	-1.529732
H	-4.460745	3.237433	-0.094882
H	-2.597112	4.286653	1.156169
H	-0.320671	3.314570	1.074392
H	2.764837	3.750283	1.211578
H	-1.256508	-2.280162	2.158303

VIA-dba_{exo}

	Num. Imaginary Frequencies: 0		
C	-7.402563	0.766071	-0.434857
C	-6.372738	-0.182691	-0.479144
C	-6.692505	-1.527453	-0.239637
C	-7.998713	-1.904845	0.039932
C	-9.012224	-0.947708	0.085980
C	-8.711315	0.389667	-0.153276
C	-5.011431	0.276352	-0.768552
C	-3.881475	-0.446007	-0.764797
C	-2.581473	0.199576	-1.069212
O	-2.500867	1.382787	-1.375629
C	-1.380244	-0.680593	-0.985932
C	-0.165967	-0.246463	-1.482579
C	0.994678	-1.075843	-1.840957
C	2.120818	-0.436382	-2.373653
C	3.263512	-1.158170	-2.694242
C	3.294250	-2.535656	-2.492474
C	2.174348	-3.186076	-1.979936
C	1.034637	-2.461777	-1.654778
Pd	-0.339014	0.184440	0.824733
C	-0.153863	0.974222	2.782458
C	-1.108309	-0.080229	2.871314
C	-2.257402	-0.066008	2.086856
C	1.535447	1.027335	0.521132
C	2.628061	0.252485	0.599320
C	2.803467	-1.155932	0.967128
C	4.130570	-1.499977	0.714201
C	4.807039	-0.309622	0.197526
O	3.894995	0.713097	0.197889
C	4.623751	-2.778803	0.931826
C	3.748179	-3.735127	1.433251
C	2.416495	-3.399997	1.707651
C	1.932135	-2.116800	1.480165
N	6.004194	-0.200941	-0.195294
C	6.427120	1.099203	-0.683101
C	1.564956	2.464414	0.177430
C	2.684915	3.278246	0.434227
C	2.674944	4.633646	0.127286
C	1.550890	5.223260	-0.445734
C	0.427863	4.440071	-0.694168
C	0.431089	3.085845	-0.376629
H	-0.470974	2.508215	-0.562542
H	-0.463153	4.881592	-1.131366
H	1.547940	6.282581	-0.686116
H	3.555128	5.233900	0.341377
H	3.569529	2.842377	0.880824
H	7.403840	1.000202	-1.163913
H	6.524126	1.819792	0.140539
H	5.716712	1.528125	-1.403453
H	5.662543	-3.005319	0.714794
H	4.097479	-4.746253	1.619768
H	1.746587	-4.158903	2.102579
H	0.893135	-1.874653	1.682261
H	0.798755	0.861811	3.288698
H	-0.809080	-1.012988	3.346414
H	-0.486931	2.000738	2.638543
H	-2.897404	-0.941199	2.042097
H	-2.705947	0.872396	1.767288
H	-1.556239	-1.734304	-0.784650
H	-0.146843	0.769857	-1.869569

H	2.107983	0.642980	-2.498035
H	4.138326	-0.643788	-3.079059
H	4.193781	-3.098116	-2.722456
H	2.197958	-4.257892	-1.809798
H	0.179350	-2.980456	-1.231791
H	-3.872362	-1.507476	-0.529612
H	-4.900988	1.334044	-1.006218
H	-7.169742	1.811101	-0.622284
H	-9.494781	1.140443	-0.122270
H	-8.229548	-2.950335	0.220670
H	-5.917240	-2.286575	-0.279316

V1a-dba_{exc}-Me3N

	Num. Imaginary Frequencies: 0		
C	0.827424	4.136750	0.177187
C	-0.085491	3.082499	-0.013267
C	-1.229801	3.351483	-0.785383
C	-1.430993	4.596108	-1.372896
C	-0.506277	5.619531	-1.187572
C	0.618976	5.382809	-0.401825
C	0.101458	1.755036	0.607759
C	1.299711	1.235476	0.910573
C	1.693601	-0.032088	1.527301
C	3.069707	-0.185024	1.351343
C	3.555280	1.016637	0.676976
O	2.500544	1.853425	0.494469
C	3.745984	-1.331660	1.743327
C	3.014451	-2.336512	2.364518
C	1.644003	-2.173175	2.595134
C	0.969922	-1.030002	2.178625
N	4.739346	1.291851	0.299721
C	4.939248	2.569892	-0.360696
Pd	-1.597966	0.611253	0.929616
C	-2.560063	0.561809	2.909459
C	-3.572732	0.157842	2.045559
C	-2.199287	-0.782414	-0.760704
C	-1.051603	-0.190839	-1.248901
C	0.281005	-0.796882	-1.365788
C	1.290069	-0.055919	-1.991979
C	2.573470	-0.575451	-2.123126
C	2.870376	-1.839340	-1.621097
C	1.871492	-2.587407	-1.000471
C	0.588663	-2.073209	-0.877344
C	-3.534589	-0.219678	-1.110987
O	-3.660245	0.875214	-1.646450
C	-4.703042	-1.073113	-0.784688
C	-5.945660	-0.654808	-1.065801
C	-7.207718	-1.356259	-0.814597
C	-7.277272	-2.600715	-0.170732
C	-8.500643	-3.221745	0.038858
C	-9.680340	-2.613428	-0.389797
C	-9.627859	-1.378347	-1.028616
C	-8.401503	-0.756807	-1.236668
C	-1.849568	1.775431	2.679279
C1	5.743394	-3.638913	-0.083641
N	7.184270	-1.277795	-0.956245
C	6.365935	-0.545505	-1.944952
C	7.555051	-0.434771	0.202920
C	8.351149	-1.944016	-1.568086
H	-1.981513	2.579137	-0.929848
H	-2.322216	4.764128	-1.970801
H	-0.664831	6.593353	-1.641842
H	1.342533	6.176113	-0.234172
H	1.707174	3.976488	0.787925
H	5.931320	2.581136	-0.824007
H	4.894270	3.399421	0.357535
H	4.184374	2.768759	-1.133393
H	4.801207	-1.470054	1.537877
H	3.513812	-3.255490	2.652334
H	1.090638	-2.964823	3.093081
H	-0.098936	-0.926912	2.337589
H	-0.972859	1.992122	3.280283
H	-2.136412	-0.166905	3.598631
H	-2.372356	2.647443	2.289521
H	-3.999562	-0.836010	2.132823
H	-4.164409	0.886687	1.495591
H	6.965793	0.243906	-2.408094
H	6.024254	-1.253461	-2.702873
H	5.513063	-0.109384	-1.419855
H	8.309701	0.295353	-0.105639
H	6.656993	0.082091	0.555859
H	7.957696	-1.086789	0.980732
H	9.021671	-1.196287	-2.001146
H	8.865854	-2.517297	-0.795535
H	7.994880	-2.633437	-2.335090
H	-2.178150	-1.795058	-0.366022
H	-1.197679	0.724795	-1.817804
H	1.067851	0.945459	-2.351557

H	3.343794	0.021052	-2.604442
H	3.873555	-2.253424	-1.668886
H	2.116614	-3.560379	-0.588283
H	-0.171590	-2.660433	-0.370551
H	-4.507571	-2.034703	-0.316763
H	-6.025724	0.322005	-1.542025
H	-8.361740	0.207743	-1.736108
H	-8.537192	-4.185102	0.538437
H	-6.369278	-3.088411	0.170930
H	6.567917	-2.108994	-0.579581

VIA_{exo}

Num. Imaginary Frequencies: 0

C	-2.066628	1.445979	-1.085331
C	-1.049790	1.350388	-0.101308
C	-1.142701	2.192929	1.037118
C	-2.174684	3.097530	1.159039
C	-3.177110	3.182068	0.176196
C	-3.121864	2.364039	-0.934332
C	-0.129640	0.221105	-0.163175
Pd	-1.860031	-0.842764	-0.088731
C	-1.620114	-2.869714	0.471506
C	-2.905202	-2.735899	-0.143743
C	-3.844270	-1.842411	0.359304
C	1.197267	0.235815	-0.114947
C	2.193494	-0.833124	-0.042523
C	3.450579	-0.235055	-0.012522
C	3.254916	1.217447	-0.075092
O	1.898764	1.449105	-0.132739
C	4.618652	-0.982183	0.063904
C	4.496929	-2.366945	0.110861
C	3.234731	-2.974986	0.079667
C	2.070122	-2.217989	0.003038
N	4.138397	2.119346	-0.077352
C	3.697941	3.500841	-0.148047
H	-1.954850	0.903611	-2.022090
H	-3.878713	2.436175	-1.709460
H	-3.985939	3.897407	0.289283
H	-2.217162	3.751475	2.025396
H	-0.373947	2.115589	1.799045
H	2.937741	3.662295	-0.923474
H	4.559851	4.138929	-0.359448
H	3.262069	3.822004	0.807438
H	5.584398	-0.488267	0.086692
H	5.387283	-2.985514	0.171691
H	3.165255	-4.058355	0.117956
H	1.092145	-2.682494	-0.021577
H	-0.881895	-3.486821	-0.030820
H	-3.044646	-3.132105	-1.148196
H	-1.534637	-2.844431	1.556846
H	-4.739907	-1.616890	-0.210310
H	-3.870295	-1.592746	1.418357

VIB-PPh_{3endo}

Num. Imaginary Frequencies: 0

C	-3.301587	-0.219003	2.287642
C	-3.417600	0.023560	0.916596
C	-4.673873	-0.076395	0.308552
C	-5.791737	-0.415624	1.061266
C	-5.666368	-0.659373	2.428733
C	-4.421968	-0.560650	3.041991
P	-1.897586	0.423327	-0.019934
C	-1.672257	-0.992929	-1.151878
C	-0.824318	-0.846964	-2.256937
C	-0.458118	-1.953690	-3.012833
C	-0.929588	-3.219454	-2.672143
C	-1.779481	-3.370386	-1.581993
C	-2.147750	-2.263455	-0.821573
Pd	0.137390	0.809971	1.269292
C	1.216323	-0.584030	0.318360
C	2.029052	-0.301238	-0.713556
O	2.617949	-1.287122	-1.483836
C	2.350897	-2.616084	-1.313496
C	1.501303	-2.985953	-0.173842
C	0.954791	-1.981452	0.642894
C	0.142352	-2.375195	1.719614
C	-0.128091	-3.711538	1.960737
C	0.410829	-4.698619	1.130515
C	1.224307	-4.333579	0.070857
C	2.452679	1.031332	-1.193286
C	1.533466	2.065435	-1.390403
C	1.955882	3.324622	-1.804786
C	3.306909	3.565174	-2.036880
C	4.228504	2.533382	-1.866599
C	3.804720	1.274274	-1.457555
N	2.831496	-3.470154	-2.121785
C	3.645342	-2.977555	-3.214006
C	1.851908	1.076849	2.265054

C	2.598292	2.233120	1.999222
C	3.666135	2.594310	2.819904
C	4.019925	1.793494	3.902494
C	3.304670	0.625749	4.158122
C	2.235170	0.265025	3.340047
C	-2.373422	1.811625	-1.116049
C	-2.060843	3.109485	-0.697233
C	-2.404377	4.208310	-1.479032
C	-3.054979	4.018764	-2.695398
C	-3.361216	2.730057	-3.126324
C	-3.022376	1.631591	-2.342306
H	1.658700	-5.072429	-0.594043
H	0.199041	-5.747061	1.317683
H	-0.763278	-3.990302	2.796901
H	-0.280158	-1.603735	2.358142
H	0.477890	1.888405	-1.218183
H	1.221311	4.111303	-1.953056
H	3.641182	4.547754	-2.357130
H	5.284191	2.711834	-2.048544
H	4.524626	0.473730	-1.321544
H	3.110026	-2.240088	-3.829350
H	4.559670	-2.485378	-2.854355
H	3.935555	-3.817999	-3.850339
H	2.359649	2.854284	1.139209
H	4.229685	3.498190	2.602715
H	4.857523	2.070624	4.536824
H	3.586988	-0.014010	4.990515
H	1.708901	-0.665828	3.535678
H	-2.785967	-2.398601	0.046194
H	-2.139700	-4.355494	-1.302895
H	-0.614259	-4.086694	-3.243429
H	0.218398	-1.830848	-3.852939
H	-0.429142	0.130436	-2.519080
H	-3.242402	0.628102	-2.695672
H	-3.859309	2.578623	-4.079179
H	-3.316859	4.874167	-3.310971
H	-2.156930	5.210253	-1.141552
H	-1.535240	3.260409	0.243340
H	-4.779215	0.113452	-0.755622
H	-6.763040	-0.491024	0.581917
H	-6.541804	-0.924221	3.014323
H	-4.319541	-0.746091	4.106803
H	-2.327755	-0.140240	2.765444

VIB-PPh₃exo

Num.	Imaginary Frequencies:	0
C	0.124182	2.506119
C	1.235120	1.755655
C	1.843499	2.035189
C	1.334563	3.040352
C	0.211050	3.762425
C	-0.391356	3.499007
P	1.749175	0.360415
Pd	-0.003972	-1.278680
C	-1.231217	-0.652349
C	-0.828928	-1.106355
C	-0.645788	-2.468589
C	-0.160816	-2.880622
C	0.166960	-1.940072
C	-0.020661	-0.585709
C	-0.522259	-0.170829
C	3.146800	-0.396708
C	4.486088	-0.096915
C	5.495492	-0.690024
C	5.175635	-1.576446
C	3.841870	-1.877192
C	2.831322	-1.298361
C	2.510210	1.172801
C	2.508385	0.493056
C	3.097534	1.061550
C	3.686183	2.320426
C	3.685320	3.008658
C	3.099814	2.439073
C	-1.315576	-2.763504
C	-0.687730	-0.412589
C	-1.397677	-5.139249
C	-2.755305	-5.037205
C	-3.396201	-3.807225
C	-2.685393	-2.683324
C	-2.149982	0.291221
O	-2.820086	0.901414
C	-3.564807	1.963013
C	-3.460356	1.992052
C	-2.602612	0.961658
C	-2.304687	0.773302
C	-2.882772	1.634461
C	-3.738973	2.668755
C	-4.036372	2.858790

N	-4.189569	2.763792	1.730851
C	-4.090243	2.536999	3.162015
H	-3.062357	2.697525	3.516520
H	-4.369993	1.512874	3.441448
H	-4.748741	3.236805	3.682667
H	-4.695611	3.651866	-1.064475
H	-4.171214	3.325583	-3.496013
H	-2.666566	1.498200	-4.201112
H	-1.642274	-0.027042	-2.534330
H	-0.667760	0.884852	2.733987
H	0.229242	0.157142	4.911658
H	0.562573	-2.261763	5.382376
H	-0.027397	-3.940481	3.645202
H	-0.872948	-3.198956	1.440881
H	-3.207313	-1.737940	-1.355778
H	-4.458821	-3.722397	-2.095546
H	-3.313547	-5.913298	-2.336860
H	-0.890639	-6.096588	-1.821700
H	0.369326	-4.124686	-1.069403
H	2.700386	1.456445	2.212839
H	1.810593	3.246007	3.657482
H	-0.197129	4.530141	2.962589
H	-1.274587	4.050074	0.772960
H	-0.353354	2.300762	-0.696169
H	3.093442	2.980770	-0.838212
H	4.139211	3.992677	-2.837886
H	4.140271	2.768509	-4.995967
H	3.088993	0.525900	-5.147811
H	2.037691	-0.485031	-3.153506
H	4.744967	0.598065	-0.553521
H	6.534449	-0.456574	0.781064
H	5.965711	-2.034170	2.607240
H	3.579752	-2.566474	3.082917
H	1.794473	-1.541343	1.741096

VIIa-dba_{endo}

	Num. Imaginary Frequencies: 0		
C	-0.697867	2.546541	-1.042574
C	0.222695	2.999540	-0.093756
C	0.045094	4.250848	0.500147
C	-1.054560	5.035050	0.162317
C	-1.979230	4.573314	-0.771203
C	-1.798294	3.329629	-1.372948
C	1.377016	2.139332	0.271252
C	1.573341	1.521060	1.460503
C	2.754400	0.662265	1.611347
C	3.633277	0.519636	0.522920
C	3.377003	1.245509	-0.727743
O	2.241543	2.023596	-0.776353
C	4.739113	-0.327692	0.607424
C	4.983547	-1.040488	1.769308
C	4.125203	-0.898604	2.860622
C	3.026118	-0.056938	2.784868
C	0.532200	1.609863	2.565121
C	-0.302571	0.337764	2.604847
C	-1.521582	0.222103	1.991581
Pd	0.095874	-0.497507	0.548763
C	-0.643238	-1.821614	-0.996261
C	-1.855320	-1.096323	-1.449722
O	-1.823916	-0.212410	-2.301665
N	4.133770	1.180760	-1.740615
C	3.755840	1.919651	-2.928874
C	0.627579	-1.363716	-1.353770
C	1.882903	-2.130993	-1.202367
C	2.942797	-1.877657	-2.080151
C	4.142911	-2.570984	-1.973178
C	4.309191	-3.530158	-0.978632
C	3.266865	-3.785353	-0.089263
C	2.066331	-3.094786	-0.198909
C	-3.122791	-1.483869	-0.775148
H	-2.158347	-0.639262	2.169249
H	-1.978431	1.064154	1.475668
H	0.030607	-0.456903	3.271011
H	1.015478	1.784001	3.533037
H	2.367720	0.034956	3.642187
H	4.313589	-1.450480	3.776857
H	5.835233	-1.710728	1.825904
H	5.381441	-0.418834	-0.260473
H	3.628319	2.991657	-2.729662
H	4.533017	1.794648	-3.686827
H	-0.576791	1.572383	-1.507326
H	-2.513441	2.955158	-2.098519
H	-2.839891	5.183417	-1.029693
H	-1.187872	6.006422	0.629020
H	0.769385	4.605833	1.228316
H	2.804362	1.557403	-3.343423
H	-0.123826	2.462781	2.382600
H	-0.786697	-2.809597	-0.562540

H	0.663572	-0.546124	-2.074338
H	1.268806	-3.288436	0.513544
H	3.391271	-4.523186	0.698110
H	5.248533	-4.067874	-0.888377
H	4.951036	-2.349987	-2.663893
H	2.826114	-1.122069	-2.851397
C	-4.255786	-0.812032	-1.017800
H	-3.071690	-2.294210	-0.051906
C	-5.571066	-1.020773	-0.402303
H	-4.188476	-0.008322	-1.750334
C	-6.628065	-0.178803	-0.771319
C	-7.891799	-0.324322	-0.208852
C	-8.121633	-1.319421	0.736246
C	-7.080290	-2.167516	1.112246
C	-5.819632	-2.020377	0.549934
H	-6.451435	0.599283	-1.509643
H	-8.696003	0.340757	-0.509016
H	-9.106116	-1.436337	1.179253
H	-7.253458	-2.946705	1.848670
H	-5.021811	-2.691408	0.853837

VIIa_{endo}

Num. Imaginary Frequencies: 0

C	-1.414506	3.011329	0.868833
C	-1.309455	1.675487	0.461348
C	-2.472322	0.980142	0.119796
C	-3.716497	1.596860	0.210974
C	-3.814012	2.918027	0.636559
C	-2.657698	3.624675	0.961689
C	0.038538	1.063058	0.372528
O	0.880357	1.926360	-0.279812
C	2.201497	1.652718	-0.529221
C	2.733746	0.405947	0.033982
C	1.882900	-0.455428	0.747549
C	0.463948	-0.111056	0.887643
C	2.446977	-1.607155	1.321221
C	3.793475	-1.896895	1.163529
C	4.619916	-1.044264	0.429071
C	4.089001	0.107252	-0.127583
N	2.900358	2.467679	-1.201722
C	2.264558	3.673213	-1.694201
Pd	-1.394052	-2.096228	-1.125933
C	-0.746446	-2.354129	0.901742
C	-2.026565	-2.885711	0.765067
C	-0.462168	-1.048883	1.628648
H	-2.168220	-3.953835	0.613745
H	-2.892098	-2.345340	1.147175
H	0.098309	-3.036693	0.808325
H	-0.015373	-1.286395	2.605554
H	1.831849	-2.280917	1.906706
H	4.203838	-2.794281	1.617170
H	5.672868	-1.275354	0.302309
H	4.702266	0.801654	-0.691220
H	2.969326	4.211277	-2.332863
H	1.355929	3.458541	-2.272520
H	-2.396605	-0.047019	-0.238949
H	-4.610181	1.043075	-0.061595
H	-4.785007	3.398887	0.708322
H	-2.724927	4.658245	1.288034
H	-0.513821	3.565191	1.113920
H	1.970174	4.338548	-0.870755
H	-1.406628	-0.544847	1.845055

VIIa-dba_{exo}

Num. Imaginary Frequencies: 0

C	6.174671	-1.990183	-0.299228
C	5.849049	-0.848409	0.447370
C	6.850824	0.103467	0.676950
C	8.132270	-0.066783	0.163946
C	8.437710	-1.200849	-0.582737
C	7.454363	-2.163456	-0.809189
C	4.508303	-0.608939	0.993373
C	3.382273	-1.274746	0.706042
C	2.090700	-0.880041	1.331672
O	2.027925	0.027804	2.155186
C	0.898471	-1.635562	0.875338
C	-0.377006	-1.255901	1.315665
C	-1.587551	-2.099976	1.222942
C	-2.599605	-1.941229	2.174918
C	-3.753926	-2.716125	2.132677
C	-3.917933	-3.668094	1.132169
C	-2.923341	-3.830305	0.168166
C	-1.773300	-3.053980	0.210258
Pd	0.047788	-0.263049	-0.552586
C	-0.486297	1.723306	-2.610520
C	0.476310	0.544018	-2.638907
C	1.673807	0.523677	-1.978398
C	-1.028418	1.894889	-1.195383

C	-2.071821	1.154183	-0.729580
C	-2.955827	0.149507	-1.346700
C	-3.990532	-0.080987	-0.439287
C	-3.753783	0.748003	0.742866
O	-2.590431	1.455409	0.518802
C	-5.011725	-0.982852	-0.693239
C	-4.981462	-1.674220	-1.898729
C	-3.943160	-1.462679	-2.811116
C	-2.919125	-0.557160	-2.548817
N	-4.441550	0.832954	1.795413
C	-3.960983	1.711390	2.847060
C	-0.447152	2.993288	-0.368223
C	0.188370	2.760595	0.855726
C	0.733397	3.817786	1.577722
C	0.645729	5.120363	1.094470
C	0.013176	5.362082	-0.122420
C	-0.523561	4.305216	-0.849615
H	0.286107	1.748205	1.237097
H	1.234498	3.613054	2.518764
H	1.072853	5.943532	1.659630
H	-0.063452	6.374401	-0.508416
H	-1.020227	4.501865	-1.796734
H	-4.514817	1.503229	3.765806
H	-4.120664	2.764343	2.582000
H	-2.887453	1.584238	3.040079
H	-5.791586	-1.140955	0.043320
H	-5.759749	-2.394492	-2.130262
H	-3.928850	-2.020693	-3.742624
H	-2.112436	-0.435174	-3.261551
H	-1.300521	1.566080	-3.324148
H	0.239761	-0.274411	-3.317263
H	0.024809	2.643383	-2.910006
H	2.381968	-0.283312	-2.136224
H	2.041896	1.392234	-1.436768
H	1.069324	-2.604993	0.411174
H	-0.410410	-0.477646	2.077757
H	-2.481507	-1.194740	2.955793
H	-4.528790	-2.563206	2.877560
H	-4.820096	-4.271769	1.093251
H	-3.050612	-4.558740	-0.627494
H	-1.016554	-3.171493	-0.560941
H	3.360919	-2.093312	-0.010031
H	4.411988	0.214332	1.700686
H	6.614635	0.990170	1.259822
H	7.689641	-3.056425	-1.380896
H	5.424106	-2.756281	-0.470215
H	8.892777	0.685786	0.349661
H	9.437622	-1.339084	-0.983113

VIIa_{exo}

Num. Imaginary Frequencies: 0			
C	-3.228617	-0.556469	-0.296392
C	-2.082568	-0.103005	0.365266
C	-2.221461	0.914431	1.315657
C	-3.467488	1.476716	1.576352
C	-4.597668	1.027611	0.898922
C	-4.474434	0.004975	-0.038358
C	-0.760203	-0.773898	0.125407
Pd	-0.225731	-0.807721	-1.951815
C	-0.674672	-2.176827	0.736931
C	-0.573869	-2.097032	2.238847
C	0.436153	-2.582325	2.955658
C	0.396168	0.004813	-0.080106
C	1.829521	-0.264190	0.182341
C	2.463710	0.972042	0.295045
C	1.460247	2.022521	0.111206
O	0.251863	1.400164	-0.097582
C	3.825913	1.092686	0.536156
C	4.569115	-0.074353	0.660236
C	3.948442	-1.322866	0.532531
C	2.584031	-1.433727	0.288721
N	1.638911	3.271104	0.137996
C	0.508606	4.155643	-0.068936
H	-3.133906	-1.351704	-1.032544
H	-5.349504	-0.355745	-0.571062
H	-5.568369	1.470908	1.100107
H	-3.553909	2.267755	2.315702
H	-1.345672	1.270180	1.847771
H	-0.467689	3.657571	-0.035092
H	0.614726	4.646904	-1.043555
H	0.535132	4.942069	0.692414
H	4.276966	2.075900	0.619573
H	5.636884	-0.021056	0.848504
H	4.544463	-2.226585	0.619089
H	2.136131	-2.412002	0.165958
H	-1.584824	-2.720751	0.457599
H	-1.392433	-1.581671	2.740334
H	0.162251	-2.749005	0.333205

H	0.464840	-2.483494	4.036970
H	1.275685	-3.093611	2.490285

VIIb-PPh_{3endo}

Num. Imaginary Frequencies:	0		
C	-3.122082	-0.336547	2.214056
C	-3.294912	-0.526905	0.840452
C	-4.288318	-1.409015	0.400746
C	-5.068794	-2.107535	1.316229
C	-4.874896	-1.923833	2.683986
C	-3.905218	-1.031726	3.132413
P	-2.205138	0.414509	-0.303911
C	-1.149157	-0.871198	-1.093476
C	-0.094667	-0.417027	-1.896116
C	0.751086	-1.315355	-2.536141
C	0.559361	-2.686499	-2.379554
C	-0.477274	-3.146420	-1.575098
C	-1.327319	-2.246785	-0.935375
Pd	-0.883472	2.068738	0.548398
C	2.218616	-0.202400	0.930507
C	3.240407	-0.348336	0.060504
O	3.571582	-1.558457	-0.481300
C	2.955068	-2.735208	-0.136981
C	1.862831	-2.648871	0.836763
C	1.459939	-1.395829	1.324578
C	0.326797	-1.340509	2.151480
C	-0.346579	-2.497061	2.510059
C	0.096634	-3.742982	2.059920
C	1.193003	-3.814314	1.218248
C	4.132103	0.705926	-0.470301
C	4.503483	0.670867	-1.819275
C	5.335911	1.651441	-2.346879
C	5.817674	2.672375	-1.531327
C	5.467470	2.702525	-0.183656
C	4.632450	1.725601	0.346128
N	3.325701	-3.819672	-0.678995
C	4.390808	-3.760738	-1.659160
C	1.808166	1.131099	1.444809
C	1.396745	2.141653	0.540625
C	0.928428	3.380682	1.030036
C	0.859167	3.595553	2.424214
C	1.297741	2.616172	3.300215
C	1.777318	1.393536	2.809364
C	-3.364782	0.851828	-1.663169
C	-4.033753	2.076606	-1.571270
C	-4.953935	2.455842	-2.542958
C	-5.205990	1.619329	-3.627789
C	-4.533654	0.405030	-3.736385
C	-3.617334	0.021994	-2.759991
H	1.544804	-4.759168	0.818593
H	-0.427278	-4.648270	2.351088
H	-1.232544	-2.426568	3.133865
H	-0.035967	-0.378157	2.494854
H	4.136150	-0.131565	-2.450886
H	5.608988	1.616828	-3.397367
H	6.470512	3.436836	-1.942058
H	5.850923	3.486336	0.462560
H	4.369857	1.751441	1.398120
H	4.091132	-3.181564	-2.545158
H	5.299952	-3.289914	-1.261914
H	4.634284	-4.776519	-1.980836
H	1.593771	2.007218	-0.518530
H	0.758828	4.207434	0.344276
H	0.495143	4.546559	2.801043
H	1.271619	2.792368	4.371246
H	2.112216	0.628435	3.504346
H	-2.114019	-2.625269	-0.291307
H	-0.615310	-4.212605	-1.424647
H	1.232322	-3.392889	-2.855216
H	1.565526	-0.943817	-3.151640
H	0.065138	0.652263	-2.009720
H	-3.090720	-0.923354	-2.858349
H	-4.719863	-0.246843	-4.585078
H	-5.919049	1.917254	-4.390890
H	-5.466658	3.409458	-2.458029
H	-3.819490	2.737930	-0.734838
H	-4.457595	-1.547095	-0.663526
H	-5.833440	-2.792637	0.962002
H	-5.487847	-2.467414	3.397103
H	-3.760857	-0.870536	4.196841
H	-2.371572	0.371816	2.557190

VIIb-PPh_{3exo}

Num. Imaginary Frequencies:	0		
C	1.302500	2.303507	0.997025
C	1.075303	0.931757	1.123012
C	-0.018420	0.494763	1.881342
C	-0.847366	1.409421	2.520518

C	-0.612659	2.776740	2.390934
C	0.458564	3.218751	1.622558
P	2.117710	-0.365786	0.340341
Pd	0.865624	-1.953160	-0.718638
C	-2.792225	-0.578689	-0.529651
C	-3.829719	-1.194801	0.336925
C	-4.579370	-2.273801	-0.151140
C	-5.539708	-2.894270	0.639623
C	-5.763011	-2.455771	1.942047
C	-5.017156	-1.392116	2.443613
C	-4.060901	-0.767334	1.651210
C	3.158975	-0.931552	1.746421
C	3.359865	-0.183838	2.910614
C	4.190219	-0.664545	3.920410
C	4.827820	-1.893889	3.776921
C	4.627538	-2.647874	2.622927
C	3.791901	-2.172301	1.618177
C	3.325968	0.574603	-0.678155
C	3.229528	0.473634	-2.068702
C	4.104273	1.174821	-2.895047
C	5.091340	1.981583	-2.336603
C	5.207906	2.076088	-0.951021
C	4.334541	1.373082	-0.127135
C	-2.022399	-1.496716	-1.405959
C	-1.348953	-2.599630	-0.824857
C	-0.569852	-3.456291	-1.629367
C	-0.472296	-3.206191	-3.016835
C	-1.187617	-2.164471	-3.586479
C	-1.971704	-1.324821	-2.784926
C	-2.542627	0.746624	-0.535638
O	-3.348203	1.586787	0.212335
C	-2.965187	2.901005	0.057310
C	-1.825650	2.909813	-0.858733
C	-1.533549	1.589336	-1.200157
C	-0.414535	1.316414	-1.990089
C	0.351213	2.387691	-2.437090
C	0.024803	3.710108	-2.114868
C	-1.071560	3.984591	-1.308019
N	-3.505888	3.880149	0.640088
C	-4.598892	3.632524	1.560397
H	-5.070247	2.649049	1.444888
H	-5.356690	4.410930	1.428238
H	-4.224720	3.716888	2.588944
H	-1.336016	4.995283	-1.015002
H	0.644860	4.520835	-2.485288
H	1.233661	2.189941	-3.037193
H	-0.124886	0.299682	-2.228740
H	-3.485490	0.059610	2.049665
H	-5.176752	-1.047846	3.461465
H	-6.509536	-2.941884	2.563185
H	-6.113557	-3.723599	0.236492
H	-4.406278	-2.625211	-1.164378
H	-2.525545	-0.506295	-3.235197
H	-1.145054	-1.998330	-4.658644
H	0.127115	-3.865268	-3.637175
H	-0.165431	-4.377226	-1.215358
H	-1.541585	-2.844121	0.215936
H	-0.224982	-0.569945	1.959817
H	-1.684007	1.054613	3.115058
H	-1.276790	3.493685	2.863650
H	0.633098	4.282631	1.494381
H	2.125278	2.667191	0.390524
H	4.442170	1.442681	0.951848
H	5.984897	2.694410	-0.511104
H	5.775672	2.529126	-2.978090
H	4.017722	1.083213	-3.973937
H	2.463467	-0.168688	-2.497949
H	2.859899	0.772956	3.034002
H	4.335708	-0.078456	4.823235
H	5.474331	-2.266935	4.565938
H	5.114299	-3.612065	2.509502
H	3.616504	-2.767788	0.725164

VIIIa-dba_{endo}-Me3N

Num. Imaginary Frequencies: 0

C	-4.842042	-0.699284	-2.400785
C	-4.210424	0.546303	-2.520392
C	-4.991124	1.664374	-2.840900
C	-6.359647	1.540737	-3.056897
C	-6.972176	0.295338	-2.943533
C	-6.208787	-0.823570	-2.613183
C	-2.781185	0.724221	-2.244731
C	-1.837961	-0.225528	-2.218792
C	-0.464648	0.092354	-1.741614
O	-0.206053	1.197776	-1.267125
C	0.530549	-0.995497	-1.855212
Pd	0.346803	-1.953699	0.110862
C	-0.787341	-0.743423	2.515662

C	0.667571	-0.616100	2.370155
C	1.226068	0.644646	2.077342
C	0.332896	1.784140	1.845046
O	-1.006989	1.572996	2.012649
C	-1.544977	0.351654	2.318725
C	2.606029	0.792482	1.932082
C	3.451238	-0.303325	2.038590
C	2.913957	-1.559720	2.304859
C	1.541183	-1.720554	2.483418
N	0.739938	2.932992	1.485516
C	-0.260626	3.940006	1.190832
C	-3.023271	0.415644	2.267854
C	-3.825519	-0.000010	3.332532
C	-5.212683	0.037043	3.218023
C	-5.805800	0.492140	2.043402
C	-5.010492	0.925242	0.983907
C	-3.625816	0.897600	1.101304
C	1.750335	-0.913958	-1.185316
C	2.936317	-1.749440	-1.454353
C	4.201354	-1.230966	-1.150984
C	5.349915	-1.975952	-1.395235
C	5.252422	-3.253404	-1.940723
C	3.997293	-3.782263	-2.240917
C	2.848150	-3.038314	-2.000767
C	-1.769390	-2.645784	0.197631
C	-1.178781	-2.968484	1.399821
C	-1.372786	-2.129165	2.662657
C	3.250545	4.536827	-0.039544
N	3.601894	3.474334	-1.007786
C	2.416460	2.709611	-1.456309
C	4.409981	3.981563	-2.135157
C1	5.655389	1.847854	0.281277
H	-1.874305	-3.391380	-0.585945
H	-2.384615	-1.752245	0.103383
H	-0.810174	-3.983948	1.542361
H	-0.908426	-2.637825	3.514578
H	1.158241	-2.694502	2.769717
H	3.564728	-2.425463	2.377307
H	4.515193	-0.160247	1.883013
H	3.026107	1.767575	1.713175
H	0.241728	4.886202	0.967845
H	-0.857157	3.645750	0.316953
H	-2.992481	1.231368	0.286183
H	-5.467032	1.277869	0.063640
H	-6.887822	0.513616	1.953278
H	-5.830344	-0.286403	4.050579
H	-3.360862	-0.342918	4.252573
H	-0.954820	4.103556	2.024874
H	-2.439885	-2.069344	2.887675
H	0.356295	-1.743645	-2.626109
H	1.949004	0.007591	-0.640347
H	1.873443	-3.467255	-2.218850
H	3.913060	-4.780010	-2.662522
H	6.148814	-3.836948	-2.130332
H	6.316925	-1.544243	-1.155374
H	4.303805	-0.236701	-0.720737
H	-2.048112	-1.256719	-2.491735
H	-2.456406	1.735502	-1.999279
H	-4.515343	2.638410	-2.921811
H	-6.948275	2.417742	-3.309163
H	-8.041588	0.196432	-3.103270
H	-6.684270	-1.793830	-2.506208
H	-4.263353	-1.570013	-2.106718
H	4.273683	2.795750	-0.482998
H	1.781944	3.344851	-2.080314
H	2.754030	1.842858	-2.027294
H	1.845896	2.385209	-0.586698
H	2.681205	5.319771	-0.549571
H	2.645558	4.089652	0.753753
H	4.175883	4.944492	0.371755
H	3.826095	4.704110	-2.711974
H	5.312234	4.444841	-1.733339
H	4.697642	3.136569	-2.762698

VIIIa_{endo}-Me3N

Num. Imaginary Frequencies: 0

C	-2.696614	-1.208524	-1.711441
C	-1.378887	-0.793883	-1.458828
C	-0.344317	-1.729042	-1.264299
C	-0.685132	-3.093432	-1.265652
C	-1.988998	-3.494295	-1.485449
C	-3.001294	-2.553259	-1.723838
C	1.016473	-1.256441	-1.071270
C	1.270849	0.048496	-1.294291
O	0.240982	0.943490	-1.533032
C	-1.021755	0.600979	-1.412944
C	2.555249	0.762054	-1.197139
C	3.645865	0.384321	-1.983650

C	4.858850	1.053635	-1.858858
C	4.982575	2.101816	-0.949749
C	3.893567	2.481447	-0.167260
C	2.677553	1.818230	-0.287341
N	-1.887378	1.582194	-1.338451
C	-1.443773	2.966621	-1.232334
Pd	0.932322	-0.580520	1.911210
C	2.039969	-2.150873	-0.406855
C	1.618150	-2.381445	1.042305
C	2.433493	-2.053630	2.131771
C1	-0.488361	1.403984	1.782473
N	-4.155929	1.158948	0.292174
C	-4.050079	2.428850	1.014210
C	-5.485767	1.000447	-0.282485
C	-3.836399	0.050228	1.198084
H	2.300111	-2.564986	3.083436
H	3.419621	-1.617706	1.971818
H	0.839895	-3.133322	1.180794
H	2.149858	-3.100848	-0.947897
H	0.084254	-3.838354	-1.098782
H	-2.228516	-4.553261	-1.488240
H	-4.016355	-2.881004	-1.922454
H	-3.465184	-0.469891	-1.913031
H	-0.779147	3.215513	-2.062042
H	-2.326870	3.604801	-1.274587
H	-2.811046	1.351496	-0.890644
H	1.830398	2.080253	0.341801
H	3.993478	3.288875	0.551491
H	5.931244	2.620726	-0.848074
H	5.704912	0.758628	-2.472156
H	3.537851	-0.431031	-2.693760
H	-0.919697	3.108105	-0.280754
H	3.016521	-1.663751	-0.424443
H	-6.273578	1.006809	0.490064
H	-5.687520	1.813005	-0.988312
H	-5.546590	0.048289	-0.820243
H	-4.775336	2.484467	1.843217
H	-3.040217	2.525041	1.424365
H	-4.248171	3.260566	0.329040
H	-4.527519	0.027514	2.057454
H	-3.917707	-0.899349	0.662065
H	-2.811517	0.165878	1.564250

VIIIfa-dba_{exo}-Me3N

Num. Imaginary Frequencies: 0			
C	-6.955282	-3.055914	-0.604189
C	-5.599020	-3.287869	-0.341546
C	-5.256530	-4.379306	0.470260
C	-6.238167	-5.201242	1.007080
C	-7.584628	-4.952192	0.743144
C	-7.940346	-3.876827	-0.065396
C	-4.600895	-2.383027	-0.924225
C	-3.289843	-2.336917	-0.655112
C	-2.409418	-1.340091	-1.325341
O	-2.843323	-0.568321	-2.175029
C	-0.997339	-1.333440	-0.875266
C	-0.108268	-0.362339	-1.360592
C	1.363355	-0.438631	-1.243188
C	2.162986	0.151192	-2.227135
C	3.552148	0.143871	-2.125818
C	4.167222	-0.446518	-1.026991
C	3.382685	-1.041468	-0.036336
C	1.999852	-1.044968	-0.147033
Pd	-0.985989	0.336215	0.481803
C	-1.446071	2.324177	2.542947
C	-1.743063	0.831655	2.575320
C	-2.790913	0.249769	1.918746
C	-1.030320	2.720365	1.129474
C	0.252526	2.578390	0.691563
C	1.499910	2.140291	1.343639
C	2.540964	2.481377	0.479808
C	1.959397	3.088825	-0.717621
O	0.587560	3.096216	-0.546178
C	3.867997	2.212001	0.776407
C	4.149947	1.559134	1.971336
C	3.113347	1.199614	2.838027
C	1.782660	1.482211	2.540339
N	2.548506	3.530653	-1.740010
C	1.742343	4.053791	-2.826601
C	-2.045985	3.423850	0.289638
C	-2.561350	4.641685	0.748189
C	-3.519848	5.330623	0.013209
C	-3.986006	4.805408	-1.189531
C	-3.483508	3.592171	-1.651337
C	-2.518332	2.905802	-0.920375
C1	6.565408	-1.781369	1.366528
N	5.796315	-3.852111	-0.500425
C	4.440630	-4.356954	-0.200880

C	5.927886	-3.369764	-1.890587
C	6.846226	-4.830399	-0.145109
H	-2.150340	1.949341	-1.282144
H	-3.846545	3.165910	-2.581567
H	-4.739987	5.338190	-1.761577
H	-3.903803	6.277425	0.381884
H	-2.196865	5.060427	1.683235
H	0.848838	4.592161	-2.487324
H	1.406335	3.230051	-3.471113
H	2.356551	4.722881	-3.434921
H	4.647440	2.479362	0.071755
H	5.171862	1.285716	2.212621
H	3.350398	0.671077	3.756276
H	1.000239	1.161039	3.217623
H	-0.661801	2.571666	3.264139
H	-1.141047	0.218021	3.243870
H	-2.333670	2.898222	2.826833
H	-3.028177	-0.798399	2.069551
H	-3.526516	0.842608	1.379511
H	4.255855	-5.279229	-0.759584
H	4.374270	-4.545537	0.872308
H	3.711747	-3.593359	-0.476479
H	5.832255	-4.208513	-2.586408
H	5.149293	-2.628681	-2.078906
H	6.906131	-2.897855	-1.999133
H	6.745642	-5.727733	-0.762165
H	7.819558	-4.362618	-0.299177
H	6.742717	-5.076414	0.912604
H	-0.631189	-2.224491	-0.368192
H	-0.482296	0.281015	-2.156600
H	1.686686	0.638523	-3.074200
H	4.146287	0.640001	-2.887469
H	5.244822	-0.411286	-0.889918
H	3.873996	-1.447533	0.843599
H	1.398251	-1.467253	0.654111
H	-2.826058	-2.996939	0.074756
H	-4.967870	-1.658424	-1.650628
H	-7.236169	-2.217648	-1.236750
H	-8.986322	-3.677659	-0.278554
H	-8.350632	-5.597975	1.161992
H	-5.953337	-6.043108	1.631411
H	-4.211864	-4.594583	0.674111
H	5.999525	-2.993987	0.175879

VIIIa_{exo}-Me3N

Num. Imaginary Frequencies: 0

C	0.627298	-0.517049	-1.191725
O	-0.020656	0.723975	-1.263873
C	-1.322182	0.545473	-1.292339
C	-1.624736	-0.841638	-1.418392
C	-0.384670	-1.514675	-1.326372
C	-0.381935	-2.924099	-1.346615
C	-1.584459	-3.583379	-1.499805
C	-2.809669	-2.894418	-1.641968
C	-2.837206	-1.517061	-1.599224
H	-3.766008	-0.965829	-1.709092
H	-3.727550	-3.455286	-1.782940
H	-1.589441	-4.669337	-1.519399
H	0.535442	-3.489938	-1.240878
N	-2.122469	1.596012	-1.235656
C	-1.559695	2.898456	-0.903155
H	-0.786905	3.167220	-1.626890
H	-1.119256	2.875994	0.100998
H	-2.360225	3.637866	-0.947054
H	-3.067988	1.390408	-0.853100
N	-4.453130	1.143103	0.398701
C	-5.801408	1.254850	-0.139860
H	-6.570806	1.235970	0.652099
H	-5.902612	2.193317	-0.694611
H	-5.996859	0.424973	-0.827113
C	-4.146213	2.270788	1.278162
H	-4.227455	3.210440	0.720851
H	-4.838005	2.318264	2.136906
H	-3.125945	2.162701	1.658644
C	-4.277986	-0.109426	1.136031
H	-3.233860	-0.203905	1.450447
H	-4.532728	-0.958146	0.495264
C	1.929098	-0.502836	-0.709133
Pd	1.197841	-0.822151	1.469579
C	2.725095	-1.805735	-0.639745
H	3.786552	-1.608917	-0.812787
H	2.402594	-2.516494	-1.404429
C	2.505525	-2.346490	0.768426
H	2.007135	-3.308881	0.870921
C	3.125140	-1.768846	1.867961
H	3.115134	-2.271400	2.830612
H	3.878349	-0.993281	1.742819
Cl	-0.687003	0.669849	1.940943

C	2.697874	0.785343	-0.739612
C	3.821545	0.884391	-1.567803
C	4.540951	2.072380	-1.653737
C	4.151915	3.178594	-0.904939
C	3.033471	3.090128	-0.079594
C	2.306403	1.907684	0.000723
H	1.438827	1.843016	0.650850
H	2.723490	3.945977	0.512779
H	4.716716	4.104422	-0.963746
H	5.405944	2.130210	-2.308015
H	4.129540	0.035901	-2.172771
H	-4.926219	-0.143951	2.028942

VIIa-AC_{endo}-Me3N

Num. Imaginary Frequencies: 0

C	-1.159102	-1.688253	2.493490
N	-1.501256	-0.491994	1.747328
C	-0.555590	0.275201	1.376678
O	0.727909	-0.037618	1.731357
C	1.819726	0.587512	1.189630
C	1.707667	1.632412	0.334264
Pd	1.861303	-0.255635	-1.566020
C	2.927988	2.216811	-0.357732
C	2.953800	1.736427	-1.797396
C	3.813535	0.777832	-2.250948
C	3.067406	-0.010680	1.723914
C	3.318163	-1.374407	1.548213
C	4.476757	-1.944532	2.062472
C	5.389247	-1.160137	2.765598
C	5.137028	0.195285	2.957796
C	3.977767	0.767687	2.442444
C	-0.754138	1.482175	0.569615
C	0.366194	2.145454	0.033369
C	0.148712	3.273608	-0.769455
C	-1.138862	3.721814	-1.028532
C	-2.243344	3.059035	-0.491199
C	-2.045786	1.944454	0.307246
C	1.466634	-2.000827	-2.733754
C	0.685273	-2.045083	-1.574316
C	-0.769302	-1.697542	-1.592653
C	-4.246464	-1.470382	0.001787
N	-5.247992	-0.779719	0.842780
C	-6.617062	-1.287935	0.628323
C	-4.867061	-0.760572	2.270682
H	-3.850034	-0.369051	2.348736
H	-5.560173	-0.105673	2.801904
H	-4.913167	-1.775051	2.678674
Cl	-5.609719	1.984453	0.065977
H	-7.308880	-0.667961	1.200668
H	-6.681529	-2.332807	0.945262
H	-6.857211	-1.195643	-0.431929
H	-3.263108	-1.059017	0.236649
H	-4.257294	-2.543274	0.212564
H	-4.487270	-1.293858	-1.047656
H	-2.077800	-2.238022	2.717157
H	-0.495428	-2.347885	1.917988
H	-0.651596	-1.458205	3.438817
H	-2.907843	1.441563	0.729671
H	-3.260399	3.387000	-0.681146
H	-1.283300	4.598247	-1.653321
H	0.993144	-2.687786	-0.749722
H	2.381170	-2.583818	-2.807738
H	1.021437	-1.707050	-3.683052
H	-1.026525	-1.034590	-2.419712
H	-1.110033	-1.260136	-0.655363
Cl	-8.12467	-3.193279	-1.809531
H	3.837555	1.882879	0.143968
H	2.918490	3.311593	-0.305828
H	2.323275	2.266668	-2.509184
H	4.577499	0.354259	-1.602356
H	3.890957	0.551588	-3.309823
H	2.605667	-1.976802	0.993541
H	4.668722	-3.002544	1.912649
H	6.293306	-1.606996	3.168070
H	5.837605	0.807558	3.517238
H	3.769655	1.821555	2.604563
H	0.991248	3.807974	-1.195543
H	-5.294571	0.275313	0.522776

VIIa-AC_{exo}-Me3N

Num. Imaginary Frequencies: 0

C	0.113977	3.141344	0.683497
C	0.108478	1.769967	0.935596
C	-1.108890	1.116059	1.148839
C	-2.329270	1.769878	1.079143
C	-2.320408	3.130238	0.790850
C	-1.109334	3.804753	0.610537
C	-0.816386	-0.284829	1.442295

O	0.546451	-0.437606	1.433199
C	1.166969	0.756853	1.079170
C	2.523023	0.795103	1.015091
Pd	1.949384	0.462142	-1.476273
C	3.267475	2.055962	0.570736
C	2.976256	2.373835	-0.888707
C	3.702473	1.890816	-1.942087
N	-1.624050	-1.239296	1.642452
C	-1.069265	-2.564969	1.860242
C	3.337364	-0.373015	1.458272
C	4.385909	-0.857727	0.668290
C	5.172279	-1.919851	1.099820
C	4.930883	-2.510208	2.337361
C	3.896992	-2.030516	3.136980
C	3.106995	-0.971569	2.701987
C	1.549842	-0.650967	-3.259637
C	0.911325	-1.271293	-2.180489
C	-0.556225	-1.119574	-1.945863
C1	-1.515920	-2.453744	-2.767347
C	-4.992517	-1.661873	1.503277
N	-5.251987	-1.061401	0.176323
C	-6.556787	-1.471557	-0.380660
C	-4.138107	-1.285385	-0.770043
C1	-5.772362	1.758648	0.618943
H	2.486584	-1.043787	-3.646358
H	2.305619	-0.600929	3.332819
H	3.706012	-2.479493	4.107192
H	5.546031	-3.337840	2.677502
H	5.972800	-2.288268	0.465246
H	4.568788	-0.415266	-0.306183
H	-0.649601	-2.970736	0.929588
H	-1.866926	-3.233599	2.193696
H	-0.268370	-2.567821	2.609265
H	-3.276499	1.265225	1.240428
H	-3.270053	3.649792	0.714404
H	-1.117711	4.871766	0.408927
H	1.033532	3.697586	0.552075
H	3.005202	2.903702	1.214913
H	2.212839	3.120219	-1.095997
H	4.338142	1.882949	0.708616
H	3.526612	2.257440	-2.948193
H	4.609345	1.309203	-1.794155
H	-4.059881	-2.348412	-1.011845
H	-4.325773	-0.708641	-1.677018
H	-3.212702	-0.953399	-0.297496
H	-5.036883	-2.752417	1.424070
H	-3.998007	-1.353113	1.835577
H	-5.753388	-1.298910	2.196794
H	-6.564695	-2.551694	-0.551908
H	-7.337604	-1.187254	0.326325
H	-6.718771	-0.936298	-1.317421
H	0.978469	-0.037065	-3.954196
H	1.364585	-2.150137	-1.723736
H	-5.355099	0.022863	0.336894
H	-0.949271	-0.184949	-2.348774
H	-0.821832	-1.205727	-0.893632